



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:30 PM EDT

PDB ID : 2FRV / pdb_00002frv
Title : CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDRO-
GENASE
Authors : Volbeda, A.; Frey, M.; Fontecilla-Camps, J.C.
Deposited on : 1997-06-10
Resolution : 2.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

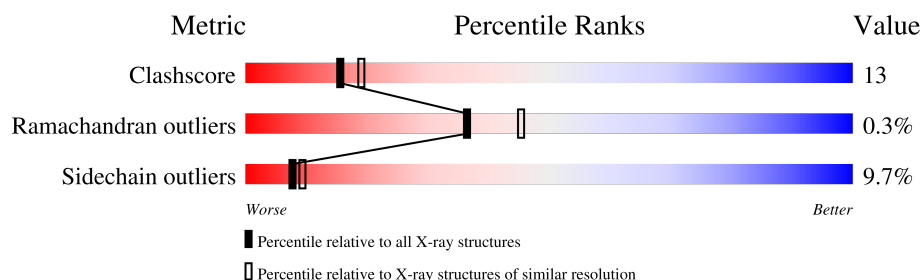
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	C	264	
1	E	264	
1	G	264	
1	I	264	
1	S	264	
2	B	536	
2	D	536	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	536	
2	H	536	
2	J	536	
2	L	536	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FCO	B	537	-	-	X	-
7	FCO	D	537	-	-	X	-
7	FCO	F	537	-	-	X	-
7	FCO	H	537	-	-	X	-
7	FCO	J	537	-	-	X	-
7	FCO	L	537	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 38040 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PERIPLASMIC HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	A	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	C	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	E	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	G	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			
1	I	261	Total	C	N	O	S	0	0	0
			1964	1249	329	367	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	24	VAL	LEU	conflict	UNP P12943
S	89	GLY	ARG	conflict	UNP P12943
A	24	VAL	LEU	conflict	UNP P12943
A	89	GLY	ARG	conflict	UNP P12943
C	24	VAL	LEU	conflict	UNP P12943
C	89	GLY	ARG	conflict	UNP P12943
E	24	VAL	LEU	conflict	UNP P12943
E	89	GLY	ARG	conflict	UNP P12943
G	24	VAL	LEU	conflict	UNP P12943
G	89	GLY	ARG	conflict	UNP P12943
I	24	VAL	LEU	conflict	UNP P12943
I	89	GLY	ARG	conflict	UNP P12943

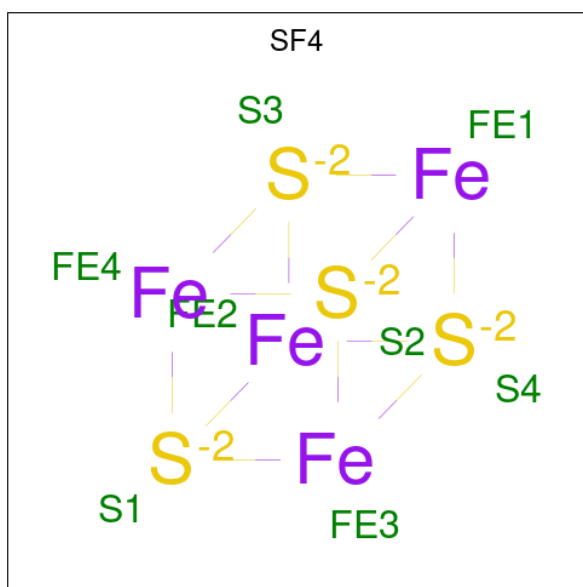
- Molecule 2 is a protein called PERIPLASMIC HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	B	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	D	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	F	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	H	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			
2	J	530	Total	C	N	O	S	0	0	0
			4152	2653	725	757	17			

There are 24 discrepancies between the modelled and reference sequences:

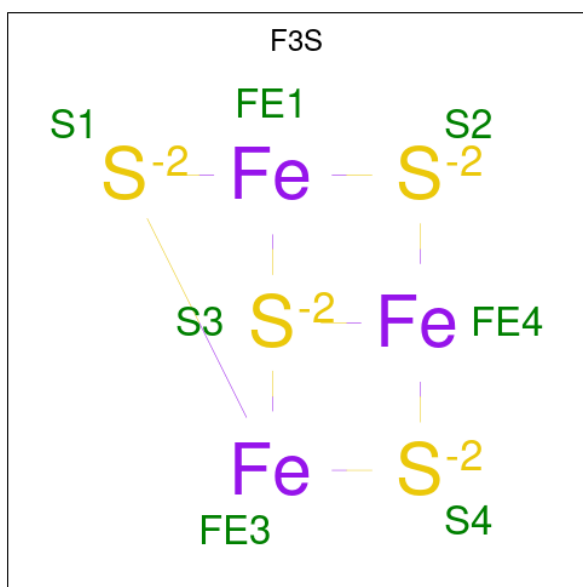
Chain	Residue	Modelled	Actual	Comment	Reference
L	144	LYS	ARG	conflict	UNP P12944
L	332	GLY	ASP	conflict	UNP P12944
L	482	LEU	HIS	conflict	UNP P12944
L	497	GLY	ARG	conflict	UNP P12944
B	144	LYS	ARG	conflict	UNP P12944
B	332	GLY	ASP	conflict	UNP P12944
B	482	LEU	HIS	conflict	UNP P12944
B	497	GLY	ARG	conflict	UNP P12944
D	144	LYS	ARG	conflict	UNP P12944
D	332	GLY	ASP	conflict	UNP P12944
D	482	LEU	HIS	conflict	UNP P12944
D	497	GLY	ARG	conflict	UNP P12944
F	144	LYS	ARG	conflict	UNP P12944
F	332	GLY	ASP	conflict	UNP P12944
F	482	LEU	HIS	conflict	UNP P12944
F	497	GLY	ARG	conflict	UNP P12944
H	144	LYS	ARG	conflict	UNP P12944
H	332	GLY	ASP	conflict	UNP P12944
H	482	LEU	HIS	conflict	UNP P12944
H	497	GLY	ARG	conflict	UNP P12944
J	144	LYS	ARG	conflict	UNP P12944
J	332	GLY	ASP	conflict	UNP P12944
J	482	LEU	HIS	conflict	UNP P12944
J	497	GLY	ARG	conflict	UNP P12944

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	C	1	Total	Fe	S	0	0
			7	3	4		
4	E	1	Total	Fe	S	0	0
			7	3	4		
4	G	1	Total	Fe	S	0	0
			7	3	4		
4	I	1	Total	Fe	S	0	0
			7	3	4		

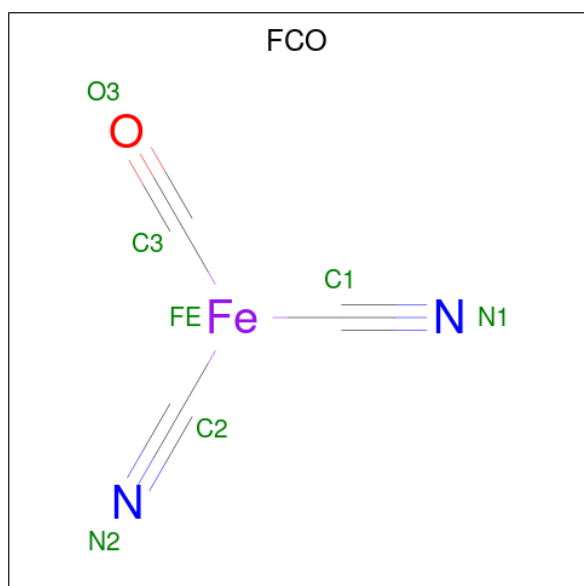
- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	Ni	0	0
			1	1		
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		
5	F	1	Total	Ni	0	0
			1	1		
5	H	1	Total	Ni	0	0
			1	1		
5	J	1	Total	Ni	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		
6	H	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	B	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	D	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	F	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	H	1	Total 7	C 3	Fe 1	N 2	O 1	0	0
7	J	1	Total 7	C 3	Fe 1	N 2	O 1	0	0

- Molecule 8 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total 1	O 1	0	0
8	B	1	Total 1	O 1	0	0
8	D	1	Total 1	O 1	0	0
8	F	1	Total 1	O 1	0	0
8	H	1	Total 1	O 1	0	0
8	J	1	Total 1	O 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	77	Total 77	O 77	0	0
9	L	110	Total 110	O 110	0	0
9	A	78	Total 78	O 78	0	0
9	B	114	Total 114	O 114	0	0
9	C	76	Total 76	O 76	0	0
9	D	114	Total 114	O 114	0	0
9	E	81	Total 81	O 81	0	0
9	F	115	Total 115	O 115	0	0
9	G	76	Total 76	O 76	0	0

Continued on next page...

Continued from previous page...

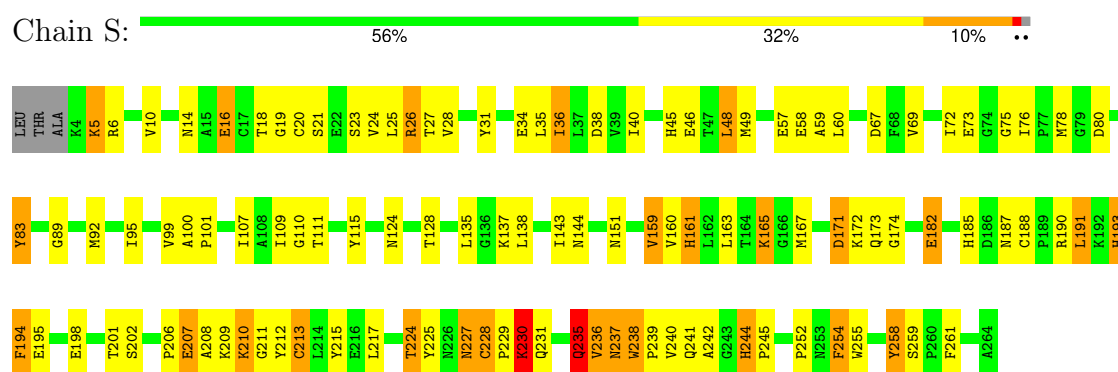
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	112	Total 112	O 112	0	0
9	I	80	Total 80	O 80	0	0
9	J	113	Total 113	O 113	0	0

3 Residue-property plots

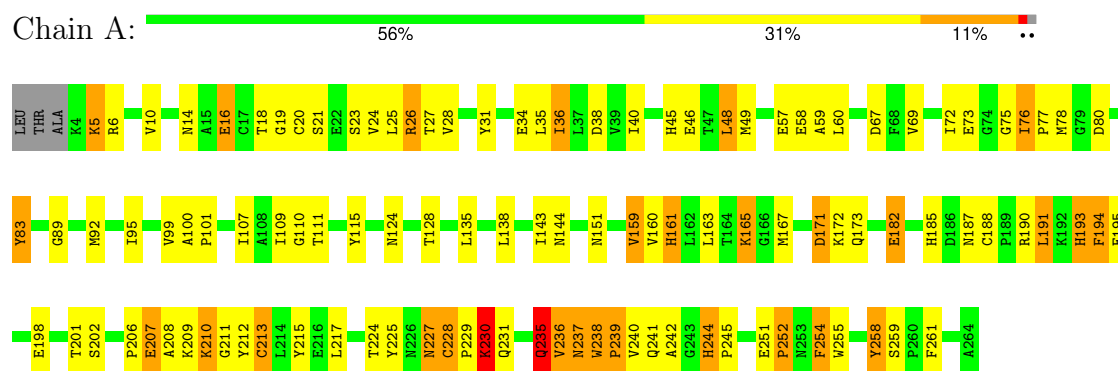
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

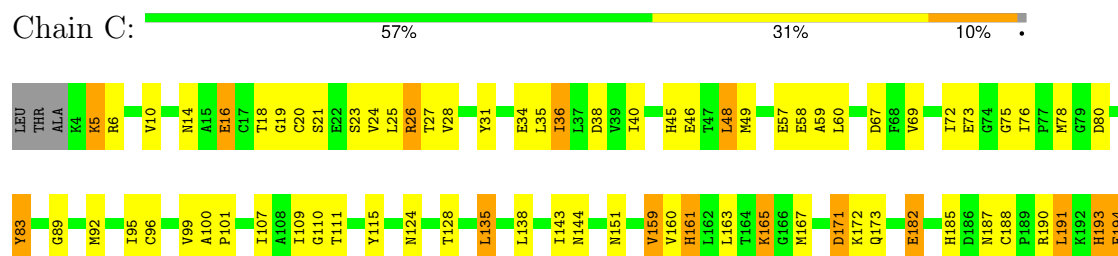
• Molecule 1: PERIPLASMIC HYDROGENASE



• Molecule 1: PERIPLASMIC HYDROGENASE



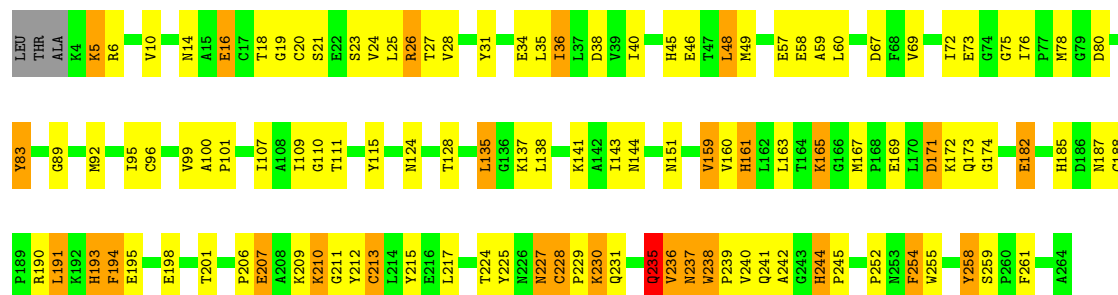
• Molecule 1: PERIPLASMIC HYDROGENASE





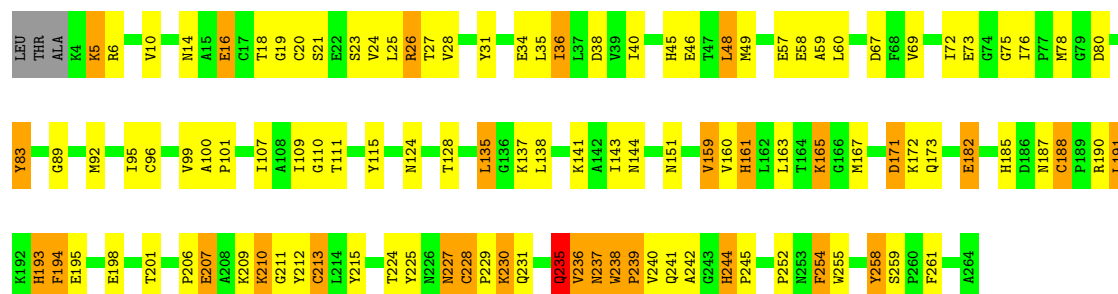
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain E: 56% 32% 10% .



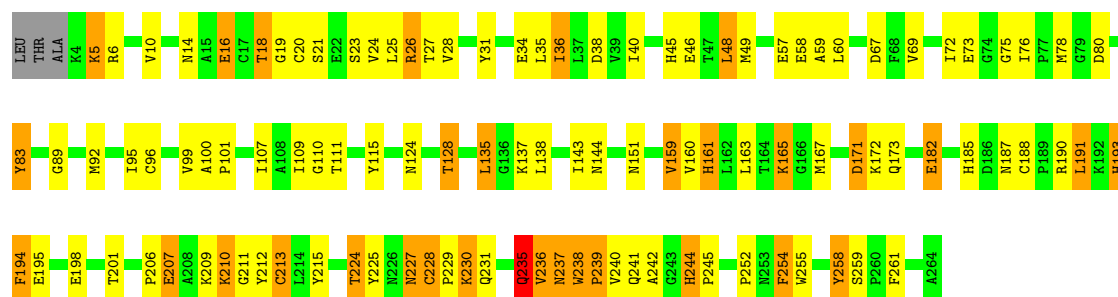
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain G: 57% 30% 11% .



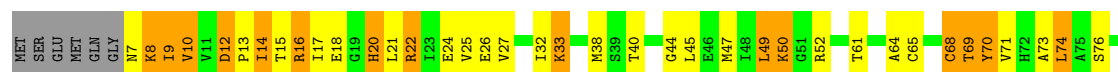
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain I: 58% 29% 12% .

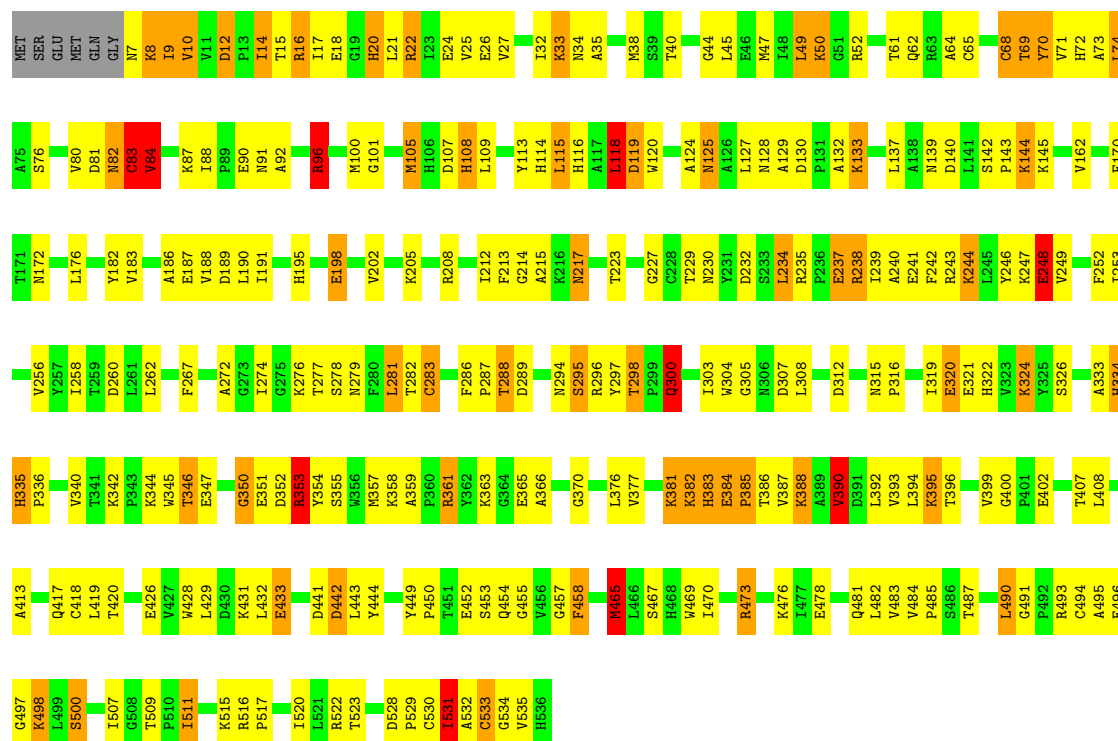


• Molecule 2: PERIPLASMIC HYDROGENASE

Chain L: 49% 37% 11% ..

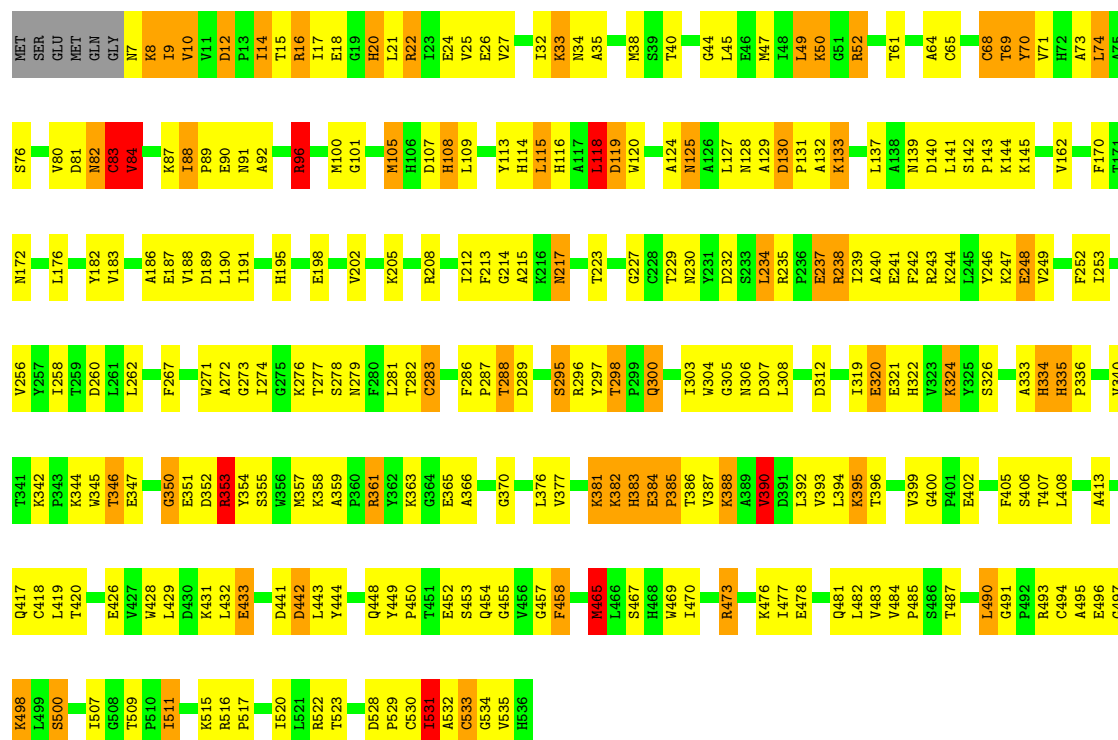






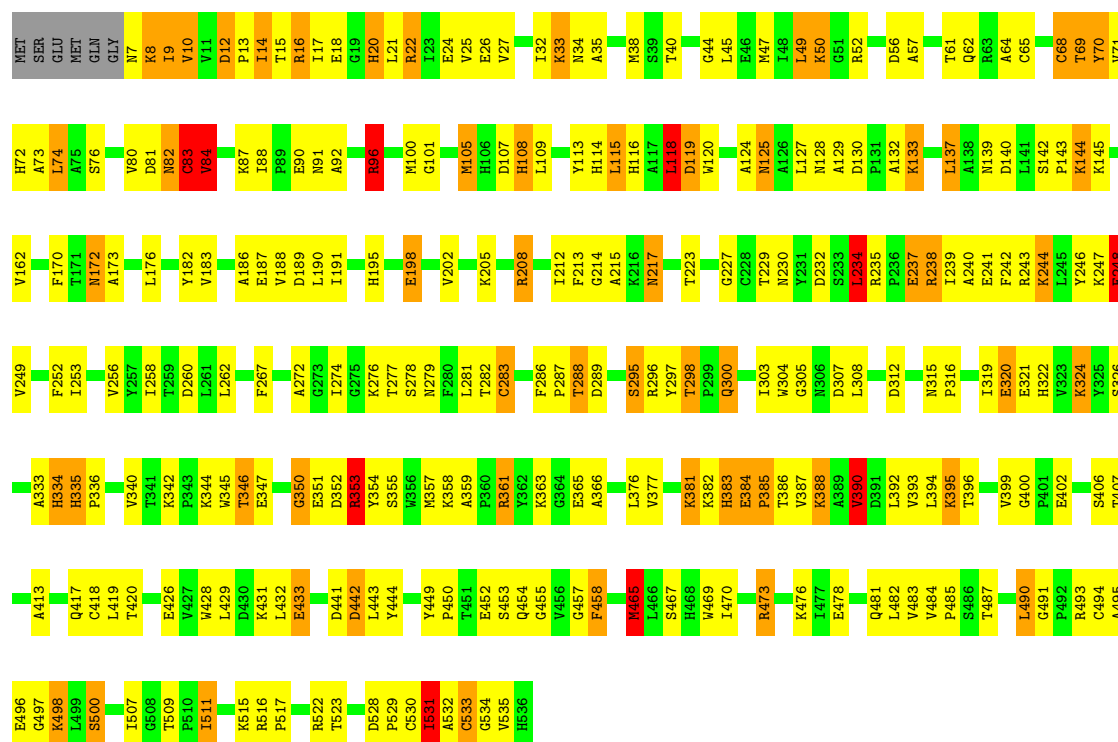
- Molecule 2: PERIPLASMIC HYDROGENASE

Chain F:  48% 39% 11% ..



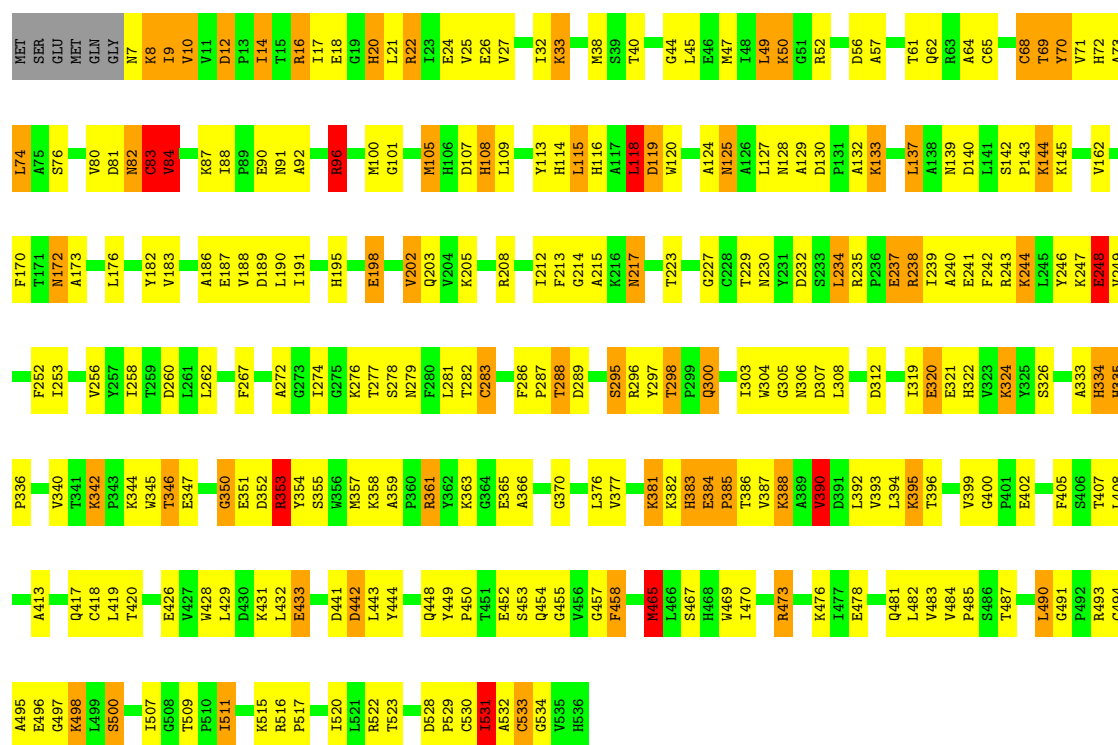
- Molecule 2: PERIPLASMIC HYDROGENASE

Chain H: 



• Molecule 2: PERIPLASMIC HYDROGENASE

Chain J: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.78Å 113.16Å 133.91Å 90.03° 90.02° 119.99°	Depositor
Resolution (Å)	8.00 – 2.54	Depositor
% Data completeness (in resolution range)	92.5 (8.00-2.54)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.201 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	38040	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, FCO, MG, SF4, O, F3S

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.28	3/2017 (0.1%)	2.30	108/2742 (3.9%)
1	C	1.28	3/2017 (0.1%)	2.30	109/2742 (4.0%)
1	E	1.28	3/2017 (0.1%)	2.30	111/2742 (4.0%)
1	G	1.28	3/2017 (0.1%)	2.30	111/2742 (4.0%)
1	I	1.28	3/2017 (0.1%)	2.30	112/2742 (4.1%)
1	S	1.28	3/2017 (0.1%)	2.30	111/2742 (4.0%)
2	B	1.23	5/4257 (0.1%)	2.33	231/5786 (4.0%)
2	D	1.23	5/4257 (0.1%)	2.33	232/5786 (4.0%)
2	F	1.23	5/4257 (0.1%)	2.33	233/5786 (4.0%)
2	H	1.23	5/4257 (0.1%)	2.33	230/5786 (4.0%)
2	J	1.23	5/4257 (0.1%)	2.33	229/5786 (4.0%)
2	L	1.23	5/4257 (0.1%)	2.33	233/5786 (4.0%)
All	All	1.25	48/37644 (0.1%)	2.32	2050/51168 (4.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1
2	L	0	1
All	All	0	6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	528	ASP	C-O	10.80	1.29	1.23
2	D	528	ASP	C-O	10.72	1.28	1.23
2	L	528	ASP	C-O	10.69	1.28	1.23
2	J	528	ASP	C-O	10.69	1.28	1.23
2	H	528	ASP	C-O	10.66	1.28	1.23
2	B	528	ASP	C-O	10.56	1.28	1.23
1	G	23	SER	C-N	-6.06	1.26	1.33
1	C	23	SER	C-N	-6.04	1.26	1.33
1	S	23	SER	C-N	-6.03	1.26	1.33
1	E	23	SER	C-N	-6.00	1.26	1.33
1	I	23	SER	C-N	-5.99	1.26	1.33
1	A	23	SER	C-N	-5.97	1.26	1.33
1	E	76	ILE	CA-CB	5.95	1.61	1.54
1	G	76	ILE	CA-CB	5.89	1.61	1.54
1	S	76	ILE	CA-CB	5.88	1.61	1.54
1	I	76	ILE	CA-CB	5.88	1.61	1.54
1	C	76	ILE	CA-CB	5.87	1.61	1.54
1	A	76	ILE	CA-CB	5.85	1.61	1.54
2	B	528	ASP	N-CA	5.77	1.50	1.46
2	D	528	ASP	N-CA	5.72	1.50	1.46
2	F	528	ASP	N-CA	5.72	1.50	1.46
2	B	40	THR	CA-CB	5.70	1.61	1.53
2	L	528	ASP	N-CA	5.70	1.50	1.46
2	J	528	ASP	N-CA	5.70	1.50	1.46
2	L	40	THR	CA-CB	5.65	1.61	1.53
2	J	40	THR	CA-CB	5.65	1.61	1.53
2	H	40	THR	CA-CB	5.64	1.61	1.53
2	F	40	THR	CA-CB	5.63	1.61	1.53
2	D	40	THR	CA-CB	5.62	1.61	1.53
2	H	528	ASP	N-CA	5.62	1.50	1.46
2	J	130	ASP	N-CA	5.42	1.52	1.45
2	F	130	ASP	N-CA	5.42	1.52	1.45
2	L	130	ASP	N-CA	5.41	1.52	1.45
2	H	130	ASP	N-CA	5.41	1.52	1.45
2	D	130	ASP	N-CA	5.40	1.52	1.45
2	B	130	ASP	N-CA	5.37	1.52	1.45
2	F	229	THR	CA-CB	5.25	1.61	1.54
2	B	229	THR	CA-CB	5.23	1.61	1.54
2	L	229	THR	CA-CB	5.20	1.61	1.54
2	H	229	THR	CA-CB	5.20	1.61	1.54
2	J	229	THR	CA-CB	5.17	1.61	1.54
2	D	229	THR	CA-CB	5.16	1.61	1.54
1	G	238	TRP	CA-CB	-5.11	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	TRP	CA-CB	-5.09	1.47	1.53
1	S	238	TRP	CA-CB	-5.08	1.47	1.53
1	I	238	TRP	CA-CB	-5.08	1.47	1.53
1	C	238	TRP	CA-CB	-5.07	1.47	1.53
1	E	238	TRP	CA-CB	-5.07	1.47	1.53

All (2050) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	353	ARG	CD-NE-CZ	16.53	147.54	124.40
2	F	353	ARG	CD-NE-CZ	16.53	147.54	124.40
2	D	353	ARG	CD-NE-CZ	16.52	147.52	124.40
2	B	353	ARG	CD-NE-CZ	16.50	147.50	124.40
2	J	353	ARG	CD-NE-CZ	16.50	147.50	124.40
2	H	353	ARG	CD-NE-CZ	16.48	147.47	124.40
2	H	81	ASP	CA-CB-CG	14.51	127.11	112.60
2	F	81	ASP	CA-CB-CG	14.51	127.11	112.60
2	J	81	ASP	CA-CB-CG	14.50	127.10	112.60
2	L	81	ASP	CA-CB-CG	14.49	127.09	112.60
2	B	81	ASP	CA-CB-CG	14.48	127.08	112.60
2	D	81	ASP	CA-CB-CG	14.47	127.07	112.60
2	B	288	THR	N-CA-C	-10.22	100.68	113.55
2	H	288	THR	N-CA-C	-10.21	100.69	113.55
2	L	288	THR	N-CA-C	-10.20	100.70	113.55
2	F	288	THR	N-CA-C	-10.18	100.72	113.55
2	D	288	THR	N-CA-C	-10.18	100.73	113.55
2	J	288	THR	N-CA-C	-10.18	100.73	113.55
2	B	96	ARG	NE-CZ-NH1	10.01	131.51	121.50
2	H	96	ARG	NE-CZ-NH1	9.98	131.48	121.50
2	F	96	ARG	NE-CZ-NH1	9.97	131.47	121.50
2	L	96	ARG	NE-CZ-NH1	9.96	131.46	121.50
2	D	96	ARG	NE-CZ-NH1	9.96	131.46	121.50
2	J	96	ARG	NE-CZ-NH1	9.90	131.40	121.50
1	E	40	ILE	O-C-N	9.82	133.16	122.75
1	A	40	ILE	O-C-N	9.81	133.15	122.75
1	G	40	ILE	O-C-N	9.80	133.14	122.75
1	C	40	ILE	O-C-N	9.80	133.14	122.75
1	S	40	ILE	O-C-N	9.79	133.13	122.75
1	I	40	ILE	O-C-N	9.77	133.11	122.75
2	H	52	ARG	NE-CZ-NH2	9.53	127.78	119.20
2	L	52	ARG	NE-CZ-NH2	9.47	127.72	119.20
2	B	52	ARG	NE-CZ-NH2	9.47	127.72	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	52	ARG	NE-CZ-NH2	9.46	127.71	119.20
2	J	52	ARG	NE-CZ-NH2	9.45	127.71	119.20
2	F	52	ARG	NE-CZ-NH2	9.44	127.70	119.20
2	J	40	THR	N-CA-C	8.93	123.48	112.59
2	B	40	THR	N-CA-C	8.92	123.47	112.59
2	H	40	THR	N-CA-C	8.91	123.46	112.59
2	L	40	THR	N-CA-C	8.91	123.46	112.59
2	D	40	THR	N-CA-C	8.89	123.44	112.59
1	E	36	ILE	CA-CB-CG2	8.89	125.61	110.50
1	G	36	ILE	CA-CB-CG2	8.89	125.61	110.50
1	S	36	ILE	CA-CB-CG2	8.88	125.60	110.50
1	I	36	ILE	CA-CB-CG2	8.88	125.60	110.50
1	A	36	ILE	CA-CB-CG2	8.88	125.60	110.50
1	C	36	ILE	CA-CB-CG2	8.87	125.58	110.50
2	F	40	THR	N-CA-C	8.87	123.42	112.59
2	F	16	ARG	NE-CZ-NH2	8.85	127.16	119.20
1	I	241	GLN	CG-CD-NE2	8.83	129.65	116.40
1	C	241	GLN	CG-CD-NE2	8.82	129.64	116.40
1	E	241	GLN	CG-CD-NE2	8.82	129.64	116.40
1	G	241	GLN	CG-CD-NE2	8.82	129.64	116.40
2	B	16	ARG	NE-CZ-NH2	8.82	127.14	119.20
2	J	16	ARG	NE-CZ-NH2	8.82	127.14	119.20
1	S	241	GLN	CG-CD-NE2	8.82	129.63	116.40
2	H	399	VAL	CA-C-O	-8.82	112.18	121.44
1	A	241	GLN	CG-CD-NE2	8.81	129.62	116.40
2	L	16	ARG	NE-CZ-NH2	8.80	127.12	119.20
2	L	399	VAL	CA-C-O	-8.78	112.22	121.44
2	D	16	ARG	NE-CZ-NH2	8.78	127.10	119.20
2	H	16	ARG	NE-CZ-NH2	8.78	127.10	119.20
2	B	399	VAL	CA-C-O	-8.77	112.23	121.44
2	F	399	VAL	CA-C-O	-8.76	112.24	121.44
2	J	399	VAL	CA-C-O	-8.74	112.27	121.44
2	D	399	VAL	CA-C-O	-8.74	112.27	121.44
1	E	207	GLU	CA-C-N	8.70	131.75	120.44
1	E	207	GLU	C-N-CA	8.70	131.75	120.44
1	G	207	GLU	CA-C-N	8.70	131.75	120.44
1	G	207	GLU	C-N-CA	8.70	131.75	120.44
1	A	207	GLU	CA-C-N	8.70	131.75	120.44
1	A	207	GLU	C-N-CA	8.70	131.75	120.44
1	I	207	GLU	CA-C-N	8.68	131.73	120.44
1	I	207	GLU	C-N-CA	8.68	131.73	120.44
1	S	207	GLU	CA-C-N	8.68	131.72	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	207	GLU	C-N-CA	8.68	131.72	120.44
1	C	207	GLU	CA-C-N	8.66	131.70	120.44
1	C	207	GLU	C-N-CA	8.66	131.70	120.44
2	F	105	MET	CA-C-N	8.65	132.40	120.63
2	F	105	MET	C-N-CA	8.65	132.40	120.63
2	J	105	MET	CA-C-N	8.65	132.40	120.63
2	J	105	MET	C-N-CA	8.65	132.40	120.63
2	D	105	MET	CA-C-N	8.65	132.40	120.63
2	D	105	MET	C-N-CA	8.65	132.40	120.63
2	L	105	MET	CA-C-N	8.63	132.37	120.63
2	L	105	MET	C-N-CA	8.63	132.37	120.63
2	H	105	MET	CA-C-N	8.62	132.36	120.63
2	H	105	MET	C-N-CA	8.62	132.36	120.63
2	B	105	MET	CA-C-N	8.59	132.31	120.63
2	B	105	MET	C-N-CA	8.59	132.31	120.63
2	B	16	ARG	NE-CZ-NH1	-8.59	112.91	121.50
2	J	16	ARG	NE-CZ-NH1	-8.58	112.92	121.50
2	H	16	ARG	NE-CZ-NH1	-8.57	112.93	121.50
2	F	16	ARG	NE-CZ-NH1	-8.56	112.94	121.50
2	L	16	ARG	NE-CZ-NH1	-8.55	112.95	121.50
2	B	516	ARG	O-C-N	8.54	127.42	121.19
2	D	16	ARG	NE-CZ-NH1	-8.54	112.97	121.50
1	C	242	ALA	CA-C-O	8.53	130.08	119.59
2	J	516	ARG	O-C-N	8.53	127.42	121.19
2	H	69	THR	CA-C-O	-8.53	112.26	121.56
2	F	516	ARG	O-C-N	8.53	127.42	121.19
2	H	516	ARG	O-C-N	8.53	127.41	121.19
1	G	242	ALA	CA-C-O	8.51	130.05	119.59
2	D	516	ARG	O-C-N	8.51	127.40	121.19
2	L	69	THR	CA-C-O	-8.50	112.29	121.56
2	B	69	THR	CA-C-O	-8.50	112.29	121.56
1	S	242	ALA	CA-C-O	8.50	130.04	119.59
2	H	119	ASP	CA-CB-CG	8.49	121.09	112.60
1	E	242	ALA	CA-C-O	8.49	130.03	119.59
2	F	69	THR	CA-C-O	-8.49	112.31	121.56
2	L	516	ARG	O-C-N	8.48	127.38	121.19
1	A	242	ALA	CA-C-O	8.48	130.02	119.59
2	D	69	THR	CA-C-O	-8.48	112.32	121.56
2	J	69	THR	CA-C-O	-8.47	112.33	121.56
1	I	242	ALA	CA-C-O	8.47	130.01	119.59
2	J	119	ASP	CA-CB-CG	8.47	121.07	112.60
2	L	119	ASP	CA-CB-CG	8.45	121.05	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	119	ASP	CA-CB-CG	8.45	121.05	112.60
2	B	119	ASP	CA-CB-CG	8.43	121.03	112.60
2	D	119	ASP	CA-CB-CG	8.42	121.02	112.60
2	H	26	GLU	CA-CB-CG	8.41	130.93	114.10
2	J	26	GLU	CA-CB-CG	8.40	130.91	114.10
2	F	26	GLU	CA-CB-CG	8.40	130.90	114.10
2	L	26	GLU	CA-CB-CG	8.40	130.90	114.10
2	D	213	PHE	CA-CB-CG	-8.39	105.41	113.80
2	F	213	PHE	CA-CB-CG	-8.39	105.41	113.80
2	D	26	GLU	CA-CB-CG	8.39	130.87	114.10
2	B	26	GLU	CA-CB-CG	8.38	130.86	114.10
2	J	213	PHE	CA-CB-CG	-8.37	105.43	113.80
2	L	213	PHE	CA-CB-CG	-8.36	105.44	113.80
2	B	213	PHE	CA-CB-CG	-8.36	105.44	113.80
2	H	213	PHE	CA-CB-CG	-8.36	105.44	113.80
1	C	24	VAL	N-CA-CB	8.33	120.30	110.55
1	I	24	VAL	N-CA-CB	8.32	120.28	110.55
2	B	183	VAL	N-CA-CB	-8.31	101.23	112.28
1	A	24	VAL	N-CA-CB	8.30	120.26	110.55
1	S	24	VAL	N-CA-CB	8.30	120.26	110.55
1	G	24	VAL	N-CA-CB	8.30	120.26	110.55
2	H	183	VAL	N-CA-CB	-8.30	101.24	112.28
2	L	183	VAL	N-CA-CB	-8.29	101.26	112.28
2	H	449	TYR	CA-C-O	-8.28	111.78	120.23
1	E	24	VAL	N-CA-CB	8.28	120.24	110.55
2	F	183	VAL	N-CA-CB	-8.28	101.27	112.28
2	D	183	VAL	N-CA-CB	-8.27	101.28	112.28
2	J	449	TYR	CA-C-O	-8.27	111.79	120.23
2	J	183	VAL	N-CA-CB	-8.26	101.29	112.28
2	D	449	TYR	CA-C-O	-8.25	111.82	120.23
2	L	449	TYR	CA-C-O	-8.23	111.83	120.23
2	B	449	TYR	CA-C-O	-8.23	111.83	120.23
2	F	449	TYR	CA-C-O	-8.22	111.85	120.23
2	B	38	MET	CA-C-O	-8.19	111.70	120.46
2	J	38	MET	CA-C-O	-8.17	111.71	120.46
2	D	38	MET	CA-C-O	-8.16	111.73	120.46
2	L	38	MET	CA-C-O	-8.16	111.73	120.46
2	F	38	MET	CA-C-O	-8.15	111.74	120.46
1	S	49	MET	CA-CB-CG	-8.13	97.84	114.10
1	G	49	MET	CA-CB-CG	-8.13	97.84	114.10
1	A	49	MET	CA-CB-CG	-8.13	97.85	114.10
2	H	38	MET	CA-C-O	-8.13	111.77	120.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	49	MET	CA-CB-CG	-8.13	97.85	114.10
2	F	531	ILE	CB-CG1-CD1	8.12	130.86	113.80
2	B	531	ILE	CB-CG1-CD1	8.12	130.85	113.80
2	J	531	ILE	CB-CG1-CD1	8.12	130.85	113.80
1	E	49	MET	CA-CB-CG	-8.12	97.87	114.10
1	C	49	MET	CA-CB-CG	-8.11	97.88	114.10
2	L	531	ILE	CB-CG1-CD1	8.11	130.82	113.80
2	H	531	ILE	CB-CG1-CD1	8.10	130.81	113.80
2	D	531	ILE	CB-CG1-CD1	8.10	130.81	113.80
2	J	223	THR	CA-CB-CG2	8.03	124.15	110.50
1	I	83	TYR	CA-C-N	8.03	131.84	120.28
1	I	83	TYR	C-N-CA	8.03	131.84	120.28
2	D	223	THR	CA-CB-CG2	8.02	124.14	110.50
2	B	223	THR	CA-CB-CG2	8.02	124.12	110.50
1	C	83	TYR	CA-C-N	8.02	131.82	120.28
1	C	83	TYR	C-N-CA	8.02	131.82	120.28
2	L	223	THR	CA-CB-CG2	8.00	124.11	110.50
2	F	223	THR	CA-CB-CG2	8.00	124.11	110.50
1	S	83	TYR	CA-C-N	8.00	131.80	120.28
1	S	83	TYR	C-N-CA	8.00	131.80	120.28
1	A	83	TYR	CA-C-N	7.99	131.79	120.28
1	A	83	TYR	C-N-CA	7.99	131.79	120.28
1	E	83	TYR	CA-C-N	7.99	131.79	120.28
1	E	83	TYR	C-N-CA	7.99	131.79	120.28
2	H	223	THR	CA-CB-CG2	7.98	124.06	110.50
1	G	83	TYR	CA-C-N	7.97	131.76	120.28
1	G	83	TYR	C-N-CA	7.97	131.76	120.28
2	J	429	LEU	CA-C-O	7.97	129.19	120.82
2	B	429	LEU	CA-C-O	7.97	129.19	120.82
2	L	429	LEU	CA-C-O	7.96	129.18	120.82
2	D	429	LEU	CA-C-O	7.96	129.18	120.82
2	F	429	LEU	CA-C-O	7.95	129.16	120.82
2	H	429	LEU	CA-C-O	7.95	129.16	120.82
1	E	231	GLN	OE1-CD-NE2	7.92	130.52	122.60
1	A	231	GLN	OE1-CD-NE2	7.91	130.51	122.60
1	S	231	GLN	OE1-CD-NE2	7.91	130.51	122.60
1	I	231	GLN	OE1-CD-NE2	7.91	130.51	122.60
1	G	231	GLN	OE1-CD-NE2	7.89	130.49	122.60
1	C	231	GLN	OE1-CD-NE2	7.86	130.46	122.60
1	I	190	ARG	NH1-CZ-NH2	-7.85	109.10	119.30
2	B	205	LYS	CA-C-N	7.84	131.43	120.29
2	B	205	LYS	C-N-CA	7.84	131.43	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	107	ILE	CA-C-O	-7.84	112.24	120.39
2	F	205	LYS	CA-C-N	7.84	131.42	120.29
2	F	205	LYS	C-N-CA	7.84	131.42	120.29
2	H	205	LYS	CA-C-N	7.82	131.40	120.29
2	H	205	LYS	C-N-CA	7.82	131.40	120.29
2	D	205	LYS	CA-C-N	7.82	131.40	120.29
2	D	205	LYS	C-N-CA	7.82	131.40	120.29
1	C	190	ARG	NH1-CZ-NH2	-7.82	109.14	119.30
1	S	190	ARG	NH1-CZ-NH2	-7.82	109.14	119.30
1	G	190	ARG	NH1-CZ-NH2	-7.81	109.15	119.30
2	L	205	LYS	CA-C-N	7.80	131.37	120.29
2	L	205	LYS	C-N-CA	7.80	131.37	120.29
1	G	107	ILE	CA-C-O	-7.80	112.28	120.39
1	E	107	ILE	CA-C-O	-7.80	112.28	120.39
1	A	190	ARG	NH1-CZ-NH2	-7.80	109.16	119.30
1	E	190	ARG	NH1-CZ-NH2	-7.80	109.16	119.30
2	B	22	ARG	CD-NE-CZ	-7.79	113.49	124.40
2	J	205	LYS	CA-C-N	7.79	131.35	120.29
2	J	205	LYS	C-N-CA	7.79	131.35	120.29
2	J	276	LYS	CA-C-N	7.79	134.82	122.59
2	J	276	LYS	C-N-CA	7.79	134.82	122.59
2	F	22	ARG	CD-NE-CZ	-7.78	113.51	124.40
1	A	107	ILE	CA-C-O	-7.78	112.30	120.39
2	H	22	ARG	CD-NE-CZ	-7.77	113.52	124.40
1	S	107	ILE	CA-C-O	-7.76	112.31	120.39
2	L	22	ARG	CD-NE-CZ	-7.76	113.53	124.40
1	C	107	ILE	CA-C-O	-7.76	112.32	120.39
2	L	276	LYS	CA-C-N	7.75	134.75	122.59
2	L	276	LYS	C-N-CA	7.75	134.75	122.59
2	D	22	ARG	CD-NE-CZ	-7.75	113.56	124.40
2	J	22	ARG	CD-NE-CZ	-7.74	113.56	124.40
2	F	276	LYS	CA-C-N	7.74	134.74	122.59
2	F	276	LYS	C-N-CA	7.74	134.74	122.59
2	F	113	TYR	N-CA-C	7.74	120.84	111.40
2	B	276	LYS	CA-C-N	7.73	134.73	122.59
2	B	276	LYS	C-N-CA	7.73	134.73	122.59
2	H	276	LYS	CA-C-N	7.73	134.73	122.21
2	H	276	LYS	C-N-CA	7.73	134.73	122.21
2	D	276	LYS	CA-C-N	7.72	134.71	122.59
2	D	276	LYS	C-N-CA	7.72	134.71	122.59
2	J	528	ASP	CB-CA-C	7.72	117.72	111.00
2	B	528	ASP	CB-CA-C	7.72	117.71	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	528	ASP	CB-CA-C	7.71	117.71	111.00
2	H	113	TYR	N-CA-C	7.71	120.80	111.40
2	L	113	TYR	N-CA-C	7.71	120.80	111.40
2	F	528	ASP	CB-CA-C	7.71	117.70	111.00
2	J	113	TYR	N-CA-C	7.70	120.80	111.40
1	I	236	VAL	N-CA-CB	-7.70	98.53	111.23
1	G	236	VAL	N-CA-CB	-7.70	98.53	111.23
1	C	99	VAL	N-CA-C	7.69	118.28	110.82
2	L	528	ASP	CB-CA-C	7.69	117.69	111.00
2	J	107	ASP	CA-CB-CG	7.69	120.29	112.60
1	C	236	VAL	N-CA-CB	-7.69	98.55	111.23
1	E	236	VAL	N-CA-CB	-7.69	98.55	111.23
1	S	236	VAL	N-CA-CB	-7.68	98.55	111.23
2	B	113	TYR	N-CA-C	7.68	120.76	111.40
1	A	236	VAL	N-CA-CB	-7.67	98.58	111.23
2	B	107	ASP	CA-CB-CG	7.67	120.27	112.60
2	F	107	ASP	CA-CB-CG	7.67	120.27	112.60
2	F	14	ILE	N-CA-C	-7.66	98.77	108.89
2	D	113	TYR	N-CA-C	7.66	120.75	111.40
2	D	465	MET	N-CA-C	7.66	120.18	109.15
2	D	14	ILE	N-CA-C	-7.66	98.78	108.89
2	J	14	ILE	N-CA-C	-7.66	98.78	108.89
2	L	107	ASP	CA-CB-CG	7.66	120.25	112.60
2	H	465	MET	N-CA-C	7.66	120.17	109.15
2	F	465	MET	N-CA-C	7.65	120.17	109.15
1	S	99	VAL	N-CA-C	7.65	118.24	110.82
2	L	14	ILE	N-CA-C	-7.65	98.79	108.89
1	G	99	VAL	N-CA-C	7.65	118.24	110.82
2	L	465	MET	N-CA-C	7.64	120.16	109.15
2	J	465	MET	N-CA-C	7.64	120.16	109.15
2	H	14	ILE	N-CA-C	-7.64	98.80	108.89
2	B	14	ILE	N-CA-C	-7.64	98.81	108.89
2	H	107	ASP	CA-CB-CG	7.64	120.24	112.60
2	H	444	TYR	N-CA-C	7.63	122.04	109.06
1	I	99	VAL	N-CA-C	7.63	118.22	110.82
2	J	444	TYR	N-CA-C	7.63	122.04	109.06
2	D	107	ASP	CA-CB-CG	7.63	120.23	112.60
2	B	444	TYR	N-CA-C	7.62	122.02	109.06
2	B	465	MET	N-CA-C	7.62	120.12	109.15
2	D	444	TYR	N-CA-C	7.62	122.02	109.06
2	H	528	ASP	CB-CA-C	7.62	117.63	111.00
2	F	444	TYR	N-CA-C	7.62	122.00	109.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	444	TYR	N-CA-C	7.61	122.00	109.06
1	A	99	VAL	N-CA-C	7.61	118.20	110.82
1	E	99	VAL	N-CA-C	7.61	118.20	110.82
2	D	212	ILE	CA-C-O	-7.53	112.69	121.05
2	F	81	ASP	N-CA-C	-7.53	103.01	111.07
2	H	212	ILE	CA-C-O	-7.52	112.70	121.05
2	B	212	ILE	CA-C-O	-7.52	112.71	121.05
2	B	298	THR	CB-CA-C	7.52	120.28	109.08
2	D	81	ASP	N-CA-C	-7.51	103.03	111.07
2	H	81	ASP	N-CA-C	-7.51	103.03	111.07
2	B	392	LEU	CA-C-N	7.51	130.09	120.70
2	B	392	LEU	C-N-CA	7.51	130.09	120.70
2	F	212	ILE	CA-C-O	-7.51	112.72	121.05
2	L	212	ILE	CA-C-O	-7.51	112.72	121.05
2	F	392	LEU	CA-C-N	7.51	130.08	120.70
2	F	392	LEU	C-N-CA	7.51	130.08	120.70
2	F	298	THR	CB-CA-C	7.50	120.25	109.08
2	J	298	THR	CB-CA-C	7.50	120.25	109.08
2	L	81	ASP	N-CA-C	-7.50	103.05	111.07
2	B	81	ASP	N-CA-C	-7.49	103.06	111.07
2	H	353	ARG	NE-CZ-NH1	7.49	128.99	121.50
2	J	81	ASP	N-CA-C	-7.49	103.06	111.07
2	L	298	THR	CB-CA-C	7.48	120.23	109.08
2	H	298	THR	CB-CA-C	7.48	120.23	109.08
2	J	212	ILE	CA-C-O	-7.48	112.75	121.05
2	D	392	LEU	CA-C-N	7.47	130.04	120.70
2	D	392	LEU	C-N-CA	7.47	130.04	120.70
2	D	298	THR	CB-CA-C	7.47	120.21	109.08
2	L	392	LEU	CA-C-N	7.46	130.03	120.70
2	L	392	LEU	C-N-CA	7.46	130.03	120.70
2	H	392	LEU	CA-C-N	7.45	130.02	120.70
2	H	392	LEU	C-N-CA	7.45	130.02	120.70
2	J	353	ARG	NE-CZ-NH1	7.45	128.95	121.50
1	I	38	ASP	CA-CB-CG	7.44	120.04	112.60
1	C	38	ASP	CA-CB-CG	7.44	120.04	112.60
2	D	353	ARG	NE-CZ-NH1	7.43	128.93	121.50
2	J	392	LEU	CA-C-N	7.43	129.99	120.70
2	J	392	LEU	C-N-CA	7.43	129.99	120.70
2	F	353	ARG	NE-CZ-NH1	7.42	128.92	121.50
2	L	353	ARG	NE-CZ-NH1	7.41	128.91	121.50
1	A	38	ASP	CA-CB-CG	7.41	120.01	112.60
2	H	267	PHE	CA-CB-CG	-7.40	106.40	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	38	ASP	CA-CB-CG	7.39	120.00	112.60
2	B	353	ARG	NE-CZ-NH1	7.39	128.90	121.50
1	G	38	ASP	CA-CB-CG	7.39	119.99	112.60
2	F	267	PHE	CA-CB-CG	-7.38	106.42	113.80
2	B	267	PHE	CA-CB-CG	-7.38	106.42	113.80
2	L	267	PHE	CA-CB-CG	-7.38	106.42	113.80
1	E	38	ASP	CA-CB-CG	7.37	119.97	112.60
2	J	267	PHE	CA-CB-CG	-7.36	106.44	113.80
2	D	267	PHE	CA-CB-CG	-7.35	106.45	113.80
2	L	27	VAL	CB-CA-C	7.34	122.77	110.95
2	D	27	VAL	CB-CA-C	7.34	122.77	110.95
2	J	27	VAL	CB-CA-C	7.34	122.77	110.95
2	F	84	VAL	N-CA-CB	-7.34	102.79	112.26
2	F	27	VAL	CB-CA-C	7.34	122.77	110.95
2	D	84	VAL	N-CA-CB	-7.33	102.80	112.26
2	B	84	VAL	N-CA-CB	-7.32	102.82	112.26
2	H	27	VAL	CB-CA-C	7.32	122.73	110.95
2	B	27	VAL	CB-CA-C	7.32	122.73	110.95
2	H	84	VAL	N-CA-CB	-7.32	102.82	112.26
2	L	84	VAL	N-CA-CB	-7.31	102.82	112.26
2	J	84	VAL	N-CA-CB	-7.31	102.82	112.26
1	A	138	LEU	N-CA-C	-7.24	104.02	112.92
1	C	138	LEU	N-CA-C	-7.23	104.03	112.92
1	E	238	TRP	O-C-N	7.21	126.91	121.65
1	E	241	GLN	CB-CG-CD	7.20	124.84	112.60
2	H	139	ASN	CB-CG-ND2	7.20	127.20	116.40
1	I	241	GLN	CB-CG-CD	7.20	124.83	112.60
1	A	135	LEU	N-CA-CB	-7.19	99.75	110.61
2	J	413	ALA	O-C-N	-7.19	113.80	122.22
1	S	135	LEU	N-CA-CB	-7.19	99.75	110.61
1	G	135	LEU	N-CA-CB	-7.19	99.76	110.61
2	B	139	ASN	CB-CG-ND2	7.19	127.18	116.40
1	G	238	TRP	O-C-N	7.19	126.90	121.65
1	S	241	GLN	CB-CG-CD	7.18	124.81	112.60
2	B	413	ALA	O-C-N	-7.18	113.82	122.22
1	C	135	LEU	N-CA-CB	-7.18	99.77	110.61
1	E	135	LEU	N-CA-CB	-7.18	99.77	110.61
1	G	241	GLN	CB-CG-CD	7.18	124.81	112.60
2	L	413	ALA	O-C-N	-7.18	113.82	122.22
2	L	139	ASN	CB-CG-ND2	7.17	127.16	116.40
1	A	241	GLN	CB-CG-CD	7.17	124.80	112.60
2	J	139	ASN	CB-CG-ND2	7.17	127.16	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	238	TRP	O-C-N	7.17	126.89	121.65
1	I	135	LEU	N-CA-CB	-7.17	99.79	110.61
1	A	238	TRP	O-C-N	7.17	126.88	121.65
1	I	238	TRP	O-C-N	7.16	126.88	121.65
1	C	241	GLN	CB-CG-CD	7.16	124.77	112.60
1	C	238	TRP	O-C-N	7.16	126.87	121.65
2	D	139	ASN	CB-CG-ND2	7.16	127.13	116.40
2	F	139	ASN	CB-CG-ND2	7.16	127.13	116.40
2	F	413	ALA	O-C-N	-7.15	113.85	122.22
2	B	277	THR	CA-C-N	7.15	134.03	122.81
2	B	277	THR	C-N-CA	7.15	134.03	122.81
2	D	413	ALA	O-C-N	-7.15	113.86	122.22
2	H	413	ALA	O-C-N	-7.14	113.86	122.22
2	F	277	THR	CA-C-N	7.13	134.01	122.81
2	F	277	THR	C-N-CA	7.13	134.01	122.81
2	L	277	THR	CA-C-N	7.13	134.00	122.81
2	L	277	THR	C-N-CA	7.13	134.00	122.81
2	D	277	THR	CA-C-N	7.13	134.00	122.81
2	D	277	THR	C-N-CA	7.13	134.00	122.81
2	H	277	THR	CA-C-N	7.13	134.00	122.81
2	H	277	THR	C-N-CA	7.13	134.00	122.81
2	J	277	THR	CA-C-N	7.11	133.97	122.81
2	J	277	THR	C-N-CA	7.11	133.97	122.81
2	D	247	LYS	CA-C-O	-7.08	113.39	120.82
2	F	247	LYS	CA-C-O	-7.07	113.39	120.82
1	G	190	ARG	NE-CZ-NH2	7.07	125.56	119.20
2	L	247	LYS	CA-C-O	-7.06	113.41	120.82
2	H	247	LYS	CA-C-O	-7.06	113.41	120.82
2	B	247	LYS	CA-C-O	-7.04	113.42	120.82
1	C	190	ARG	NE-CZ-NH2	7.04	125.53	119.20
2	J	247	LYS	CA-C-O	-7.04	113.43	120.82
1	S	190	ARG	NE-CZ-NH2	7.04	125.53	119.20
1	I	190	ARG	NE-CZ-NH2	7.04	125.53	119.20
2	B	24	GLU	CB-CG-CD	7.03	124.55	112.60
1	E	190	ARG	NE-CZ-NH2	7.03	125.52	119.20
2	D	24	GLU	CB-CG-CD	7.02	124.54	112.60
1	A	190	ARG	NE-CZ-NH2	7.01	125.51	119.20
2	J	24	GLU	CB-CG-CD	7.01	124.52	112.60
2	J	238	ARG	CD-NE-CZ	-7.01	114.59	124.40
2	H	24	GLU	CB-CG-CD	7.01	124.51	112.60
2	L	24	GLU	CB-CG-CD	7.00	124.51	112.60
1	I	78	MET	N-CA-CB	-7.00	100.86	110.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	298	THR	N-CA-C	-7.00	100.97	109.72
2	H	298	THR	N-CA-C	-7.00	100.97	109.72
2	D	238	ARG	CD-NE-CZ	-7.00	114.60	124.40
2	J	298	THR	N-CA-C	-7.00	100.97	109.72
2	L	298	THR	N-CA-C	-7.00	100.97	109.72
2	D	298	THR	N-CA-C	-6.99	100.98	109.72
1	E	78	MET	N-CA-CB	-6.99	100.89	110.95
2	L	238	ARG	CD-NE-CZ	-6.99	114.62	124.40
2	B	298	THR	N-CA-C	-6.99	100.99	109.72
2	F	24	GLU	CB-CG-CD	6.99	124.47	112.60
2	B	238	ARG	CD-NE-CZ	-6.98	114.62	124.40
1	A	78	MET	N-CA-CB	-6.98	100.90	110.95
1	G	78	MET	N-CA-CB	-6.97	100.91	110.95
2	H	238	ARG	CD-NE-CZ	-6.97	114.64	124.40
1	S	78	MET	N-CA-CB	-6.97	100.92	110.95
2	F	238	ARG	CD-NE-CZ	-6.96	114.65	124.40
1	C	78	MET	N-CA-CB	-6.95	100.94	110.95
1	E	138	LEU	N-CA-C	-6.93	103.93	112.88
2	H	399	VAL	O-C-N	6.93	130.10	122.75
2	L	399	VAL	O-C-N	6.92	130.08	122.75
2	F	399	VAL	O-C-N	6.92	130.08	122.75
1	A	40	ILE	CA-C-O	-6.91	114.19	121.44
1	E	40	ILE	CA-C-O	-6.91	114.19	121.44
1	G	138	LEU	N-CA-C	-6.91	103.97	112.88
1	G	230	LYS	CA-C-O	-6.91	112.57	120.24
1	E	230	LYS	CA-C-O	-6.90	112.58	120.24
1	S	138	LEU	N-CA-C	-6.90	103.98	112.88
2	B	399	VAL	O-C-N	6.90	130.06	122.75
1	G	241	GLN	OE1-CD-NE2	-6.89	115.70	122.60
1	S	40	ILE	CA-C-O	-6.89	114.20	121.44
2	F	61	THR	O-C-N	6.88	129.42	122.12
1	C	40	ILE	CA-C-O	-6.88	114.21	121.44
2	J	399	VAL	O-C-N	6.88	130.04	122.75
1	S	230	LYS	CA-C-O	-6.88	112.60	120.24
2	B	61	THR	O-C-N	6.88	129.41	122.12
2	H	130	ASP	CB-CA-C	6.87	116.98	110.17
1	C	230	LYS	CA-C-O	-6.87	112.61	120.24
1	I	230	LYS	CA-C-O	-6.87	112.61	120.24
1	G	40	ILE	CA-C-O	-6.87	114.23	121.44
1	I	40	ILE	CA-C-O	-6.87	114.23	121.44
1	I	138	LEU	N-CA-C	-6.87	104.02	112.88
1	E	144	ASN	CA-C-O	-6.87	113.40	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	399	VAL	O-C-N	6.86	130.03	122.75
2	L	61	THR	O-C-N	6.86	129.39	122.12
2	L	130	ASP	CB-CA-C	6.85	116.95	110.17
1	A	230	LYS	CA-C-O	-6.85	112.64	120.24
2	H	61	THR	O-C-N	6.85	129.38	122.12
1	C	241	GLN	OE1-CD-NE2	-6.84	115.76	122.60
2	D	61	THR	O-C-N	6.84	129.37	122.12
1	S	241	GLN	OE1-CD-NE2	-6.84	115.76	122.60
2	D	130	ASP	CB-CA-C	6.84	116.94	110.17
2	F	130	ASP	CB-CA-C	6.84	116.94	110.17
1	I	241	GLN	OE1-CD-NE2	-6.84	115.76	122.60
2	J	61	THR	O-C-N	6.84	129.37	122.12
1	A	241	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	E	241	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	I	144	ASN	CA-C-O	-6.83	113.44	120.54
1	S	144	ASN	CA-C-O	-6.83	113.44	120.54
2	B	130	ASP	CB-CA-C	6.82	116.92	110.17
1	G	144	ASN	CA-C-O	-6.82	113.45	120.54
2	J	130	ASP	CB-CA-C	6.81	116.91	110.17
1	C	144	ASN	CA-C-O	-6.80	113.47	120.54
1	A	144	ASN	CA-C-O	-6.79	113.47	120.54
2	D	212	ILE	O-C-N	6.79	128.96	121.90
2	H	212	ILE	O-C-N	6.79	128.96	121.90
2	F	212	ILE	O-C-N	6.78	128.95	121.90
2	L	212	ILE	O-C-N	6.78	128.95	121.90
2	L	133	LYS	CB-CA-C	6.76	124.17	110.38
2	B	212	ILE	O-C-N	6.76	128.93	121.90
2	D	300	GLN	CA-CB-CG	6.76	127.61	114.10
2	F	133	LYS	CB-CA-C	6.76	124.17	110.38
2	J	300	GLN	CA-CB-CG	6.76	127.61	114.10
2	B	300	GLN	CA-CB-CG	6.75	127.61	114.10
2	H	133	LYS	CB-CA-C	6.75	124.16	110.38
2	D	133	LYS	CB-CA-C	6.75	124.15	110.38
2	J	133	LYS	CB-CA-C	6.75	124.14	110.38
2	F	300	GLN	CA-CB-CG	6.74	127.58	114.10
2	L	300	GLN	CA-CB-CG	6.74	127.58	114.10
2	B	133	LYS	CB-CA-C	6.74	124.13	110.38
2	H	300	GLN	CA-CB-CG	6.74	127.58	114.10
1	E	161	HIS	CA-C-O	6.72	127.62	120.70
1	S	161	HIS	CA-C-O	6.71	127.61	120.70
2	J	212	ILE	O-C-N	6.71	128.88	121.90
2	J	523	THR	N-CA-CB	6.71	119.79	110.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	523	THR	N-CA-CB	6.70	119.79	110.07
2	F	523	THR	N-CA-CB	6.70	119.78	110.07
1	C	161	HIS	CA-C-O	6.70	127.60	120.70
1	G	161	HIS	CA-C-O	6.69	127.59	120.70
2	H	523	THR	N-CA-CB	6.69	119.77	110.07
2	B	183	VAL	CA-C-O	-6.69	113.29	119.91
2	H	183	VAL	CA-C-O	-6.69	113.29	119.91
2	B	523	THR	N-CA-CB	6.69	119.77	110.07
1	I	161	HIS	CA-C-O	6.68	127.58	120.70
2	D	183	VAL	CA-C-O	-6.68	113.29	119.91
1	I	49	MET	N-CA-C	6.68	120.17	110.28
2	D	523	THR	N-CA-CB	6.68	119.75	110.07
1	G	49	MET	N-CA-C	6.67	120.14	110.28
1	A	49	MET	N-CA-C	6.66	120.14	110.28
1	S	49	MET	N-CA-C	6.66	120.14	110.28
1	C	49	MET	N-CA-C	6.66	120.14	110.28
1	C	224	THR	O-C-N	6.66	131.15	123.29
2	L	183	VAL	CA-C-O	-6.65	113.33	119.91
1	E	49	MET	N-CA-C	6.65	120.12	110.28
1	A	161	HIS	CA-C-O	6.64	127.54	120.70
2	F	183	VAL	CA-C-O	-6.64	113.33	119.91
1	S	224	THR	O-C-N	6.63	131.12	123.29
1	A	224	THR	O-C-N	6.63	131.12	123.29
1	E	224	THR	O-C-N	6.63	131.12	123.29
2	J	183	VAL	CA-C-O	-6.63	113.34	119.91
2	B	533	CYS	CB-CA-C	-6.62	100.44	110.90
2	L	533	CYS	CB-CA-C	-6.61	100.45	110.90
2	J	533	CYS	CB-CA-C	-6.61	100.45	110.90
2	H	533	CYS	CB-CA-C	-6.61	100.45	110.90
2	H	17	ILE	N-CA-CB	6.61	119.92	112.32
1	G	224	THR	O-C-N	6.61	131.08	123.29
2	D	533	CYS	CB-CA-C	-6.60	100.47	110.90
1	I	224	THR	O-C-N	6.60	131.08	123.29
2	J	17	ILE	N-CA-CB	6.59	119.90	112.32
2	F	533	CYS	CB-CA-C	-6.59	100.49	110.90
1	A	225	TYR	O-C-N	6.58	130.88	123.05
2	B	183	VAL	N-CA-C	6.58	118.42	112.17
1	G	225	TYR	O-C-N	6.58	130.88	123.05
2	H	183	VAL	N-CA-C	6.58	118.42	112.17
1	E	69	VAL	O-C-N	6.57	129.90	122.93
2	F	183	VAL	N-CA-C	6.57	118.41	112.17
2	D	17	ILE	N-CA-CB	6.57	119.87	112.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	183	VAL	N-CA-C	6.57	118.41	112.17
1	E	225	TYR	O-C-N	6.57	130.87	123.05
2	F	17	ILE	N-CA-CB	6.57	119.87	112.32
2	D	183	VAL	N-CA-C	6.57	118.41	112.17
1	I	225	TYR	O-C-N	6.57	130.86	123.05
2	J	183	VAL	N-CA-C	6.56	118.40	112.17
2	D	241	GLU	CB-CA-C	-6.56	100.58	110.88
2	L	17	ILE	N-CA-CB	6.56	119.86	112.32
1	A	259	SER	N-CA-C	-6.56	101.03	110.40
1	C	259	SER	N-CA-C	-6.55	101.03	110.40
2	F	241	GLU	CB-CA-C	-6.55	100.59	110.88
1	E	259	SER	N-CA-C	-6.55	101.03	110.40
1	S	225	TYR	O-C-N	6.55	130.85	123.05
1	C	60	LEU	N-CA-C	-6.55	104.06	111.07
1	I	259	SER	N-CA-C	-6.55	101.03	110.40
1	S	259	SER	N-CA-C	-6.55	101.04	110.40
2	F	248	GLU	CA-CB-CG	6.55	127.19	114.10
2	H	241	GLU	CB-CA-C	-6.55	100.60	110.88
2	B	17	ILE	N-CA-CB	6.54	119.85	112.32
1	A	35	LEU	CA-C-N	6.54	130.81	120.47
1	A	35	LEU	C-N-CA	6.54	130.81	120.47
1	G	259	SER	N-CA-C	-6.54	101.05	110.40
2	L	248	GLU	CA-CB-CG	6.54	127.17	114.10
2	J	248	GLU	CA-CB-CG	6.54	127.17	114.10
1	I	69	VAL	O-C-N	6.53	129.86	122.93
2	L	241	GLU	CB-CA-C	-6.53	100.63	110.88
1	C	225	TYR	O-C-N	6.53	130.82	123.05
2	H	248	GLU	CA-CB-CG	6.53	127.16	114.10
2	J	241	GLU	CB-CA-C	-6.53	100.63	110.88
1	A	60	LEU	N-CA-C	-6.52	104.09	111.07
2	D	248	GLU	CA-CB-CG	6.52	127.14	114.10
2	B	248	GLU	CA-CB-CG	6.52	127.13	114.10
1	I	60	LEU	N-CA-C	-6.52	104.10	111.07
1	G	35	LEU	CA-C-N	6.51	130.76	120.47
1	G	35	LEU	C-N-CA	6.51	130.76	120.47
1	S	69	VAL	O-C-N	6.50	129.82	122.93
1	S	35	LEU	CA-C-N	6.50	130.74	120.47
1	S	35	LEU	C-N-CA	6.50	130.74	120.47
1	A	69	VAL	O-C-N	6.50	129.82	122.93
1	I	35	LEU	CA-C-N	6.50	130.74	120.47
1	I	35	LEU	C-N-CA	6.50	130.74	120.47
1	G	60	LEU	N-CA-C	-6.50	104.11	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	60	LEU	N-CA-C	-6.50	104.11	111.07
2	B	241	GLU	CB-CA-C	-6.50	100.67	110.88
2	D	312	ASP	CA-C-O	6.50	129.41	121.94
2	B	312	ASP	CA-C-O	6.49	129.40	121.94
1	C	69	VAL	O-C-N	6.49	129.81	122.93
1	E	60	LEU	N-CA-C	-6.49	104.13	111.07
1	E	35	LEU	CA-C-N	6.49	130.72	120.47
1	E	35	LEU	C-N-CA	6.49	130.72	120.47
2	H	312	ASP	CA-C-O	6.48	129.39	121.94
2	L	312	ASP	CA-C-O	6.48	129.39	121.94
2	H	84	VAL	CA-C-N	6.48	133.34	120.77
2	H	84	VAL	C-N-CA	6.48	133.34	120.77
2	J	312	ASP	CA-C-O	6.48	129.39	121.94
2	D	84	VAL	CA-C-N	6.47	133.32	120.77
2	D	84	VAL	C-N-CA	6.47	133.32	120.77
2	L	84	VAL	CA-C-N	6.47	133.31	120.77
2	L	84	VAL	C-N-CA	6.47	133.31	120.77
2	J	276	LYS	CA-C-O	6.47	128.42	121.05
2	F	443	LEU	O-C-N	6.46	128.85	122.19
2	H	276	LYS	CA-C-O	6.46	128.42	121.05
1	C	35	LEU	CA-C-N	6.46	130.68	120.47
1	C	35	LEU	C-N-CA	6.46	130.68	120.47
2	F	84	VAL	CA-C-N	6.46	133.30	120.77
2	F	84	VAL	C-N-CA	6.46	133.30	120.77
2	B	276	LYS	CA-C-O	6.45	128.41	121.05
2	D	276	LYS	CA-C-O	6.45	128.40	121.05
2	J	84	VAL	CA-C-N	6.45	133.28	120.77
2	J	84	VAL	C-N-CA	6.45	133.28	120.77
2	L	443	LEU	O-C-N	6.45	128.83	122.19
2	B	84	VAL	CA-C-N	6.45	133.28	120.77
2	B	84	VAL	C-N-CA	6.45	133.28	120.77
2	L	276	LYS	CA-C-O	6.44	128.40	121.05
2	D	82	ASN	CB-CG-ND2	6.44	126.06	116.40
1	G	69	VAL	O-C-N	6.44	129.76	122.93
2	H	443	LEU	O-C-N	6.44	128.82	122.19
2	F	312	ASP	CA-C-O	6.44	129.34	121.94
2	F	82	ASN	CB-CG-ND2	6.44	126.05	116.40
2	D	443	LEU	O-C-N	6.43	128.82	122.19
2	H	82	ASN	CB-CG-ND2	6.43	126.05	116.40
2	H	137	LEU	N-CA-CB	-6.43	100.66	110.12
2	J	82	ASN	CB-CG-ND2	6.43	126.05	116.40
2	B	443	LEU	O-C-N	6.43	128.81	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	137	LEU	N-CA-CB	-6.43	100.67	110.12
2	L	82	ASN	CB-CG-ND2	6.42	126.03	116.40
2	D	137	LEU	N-CA-CB	-6.42	100.68	110.12
1	G	27	THR	CA-C-O	6.42	128.21	121.15
2	L	137	LEU	N-CA-CB	-6.41	100.70	110.12
1	A	27	THR	CA-C-O	6.41	128.20	121.15
2	J	137	LEU	N-CA-CB	-6.41	100.70	110.12
1	E	27	THR	CA-C-O	6.41	128.20	121.15
2	F	276	LYS	CA-C-O	6.40	128.35	121.05
2	J	241	GLU	CA-C-N	6.40	128.76	120.44
2	J	241	GLU	C-N-CA	6.40	128.76	120.44
1	S	27	THR	CA-C-O	6.40	128.19	121.15
2	B	137	LEU	N-CA-CB	-6.40	100.72	110.12
2	J	443	LEU	O-C-N	6.39	128.78	122.19
2	B	82	ASN	CB-CG-ND2	6.39	125.99	116.40
2	F	241	GLU	CA-C-N	6.39	128.75	120.44
2	F	241	GLU	C-N-CA	6.39	128.75	120.44
1	I	27	THR	CA-C-O	6.39	128.18	121.15
2	F	9	ILE	CA-C-O	-6.38	113.60	120.36
2	L	241	GLU	CA-C-N	6.37	128.72	120.44
2	L	241	GLU	C-N-CA	6.37	128.72	120.44
1	C	27	THR	CA-C-O	6.37	128.15	121.15
2	D	241	GLU	CA-C-N	6.37	128.72	120.44
2	D	241	GLU	C-N-CA	6.37	128.72	120.44
2	B	241	GLU	CA-C-N	6.36	128.71	120.44
2	B	241	GLU	C-N-CA	6.36	128.71	120.44
1	C	16	GLU	CA-CB-CG	6.36	126.82	114.10
1	S	16	GLU	CA-CB-CG	6.36	126.81	114.10
1	E	16	GLU	CA-CB-CG	6.36	126.81	114.10
2	H	9	ILE	CA-C-O	-6.36	113.62	120.36
1	I	16	GLU	CA-CB-CG	6.36	126.81	114.10
2	H	188	VAL	N-CA-C	-6.35	104.08	111.00
2	H	241	GLU	CA-C-N	6.35	128.70	120.44
2	H	241	GLU	C-N-CA	6.35	128.70	120.44
1	G	16	GLU	CA-CB-CG	6.35	126.79	114.10
1	A	16	GLU	CA-CB-CG	6.34	126.78	114.10
2	D	188	VAL	N-CA-C	-6.34	104.09	111.00
2	F	170	PHE	CA-CB-CG	-6.34	107.46	113.80
2	L	188	VAL	N-CA-C	-6.34	104.09	111.00
2	J	9	ILE	CA-C-O	-6.33	113.64	120.36
2	D	170	PHE	CA-CB-CG	-6.33	107.47	113.80
2	B	170	PHE	CA-CB-CG	-6.33	107.47	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	ILE	CA-C-O	-6.32	113.66	120.36
2	F	188	VAL	N-CA-C	-6.32	104.11	111.00
2	J	170	PHE	CA-CB-CG	-6.32	107.48	113.80
2	L	9	ILE	CA-C-O	-6.32	113.66	120.36
2	B	188	VAL	N-CA-C	-6.31	104.12	111.00
2	J	188	VAL	N-CA-C	-6.30	104.13	111.00
2	F	248	GLU	CB-CG-CD	6.30	123.31	112.60
2	D	296	ARG	CD-NE-CZ	6.30	133.22	124.40
2	B	9	ILE	CA-C-O	-6.30	113.68	120.36
2	L	170	PHE	CA-CB-CG	-6.29	107.50	113.80
2	H	248	GLU	CB-CG-CD	6.29	123.30	112.60
2	H	296	ARG	CD-NE-CZ	6.29	133.21	124.40
2	L	248	GLU	CB-CG-CD	6.29	123.29	112.60
2	D	20	HIS	CA-CB-CG	-6.29	107.51	113.80
1	I	187	ASN	CA-CB-CG	-6.28	106.32	112.60
1	G	187	ASN	CA-CB-CG	-6.28	106.32	112.60
2	H	170	PHE	CA-CB-CG	-6.28	107.52	113.80
2	J	248	GLU	CB-CG-CD	6.28	123.27	112.60
2	L	296	ARG	CD-NE-CZ	6.27	133.18	124.40
2	B	20	HIS	CA-CB-CG	-6.27	107.53	113.80
1	A	187	ASN	CA-CB-CG	-6.27	106.33	112.60
1	G	198	GLU	CA-C-N	6.27	132.34	122.94
1	G	198	GLU	C-N-CA	6.27	132.34	122.94
2	H	20	HIS	CA-CB-CG	-6.27	107.53	113.80
2	B	248	GLU	CB-CG-CD	6.26	123.25	112.60
2	B	296	ARG	CD-NE-CZ	6.26	133.17	124.40
2	F	296	ARG	CD-NE-CZ	6.26	133.17	124.40
2	D	248	GLU	CB-CG-CD	6.26	123.24	112.60
2	F	20	HIS	CA-CB-CG	-6.25	107.55	113.80
2	J	296	ARG	CD-NE-CZ	6.25	133.15	124.40
1	S	187	ASN	CA-CB-CG	-6.25	106.35	112.60
2	L	20	HIS	CA-CB-CG	-6.25	107.55	113.80
2	J	20	HIS	CA-CB-CG	-6.25	107.55	113.80
2	D	352	ASP	O-C-N	6.24	129.81	122.00
2	H	352	ASP	O-C-N	6.24	129.80	122.00
2	B	272	ALA	N-CA-C	-6.24	105.65	113.20
2	F	272	ALA	N-CA-C	-6.23	105.66	113.20
2	J	533	CYS	CA-C-O	-6.23	114.28	120.70
2	H	272	ALA	N-CA-C	-6.23	105.66	113.20
1	C	89	GLY	N-CA-C	-6.23	106.82	114.92
1	C	187	ASN	CA-CB-CG	-6.23	106.37	112.60
1	I	21	SER	CA-C-O	-6.23	114.28	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	89	GLY	N-CA-C	-6.23	106.82	114.92
2	J	272	ALA	N-CA-C	-6.23	105.67	113.20
2	L	272	ALA	N-CA-C	-6.23	105.67	113.20
1	G	190	ARG	N-CA-C	-6.22	105.67	113.20
1	S	198	GLU	CA-C-N	6.22	132.27	122.94
1	S	198	GLU	C-N-CA	6.22	132.27	122.94
1	I	198	GLU	CA-C-N	6.22	132.27	122.94
1	I	198	GLU	C-N-CA	6.22	132.27	122.94
2	D	272	ALA	N-CA-C	-6.22	105.68	113.20
1	C	21	SER	CA-C-O	-6.21	114.30	120.70
1	E	187	ASN	CA-CB-CG	-6.21	106.39	112.60
1	C	198	GLU	CA-C-N	6.21	132.26	122.94
1	C	198	GLU	C-N-CA	6.21	132.26	122.94
2	H	248	GLU	O-C-N	-6.21	115.63	122.09
1	G	89	GLY	N-CA-C	-6.21	106.85	114.92
1	E	190	ARG	N-CA-C	-6.21	105.69	113.20
2	F	198	GLU	CA-C-O	-6.21	113.97	120.55
1	A	198	GLU	CA-C-N	6.21	132.25	122.94
1	A	198	GLU	C-N-CA	6.21	132.25	122.94
2	J	248	GLU	O-C-N	-6.21	115.64	122.09
1	S	21	SER	CA-C-O	-6.20	114.31	120.70
2	L	352	ASP	O-C-N	6.20	129.75	122.00
1	A	190	ARG	N-CA-C	-6.20	105.70	113.20
1	E	198	GLU	CA-C-N	6.20	132.24	122.94
1	E	198	GLU	C-N-CA	6.20	132.24	122.94
2	J	352	ASP	O-C-N	6.20	129.75	122.00
2	B	533	CYS	CA-C-O	-6.20	114.31	120.70
1	S	190	ARG	N-CA-C	-6.20	105.70	113.20
2	H	533	CYS	CA-C-O	-6.20	114.32	120.70
1	I	111	THR	CA-CB-OG1	-6.19	100.31	109.60
1	S	89	GLY	N-CA-C	-6.19	106.87	114.92
2	B	352	ASP	O-C-N	6.19	129.74	122.00
1	I	89	GLY	N-CA-C	-6.19	106.87	114.92
1	E	21	SER	CA-C-O	-6.19	114.33	120.70
1	G	21	SER	CA-C-O	-6.19	114.33	120.70
1	G	182	GLU	CA-CB-CG	6.19	126.47	114.10
2	D	243	ARG	CA-C-N	6.19	128.48	120.44
2	D	243	ARG	C-N-CA	6.19	128.48	120.44
1	A	182	GLU	CA-CB-CG	6.18	126.46	114.10
1	A	89	GLY	N-CA-C	-6.18	106.89	114.92
2	B	243	ARG	CA-C-N	6.18	128.47	120.44
2	B	243	ARG	C-N-CA	6.18	128.47	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	114	HIS	CA-CB-CG	-6.18	107.62	113.80
2	L	533	CYS	CA-C-O	-6.18	114.34	120.70
1	S	182	GLU	CA-CB-CG	6.17	126.45	114.10
1	E	111	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	21	SER	CA-C-O	-6.17	114.34	120.70
1	C	190	ARG	N-CA-C	-6.17	105.73	113.20
2	F	248	GLU	O-C-N	-6.17	115.67	122.09
1	S	111	THR	CA-CB-OG1	-6.17	100.35	109.60
1	A	111	THR	CA-CB-OG1	-6.17	100.35	109.60
1	E	182	GLU	CA-CB-CG	6.17	126.43	114.10
2	F	473	ARG	CA-CB-CG	6.17	126.43	114.10
2	L	248	GLU	O-C-N	-6.17	115.68	122.09
1	E	215	TYR	CA-CB-CG	-6.17	102.80	113.90
2	B	473	ARG	CA-CB-CG	6.16	126.43	114.10
1	C	182	GLU	CA-CB-CG	6.16	126.43	114.10
2	F	114	HIS	CA-CB-CG	-6.16	107.64	113.80
1	I	182	GLU	CA-CB-CG	6.16	126.43	114.10
2	B	500	SER	CA-C-O	-6.16	114.97	121.99
1	C	215	TYR	CA-CB-CG	-6.16	102.81	113.90
2	D	473	ARG	CA-CB-CG	6.16	126.42	114.10
2	L	473	ARG	CA-CB-CG	6.16	126.41	114.10
2	B	114	HIS	CA-CB-CG	-6.16	107.64	113.80
1	C	111	THR	CA-CB-OG1	-6.16	100.37	109.60
2	F	352	ASP	O-C-N	6.16	129.70	122.00
1	G	215	TYR	CA-CB-CG	-6.15	102.83	113.90
2	L	114	HIS	CA-CB-CG	-6.15	107.65	113.80
2	B	248	GLU	O-C-N	-6.15	115.69	122.09
2	F	91	ASN	CA-CB-CG	6.15	118.75	112.60
1	I	190	ARG	N-CA-C	-6.15	105.76	113.20
2	L	198	GLU	CA-C-O	-6.15	114.03	120.55
2	H	114	HIS	CA-CB-CG	-6.15	107.65	113.80
2	J	198	GLU	CA-C-O	-6.15	114.03	120.55
1	S	215	TYR	CA-CB-CG	-6.14	102.84	113.90
2	H	366	ALA	CA-C-O	-6.14	114.05	121.05
2	L	243	ARG	CA-C-N	6.14	128.43	120.44
2	L	243	ARG	C-N-CA	6.14	128.43	120.44
2	B	198	GLU	CA-C-O	-6.14	114.04	120.55
2	F	243	ARG	CA-C-N	6.14	128.42	120.44
2	F	243	ARG	C-N-CA	6.14	128.42	120.44
2	H	198	GLU	CA-C-O	-6.14	114.04	120.55
2	H	473	ARG	CA-CB-CG	6.14	126.38	114.10
1	I	215	TYR	CA-CB-CG	-6.14	102.85	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	500	SER	CA-C-O	-6.14	114.99	121.99
1	A	215	TYR	CA-CB-CG	-6.14	102.85	113.90
2	F	533	CYS	CA-C-O	-6.14	114.38	120.70
2	H	243	ARG	CA-C-N	6.14	128.42	120.44
2	H	243	ARG	C-N-CA	6.14	128.42	120.44
1	G	235	GLN	N-CA-C	-6.13	105.38	112.86
1	I	236	VAL	N-CA-C	6.13	122.10	109.34
1	I	255	TRP	O-C-N	6.13	128.62	122.12
2	J	139	ASN	OD1-CG-ND2	-6.13	116.47	122.60
2	L	500	SER	CA-C-O	-6.13	115.00	121.99
1	E	6	ARG	NE-CZ-NH2	6.13	124.72	119.20
2	D	248	GLU	O-C-N	-6.13	115.72	122.09
1	G	111	THR	CA-CB-OG1	-6.13	100.41	109.60
2	H	139	ASN	OD1-CG-ND2	-6.13	116.47	122.60
2	B	91	ASN	CA-CB-CG	6.13	118.73	112.60
1	G	6	ARG	NE-CZ-NH2	6.13	124.71	119.20
1	G	236	VAL	N-CA-C	6.13	122.08	109.34
2	H	500	SER	CA-C-O	-6.13	115.01	121.99
2	J	114	HIS	CA-CB-CG	-6.13	107.67	113.80
2	J	243	ARG	CA-C-N	6.13	128.41	120.44
2	J	243	ARG	C-N-CA	6.13	128.41	120.44
2	L	139	ASN	OD1-CG-ND2	-6.12	116.48	122.60
2	D	458	PHE	CA-CB-CG	-6.12	107.68	113.80
2	J	473	ARG	CA-CB-CG	6.12	126.35	114.10
2	F	500	SER	CA-C-O	-6.12	115.01	121.99
1	E	236	VAL	N-CA-C	6.12	122.07	109.34
1	S	236	VAL	N-CA-C	6.12	122.06	109.34
2	D	366	ALA	CA-C-O	-6.12	114.08	121.05
2	D	533	CYS	CA-C-O	-6.12	114.40	120.70
2	D	500	SER	CA-C-O	-6.12	115.02	121.99
2	L	91	ASN	CA-CB-CG	6.12	118.72	112.60
2	B	139	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	S	235	GLN	N-CA-C	-6.11	105.40	112.86
2	F	458	PHE	CA-CB-CG	-6.11	107.69	113.80
2	H	458	PHE	CA-CB-CG	-6.11	107.69	113.80
1	I	235	GLN	N-CA-C	-6.11	105.40	112.86
2	L	458	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	236	VAL	N-CA-C	6.11	122.05	109.34
1	C	235	GLN	N-CA-C	-6.11	105.41	112.86
1	I	19	GLY	N-CA-C	-6.11	107.08	114.66
2	D	198	GLU	CA-C-O	-6.11	114.07	120.55
2	J	91	ASN	CA-CB-CG	6.10	118.70	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	458	PHE	CA-CB-CG	-6.10	107.70	113.80
2	L	366	ALA	CA-C-O	-6.10	114.09	121.05
2	D	483	VAL	CB-CA-C	6.10	117.99	110.73
2	D	530	CYS	O-C-N	6.10	130.95	123.14
2	H	91	ASN	CA-CB-CG	6.10	118.70	112.60
1	A	235	GLN	N-CA-C	-6.10	105.42	112.86
1	E	235	GLN	N-CA-C	-6.10	105.42	112.86
2	D	91	ASN	CA-CB-CG	6.10	118.70	112.60
2	B	366	ALA	CA-C-O	-6.09	114.10	121.05
2	B	458	PHE	CA-CB-CG	-6.09	107.70	113.80
1	G	19	GLY	N-CA-C	-6.09	107.10	114.66
2	B	528	ASP	N-CA-CB	-6.09	102.80	111.51
2	J	483	VAL	CB-CA-C	6.09	117.98	110.73
1	S	6	ARG	NE-CZ-NH2	6.09	124.68	119.20
2	F	366	ALA	CA-C-O	-6.09	114.11	121.05
1	C	236	VAL	N-CA-C	6.09	122.00	109.34
1	C	6	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	E	78	MET	CA-CB-CG	-6.09	101.92	114.10
2	F	528	ASP	N-CA-CB	-6.09	102.81	111.51
2	J	366	ALA	CA-C-O	-6.08	114.11	121.05
2	L	483	VAL	CB-CA-C	6.08	117.97	110.73
2	D	139	ASN	OD1-CG-ND2	-6.08	116.52	122.60
2	F	139	ASN	OD1-CG-ND2	-6.08	116.52	122.60
2	B	483	VAL	CB-CA-C	6.08	117.97	110.73
2	D	528	ASP	N-CA-CB	-6.08	102.81	111.51
1	S	19	GLY	N-CA-C	-6.08	107.12	114.66
2	F	530	CYS	O-C-N	6.08	130.92	123.14
1	I	78	MET	CA-CB-CG	-6.08	101.94	114.10
2	J	528	ASP	N-CA-CB	-6.08	102.82	111.51
1	E	19	GLY	N-CA-C	-6.08	107.13	114.66
1	I	6	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	S	78	MET	CA-CB-CG	-6.07	101.95	114.10
2	L	528	ASP	N-CA-CB	-6.07	102.83	111.51
1	A	160	VAL	O-C-N	-6.07	115.74	121.87
2	D	81	ASP	CA-C-N	6.07	128.42	120.28
2	D	81	ASP	C-N-CA	6.07	128.42	120.28
1	A	19	GLY	N-CA-C	-6.07	107.13	114.66
2	B	530	CYS	O-C-N	6.07	130.91	123.14
1	C	19	GLY	N-CA-C	-6.07	107.13	114.66
2	H	283	CYS	CA-C-N	6.07	129.38	121.85
2	H	283	CYS	C-N-CA	6.07	129.38	121.85
2	J	283	CYS	CA-C-N	6.07	129.38	121.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	283	CYS	C-N-CA	6.07	129.38	121.85
1	A	78	MET	CA-CB-CG	-6.07	101.96	114.10
2	B	344	LYS	CB-CA-C	-6.07	103.45	111.82
2	J	183	VAL	O-C-N	-6.07	115.68	122.05
2	L	530	CYS	O-C-N	6.07	130.90	123.14
1	A	6	ARG	NE-CZ-NH2	6.07	124.66	119.20
2	F	483	VAL	CB-CA-C	6.07	117.95	110.73
2	L	81	ASP	CA-C-N	6.06	128.40	120.28
2	L	81	ASP	C-N-CA	6.06	128.40	120.28
1	C	78	MET	CA-CB-CG	-6.06	101.97	114.10
1	C	160	VAL	O-C-N	-6.06	115.75	121.87
2	J	81	ASP	CA-C-N	6.06	128.40	120.28
2	J	81	ASP	C-N-CA	6.06	128.40	120.28
1	G	78	MET	CA-CB-CG	-6.06	101.98	114.10
1	E	160	VAL	O-C-N	-6.06	115.75	121.87
2	B	81	ASP	CA-C-N	6.06	128.40	120.28
2	B	81	ASP	C-N-CA	6.06	128.40	120.28
2	H	344	LYS	CB-CA-C	-6.06	103.46	111.82
2	D	344	LYS	CB-CA-C	-6.06	103.46	111.82
2	F	283	CYS	CA-C-N	6.06	129.36	121.85
2	F	283	CYS	C-N-CA	6.06	129.36	121.85
2	H	528	ASP	N-CA-CB	-6.05	102.85	111.51
2	J	530	CYS	O-C-N	6.05	130.89	123.14
1	S	160	VAL	O-C-N	-6.05	115.76	121.87
2	H	16	ARG	CA-C-N	6.05	131.75	123.46
2	H	16	ARG	C-N-CA	6.05	131.75	123.46
2	L	183	VAL	O-C-N	-6.05	115.70	122.05
2	F	183	VAL	O-C-N	-6.05	115.70	122.05
1	I	160	VAL	O-C-N	-6.05	115.76	121.87
2	D	283	CYS	CA-C-N	6.04	129.35	121.85
2	D	283	CYS	C-N-CA	6.04	129.35	121.85
2	J	344	LYS	CB-CA-C	-6.04	103.48	111.82
2	L	344	LYS	CB-CA-C	-6.04	103.48	111.82
2	H	530	CYS	O-C-N	6.04	130.87	123.14
2	F	344	LYS	CB-CA-C	-6.04	103.48	111.82
2	H	483	VAL	CB-CA-C	6.04	117.92	110.73
2	L	283	CYS	CA-C-N	6.04	129.34	121.85
2	L	283	CYS	C-N-CA	6.04	129.34	121.85
2	H	81	ASP	CA-C-N	6.04	128.37	120.28
2	H	81	ASP	C-N-CA	6.04	128.37	120.28
2	D	144	LYS	CB-CA-C	6.04	119.70	109.80
2	D	183	VAL	O-C-N	-6.03	115.72	122.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	16	ARG	CA-C-N	6.03	131.73	123.46
2	J	16	ARG	C-N-CA	6.03	131.73	123.46
2	F	82	ASN	CA-CB-CG	6.03	118.63	112.60
2	D	212	ILE	N-CA-C	-6.03	104.86	110.53
2	D	319	ILE	CB-CA-C	-6.03	103.43	110.91
1	G	160	VAL	O-C-N	-6.03	115.78	121.87
2	F	81	ASP	CA-C-N	6.03	128.36	120.28
2	F	81	ASP	C-N-CA	6.03	128.36	120.28
2	B	212	ILE	N-CA-C	-6.03	104.86	110.53
2	B	183	VAL	O-C-N	-6.03	115.72	122.05
2	D	248	GLU	CG-CD-OE1	6.02	132.24	118.40
2	B	283	CYS	CA-C-N	6.02	129.31	121.85
2	B	283	CYS	C-N-CA	6.02	129.31	121.85
2	H	144	LYS	CB-CA-C	6.02	119.67	109.80
2	L	144	LYS	CB-CA-C	6.01	119.66	109.80
2	H	82	ASN	CA-CB-CG	6.01	118.61	112.60
2	J	144	LYS	CB-CA-C	6.01	119.65	109.80
2	L	82	ASN	CA-CB-CG	6.00	118.61	112.60
2	L	248	GLU	CG-CD-OE1	6.00	132.21	118.40
2	F	107	ASP	CA-C-N	6.00	128.65	120.54
2	F	107	ASP	C-N-CA	6.00	128.65	120.54
1	S	135	LEU	CA-C-N	6.00	126.75	120.03
1	S	135	LEU	C-N-CA	6.00	126.75	120.03
2	D	490	LEU	N-CA-C	6.00	120.62	112.88
1	I	135	LEU	CA-C-N	6.00	126.75	120.03
1	I	135	LEU	C-N-CA	6.00	126.75	120.03
2	J	490	LEU	N-CA-C	6.00	120.62	112.88
1	G	57	GLU	CB-CG-CD	6.00	122.80	112.60
2	H	212	ILE	N-CA-C	-6.00	104.89	110.53
2	B	16	ARG	CA-C-N	6.00	131.68	123.46
2	B	16	ARG	C-N-CA	6.00	131.68	123.46
2	B	144	LYS	CB-CA-C	6.00	119.64	109.80
2	D	16	ARG	CA-C-N	6.00	131.68	123.46
2	D	16	ARG	C-N-CA	6.00	131.68	123.46
2	F	144	LYS	CB-CA-C	6.00	119.64	109.80
2	F	248	GLU	CG-CD-OE1	6.00	132.20	118.40
2	J	52	ARG	CA-C-N	6.00	129.60	121.20
2	J	52	ARG	C-N-CA	6.00	129.60	121.20
2	J	107	ASP	CA-C-N	6.00	128.64	120.54
2	J	107	ASP	C-N-CA	6.00	128.64	120.54
2	L	16	ARG	CA-C-N	6.00	131.68	123.46
2	L	16	ARG	C-N-CA	6.00	131.68	123.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	248	GLU	CG-CD-OE1	6.00	132.19	118.40
1	I	57	GLU	CB-CG-CD	6.00	122.80	112.60
2	L	319	ILE	CB-CA-C	-6.00	103.48	110.91
2	B	248	GLU	CG-CD-OE1	6.00	132.19	118.40
2	B	319	ILE	CB-CA-C	-6.00	103.48	110.91
2	F	212	ILE	N-CA-C	-6.00	104.89	110.53
2	L	212	ILE	N-CA-C	-5.99	104.90	110.53
1	A	57	GLU	CB-CG-CD	5.99	122.79	112.60
2	F	319	ILE	CB-CA-C	-5.99	103.48	110.91
1	S	57	GLU	CB-CG-CD	5.99	122.78	112.60
1	C	57	GLU	CB-CG-CD	5.99	122.78	112.60
2	D	107	ASP	CA-C-N	5.99	128.62	120.54
2	D	107	ASP	C-N-CA	5.99	128.62	120.54
2	J	82	ASN	CA-CB-CG	5.99	118.59	112.60
1	E	57	GLU	CB-CG-CD	5.99	122.78	112.60
2	J	248	GLU	CG-CD-OE1	5.99	132.17	118.40
1	A	135	LEU	CA-C-N	5.98	126.73	120.03
1	A	135	LEU	C-N-CA	5.98	126.73	120.03
2	B	172	ASN	CB-CG-ND2	5.98	125.37	116.40
1	C	135	LEU	CA-C-N	5.98	126.73	120.03
1	C	135	LEU	C-N-CA	5.98	126.73	120.03
2	J	212	ILE	N-CA-C	-5.98	104.91	110.53
2	D	82	ASN	CA-CB-CG	5.98	118.58	112.60
1	I	207	GLU	CB-CG-CD	5.98	122.76	112.60
2	F	490	LEU	N-CA-C	5.98	120.59	112.88
2	F	16	ARG	CA-C-N	5.97	131.65	123.46
2	F	16	ARG	C-N-CA	5.97	131.65	123.46
2	H	107	ASP	CA-C-N	5.97	128.61	120.54
2	H	107	ASP	C-N-CA	5.97	128.61	120.54
2	L	107	ASP	CA-C-N	5.97	128.60	120.54
2	L	107	ASP	C-N-CA	5.97	128.60	120.54
1	G	135	LEU	CA-C-N	5.97	126.72	120.03
1	G	135	LEU	C-N-CA	5.97	126.72	120.03
2	H	183	VAL	O-C-N	-5.97	115.78	122.05
2	H	319	ILE	CB-CA-C	-5.97	103.50	110.91
2	J	319	ILE	CB-CA-C	-5.97	103.50	110.91
2	D	172	ASN	CB-CG-ND2	5.97	125.36	116.40
2	H	52	ARG	CA-C-N	5.97	129.56	121.20
2	H	52	ARG	C-N-CA	5.97	129.56	121.20
1	A	207	GLU	CB-CG-CD	5.97	122.75	112.60
1	G	207	GLU	CB-CG-CD	5.97	122.75	112.60
2	L	52	ARG	CA-C-N	5.97	129.55	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	52	ARG	C-N-CA	5.97	129.55	121.20
2	F	52	ARG	CA-C-N	5.97	129.55	121.20
2	F	52	ARG	C-N-CA	5.97	129.55	121.20
2	H	490	LEU	N-CA-C	5.97	120.58	112.88
2	H	361	ARG	CA-C-O	-5.96	114.26	120.70
2	B	82	ASN	CA-CB-CG	5.96	118.56	112.60
2	L	490	LEU	N-CA-C	5.96	120.57	112.88
2	J	487	THR	N-CA-C	-5.96	104.86	111.36
1	E	135	LEU	CA-C-N	5.96	126.70	120.03
1	E	135	LEU	C-N-CA	5.96	126.70	120.03
2	L	487	THR	N-CA-C	-5.96	104.87	111.36
2	B	52	ARG	CA-C-N	5.95	129.53	121.20
2	B	52	ARG	C-N-CA	5.95	129.53	121.20
2	B	487	THR	N-CA-C	-5.95	104.87	111.36
2	B	490	LEU	N-CA-C	5.95	120.56	112.88
2	H	487	THR	N-CA-C	-5.95	104.87	111.36
1	S	207	GLU	CB-CG-CD	5.95	122.72	112.60
2	D	361	ARG	CA-C-O	-5.95	114.27	120.70
2	D	52	ARG	CA-C-N	5.95	129.53	121.20
2	D	52	ARG	C-N-CA	5.95	129.53	121.20
2	F	487	THR	N-CA-C	-5.95	104.88	111.36
1	E	207	GLU	CB-CG-CD	5.95	122.71	112.60
2	H	172	ASN	CB-CG-ND2	5.95	125.32	116.40
2	B	107	ASP	CA-C-N	5.94	128.56	120.54
2	B	107	ASP	C-N-CA	5.94	128.56	120.54
2	L	172	ASN	CB-CG-ND2	5.94	125.31	116.40
2	L	361	ARG	CA-C-O	-5.94	114.28	120.70
2	D	487	THR	N-CA-C	-5.94	104.89	111.36
2	J	361	ARG	CA-C-O	-5.94	114.29	120.70
1	C	207	GLU	CB-CG-CD	5.93	122.68	112.60
2	F	361	ARG	CA-C-O	-5.93	114.29	120.70
2	D	419	LEU	N-CA-CB	-5.93	101.43	110.33
2	L	419	LEU	N-CA-CB	-5.93	101.44	110.33
2	J	419	LEU	N-CA-CB	-5.93	101.44	110.33
2	F	419	LEU	N-CA-CB	-5.92	101.44	110.33
2	F	172	ASN	CB-CG-ND2	5.92	125.28	116.40
2	J	172	ASN	CB-CG-ND2	5.92	125.28	116.40
2	D	243	ARG	CA-C-O	-5.92	114.61	120.82
2	B	361	ARG	CA-C-O	-5.91	114.31	120.70
2	D	108	HIS	CA-CB-CG	-5.91	107.89	113.80
2	B	419	LEU	N-CA-CB	-5.91	101.47	110.33
2	H	419	LEU	N-CA-CB	-5.91	101.47	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	307	ASP	O-C-N	5.91	130.19	122.68
2	B	307	ASP	O-C-N	5.91	130.14	122.87
1	C	24	VAL	CA-C-N	5.91	130.05	120.60
1	C	24	VAL	C-N-CA	5.91	130.05	120.60
2	J	108	HIS	CA-CB-CG	-5.91	107.89	113.80
1	S	24	VAL	CA-C-N	5.90	130.04	120.60
1	S	24	VAL	C-N-CA	5.90	130.04	120.60
1	G	24	VAL	CA-C-N	5.90	130.04	120.60
1	G	24	VAL	C-N-CA	5.90	130.04	120.60
2	L	223	THR	CA-C-N	5.90	130.23	122.51
2	L	223	THR	C-N-CA	5.90	130.23	122.51
2	D	223	THR	CA-C-N	5.90	130.23	122.51
2	D	223	THR	C-N-CA	5.90	130.23	122.51
2	D	307	ASP	O-C-N	5.89	130.12	122.87
1	E	24	VAL	CA-C-N	5.89	130.03	120.60
1	E	24	VAL	C-N-CA	5.89	130.03	120.60
1	I	24	VAL	CA-C-N	5.89	130.03	120.60
1	I	24	VAL	C-N-CA	5.89	130.03	120.60
2	B	223	THR	CA-C-N	5.89	130.23	122.51
2	B	223	THR	C-N-CA	5.89	130.23	122.51
2	F	243	ARG	CA-C-O	-5.89	114.63	120.82
2	F	223	THR	CA-C-N	5.89	130.22	122.51
2	F	223	THR	C-N-CA	5.89	130.22	122.51
2	H	223	THR	CA-C-N	5.89	130.22	122.51
2	H	223	THR	C-N-CA	5.89	130.22	122.51
1	I	143	ILE	CA-C-O	-5.89	114.14	120.85
1	A	143	ILE	CA-C-O	-5.88	114.14	120.85
1	S	172	LYS	O-C-N	5.88	130.58	122.46
1	C	143	ILE	CA-C-O	-5.88	114.14	120.85
1	I	172	LYS	O-C-N	5.88	130.58	122.46
2	J	324	LYS	CA-C-O	-5.88	114.31	120.55
2	L	243	ARG	CA-C-O	-5.88	114.64	120.82
2	L	307	ASP	O-C-N	5.88	130.15	122.68
1	A	24	VAL	CA-C-N	5.88	130.01	120.60
1	A	24	VAL	C-N-CA	5.88	130.01	120.60
2	H	277	THR	N-CA-CB	-5.88	101.46	111.69
2	L	108	HIS	CA-CB-CG	-5.88	107.92	113.80
2	D	407	THR	CA-CB-OG1	-5.88	100.79	109.60
2	H	307	ASP	O-C-N	5.88	130.14	122.68
2	H	108	HIS	CA-CB-CG	-5.88	107.92	113.80
1	S	143	ILE	CA-C-O	-5.87	114.16	120.85
2	H	243	ARG	CA-C-O	-5.87	114.65	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	223	THR	CA-C-N	5.87	130.20	122.51
2	J	223	THR	C-N-CA	5.87	130.20	122.51
2	B	243	ARG	CA-C-O	-5.87	114.66	120.82
2	F	407	THR	CA-CB-OG1	-5.87	100.79	109.60
1	A	172	LYS	O-C-N	5.87	130.56	122.46
2	F	191	ILE	N-CA-CB	-5.87	103.06	110.57
2	L	407	THR	CA-CB-OG1	-5.87	100.80	109.60
2	H	191	ILE	N-CA-CB	-5.87	103.06	110.57
1	C	172	LYS	O-C-N	5.86	130.55	122.46
1	E	143	ILE	CA-C-O	-5.86	114.17	120.85
2	F	108	HIS	CA-CB-CG	-5.86	107.94	113.80
2	F	307	ASP	O-C-N	5.86	130.12	122.68
1	G	172	LYS	O-C-N	5.86	130.55	122.46
1	E	172	LYS	O-C-N	5.86	130.54	122.46
2	J	407	THR	CA-CB-OG1	-5.86	100.82	109.60
2	B	191	ILE	N-CA-CB	-5.85	103.08	110.57
2	H	407	THR	CA-CB-OG1	-5.85	100.83	109.60
2	J	399	VAL	N-CA-C	-5.85	101.39	108.53
2	J	243	ARG	CA-C-O	-5.85	114.68	120.82
2	L	324	LYS	CA-C-O	-5.85	114.35	120.55
2	L	191	ILE	N-CA-CB	-5.84	103.09	110.57
2	D	324	LYS	CA-C-O	-5.84	114.36	120.55
2	J	191	ILE	N-CA-CB	-5.84	103.09	110.57
2	B	324	LYS	CA-C-O	-5.84	114.36	120.55
2	F	324	LYS	CA-C-O	-5.84	114.36	120.55
1	G	143	ILE	CA-C-O	-5.84	114.20	120.85
2	B	407	THR	CA-CB-OG1	-5.83	100.85	109.60
2	B	108	HIS	CA-CB-CG	-5.83	107.97	113.80
2	D	191	ILE	N-CA-CB	-5.82	103.12	110.57
2	H	324	LYS	CA-C-O	-5.82	114.38	120.55
2	B	120	TRP	O-C-N	5.82	128.74	122.34
2	D	399	VAL	N-CA-C	-5.82	101.43	108.53
1	I	151	ASN	O-C-N	-5.82	115.46	121.28
2	F	399	VAL	N-CA-C	-5.81	101.44	108.53
2	L	399	VAL	N-CA-C	-5.81	101.44	108.53
2	B	399	VAL	N-CA-C	-5.81	101.44	108.53
1	G	151	ASN	O-C-N	-5.81	115.47	121.28
2	H	288	THR	N-CA-CB	5.81	118.82	110.40
2	D	288	THR	N-CA-CB	5.80	118.82	110.40
2	D	277	THR	N-CA-CB	-5.80	101.46	111.55
2	D	120	TRP	O-C-N	5.80	128.72	122.34
2	F	288	THR	N-CA-CB	5.80	118.81	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	120	TRP	O-C-N	5.80	128.72	122.34
1	E	151	ASN	O-C-N	-5.80	115.48	121.28
2	B	277	THR	N-CA-CB	-5.79	101.47	111.55
2	F	277	THR	N-CA-CB	-5.79	101.47	111.55
2	L	277	THR	N-CA-CB	-5.79	101.47	111.55
2	B	288	THR	N-CA-CB	5.79	118.80	110.40
2	L	288	THR	N-CA-CB	5.79	118.80	110.40
2	J	120	TRP	O-C-N	5.79	128.71	122.34
2	J	277	THR	N-CA-CB	-5.79	101.48	111.55
2	F	120	TRP	O-C-N	5.78	128.69	122.34
1	S	151	ASN	O-C-N	-5.78	115.50	121.28
2	J	288	THR	N-CA-CB	5.77	118.77	110.40
1	C	151	ASN	O-C-N	-5.77	115.51	121.28
2	H	399	VAL	N-CA-C	-5.76	101.50	108.53
2	H	145	LYS	CA-C-N	5.75	131.27	122.93
2	H	145	LYS	C-N-CA	5.75	131.27	122.93
1	A	151	ASN	O-C-N	-5.75	115.53	121.28
2	J	334	HIS	CA-CB-CG	-5.75	108.05	113.80
2	B	145	LYS	CA-C-N	5.74	131.26	122.93
2	B	145	LYS	C-N-CA	5.74	131.26	122.93
2	F	145	LYS	CA-C-N	5.74	131.25	122.93
2	F	145	LYS	C-N-CA	5.74	131.25	122.93
2	H	458	PHE	O-C-N	5.74	130.04	123.27
2	L	145	LYS	CA-C-N	5.74	131.25	122.93
2	L	145	LYS	C-N-CA	5.74	131.25	122.93
2	J	145	LYS	CA-C-N	5.74	131.25	122.93
2	J	145	LYS	C-N-CA	5.74	131.25	122.93
2	B	274	ILE	O-C-N	5.74	129.37	123.18
2	J	458	PHE	O-C-N	5.74	130.04	123.27
2	D	125	ASN	OD1-CG-ND2	5.73	128.33	122.60
2	L	125	ASN	OD1-CG-ND2	5.73	128.33	122.60
1	C	75	GLY	N-CA-C	-5.73	103.84	112.89
2	L	361	ARG	NH1-CZ-NH2	-5.73	111.85	119.30
1	C	193	HIS	CA-CB-CG	-5.73	108.07	113.80
1	G	261	PHE	N-CA-C	5.73	118.30	111.71
2	B	458	PHE	O-C-N	5.72	130.02	123.27
2	D	334	HIS	CA-CB-CG	-5.72	108.08	113.80
2	F	361	ARG	NH1-CZ-NH2	-5.72	111.86	119.30
1	G	193	HIS	CA-CB-CG	-5.72	108.08	113.80
1	G	228	CYS	O-C-N	5.72	125.99	120.55
1	E	193	HIS	CA-CB-CG	-5.72	108.08	113.80
2	L	458	PHE	O-C-N	5.72	130.02	123.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	145	LYS	CA-C-N	5.72	131.22	122.93
2	D	145	LYS	C-N-CA	5.72	131.22	122.93
2	H	105	MET	O-C-N	-5.72	116.14	122.09
2	B	334	HIS	CA-CB-CG	-5.72	108.08	113.80
2	H	125	ASN	OD1-CG-ND2	5.72	128.32	122.60
2	H	334	HIS	CA-CB-CG	-5.72	108.08	113.80
1	G	75	GLY	N-CA-C	-5.72	103.86	112.89
1	E	75	GLY	N-CA-C	-5.71	103.86	112.89
1	E	228	CYS	O-C-N	5.71	125.98	120.55
1	C	237	ASN	N-CA-CB	-5.71	102.66	111.46
2	F	125	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	S	193	HIS	CA-CB-CG	-5.71	108.09	113.80
2	B	125	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	G	237	ASN	N-CA-CB	-5.71	102.67	111.46
1	I	193	HIS	CA-CB-CG	-5.71	108.09	113.80
1	S	75	GLY	N-CA-C	-5.71	103.87	112.89
2	F	234	LEU	N-CA-C	-5.71	106.29	113.20
2	F	458	PHE	O-C-N	5.71	130.01	123.27
1	I	228	CYS	O-C-N	5.71	125.97	120.55
1	S	228	CYS	O-C-N	5.71	125.97	120.55
2	L	334	HIS	CA-CB-CG	-5.71	108.09	113.80
1	E	261	PHE	N-CA-C	5.71	118.27	111.71
2	F	105	MET	O-C-N	-5.71	116.16	122.09
1	E	237	ASN	N-CA-CB	-5.70	102.68	111.46
1	I	237	ASN	N-CA-CB	-5.70	102.67	111.46
1	S	237	ASN	N-CA-CB	-5.70	102.68	111.46
1	S	261	PHE	N-CA-C	5.70	118.27	111.71
2	B	335	HIS	N-CA-C	-5.70	102.22	110.08
2	J	234	LEU	N-CA-C	-5.70	106.30	113.20
2	J	361	ARG	NH1-CZ-NH2	-5.70	111.89	119.30
2	H	361	ARG	NH1-CZ-NH2	-5.70	111.89	119.30
1	A	75	GLY	N-CA-C	-5.69	103.89	112.89
2	B	361	ARG	NH1-CZ-NH2	-5.69	111.90	119.30
1	I	75	GLY	N-CA-C	-5.69	103.89	112.89
2	J	125	ASN	OD1-CG-ND2	5.69	128.29	122.60
2	D	289	ASP	CA-C-O	5.69	126.55	120.46
2	D	458	PHE	O-C-N	5.69	129.99	123.27
1	A	193	HIS	CA-CB-CG	-5.69	108.11	113.80
1	A	261	PHE	N-CA-C	5.69	118.25	111.71
2	D	361	ARG	NH1-CZ-NH2	-5.69	111.90	119.30
1	C	228	CYS	O-C-N	5.69	125.95	120.55
1	A	237	ASN	N-CA-CB	-5.69	102.70	111.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	105	MET	O-C-N	-5.69	116.18	122.09
1	G	58	GLU	CB-CG-CD	5.69	122.27	112.60
2	F	334	HIS	CA-CB-CG	-5.68	108.12	113.80
1	S	58	GLU	CB-CG-CD	5.68	122.26	112.60
2	L	105	MET	O-C-N	-5.68	116.18	122.09
1	A	58	GLU	CB-CG-CD	5.68	122.26	112.60
1	A	228	CYS	O-C-N	5.68	125.95	120.55
2	B	289	ASP	CA-C-O	5.68	126.54	120.46
1	E	58	GLU	CB-CG-CD	5.68	122.26	112.60
2	J	105	MET	O-C-N	-5.68	116.18	122.09
1	C	58	GLU	CB-CG-CD	5.68	122.26	112.60
2	D	335	HIS	N-CA-C	-5.68	102.24	110.08
2	L	234	LEU	N-CA-C	-5.68	106.33	113.20
2	L	335	HIS	N-CA-C	-5.68	102.24	110.08
2	D	234	LEU	N-CA-C	-5.68	106.33	113.20
2	H	267	PHE	CB-CA-C	-5.68	100.96	110.56
1	I	31	TYR	CA-C-O	-5.68	115.11	121.81
2	J	335	HIS	N-CA-C	-5.68	102.24	110.08
2	H	335	HIS	N-CA-C	-5.68	102.24	110.08
2	L	274	ILE	O-C-N	5.68	129.31	123.18
2	D	274	ILE	O-C-N	5.68	129.31	123.18
2	D	383	HIS	CA-CB-CG	5.68	119.48	113.80
2	J	274	ILE	O-C-N	5.68	129.31	123.18
2	B	267	PHE	CB-CA-C	-5.67	100.97	110.56
1	E	31	TYR	CA-C-O	-5.67	115.11	121.81
2	F	390	VAL	N-CA-C	-5.67	104.97	110.42
2	L	267	PHE	CB-CA-C	-5.67	100.98	110.56
2	B	234	LEU	N-CA-C	-5.67	106.34	113.20
2	F	358	LYS	N-CA-C	-5.67	103.21	110.53
2	F	433	GLU	N-CA-C	5.67	117.46	111.28
2	H	358	LYS	N-CA-C	-5.67	103.22	110.53
2	L	383	HIS	CA-CB-CG	5.67	119.47	113.80
2	F	267	PHE	CB-CA-C	-5.67	100.98	110.56
2	H	90	GLU	CA-C-O	-5.67	114.51	120.63
1	I	261	PHE	N-CA-C	5.67	118.23	111.71
2	J	358	LYS	N-CA-C	-5.67	103.22	110.53
2	L	358	LYS	N-CA-C	-5.67	103.22	110.53
2	B	358	LYS	N-CA-C	-5.67	103.22	110.53
2	F	140	ASP	CB-CA-C	5.66	120.59	109.72
2	L	449	TYR	CB-CA-C	-5.66	100.94	109.26
2	B	383	HIS	CA-CB-CG	5.66	119.46	113.80
2	B	449	TYR	CB-CA-C	-5.66	100.94	109.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	449	TYR	CB-CA-C	-5.66	100.94	109.26
2	J	449	TYR	CB-CA-C	-5.66	100.94	109.26
1	C	261	PHE	N-CA-C	5.66	118.22	111.71
2	H	449	TYR	CB-CA-C	-5.66	100.94	109.26
1	I	58	GLU	CB-CG-CD	5.66	122.22	112.60
2	J	267	PHE	CB-CA-C	-5.66	101.00	110.56
2	F	449	TYR	CB-CA-C	-5.66	100.94	109.26
2	J	140	ASP	CB-CA-C	5.66	120.58	109.72
2	L	433	GLU	N-CA-C	5.66	117.44	111.28
2	H	383	HIS	CA-CB-CG	5.66	119.46	113.80
2	D	433	GLU	N-CA-C	5.65	117.44	111.28
1	A	31	TYR	CA-C-O	-5.65	115.14	121.81
2	J	390	VAL	N-CA-C	-5.65	104.99	110.42
2	L	140	ASP	CB-CA-C	5.65	120.57	109.72
2	D	390	VAL	N-CA-C	-5.65	105.00	110.42
2	H	234	LEU	N-CA-C	-5.65	106.37	113.20
1	G	194	PHE	CA-C-O	5.65	126.75	120.82
2	B	105	MET	O-C-N	-5.64	116.22	122.09
2	F	90	GLU	CA-C-O	-5.64	114.53	120.63
2	F	335	HIS	N-CA-C	-5.64	102.29	110.08
2	B	140	ASP	CB-CA-C	5.64	120.55	109.72
2	D	267	PHE	CB-CA-C	-5.64	101.02	110.56
2	H	140	ASP	CB-CA-C	5.64	120.55	109.72
2	H	274	ILE	O-C-N	5.64	129.28	123.18
2	H	289	ASP	CA-C-O	5.64	126.50	120.46
2	L	289	ASP	CA-C-O	5.64	126.50	120.46
2	B	12	ASP	CB-CG-OD2	5.64	131.37	118.40
1	S	31	TYR	CA-C-O	-5.64	115.16	121.81
2	B	433	GLU	N-CA-C	5.64	117.43	111.28
1	C	31	TYR	CA-C-O	-5.64	115.16	121.81
2	D	140	ASP	CB-CA-C	5.64	120.55	109.72
1	E	95	ILE	CA-C-N	5.64	127.84	120.28
1	E	95	ILE	C-N-CA	5.64	127.84	120.28
2	L	90	GLU	CA-C-O	-5.64	114.54	120.63
2	D	90	GLU	CA-C-O	-5.64	114.54	120.63
2	L	390	VAL	N-CA-C	-5.63	105.01	110.42
2	D	452	GLU	CA-C-O	-5.63	113.36	120.28
1	S	95	ILE	CA-C-N	5.63	127.82	120.28
1	S	95	ILE	C-N-CA	5.63	127.82	120.28
2	D	358	LYS	N-CA-C	-5.63	103.27	110.53
1	I	95	ILE	CA-C-N	5.63	127.82	120.28
1	I	95	ILE	C-N-CA	5.63	127.82	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	274	ILE	O-C-N	5.63	129.26	123.18
2	F	452	GLU	CA-C-O	-5.63	113.36	120.28
1	G	239	PRO	CA-C-N	5.62	129.52	120.30
1	G	239	PRO	C-N-CA	5.62	129.52	120.30
2	H	433	GLU	N-CA-C	5.62	117.41	111.28
2	H	452	GLU	CA-C-O	-5.62	113.36	120.28
1	A	239	PRO	CA-C-N	5.62	129.52	120.30
1	A	239	PRO	C-N-CA	5.62	129.52	120.30
2	J	383	HIS	CA-CB-CG	5.62	119.42	113.80
2	J	433	GLU	N-CA-C	5.62	117.41	111.28
2	L	12	ASP	CB-CG-OD2	5.62	131.32	118.40
1	G	31	TYR	CA-C-O	-5.62	115.18	121.81
2	B	90	GLU	CA-C-O	-5.62	114.56	120.63
1	C	194	PHE	CA-C-O	5.62	126.72	120.82
2	D	12	ASP	CB-CG-OD2	5.62	131.31	118.40
2	F	289	ASP	CA-C-O	5.62	126.47	120.46
2	F	383	HIS	CA-CB-CG	5.62	119.42	113.80
1	I	239	PRO	CA-C-N	5.62	129.51	120.30
1	I	239	PRO	C-N-CA	5.62	129.51	120.30
1	A	95	ILE	CA-C-N	5.61	127.80	120.28
1	A	95	ILE	C-N-CA	5.61	127.80	120.28
2	B	390	VAL	N-CA-C	-5.61	105.03	110.42
2	F	12	ASP	CB-CG-OD2	5.61	131.30	118.40
1	S	239	PRO	CA-C-N	5.61	129.49	120.30
1	S	239	PRO	C-N-CA	5.61	129.49	120.30
1	C	95	ILE	CA-C-N	5.61	127.79	120.28
1	C	95	ILE	C-N-CA	5.61	127.79	120.28
2	J	12	ASP	CB-CG-OD2	5.60	131.29	118.40
2	H	12	ASP	CB-CG-OD2	5.60	131.28	118.40
1	E	194	PHE	CA-C-O	5.60	126.70	120.82
2	H	390	VAL	N-CA-C	-5.60	105.04	110.42
1	S	194	PHE	CA-C-O	5.60	126.70	120.82
2	J	289	ASP	CA-C-O	5.60	126.45	120.46
1	E	239	PRO	CA-C-N	5.60	129.48	120.30
1	E	239	PRO	C-N-CA	5.60	129.48	120.30
2	J	90	GLU	CA-C-O	-5.59	114.59	120.63
2	D	272	ALA	CA-C-O	5.59	126.45	119.12
2	D	320	GLU	CB-CG-CD	5.59	122.11	112.60
2	F	342	LYS	O-C-N	5.59	126.52	121.04
2	B	452	GLU	CA-C-O	-5.59	113.41	120.28
1	C	239	PRO	CA-C-N	5.59	129.47	120.30
1	C	239	PRO	C-N-CA	5.59	129.47	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	95	ILE	CA-C-N	5.59	127.77	120.28
1	G	95	ILE	C-N-CA	5.59	127.77	120.28
1	I	171	ASP	CA-CB-CG	5.59	118.19	112.60
2	J	320	GLU	CB-CG-CD	5.59	122.10	112.60
2	F	320	GLU	CB-CG-CD	5.59	122.10	112.60
2	H	342	LYS	O-C-N	5.59	126.51	121.04
1	C	171	ASP	CA-CB-CG	5.58	118.19	112.60
2	L	452	GLU	CA-C-O	-5.58	113.41	120.28
2	B	241	GLU	CB-CG-CD	5.58	122.09	112.60
1	A	194	PHE	CA-C-O	5.58	126.68	120.82
1	A	171	ASP	CA-CB-CG	5.58	118.18	112.60
1	G	171	ASP	CA-CB-CG	5.58	118.18	112.60
1	S	171	ASP	CA-CB-CG	5.58	118.18	112.60
2	B	320	GLU	CB-CG-CD	5.58	122.08	112.60
1	E	225	TYR	CA-C-O	-5.58	114.74	120.54
2	D	241	GLU	CB-CG-CD	5.57	122.08	112.60
2	F	272	ALA	CA-C-O	5.57	126.42	119.12
1	I	194	PHE	CA-C-O	5.57	126.67	120.82
2	B	452	GLU	CB-CA-C	-5.57	99.90	109.65
2	L	241	GLU	CB-CG-CD	5.57	122.07	112.60
2	L	320	GLU	CB-CG-CD	5.57	122.07	112.60
2	D	189	ASP	CA-CB-CG	5.57	118.17	112.60
2	H	272	ALA	CA-C-O	5.57	126.41	119.12
1	G	225	TYR	CA-C-O	-5.56	114.75	120.54
2	L	272	ALA	CA-C-O	5.56	126.41	119.12
2	L	452	GLU	CB-CA-C	-5.56	99.92	109.65
2	J	272	ALA	CA-C-O	5.56	126.41	119.12
2	J	452	GLU	CA-C-O	-5.56	113.44	120.28
2	H	241	GLU	CB-CG-CD	5.56	122.05	112.60
2	J	342	LYS	O-C-N	5.56	126.49	121.04
2	H	189	ASP	CA-CB-CG	5.56	118.16	112.60
2	J	452	GLU	CB-CA-C	-5.56	99.92	109.65
2	J	241	GLU	CB-CG-CD	5.56	122.05	112.60
1	S	225	TYR	CA-C-O	-5.55	114.76	120.54
2	B	240	ALA	CA-C-N	5.55	127.66	120.44
2	B	240	ALA	C-N-CA	5.55	127.66	120.44
1	C	225	TYR	CA-C-O	-5.55	114.76	120.54
1	E	171	ASP	CA-CB-CG	5.55	118.15	112.60
2	L	342	LYS	O-C-N	5.55	126.48	121.04
2	B	272	ALA	CA-C-O	5.55	126.39	119.12
2	D	452	GLU	CB-CA-C	-5.55	99.94	109.65
2	D	530	CYS	CA-C-O	-5.55	112.97	120.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	320	GLU	CB-CG-CD	5.55	122.04	112.60
2	J	240	ALA	CA-C-N	5.55	127.66	120.44
2	J	240	ALA	C-N-CA	5.55	127.66	120.44
1	A	225	TYR	CA-C-O	-5.55	114.77	120.54
2	H	452	GLU	CB-CA-C	-5.55	99.94	109.65
2	B	342	LYS	O-C-N	5.55	126.48	121.04
2	F	241	GLU	CB-CG-CD	5.55	122.03	112.60
2	F	350	GLY	N-CA-C	-5.55	102.32	110.97
2	F	387	VAL	O-C-N	-5.55	116.47	121.91
1	E	244	HIS	CA-CB-CG	5.54	119.34	113.80
2	B	189	ASP	CA-CB-CG	5.54	118.14	112.60
2	F	96	ARG	NH1-CZ-NH2	-5.54	112.10	119.30
2	J	395	LYS	O-C-N	5.54	128.47	122.15
2	L	96	ARG	NH1-CZ-NH2	-5.54	112.10	119.30
2	J	387	VAL	O-C-N	-5.54	116.48	121.91
2	D	240	ALA	CA-C-N	5.54	127.64	120.44
2	D	240	ALA	C-N-CA	5.54	127.64	120.44
2	F	189	ASP	CA-CB-CG	5.54	118.14	112.60
2	H	240	ALA	CA-C-N	5.54	127.64	120.44
2	H	240	ALA	C-N-CA	5.54	127.64	120.44
2	B	96	ARG	NH1-CZ-NH2	-5.54	112.11	119.30
2	D	96	ARG	NH1-CZ-NH2	-5.54	112.10	119.30
2	L	240	ALA	CA-C-N	5.53	127.64	120.44
2	L	240	ALA	C-N-CA	5.53	127.64	120.44
2	B	118	LEU	CA-C-O	-5.53	112.60	120.51
2	D	395	LYS	O-C-N	5.53	128.46	122.15
2	B	530	CYS	CA-C-O	-5.53	113.00	120.47
2	F	118	LEU	CA-C-O	-5.53	112.60	120.51
1	G	171	ASP	N-CA-C	-5.53	101.82	110.17
2	H	96	ARG	NH1-CZ-NH2	-5.53	112.11	119.30
1	I	252	PRO	CA-C-O	5.53	127.35	121.32
2	J	65	CYS	N-CA-C	5.53	117.39	108.32
2	F	395	LYS	O-C-N	5.53	128.45	122.15
1	C	252	PRO	CA-C-O	5.53	127.34	121.32
2	D	350	GLY	N-CA-C	-5.53	102.35	110.97
2	F	452	GLU	CB-CA-C	-5.53	99.98	109.65
2	H	65	CYS	N-CA-C	5.53	117.38	108.32
1	I	225	TYR	CA-C-O	-5.53	114.79	120.54
2	B	395	LYS	O-C-N	5.53	128.45	122.15
2	B	516	ARG	NE-CZ-NH2	-5.53	114.23	119.20
2	D	342	LYS	O-C-N	5.53	126.45	121.04
2	J	96	ARG	NH1-CZ-NH2	-5.53	112.12	119.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	189	ASP	CA-CB-CG	5.52	118.12	112.60
2	J	189	ASP	CA-CB-CG	5.52	118.12	112.60
2	F	300	GLN	CB-CG-CD	5.52	121.99	112.60
2	L	395	LYS	O-C-N	5.52	128.44	122.15
2	D	118	LEU	CA-C-O	-5.52	112.62	120.51
1	G	244	HIS	CA-CB-CG	5.52	119.32	113.80
1	A	252	PRO	CA-C-O	5.52	127.33	121.32
2	B	65	CYS	N-CA-C	5.52	117.37	108.32
2	D	182	TYR	O-C-N	5.52	129.66	122.87
1	G	252	PRO	CA-C-O	5.52	127.33	121.32
1	A	244	HIS	CA-CB-CG	5.52	119.32	113.80
2	J	350	GLY	N-CA-C	-5.52	102.36	110.97
2	L	350	GLY	N-CA-C	-5.51	102.37	110.97
2	L	530	CYS	CA-C-O	-5.51	113.03	120.47
1	E	171	ASP	N-CA-C	-5.51	101.85	110.17
2	F	240	ALA	CA-C-N	5.51	127.61	120.44
2	F	240	ALA	C-N-CA	5.51	127.61	120.44
2	L	118	LEU	CA-C-O	-5.51	112.63	120.51
1	C	171	ASP	N-CA-C	-5.51	101.85	110.17
2	J	118	LEU	CA-C-O	-5.51	112.63	120.51
2	L	300	GLN	CB-CG-CD	5.51	121.97	112.60
1	C	244	HIS	CA-CB-CG	5.51	119.31	113.80
1	E	27	THR	CA-CB-OG1	-5.51	101.33	109.60
1	S	171	ASP	N-CA-C	-5.51	101.85	110.17
2	L	65	CYS	N-CA-C	5.51	117.35	108.32
1	I	171	ASP	N-CA-C	-5.51	101.85	110.17
2	H	182	TYR	O-C-N	5.51	129.64	122.87
2	H	350	GLY	N-CA-C	-5.51	102.38	110.97
2	H	530	CYS	CA-C-O	-5.51	113.04	120.47
2	H	395	LYS	O-C-N	5.50	128.43	122.15
1	S	252	PRO	CA-C-O	5.50	127.32	121.32
2	B	300	GLN	CB-CG-CD	5.50	121.95	112.60
2	B	387	VAL	O-C-N	-5.50	116.52	121.91
1	A	171	ASP	N-CA-C	-5.50	101.86	110.17
1	I	45	HIS	CA-C-N	5.50	128.41	120.38
1	I	45	HIS	C-N-CA	5.50	128.41	120.38
2	B	350	GLY	N-CA-C	-5.50	102.39	110.97
2	F	65	CYS	N-CA-C	5.50	117.34	108.32
2	L	387	VAL	O-C-N	-5.50	116.52	121.91
2	H	300	GLN	CB-CG-CD	5.50	121.95	112.60
2	B	182	TYR	O-C-N	5.50	129.63	122.87
1	E	252	PRO	CA-C-O	5.50	127.31	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	244	HIS	CA-CB-CG	5.49	119.29	113.80
2	D	387	VAL	O-C-N	-5.49	116.53	121.91
1	I	244	HIS	CA-CB-CG	5.49	119.29	113.80
2	J	300	GLN	CB-CG-CD	5.49	121.94	112.60
2	J	530	CYS	CA-C-O	-5.49	113.06	120.47
2	D	191	ILE	N-CA-C	-5.49	105.37	110.53
2	D	65	CYS	N-CA-C	5.49	117.32	108.32
2	L	182	TYR	O-C-N	5.49	129.62	122.87
2	F	530	CYS	CA-C-O	-5.49	113.06	120.47
2	F	132	ALA	CA-C-O	5.48	126.28	119.97
1	I	254	PHE	CA-C-N	5.48	127.62	120.28
1	I	254	PHE	C-N-CA	5.48	127.62	120.28
1	S	45	HIS	CA-C-N	5.48	128.38	120.38
1	S	45	HIS	C-N-CA	5.48	128.38	120.38
2	H	83	CYS	CA-C-N	5.48	130.85	122.69
2	H	83	CYS	C-N-CA	5.48	130.85	122.69
1	E	167	MET	CA-CB-CG	-5.48	103.14	114.10
2	H	387	VAL	O-C-N	-5.48	116.54	121.91
1	S	27	THR	CA-CB-OG1	-5.48	101.38	109.60
2	D	83	CYS	CA-C-N	5.48	130.85	122.69
2	D	83	CYS	C-N-CA	5.48	130.85	122.69
2	D	300	GLN	CB-CG-CD	5.48	121.91	112.60
2	L	516	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	C	27	THR	CA-CB-OG1	-5.48	101.39	109.60
2	H	191	ILE	N-CA-C	-5.47	105.39	110.53
1	I	27	THR	CA-CB-OG1	-5.47	101.39	109.60
1	E	45	HIS	CA-C-N	5.47	128.37	120.38
1	E	45	HIS	C-N-CA	5.47	128.37	120.38
2	L	83	CYS	CA-C-N	5.47	130.84	122.69
2	L	83	CYS	C-N-CA	5.47	130.84	122.69
1	C	45	HIS	CA-C-N	5.47	128.37	120.38
1	C	45	HIS	C-N-CA	5.47	128.37	120.38
1	A	45	HIS	CA-C-N	5.47	128.36	120.38
1	A	45	HIS	C-N-CA	5.47	128.36	120.38
1	G	45	HIS	CA-C-N	5.47	128.36	120.38
1	G	45	HIS	C-N-CA	5.47	128.36	120.38
2	L	191	ILE	N-CA-C	-5.47	105.39	110.53
2	B	230	ASN	N-CA-C	5.47	118.03	108.52
2	H	132	ALA	CA-C-O	5.47	126.26	119.97
1	A	27	THR	CA-CB-OG1	-5.46	101.40	109.60
1	G	27	THR	CA-CB-OG1	-5.46	101.40	109.60
2	B	83	CYS	CA-C-N	5.46	130.83	122.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	CYS	C-N-CA	5.46	130.83	122.69
1	G	167	MET	CA-CB-CG	-5.46	103.17	114.10
2	D	516	ARG	NE-CZ-NH2	-5.46	114.28	119.20
2	H	118	LEU	CA-C-O	-5.46	112.70	120.51
2	J	73	ALA	N-CA-C	-5.46	105.23	111.07
2	B	132	ALA	CA-C-O	5.46	126.25	119.97
1	E	10	VAL	CB-CA-C	5.46	118.52	110.77
2	F	230	ASN	N-CA-C	5.46	118.02	108.52
2	H	73	ALA	N-CA-C	-5.46	105.23	111.07
2	J	230	ASN	N-CA-C	5.46	118.02	108.52
2	H	516	ARG	NE-CZ-NH2	-5.46	114.29	119.20
2	B	191	ILE	N-CA-C	-5.46	105.40	110.53
1	S	167	MET	CA-CB-CG	-5.45	103.19	114.10
1	A	167	MET	CA-CB-CG	-5.45	103.19	114.10
1	C	167	MET	CA-CB-CG	-5.45	103.19	114.10
2	F	83	CYS	CA-C-N	5.45	130.81	122.69
2	F	83	CYS	C-N-CA	5.45	130.81	122.69
2	J	10	VAL	CA-CB-CG1	5.45	119.67	110.40
1	G	255	TRP	O-C-N	5.45	128.60	122.22
1	A	10	VAL	CB-CA-C	5.45	118.51	110.77
2	D	132	ALA	CA-C-O	5.45	126.24	119.97
2	F	516	ARG	NE-CZ-NH2	-5.45	114.30	119.20
2	H	400	GLY	CA-C-N	5.45	125.07	119.56
2	H	400	GLY	C-N-CA	5.45	125.07	119.56
2	J	191	ILE	N-CA-C	-5.45	105.41	110.53
2	L	73	ALA	N-CA-C	-5.45	105.24	111.07
2	L	132	ALA	CA-C-O	5.45	126.23	119.97
2	J	132	ALA	CA-C-O	5.45	126.23	119.97
1	G	10	VAL	CB-CA-C	5.44	118.50	110.77
2	L	230	ASN	N-CA-C	5.44	117.99	108.52
2	J	182	TYR	O-C-N	5.44	129.56	122.87
2	J	516	ARG	NE-CZ-NH2	-5.44	114.30	119.20
2	F	182	TYR	O-C-N	5.44	129.56	122.87
2	F	191	ILE	N-CA-C	-5.44	105.42	110.53
2	D	400	GLY	CA-C-N	5.44	125.05	119.56
2	D	400	GLY	C-N-CA	5.44	125.05	119.56
1	S	10	VAL	CB-CA-C	5.44	118.49	110.77
1	S	255	TRP	O-C-N	5.44	128.58	122.22
2	H	119	ASP	N-CA-C	-5.44	106.65	113.72
1	I	167	MET	CA-CB-CG	-5.44	103.23	114.10
2	D	388	LYS	CA-C-N	5.43	128.01	120.29
2	D	388	LYS	C-N-CA	5.43	128.01	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	10	VAL	CA-CB-CG1	5.43	119.64	110.40
2	D	73	ALA	N-CA-C	-5.43	105.26	111.07
1	A	255	TRP	O-C-N	5.43	128.57	122.22
2	H	230	ASN	N-CA-C	5.43	117.97	108.52
2	J	83	CYS	CA-C-N	5.43	130.78	122.69
2	J	83	CYS	C-N-CA	5.43	130.78	122.69
2	F	400	GLY	CA-C-N	5.43	125.04	119.56
2	F	400	GLY	C-N-CA	5.43	125.04	119.56
2	L	400	GLY	CA-C-N	5.43	125.04	119.56
2	L	400	GLY	C-N-CA	5.43	125.04	119.56
2	B	73	ALA	N-CA-C	-5.43	105.26	111.07
1	C	10	VAL	CB-CA-C	5.43	118.48	110.77
2	D	230	ASN	N-CA-C	5.43	117.96	108.52
2	F	119	ASP	N-CA-C	-5.43	106.67	113.72
1	I	10	VAL	CB-CA-C	5.43	118.47	110.77
2	L	119	ASP	N-CA-C	-5.42	106.67	113.72
2	B	400	GLY	CA-C-N	5.42	125.04	119.56
2	B	400	GLY	C-N-CA	5.42	125.04	119.56
1	C	255	TRP	O-C-N	5.42	128.57	122.22
2	F	73	ALA	N-CA-C	-5.42	105.27	111.07
2	J	119	ASP	N-CA-C	-5.42	106.67	113.72
1	G	26	ARG	CD-NE-CZ	-5.42	116.81	124.40
2	L	10	VAL	CA-CB-CG1	5.42	119.62	110.40
2	B	119	ASP	N-CA-C	-5.42	106.67	113.72
1	E	255	TRP	O-C-N	5.42	128.56	122.22
2	D	119	ASP	N-CA-C	-5.42	106.68	113.72
2	H	10	VAL	CA-CB-CG1	5.42	119.61	110.40
2	J	400	GLY	CA-C-N	5.41	125.03	119.56
2	J	400	GLY	C-N-CA	5.41	125.03	119.56
2	B	388	LYS	CA-C-N	5.41	127.97	120.29
2	B	388	LYS	C-N-CA	5.41	127.97	120.29
1	A	143	ILE	N-CA-C	-5.41	101.75	108.89
1	C	26	ARG	CD-NE-CZ	-5.41	116.83	124.40
2	L	388	LYS	CA-C-N	5.41	127.97	120.29
2	L	388	LYS	C-N-CA	5.41	127.97	120.29
2	D	10	VAL	CA-CB-CG1	5.40	119.59	110.40
1	E	143	ILE	N-CA-C	-5.40	101.76	108.89
1	S	26	ARG	CD-NE-CZ	-5.40	116.84	124.40
1	A	26	ARG	CD-NE-CZ	-5.40	116.84	124.40
1	I	26	ARG	CD-NE-CZ	-5.40	116.84	124.40
2	B	10	VAL	CA-CB-CG1	5.40	119.58	110.40
2	B	68	CYS	CA-C-N	5.40	129.42	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	68	CYS	C-N-CA	5.40	129.42	120.94
2	H	68	CYS	CA-C-N	5.39	129.41	120.94
2	H	68	CYS	C-N-CA	5.39	129.41	120.94
1	S	143	ILE	N-CA-C	-5.38	101.78	108.89
2	D	346	THR	OG1-CB-CG2	5.38	120.07	109.30
2	L	68	CYS	CA-C-N	5.38	129.39	120.94
2	L	68	CYS	C-N-CA	5.38	129.39	120.94
2	H	388	LYS	CA-C-N	5.38	127.93	120.29
2	H	388	LYS	C-N-CA	5.38	127.93	120.29
1	E	26	ARG	CD-NE-CZ	-5.38	116.87	124.40
1	G	143	ILE	N-CA-C	-5.38	101.79	108.89
2	H	345	TRP	CA-CB-CG	5.38	123.82	113.60
2	J	346	THR	OG1-CB-CG2	5.38	120.06	109.30
2	L	346	THR	OG1-CB-CG2	5.38	120.05	109.30
1	C	143	ILE	N-CA-C	-5.38	101.79	108.89
1	I	34	GLU	CG-CD-OE2	5.38	130.76	118.40
2	J	388	LYS	CA-C-N	5.38	127.92	120.29
2	J	388	LYS	C-N-CA	5.38	127.92	120.29
2	J	345	TRP	CA-CB-CG	5.37	123.81	113.60
1	C	34	GLU	CG-CD-OE2	5.37	130.75	118.40
2	F	388	LYS	CA-C-N	5.37	127.92	120.29
2	F	388	LYS	C-N-CA	5.37	127.92	120.29
2	D	68	CYS	CA-C-N	5.37	129.37	120.94
2	D	68	CYS	C-N-CA	5.37	129.37	120.94
2	H	346	THR	OG1-CB-CG2	5.37	120.04	109.30
1	G	34	GLU	CG-CD-OE2	5.37	130.74	118.40
2	F	346	THR	OG1-CB-CG2	5.37	120.03	109.30
2	J	81	ASP	OD1-CG-OD2	-5.37	110.02	122.90
1	S	34	GLU	CG-CD-OE2	5.36	130.74	118.40
2	F	345	TRP	CA-CB-CG	5.36	123.79	113.60
2	F	385	PRO	CA-C-N	5.36	127.41	120.44
2	F	385	PRO	C-N-CA	5.36	127.41	120.44
2	B	345	TRP	CA-CB-CG	5.36	123.78	113.60
1	I	143	ILE	N-CA-C	-5.36	101.82	108.89
2	F	295	SER	N-CA-C	-5.36	106.33	112.92
2	J	68	CYS	CA-C-N	5.36	129.35	120.94
2	J	68	CYS	C-N-CA	5.36	129.35	120.94
2	B	346	THR	OG1-CB-CG2	5.36	120.01	109.30
2	L	345	TRP	CA-CB-CG	5.35	123.77	113.60
2	B	385	PRO	CA-C-N	5.35	127.40	120.44
2	B	385	PRO	C-N-CA	5.35	127.40	120.44
2	D	345	TRP	CA-CB-CG	5.35	123.77	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	GLU	CG-CD-OE2	5.35	130.70	118.40
2	H	120	TRP	O-C-N	5.35	128.67	122.25
2	F	68	CYS	CA-C-N	5.34	129.33	120.94
2	F	68	CYS	C-N-CA	5.34	129.33	120.94
2	H	295	SER	N-CA-C	-5.34	106.35	112.92
1	E	34	GLU	CG-CD-OE2	5.34	130.69	118.40
2	J	295	SER	N-CA-C	-5.34	106.36	112.92
2	L	81	ASP	OD1-CG-OD2	-5.33	110.09	122.90
2	L	295	SER	N-CA-C	-5.33	106.37	112.92
2	B	295	SER	N-CA-C	-5.32	106.37	112.92
2	H	81	ASP	OD1-CG-OD2	-5.32	110.12	122.90
2	D	81	ASP	OD1-CG-OD2	-5.32	110.13	122.90
2	H	385	PRO	CA-C-N	5.32	127.36	120.44
2	H	385	PRO	C-N-CA	5.32	127.36	120.44
2	D	295	SER	N-CA-C	-5.32	106.38	112.92
2	L	385	PRO	CA-C-N	5.32	127.35	120.44
2	L	385	PRO	C-N-CA	5.32	127.35	120.44
2	F	81	ASP	OD1-CG-OD2	-5.32	110.14	122.90
2	B	81	ASP	OD1-CG-OD2	-5.31	110.16	122.90
2	J	96	ARG	CD-NE-CZ	5.31	131.83	124.40
1	E	235	GLN	CA-C-O	-5.30	114.06	120.32
1	G	235	GLN	CA-C-O	-5.30	114.06	120.32
2	F	96	ARG	CD-NE-CZ	5.30	131.82	124.40
2	H	70	TYR	CA-C-N	5.30	128.00	120.53
2	H	70	TYR	C-N-CA	5.30	128.00	120.53
2	H	22	ARG	CA-C-O	-5.30	114.44	120.32
2	D	96	ARG	CD-NE-CZ	5.29	131.81	124.40
2	F	22	ARG	CA-C-O	-5.29	114.45	120.32
2	B	70	TYR	CA-C-N	5.29	127.99	120.53
2	B	70	TYR	C-N-CA	5.29	127.99	120.53
2	J	227	GLY	CA-C-N	5.29	130.89	122.59
2	J	227	GLY	C-N-CA	5.29	130.89	122.59
1	S	235	GLN	CA-C-O	-5.29	114.08	120.32
1	C	235	GLN	CA-C-O	-5.29	114.08	120.32
2	J	385	PRO	CA-C-N	5.28	127.31	120.44
2	J	385	PRO	C-N-CA	5.28	127.31	120.44
2	L	96	ARG	CD-NE-CZ	5.28	131.79	124.40
1	A	235	GLN	CA-C-O	-5.28	114.09	120.32
1	C	258	TYR	O-C-N	5.28	128.53	122.25
2	B	22	ARG	CA-C-O	-5.28	114.46	120.32
2	D	385	PRO	CA-C-N	5.28	127.30	120.44
2	D	385	PRO	C-N-CA	5.28	127.30	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	193	HIS	CA-C-N	5.27	127.30	120.44
1	G	193	HIS	C-N-CA	5.27	127.30	120.44
2	D	70	TYR	CA-C-N	5.27	127.96	120.53
2	D	70	TYR	C-N-CA	5.27	127.96	120.53
2	F	70	TYR	CA-C-N	5.27	127.96	120.53
2	F	70	TYR	C-N-CA	5.27	127.96	120.53
2	H	96	ARG	CD-NE-CZ	5.27	131.78	124.40
2	L	70	TYR	CA-C-N	5.27	127.96	120.53
2	L	70	TYR	C-N-CA	5.27	127.96	120.53
1	I	258	TYR	O-C-N	5.27	128.52	122.25
2	L	227	GLY	CA-C-N	5.26	130.85	122.59
2	L	227	GLY	C-N-CA	5.26	130.85	122.59
2	J	70	TYR	CA-C-N	5.26	127.95	120.53
2	J	70	TYR	C-N-CA	5.26	127.95	120.53
2	F	227	GLY	CA-C-N	5.26	130.85	122.59
2	F	227	GLY	C-N-CA	5.26	130.85	122.59
2	F	442	ASP	CA-CB-CG	-5.26	107.34	112.60
2	J	516	ARG	CA-C-O	-5.26	116.40	121.34
2	F	516	ARG	CA-C-O	-5.25	116.40	121.34
2	D	227	GLY	CA-C-N	5.25	130.84	122.59
2	D	227	GLY	C-N-CA	5.25	130.84	122.59
2	H	516	ARG	CA-C-O	-5.25	116.40	121.34
1	S	258	TYR	O-C-N	5.25	128.50	122.25
1	I	225	TYR	CA-CB-CG	-5.25	104.45	113.90
2	D	516	ARG	CA-C-O	-5.25	116.41	121.34
1	A	193	HIS	CA-C-N	5.25	127.26	120.44
1	A	193	HIS	C-N-CA	5.25	127.26	120.44
1	A	258	TYR	O-C-N	5.25	128.50	122.25
1	E	193	HIS	CA-C-N	5.25	127.26	120.44
1	E	193	HIS	C-N-CA	5.25	127.26	120.44
1	G	258	TYR	O-C-N	5.25	128.50	122.25
1	I	235	GLN	CA-C-O	-5.25	114.13	120.32
2	L	22	ARG	CA-C-O	-5.25	114.50	120.32
2	B	516	ARG	CA-C-O	-5.25	116.41	121.34
2	D	22	ARG	CA-C-O	-5.25	114.50	120.32
1	S	193	HIS	CA-C-N	5.25	127.26	120.44
1	S	193	HIS	C-N-CA	5.25	127.26	120.44
2	B	227	GLY	CA-C-N	5.25	130.82	122.59
2	B	227	GLY	C-N-CA	5.25	130.82	122.59
1	G	225	TYR	CA-CB-CG	-5.25	104.46	113.90
2	F	198	GLU	O-C-N	5.24	127.68	122.12
2	B	96	ARG	CD-NE-CZ	5.24	131.74	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	225	TYR	CA-CB-CG	-5.24	104.47	113.90
1	I	48	LEU	N-CA-CB	-5.24	102.99	110.80
1	S	225	TYR	CA-CB-CG	-5.24	104.47	113.90
1	A	225	TYR	CA-CB-CG	-5.23	104.48	113.90
1	S	48	LEU	N-CA-CB	-5.23	103.00	110.80
2	L	320	GLU	CA-C-O	-5.23	114.32	120.60
2	H	227	GLY	CA-C-N	5.23	130.81	122.59
2	H	227	GLY	C-N-CA	5.23	130.81	122.59
2	B	320	GLU	CA-C-O	-5.23	114.32	120.60
1	C	48	LEU	N-CA-CB	-5.23	103.00	110.80
1	E	258	TYR	O-C-N	5.23	128.47	122.25
2	F	346	THR	CA-CB-OG1	-5.23	101.76	109.60
1	A	48	LEU	N-CA-CB	-5.23	103.01	110.80
1	E	48	LEU	N-CA-CB	-5.23	103.01	110.80
2	H	443	LEU	CA-C-O	-5.23	112.68	118.69
1	G	48	LEU	N-CA-CB	-5.23	103.01	110.80
1	I	193	HIS	CA-C-N	5.23	127.23	120.44
1	I	193	HIS	C-N-CA	5.23	127.23	120.44
2	F	443	LEU	CA-C-O	-5.22	112.69	118.69
1	C	225	TYR	CA-CB-CG	-5.22	104.50	113.90
2	L	516	ARG	CA-C-O	-5.22	116.44	121.34
2	B	346	THR	CA-CB-OG1	-5.22	101.78	109.60
1	E	213	CYS	CB-CA-C	5.22	118.38	109.72
2	J	442	ASP	CA-CB-CG	-5.22	107.38	112.60
1	C	193	HIS	CA-C-N	5.21	127.22	120.44
1	C	193	HIS	C-N-CA	5.21	127.22	120.44
2	H	320	GLU	CA-C-O	-5.21	114.34	120.60
2	D	443	LEU	CA-C-O	-5.21	112.69	118.69
2	J	346	THR	CA-CB-OG1	-5.21	101.78	109.60
1	C	213	CYS	CB-CA-C	5.21	118.37	109.72
2	F	130	ASP	N-CA-C	-5.21	99.31	108.69
2	B	442	ASP	CA-CB-CG	-5.21	107.39	112.60
2	D	442	ASP	CA-CB-CG	-5.21	107.39	112.60
2	D	320	GLU	CA-C-O	-5.21	114.35	120.60
2	F	320	GLU	CA-C-O	-5.21	114.35	120.60
2	J	22	ARG	CA-C-O	-5.21	114.54	120.32
2	J	320	GLU	CA-C-O	-5.21	114.35	120.60
2	H	346	THR	CA-CB-OG1	-5.21	101.79	109.60
1	S	213	CYS	CB-CA-C	5.20	118.36	109.72
2	L	346	THR	CA-CB-OG1	-5.20	101.80	109.60
2	L	442	ASP	CA-CB-CG	-5.20	107.40	112.60
1	A	213	CYS	CB-CA-C	5.20	118.36	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	47	MET	CA-C-N	5.20	129.24	120.29
2	F	47	MET	C-N-CA	5.20	129.24	120.29
1	I	213	CYS	CB-CA-C	5.20	118.36	109.72
2	J	130	ASP	N-CA-C	-5.20	99.32	108.69
2	J	47	MET	CA-C-N	5.20	129.23	120.29
2	J	47	MET	C-N-CA	5.20	129.23	120.29
2	B	47	MET	CA-C-N	5.20	129.23	120.29
2	B	47	MET	C-N-CA	5.20	129.23	120.29
2	B	443	LEU	CA-C-O	-5.20	112.71	118.69
2	L	443	LEU	CA-C-O	-5.20	112.71	118.69
2	H	47	MET	CA-C-N	5.20	129.23	120.29
2	H	47	MET	C-N-CA	5.20	129.23	120.29
2	D	47	MET	CA-C-N	5.19	129.22	120.29
2	D	47	MET	C-N-CA	5.19	129.22	120.29
1	C	45	HIS	CA-C-O	-5.19	114.84	120.09
1	G	45	HIS	CA-C-O	-5.19	114.84	120.09
2	L	130	ASP	N-CA-C	-5.19	99.35	108.69
2	D	130	ASP	N-CA-C	-5.19	99.35	108.69
2	D	346	THR	CA-CB-OG1	-5.19	101.81	109.60
2	B	198	GLU	O-C-N	5.19	127.62	122.12
1	I	45	HIS	CA-C-O	-5.19	114.85	120.09
2	L	47	MET	CA-C-N	5.18	129.21	120.29
2	L	47	MET	C-N-CA	5.18	129.21	120.29
1	G	213	CYS	CB-CA-C	5.18	118.33	109.72
2	H	442	ASP	CA-CB-CG	-5.18	107.42	112.60
2	D	532	ALA	CA-C-N	5.18	127.49	120.44
2	D	532	ALA	C-N-CA	5.18	127.49	120.44
2	D	130	ASP	O-C-N	5.18	126.06	121.19
2	L	198	GLU	O-C-N	5.18	127.61	122.12
1	C	72	ILE	CA-C-O	-5.18	114.99	120.53
2	F	532	ALA	CA-C-N	5.18	127.48	120.44
2	F	532	ALA	C-N-CA	5.18	127.48	120.44
2	J	198	GLU	O-C-N	5.18	127.61	122.12
2	J	441	ASP	N-CA-CB	-5.18	102.66	111.20
2	B	45	LEU	CA-C-O	-5.17	114.94	120.42
2	B	130	ASP	N-CA-C	-5.17	99.39	108.69
2	D	287	PRO	CB-CA-C	-5.17	103.47	110.60
2	H	130	ASP	N-CA-C	-5.17	99.39	108.69
2	B	441	ASP	N-CA-CB	-5.17	102.67	111.20
1	E	38	ASP	CA-C-N	-5.17	116.25	122.35
1	E	38	ASP	C-N-CA	-5.17	116.25	122.35
1	I	38	ASP	CA-C-N	-5.17	116.25	122.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	38	ASP	C-N-CA	-5.17	116.25	122.35
2	F	130	ASP	O-C-N	5.17	126.05	121.19
2	D	198	GLU	O-C-N	5.16	127.59	122.12
2	H	441	ASP	N-CA-CB	-5.16	102.68	111.20
1	S	72	ILE	CA-C-O	-5.16	115.01	120.53
2	L	441	ASP	N-CA-CB	-5.16	102.68	111.20
2	L	532	ALA	CA-C-N	5.16	127.46	120.44
2	L	532	ALA	C-N-CA	5.16	127.46	120.44
1	C	38	ASP	CA-C-N	-5.16	116.26	122.35
1	C	38	ASP	C-N-CA	-5.16	116.26	122.35
2	D	9	ILE	O-C-N	5.16	128.77	123.20
2	F	441	ASP	N-CA-CB	-5.16	102.69	111.20
1	G	72	ILE	CA-C-O	-5.16	115.01	120.53
1	S	45	HIS	CA-C-O	-5.16	114.88	120.09
2	L	45	LEU	CA-C-O	-5.16	114.95	120.42
2	J	45	LEU	CA-C-O	-5.16	114.95	120.42
2	J	287	PRO	CB-CA-C	-5.15	103.49	110.60
2	F	9	ILE	O-C-N	5.15	128.76	123.20
1	E	45	HIS	CA-C-O	-5.15	114.89	120.09
2	H	532	ALA	CA-C-N	5.15	127.44	120.44
2	H	532	ALA	C-N-CA	5.15	127.44	120.44
2	F	45	LEU	CA-C-O	-5.15	114.96	120.42
2	D	441	ASP	N-CA-CB	-5.14	102.71	111.20
2	J	443	LEU	CA-C-O	-5.14	112.77	118.69
1	S	59	ALA	CA-C-O	5.14	126.00	120.70
1	E	72	ILE	CA-C-O	-5.14	115.03	120.53
2	H	44	GLY	CA-C-N	5.14	127.59	120.29
2	H	44	GLY	C-N-CA	5.14	127.59	120.29
2	H	45	LEU	CA-C-O	-5.14	114.97	120.42
2	J	64	ALA	N-CA-C	-5.14	106.27	112.54
2	B	64	ALA	N-CA-C	-5.14	106.27	112.54
2	F	64	ALA	N-CA-C	-5.14	106.27	112.54
1	I	59	ALA	CA-C-O	5.14	125.99	120.70
2	D	115	LEU	CB-CA-C	5.14	118.82	110.24
2	H	9	ILE	O-C-N	5.14	128.75	123.20
2	H	115	LEU	CB-CA-C	5.14	118.82	110.24
2	H	287	PRO	CB-CA-C	-5.14	103.51	110.60
2	L	287	PRO	CB-CA-C	-5.13	103.51	110.60
1	A	72	ILE	CA-C-O	-5.13	115.03	120.53
1	C	36	ILE	N-CA-CB	-5.13	101.87	110.65
2	H	198	GLU	O-C-N	5.13	127.56	122.12
2	J	115	LEU	CB-CA-C	5.13	118.81	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	532	ALA	CA-C-N	5.13	127.42	120.44
2	B	532	ALA	C-N-CA	5.13	127.42	120.44
2	D	45	LEU	CA-C-O	-5.13	114.98	120.42
2	D	64	ALA	N-CA-C	-5.13	106.28	112.54
2	J	532	ALA	CA-C-N	5.13	127.42	120.44
2	J	532	ALA	C-N-CA	5.13	127.42	120.44
2	L	115	LEU	CB-CA-C	5.13	118.81	110.24
2	L	9	ILE	O-C-N	5.13	128.74	123.20
2	J	9	ILE	O-C-N	5.13	128.74	123.20
2	J	44	GLY	CA-C-N	5.13	127.57	120.29
2	J	44	GLY	C-N-CA	5.13	127.57	120.29
1	S	38	ASP	CA-C-N	-5.13	116.30	122.35
1	S	38	ASP	C-N-CA	-5.13	116.30	122.35
2	L	130	ASP	O-C-N	5.13	126.01	121.19
2	B	182	TYR	CA-C-O	-5.13	115.30	120.84
2	D	182	TYR	CA-C-O	-5.13	115.30	120.84
2	H	130	ASP	O-C-N	5.12	126.01	121.19
2	J	420	THR	CB-CA-C	5.12	119.56	110.85
2	L	44	GLY	CA-C-N	5.12	127.56	120.29
2	L	44	GLY	C-N-CA	5.12	127.56	120.29
2	L	64	ALA	N-CA-C	-5.12	106.29	112.54
1	A	59	ALA	CA-C-O	5.12	125.98	120.70
2	F	420	THR	CB-CA-C	5.12	119.56	110.85
2	B	101	GLY	N-CA-C	-5.12	106.56	112.50
2	B	420	THR	CB-CA-C	5.12	119.56	110.85
2	B	520	ILE	CA-C-N	5.12	127.14	120.28
2	B	520	ILE	C-N-CA	5.12	127.14	120.28
2	D	420	THR	CB-CA-C	5.12	119.56	110.85
2	F	287	PRO	CB-CA-C	-5.12	103.53	110.60
1	G	159	VAL	N-CA-C	-5.12	105.33	110.30
2	H	202	VAL	N-CA-C	-5.12	105.72	110.53
2	D	44	GLY	CA-C-N	5.12	127.56	120.29
2	D	44	GLY	C-N-CA	5.12	127.56	120.29
2	J	507	ILE	CB-CG1-CD1	5.12	124.55	113.80
2	B	287	PRO	CB-CA-C	-5.12	103.54	110.60
1	E	254	PHE	CA-C-N	5.12	127.65	120.28
1	E	254	PHE	C-N-CA	5.12	127.65	120.28
1	A	38	ASP	CA-C-N	-5.12	116.31	122.35
1	A	38	ASP	C-N-CA	-5.12	116.31	122.35
2	B	130	ASP	O-C-N	5.12	126.00	121.19
2	B	115	LEU	CB-CA-C	5.11	118.78	110.24
2	D	363	LYS	N-CA-C	-5.11	104.59	111.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	115	LEU	CB-CA-C	5.11	118.78	110.24
2	F	520	ILE	CA-C-N	5.11	127.13	120.28
2	F	520	ILE	C-N-CA	5.11	127.13	120.28
1	A	159	VAL	N-CA-C	-5.11	105.34	110.30
1	I	72	ILE	CA-C-O	-5.11	115.06	120.53
2	F	44	GLY	CA-C-N	5.11	127.55	120.29
2	F	44	GLY	C-N-CA	5.11	127.55	120.29
2	F	507	ILE	CB-CG1-CD1	5.11	124.53	113.80
1	G	38	ASP	CA-C-N	-5.11	116.32	122.35
1	G	38	ASP	C-N-CA	-5.11	116.32	122.35
2	H	420	THR	CB-CA-C	5.11	119.54	110.85
2	J	182	TYR	CA-C-O	-5.11	115.32	120.84
2	B	44	GLY	CA-C-N	5.11	127.54	120.29
2	B	44	GLY	C-N-CA	5.11	127.54	120.29
1	C	59	ALA	CA-C-O	5.11	125.96	120.70
2	L	420	THR	CB-CA-C	5.11	119.53	110.85
2	L	182	TYR	CA-C-O	-5.11	115.33	120.84
2	H	176	LEU	CA-C-O	5.11	126.57	120.70
1	G	36	ILE	N-CA-CB	-5.10	101.92	110.65
1	E	36	ILE	N-CA-CB	-5.10	101.92	110.65
2	F	363	LYS	N-CA-C	-5.10	104.60	111.54
1	G	59	ALA	CA-C-O	5.10	125.95	120.70
2	H	182	TYR	CA-C-O	-5.10	115.33	120.84
1	S	36	ILE	N-CA-CB	-5.10	101.93	110.65
1	S	254	PHE	CA-C-N	5.10	127.62	120.28
1	S	254	PHE	C-N-CA	5.10	127.62	120.28
2	D	520	ILE	CA-C-N	5.10	127.11	120.28
2	D	520	ILE	C-N-CA	5.10	127.11	120.28
1	I	36	ILE	N-CA-CB	-5.10	101.93	110.65
2	L	507	ILE	CB-CG1-CD1	5.10	124.51	113.80
1	A	143	ILE	CA-C-N	-5.10	116.21	122.84
1	A	143	ILE	C-N-CA	-5.10	116.21	122.84
2	H	64	ALA	N-CA-C	-5.10	106.32	112.54
1	A	48	LEU	O-C-N	5.10	128.22	122.20
2	D	507	ILE	CB-CG1-CD1	5.10	124.50	113.80
2	H	101	GLY	N-CA-C	-5.10	106.59	112.50
2	J	130	ASP	O-C-N	5.10	125.98	121.19
2	J	176	LEU	CA-C-O	5.10	126.56	120.70
2	L	363	LYS	N-CA-C	-5.10	104.61	111.54
2	D	176	LEU	CA-C-O	5.10	126.56	120.70
2	B	9	ILE	O-C-N	5.09	128.70	123.20
1	C	159	VAL	N-CA-C	-5.09	105.36	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48	LEU	O-C-N	5.09	128.21	122.20
2	H	507	ILE	CB-CG1-CD1	5.09	124.50	113.80
2	J	363	LYS	N-CA-C	-5.09	104.61	111.54
1	A	45	HIS	CA-C-O	-5.09	114.95	120.09
2	L	101	GLY	N-CA-C	-5.09	106.59	112.50
2	L	176	LEU	CA-C-O	5.09	126.56	120.70
2	B	363	LYS	N-CA-C	-5.09	104.61	111.54
1	E	159	VAL	N-CA-C	-5.09	105.36	110.30
1	S	137	LYS	CA-C-N	5.09	130.54	122.60
1	S	137	LYS	C-N-CA	5.09	130.54	122.60
1	E	137	LYS	CA-C-N	5.09	130.54	122.60
1	E	137	LYS	C-N-CA	5.09	130.54	122.60
1	S	159	VAL	N-CA-C	-5.08	105.37	110.30
1	E	59	ALA	CA-C-O	5.08	125.94	120.70
1	A	36	ILE	N-CA-CB	-5.08	101.96	110.65
1	A	254	PHE	CA-C-N	5.08	127.60	120.28
1	A	254	PHE	C-N-CA	5.08	127.60	120.28
1	C	48	LEU	O-C-N	5.08	128.20	122.20
1	C	254	PHE	CA-C-N	5.08	127.60	120.28
1	C	254	PHE	C-N-CA	5.08	127.60	120.28
1	G	137	LYS	CA-C-N	5.08	130.53	122.60
1	G	137	LYS	C-N-CA	5.08	130.53	122.60
2	L	520	ILE	CA-C-N	5.08	127.09	120.28
2	L	520	ILE	C-N-CA	5.08	127.09	120.28
1	G	201	THR	N-CA-CB	5.08	118.28	110.61
1	G	254	PHE	CA-C-N	5.08	127.60	120.28
1	G	254	PHE	C-N-CA	5.08	127.60	120.28
2	B	507	ILE	CB-CG1-CD1	5.08	124.47	113.80
2	D	381	LYS	CG-CD-CE	5.08	122.98	111.30
2	J	520	ILE	CA-C-N	5.08	127.08	120.28
2	J	520	ILE	C-N-CA	5.08	127.08	120.28
2	F	101	GLY	N-CA-C	-5.08	106.61	112.50
2	F	176	LEU	CA-C-O	5.08	126.54	120.70
2	B	381	LYS	CG-CD-CE	5.08	122.97	111.30
2	J	101	GLY	N-CA-C	-5.08	106.61	112.50
1	E	201	THR	N-CA-CB	5.07	118.27	110.61
1	I	159	VAL	N-CA-C	-5.07	105.38	110.30
2	B	176	LEU	CA-C-O	5.07	126.53	120.70
1	E	143	ILE	CA-C-N	-5.07	116.25	122.84
1	E	143	ILE	C-N-CA	-5.07	116.25	122.84
1	S	201	THR	N-CA-CB	5.07	118.27	110.61
1	A	201	THR	N-CA-CB	5.07	118.27	110.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	143	ILE	CA-C-N	-5.07	116.25	122.84
1	S	143	ILE	C-N-CA	-5.07	116.25	122.84
2	H	363	LYS	N-CA-C	-5.07	104.65	111.54
1	I	137	LYS	CA-C-N	5.07	130.51	122.60
1	I	137	LYS	C-N-CA	5.07	130.51	122.60
1	I	201	THR	N-CA-CB	5.07	118.26	110.61
2	J	202	VAL	N-CA-C	-5.07	105.77	110.53
1	C	201	THR	N-CA-CB	5.07	118.26	110.61
2	F	381	LYS	CG-CD-CE	5.07	122.95	111.30
1	C	115	TYR	O-C-N	-5.06	116.40	122.27
2	F	182	TYR	CA-C-O	-5.06	115.37	120.84
2	H	381	LYS	CG-CD-CE	5.06	122.94	111.30
2	J	381	LYS	CG-CD-CE	5.06	122.94	111.30
1	S	48	LEU	O-C-N	5.06	128.17	122.20
2	D	101	GLY	N-CA-C	-5.06	106.63	112.50
2	D	535	VAL	N-CA-C	5.06	116.16	111.81
2	L	381	LYS	CG-CD-CE	5.06	122.93	111.30
2	J	528	ASP	O-C-N	-5.05	115.51	121.32
1	C	143	ILE	CA-C-N	-5.05	116.27	122.84
1	C	143	ILE	C-N-CA	-5.05	116.27	122.84
1	G	143	ILE	CA-C-N	-5.05	116.27	122.84
1	G	143	ILE	C-N-CA	-5.05	116.27	122.84
2	D	116	HIS	N-CA-C	5.05	119.43	113.12
2	F	382	LYS	N-CA-C	5.05	118.59	111.52
2	H	535	VAL	N-CA-C	5.05	116.15	111.81
2	J	478	GLU	N-CA-C	-5.05	106.81	113.12
2	F	478	GLU	N-CA-C	-5.04	106.81	113.12
2	L	202	VAL	N-CA-C	-5.04	105.79	110.53
1	G	48	LEU	O-C-N	5.04	128.15	122.20
1	I	143	ILE	CA-C-N	-5.04	116.28	122.84
1	I	143	ILE	C-N-CA	-5.04	116.28	122.84
2	B	69	THR	CA-CB-OG1	-5.04	102.04	109.60
2	H	69	THR	CA-CB-OG1	-5.04	102.04	109.60
2	D	202	VAL	N-CA-C	-5.04	105.80	110.53
2	D	382	LYS	N-CA-C	5.04	118.57	111.52
2	H	15	THR	CA-CB-OG1	-5.04	102.05	109.60
2	J	116	HIS	N-CA-C	5.04	119.41	113.12
2	L	478	GLU	N-CA-C	-5.03	106.83	113.12
2	B	202	VAL	N-CA-C	-5.03	105.80	110.53
2	D	528	ASP	O-C-N	-5.03	115.54	121.32
1	I	48	LEU	O-C-N	5.03	128.13	122.20
2	L	69	THR	CA-CB-OG1	-5.03	102.06	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	LYS	N-CA-C	5.03	118.56	111.52
2	J	69	THR	CA-CB-OG1	-5.03	102.06	109.60
2	L	528	ASP	O-C-N	-5.03	115.54	121.32
2	B	370	GLY	O-C-N	5.03	126.80	121.77
2	F	528	ASP	O-C-N	-5.03	115.54	121.32
1	G	115	TYR	O-C-N	-5.03	116.44	122.27
2	H	478	GLU	N-CA-C	-5.02	106.84	113.12
1	C	213	CYS	O-C-N	-5.02	116.69	122.87
2	D	15	THR	CA-CB-OG1	-5.02	102.06	109.60
2	L	15	THR	CA-CB-OG1	-5.02	102.07	109.60
2	F	15	THR	CA-CB-OG1	-5.02	102.07	109.60
2	H	528	ASP	O-C-N	-5.02	115.55	121.32
1	S	115	TYR	O-C-N	-5.02	116.45	122.27
2	B	208	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	D	69	THR	CA-CB-OG1	-5.02	102.07	109.60
2	F	370	GLY	O-C-N	5.02	126.79	121.77
1	I	115	TYR	O-C-N	-5.02	116.45	122.27
2	D	478	GLU	N-CA-C	-5.02	106.85	113.12
2	F	69	THR	CA-CB-OG1	-5.02	102.08	109.60
1	I	128	THR	CA-CB-OG1	-5.02	102.07	109.60
1	E	115	TYR	O-C-N	-5.01	116.45	122.27
2	D	370	GLY	O-C-N	5.01	126.78	121.77
2	B	478	GLU	N-CA-C	-5.01	106.86	113.12
2	H	116	HIS	N-CA-C	5.01	119.38	113.12
2	L	116	HIS	N-CA-C	5.01	119.38	113.12
2	F	406	SER	N-CA-CB	-5.01	103.32	111.24
1	G	188	CYS	CA-C-O	-5.01	115.04	119.75
2	L	382	LYS	N-CA-C	5.01	118.53	111.52
2	H	208	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	J	370	GLY	O-C-N	5.01	126.78	121.77
2	B	406	SER	N-CA-CB	-5.01	103.33	111.24
2	F	116	HIS	N-CA-C	5.01	119.38	113.12
2	F	202	VAL	N-CA-C	-5.01	105.82	110.53
2	L	370	GLY	O-C-N	5.00	126.78	121.77
2	L	406	SER	N-CA-CB	-5.00	103.33	111.24
1	I	18	THR	CA-CB-OG1	-5.00	102.09	109.60
2	L	535	VAL	N-CA-C	5.00	116.11	111.81
2	B	15	THR	CA-CB-OG1	-5.00	102.09	109.60
1	E	174	GLY	CA-C-O	-5.00	113.03	119.13
1	S	174	GLY	CA-C-O	-5.00	113.03	119.13
1	A	115	TYR	O-C-N	-5.00	116.47	122.27
2	F	535	VAL	N-CA-C	5.00	116.11	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	406	SER	N-CA-CB	-5.00	103.34	111.24

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	353	ARG	Sidechain
2	D	353	ARG	Sidechain
2	F	353	ARG	Sidechain
2	H	353	ARG	Sidechain
2	J	353	ARG	Sidechain
2	L	353	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1964	0	1895	46	0
1	C	1964	0	1895	40	0
1	E	1964	0	1895	44	0
1	G	1964	0	1895	43	0
1	I	1964	0	1895	41	0
1	S	1964	0	1895	43	0
2	B	4152	0	4114	132	0
2	D	4152	0	4114	125	0
2	F	4152	0	4114	127	0
2	H	4152	0	4114	128	0
2	J	4152	0	4114	129	0
2	L	4152	0	4114	127	0
3	A	16	0	0	0	0
3	C	16	0	0	0	0
3	E	16	0	0	0	0
3	G	16	0	0	0	0
3	I	16	0	0	0	0
3	S	16	0	0	0	0
4	A	7	0	0	0	0
4	C	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	7	0	0	0	0
4	G	7	0	0	0	0
4	I	7	0	0	1	0
4	S	7	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
7	B	7	0	0	2	0
7	D	7	0	0	2	0
7	F	7	0	0	2	0
7	H	7	0	0	2	0
7	J	7	0	0	2	0
7	L	7	0	0	2	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
8	J	1	0	0	0	0
8	L	1	0	0	0	0
9	A	78	0	0	0	2
9	B	114	0	0	0	0
9	C	76	0	0	0	1
9	D	114	0	0	0	0
9	E	81	0	0	0	1
9	F	115	0	0	0	0
9	G	76	0	0	0	0
9	H	112	0	0	0	0
9	I	80	0	0	0	1
9	J	113	0	0	0	0
9	L	110	0	0	0	0
9	S	77	0	0	0	1
All	All	38040	0	36054	964	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 13.

All (964) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:GLN:NE2	2:J:208:ARG:HH21	1.56	1.03
1:E:235:GLN:NE2	2:F:208:ARG:HH21	1.56	1.03
1:C:235:GLN:NE2	2:D:208:ARG:HH21	1.56	1.02
1:A:235:GLN:NE2	2:B:208:ARG:HH21	1.56	1.02
1:G:235:GLN:NE2	2:H:208:ARG:HH21	1.56	1.02
1:S:235:GLN:NE2	2:L:208:ARG:HH21	1.56	1.01
1:C:235:GLN:HE21	2:D:208:ARG:NH2	1.62	0.96
1:S:235:GLN:HE21	2:L:208:ARG:NH2	1.62	0.96
1:G:235:GLN:HE21	2:H:208:ARG:NH2	1.62	0.96
1:A:235:GLN:HE21	2:B:208:ARG:NH2	1.62	0.95
1:I:235:GLN:HE21	2:J:208:ARG:NH2	1.62	0.95
1:E:235:GLN:HE21	2:F:208:ARG:NH2	1.62	0.95
2:B:142:SER:HB2	2:B:143:PRO:CD	2.08	0.84
2:D:142:SER:HB2	2:D:143:PRO:CD	2.08	0.84
2:L:142:SER:HB2	2:L:143:PRO:CD	2.08	0.84
2:H:142:SER:HB2	2:H:143:PRO:CD	2.08	0.84
1:E:26:ARG:HH21	2:F:217:ASN:HD21	1.24	0.84
1:C:26:ARG:HH21	2:D:217:ASN:HD21	1.24	0.83
2:J:142:SER:HB2	2:J:143:PRO:CD	2.08	0.83
1:A:26:ARG:HH21	2:B:217:ASN:HD21	1.24	0.83
2:F:142:SER:HB2	2:F:143:PRO:CD	2.08	0.83
1:G:26:ARG:HH21	2:H:217:ASN:HD21	1.24	0.83
1:I:26:ARG:HH21	2:J:217:ASN:HD21	1.24	0.82
1:S:26:ARG:HH21	2:L:217:ASN:HD21	1.24	0.82
2:F:108:HIS:CE1	2:F:417:GLN:HE21	2.00	0.80
2:L:108:HIS:CE1	2:L:417:GLN:HE21	2.00	0.80
2:J:108:HIS:CE1	2:J:417:GLN:HE21	2.00	0.80
2:D:108:HIS:CE1	2:D:417:GLN:HE21	2.00	0.80
1:G:141:LYS:HD2	2:J:384:GLU:HG3	1.64	0.80
2:D:484:VAL:HG11	2:D:533:CYS:HB3	1.63	0.79
2:H:108:HIS:CE1	2:H:417:GLN:HE21	2.00	0.79
2:H:484:VAL:HG11	2:H:533:CYS:HB3	1.63	0.79
2:B:108:HIS:CE1	2:B:417:GLN:HE21	2.00	0.79
2:B:217:ASN:C	2:B:217:ASN:HD22	1.91	0.79
2:J:217:ASN:C	2:J:217:ASN:HD22	1.91	0.78
2:H:217:ASN:C	2:H:217:ASN:HD22	1.91	0.78
2:D:217:ASN:C	2:D:217:ASN:HD22	1.91	0.78
2:B:484:VAL:HG11	2:B:533:CYS:HB3	1.63	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:217:ASN:C	2:L:217:ASN:HD22	1.91	0.78
2:L:484:VAL:HG11	2:L:533:CYS:HB3	1.63	0.78
2:F:217:ASN:C	2:F:217:ASN:HD22	1.91	0.78
2:J:484:VAL:HG11	2:J:533:CYS:HB3	1.63	0.77
2:F:484:VAL:HG11	2:F:533:CYS:HB3	1.63	0.77
2:H:484:VAL:CG1	2:H:485:PRO:HD2	2.15	0.77
1:I:227:ASN:HD22	1:I:227:ASN:H	1.33	0.77
2:J:484:VAL:CG1	2:J:485:PRO:HD2	2.15	0.77
2:B:484:VAL:CG1	2:B:485:PRO:HD2	2.15	0.76
1:E:227:ASN:H	1:E:227:ASN:HD22	1.33	0.76
2:D:484:VAL:CG1	2:D:485:PRO:HD2	2.15	0.76
1:G:227:ASN:H	1:G:227:ASN:HD22	1.33	0.76
2:L:484:VAL:CG1	2:L:485:PRO:HD2	2.15	0.76
2:F:484:VAL:CG1	2:F:485:PRO:HD2	2.15	0.76
1:C:227:ASN:HD22	1:C:227:ASN:H	1.33	0.75
1:A:227:ASN:HD22	1:A:227:ASN:H	1.33	0.74
1:S:227:ASN:H	1:S:227:ASN:HD22	1.33	0.74
2:J:32:ILE:HD12	2:J:509:THR:HB	1.71	0.73
2:L:32:ILE:HD12	2:L:509:THR:HB	1.71	0.73
2:B:32:ILE:HD12	2:B:509:THR:HB	1.71	0.73
2:D:32:ILE:HD12	2:D:509:THR:HB	1.71	0.72
2:H:32:ILE:HD12	2:H:509:THR:HB	1.71	0.72
2:H:346:THR:O	2:H:350:GLY:HA3	1.89	0.72
2:J:346:THR:O	2:J:350:GLY:HA3	1.89	0.72
2:L:346:THR:O	2:L:350:GLY:HA3	1.89	0.72
2:F:32:ILE:HD12	2:F:509:THR:HB	1.71	0.72
2:B:346:THR:O	2:B:350:GLY:HA3	1.89	0.72
2:F:346:THR:O	2:F:350:GLY:HA3	1.89	0.71
2:D:346:THR:O	2:D:350:GLY:HA3	1.89	0.71
2:F:108:HIS:HE1	2:F:417:GLN:HG2	1.55	0.71
1:E:124:ASN:HD21	1:E:128:THR:H	1.39	0.71
1:A:124:ASN:HD21	1:A:128:THR:H	1.39	0.70
2:J:108:HIS:HE1	2:J:417:GLN:HG2	1.55	0.70
1:I:124:ASN:HD21	1:I:128:THR:H	1.39	0.70
2:L:108:HIS:HE1	2:L:417:GLN:HE21	1.40	0.70
2:L:108:HIS:HE1	2:L:417:GLN:HG2	1.55	0.70
2:D:108:HIS:HE1	2:D:417:GLN:HG2	1.55	0.70
1:S:124:ASN:HD21	1:S:128:THR:H	1.39	0.69
2:D:108:HIS:HE1	2:D:417:GLN:HE21	1.40	0.69
2:B:108:HIS:HE1	2:B:417:GLN:HE21	1.40	0.69
2:H:108:HIS:HE1	2:H:417:GLN:HE21	1.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:ASN:HD21	1:G:128:THR:H	1.39	0.69
2:B:108:HIS:HE1	2:B:417:GLN:HG2	1.55	0.69
1:C:124:ASN:HD21	1:C:128:THR:H	1.39	0.69
2:F:108:HIS:HE1	2:F:417:GLN:HE21	1.40	0.69
2:H:108:HIS:HE1	2:H:417:GLN:HG2	1.55	0.69
2:J:108:HIS:HE1	2:J:417:GLN:HE21	1.40	0.69
2:H:357:MET:HE2	2:H:534:GLY:HA3	1.76	0.68
2:B:384:GLU:HG3	1:E:141:LYS:HD2	1.76	0.68
2:D:357:MET:HE2	2:D:534:GLY:HA3	1.76	0.68
2:J:357:MET:HE2	2:J:534:GLY:HA3	1.76	0.68
1:C:235:GLN:HE21	2:D:208:ARG:HH21	0.77	0.67
1:S:235:GLN:HE21	2:L:208:ARG:HH21	0.77	0.67
2:L:357:MET:HE2	2:L:534:GLY:HA3	1.76	0.67
2:F:357:MET:HE2	2:F:534:GLY:HA3	1.76	0.67
2:B:357:MET:HE2	2:B:534:GLY:HA3	1.76	0.66
2:H:253:ILE:O	2:H:258:ILE:HG12	1.95	0.66
2:D:253:ILE:O	2:D:258:ILE:HG12	1.96	0.66
2:J:278:SER:O	2:J:279:ASN:HB2	1.96	0.66
1:A:235:GLN:HE21	2:B:208:ARG:HH21	0.77	0.65
2:D:195:HIS:ND1	2:D:260:ASP:OD2	2.24	0.65
2:J:253:ILE:O	2:J:258:ILE:HG12	1.96	0.65
2:B:253:ILE:O	2:B:258:ILE:HG12	1.96	0.65
2:L:253:ILE:O	2:L:258:ILE:HG12	1.96	0.65
2:F:278:SER:O	2:F:279:ASN:HB2	1.96	0.65
2:D:278:SER:O	2:D:279:ASN:HB2	1.96	0.65
1:C:206:PRO:O	1:C:210:LYS:HD3	1.97	0.65
2:H:278:SER:O	2:H:279:ASN:HB2	1.96	0.65
1:G:206:PRO:O	1:G:210:LYS:HD3	1.97	0.65
2:H:133:LYS:HG2	2:H:187:GLU:HG2	1.80	0.64
2:L:278:SER:O	2:L:279:ASN:HB2	1.96	0.64
1:G:235:GLN:HE21	2:H:208:ARG:HH21	0.77	0.64
2:L:133:LYS:HG2	2:L:187:GLU:HG2	1.80	0.64
2:F:253:ILE:O	2:F:258:ILE:HG12	1.96	0.64
2:B:133:LYS:HG2	2:B:187:GLU:HG2	1.80	0.64
2:H:195:HIS:ND1	2:H:260:ASP:OD2	2.24	0.64
2:B:278:SER:O	2:B:279:ASN:HB2	1.96	0.64
2:J:133:LYS:HG2	2:J:187:GLU:HG2	1.80	0.64
1:S:206:PRO:O	1:S:210:LYS:HD3	1.97	0.64
2:D:133:LYS:HG2	2:D:187:GLU:HG2	1.80	0.64
1:I:206:PRO:O	1:I:210:LYS:HD3	1.97	0.64
2:L:105:MET:HE2	2:L:249:VAL:HG12	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:MET:HE2	2:F:249:VAL:HG12	1.80	0.64
2:F:133:LYS:HG2	2:F:187:GLU:HG2	1.80	0.64
2:L:195:HIS:ND1	2:L:260:ASP:OD2	2.24	0.63
2:B:105:MET:HE2	2:B:249:VAL:HG12	1.80	0.63
1:G:141:LYS:CD	2:J:384:GLU:HG3	2.29	0.63
1:A:206:PRO:O	1:A:210:LYS:HD3	1.97	0.63
2:J:217:ASN:C	2:J:217:ASN:ND2	2.57	0.63
2:L:383:HIS:HD2	2:L:386:THR:OG1	1.82	0.63
1:I:235:GLN:HE21	2:J:208:ARG:HH21	0.76	0.63
1:A:171:ASP:OD1	1:A:173:GLN:N	2.31	0.63
2:D:383:HIS:HD2	2:D:386:THR:OG1	1.82	0.63
2:B:217:ASN:C	2:B:217:ASN:ND2	2.56	0.63
2:D:129:ALA:HB2	2:D:186:ALA:O	1.99	0.63
1:G:228:CYS:HB2	1:G:229:PRO:HD3	1.81	0.63
2:H:383:HIS:HD2	2:H:386:THR:OG1	1.82	0.63
2:F:484:VAL:HG12	2:F:485:PRO:HD2	1.81	0.62
2:H:129:ALA:HB2	2:H:186:ALA:O	1.99	0.62
2:J:484:VAL:HG12	2:J:485:PRO:HD2	1.81	0.62
2:B:129:ALA:HB2	2:B:186:ALA:O	1.99	0.62
2:B:383:HIS:HD2	2:B:386:THR:OG1	1.82	0.62
1:E:235:GLN:HE21	2:F:208:ARG:HH21	0.77	0.62
2:H:217:ASN:C	2:H:217:ASN:ND2	2.57	0.62
2:J:383:HIS:HD2	2:J:386:THR:OG1	1.82	0.62
1:E:206:PRO:O	1:E:210:LYS:HD3	1.97	0.62
2:J:195:HIS:ND1	2:J:260:ASP:OD2	2.24	0.62
2:L:129:ALA:HB2	2:L:186:ALA:O	1.99	0.62
2:F:129:ALA:HB2	2:F:186:ALA:O	1.99	0.62
2:F:383:HIS:HD2	2:F:386:THR:OG1	1.82	0.62
2:D:105:MET:HE2	2:D:249:VAL:HG12	1.80	0.62
2:H:105:MET:HE2	2:H:249:VAL:HG12	1.80	0.62
2:J:105:MET:HE2	2:J:249:VAL:HG12	1.80	0.62
1:A:228:CYS:HB2	1:A:229:PRO:HD3	1.81	0.62
1:C:14:ASN:OD1	1:C:92:MET:HB3	2.00	0.62
2:D:351:GLU:HB2	2:D:353:ARG:HD2	1.82	0.62
2:L:217:ASN:C	2:L:217:ASN:ND2	2.57	0.62
2:B:484:VAL:HG12	2:B:485:PRO:HD2	1.81	0.62
2:D:484:VAL:HG12	2:D:485:PRO:HD2	1.81	0.62
1:G:171:ASP:OD1	1:G:173:GLN:N	2.31	0.62
1:C:171:ASP:OD1	1:C:173:GLN:N	2.31	0.62
1:E:161:HIS:HD2	1:E:165:LYS:NZ	1.98	0.62
1:I:228:CYS:HB2	1:I:229:PRO:HD3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:171:ASP:OD1	1:S:173:GLN:N	2.31	0.61
1:E:171:ASP:OD1	1:E:173:GLN:N	2.31	0.61
1:E:228:CYS:HB2	1:E:229:PRO:HD3	1.81	0.61
2:J:129:ALA:HB2	2:J:186:ALA:O	1.99	0.61
1:E:14:ASN:OD1	1:E:92:MET:HB3	2.00	0.61
1:G:14:ASN:OD1	1:G:92:MET:HB3	2.00	0.61
2:H:351:GLU:HB2	2:H:353:ARG:HD2	1.82	0.61
1:S:228:CYS:HB2	1:S:229:PRO:HD3	1.81	0.61
1:S:14:ASN:OD1	1:S:92:MET:HB3	2.00	0.61
2:F:195:HIS:ND1	2:F:260:ASP:OD2	2.24	0.61
2:D:217:ASN:C	2:D:217:ASN:ND2	2.57	0.61
2:L:484:VAL:HG12	2:L:485:PRO:HD2	1.81	0.61
1:C:161:HIS:HD2	1:C:165:LYS:NZ	1.98	0.61
1:S:161:HIS:HD2	1:S:165:LYS:NZ	1.98	0.61
1:E:188:CYS:O	1:E:191:LEU:HB2	2.01	0.61
2:F:351:GLU:HB2	2:F:353:ARG:HD2	1.82	0.61
2:B:351:GLU:HB2	2:B:353:ARG:HD2	1.82	0.61
2:L:351:GLU:HB2	2:L:353:ARG:HD2	1.82	0.61
1:A:161:HIS:HD2	1:A:165:LYS:NZ	1.98	0.61
1:I:161:HIS:HD2	1:I:165:LYS:NZ	1.98	0.61
1:I:188:CYS:O	1:I:191:LEU:HB2	2.01	0.61
1:A:14:ASN:OD1	1:A:92:MET:HB3	2.00	0.60
1:G:161:HIS:HD2	1:G:165:LYS:NZ	1.98	0.60
1:C:188:CYS:O	1:C:191:LEU:HB2	2.01	0.60
2:J:351:GLU:HB2	2:J:353:ARG:HD2	1.82	0.60
1:C:228:CYS:HB2	1:C:229:PRO:HD3	1.81	0.60
2:H:484:VAL:HG12	2:H:485:PRO:HD2	1.81	0.60
1:S:188:CYS:O	1:S:191:LEU:HB2	2.01	0.60
1:I:14:ASN:OD1	1:I:92:MET:HB3	2.00	0.60
2:F:458:PHE:CD1	2:F:465:MET:HE3	2.37	0.60
1:A:188:CYS:O	1:A:191:LEU:HB2	2.01	0.60
2:B:195:HIS:ND1	2:B:260:ASP:OD2	2.24	0.60
2:J:458:PHE:CD1	2:J:465:MET:HE3	2.37	0.60
1:S:26:ARG:NH2	2:L:217:ASN:HD21	1.98	0.60
2:B:458:PHE:CD1	2:B:465:MET:HE3	2.37	0.60
2:H:458:PHE:CD1	2:H:465:MET:HE3	2.37	0.60
2:L:458:PHE:CD1	2:L:465:MET:HE3	2.37	0.60
2:D:458:PHE:CD1	2:D:465:MET:HE3	2.37	0.60
2:F:108:HIS:CE1	2:F:417:GLN:HG2	2.37	0.59
2:D:108:HIS:CE1	2:D:417:GLN:HG2	2.36	0.59
2:H:108:HIS:CE1	2:H:417:GLN:HG2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:322:HIS:HB2	2:L:359:ALA:HB3	1.84	0.59
2:F:217:ASN:C	2:F:217:ASN:ND2	2.57	0.59
2:D:322:HIS:HB2	2:D:359:ALA:HB3	1.84	0.59
2:H:237:GLU:CD	2:H:237:GLU:H	2.11	0.59
2:J:108:HIS:CE1	2:J:417:GLN:HG2	2.36	0.59
2:B:108:HIS:CE1	2:B:417:GLN:HG2	2.36	0.59
1:G:188:CYS:O	1:G:191:LEU:HB2	2.01	0.59
2:J:232:ASP:O	2:J:235:ARG:HG3	2.03	0.59
2:J:322:HIS:HB2	2:J:359:ALA:HB3	1.84	0.59
2:B:142:SER:HB2	2:B:143:PRO:HD3	1.85	0.59
2:D:232:ASP:O	2:D:235:ARG:HG3	2.03	0.58
2:F:232:ASP:O	2:F:235:ARG:HG3	2.03	0.58
1:C:26:ARG:NH2	2:D:217:ASN:HD21	1.98	0.58
2:F:484:VAL:CG1	2:F:533:CYS:HB3	2.33	0.58
2:J:237:GLU:CD	2:J:237:GLU:H	2.11	0.58
2:B:232:ASP:O	2:B:235:ARG:HG3	2.03	0.58
2:D:142:SER:HB2	2:D:143:PRO:HD2	1.85	0.58
2:F:322:HIS:HB2	2:F:359:ALA:HB3	1.84	0.58
2:L:232:ASP:O	2:L:235:ARG:HG3	2.03	0.58
2:F:237:GLU:H	2:F:237:GLU:CD	2.11	0.58
2:F:142:SER:HB2	2:F:143:PRO:HD3	1.85	0.58
1:I:171:ASP:OD1	1:I:173:GLN:N	2.31	0.58
2:L:32:ILE:HD11	2:L:511:ILE:HD11	1.86	0.58
2:D:237:GLU:H	2:D:237:GLU:CD	2.11	0.58
2:L:237:GLU:CD	2:L:237:GLU:H	2.11	0.58
2:H:322:HIS:HB2	2:H:359:ALA:HB3	1.84	0.58
2:D:8:LYS:HG3	2:D:25:VAL:O	2.04	0.58
2:D:32:ILE:HD11	2:D:511:ILE:HD11	1.86	0.58
2:L:8:LYS:HG3	2:L:25:VAL:O	2.04	0.58
2:L:108:HIS:CE1	2:L:417:GLN:HG2	2.37	0.58
2:B:32:ILE:HD11	2:B:511:ILE:HD11	1.86	0.58
2:B:142:SER:HB2	2:B:143:PRO:HD2	1.85	0.58
2:B:237:GLU:CD	2:B:237:GLU:H	2.11	0.58
1:G:26:ARG:NH2	2:H:217:ASN:HD21	1.98	0.58
2:H:484:VAL:CG1	2:H:533:CYS:HB3	2.33	0.58
2:D:484:VAL:CG1	2:D:533:CYS:HB3	2.33	0.57
2:J:484:VAL:CG1	2:J:533:CYS:HB3	2.33	0.57
2:H:8:LYS:HG3	2:H:25:VAL:O	2.04	0.57
2:H:232:ASP:O	2:H:235:ARG:HG3	2.03	0.57
2:B:322:HIS:HB2	2:B:359:ALA:HB3	1.84	0.57
2:H:32:ILE:HD11	2:H:511:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:ARG:NH2	2:F:217:ASN:HD21	1.98	0.57
2:B:8:LYS:HG3	2:B:25:VAL:O	2.04	0.57
2:F:32:ILE:HD11	2:F:511:ILE:HD11	1.86	0.57
2:J:8:LYS:HG3	2:J:25:VAL:O	2.04	0.57
2:J:142:SER:HB2	2:J:143:PRO:HD3	1.85	0.57
2:D:308:LEU:HD21	2:D:376:LEU:HD22	1.87	0.57
2:F:142:SER:HB2	2:F:143:PRO:HD2	1.85	0.57
2:J:32:ILE:HD11	2:J:511:ILE:HD11	1.86	0.57
2:J:308:LEU:HD21	2:J:376:LEU:HD22	1.87	0.57
1:S:18:THR:O	1:S:18:THR:HG22	2.05	0.56
2:L:308:LEU:HD21	2:L:376:LEU:HD22	1.87	0.56
2:H:308:LEU:HD21	2:H:376:LEU:HD22	1.87	0.56
2:J:142:SER:HB2	2:J:143:PRO:HD2	1.85	0.56
1:A:26:ARG:NH2	2:B:217:ASN:HD21	1.98	0.56
1:E:18:THR:HG22	1:E:18:THR:O	2.05	0.56
2:F:8:LYS:HG3	2:F:25:VAL:O	2.04	0.56
1:G:18:THR:O	1:G:18:THR:HG22	2.05	0.56
2:L:484:VAL:CG1	2:L:533:CYS:HB3	2.33	0.56
2:F:308:LEU:HD21	2:F:376:LEU:HD22	1.87	0.56
1:G:141:LYS:HD2	2:J:384:GLU:CG	2.35	0.56
1:I:18:THR:O	1:I:18:THR:HG22	2.06	0.56
2:B:308:LEU:HD21	2:B:376:LEU:HD22	1.87	0.56
1:A:18:THR:HG22	1:A:18:THR:O	2.05	0.56
1:C:18:THR:HG22	1:C:18:THR:O	2.05	0.56
2:F:195:HIS:HD1	2:F:260:ASP:CG	2.14	0.56
2:F:283:CYS:SG	2:F:465:MET:HG3	2.46	0.56
1:I:26:ARG:NH2	2:J:217:ASN:HD21	1.98	0.56
2:J:283:CYS:SG	2:J:465:MET:HG3	2.46	0.56
2:H:142:SER:HB2	2:H:143:PRO:HD3	1.85	0.55
2:B:69:THR:O	2:B:70:TYR:HB3	2.06	0.55
2:J:119:ASP:O	2:J:522:ARG:NE	2.36	0.55
2:B:283:CYS:SG	2:B:465:MET:HG3	2.46	0.55
2:J:69:THR:O	2:J:70:TYR:HB3	2.06	0.55
2:L:283:CYS:SG	2:L:465:MET:HG3	2.46	0.55
2:B:195:HIS:HD1	2:B:260:ASP:CG	2.14	0.55
2:D:283:CYS:SG	2:D:465:MET:HG3	2.46	0.55
2:L:69:THR:O	2:L:70:TYR:HB3	2.06	0.55
2:L:278:SER:HB3	2:L:305:GLY:HA2	1.88	0.55
2:L:142:SER:HB2	2:L:143:PRO:HD2	1.85	0.55
2:B:278:SER:HB3	2:B:305:GLY:HA2	1.89	0.55
2:B:297:TYR:CD2	2:B:298:THR:HG23	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:LYS:HA	2:F:25:VAL:O	2.07	0.55
2:H:69:THR:O	2:H:70:TYR:HB3	2.06	0.55
2:L:8:LYS:HA	2:L:25:VAL:O	2.08	0.54
2:F:297:TYR:CD2	2:F:298:THR:HG23	2.42	0.54
2:H:278:SER:HB3	2:H:305:GLY:HA2	1.88	0.54
2:J:8:LYS:HA	2:J:25:VAL:O	2.08	0.54
2:J:278:SER:HB3	2:J:305:GLY:HA2	1.88	0.54
2:F:69:THR:O	2:F:70:TYR:HB3	2.06	0.54
2:B:484:VAL:CG1	2:B:533:CYS:HB3	2.33	0.54
2:D:142:SER:HB2	2:D:143:PRO:HD3	1.85	0.54
1:E:26:ARG:HE	2:F:217:ASN:ND2	2.06	0.54
2:L:297:TYR:CD2	2:L:298:THR:HG23	2.42	0.54
2:B:8:LYS:HA	2:B:25:VAL:O	2.07	0.54
2:D:8:LYS:HA	2:D:25:VAL:O	2.08	0.54
2:H:8:LYS:HA	2:H:25:VAL:O	2.07	0.54
1:A:238:TRP:CH2	1:A:240:VAL:HB	2.43	0.54
2:H:283:CYS:SG	2:H:465:MET:HG3	2.46	0.54
2:J:297:TYR:CD2	2:J:298:THR:HG23	2.42	0.54
1:C:238:TRP:CH2	1:C:240:VAL:HB	2.43	0.54
1:G:238:TRP:CH2	1:G:240:VAL:HB	2.43	0.54
2:H:142:SER:HB2	2:H:143:PRO:HD2	1.85	0.54
2:L:195:HIS:HD1	2:L:260:ASP:CG	2.14	0.54
2:L:484:VAL:HG13	2:L:485:PRO:HD2	1.89	0.54
2:D:278:SER:HB3	2:D:305:GLY:HA2	1.89	0.54
1:S:238:TRP:CH2	1:S:240:VAL:HB	2.43	0.54
1:A:26:ARG:HE	2:B:217:ASN:ND2	2.06	0.54
2:D:69:THR:O	2:D:70:TYR:HB3	2.06	0.54
2:D:297:TYR:CD2	2:D:298:THR:HG23	2.42	0.54
2:F:278:SER:HB3	2:F:305:GLY:HA2	1.89	0.54
1:E:227:ASN:H	1:E:227:ASN:ND2	2.04	0.53
1:I:238:TRP:CH2	1:I:240:VAL:HB	2.43	0.53
2:D:494:CYS:SG	2:D:498:LYS:HG3	2.48	0.53
2:H:297:TYR:CD2	2:H:298:THR:HG23	2.42	0.53
2:H:484:VAL:HG13	2:H:485:PRO:HD2	1.89	0.53
2:L:494:CYS:SG	2:L:498:LYS:HG3	2.48	0.53
2:H:282:THR:HG22	2:H:377:VAL:HG21	1.90	0.53
2:L:142:SER:HB2	2:L:143:PRO:HD3	1.85	0.53
1:C:26:ARG:HE	2:D:217:ASN:ND2	2.06	0.53
1:E:238:TRP:CH2	1:E:240:VAL:HB	2.43	0.53
2:H:108:HIS:ND1	2:H:418:CYS:HB2	2.24	0.53
2:J:282:THR:HG22	2:J:377:VAL:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:CYS:SG	1:C:110:GLY:HA3	2.49	0.53
1:E:237:ASN:HB3	2:F:215:ALA:O	2.09	0.53
1:S:26:ARG:HE	2:L:217:ASN:ND2	2.06	0.53
2:B:108:HIS:ND1	2:B:418:CYS:HB2	2.24	0.53
1:C:237:ASN:HB3	2:D:215:ALA:O	2.09	0.53
2:F:494:CYS:SG	2:F:498:LYS:HG3	2.48	0.53
1:S:227:ASN:H	1:S:227:ASN:ND2	2.04	0.53
1:S:227:ASN:HD22	1:S:227:ASN:N	2.04	0.53
2:H:119:ASP:O	2:H:522:ARG:NE	2.36	0.53
1:I:237:ASN:HB3	2:J:215:ALA:O	2.09	0.53
2:J:108:HIS:ND1	2:J:418:CYS:HB2	2.24	0.53
1:A:20:CYS:SG	1:A:110:GLY:HA3	2.49	0.53
2:H:494:CYS:SG	2:H:498:LYS:HG3	2.48	0.53
2:B:484:VAL:HG13	2:B:485:PRO:HD2	1.89	0.53
2:B:494:CYS:SG	2:B:498:LYS:HG3	2.48	0.53
2:D:484:VAL:HG13	2:D:485:PRO:HD2	1.89	0.53
2:F:354:TYR:OH	2:F:493:ARG:HD2	2.09	0.53
1:G:20:CYS:SG	1:G:110:GLY:HA3	2.49	0.53
2:J:195:HIS:HD1	2:J:260:ASP:CG	2.14	0.53
1:S:20:CYS:SG	1:S:110:GLY:HA3	2.49	0.52
1:A:237:ASN:HB3	2:B:215:ALA:O	2.09	0.52
2:B:282:THR:HG22	2:B:377:VAL:HG21	1.90	0.52
2:B:354:TYR:OH	2:B:493:ARG:HD2	2.09	0.52
1:E:20:CYS:SG	1:E:110:GLY:HA3	2.49	0.52
1:G:26:ARG:HE	2:H:217:ASN:ND2	2.06	0.52
1:S:237:ASN:HB3	2:L:215:ALA:O	2.09	0.52
2:D:282:THR:HG22	2:D:377:VAL:HG21	1.90	0.52
2:F:282:THR:HG22	2:F:377:VAL:HG21	1.90	0.52
1:I:26:ARG:HE	2:J:217:ASN:ND2	2.06	0.52
2:J:484:VAL:HG13	2:J:485:PRO:HD2	1.89	0.52
2:D:108:HIS:ND1	2:D:418:CYS:HB2	2.24	0.52
2:D:195:HIS:HD1	2:D:260:ASP:CG	2.14	0.52
2:D:383:HIS:NE2	2:D:385:PRO:HG2	2.25	0.52
2:J:494:CYS:SG	2:J:498:LYS:HG3	2.49	0.52
2:L:108:HIS:ND1	2:L:418:CYS:HB2	2.24	0.52
2:L:383:HIS:NE2	2:L:385:PRO:HG2	2.25	0.52
1:A:227:ASN:H	1:A:227:ASN:ND2	2.04	0.52
1:I:20:CYS:SG	1:I:110:GLY:HA3	2.49	0.52
1:G:237:ASN:HB3	2:H:215:ALA:O	2.09	0.52
2:L:354:TYR:OH	2:L:493:ARG:HD2	2.09	0.52
1:G:185:HIS:CE1	1:G:191:LEU:HD23	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ASN:H	1:C:227:ASN:ND2	2.05	0.52
2:F:108:HIS:ND1	2:F:418:CYS:HB2	2.24	0.52
2:H:383:HIS:NE2	2:H:385:PRO:HG2	2.25	0.52
2:J:354:TYR:OH	2:J:493:ARG:HD2	2.09	0.52
1:A:185:HIS:CE1	1:A:191:LEU:HD23	2.45	0.52
2:D:354:TYR:OH	2:D:493:ARG:HD2	2.09	0.52
1:S:185:HIS:CE1	1:S:191:LEU:HD23	2.45	0.51
1:C:185:HIS:CE1	1:C:191:LEU:HD23	2.45	0.51
1:C:209:LYS:NZ	2:D:442:ASP:OD1	2.43	0.51
1:I:185:HIS:CE1	1:I:191:LEU:HD23	2.45	0.51
1:A:185:HIS:CE1	1:A:191:LEU:CD2	2.94	0.51
1:E:185:HIS:CE1	1:E:191:LEU:CD2	2.94	0.51
2:F:484:VAL:HG13	2:F:485:PRO:HD2	1.89	0.51
1:G:244:HIS:CG	1:G:245:PRO:HD2	2.46	0.51
1:I:185:HIS:CE1	1:I:191:LEU:CD2	2.94	0.51
2:J:320:GLU:OE1	2:J:333:ALA:C	2.54	0.51
2:J:383:HIS:NE2	2:J:385:PRO:HG2	2.25	0.51
2:B:383:HIS:NE2	2:B:385:PRO:HG2	2.25	0.51
1:C:244:HIS:CG	1:C:245:PRO:HD2	2.46	0.51
2:L:282:THR:HG22	2:L:377:VAL:HG21	1.90	0.51
2:L:320:GLU:OE1	2:L:333:ALA:C	2.54	0.51
1:A:244:HIS:CG	1:A:245:PRO:HD2	2.46	0.51
1:E:185:HIS:CE1	1:E:191:LEU:HD23	2.45	0.51
2:F:383:HIS:NE2	2:F:385:PRO:HG2	2.25	0.51
2:H:354:TYR:OH	2:H:493:ARG:HD2	2.09	0.51
1:A:207:GLU:HB3	1:A:212:TYR:CD2	2.46	0.51
1:S:185:HIS:CE1	1:S:191:LEU:CD2	2.94	0.51
1:E:244:HIS:CG	1:E:245:PRO:HD2	2.46	0.51
2:J:458:PHE:HD1	2:J:465:MET:HE3	1.76	0.51
2:L:346:THR:O	2:L:347:GLU:HB2	2.10	0.51
2:F:346:THR:O	2:F:347:GLU:HB2	2.10	0.51
1:G:207:GLU:HB3	1:G:212:TYR:CD2	2.46	0.51
2:H:458:PHE:HD1	2:H:465:MET:HE3	1.75	0.51
1:I:207:GLU:HB3	1:I:212:TYR:CD2	2.46	0.51
1:I:227:ASN:H	1:I:227:ASN:ND2	2.04	0.51
1:A:209:LYS:NZ	2:B:442:ASP:OD1	2.43	0.51
2:B:119:ASP:O	2:B:522:ARG:NE	2.36	0.51
1:G:185:HIS:CE1	1:G:191:LEU:CD2	2.94	0.51
2:H:320:GLU:OE1	2:H:333:ALA:C	2.54	0.51
1:S:207:GLU:HB3	1:S:212:TYR:CD2	2.46	0.50
1:S:244:HIS:CG	1:S:245:PRO:HD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:485:PRO:HG2	7:L:537:FCO:N1	2.26	0.50
2:D:320:GLU:OE1	2:D:333:ALA:C	2.54	0.50
2:F:119:ASP:O	2:F:522:ARG:NE	2.36	0.50
1:G:227:ASN:H	1:G:227:ASN:ND2	2.04	0.50
2:H:346:THR:O	2:H:347:GLU:HB2	2.11	0.50
2:J:346:THR:O	2:J:347:GLU:HB2	2.10	0.50
2:H:20:HIS:O	2:H:531:ILE:HG21	2.12	0.50
1:I:244:HIS:CG	1:I:245:PRO:HD2	2.46	0.50
2:B:346:THR:O	2:B:347:GLU:HB2	2.10	0.50
2:B:485:PRO:HG2	7:B:537:FCO:N1	2.26	0.50
1:E:207:GLU:HB3	1:E:212:TYR:CD2	2.46	0.50
2:H:195:HIS:HD1	2:H:260:ASP:CG	2.14	0.50
2:J:20:HIS:O	2:J:531:ILE:HG21	2.12	0.50
2:D:20:HIS:O	2:D:531:ILE:HG21	2.12	0.50
2:D:491:GLY:O	2:D:500:SER:HB3	2.12	0.50
1:E:161:HIS:HD2	1:E:165:LYS:HZ3	1.58	0.50
2:F:20:HIS:O	2:F:531:ILE:HG21	2.12	0.50
2:J:491:GLY:O	2:J:500:SER:HB3	2.12	0.50
2:B:320:GLU:OE1	2:B:333:ALA:C	2.54	0.50
1:C:185:HIS:CE1	1:C:191:LEU:CD2	2.94	0.50
2:D:119:ASP:O	2:D:522:ARG:NE	2.36	0.50
2:H:262:LEU:HD21	2:H:393:VAL:HG22	1.93	0.50
2:J:262:LEU:HD21	2:J:393:VAL:HG22	1.93	0.50
2:D:458:PHE:HD1	2:D:465:MET:HE3	1.75	0.50
2:F:320:GLU:OE1	2:F:333:ALA:C	2.54	0.50
2:L:20:HIS:O	2:L:531:ILE:HG21	2.12	0.50
2:B:262:LEU:HD21	2:B:393:VAL:HG22	1.93	0.50
1:C:207:GLU:HB3	1:C:212:TYR:CD2	2.46	0.50
2:L:262:LEU:HD21	2:L:393:VAL:HG22	1.93	0.50
2:B:20:HIS:O	2:B:531:ILE:HG21	2.12	0.50
2:D:346:THR:O	2:D:347:GLU:HB2	2.10	0.50
2:B:491:GLY:O	2:B:500:SER:HB3	2.12	0.49
2:H:491:GLY:O	2:H:500:SER:HB3	2.12	0.49
2:J:214:GLY:O	2:J:215:ALA:HB3	2.12	0.49
1:S:209:LYS:NZ	2:L:442:ASP:OD1	2.43	0.49
2:J:74:LEU:HD12	2:J:100:MET:HE2	1.94	0.49
2:D:92:ALA:O	2:D:96:ARG:HD3	2.12	0.49
2:F:214:GLY:O	2:F:215:ALA:HB3	2.12	0.49
2:J:485:PRO:HG2	7:J:537:FCO:N1	2.26	0.49
2:D:262:LEU:HD21	2:D:393:VAL:HG22	1.93	0.49
1:I:36:ILE:CD1	1:I:36:ILE:N	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:N	1:A:36:ILE:CD1	2.76	0.49
1:A:100:ALA:HB3	1:A:101:PRO:HD3	1.95	0.49
1:E:36:ILE:N	1:E:36:ILE:CD1	2.76	0.49
1:E:235:GLN:NE2	2:F:208:ARG:NH2	2.39	0.49
2:F:74:LEU:HD12	2:F:100:MET:HE2	1.94	0.49
2:F:491:GLY:O	2:F:500:SER:HB3	2.12	0.49
2:H:485:PRO:HG2	7:H:537:FCO:N1	2.26	0.49
1:S:36:ILE:CD1	1:S:36:ILE:N	2.76	0.49
2:L:431:LYS:O	2:L:432:LEU:C	2.55	0.49
2:L:458:PHE:HD1	2:L:465:MET:HE3	1.75	0.49
1:C:100:ALA:HB3	1:C:101:PRO:HD3	1.95	0.49
2:D:321:GLU:O	2:D:333:ALA:HA	2.13	0.49
2:D:431:LYS:O	2:D:432:LEU:C	2.55	0.49
2:F:458:PHE:HD1	2:F:465:MET:HE3	1.75	0.49
1:G:100:ALA:HB3	1:G:101:PRO:HD3	1.95	0.49
1:I:100:ALA:HB3	1:I:101:PRO:HD3	1.95	0.49
1:I:235:GLN:NE2	2:J:208:ARG:NH2	2.39	0.49
1:S:100:ALA:HB3	1:S:101:PRO:HD3	1.95	0.49
2:L:491:GLY:O	2:L:500:SER:HB3	2.12	0.49
1:A:235:GLN:NE2	2:B:208:ARG:NH2	2.39	0.49
2:D:214:GLY:O	2:D:215:ALA:HB3	2.13	0.49
2:D:485:PRO:HG2	7:D:537:FCO:N1	2.26	0.49
2:F:321:GLU:O	2:F:333:ALA:HA	2.13	0.49
2:F:485:PRO:HG2	7:F:537:FCO:N1	2.26	0.49
2:H:214:GLY:O	2:H:215:ALA:HB3	2.13	0.49
2:L:92:ALA:O	2:L:96:ARG:HD3	2.12	0.49
2:H:82:ASN:HD22	2:H:455:GLY:HA2	1.77	0.49
2:H:92:ALA:O	2:H:96:ARG:HD3	2.12	0.49
2:J:92:ALA:O	2:J:96:ARG:HD3	2.12	0.49
2:B:92:ALA:O	2:B:96:ARG:HD3	2.12	0.49
2:B:431:LYS:O	2:B:432:LEU:C	2.55	0.49
1:E:100:ALA:HB3	1:E:101:PRO:HD3	1.95	0.49
2:F:262:LEU:HD21	2:F:393:VAL:HG22	1.93	0.49
2:H:431:LYS:O	2:H:432:LEU:C	2.55	0.49
2:L:321:GLU:O	2:L:333:ALA:HA	2.13	0.49
2:B:82:ASN:HD22	2:B:455:GLY:HA2	1.77	0.49
2:F:92:ALA:O	2:F:96:ARG:HD3	2.12	0.49
2:H:74:LEU:HD12	2:H:100:MET:HE2	1.94	0.49
2:B:321:GLU:O	2:B:333:ALA:HA	2.13	0.48
2:J:82:ASN:HD22	2:J:455:GLY:HA2	1.77	0.48
2:D:82:ASN:HD22	2:D:455:GLY:HA2	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:LYS:NZ	2:F:442:ASP:OD1	2.43	0.48
1:G:36:ILE:CD1	1:G:36:ILE:N	2.76	0.48
2:H:321:GLU:O	2:H:333:ALA:HA	2.13	0.48
2:J:303:ILE:HD13	2:J:308:LEU:HD23	1.95	0.48
2:L:74:LEU:HD12	2:L:100:MET:HE2	1.94	0.48
1:A:36:ILE:N	1:A:36:ILE:HD12	2.29	0.48
2:B:384:GLU:HG3	1:E:141:LYS:CD	2.43	0.48
2:D:74:LEU:HD12	2:D:100:MET:HE2	1.94	0.48
2:F:82:ASN:HD22	2:F:455:GLY:HA2	1.77	0.48
2:L:82:ASN:HD22	2:L:455:GLY:HA2	1.77	0.48
2:B:214:GLY:O	2:B:215:ALA:HB3	2.12	0.48
2:B:334:HIS:CD2	2:B:340:VAL:HG22	2.49	0.48
2:B:458:PHE:HD1	2:B:465:MET:HE3	1.76	0.48
2:H:303:ILE:HD13	2:H:308:LEU:HD23	1.95	0.48
2:J:321:GLU:O	2:J:333:ALA:HA	2.13	0.48
2:J:431:LYS:O	2:J:432:LEU:C	2.56	0.48
2:L:334:HIS:CD2	2:L:340:VAL:HG22	2.49	0.48
2:F:303:ILE:HD13	2:F:308:LEU:HD23	1.95	0.48
2:F:431:LYS:O	2:F:432:LEU:C	2.55	0.48
1:G:36:ILE:N	1:G:36:ILE:HD12	2.29	0.48
1:I:36:ILE:N	1:I:36:ILE:HD12	2.29	0.48
2:B:74:LEU:HD12	2:B:100:MET:HE2	1.94	0.48
1:C:36:ILE:N	1:C:36:ILE:CD1	2.76	0.48
2:F:457:GLY:O	2:F:467:SER:HA	2.14	0.48
2:J:334:HIS:CD2	2:J:340:VAL:HG22	2.49	0.48
2:L:214:GLY:O	2:L:215:ALA:HB3	2.12	0.48
2:B:283:CYS:SG	2:B:465:MET:CG	3.02	0.48
2:J:283:CYS:SG	2:J:465:MET:CG	3.02	0.48
2:J:457:GLY:O	2:J:467:SER:HA	2.14	0.48
2:B:303:ILE:HD13	2:B:308:LEU:HD23	1.95	0.48
2:D:283:CYS:SG	2:D:465:MET:CG	3.02	0.48
2:D:303:ILE:HD13	2:D:308:LEU:HD23	1.95	0.48
2:H:334:HIS:CD2	2:H:340:VAL:HG22	2.49	0.48
2:F:283:CYS:SG	2:F:465:MET:CG	3.02	0.48
1:S:36:ILE:N	1:S:36:ILE:HD12	2.29	0.47
2:F:334:HIS:CD2	2:F:340:VAL:HG22	2.49	0.47
2:L:283:CYS:SG	2:L:465:MET:CG	3.02	0.47
2:B:457:GLY:O	2:B:467:SER:HA	2.14	0.47
2:H:457:GLY:O	2:H:467:SER:HA	2.14	0.47
2:J:390:VAL:O	2:J:394:LEU:HG	2.15	0.47
2:D:334:HIS:CD2	2:D:340:VAL:HG22	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:119:ASP:O	2:L:522:ARG:NE	2.36	0.47
2:L:303:ILE:HD13	2:L:308:LEU:HD23	1.95	0.47
2:H:242:PHE:CD1	2:H:242:PHE:C	2.92	0.47
2:H:390:VAL:O	2:H:394:LEU:HG	2.15	0.47
2:H:493:ARG:HA	2:H:498:LYS:O	2.15	0.47
2:L:457:GLY:O	2:L:467:SER:HA	2.14	0.47
2:B:68:CYS:CB	7:B:537:FCO:C2	2.93	0.47
1:C:161:HIS:HD2	1:C:165:LYS:HZ3	1.61	0.47
2:D:390:VAL:O	2:D:394:LEU:HG	2.15	0.47
1:E:36:ILE:N	1:E:36:ILE:HD12	2.29	0.47
2:F:390:VAL:O	2:F:394:LEU:HG	2.15	0.47
2:F:493:ARG:HA	2:F:498:LYS:O	2.15	0.47
1:G:209:LYS:NZ	2:H:442:ASP:OD1	2.43	0.47
2:H:283:CYS:SG	2:H:465:MET:CG	3.02	0.47
2:L:304:TRP:HZ3	2:L:365:GLU:HG3	1.80	0.47
2:B:242:PHE:CD1	2:B:242:PHE:C	2.92	0.47
2:D:242:PHE:CD1	2:D:242:PHE:C	2.92	0.47
2:F:242:PHE:CD1	2:F:242:PHE:C	2.92	0.47
1:S:124:ASN:HD21	1:S:128:THR:N	2.10	0.47
2:D:304:TRP:HZ3	2:D:365:GLU:HG3	1.80	0.47
2:J:68:CYS:CB	7:J:537:FCO:C2	2.93	0.47
2:J:335:HIS:HE1	2:J:469:TRP:CZ3	2.33	0.47
2:L:390:VAL:O	2:L:394:LEU:HG	2.15	0.47
2:B:304:TRP:HZ3	2:B:365:GLU:HG3	1.80	0.47
1:C:36:ILE:N	1:C:36:ILE:HD12	2.29	0.47
2:D:457:GLY:O	2:D:467:SER:HA	2.14	0.47
2:D:493:ARG:HA	2:D:498:LYS:O	2.15	0.47
1:G:235:GLN:NE2	2:H:208:ARG:NH2	2.39	0.47
2:H:335:HIS:HE1	2:H:469:TRP:CZ3	2.33	0.47
1:I:209:LYS:NZ	2:J:442:ASP:OD1	2.43	0.47
2:L:239:ILE:HG21	2:L:433:GLU:HG3	1.97	0.46
2:L:242:PHE:CD1	2:L:242:PHE:C	2.92	0.46
2:D:239:ILE:HG21	2:D:433:GLU:HG3	1.97	0.46
2:F:68:CYS:CB	7:F:537:FCO:C2	2.93	0.46
2:H:68:CYS:CB	7:H:537:FCO:C2	2.93	0.46
2:J:304:TRP:HZ3	2:J:365:GLU:HG3	1.80	0.46
2:D:458:PHE:HD1	2:D:465:MET:CE	2.29	0.46
1:G:161:HIS:HD2	1:G:165:LYS:HZ3	1.62	0.46
2:B:408:LEU:HD12	2:B:408:LEU:HA	1.65	0.46
2:F:304:TRP:HZ3	2:F:365:GLU:HG3	1.80	0.46
2:F:335:HIS:HE1	2:F:469:TRP:CZ3	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:68:CYS:CB	7:L:537:FCO:C2	2.93	0.46
2:L:493:ARG:HA	2:L:498:LYS:O	2.15	0.46
2:B:493:ARG:HA	2:B:498:LYS:O	2.15	0.46
1:A:124:ASN:HD21	1:A:128:THR:N	2.10	0.46
1:A:217:LEU:HA	1:A:217:LEU:HD23	1.72	0.46
1:C:124:ASN:HD21	1:C:128:THR:N	2.10	0.46
2:H:304:TRP:HZ3	2:H:365:GLU:HG3	1.80	0.46
2:J:242:PHE:CD1	2:J:242:PHE:C	2.92	0.46
2:J:493:ARG:HA	2:J:498:LYS:O	2.15	0.46
1:S:217:LEU:HD23	1:S:217:LEU:HA	1.73	0.46
2:L:458:PHE:CD1	2:L:465:MET:CE	2.99	0.46
1:A:161:HIS:HD2	1:A:165:LYS:HZ3	1.62	0.46
2:B:278:SER:O	2:B:279:ASN:CB	2.63	0.46
2:B:390:VAL:O	2:B:394:LEU:HG	2.15	0.46
2:D:335:HIS:HE1	2:D:469:TRP:CZ3	2.33	0.46
2:F:34:ASN:OD1	2:F:35:ALA:N	2.49	0.46
2:F:458:PHE:HD1	2:F:465:MET:CE	2.28	0.46
2:H:76:SER:O	2:H:80:VAL:HG23	2.16	0.46
2:J:458:PHE:HD1	2:J:465:MET:CE	2.29	0.46
2:B:239:ILE:HG21	2:B:433:GLU:HG3	1.97	0.46
2:B:335:HIS:HE1	2:B:469:TRP:CZ3	2.33	0.46
1:C:217:LEU:HA	1:C:217:LEU:HD23	1.72	0.46
1:C:235:GLN:NE2	2:D:208:ARG:NH2	2.39	0.46
2:F:239:ILE:HG21	2:F:433:GLU:HG3	1.97	0.46
2:B:34:ASN:OD1	2:B:35:ALA:N	2.49	0.45
2:D:68:CYS:CB	7:D:537:FCO:C2	2.93	0.45
2:D:76:SER:O	2:D:80:VAL:HG23	2.16	0.45
2:F:458:PHE:CD1	2:F:465:MET:CE	2.99	0.45
2:H:18:GLU:C	2:H:18:GLU:CD	2.84	0.45
2:H:235:ARG:HH11	2:H:235:ARG:HD2	1.64	0.45
2:H:239:ILE:HG21	2:H:433:GLU:HG3	1.97	0.45
2:J:16:ARG:HH11	2:J:16:ARG:HD2	1.47	0.45
2:J:83:CYS:HB2	2:J:454:GLN:C	2.41	0.45
2:J:239:ILE:HG21	2:J:433:GLU:HG3	1.97	0.45
2:J:408:LEU:HD12	2:J:408:LEU:HA	1.65	0.45
2:L:83:CYS:HB2	2:L:454:GLN:C	2.41	0.45
2:L:335:HIS:HE1	2:L:469:TRP:CZ3	2.33	0.45
2:D:83:CYS:HB2	2:D:454:GLN:C	2.42	0.45
2:F:76:SER:O	2:F:80:VAL:HG23	2.16	0.45
2:F:83:CYS:HB2	2:F:454:GLN:C	2.41	0.45
2:J:458:PHE:CD1	2:J:465:MET:CE	2.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASN:ND2	2:B:405:PHE:CD1	2.80	0.45
2:B:458:PHE:CD1	2:B:465:MET:CE	2.99	0.45
2:J:18:GLU:C	2:J:18:GLU:CD	2.84	0.45
2:L:458:PHE:HD1	2:L:465:MET:CE	2.29	0.45
2:B:288:THR:OG1	2:B:295:SER:HB2	2.17	0.45
2:B:458:PHE:HD1	2:B:465:MET:CE	2.29	0.45
1:E:217:LEU:HA	1:E:217:LEU:HD23	1.72	0.45
2:H:83:CYS:HB2	2:H:454:GLN:C	2.42	0.45
1:S:254:PHE:HA	1:S:258:TYR:HD2	1.82	0.45
2:L:491:GLY:O	2:L:500:SER:CB	2.65	0.45
2:B:76:SER:O	2:B:80:VAL:HG23	2.16	0.45
2:D:458:PHE:CD1	2:D:465:MET:CE	2.99	0.45
2:D:491:GLY:O	2:D:500:SER:CB	2.65	0.45
2:F:288:THR:OG1	2:F:295:SER:HB2	2.17	0.45
2:F:491:GLY:O	2:F:500:SER:CB	2.65	0.45
2:L:18:GLU:C	2:L:18:GLU:CD	2.84	0.45
1:A:254:PHE:HA	1:A:258:TYR:HD2	1.82	0.45
2:B:491:GLY:O	2:B:500:SER:CB	2.65	0.45
2:D:16:ARG:HH11	2:D:16:ARG:HD2	1.47	0.45
2:D:18:GLU:CD	2:D:18:GLU:C	2.85	0.45
2:D:80:VAL:O	2:D:84:VAL:HB	2.17	0.45
2:D:408:LEU:HA	2:D:408:LEU:HD12	1.65	0.45
2:F:278:SER:O	2:F:279:ASN:CB	2.63	0.45
1:I:161:HIS:HD2	1:I:165:LYS:HZ3	1.64	0.45
2:L:235:ARG:HH11	2:L:235:ARG:HD2	1.64	0.45
2:B:83:CYS:HB2	2:B:454:GLN:C	2.42	0.45
2:L:278:SER:O	2:L:279:ASN:CB	2.63	0.45
2:B:18:GLU:C	2:B:18:GLU:CD	2.84	0.45
2:F:335:HIS:CE1	2:F:469:TRP:CZ3	3.05	0.45
2:H:80:VAL:O	2:H:84:VAL:HB	2.17	0.45
2:B:335:HIS:CE1	2:B:469:TRP:CZ3	3.05	0.45
1:E:124:ASN:HD21	1:E:128:THR:N	2.10	0.45
2:J:76:SER:O	2:J:80:VAL:HG23	2.16	0.45
2:J:491:GLY:O	2:J:500:SER:CB	2.65	0.45
2:L:76:SER:O	2:L:80:VAL:HG23	2.16	0.44
2:L:336:PRO:O	2:L:481:GLN:HG3	2.17	0.44
1:C:254:PHE:HA	1:C:258:TYR:HD2	1.82	0.44
2:D:288:THR:OG1	2:D:295:SER:HB2	2.16	0.44
2:D:335:HIS:CE1	2:D:469:TRP:CZ3	3.05	0.44
2:F:408:LEU:HD12	2:F:408:LEU:HA	1.65	0.44
1:G:124:ASN:HD21	1:G:128:THR:N	2.10	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:288:THR:OG1	2:H:295:SER:HB2	2.16	0.44
2:J:288:THR:OG1	2:J:295:SER:HB2	2.17	0.44
2:J:336:PRO:O	2:J:481:GLN:HG3	2.18	0.44
2:D:142:SER:CB	2:D:143:PRO:CD	2.81	0.44
2:F:336:PRO:O	2:F:481:GLN:HG3	2.17	0.44
2:H:458:PHE:HD1	2:H:465:MET:CE	2.29	0.44
2:J:244:LYS:NZ	2:J:248:GLU:OE1	2.44	0.44
2:L:80:VAL:O	2:L:84:VAL:HB	2.17	0.44
2:H:336:PRO:O	2:H:481:GLN:HG3	2.17	0.44
2:H:458:PHE:CD1	2:H:465:MET:CE	2.99	0.44
2:J:80:VAL:O	2:J:84:VAL:HB	2.17	0.44
2:B:326:SER:HA	2:B:355:SER:O	2.18	0.44
2:H:335:HIS:CE1	2:H:469:TRP:CZ3	3.05	0.44
2:B:384:GLU:CG	1:E:141:LYS:HD2	2.45	0.44
1:C:20:CYS:HB2	1:C:73:GLU:CD	2.42	0.44
2:D:315:ASN:HA	2:D:316:PRO:HD2	1.95	0.44
2:F:18:GLU:C	2:F:18:GLU:CD	2.84	0.44
1:G:254:PHE:HA	1:G:258:TYR:HD2	1.82	0.44
2:H:491:GLY:O	2:H:500:SER:CB	2.65	0.44
2:H:124:ALA:O	2:H:127:LEU:HB2	2.18	0.44
2:J:335:HIS:CE1	2:J:469:TRP:CZ3	3.05	0.44
1:S:83:TYR:C	1:S:83:TYR:CD1	2.96	0.44
2:L:326:SER:HA	2:L:355:SER:O	2.18	0.44
2:B:235:ARG:HH11	2:B:235:ARG:HD2	1.64	0.44
2:B:244:LYS:NZ	2:B:248:GLU:OE1	2.44	0.44
2:F:454:GLN:HA	2:F:470:ILE:O	2.18	0.44
1:G:83:TYR:C	1:G:83:TYR:CD1	2.96	0.44
2:H:84:VAL:O	2:H:84:VAL:HG13	2.18	0.44
2:H:454:GLN:HA	2:H:470:ILE:O	2.18	0.44
1:I:254:PHE:HA	1:I:258:TYR:HD2	1.82	0.44
2:J:454:GLN:HA	2:J:470:ILE:O	2.18	0.44
2:L:335:HIS:CE1	2:L:469:TRP:CZ3	3.05	0.44
1:A:80:ASP:HB3	1:A:83:TYR:CE2	2.53	0.44
2:B:119:ASP:HB3	2:B:522:ARG:HG3	2.00	0.44
2:B:336:PRO:O	2:B:481:GLN:HG3	2.17	0.44
2:B:454:GLN:HA	2:B:470:ILE:O	2.18	0.44
2:F:324:LYS:O	2:F:324:LYS:HG2	2.18	0.44
2:L:454:GLN:HA	2:L:470:ILE:O	2.18	0.44
2:D:124:ALA:O	2:D:127:LEU:HB2	2.18	0.44
2:D:450:PRO:HG2	2:D:453:SER:HB3	2.00	0.44
1:I:20:CYS:HB2	1:I:73:GLU:CD	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:84:VAL:O	2:J:84:VAL:HG13	2.18	0.44
2:L:324:LYS:O	2:L:324:LYS:HG2	2.18	0.43
2:B:431:LYS:NZ	1:E:169:GLU:OE1	2.43	0.43
1:C:194:PHE:HD1	1:C:213:CYS:SG	2.41	0.43
1:E:20:CYS:HB2	1:E:73:GLU:CD	2.42	0.43
1:E:83:TYR:CD1	1:E:83:TYR:C	2.95	0.43
2:F:16:ARG:HH11	2:F:16:ARG:HD2	1.47	0.43
2:F:326:SER:HA	2:F:355:SER:O	2.18	0.43
2:F:450:PRO:HG2	2:F:453:SER:HB3	2.00	0.43
1:G:20:CYS:HB2	1:G:73:GLU:CD	2.42	0.43
1:A:83:TYR:CD1	1:A:83:TYR:C	2.96	0.43
1:C:83:TYR:CD1	1:C:83:TYR:C	2.96	0.43
2:D:454:GLN:HA	2:D:470:ILE:O	2.18	0.43
2:F:80:VAL:O	2:F:84:VAL:HB	2.17	0.43
2:J:124:ALA:O	2:J:127:LEU:HB2	2.18	0.43
2:B:124:ALA:O	2:B:127:LEU:HB2	2.18	0.43
2:B:324:LYS:O	2:B:324:LYS:HG2	2.18	0.43
1:C:80:ASP:HB3	1:C:83:TYR:CE2	2.53	0.43
2:F:246:TYR:HE2	2:F:426:GLU:OE1	2.02	0.43
2:H:246:TYR:HE2	2:H:426:GLU:OE1	2.02	0.43
2:H:326:SER:HA	2:H:355:SER:O	2.18	0.43
1:I:83:TYR:CD1	1:I:83:TYR:C	2.96	0.43
2:L:12:ASP:OD2	2:L:22:ARG:HB2	2.18	0.43
1:A:20:CYS:HB2	1:A:73:GLU:CD	2.42	0.43
2:B:80:VAL:O	2:B:84:VAL:HB	2.17	0.43
2:B:246:TYR:HE2	2:B:426:GLU:OE1	2.02	0.43
2:D:246:TYR:HE2	2:D:426:GLU:OE1	2.02	0.43
2:D:252:PHE:CE1	2:D:256:VAL:HG11	2.54	0.43
2:F:119:ASP:HB3	2:F:522:ARG:HG3	2.00	0.43
2:F:448:GLN:HE21	2:F:448:GLN:HB3	1.67	0.43
2:H:239:ILE:HD11	2:H:432:LEU:HD23	2.00	0.43
2:H:252:PHE:CE1	2:H:256:VAL:HG11	2.54	0.43
2:H:450:PRO:HG2	2:H:453:SER:HB3	2.00	0.43
2:J:12:ASP:OD2	2:J:22:ARG:HB2	2.18	0.43
2:J:246:TYR:HE2	2:J:426:GLU:OE1	2.02	0.43
2:L:124:ALA:O	2:L:127:LEU:HB2	2.18	0.43
2:B:12:ASP:OD2	2:B:22:ARG:HB2	2.18	0.43
2:B:235:ARG:NH2	2:B:238:ARG:HD3	2.34	0.43
2:B:262:LEU:HD13	2:B:396:THR:HG21	2.01	0.43
1:E:254:PHE:HA	1:E:258:TYR:HD2	1.82	0.43
2:H:16:ARG:HH11	2:H:16:ARG:HD2	1.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:ASP:HB3	1:I:83:TYR:CE2	2.53	0.43
1:I:124:ASN:HD21	1:I:128:THR:N	2.10	0.43
1:I:194:PHE:HD1	1:I:213:CYS:SG	2.41	0.43
2:J:278:SER:O	2:J:279:ASN:CB	2.63	0.43
2:L:84:VAL:O	2:L:84:VAL:HG13	2.18	0.43
2:L:246:TYR:HE2	2:L:426:GLU:OE1	2.02	0.43
1:A:194:PHE:HD1	1:A:213:CYS:SG	2.41	0.43
2:B:239:ILE:HD11	2:B:432:LEU:HD23	2.00	0.43
2:D:278:SER:O	2:D:279:ASN:CB	2.63	0.43
2:D:336:PRO:O	2:D:481:GLN:HG3	2.17	0.43
2:F:12:ASP:OD2	2:F:22:ARG:HB2	2.18	0.43
2:F:252:PHE:CE1	2:F:256:VAL:HG11	2.54	0.43
2:L:71:VAL:HG12	2:L:100:MET:HE1	2.01	0.43
2:L:235:ARG:NH2	2:L:238:ARG:HD3	2.34	0.43
2:B:450:PRO:HG2	2:B:453:SER:HB3	2.00	0.43
2:D:262:LEU:HD13	2:D:396:THR:HG21	2.01	0.43
1:E:80:ASP:HB3	1:E:83:TYR:CE2	2.53	0.43
2:F:124:ALA:O	2:F:127:LEU:HB2	2.18	0.43
2:H:12:ASP:OD2	2:H:22:ARG:HB2	2.19	0.43
2:J:450:PRO:HG2	2:J:453:SER:HB3	2.00	0.43
2:B:495:ALA:C	2:B:497:GLY:H	2.27	0.43
2:F:84:VAL:O	2:F:84:VAL:HG13	2.18	0.43
2:F:495:ALA:C	2:F:497:GLY:H	2.27	0.43
2:J:239:ILE:HD11	2:J:432:LEU:HD23	2.00	0.43
1:S:80:ASP:HB3	1:S:83:TYR:CE2	2.53	0.43
2:L:119:ASP:HB3	2:L:522:ARG:HG3	2.00	0.43
2:L:288:THR:OG1	2:L:295:SER:HB2	2.17	0.43
2:B:119:ASP:O	2:B:522:ARG:NH2	2.51	0.43
2:D:12:ASP:OD2	2:D:22:ARG:HB2	2.18	0.43
2:D:239:ILE:HD11	2:D:432:LEU:HD23	2.00	0.43
2:D:324:LYS:HG2	2:D:324:LYS:O	2.18	0.43
1:G:80:ASP:HB3	1:G:83:TYR:CE2	2.53	0.43
2:H:262:LEU:HD13	2:H:396:THR:HG21	2.01	0.43
2:J:119:ASP:O	2:J:522:ARG:NH2	2.51	0.43
2:J:252:PHE:CE1	2:J:256:VAL:HG11	2.54	0.43
2:J:262:LEU:HD13	2:J:396:THR:HG21	2.01	0.43
2:L:262:LEU:HD13	2:L:396:THR:HG21	2.01	0.43
2:B:71:VAL:HG12	2:B:100:MET:HE1	2.01	0.43
2:B:450:PRO:HG2	2:B:453:SER:CB	2.49	0.43
2:D:84:VAL:O	2:D:84:VAL:HG13	2.18	0.43
2:D:119:ASP:HB3	2:D:522:ARG:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:VAL:HG12	2:F:100:MET:HE1	2.01	0.43
2:F:262:LEU:HD13	2:F:396:THR:HG21	2.01	0.43
2:F:306:ASN:ND2	2:F:405:PHE:CD1	2.80	0.43
1:G:193:HIS:CD2	1:G:211:GLY:O	2.72	0.43
2:H:278:SER:O	2:H:279:ASN:CB	2.63	0.43
2:H:324:LYS:O	2:H:324:LYS:HG2	2.18	0.43
2:H:450:PRO:HG2	2:H:453:SER:CB	2.49	0.43
2:J:326:SER:HA	2:J:355:SER:O	2.18	0.43
2:J:495:ALA:C	2:J:497:GLY:H	2.27	0.43
1:S:20:CYS:HB2	1:S:73:GLU:CD	2.42	0.42
1:S:194:PHE:HD1	1:S:213:CYS:SG	2.41	0.42
2:L:252:PHE:CE1	2:L:256:VAL:HG11	2.54	0.42
2:D:326:SER:HA	2:D:355:SER:O	2.18	0.42
2:D:450:PRO:HG2	2:D:453:SER:CB	2.49	0.42
1:E:194:PHE:HD1	1:E:213:CYS:SG	2.41	0.42
2:F:235:ARG:NH2	2:F:238:ARG:HD3	2.34	0.42
2:H:12:ASP:HA	2:H:13:PRO:HA	1.91	0.42
1:I:193:HIS:CD2	1:I:211:GLY:O	2.72	0.42
2:J:235:ARG:HH11	2:J:235:ARG:HD2	1.64	0.42
2:D:71:VAL:HG12	2:D:100:MET:HE1	2.01	0.42
2:D:235:ARG:NH2	2:D:238:ARG:HD3	2.34	0.42
2:F:239:ILE:HD11	2:F:432:LEU:HD23	2.00	0.42
1:G:194:PHE:HD1	1:G:213:CYS:SG	2.41	0.42
2:H:119:ASP:O	2:H:522:ARG:NH2	2.51	0.42
2:H:495:ALA:C	2:H:497:GLY:H	2.27	0.42
2:J:9:ILE:HB	2:J:25:VAL:CG2	2.50	0.42
2:J:286:PHE:CD1	2:J:428:TRP:CH2	3.07	0.42
2:J:306:ASN:ND2	2:J:405:PHE:CD1	2.80	0.42
2:L:450:PRO:HG2	2:L:453:SER:HB3	2.00	0.42
2:L:495:ALA:C	2:L:497:GLY:H	2.27	0.42
1:C:193:HIS:CD2	1:C:211:GLY:O	2.72	0.42
2:F:286:PHE:CD1	2:F:428:TRP:CH2	3.07	0.42
2:F:450:PRO:HG2	2:F:453:SER:CB	2.49	0.42
2:H:9:ILE:HB	2:H:25:VAL:CG2	2.50	0.42
1:A:230:LYS:H	1:A:230:LYS:HG3	1.68	0.42
2:H:9:ILE:HB	2:H:25:VAL:HG22	2.01	0.42
1:S:193:HIS:CD2	1:S:211:GLY:O	2.72	0.42
2:L:239:ILE:HD11	2:L:432:LEU:HD23	2.00	0.42
2:L:450:PRO:HG2	2:L:453:SER:CB	2.49	0.42
2:D:9:ILE:HB	2:D:25:VAL:HG22	2.01	0.42
2:D:286:PHE:CD1	2:D:428:TRP:CH2	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:119:ASP:HB3	2:H:522:ARG:HG3	2.00	0.42
2:H:244:LYS:NZ	2:H:248:GLU:OE1	2.44	0.42
2:J:450:PRO:HG2	2:J:453:SER:CB	2.49	0.42
2:B:252:PHE:CE1	2:B:256:VAL:HG11	2.54	0.42
2:B:383:HIS:CD2	2:B:386:THR:OG1	2.70	0.42
2:D:495:ALA:C	2:D:497:GLY:H	2.27	0.42
2:H:71:VAL:HG12	2:H:100:MET:HE1	2.01	0.42
2:L:286:PHE:CD1	2:L:428:TRP:CH2	3.07	0.42
2:B:286:PHE:CD1	2:B:428:TRP:CH2	3.07	0.42
2:D:490:LEU:HD13	2:D:529:PRO:HB3	2.02	0.42
2:H:235:ARG:NH2	2:H:238:ARG:HD3	2.34	0.42
2:J:119:ASP:HB3	2:J:522:ARG:HG3	2.00	0.42
2:L:9:ILE:HB	2:L:25:VAL:CG2	2.50	0.42
2:L:384:GLU:N	2:L:385:PRO:CD	2.83	0.42
2:B:9:ILE:HB	2:B:25:VAL:CG2	2.50	0.42
2:D:9:ILE:HB	2:D:25:VAL:CG2	2.50	0.42
2:H:33:LYS:CD	2:H:33:LYS:C	2.93	0.42
2:H:490:LEU:HD13	2:H:529:PRO:HB3	2.02	0.42
2:J:71:VAL:HG12	2:J:100:MET:HE1	2.01	0.42
2:L:12:ASP:HA	2:L:13:PRO:HA	1.91	0.42
1:A:193:HIS:CD2	1:A:211:GLY:O	2.72	0.42
2:B:84:VAL:O	2:B:84:VAL:HG13	2.18	0.42
2:F:33:LYS:CD	2:F:33:LYS:C	2.93	0.42
2:J:324:LYS:O	2:J:324:LYS:HG2	2.18	0.42
1:S:235:GLN:NE2	2:L:208:ARG:NH2	2.39	0.42
2:L:306:ASN:ND2	2:L:405:PHE:CD1	2.80	0.42
2:B:141:LEU:HD23	2:B:141:LEU:HA	1.78	0.42
2:F:9:ILE:HB	2:F:25:VAL:CG2	2.50	0.42
2:J:490:LEU:HD13	2:J:529:PRO:HB3	2.02	0.42
2:L:144:LYS:NZ	2:L:198:GLU:OE2	2.53	0.41
2:B:33:LYS:CD	2:B:33:LYS:C	2.93	0.41
2:B:315:ASN:HA	2:B:316:PRO:HD2	1.95	0.41
2:F:125:ASN:HA	2:F:128:ASN:ND2	2.35	0.41
2:H:286:PHE:CD1	2:H:428:TRP:CH2	3.07	0.41
2:J:125:ASN:HA	2:J:128:ASN:ND2	2.35	0.41
2:J:172:ASN:O	2:J:173:ALA:C	2.63	0.41
2:L:490:LEU:HD13	2:L:529:PRO:HB3	2.02	0.41
2:B:384:GLU:N	2:B:385:PRO:CD	2.83	0.41
2:D:21:LEU:HB2	2:D:531:ILE:HG12	2.02	0.41
2:D:33:LYS:CD	2:D:33:LYS:C	2.93	0.41
2:D:125:ASN:HA	2:D:128:ASN:ND2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:384:GLU:N	2:D:385:PRO:CD	2.83	0.41
1:E:193:HIS:CD2	1:E:211:GLY:O	2.72	0.41
2:F:119:ASP:O	2:F:522:ARG:NH2	2.51	0.41
1:G:244:HIS:ND1	1:G:245:PRO:HD2	2.36	0.41
2:H:125:ASN:HA	2:H:128:ASN:ND2	2.35	0.41
2:J:21:LEU:HB2	2:J:531:ILE:HG12	2.02	0.41
2:L:33:LYS:CD	2:L:33:LYS:C	2.93	0.41
2:J:9:ILE:HB	2:J:25:VAL:HG22	2.01	0.41
2:L:49:LEU:O	2:L:50:LYS:C	2.64	0.41
2:L:125:ASN:HA	2:L:128:ASN:ND2	2.35	0.41
2:B:125:ASN:HA	2:B:128:ASN:ND2	2.35	0.41
1:E:244:HIS:ND1	1:E:245:PRO:HD2	2.36	0.41
2:H:49:LEU:O	2:H:50:LYS:C	2.64	0.41
2:L:16:ARG:HH11	2:L:16:ARG:HD2	1.47	0.41
2:B:271:TRP:C	2:B:273:GLY:H	2.29	0.41
1:C:244:HIS:ND1	1:C:245:PRO:HD2	2.36	0.41
2:D:119:ASP:O	2:D:522:ARG:NH2	2.51	0.41
2:F:384:GLU:N	2:F:385:PRO:CD	2.83	0.41
2:H:21:LEU:HB2	2:H:531:ILE:HG12	2.02	0.41
2:H:137:LEU:C	2:H:137:LEU:HD12	2.46	0.41
2:H:315:ASN:HA	2:H:316:PRO:HD2	1.95	0.41
1:I:18:THR:O	1:I:18:THR:CG2	2.69	0.41
2:J:235:ARG:NH2	2:J:238:ARG:HD3	2.34	0.41
1:S:230:LYS:H	1:S:230:LYS:HG3	1.68	0.41
2:L:9:ILE:HB	2:L:25:VAL:HG22	2.01	0.41
2:L:172:ASN:O	2:L:173:ALA:C	2.63	0.41
2:B:490:LEU:HD13	2:B:529:PRO:HB3	2.02	0.41
1:E:228:CYS:HB2	1:E:229:PRO:CD	2.50	0.41
2:L:130:ASP:HA	2:L:131:PRO:HD2	1.93	0.41
2:L:244:LYS:NZ	2:L:248:GLU:OE1	2.44	0.41
2:D:244:LYS:NZ	2:D:248:GLU:OE1	2.44	0.41
2:F:141:LEU:HA	2:F:141:LEU:HD23	1.78	0.41
2:J:448:GLN:HE21	2:J:448:GLN:HB3	1.67	0.41
2:L:141:LEU:HD23	2:L:141:LEU:HA	1.78	0.41
1:A:227:ASN:HD22	1:A:227:ASN:N	2.04	0.41
2:B:9:ILE:HB	2:B:25:VAL:HG22	2.01	0.41
2:F:271:TRP:C	2:F:273:GLY:H	2.29	0.41
2:F:490:LEU:HD13	2:F:529:PRO:HB3	2.02	0.41
2:H:384:GLU:N	2:H:385:PRO:CD	2.83	0.41
1:I:96:CYS:HB3	1:I:135:LEU:HD11	2.03	0.41
1:I:244:HIS:ND1	1:I:245:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:137:LEU:C	2:J:137:LEU:HD12	2.46	0.41
1:S:18:THR:O	1:S:18:THR:CG2	2.69	0.41
2:L:137:LEU:C	2:L:137:LEU:HD12	2.46	0.41
1:A:18:THR:O	1:A:18:THR:CG2	2.69	0.41
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.95	0.41
1:A:251:GLU:HA	1:A:252:PRO:HD3	1.95	0.41
2:B:49:LEU:O	2:B:50:LYS:C	2.64	0.41
2:B:144:LYS:NZ	2:B:198:GLU:OE2	2.53	0.41
2:B:172:ASN:O	2:B:173:ALA:C	2.63	0.41
2:D:34:ASN:OD1	2:D:35:ALA:N	2.49	0.41
2:D:49:LEU:O	2:D:50:LYS:C	2.64	0.41
2:D:144:LYS:NZ	2:D:198:GLU:OE2	2.53	0.41
2:D:294:ASN:OD1	2:D:300:GLN:NE2	2.47	0.41
2:F:52:ARG:HH11	2:F:52:ARG:HD3	1.69	0.41
2:F:477:ILE:HD13	2:F:477:ILE:HG21	1.90	0.41
1:G:96:CYS:HB3	1:G:135:LEU:HD11	2.03	0.41
2:H:62:GLN:HA	2:H:72:HIS:HB2	2.03	0.41
2:H:383:HIS:CD2	2:H:386:THR:OG1	2.70	0.41
2:J:33:LYS:CD	2:J:33:LYS:C	2.93	0.41
2:J:62:GLN:HA	2:J:72:HIS:HB2	2.03	0.41
1:S:202:SER:O	1:S:208:ALA:HB2	2.22	0.41
2:L:21:LEU:HB2	2:L:531:ILE:HG12	2.02	0.41
1:A:244:HIS:ND1	1:A:245:PRO:HD2	2.36	0.41
2:F:9:ILE:HB	2:F:25:VAL:HG22	2.01	0.41
2:F:21:LEU:HB2	2:F:531:ILE:HG12	2.02	0.41
2:H:34:ASN:OD1	2:H:35:ALA:N	2.48	0.41
1:A:238:TRP:HB2	1:A:239:PRO:HD2	2.04	0.40
2:B:281:LEU:HD12	2:B:281:LEU:C	2.47	0.40
1:E:96:CYS:HB3	1:E:135:LEU:HD11	2.03	0.40
1:I:224:THR:HG21	4:I:266:F3S:S3	2.62	0.40
2:J:49:LEU:O	2:J:50:LYS:C	2.64	0.40
2:L:281:LEU:HD12	2:L:281:LEU:C	2.47	0.40
2:F:49:LEU:O	2:F:50:LYS:C	2.64	0.40
1:S:228:CYS:HB2	1:S:229:PRO:CD	2.50	0.40
2:L:12:ASP:C	2:L:12:ASP:OD1	2.65	0.40
2:L:315:ASN:HA	2:L:316:PRO:HD2	1.95	0.40
2:D:281:LEU:C	2:D:281:LEU:HD12	2.47	0.40
2:F:12:ASP:OD1	2:F:12:ASP:C	2.65	0.40
2:F:130:ASP:HA	2:F:131:PRO:HD2	1.93	0.40
1:G:238:TRP:HB2	1:G:239:PRO:HD2	2.03	0.40
1:I:238:TRP:HB2	1:I:239:PRO:HD2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:144:LYS:NZ	2:J:198:GLU:OE2	2.53	0.40
2:J:202:VAL:O	2:J:203:GLN:C	2.64	0.40
2:J:384:GLU:N	2:J:385:PRO:CD	2.83	0.40
1:S:224:THR:HG21	4:S:266:F3S:S3	2.62	0.40
1:S:244:HIS:ND1	1:S:245:PRO:HD2	2.36	0.40
2:L:119:ASP:O	2:L:522:ARG:NH2	2.51	0.40
1:A:202:SER:O	1:A:208:ALA:HB2	2.21	0.40
1:A:228:CYS:HB2	1:A:229:PRO:CD	2.51	0.40
2:B:12:ASP:OD1	2:B:12:ASP:C	2.65	0.40
2:B:62:GLN:HA	2:B:72:HIS:HB2	2.03	0.40
2:B:137:LEU:C	2:B:137:LEU:HD12	2.46	0.40
2:D:62:GLN:HA	2:D:72:HIS:HB2	2.03	0.40
2:F:88:ILE:HA	2:F:89:PRO:HD3	1.90	0.40
2:H:56:ASP:O	2:H:57:ALA:C	2.65	0.40
2:H:172:ASN:O	2:H:173:ALA:C	2.63	0.40
2:J:56:ASP:O	2:J:57:ALA:C	2.65	0.40
1:C:96:CYS:HB3	1:C:135:LEU:HD11	2.03	0.40
1:C:202:SER:O	1:C:208:ALA:HB2	2.22	0.40
2:D:320:GLU:OE1	2:D:334:HIS:CA	2.70	0.40
2:F:235:ARG:HH11	2:F:235:ARG:HD2	1.64	0.40
1:G:18:THR:O	1:G:18:THR:CG2	2.69	0.40
2:H:12:ASP:OD1	2:H:12:ASP:C	2.65	0.40
2:H:144:LYS:NZ	2:H:198:GLU:OE2	2.53	0.40
2:H:234:LEU:HD12	2:H:234:LEU:HA	1.95	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:340:HOH:O	9:I:1015:HOH:O[1_445]	1.32	0.88
9:A:341:HOH:O	9:C:450:HOH:O[1_444]	1.34	0.86
9:S:338:HOH:O	9:E:639:HOH:O[1_556]	1.41	0.79

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	C	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	E	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	G	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	I	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
1	S	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	39
2	B	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	D	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	F	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	H	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	J	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
2	L	528/536 (98%)	506 (96%)	21 (4%)	1 (0%)	43	56
All	All	4722/4800 (98%)	4500 (95%)	210 (4%)	12 (0%)	36	45

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	5	LYS
2	L	118	LEU
1	A	5	LYS
2	B	118	LEU
1	C	5	LYS
2	D	118	LEU
1	E	5	LYS
2	F	118	LEU
1	G	5	LYS
2	H	118	LEU
1	I	5	LYS
2	J	118	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	189 (91%)	19 (9%)	9	11
1	C	208/210 (99%)	189 (91%)	19 (9%)	9	11
1	E	208/210 (99%)	189 (91%)	19 (9%)	9	11
1	G	208/210 (99%)	189 (91%)	19 (9%)	9	11
1	I	208/210 (99%)	189 (91%)	19 (9%)	9	11
1	S	208/210 (99%)	189 (91%)	19 (9%)	9	11
2	B	434/439 (99%)	391 (90%)	43 (10%)	7	9
2	D	434/439 (99%)	391 (90%)	43 (10%)	7	9
2	F	434/439 (99%)	391 (90%)	43 (10%)	7	9
2	H	434/439 (99%)	391 (90%)	43 (10%)	7	9
2	J	434/439 (99%)	390 (90%)	44 (10%)	7	8
2	L	434/439 (99%)	391 (90%)	43 (10%)	7	9
All	All	3852/3894 (99%)	3479 (90%)	373 (10%)	8	9

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	5	LYS
1	S	16	GLU
1	S	25	LEU
1	S	28	VAL
1	S	46	GLU
1	S	48	LEU
1	S	67	ASP
1	S	109	ILE
1	S	159	VAL
1	S	163	LEU
1	S	165	LYS
1	S	182	GLU
1	S	191	LEU
1	S	195	GLU
1	S	210	LYS
1	S	227	ASN
1	S	230	LYS
1	S	235	GLN
1	S	236	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	7	ASN
2	L	8	LYS
2	L	10	VAL
2	L	14	ILE
2	L	33	LYS
2	L	49	LEU
2	L	50	LYS
2	L	74	LEU
2	L	83	CYS
2	L	84	VAL
2	L	87	LYS
2	L	88	ILE
2	L	96	ARG
2	L	109	LEU
2	L	115	LEU
2	L	118	LEU
2	L	162	VAL
2	L	190	LEU
2	L	217	ASN
2	L	234	LEU
2	L	237	GLU
2	L	244	LYS
2	L	248	GLU
2	L	281	LEU
2	L	300	GLN
2	L	361	ARG
2	L	381	LYS
2	L	382	LYS
2	L	384	GLU
2	L	388	LYS
2	L	390	VAL
2	L	395	LYS
2	L	402	GLU
2	L	465	MET
2	L	473	ARG
2	L	476	LYS
2	L	482	LEU
2	L	496	GLU
2	L	498	LYS
2	L	511	ILE
2	L	515	LYS
2	L	517	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	531	ILE
1	A	5	LYS
1	A	16	GLU
1	A	25	LEU
1	A	28	VAL
1	A	46	GLU
1	A	48	LEU
1	A	67	ASP
1	A	109	ILE
1	A	159	VAL
1	A	163	LEU
1	A	165	LYS
1	A	182	GLU
1	A	191	LEU
1	A	195	GLU
1	A	210	LYS
1	A	227	ASN
1	A	230	LYS
1	A	235	GLN
1	A	236	VAL
2	B	7	ASN
2	B	8	LYS
2	B	10	VAL
2	B	14	ILE
2	B	33	LYS
2	B	49	LEU
2	B	50	LYS
2	B	74	LEU
2	B	83	CYS
2	B	84	VAL
2	B	87	LYS
2	B	88	ILE
2	B	96	ARG
2	B	109	LEU
2	B	115	LEU
2	B	118	LEU
2	B	162	VAL
2	B	190	LEU
2	B	217	ASN
2	B	234	LEU
2	B	237	GLU
2	B	244	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	248	GLU
2	B	281	LEU
2	B	300	GLN
2	B	361	ARG
2	B	381	LYS
2	B	382	LYS
2	B	384	GLU
2	B	388	LYS
2	B	390	VAL
2	B	395	LYS
2	B	402	GLU
2	B	465	MET
2	B	473	ARG
2	B	476	LYS
2	B	482	LEU
2	B	496	GLU
2	B	498	LYS
2	B	511	ILE
2	B	515	LYS
2	B	517	PRO
2	B	531	ILE
1	C	5	LYS
1	C	16	GLU
1	C	25	LEU
1	C	28	VAL
1	C	46	GLU
1	C	48	LEU
1	C	67	ASP
1	C	109	ILE
1	C	159	VAL
1	C	163	LEU
1	C	165	LYS
1	C	182	GLU
1	C	191	LEU
1	C	195	GLU
1	C	210	LYS
1	C	227	ASN
1	C	230	LYS
1	C	235	GLN
1	C	236	VAL
2	D	7	ASN
2	D	8	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	10	VAL
2	D	14	ILE
2	D	33	LYS
2	D	49	LEU
2	D	50	LYS
2	D	74	LEU
2	D	83	CYS
2	D	84	VAL
2	D	87	LYS
2	D	88	ILE
2	D	96	ARG
2	D	109	LEU
2	D	115	LEU
2	D	118	LEU
2	D	162	VAL
2	D	190	LEU
2	D	217	ASN
2	D	234	LEU
2	D	237	GLU
2	D	244	LYS
2	D	248	GLU
2	D	281	LEU
2	D	300	GLN
2	D	361	ARG
2	D	381	LYS
2	D	382	LYS
2	D	384	GLU
2	D	388	LYS
2	D	390	VAL
2	D	395	LYS
2	D	402	GLU
2	D	465	MET
2	D	473	ARG
2	D	476	LYS
2	D	482	LEU
2	D	496	GLU
2	D	498	LYS
2	D	511	ILE
2	D	515	LYS
2	D	517	PRO
2	D	531	ILE
1	E	5	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	16	GLU
1	E	25	LEU
1	E	28	VAL
1	E	46	GLU
1	E	48	LEU
1	E	67	ASP
1	E	109	ILE
1	E	159	VAL
1	E	163	LEU
1	E	165	LYS
1	E	182	GLU
1	E	191	LEU
1	E	195	GLU
1	E	210	LYS
1	E	227	ASN
1	E	230	LYS
1	E	235	GLN
1	E	236	VAL
2	F	7	ASN
2	F	8	LYS
2	F	10	VAL
2	F	14	ILE
2	F	33	LYS
2	F	49	LEU
2	F	50	LYS
2	F	74	LEU
2	F	83	CYS
2	F	84	VAL
2	F	87	LYS
2	F	88	ILE
2	F	96	ARG
2	F	109	LEU
2	F	115	LEU
2	F	118	LEU
2	F	162	VAL
2	F	190	LEU
2	F	217	ASN
2	F	234	LEU
2	F	237	GLU
2	F	244	LYS
2	F	248	GLU
2	F	281	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	300	GLN
2	F	361	ARG
2	F	381	LYS
2	F	382	LYS
2	F	384	GLU
2	F	388	LYS
2	F	390	VAL
2	F	395	LYS
2	F	402	GLU
2	F	465	MET
2	F	473	ARG
2	F	476	LYS
2	F	482	LEU
2	F	496	GLU
2	F	498	LYS
2	F	511	ILE
2	F	515	LYS
2	F	517	PRO
2	F	531	ILE
1	G	5	LYS
1	G	16	GLU
1	G	25	LEU
1	G	28	VAL
1	G	46	GLU
1	G	48	LEU
1	G	67	ASP
1	G	109	ILE
1	G	159	VAL
1	G	163	LEU
1	G	165	LYS
1	G	182	GLU
1	G	191	LEU
1	G	195	GLU
1	G	210	LYS
1	G	227	ASN
1	G	230	LYS
1	G	235	GLN
1	G	236	VAL
2	H	7	ASN
2	H	8	LYS
2	H	10	VAL
2	H	14	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	33	LYS
2	H	49	LEU
2	H	50	LYS
2	H	74	LEU
2	H	83	CYS
2	H	84	VAL
2	H	87	LYS
2	H	88	ILE
2	H	96	ARG
2	H	109	LEU
2	H	115	LEU
2	H	118	LEU
2	H	162	VAL
2	H	190	LEU
2	H	217	ASN
2	H	234	LEU
2	H	237	GLU
2	H	244	LYS
2	H	248	GLU
2	H	281	LEU
2	H	300	GLN
2	H	361	ARG
2	H	381	LYS
2	H	382	LYS
2	H	384	GLU
2	H	388	LYS
2	H	390	VAL
2	H	395	LYS
2	H	402	GLU
2	H	465	MET
2	H	473	ARG
2	H	476	LYS
2	H	482	LEU
2	H	496	GLU
2	H	498	LYS
2	H	511	ILE
2	H	515	LYS
2	H	517	PRO
2	H	531	ILE
1	I	5	LYS
1	I	16	GLU
1	I	25	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	28	VAL
1	I	46	GLU
1	I	48	LEU
1	I	67	ASP
1	I	109	ILE
1	I	159	VAL
1	I	163	LEU
1	I	165	LYS
1	I	182	GLU
1	I	191	LEU
1	I	195	GLU
1	I	210	LYS
1	I	227	ASN
1	I	230	LYS
1	I	235	GLN
1	I	236	VAL
2	J	7	ASN
2	J	8	LYS
2	J	10	VAL
2	J	14	ILE
2	J	33	LYS
2	J	49	LEU
2	J	50	LYS
2	J	74	LEU
2	J	83	CYS
2	J	84	VAL
2	J	87	LYS
2	J	88	ILE
2	J	96	ARG
2	J	109	LEU
2	J	115	LEU
2	J	118	LEU
2	J	162	VAL
2	J	190	LEU
2	J	217	ASN
2	J	234	LEU
2	J	237	GLU
2	J	244	LYS
2	J	248	GLU
2	J	281	LEU
2	J	300	GLN
2	J	342	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	361	ARG
2	J	381	LYS
2	J	382	LYS
2	J	384	GLU
2	J	388	LYS
2	J	390	VAL
2	J	395	LYS
2	J	402	GLU
2	J	465	MET
2	J	473	ARG
2	J	476	LYS
2	J	482	LEU
2	J	496	GLU
2	J	498	LYS
2	J	511	ILE
2	J	515	LYS
2	J	517	PRO
2	J	531	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	124	ASN
1	S	154	ASN
1	S	161	HIS
1	S	193	HIS
1	S	227	ASN
1	S	231	GLN
1	S	235	GLN
1	S	241	GLN
2	L	82	ASN
2	L	97	ASN
2	L	108	HIS
2	L	217	ASN
2	L	270	ASN
2	L	334	HIS
2	L	335	HIS
2	L	383	HIS
2	L	417	GLN
2	L	448	GLN
2	L	481	GLN
1	A	124	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	154	ASN
1	A	161	HIS
1	A	193	HIS
1	A	227	ASN
1	A	231	GLN
1	A	235	GLN
1	A	241	GLN
2	B	82	ASN
2	B	97	ASN
2	B	108	HIS
2	B	217	ASN
2	B	270	ASN
2	B	334	HIS
2	B	335	HIS
2	B	383	HIS
2	B	417	GLN
2	B	448	GLN
2	B	460	ASN
1	C	124	ASN
1	C	154	ASN
1	C	161	HIS
1	C	193	HIS
1	C	227	ASN
1	C	231	GLN
1	C	235	GLN
1	C	241	GLN
2	D	82	ASN
2	D	97	ASN
2	D	108	HIS
2	D	217	ASN
2	D	270	ASN
2	D	334	HIS
2	D	335	HIS
2	D	383	HIS
2	D	417	GLN
2	D	448	GLN
1	E	54	HIS
1	E	124	ASN
1	E	154	ASN
1	E	161	HIS
1	E	193	HIS
1	E	227	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	231	GLN
1	E	235	GLN
1	E	241	GLN
2	F	82	ASN
2	F	97	ASN
2	F	108	HIS
2	F	217	ASN
2	F	270	ASN
2	F	334	HIS
2	F	335	HIS
2	F	383	HIS
2	F	417	GLN
2	F	448	GLN
2	F	504	GLN
1	G	124	ASN
1	G	154	ASN
1	G	161	HIS
1	G	193	HIS
1	G	227	ASN
1	G	231	GLN
1	G	235	GLN
1	G	241	GLN
2	H	82	ASN
2	H	97	ASN
2	H	108	HIS
2	H	217	ASN
2	H	270	ASN
2	H	334	HIS
2	H	335	HIS
2	H	383	HIS
2	H	417	GLN
2	H	448	GLN
1	I	124	ASN
1	I	154	ASN
1	I	161	HIS
1	I	193	HIS
1	I	227	ASN
1	I	231	GLN
1	I	235	GLN
1	I	241	GLN
2	J	82	ASN
2	J	97	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	108	HIS
2	J	217	ASN
2	J	270	ASN
2	J	334	HIS
2	J	335	HIS
2	J	383	HIS
2	J	417	GLN
2	J	448	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 18 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SF4	G	267	1	0,12,12	-	-	-		
7	FCO	J	537	2,8	3,6,6	2.36	1 (33%)	-		
7	FCO	D	537	2,8	3,6,6	2.37	1 (33%)	-		
3	SF4	S	267	1	0,12,12	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	E	265	1	0,12,12	-	-	-		
7	FCO	L	537	2,8	3,6,6	2.36	1 (33%)	-		
4	F3S	G	266	1	0,9,9	-	-	-		
7	FCO	H	537	2,8	3,6,6	2.34	1 (33%)	-		
3	SF4	C	265	1	0,12,12	-	-	-		
3	SF4	I	267	1	0,12,12	-	-	-		
3	SF4	I	265	1	0,12,12	-	-	-		
3	SF4	G	265	1	0,12,12	-	-	-		
3	SF4	S	265	1	0,12,12	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
7	FCO	B	537	2,8	3,6,6	2.36	1 (33%)	-		
7	FCO	F	537	2,8	3,6,6	2.36	1 (33%)	-		
4	F3S	E	266	1	0,9,9	-	-	-		
4	F3S	C	266	1	0,9,9	-	-	-		
4	F3S	I	266	1	0,9,9	-	-	-		
3	SF4	E	267	1	0,12,12	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
4	F3S	S	266	1	0,9,9	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F3S	C	266	1	-	-	0/3/3/3
3	SF4	G	265	1	-	-	0/6/5/5
3	SF4	G	267	1	-	-	0/6/5/5
4	F3S	G	266	1	-	-	0/3/3/3
4	F3S	I	266	1	-	-	0/3/3/3
3	SF4	S	265	1	-	-	0/6/5/5
3	SF4	A	265	1	-	-	0/6/5/5
4	F3S	A	266	1	-	-	0/3/3/3
3	SF4	E	267	1	-	-	0/6/5/5
3	SF4	I	267	1	-	-	0/6/5/5
3	SF4	C	265	1	-	-	0/6/5/5
3	SF4	C	267	1	-	-	0/6/5/5
4	F3S	S	266	1	-	-	0/3/3/3
3	SF4	S	267	1	-	-	0/6/5/5
3	SF4	I	265	1	-	-	0/6/5/5
4	F3S	E	266	1	-	-	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	267	1	-	-	0/6/5/5
3	SF4	E	265	1	-	-	0/6/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	537	FCO	C1-N1	3.90	1.20	1.15
7	L	537	FCO	C1-N1	3.87	1.20	1.15
7	J	537	FCO	C1-N1	3.87	1.20	1.15
7	B	537	FCO	C1-N1	3.87	1.20	1.15
7	F	537	FCO	C1-N1	3.87	1.20	1.15
7	H	537	FCO	C1-N1	3.86	1.20	1.15

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	537	FCO	2	0
7	D	537	FCO	2	0
7	L	537	FCO	2	0
7	H	537	FCO	2	0
7	B	537	FCO	2	0
7	F	537	FCO	2	0
4	I	266	F3S	1	0
4	S	266	F3S	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.