



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:52 PM UTC

PDB ID : 2LDB / pdb_00002ldb
Title : STRUCTURE DETERMINATION AND REFINEMENT OF BACILLUS
STEAROTHERMOPHILUS LACTATE DEHYDROGENASE
Authors : Piontek, K.; Rossmann, M.G.
Deposited on : 1989-03-27
Resolution : 3.00 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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)	:	2.49

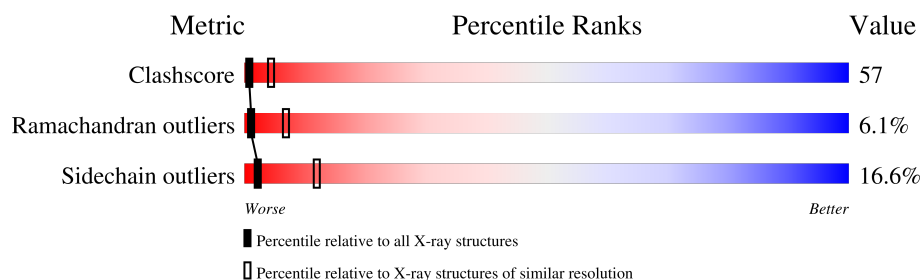
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	317	
1	B	317	
1	C	317	
1	D	317	

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
2	SO4	A	3	-	-	X	-
2	SO4	B	7	-	-	X	-
2	SO4	C	11	-	-	X	-
2	SO4	D	332	-	-	X	-

2 Entry composition [i](#)

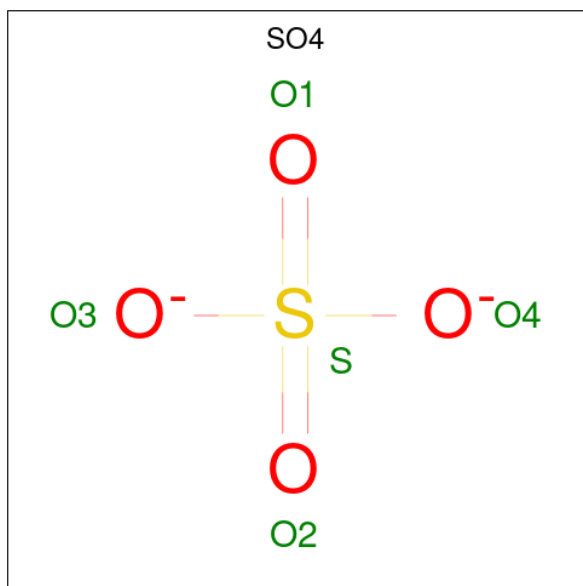
There are 5 unique types of molecules in this entry. The entry contains 9650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2336	1496	401	431	8			
1	B	301	Total	C	N	O	S	0	0	0
			2336	1496	401	431	8			
1	C	301	Total	C	N	O	S	0	0	0
			2336	1496	401	431	8			
1	D	301	Total	C	N	O	S	0	0	0
			2336	1496	401	431	8			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



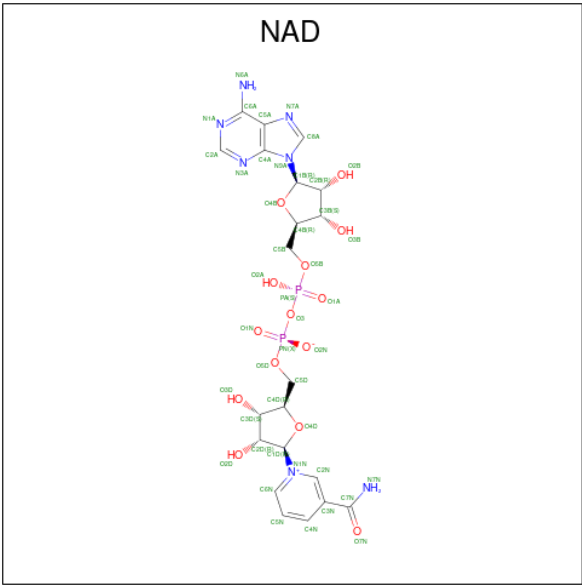
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

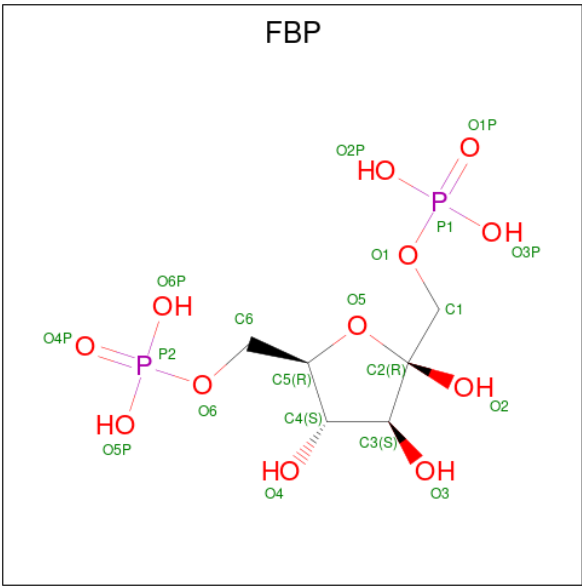
- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula:

C₆H₁₄O₁₂P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is water.

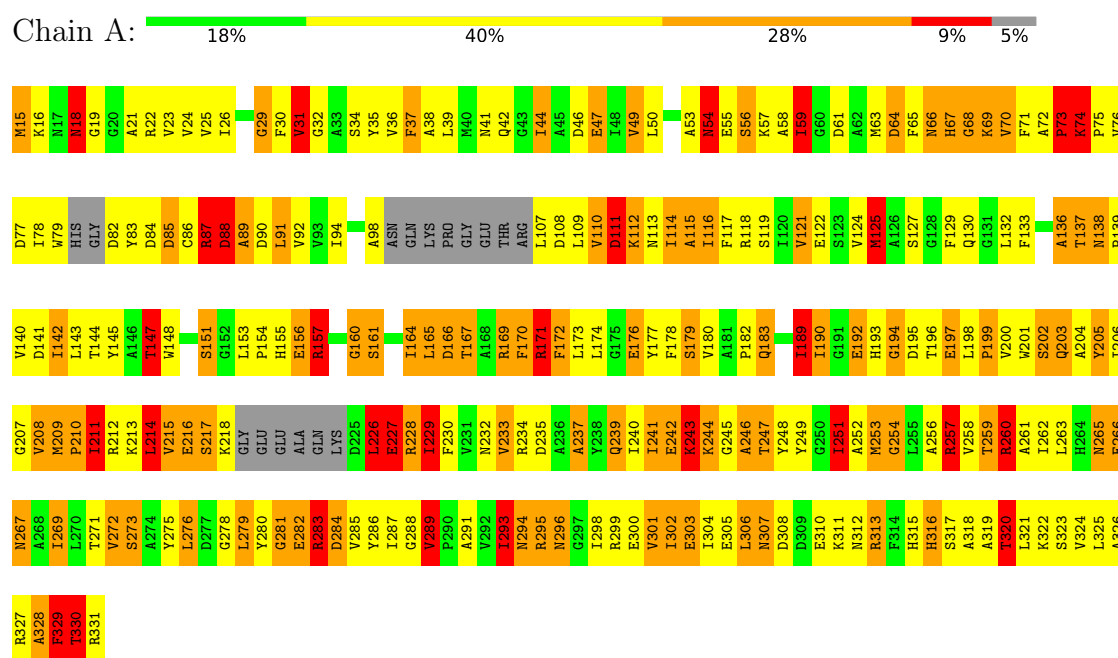
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

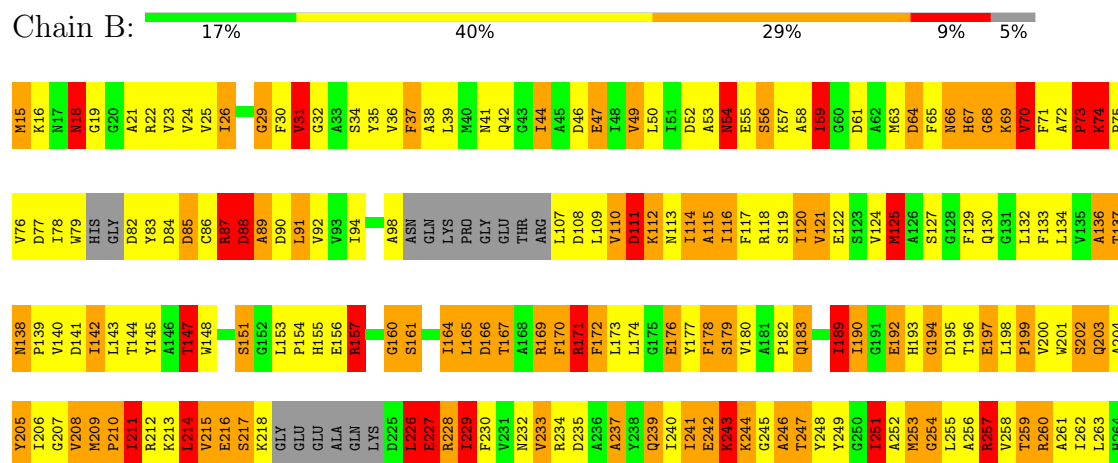
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

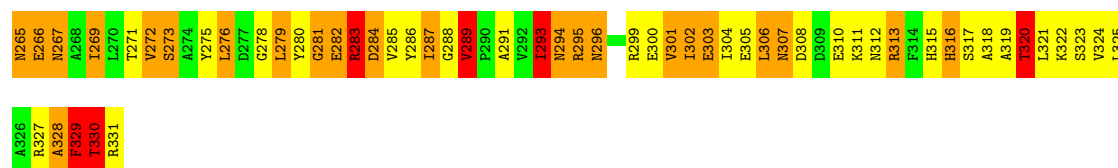
Note EDS was not executed.

• Molecule 1: L-LACTATE DEHYDROGENASE



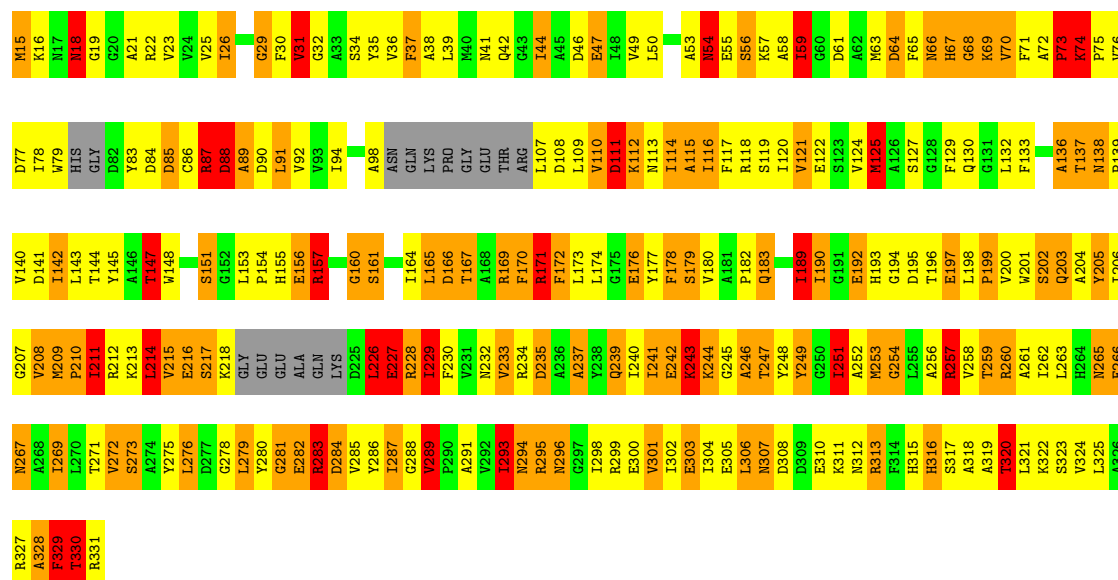
• Molecule 1: L-LACTATE DEHYDROGENASE





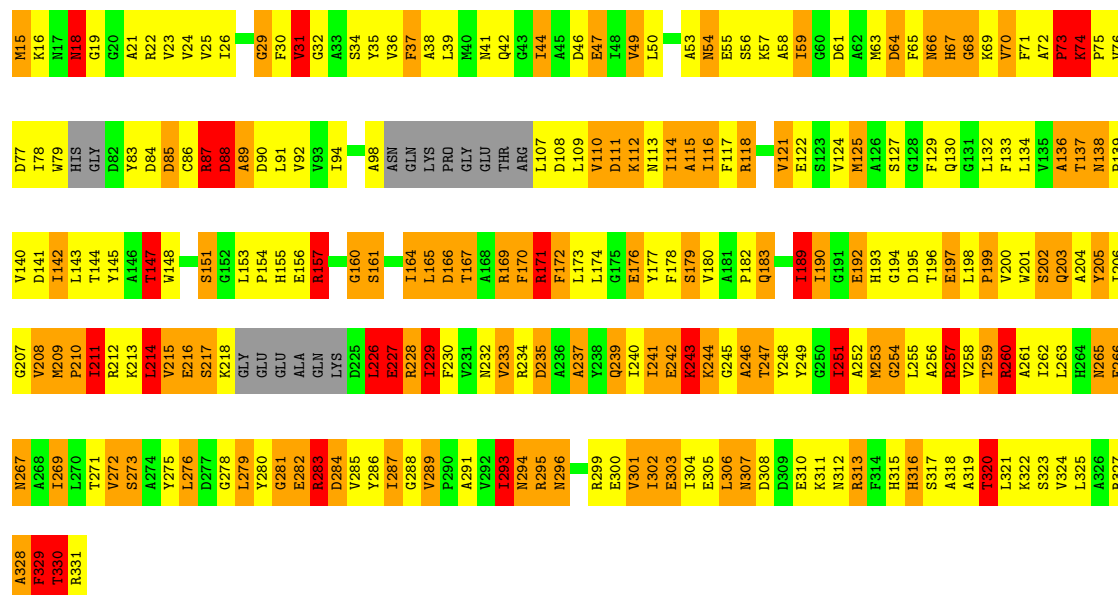
• Molecule 1: L-LACTATE DEHYDROGENASE

Chain C: 19% 39% 28% 9% 5%



• Molecule 1: L-LACTATE DEHYDROGENASE

Chain D: 19% 40% 29% 8% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	86.80 Å 86.80 Å 356.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.260 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9650	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: FBP, SO4, NAD

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	1.40	8/2379 (0.3%)	2.76	220/3223 (6.8%)
1	B	1.40	7/2379 (0.3%)	2.76	223/3223 (6.9%)
1	C	1.40	6/2379 (0.3%)	2.76	223/3223 (6.9%)
1	D	1.40	7/2379 (0.3%)	2.76	219/3223 (6.8%)
All	All	1.40	28/9516 (0.3%)	2.76	885/12892 (6.9%)

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
1	A	0	9
1	B	0	9
1	C	0	9
1	D	0	9
All	All	0	36

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	TYR	N-CA	6.07	1.53	1.45
1	A	286	TYR	N-CA	6.06	1.53	1.45
1	D	286	TYR	N-CA	5.98	1.53	1.45
1	C	286	TYR	N-CA	5.94	1.53	1.45
1	D	67	HIS	CE1-NE2	-5.69	1.26	1.32
1	C	67	HIS	CE1-NE2	-5.66	1.26	1.32
1	A	67	HIS	CE1-NE2	-5.60	1.26	1.32
1	A	44	ILE	C-O	5.59	1.30	1.24
1	B	67	HIS	CE1-NE2	-5.57	1.26	1.32
1	C	44	ILE	C-O	5.57	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	ILE	C-O	5.55	1.30	1.24
1	A	67	HIS	C-O	5.55	1.31	1.24
1	B	67	HIS	C-O	5.53	1.31	1.24
1	B	44	ILE	C-O	5.52	1.30	1.24
1	C	67	HIS	C-O	5.47	1.30	1.24
1	D	67	HIS	C-O	5.43	1.30	1.24
1	B	138	ASN	N-CA	5.30	1.53	1.45
1	A	138	ASN	N-CA	5.22	1.53	1.45
1	C	138	ASN	N-CA	5.22	1.53	1.45
1	C	137	THR	CA-CB	5.21	1.61	1.53
1	D	138	ASN	N-CA	5.19	1.53	1.45
1	D	137	THR	CA-CB	5.18	1.61	1.53
1	A	137	THR	CA-CB	5.16	1.61	1.53
1	B	137	THR	CA-CB	5.14	1.61	1.53
1	A	279	LEU	N-CA	5.04	1.52	1.46
1	B	279	LEU	N-CA	5.01	1.52	1.46
1	D	279	LEU	N-CA	5.01	1.52	1.46
1	A	283	ARG	C-O	5.00	1.29	1.23

All (885) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	ILE	CA-C-N	22.97	158.12	122.29
1	D	211	ILE	C-N-CA	22.97	158.12	122.29
1	B	211	ILE	CA-C-N	22.94	158.08	122.29
1	B	211	ILE	C-N-CA	22.94	158.08	122.29
1	C	211	ILE	CA-C-N	22.93	158.05	122.29
1	C	211	ILE	C-N-CA	22.93	158.05	122.29
1	A	211	ILE	CA-C-N	22.92	158.04	122.29
1	A	211	ILE	C-N-CA	22.92	158.04	122.29
1	A	111	ASP	CA-CB-CG	22.01	134.61	112.60
1	B	111	ASP	CA-CB-CG	22.01	134.61	112.60
1	C	111	ASP	CA-CB-CG	21.98	134.58	112.60
1	D	111	ASP	CA-CB-CG	21.95	134.55	112.60
1	A	211	ILE	CA-C-O	13.72	137.93	120.78
1	D	211	ILE	CA-C-O	13.71	137.91	120.78
1	C	211	ILE	CA-C-O	13.70	137.90	120.78
1	B	211	ILE	CA-C-O	13.69	137.90	120.78
1	C	286	TYR	CA-C-O	-12.68	106.15	121.36
1	B	286	TYR	CA-C-O	-12.65	106.18	121.36
1	D	286	TYR	CA-C-O	-12.65	106.18	121.36
1	A	286	TYR	CA-C-O	-12.62	106.22	121.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	ASN	CA-CB-CG	12.48	125.08	112.60
1	B	296	ASN	CA-CB-CG	12.47	125.07	112.60
1	A	296	ASN	CA-CB-CG	12.46	125.06	112.60
1	D	296	ASN	CA-CB-CG	12.41	125.01	112.60
1	D	276	LEU	CA-C-N	12.21	136.64	120.28
1	D	276	LEU	C-N-CA	12.21	136.64	120.28
1	B	276	LEU	CA-C-N	12.19	136.61	120.28
1	B	276	LEU	C-N-CA	12.19	136.61	120.28
1	A	276	LEU	CA-C-N	12.16	136.58	120.28
1	A	276	LEU	C-N-CA	12.16	136.58	120.28
1	C	276	LEU	CA-C-N	12.16	136.57	120.28
1	C	276	LEU	C-N-CA	12.16	136.57	120.28
1	A	166	ASP	CA-C-N	11.63	136.31	120.38
1	A	166	ASP	C-N-CA	11.63	136.31	120.38
1	C	166	ASP	CA-C-N	11.62	136.30	120.38
1	C	166	ASP	C-N-CA	11.62	136.30	120.38
1	B	166	ASP	CA-C-N	11.59	136.26	120.38
1	B	166	ASP	C-N-CA	11.59	136.26	120.38
1	D	166	ASP	CA-C-N	11.58	136.25	120.38
1	D	166	ASP	C-N-CA	11.58	136.25	120.38
1	D	211	ILE	O-C-N	-11.38	108.35	122.57
1	C	211	ILE	O-C-N	-11.37	108.36	122.57
1	A	211	ILE	O-C-N	-11.36	108.38	122.57
1	B	211	ILE	O-C-N	-11.36	108.38	122.57
1	A	276	LEU	CA-C-O	11.25	133.54	120.49
1	B	276	LEU	CA-C-O	11.23	133.52	120.49
1	D	276	LEU	CA-C-O	11.23	133.52	120.49
1	C	276	LEU	CA-C-O	11.23	133.52	120.49
1	C	78	ILE	CA-C-O	-10.85	110.61	121.67
1	D	78	ILE	CA-C-O	-10.78	110.68	121.67
1	B	78	ILE	CA-C-O	-10.76	110.69	121.67
1	A	78	ILE	CA-C-O	-10.76	110.70	121.67
1	B	260	ARG	CD-NE-CZ	-10.37	109.88	124.40
1	A	260	ARG	CD-NE-CZ	-10.34	109.93	124.40
1	C	260	ARG	CD-NE-CZ	-10.32	109.95	124.40
1	D	260	ARG	CD-NE-CZ	-10.32	109.95	124.40
1	D	118	ARG	NE-CZ-NH1	10.15	131.65	121.50
1	A	50	LEU	CA-C-N	10.09	136.98	123.06
1	A	50	LEU	C-N-CA	10.09	136.98	123.06
1	B	50	LEU	CA-C-N	10.09	136.98	123.06
1	B	50	LEU	C-N-CA	10.09	136.98	123.06
1	C	118	ARG	NE-CZ-NH1	10.08	131.58	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	NE-CZ-NH1	10.07	131.57	121.50
1	A	118	ARG	NE-CZ-NH1	10.06	131.56	121.50
1	C	50	LEU	CA-C-N	10.05	136.93	123.06
1	C	50	LEU	C-N-CA	10.05	136.93	123.06
1	D	50	LEU	CA-C-N	10.01	136.88	123.06
1	D	50	LEU	C-N-CA	10.01	136.88	123.06
1	C	282	GLU	CA-C-O	-9.97	109.79	121.46
1	D	282	GLU	CA-C-O	-9.95	109.82	121.46
1	B	282	GLU	CA-C-O	-9.94	109.83	121.46
1	A	282	GLU	CA-C-O	-9.91	109.86	121.46
1	D	272	VAL	CA-C-N	9.61	137.73	123.12
1	D	272	VAL	C-N-CA	9.61	137.73	123.12
1	C	272	VAL	CA-C-N	9.61	137.72	123.12
1	C	272	VAL	C-N-CA	9.61	137.72	123.12
1	A	272	VAL	CA-C-N	9.59	137.69	123.12
1	A	272	VAL	C-N-CA	9.59	137.69	123.12
1	B	272	VAL	CA-C-N	9.57	137.67	123.12
1	B	272	VAL	C-N-CA	9.57	137.67	123.12
1	A	170	PHE	O-C-N	9.56	133.19	122.11
1	C	170	PHE	O-C-N	9.52	133.16	122.11
1	B	170	PHE	O-C-N	9.52	133.15	122.11
1	D	170	PHE	O-C-N	9.51	133.15	122.11
1	C	260	ARG	NE-CZ-NH1	-9.50	112.00	121.50
1	D	122	GLU	CB-CG-CD	9.46	128.69	112.60
1	A	260	ARG	NE-CZ-NH1	-9.45	112.05	121.50
1	B	122	GLU	CB-CG-CD	9.45	128.67	112.60
1	C	170	PHE	CA-CB-CG	9.44	123.24	113.80
1	D	260	ARG	NE-CZ-NH1	-9.44	112.06	121.50
1	C	122	GLU	CB-CG-CD	9.44	128.64	112.60
1	A	122	GLU	CB-CG-CD	9.43	128.63	112.60
1	B	170	PHE	CA-CB-CG	9.43	123.23	113.80
1	B	260	ARG	NE-CZ-NH1	-9.43	112.07	121.50
1	A	170	PHE	CA-CB-CG	9.39	123.19	113.80
1	D	170	PHE	CA-CB-CG	9.38	123.18	113.80
1	B	286	TYR	O-C-N	9.37	133.55	123.06
1	D	286	TYR	O-C-N	9.36	133.54	123.06
1	C	286	TYR	O-C-N	9.35	133.53	123.06
1	A	286	TYR	O-C-N	9.30	133.48	123.06
1	D	203	GLN	CB-CG-CD	9.21	128.26	112.60
1	C	203	GLN	CB-CG-CD	9.21	128.26	112.60
1	B	203	GLN	CB-CG-CD	9.19	128.22	112.60
1	A	203	GLN	CB-CG-CD	9.17	128.19	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	ASP	CA-CB-CG	-9.13	103.47	112.60
1	C	64	ASP	CA-CB-CG	-9.09	103.51	112.60
1	D	300	GLU	CB-CG-CD	9.08	128.04	112.60
1	C	300	GLU	CB-CG-CD	9.08	128.03	112.60
1	A	300	GLU	CB-CG-CD	9.07	128.02	112.60
1	A	64	ASP	CA-CB-CG	-9.06	103.54	112.60
1	B	300	GLU	CB-CG-CD	9.06	128.01	112.60
1	D	64	ASP	CA-CB-CG	-9.06	103.54	112.60
1	B	22	ARG	CD-NE-CZ	-8.97	111.85	124.40
1	A	22	ARG	CD-NE-CZ	-8.96	111.86	124.40
1	D	22	ARG	CD-NE-CZ	-8.95	111.87	124.40
1	C	22	ARG	CD-NE-CZ	-8.94	111.89	124.40
1	D	266	GLU	CB-CG-CD	8.76	127.49	112.60
1	B	130	GLN	CA-C-O	-8.74	109.64	119.78
1	B	266	GLU	CB-CG-CD	8.74	127.46	112.60
1	A	266	GLU	CB-CG-CD	8.73	127.44	112.60
1	C	266	GLU	CB-CG-CD	8.73	127.44	112.60
1	C	130	GLN	CA-C-O	-8.72	109.66	119.78
1	A	130	GLN	CA-C-O	-8.69	109.69	119.78
1	D	130	GLN	CA-C-O	-8.66	109.73	119.78
1	D	140	VAL	N-CA-C	8.62	119.41	110.36
1	A	140	VAL	N-CA-C	8.61	119.40	110.36
1	C	140	VAL	N-CA-C	8.57	119.36	110.36
1	B	140	VAL	N-CA-C	8.54	119.32	110.36
1	A	76	VAL	CB-CA-C	8.50	124.30	110.69
1	C	76	VAL	CB-CA-C	8.49	124.27	110.69
1	B	76	VAL	CB-CA-C	8.48	124.26	110.69
1	D	76	VAL	CB-CA-C	8.45	124.21	110.69
1	C	307	ASN	N-CA-CB	-8.44	98.77	110.25
1	D	307	ASN	N-CA-CB	-8.44	98.78	110.25
1	B	307	ASN	N-CA-CB	-8.41	98.81	110.25
1	A	307	ASN	N-CA-CB	-8.41	98.82	110.25
1	D	257	ARG	CD-NE-CZ	8.36	136.10	124.40
1	A	179	SER	N-CA-CB	-8.33	104.67	114.17
1	A	257	ARG	CD-NE-CZ	8.33	136.06	124.40
1	B	179	SER	N-CA-CB	-8.33	104.68	114.17
1	B	257	ARG	CD-NE-CZ	8.32	136.05	124.40
1	C	257	ARG	CD-NE-CZ	8.32	136.04	124.40
1	C	179	SER	N-CA-CB	-8.31	104.69	114.17
1	D	179	SER	N-CA-CB	-8.31	104.70	114.17
1	B	235	ASP	CA-CB-CG	-8.15	104.45	112.60
1	C	235	ASP	CA-CB-CG	-8.14	104.46	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ASP	CA-CB-CG	-8.13	104.47	112.60
1	D	235	ASP	CA-CB-CG	-8.12	104.48	112.60
1	A	37	PHE	CA-CB-CG	8.11	121.91	113.80
1	C	111	ASP	N-CA-CB	8.10	122.47	110.33
1	D	111	ASP	N-CA-CB	8.09	122.47	110.33
1	D	54	ASN	CA-C-O	-8.09	113.07	122.37
1	B	111	ASP	N-CA-CB	8.09	122.46	110.33
1	C	54	ASN	CA-C-O	-8.08	113.08	122.37
1	A	111	ASP	N-CA-CB	8.08	122.45	110.33
1	D	37	PHE	CA-CB-CG	8.07	121.87	113.80
1	B	29	GLY	N-CA-C	-8.04	101.10	112.60
1	C	37	PHE	CA-CB-CG	8.04	121.84	113.80
1	D	29	GLY	N-CA-C	-8.04	101.09	112.60
1	B	37	PHE	CA-CB-CG	8.03	121.83	113.80
1	B	54	ASN	CA-C-O	-8.03	113.14	122.37
1	A	29	GLY	N-CA-C	-8.02	101.13	112.60
1	C	29	GLY	N-CA-C	-8.02	101.14	112.60
1	A	54	ASN	CA-C-O	-8.01	113.16	122.37
1	D	78	ILE	N-CA-C	-7.96	97.19	108.80
1	B	78	ILE	N-CA-C	-7.94	97.21	108.80
1	A	78	ILE	N-CA-C	-7.93	97.22	108.80
1	B	279	LEU	CA-CB-CG	7.93	144.07	116.30
1	D	279	LEU	CA-CB-CG	7.93	144.06	116.30
1	C	78	ILE	N-CA-C	-7.93	97.22	108.80
1	A	279	LEU	CA-CB-CG	7.93	144.04	116.30
1	C	279	LEU	CA-CB-CG	7.92	144.04	116.30
1	C	171	ARG	CD-NE-CZ	-7.85	113.41	124.40
1	D	171	ARG	CD-NE-CZ	-7.80	113.47	124.40
1	A	228	ARG	CD-NE-CZ	-7.80	113.48	124.40
1	D	228	ARG	CD-NE-CZ	-7.80	113.49	124.40
1	A	171	ARG	CD-NE-CZ	-7.79	113.49	124.40
1	B	228	ARG	CD-NE-CZ	-7.79	113.50	124.40
1	C	228	ARG	CD-NE-CZ	-7.78	113.51	124.40
1	B	171	ARG	CD-NE-CZ	-7.78	113.51	124.40
1	A	316	HIS	CA-C-N	7.77	130.55	120.44
1	A	316	HIS	C-N-CA	7.77	130.55	120.44
1	B	316	HIS	CA-C-N	7.77	130.54	120.44
1	B	316	HIS	C-N-CA	7.77	130.54	120.44
1	D	316	HIS	CA-C-N	7.74	130.50	120.44
1	D	316	HIS	C-N-CA	7.74	130.50	120.44
1	C	74	LYS	N-CA-C	7.73	126.89	109.81
1	D	74	LYS	N-CA-C	7.71	126.85	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	HIS	CA-C-N	7.71	130.46	120.44
1	C	316	HIS	C-N-CA	7.71	130.46	120.44
1	A	74	LYS	N-CA-C	7.71	126.84	109.81
1	B	74	LYS	N-CA-C	7.69	126.80	109.81
1	C	116	ILE	CA-C-N	7.61	130.81	120.38
1	C	116	ILE	C-N-CA	7.61	130.81	120.38
1	A	315	HIS	CA-C-N	7.61	130.47	120.28
1	A	315	HIS	C-N-CA	7.61	130.47	120.28
1	A	192	GLU	O-C-N	7.59	132.26	122.93
1	B	192	GLU	O-C-N	7.59	132.26	122.93
1	B	116	ILE	CA-C-N	7.58	130.77	120.38
1	B	116	ILE	C-N-CA	7.58	130.77	120.38
1	B	315	HIS	CA-C-N	7.58	130.44	120.28
1	B	315	HIS	C-N-CA	7.58	130.44	120.28
1	C	192	GLU	O-C-N	7.58	132.25	122.93
1	D	116	ILE	CA-C-N	7.58	130.76	120.38
1	D	116	ILE	C-N-CA	7.58	130.76	120.38
1	D	265	ASN	CA-CB-CG	7.57	120.17	112.60
1	A	116	ILE	CA-C-N	7.57	130.75	120.38
1	A	116	ILE	C-N-CA	7.57	130.75	120.38
1	A	279	LEU	CB-CA-C	7.57	122.32	109.53
1	A	265	ASN	CA-CB-CG	7.57	120.17	112.60
1	B	279	LEU	CB-CA-C	7.56	122.31	109.53
1	D	315	HIS	CA-C-N	7.56	130.41	120.28
1	D	315	HIS	C-N-CA	7.56	130.41	120.28
1	D	192	GLU	O-C-N	7.55	132.21	122.93
1	C	279	LEU	CB-CA-C	7.54	122.27	109.53
1	C	265	ASN	CA-CB-CG	7.53	120.13	112.60
1	D	279	LEU	CB-CA-C	7.53	122.26	109.53
1	C	315	HIS	CA-C-N	7.52	130.36	120.28
1	C	315	HIS	C-N-CA	7.52	130.36	120.28
1	B	265	ASN	CA-CB-CG	7.51	120.11	112.60
1	D	47	GLU	CA-C-O	-7.46	112.31	120.36
1	C	254	GLY	CA-C-N	7.43	131.60	120.31
1	C	254	GLY	C-N-CA	7.43	131.60	120.31
1	B	47	GLU	CA-C-O	-7.43	112.34	120.36
1	A	47	GLU	CA-C-O	-7.42	112.34	120.36
1	B	254	GLY	CA-C-N	7.42	131.59	120.31
1	B	254	GLY	C-N-CA	7.42	131.59	120.31
1	C	47	GLU	CA-C-O	-7.42	112.35	120.36
1	D	254	GLY	CA-C-N	7.42	131.58	120.31
1	D	254	GLY	C-N-CA	7.42	131.58	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	GLY	CA-C-N	7.41	131.57	120.31
1	A	254	GLY	C-N-CA	7.41	131.57	120.31
1	A	214	LEU	CA-C-O	-7.34	112.77	120.99
1	B	55	GLU	CB-CG-CD	7.33	125.06	112.60
1	C	214	LEU	CA-C-O	-7.32	112.80	120.99
1	C	55	GLU	CB-CG-CD	7.31	125.03	112.60
1	A	55	GLU	CB-CG-CD	7.31	125.03	112.60
1	D	55	GLU	CB-CG-CD	7.30	125.02	112.60
1	B	214	LEU	CA-C-O	-7.29	112.82	120.99
1	D	214	LEU	CA-C-O	-7.28	112.83	120.99
1	B	138	ASN	CB-CA-C	7.26	120.01	109.11
1	C	138	ASN	CB-CA-C	7.26	120.00	109.11
1	D	138	ASN	CB-CA-C	7.24	119.97	109.11
1	A	138	ASN	CB-CA-C	7.23	119.95	109.11
1	A	90	ASP	CA-C-O	-7.16	112.90	120.63
1	A	269	ILE	O-C-N	7.14	131.32	122.32
1	B	269	ILE	O-C-N	7.14	131.32	122.32
1	D	269	ILE	O-C-N	7.14	131.31	122.32
1	B	239	GLN	CA-CB-CG	7.12	128.34	114.10
1	B	90	ASP	CA-C-O	-7.12	112.94	120.63
1	C	269	ILE	O-C-N	7.12	131.29	122.32
1	C	90	ASP	CA-C-O	-7.11	112.95	120.63
1	D	54	ASN	O-C-N	7.10	130.91	122.46
1	D	239	GLN	CA-CB-CG	7.10	128.30	114.10
1	D	90	ASP	CA-C-O	-7.09	112.98	120.63
1	B	70	VAL	CA-C-N	7.08	132.72	120.68
1	B	70	VAL	C-N-CA	7.08	132.72	120.68
1	C	239	GLN	CA-CB-CG	7.08	128.26	114.10
1	A	239	GLN	CA-CB-CG	7.08	128.25	114.10
1	C	70	VAL	CA-C-N	7.07	132.71	120.68
1	C	70	VAL	C-N-CA	7.07	132.71	120.68
1	D	70	VAL	CA-C-N	7.07	132.70	120.68
1	D	70	VAL	C-N-CA	7.07	132.70	120.68
1	C	54	ASN	O-C-N	7.06	130.87	122.46
1	A	70	VAL	CA-C-N	7.06	132.68	120.68
1	A	70	VAL	C-N-CA	7.06	132.68	120.68
1	B	54	ASN	O-C-N	7.05	130.84	122.46
1	A	203	GLN	CG-CD-NE2	7.04	126.96	116.40
1	B	203	GLN	CG-CD-NE2	7.03	126.94	116.40
1	D	317	SER	O-C-N	7.02	129.30	122.07
1	A	54	ASN	O-C-N	7.01	130.80	122.46
1	C	203	GLN	CG-CD-NE2	7.00	126.89	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	GLN	CG-CD-NE2	7.00	126.89	116.40
1	A	281	GLY	O-C-N	6.97	129.65	122.54
1	C	317	SER	O-C-N	6.97	129.25	122.07
1	B	317	SER	O-C-N	6.96	129.24	122.07
1	B	144	THR	CA-C-O	-6.96	113.04	120.42
1	A	317	SER	O-C-N	6.95	129.23	122.07
1	B	281	GLY	O-C-N	6.95	129.63	122.54
1	C	144	THR	CA-C-O	-6.95	113.05	120.42
1	D	281	GLY	O-C-N	6.95	129.63	122.54
1	A	144	THR	CA-C-O	-6.94	113.07	120.42
1	C	281	GLY	O-C-N	6.92	129.60	122.54
1	D	266	GLU	CA-CB-CG	6.91	127.93	114.10
1	B	266	GLU	CA-CB-CG	6.91	127.92	114.10
1	B	88	ASP	CA-CB-CG	-6.91	105.69	112.60
1	C	266	GLU	CA-CB-CG	6.91	127.91	114.10
1	D	144	THR	CA-C-O	-6.90	113.10	120.42
1	D	108	ASP	CA-C-O	6.90	129.05	120.15
1	A	266	GLU	CA-CB-CG	6.90	127.89	114.10
1	A	88	ASP	CA-CB-CG	-6.90	105.70	112.60
1	A	108	ASP	CA-C-O	6.89	129.04	120.15
1	C	88	ASP	CA-CB-CG	-6.89	105.71	112.60
1	D	88	ASP	CA-CB-CG	-6.89	105.71	112.60
1	C	108	ASP	CA-C-O	6.88	129.03	120.15
1	C	156	GLU	CB-CG-CD	6.86	124.27	112.60
1	B	108	ASP	CA-C-O	6.86	129.00	120.15
1	B	156	GLU	CB-CG-CD	6.85	124.25	112.60
1	A	156	GLU	CB-CG-CD	6.85	124.24	112.60
1	D	156	GLU	CB-CG-CD	6.83	124.22	112.60
1	D	176	GLU	CA-C-N	6.81	129.64	120.65
1	D	176	GLU	C-N-CA	6.81	129.64	120.65
1	A	176	GLU	CA-C-N	6.78	129.60	120.65
1	A	176	GLU	C-N-CA	6.78	129.60	120.65
1	B	176	GLU	CA-C-N	6.76	129.57	120.65
1	B	176	GLU	C-N-CA	6.76	129.57	120.65
1	C	176	GLU	CA-C-N	6.75	129.56	120.65
1	C	176	GLU	C-N-CA	6.75	129.56	120.65
1	C	230	PHE	CA-CB-CG	-6.75	107.05	113.80
1	D	230	PHE	CA-CB-CG	-6.74	107.06	113.80
1	A	230	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	197	GLU	CB-CG-CD	6.71	124.00	112.60
1	D	190	ILE	CA-C-O	-6.71	114.83	121.67
1	A	74	LYS	CB-CG-CD	6.70	126.72	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	LYS	CB-CG-CD	6.70	126.72	111.30
1	D	74	LYS	CB-CG-CD	6.70	126.72	111.30
1	B	197	GLU	CB-CG-CD	6.70	123.98	112.60
1	C	190	ILE	CA-C-O	-6.70	114.84	121.67
1	B	190	ILE	CA-C-O	-6.69	114.84	121.67
1	B	230	PHE	CA-CB-CG	-6.69	107.11	113.80
1	C	197	GLU	CB-CG-CD	6.69	123.97	112.60
1	A	190	ILE	CA-C-O	-6.68	114.85	121.67
1	C	74	LYS	CB-CG-CD	6.68	126.67	111.30
1	D	197	GLU	CB-CG-CD	6.68	123.96	112.60
1	A	22	ARG	NE-CZ-NH2	-6.65	113.21	119.20
1	A	296	ASN	CB-CG-ND2	6.63	126.34	116.40
1	B	296	ASN	CB-CG-ND2	6.61	126.31	116.40
1	D	296	ASN	CB-CG-ND2	6.61	126.31	116.40
1	B	22	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	D	22	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	C	156	GLU	N-CA-C	-6.57	105.30	113.38
1	D	293	ILE	CA-C-O	-6.57	114.58	121.93
1	D	156	GLU	N-CA-C	-6.56	105.31	113.38
1	C	293	ILE	CB-CA-C	6.56	120.56	111.38
1	A	293	ILE	CB-CA-C	6.55	120.56	111.38
1	B	195	ASP	O-C-N	6.55	129.07	122.12
1	C	296	ASN	CB-CG-ND2	6.55	126.23	116.40
1	A	293	ILE	CA-C-O	-6.55	114.59	121.93
1	C	293	ILE	CA-C-O	-6.55	114.59	121.93
1	D	195	ASP	O-C-N	6.55	129.06	122.12
1	B	293	ILE	CA-C-O	-6.55	114.60	121.93
1	C	22	ARG	NE-CZ-NH2	-6.55	113.31	119.20
1	C	142	ILE	O-C-N	6.55	130.41	121.90
1	A	156	GLU	N-CA-C	-6.54	105.33	113.38
1	D	293	ILE	CB-CA-C	6.54	120.53	111.38
1	B	293	ILE	CB-CA-C	6.53	120.52	111.38
1	C	108	ASP	N-CA-C	-6.52	105.21	112.57
1	A	142	ILE	O-C-N	6.51	130.37	121.90
1	B	156	GLU	N-CA-C	-6.51	105.38	113.38
1	A	195	ASP	O-C-N	6.50	129.01	122.12
1	B	142	ILE	O-C-N	6.49	130.34	121.90
1	B	108	ASP	N-CA-C	-6.49	105.24	112.57
1	D	142	ILE	O-C-N	6.49	130.33	121.90
1	B	30	PHE	O-C-N	6.48	128.83	122.09
1	C	195	ASP	O-C-N	6.48	128.99	122.12
1	C	300	GLU	CA-CB-CG	6.48	127.05	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PHE	O-C-N	6.47	128.81	122.09
1	D	300	GLU	CA-CB-CG	6.46	127.03	114.10
1	C	30	PHE	O-C-N	6.46	128.81	122.09
1	B	300	GLU	CA-CB-CG	6.46	127.01	114.10
1	A	300	GLU	CA-CB-CG	6.45	127.00	114.10
1	D	108	ASP	N-CA-C	-6.45	105.28	112.57
1	D	211	ILE	CB-CA-C	6.45	121.86	111.29
1	A	108	ASP	N-CA-C	-6.44	105.29	112.57
1	D	30	PHE	O-C-N	6.44	128.79	122.09
1	C	211	ILE	CB-CA-C	6.44	121.85	111.29
1	A	211	ILE	CB-CA-C	6.43	121.83	111.29
1	B	211	ILE	CB-CA-C	6.42	121.82	111.29
1	A	122	GLU	CA-CB-CG	6.39	126.89	114.10
1	D	122	GLU	CA-CB-CG	6.39	126.87	114.10
1	B	87	ARG	CA-C-O	6.38	129.64	120.51
1	B	122	GLU	CA-CB-CG	6.38	126.86	114.10
1	B	207	GLY	N-CA-C	-6.38	98.07	113.18
1	C	122	GLU	CA-CB-CG	6.37	126.85	114.10
1	A	207	GLY	N-CA-C	-6.37	98.08	113.18
1	D	141	ASP	N-CA-C	-6.37	104.39	111.71
1	C	207	GLY	N-CA-C	-6.36	98.11	113.18
1	B	84	ASP	CA-CB-CG	-6.36	106.25	112.60
1	C	92	VAL	CA-C-O	-6.36	113.78	120.39
1	C	87	ARG	CA-C-O	6.35	129.60	120.51
1	A	303	GLU	CB-CG-CD	6.35	123.40	112.60
1	A	87	ARG	CA-C-O	6.35	129.59	120.51
1	C	141	ASP	N-CA-C	-6.34	104.41	111.71
1	D	207	GLY	N-CA-C	-6.34	98.15	113.18
1	B	92	VAL	CA-C-O	-6.33	113.81	120.39
1	B	303	GLU	CB-CG-CD	6.33	123.36	112.60
1	D	87	ARG	CA-C-O	6.33	129.56	120.51
1	A	84	ASP	CA-CB-CG	-6.32	106.28	112.60
1	A	141	ASP	N-CA-C	-6.31	104.46	111.71
1	D	303	GLU	CB-CG-CD	6.31	123.32	112.60
1	C	303	GLU	CB-CG-CD	6.30	123.32	112.60
1	D	92	VAL	CA-C-O	-6.30	113.83	120.39
1	D	84	ASP	CA-CB-CG	-6.30	106.30	112.60
1	D	189	ILE	CA-CB-CG2	6.29	121.20	110.50
1	A	92	VAL	CA-C-O	-6.29	113.85	120.39
1	B	141	ASP	N-CA-C	-6.28	104.49	111.71
1	C	189	ILE	CA-CB-CG2	6.28	121.17	110.50
1	C	84	ASP	CA-CB-CG	-6.25	106.35	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	MET	O-C-N	6.24	126.29	121.23
1	A	189	ILE	CA-CB-CG2	6.24	121.11	110.50
1	B	189	ILE	CA-CB-CG2	6.23	121.09	110.50
1	A	209	MET	O-C-N	6.21	126.26	121.23
1	C	78	ILE	O-C-N	6.20	129.82	123.00
1	D	209	MET	O-C-N	6.20	126.25	121.23
1	B	209	MET	O-C-N	6.19	126.24	121.23
1	B	189	ILE	CB-CA-C	6.12	119.95	110.83
1	D	78	ILE	O-C-N	6.12	129.73	123.00
1	B	291	ALA	CA-C-O	-6.12	114.48	121.58
1	A	189	ILE	CB-CA-C	6.11	119.94	110.83
1	B	78	ILE	O-C-N	6.10	129.71	123.00
1	A	291	ALA	CA-C-O	-6.10	114.50	121.58
1	C	164	ILE	CB-CG1-CD1	-6.10	100.99	113.80
1	D	291	ALA	CA-C-O	-6.10	114.51	121.58
1	C	291	ALA	CA-C-O	-6.10	114.51	121.58
1	A	78	ILE	O-C-N	6.09	129.70	123.00
1	D	125	MET	N-CA-C	-6.09	104.72	111.36
1	A	164	ILE	CB-CG1-CD1	-6.09	101.02	113.80
1	D	164	ILE	CB-CG1-CD1	-6.09	101.02	113.80
1	B	166	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	232	ASN	CA-CB-CG	-6.08	106.52	112.60
1	D	189	ILE	CB-CA-C	6.08	119.89	110.83
1	A	232	ASN	CA-CB-CG	-6.08	106.52	112.60
1	C	189	ILE	CB-CA-C	6.08	119.89	110.83
1	C	57	LYS	CA-C-O	-6.08	113.98	120.42
1	B	227	GLU	N-CA-C	-6.07	105.92	113.15
1	D	169	ARG	N-CA-C	-6.07	104.78	111.82
1	A	166	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	227	GLU	N-CA-C	-6.07	105.93	113.15
1	C	144	THR	O-C-N	6.07	129.07	122.15
1	C	125	MET	N-CA-C	-6.06	104.75	111.36
1	A	118	ARG	CD-NE-CZ	6.06	132.89	124.40
1	B	164	ILE	CB-CG1-CD1	-6.06	101.07	113.80
1	C	49	VAL	CA-C-O	-6.06	114.65	121.98
1	D	57	LYS	CA-C-O	-6.06	114.00	120.42
1	C	118	ARG	CD-NE-CZ	6.06	132.88	124.40
1	D	227	GLU	N-CA-C	-6.05	105.95	113.15
1	A	144	THR	O-C-N	6.05	129.05	122.15
1	C	166	ASP	CA-CB-CG	6.05	118.65	112.60
1	C	169	ARG	N-CA-C	-6.05	104.81	111.82
1	A	125	MET	N-CA-C	-6.04	104.77	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	CD-NE-CZ	6.04	132.86	124.40
1	B	49	VAL	CA-C-O	-6.04	114.67	121.98
1	B	283	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	B	144	THR	O-C-N	6.03	129.03	122.15
1	C	232	ASN	CA-CB-CG	-6.03	106.57	112.60
1	A	203	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	B	169	ARG	N-CA-C	-6.03	104.83	111.82
1	D	118	ARG	CD-NE-CZ	6.02	132.83	124.40
1	D	232	ASN	CA-CB-CG	-6.02	106.58	112.60
1	C	203	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	D	166	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	203	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	D	295	ARG	CD-NE-CZ	-6.01	115.98	124.40
1	A	57	LYS	CA-C-O	-6.01	114.05	120.42
1	A	49	VAL	CA-C-O	-6.01	114.71	121.98
1	B	125	MET	N-CA-C	-6.01	104.81	111.36
1	C	227	GLU	N-CA-C	-6.01	106.00	113.15
1	A	169	ARG	N-CA-C	-6.00	104.86	111.82
1	D	49	VAL	CA-C-O	-6.00	114.71	121.98
1	C	295	ARG	CD-NE-CZ	-6.00	116.00	124.40
1	A	283	ARG	NE-CZ-NH1	6.00	127.50	121.50
1	D	144	THR	O-C-N	6.00	128.99	122.15
1	B	57	LYS	CA-C-O	-5.99	114.07	120.42
1	C	192	GLU	N-CA-CB	5.99	118.77	109.85
1	B	112	LYS	CA-C-N	5.98	128.30	120.28
1	B	112	LYS	C-N-CA	5.98	128.30	120.28
1	D	203	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	D	283	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	D	192	GLU	N-CA-CB	5.98	118.75	109.85
1	A	295	ARG	CD-NE-CZ	-5.97	116.03	124.40
1	C	112	LYS	CA-C-N	5.97	128.28	120.28
1	C	112	LYS	C-N-CA	5.97	128.28	120.28
1	A	112	LYS	CA-C-N	5.97	128.28	120.28
1	A	112	LYS	C-N-CA	5.97	128.28	120.28
1	C	283	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	A	300	GLU	CA-C-O	-5.96	114.08	120.75
1	A	136	ALA	CA-C-N	5.96	129.94	121.42
1	A	136	ALA	C-N-CA	5.96	129.94	121.42
1	B	286	TYR	N-CA-C	-5.96	100.84	110.32
1	B	295	ARG	CD-NE-CZ	-5.96	116.06	124.40
1	B	300	GLU	CA-C-O	-5.96	114.08	120.75
1	A	192	GLU	N-CA-CB	5.96	118.73	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	GLU	N-CA-CB	5.95	118.72	109.85
1	A	286	TYR	N-CA-C	-5.95	100.86	110.32
1	D	112	LYS	CA-C-N	5.94	128.24	120.28
1	D	112	LYS	C-N-CA	5.94	128.24	120.28
1	C	300	GLU	CA-C-O	-5.94	114.10	120.75
1	D	300	GLU	CA-C-O	-5.93	114.11	120.75
1	D	136	ALA	CA-C-N	5.93	129.90	121.42
1	D	136	ALA	C-N-CA	5.93	129.90	121.42
1	B	136	ALA	CA-C-N	5.92	129.89	121.42
1	B	136	ALA	C-N-CA	5.92	129.89	121.42
1	C	136	ALA	CA-C-N	5.92	129.88	121.42
1	C	136	ALA	C-N-CA	5.92	129.88	121.42
1	D	286	TYR	N-CA-C	-5.92	100.92	110.32
1	C	286	TYR	N-CA-C	-5.91	100.93	110.32
1	C	151	SER	CA-C-O	5.89	126.78	120.24
1	B	151	SER	CA-C-O	5.88	126.77	120.24
1	A	182	PRO	CA-C-N	5.88	130.54	120.72
1	A	182	PRO	C-N-CA	5.88	130.54	120.72
1	A	308	ASP	O-C-N	5.87	128.14	122.03
1	B	308	ASP	O-C-N	5.87	128.13	122.03
1	D	182	PRO	CA-C-N	5.87	130.52	120.72
1	D	182	PRO	C-N-CA	5.87	130.52	120.72
1	C	182	PRO	CA-C-N	5.87	130.52	120.72
1	C	182	PRO	C-N-CA	5.87	130.52	120.72
1	A	306	LEU	CA-C-N	5.86	131.49	121.29
1	A	306	LEU	C-N-CA	5.86	131.49	121.29
1	C	280	TYR	N-CA-C	-5.86	104.81	113.72
1	D	280	TYR	N-CA-C	-5.86	104.81	113.72
1	B	306	LEU	CA-C-N	5.86	131.49	121.29
1	B	306	LEU	C-N-CA	5.86	131.49	121.29
1	B	280	TYR	N-CA-C	-5.86	104.82	113.72
1	A	151	SER	CA-C-O	5.85	126.74	120.24
1	B	182	PRO	CA-C-N	5.85	130.49	120.72
1	B	182	PRO	C-N-CA	5.85	130.49	120.72
1	A	280	TYR	N-CA-C	-5.85	104.83	113.72
1	C	89	ALA	CA-C-O	-5.85	114.32	120.58
1	C	147	THR	N-CA-C	-5.85	104.86	112.23
1	C	313	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	C	306	LEU	CA-C-N	5.85	131.47	121.29
1	C	306	LEU	C-N-CA	5.85	131.47	121.29
1	A	50	LEU	N-CA-CB	-5.83	101.26	110.77
1	B	89	ALA	CA-C-O	-5.83	114.34	120.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	ILE	CA-C-O	-5.83	115.05	121.29
1	D	147	THR	N-CA-C	-5.83	104.89	112.23
1	D	306	LEU	CA-C-N	5.83	131.43	121.29
1	D	306	LEU	C-N-CA	5.83	131.43	121.29
1	D	313	ARG	CD-NE-CZ	-5.83	116.24	124.40
1	C	308	ASP	O-C-N	5.82	128.09	122.03
1	D	151	SER	CA-C-O	5.82	126.70	120.24
1	D	89	ALA	CA-C-O	-5.82	114.35	120.58
1	A	59	ILE	CA-C-O	-5.82	115.06	121.29
1	B	283	ARG	NH1-CZ-NH2	-5.82	111.74	119.30
1	A	89	ALA	CA-C-O	-5.82	114.36	120.58
1	B	147	THR	N-CA-C	-5.82	104.90	112.23
1	B	313	ARG	CD-NE-CZ	-5.81	116.26	124.40
1	C	283	ARG	NH1-CZ-NH2	-5.81	111.75	119.30
1	D	283	ARG	NH1-CZ-NH2	-5.81	111.75	119.30
1	B	50	LEU	N-CA-CB	-5.80	101.31	110.77
1	C	251	ILE	CA-CB-CG2	5.80	120.36	110.50
1	D	251	ILE	CA-CB-CG2	5.80	120.36	110.50
1	A	147	THR	N-CA-C	-5.79	104.93	112.23
1	C	50	LEU	N-CA-CB	-5.79	101.33	110.77
1	A	283	ARG	NH1-CZ-NH2	-5.79	111.77	119.30
1	A	22	ARG	NH1-CZ-NH2	5.78	126.81	119.30
1	B	59	ILE	CA-C-O	-5.77	115.11	121.29
1	D	50	LEU	N-CA-CB	-5.77	101.36	110.77
1	C	59	ILE	CA-C-O	-5.77	115.12	121.29
1	A	313	ARG	CD-NE-CZ	-5.76	116.33	124.40
1	A	251	ILE	CA-CB-CG2	5.76	120.29	110.50
1	B	251	ILE	CA-CB-CG2	5.75	120.28	110.50
1	D	308	ASP	O-C-N	5.75	128.01	122.03
1	A	251	ILE	CA-C-O	-5.73	115.45	121.41
1	C	251	ILE	CA-C-O	-5.73	115.45	121.41
1	D	74	LYS	CA-CB-CG	5.72	125.55	114.10
1	C	190	ILE	CB-CA-C	5.72	119.29	110.82
1	D	190	ILE	CB-CA-C	5.72	119.29	110.82
1	A	266	GLU	N-CA-CB	5.72	119.03	110.22
1	B	22	ARG	NH1-CZ-NH2	5.72	126.73	119.30
1	B	74	LYS	CA-CB-CG	5.72	125.54	114.10
1	A	118	ARG	O-C-N	5.72	128.91	122.22
1	C	167	THR	CA-CB-CG2	5.72	120.22	110.50
1	D	267	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	266	GLU	N-CA-CB	5.71	119.02	110.22
1	A	74	LYS	CA-CB-CG	5.71	125.52	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	ILE	N-CA-C	-5.71	104.80	110.62
1	C	114	ILE	N-CA-C	-5.71	104.80	110.62
1	D	114	ILE	N-CA-C	-5.71	104.80	110.62
1	B	190	ILE	CB-CA-C	5.71	119.27	110.82
1	C	74	LYS	CA-CB-CG	5.71	125.51	114.10
1	C	266	GLU	N-CA-CB	5.70	119.00	110.22
1	B	251	ILE	CA-C-O	-5.70	115.48	121.41
1	A	190	ILE	CB-CA-C	5.70	119.25	110.82
1	A	167	THR	CA-CB-CG2	5.68	120.16	110.50
1	A	267	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	B	267	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	D	266	GLU	N-CA-CB	5.68	118.97	110.22
1	D	22	ARG	NH1-CZ-NH2	5.68	126.69	119.30
1	D	167	THR	CA-CB-CG2	5.68	120.16	110.50
1	C	267	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	B	167	THR	CA-CB-CG2	5.68	120.15	110.50
1	D	251	ILE	CA-C-O	-5.68	115.51	121.41
1	A	266	GLU	CA-C-O	-5.67	113.69	120.10
1	B	266	GLU	CA-C-O	-5.67	113.69	120.10
1	C	118	ARG	O-C-N	5.67	128.86	122.22
1	C	160	GLY	CA-C-O	5.67	128.69	121.94
1	D	118	ARG	O-C-N	5.67	128.85	122.22
1	B	160	GLY	CA-C-O	5.67	128.68	121.94
1	B	171	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	C	22	ARG	NH1-CZ-NH2	5.67	126.66	119.30
1	B	118	ARG	O-C-N	5.66	128.84	122.22
1	A	160	GLY	CA-C-O	5.66	128.67	121.94
1	C	29	GLY	CA-C-O	-5.65	116.14	121.90
1	A	29	GLY	CA-C-O	-5.65	116.14	121.90
1	D	212	ARG	CA-C-O	5.65	125.85	119.18
1	C	266	GLU	CA-C-O	-5.65	113.72	120.10
1	A	171	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	29	GLY	CA-C-O	-5.64	116.15	121.90
1	A	114	ILE	N-CA-C	-5.63	104.88	110.62
1	C	212	ARG	CA-C-O	5.63	125.83	119.18
1	A	212	ARG	CA-C-O	5.63	125.83	119.18
1	D	266	GLU	CA-C-O	-5.62	113.75	120.10
1	D	160	GLY	CA-C-O	5.61	128.61	121.94
1	C	110	VAL	CB-CA-C	5.61	120.23	112.05
1	A	280	TYR	CA-C-O	5.60	126.61	119.16
1	B	212	ARG	CA-C-O	5.59	125.78	119.18
1	A	110	VAL	CB-CA-C	5.59	120.21	112.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	VAL	CB-CA-C	5.59	120.21	112.05
1	D	316	HIS	CA-C-O	5.58	126.47	120.55
1	B	208	VAL	N-CA-CB	-5.58	105.11	112.36
1	D	171	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	C	171	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	B	170	PHE	N-CA-C	-5.58	104.05	111.24
1	D	29	GLY	CA-C-O	-5.58	116.21	121.90
1	A	208	VAL	N-CA-CB	-5.57	105.11	112.36
1	B	110	VAL	CB-CA-C	5.57	120.18	112.05
1	C	316	HIS	CA-C-O	5.56	126.45	120.55
1	B	280	TYR	CA-C-O	5.55	126.54	119.16
1	C	121	VAL	O-C-N	5.55	127.65	121.94
1	C	280	TYR	CA-C-O	5.54	126.53	119.16
1	C	208	VAL	N-CA-CB	-5.54	105.15	112.36
1	A	144	THR	N-CA-CB	5.54	118.36	110.16
1	B	144	THR	N-CA-CB	5.54	118.36	110.16
1	D	111	ASP	N-CA-C	-5.54	105.65	112.90
1	D	77	ASP	O-C-N	5.54	130.11	123.36
1	D	121	VAL	O-C-N	5.53	127.64	121.94
1	D	280	TYR	CA-C-O	5.53	126.52	119.16
1	A	170	PHE	N-CA-C	-5.53	104.11	111.24
1	B	169	ARG	CD-NE-CZ	-5.53	116.67	124.40
1	A	121	VAL	O-C-N	5.52	127.63	121.94
1	C	144	THR	N-CA-CB	5.52	118.33	110.16
1	D	144	THR	N-CA-CB	5.52	118.33	110.16
1	A	169	ARG	CD-NE-CZ	-5.52	116.68	124.40
1	C	77	ASP	O-C-N	5.52	130.09	123.36
1	D	208	VAL	N-CA-CB	-5.52	105.19	112.36
1	D	170	PHE	N-CA-C	-5.51	104.13	111.24
1	B	111	ASP	N-CA-C	-5.51	105.69	112.90
1	A	111	ASP	N-CA-C	-5.50	105.69	112.90
1	B	121	VAL	O-C-N	5.50	127.61	121.94
1	C	169	ARG	CD-NE-CZ	-5.50	116.70	124.40
1	A	316	HIS	CA-C-O	5.50	126.38	120.55
1	C	170	PHE	N-CA-C	-5.50	104.15	111.24
1	A	77	ASP	O-C-N	5.49	130.06	123.36
1	A	170	PHE	CA-C-O	-5.49	115.04	120.80
1	B	77	ASP	O-C-N	5.49	130.05	123.36
1	C	176	GLU	CB-CG-CD	5.49	121.93	112.60
1	D	169	ARG	CD-NE-CZ	-5.48	116.72	124.40
1	B	316	HIS	CA-C-O	5.48	126.36	120.55
1	C	115	ALA	N-CA-CB	-5.47	101.92	109.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASP	N-CA-C	-5.47	105.73	112.90
1	D	170	PHE	CA-C-O	-5.46	115.06	120.80
1	B	115	ALA	N-CA-CB	-5.46	101.94	109.91
1	B	172	PHE	CA-C-O	-5.46	112.70	120.51
1	A	329	PHE	CA-CB-CG	-5.46	108.34	113.80
1	D	176	GLU	CB-CG-CD	5.45	121.87	112.60
1	A	115	ALA	N-CA-CB	-5.45	101.96	109.91
1	A	172	PHE	CA-C-O	-5.45	112.72	120.51
1	B	170	PHE	CA-C-O	-5.44	115.08	120.80
1	B	176	GLU	CB-CG-CD	5.44	121.85	112.60
1	D	115	ALA	N-CA-CB	-5.44	101.97	109.91
1	C	142	ILE	CA-C-O	-5.44	114.49	120.96
1	C	170	PHE	CA-C-O	-5.44	115.09	120.80
1	A	176	GLU	CB-CG-CD	5.43	121.84	112.60
1	B	58	ALA	N-CA-C	5.43	117.20	111.28
1	B	237	ALA	O-C-N	5.43	127.68	122.03
1	A	58	ALA	N-CA-C	5.43	117.19	111.28
1	B	142	ILE	CA-C-O	-5.43	114.50	120.96
1	B	301	VAL	CA-CB-CG1	5.42	119.62	110.40
1	C	172	PHE	CA-C-O	-5.42	112.75	120.51
1	A	226	LEU	CA-C-O	-5.42	113.43	119.67
1	C	237	ALA	O-C-N	5.42	127.67	122.03
1	D	172	PHE	CA-C-O	-5.42	112.76	120.51
1	A	301	VAL	CA-CB-CG1	5.42	119.61	110.40
1	D	237	ALA	O-C-N	5.42	127.66	122.03
1	C	140	VAL	CA-C-O	-5.41	115.64	121.27
1	B	329	PHE	CA-CB-CG	-5.41	108.39	113.80
1	C	85	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	142	ILE	CA-C-O	-5.41	114.53	120.96
1	A	237	ALA	O-C-N	5.41	127.65	122.03
1	D	161	SER	CB-CA-C	5.40	119.86	110.68
1	C	161	SER	CB-CA-C	5.40	119.86	110.68
1	B	140	VAL	CA-C-O	-5.39	115.66	121.27
1	D	329	PHE	CA-CB-CG	-5.39	108.41	113.80
1	D	142	ILE	CA-C-O	-5.39	114.54	120.96
1	A	85	ASP	CA-CB-CG	-5.39	107.21	112.60
1	A	253	MET	N-CA-C	-5.39	105.30	111.07
1	B	253	MET	N-CA-C	-5.39	105.30	111.07
1	B	269	ILE	N-CA-CB	5.39	117.50	111.89
1	C	58	ALA	N-CA-C	5.39	117.15	111.28
1	A	140	VAL	CA-C-O	-5.39	115.67	121.27
1	B	161	SER	CA-CB-OG	5.39	121.88	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	LEU	CA-C-O	-5.39	113.47	119.67
1	C	74	LYS	CB-CA-C	-5.39	99.56	110.17
1	D	140	VAL	CA-C-O	-5.38	115.67	121.27
1	A	161	SER	CB-CA-C	5.38	119.83	110.68
1	D	269	ILE	CA-C-O	-5.38	115.13	121.64
1	C	269	ILE	CA-C-O	-5.38	115.13	121.64
1	A	74	LYS	CB-CA-C	-5.38	99.58	110.17
1	D	74	LYS	CB-CA-C	-5.38	99.58	110.17
1	C	161	SER	CA-CB-OG	5.38	121.85	111.10
1	B	85	ASP	CA-CB-CG	-5.38	107.22	112.60
1	C	329	PHE	CA-CB-CG	-5.38	108.42	113.80
1	C	301	VAL	CA-CB-CG1	5.37	119.53	110.40
1	A	161	SER	CA-CB-OG	5.37	121.83	111.10
1	A	269	ILE	CA-C-O	-5.37	115.15	121.64
1	B	269	ILE	CA-C-O	-5.37	115.15	121.64
1	D	161	SER	CA-CB-OG	5.36	121.83	111.10
1	D	301	VAL	CA-CB-CG1	5.36	119.52	110.40
1	B	161	SER	CB-CA-C	5.36	119.80	110.68
1	D	58	ALA	N-CA-C	5.36	117.12	111.28
1	A	269	ILE	N-CA-CB	5.36	117.46	111.89
1	D	226	LEU	CA-C-O	-5.36	113.51	119.67
1	B	74	LYS	CB-CA-C	-5.35	99.63	110.17
1	B	208	VAL	CB-CA-C	5.34	116.81	110.93
1	C	226	LEU	CA-C-O	-5.34	113.53	119.67
1	A	208	VAL	CB-CA-C	5.33	116.80	110.93
1	D	85	ASP	CA-CB-CG	-5.33	107.27	112.60
1	C	259	THR	O-C-N	5.33	127.63	122.09
1	B	50	LEU	CA-C-O	-5.32	113.71	120.20
1	A	50	LEU	CA-C-O	-5.32	113.72	120.20
1	D	269	ILE	N-CA-CB	5.32	117.42	111.89
1	C	269	ILE	N-CA-CB	5.31	117.42	111.89
1	B	29	GLY	O-C-N	5.30	128.44	122.82
1	C	78	ILE	CA-CB-CG1	5.30	119.42	110.40
1	C	227	GLU	CG-CD-OE1	5.30	130.60	118.40
1	D	259	THR	O-C-N	5.30	127.61	122.09
1	D	253	MET	N-CA-C	-5.30	105.40	111.07
1	B	78	ILE	CA-CB-CG1	5.29	119.40	110.40
1	C	165	LEU	CB-CA-C	5.29	119.85	110.85
1	D	165	LEU	CB-CA-C	5.29	119.85	110.85
1	D	320	THR	CA-CB-CG2	5.29	119.50	110.50
1	A	78	ILE	CA-CB-CG1	5.29	119.40	110.40
1	B	320	THR	CA-CB-CG2	5.29	119.49	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	MET	N-CA-C	-5.29	105.41	111.07
1	D	78	ILE	CA-CB-CG1	5.29	119.39	110.40
1	C	50	LEU	CA-C-O	-5.29	113.75	120.20
1	C	208	VAL	CB-CA-C	5.29	116.75	110.93
1	B	227	GLU	CG-CD-OE1	5.29	130.56	118.40
1	A	227	GLU	CG-CD-OE1	5.28	130.55	118.40
1	D	227	GLU	CG-CD-OE1	5.28	130.55	118.40
1	C	285	VAL	CA-C-O	-5.28	115.25	120.90
1	C	320	THR	CA-CB-CG2	5.28	119.47	110.50
1	A	320	THR	CA-CB-CG2	5.28	119.47	110.50
1	C	229	ILE	O-C-N	5.27	127.21	121.94
1	D	242	GLU	CB-CG-CD	5.27	121.56	112.60
1	B	165	LEU	CB-CA-C	5.26	119.80	110.85
1	D	50	LEU	CA-C-O	-5.26	113.78	120.20
1	B	259	THR	O-C-N	5.26	127.56	122.09
1	D	285	VAL	CA-C-O	-5.26	115.27	120.90
1	D	208	VAL	CB-CA-C	5.26	116.71	110.93
1	A	165	LEU	CB-CA-C	5.25	119.78	110.85
1	A	242	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	29	GLY	O-C-N	5.25	128.39	122.82
1	B	242	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	259	THR	O-C-N	5.24	127.54	122.09
1	C	242	GLU	CB-CG-CD	5.24	121.51	112.60
1	D	118	ARG	NH1-CZ-NH2	-5.24	112.49	119.30
1	C	156	GLU	N-CA-CB	5.24	118.33	110.53
1	B	194	GLY	O-C-N	5.23	128.14	123.80
1	A	312	ASN	CA-CB-CG	5.23	117.83	112.60
1	C	29	GLY	O-C-N	5.23	128.37	122.82
1	B	259	THR	CA-CB-OG1	-5.23	101.75	109.60
1	A	259	THR	CA-CB-OG1	-5.23	101.76	109.60
1	D	249	TYR	O-C-N	-5.22	116.69	122.07
1	A	156	GLU	N-CA-CB	5.22	118.31	110.53
1	B	156	GLU	N-CA-CB	5.22	118.31	110.53
1	D	29	GLY	O-C-N	5.22	128.35	122.82
1	A	194	GLY	O-C-N	5.21	128.13	123.80
1	B	229	ILE	O-C-N	5.21	127.15	121.94
1	A	229	ILE	O-C-N	5.21	127.15	121.94
1	C	249	TYR	O-C-N	-5.21	116.71	122.07
1	B	285	VAL	CA-C-O	-5.20	115.34	120.90
1	B	312	ASN	CA-CB-CG	5.20	117.80	112.60
1	C	118	ARG	NH1-CZ-NH2	-5.20	112.55	119.30
1	C	259	THR	CA-CB-OG1	-5.20	101.81	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	THR	CA-CB-OG1	-5.20	101.81	109.60
1	D	156	GLU	N-CA-CB	5.19	118.27	110.53
1	A	249	TYR	O-C-N	-5.19	116.72	122.07
1	B	118	ARG	NH1-CZ-NH2	-5.19	112.56	119.30
1	D	55	GLU	CA-C-N	5.19	127.23	120.28
1	D	55	GLU	C-N-CA	5.19	127.23	120.28
1	C	194	GLY	O-C-N	5.18	128.10	123.80
1	C	256	ALA	CB-CA-C	5.18	119.67	109.72
1	A	285	VAL	CA-C-O	-5.18	115.36	120.90
1	B	241	ILE	O-C-N	5.18	128.92	121.82
1	A	118	ARG	NH1-CZ-NH2	-5.18	112.56	119.30
1	D	229	ILE	O-C-N	5.17	127.11	121.94
1	D	241	ILE	O-C-N	5.17	128.91	121.82
1	D	256	ALA	CB-CA-C	5.17	119.65	109.72
1	B	256	ALA	CB-CA-C	5.17	119.65	109.72
1	A	55	GLU	CA-C-N	5.17	127.21	120.28
1	A	55	GLU	C-N-CA	5.17	127.21	120.28
1	C	241	ILE	O-C-N	5.17	128.91	121.82
1	A	256	ALA	CB-CA-C	5.17	119.65	109.72
1	C	73	PRO	N-CA-C	5.17	123.12	112.47
1	A	31	VAL	CB-CA-C	5.17	119.35	112.22
1	A	73	PRO	N-CA-C	5.17	123.11	112.47
1	B	73	PRO	N-CA-C	5.17	123.11	112.47
1	A	215	VAL	CA-C-O	5.16	126.45	120.67
1	A	241	ILE	O-C-N	5.16	128.89	121.82
1	B	286	TYR	N-CA-CB	5.16	118.83	110.41
1	C	176	GLU	CA-CB-CG	5.16	124.42	114.10
1	A	286	TYR	N-CA-CB	5.16	118.82	110.41
1	C	312	ASN	CA-CB-CG	5.16	117.76	112.60
1	A	66	ASN	CA-C-O	-5.16	114.28	120.10
1	D	312	ASN	CA-CB-CG	5.16	117.75	112.60
1	D	176	GLU	CA-CB-CG	5.15	124.41	114.10
1	A	256	ALA	N-CA-C	-5.15	106.99	113.28
1	B	176	GLU	CA-CB-CG	5.15	124.41	114.10
1	D	215	VAL	CA-C-O	5.15	126.44	120.67
1	D	73	PRO	N-CA-C	5.15	123.08	112.47
1	D	194	GLY	O-C-N	5.15	128.07	123.80
1	A	59	ILE	O-C-N	5.15	127.24	121.94
1	A	114	ILE	O-C-N	5.14	126.86	121.87
1	A	176	GLU	CA-CB-CG	5.14	124.39	114.10
1	B	55	GLU	CA-C-N	5.14	127.17	120.28
1	B	55	GLU	C-N-CA	5.14	127.17	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286	TYR	N-CA-CB	5.14	118.79	110.41
1	B	157	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	C	55	GLU	CA-C-N	5.14	127.17	120.28
1	C	55	GLU	C-N-CA	5.14	127.17	120.28
1	D	59	ILE	O-C-N	5.14	127.23	121.94
1	D	66	ASN	CA-C-O	-5.14	114.30	120.10
1	B	249	TYR	O-C-N	-5.13	116.78	122.07
1	D	31	VAL	CB-CA-C	5.13	119.30	112.22
1	B	114	ILE	O-C-N	5.13	126.85	121.87
1	B	59	ILE	O-C-N	5.13	127.22	121.94
1	C	114	ILE	O-C-N	5.13	126.84	121.87
1	C	31	VAL	CB-CA-C	5.12	119.29	112.22
1	B	31	VAL	CB-CA-C	5.12	119.29	112.22
1	D	286	TYR	N-CA-CB	5.12	118.76	110.41
1	B	256	ALA	N-CA-C	-5.12	107.03	113.28
1	C	256	ALA	N-CA-C	-5.12	107.03	113.28
1	D	256	ALA	N-CA-C	-5.12	107.04	113.28
1	B	66	ASN	CA-C-O	-5.11	114.32	120.10
1	C	215	VAL	CA-C-O	5.11	126.40	120.67
1	C	66	ASN	CA-C-O	-5.11	114.33	120.10
1	A	318	ALA	N-CA-C	-5.11	105.80	111.36
1	C	243	LYS	CA-C-O	-5.10	113.57	119.59
1	B	215	VAL	CA-C-O	5.09	126.38	120.67
1	B	318	ALA	N-CA-C	-5.09	105.81	111.36
1	A	157	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	C	23	VAL	CA-CB-CG2	5.08	119.04	110.40
1	C	59	ILE	O-C-N	5.08	127.17	121.94
1	D	114	ILE	O-C-N	5.08	126.80	121.87
1	B	23	VAL	CA-CB-CG2	5.08	119.04	110.40
1	D	239	GLN	N-CA-CB	-5.07	102.49	110.30
1	D	23	VAL	CA-CB-CG2	5.07	119.02	110.40
1	D	157	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	D	318	ALA	N-CA-C	-5.07	105.84	111.36
1	C	157	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	C	55	GLU	CA-CB-CG	5.06	124.22	114.10
1	C	239	GLN	N-CA-CB	-5.06	102.51	110.30
1	B	65	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	239	GLN	N-CA-CB	-5.05	102.53	110.30
1	A	23	VAL	CA-CB-CG2	5.05	118.98	110.40
1	A	243	LYS	CA-C-O	-5.05	113.63	119.59
1	B	239	GLN	N-CA-CB	-5.05	102.53	110.30
1	D	55	GLU	CA-CB-CG	5.05	124.19	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	243	LYS	CA-C-O	-5.05	113.64	119.59
1	B	243	LYS	CA-C-O	-5.04	113.64	119.59
1	B	55	GLU	CA-CB-CG	5.04	124.17	114.10
1	C	91	LEU	CB-CA-C	5.03	119.37	110.16
1	C	318	ALA	N-CA-C	-5.03	105.88	111.36
1	A	257	ARG	CG-CD-NE	5.03	123.06	112.00
1	B	257	ARG	CG-CD-NE	5.03	123.06	112.00
1	A	55	GLU	CA-CB-CG	5.03	124.16	114.10
1	B	120	ILE	O-C-N	5.03	126.83	121.91
1	B	91	LEU	CB-CA-C	5.02	119.35	110.16
1	A	65	PHE	CA-CB-CG	5.02	118.82	113.80
1	C	257	ARG	CG-CD-NE	5.02	123.04	112.00
1	C	70	VAL	N-CA-C	5.01	119.77	109.34
1	C	65	PHE	CA-CB-CG	5.01	118.81	113.80
1	D	257	ARG	CG-CD-NE	5.01	123.02	112.00
1	A	289	VAL	N-CA-CB	-5.01	104.20	111.21
1	C	178	PHE	CA-C-N	-5.01	117.59	126.45
1	C	178	PHE	C-N-CA	-5.01	117.59	126.45
1	B	178	PHE	CA-C-N	-5.00	117.59	126.45
1	B	178	PHE	C-N-CA	-5.00	117.59	126.45
1	D	65	PHE	CA-CB-CG	5.00	118.81	113.80
1	B	289	VAL	N-CA-CB	-5.00	104.20	111.21
1	C	289	VAL	N-CA-CB	-5.00	104.20	111.21
1	D	91	LEU	CB-CA-C	5.00	119.32	110.16
1	A	91	LEU	CB-CA-C	5.00	119.31	110.16

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	171	ARG	Sidechain
1	A	189	ILE	Mainchain
1	A	205	TYR	Sidechain
1	A	226	LEU	Mainchain
1	A	260	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	47	GLU	Mainchain
1	A	68	GLY	Mainchain
1	B	157	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	189	ILE	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	205	TYR	Sidechain
1	B	226	LEU	Mainchain
1	B	260	ARG	Sidechain
1	B	283	ARG	Sidechain
1	B	47	GLU	Mainchain
1	B	68	GLY	Mainchain
1	C	157	ARG	Sidechain
1	C	171	ARG	Sidechain
1	C	189	ILE	Mainchain
1	C	205	TYR	Sidechain
1	C	226	LEU	Mainchain
1	C	260	ARG	Sidechain
1	C	283	ARG	Sidechain
1	C	47	GLU	Mainchain
1	C	68	GLY	Mainchain
1	D	157	ARG	Sidechain
1	D	171	ARG	Sidechain
1	D	189	ILE	Mainchain
1	D	205	TYR	Sidechain
1	D	226	LEU	Mainchain
1	D	260	ARG	Sidechain
1	D	283	ARG	Sidechain
1	D	47	GLU	Mainchain
1	D	68	GLY	Mainchain

5.2 Too-close contacts [i](#)

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	2336	0	2328	290	49
1	B	2336	0	2328	292	4
1	C	2336	0	2328	289	10
1	D	2336	0	2328	291	59
2	A	10	0	0	4	0
2	B	10	0	0	4	0
2	C	10	0	0	4	0
2	D	10	0	0	4	0
3	A	44	0	26	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	8	0
3	C	44	0	26	8	0
3	D	44	0	26	8	0
4	C	20	0	10	3	0
4	D	20	0	10	3	0
5	A	47	0	0	1	4
5	C	3	0	0	1	0
All	All	9650	0	9436	1081	63

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 57.

All (1081) 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:A:67:HIS:CD2	1:C:169:ARG:HG2	1.63	1.33
1:B:67:HIS:CD2	1:D:169:ARG:HG2	1.63	1.32
1:B:169:ARG:HG2	1:D:67:HIS:CD2	1.63	1.31
1:A:169:ARG:HG2	1:C:67:HIS:CD2	1.63	1.30
1:B:107:LEU:HD22	1:B:327:ARG:NE	1.54	1.23
1:C:107:LEU:HD22	1:C:327:ARG:NE	1.54	1.22
1:D:107:LEU:HD22	1:D:327:ARG:NE	1.54	1.21
1:A:107:LEU:HD22	1:A:327:ARG:NE	1.54	1.20
1:B:214:LEU:HD12	1:B:215:VAL:N	1.56	1.20
1:C:214:LEU:HD12	1:C:215:VAL:N	1.56	1.20
1:A:214:LEU:HD12	1:A:215:VAL:N	1.56	1.19
1:D:214:LEU:HD12	1:D:215:VAL:N	1.56	1.18
1:D:214:LEU:HD12	1:D:215:VAL:H	0.96	1.09
1:C:214:LEU:HD12	1:C:215:VAL:H	0.96	1.09
1:A:214:LEU:HD12	1:A:215:VAL:H	0.96	1.08
1:A:107:LEU:HD22	1:A:327:ARG:HE	0.93	1.08
1:D:216:GLU:HG3	1:D:217:SER:H	1.13	1.08
1:C:107:LEU:HD22	1:C:327:ARG:HE	0.93	1.08
1:B:216:GLU:HG3	1:B:217:SER:H	1.13	1.07
1:C:216:GLU:HG3	1:C:217:SER:H	1.13	1.06
1:A:216:GLU:HG3	1:A:217:SER:H	1.13	1.06
1:B:214:LEU:HD12	1:B:215:VAL:H	0.96	1.05
1:B:107:LEU:HD22	1:B:327:ARG:HE	0.93	1.04
1:C:15:MET:CE	1:C:18:ASN:HB3	1.89	1.03
1:D:107:LEU:HD22	1:D:327:ARG:HE	0.93	1.03
1:B:15:MET:HE1	1:B:18:ASN:HB3	1.40	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:MET:CE	1:D:18:ASN:HB3	1.89	1.02
1:B:15:MET:CE	1:B:18:ASN:HB3	1.89	1.02
1:A:15:MET:HE1	1:A:18:ASN:HB3	1.40	1.01
1:A:15:MET:CE	1:A:18:ASN:HB3	1.89	1.01
1:A:261:ALA:HA	1:A:266:GLU:HG3	1.43	1.00
1:C:112:LYS:O	1:C:115:ALA:HB3	1.62	1.00
1:D:15:MET:HE1	1:D:18:ASN:HB3	1.40	1.00
1:D:112:LYS:O	1:D:115:ALA:HB3	1.62	1.00
1:C:15:MET:HE1	1:C:18:ASN:HB3	1.40	0.99
1:D:261:ALA:HA	1:D:266:GLU:HG3	1.43	0.99
1:C:107:LEU:CD2	1:C:327:ARG:HE	1.76	0.99
1:C:183:GLN:NE2	4:C:6:FBP:O3	1.96	0.99
1:B:107:LEU:CD2	1:B:327:ARG:HE	1.76	0.99
1:D:183:GLN:NE2	4:D:2:FBP:O3	1.96	0.99
1:B:112:LYS:O	1:B:115:ALA:HB3	1.62	0.98
1:A:112:LYS:O	1:A:115:ALA:HB3	1.62	0.98
1:D:107:LEU:CD2	1:D:327:ARG:HE	1.76	0.98
1:A:107:LEU:CD2	1:A:327:ARG:HE	1.76	0.97
1:C:261:ALA:HA	1:C:266:GLU:HG3	1.43	0.97
1:C:237:ALA:O	1:C:241:ILE:HG13	1.65	0.96
1:B:261:ALA:HA	1:B:266:GLU:HG3	1.43	0.96
1:A:237:ALA:O	1:A:241:ILE:HG13	1.65	0.96
1:C:87:ARG:O	1:C:88:ASP:HB2	1.66	0.96
1:D:107:LEU:HB2	1:D:327:ARG:HH21	1.31	0.96
1:B:192:GLU:O	1:B:197:GLU:HB3	1.65	0.96
1:D:192:GLU:O	1:D:197:GLU:HB3	1.65	0.96
1:A:192:GLU:O	1:A:197:GLU:HB3	1.65	0.95
1:D:237:ALA:O	1:D:241:ILE:HG13	1.65	0.95
1:D:87:ARG:O	1:D:88:ASP:HB2	1.66	0.95
1:C:192:GLU:O	1:C:197:GLU:HB3	1.65	0.94
1:D:257:ARG:NH2	1:D:266:GLU:OE2	2.01	0.94
1:A:107:LEU:HB2	1:A:327:ARG:HH21	1.31	0.94
1:B:200:VAL:HG11	1:B:304:ILE:HD12	1.50	0.94
1:B:107:LEU:HB2	1:B:327:ARG:HH21	1.31	0.94
1:B:237:ALA:O	1:B:241:ILE:HG13	1.65	0.94
1:C:107:LEU:HB2	1:C:327:ARG:HH21	1.31	0.94
1:A:87:ARG:O	1:A:88:ASP:HB2	1.66	0.94
1:B:87:ARG:O	1:B:88:ASP:HB2	1.65	0.93
1:C:257:ARG:NH2	1:C:266:GLU:OE2	2.01	0.93
1:B:257:ARG:NH2	1:B:266:GLU:OE2	2.01	0.93
1:B:295:ARG:HH11	1:B:295:ARG:HG2	1.33	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:NH2	1:A:266:GLU:OE2	2.01	0.93
1:C:216:GLU:HG3	1:C:217:SER:N	1.83	0.92
1:B:216:GLU:HG3	1:B:217:SER:N	1.83	0.92
1:C:295:ARG:HG2	1:C:295:ARG:HH11	1.33	0.92
1:A:295:ARG:HG2	1:A:295:ARG:HH11	1.33	0.92
1:D:200:VAL:HG11	1:D:304:ILE:HD12	1.50	0.92
1:A:216:GLU:HG3	1:A:217:SER:N	1.83	0.91
1:C:200:VAL:HG11	1:C:304:ILE:HD12	1.50	0.91
1:D:295:ARG:HG2	1:D:295:ARG:HH11	1.33	0.90
1:A:200:VAL:HG11	1:A:304:ILE:HD12	1.50	0.90
1:B:67:HIS:CD2	1:D:169:ARG:CG	2.54	0.90
1:A:169:ARG:CG	1:C:67:HIS:CD2	2.53	0.89
1:A:67:HIS:CD2	1:C:169:ARG:CG	2.54	0.89
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.37	0.89
1:A:67:HIS:HD2	1:C:169:ARG:HG2	1.38	0.89
1:A:307:ASN:O	1:A:311:LYS:HG3	1.73	0.89
1:C:307:ASN:O	1:C:311:LYS:HG3	1.73	0.89
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.37	0.89
1:B:67:HIS:HD2	1:D:169:ARG:HG2	1.38	0.89
1:D:244:LYS:O	1:D:244:LYS:HG2	1.73	0.89
1:B:169:ARG:HG2	1:D:67:HIS:HD2	1.38	0.89
1:D:216:GLU:HG3	1:D:217:SER:N	1.83	0.89
1:B:169:ARG:CG	1:D:67:HIS:CD2	2.54	0.89
1:D:283:ARG:H	1:D:322:LYS:HZ2	1.19	0.88
1:D:307:ASN:O	1:D:311:LYS:HG3	1.73	0.88
1:A:283:ARG:H	1:A:322:LYS:HZ2	1.19	0.88
1:B:307:ASN:O	1:B:311:LYS:HG3	1.73	0.88
1:C:313:ARG:HH11	1:C:313:ARG:HG2	1.37	0.88
1:C:160:GLY:HA3	1:C:273:SER:HB3	1.55	0.88
1:B:244:LYS:HG2	1:B:244:LYS:O	1.73	0.88
1:A:160:GLY:HA3	1:A:273:SER:HB3	1.55	0.87
1:C:283:ARG:H	1:C:322:LYS:HZ2	1.19	0.87
1:A:244:LYS:HD3	1:A:246:ALA:O	1.75	0.87
1:B:160:GLY:HA3	1:B:273:SER:HB3	1.55	0.87
1:D:313:ARG:HG2	1:D:313:ARG:HH11	1.37	0.87
1:C:244:LYS:O	1:C:244:LYS:HG2	1.73	0.87
1:A:107:LEU:HD22	1:A:327:ARG:CD	2.04	0.87
1:D:160:GLY:HA3	1:D:273:SER:HB3	1.55	0.86
1:D:107:LEU:HD22	1:D:327:ARG:CD	2.04	0.86
1:B:107:LEU:HD22	1:B:327:ARG:CD	2.04	0.86
1:B:283:ARG:H	1:B:322:LYS:HZ2	1.19	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:O	1:A:244:LYS:HG2	1.73	0.86
1:D:151:SER:OG	1:D:153:LEU:HB2	1.75	0.86
1:C:107:LEU:HD22	1:C:327:ARG:CD	2.04	0.86
1:D:244:LYS:HD3	1:D:246:ALA:O	1.75	0.86
1:B:151:SER:OG	1:B:153:LEU:HB2	1.75	0.86
1:B:244:LYS:HD3	1:B:246:ALA:O	1.75	0.85
1:A:183:GLN:HE21	1:A:183:GLN:CA	1.85	0.85
1:C:151:SER:OG	1:C:153:LEU:HB2	1.75	0.85
1:C:183:GLN:CA	1:C:183:GLN:HE21	1.85	0.85
1:A:151:SER:OG	1:A:153:LEU:HB2	1.75	0.84
1:C:244:LYS:HD3	1:C:246:ALA:O	1.75	0.84
1:B:183:GLN:CA	1:B:183:GLN:HE21	1.85	0.84
1:A:169:ARG:HG2	1:C:67:HIS:HD2	1.37	0.84
1:D:183:GLN:HE21	1:D:183:GLN:CA	1.85	0.84
1:A:183:GLN:HE21	1:A:183:GLN:HA	1.44	0.83
1:D:183:GLN:HE21	1:D:183:GLN:HA	1.44	0.83
1:B:178:PHE:O	1:B:179:SER:HB2	1.80	0.82
1:A:178:PHE:O	1:A:179:SER:HB2	1.79	0.82
1:D:178:PHE:O	1:D:179:SER:HB2	1.80	0.82
1:C:74:LYS:HE2	1:D:266:GLU:CD	2.06	0.81
1:B:183:GLN:HE21	1:B:183:GLN:HA	1.44	0.81
1:C:178:PHE:O	1:C:179:SER:HB2	1.80	0.80
1:C:266:GLU:CD	1:D:74:LYS:HE2	2.06	0.80
1:D:240:ILE:HG21	1:D:247:THR:CG2	2.11	0.80
1:A:240:ILE:HG21	1:A:247:THR:CG2	2.11	0.80
1:C:183:GLN:HE21	1:C:183:GLN:HA	1.44	0.80
1:C:240:ILE:HG21	1:C:247:THR:CG2	2.11	0.80
1:C:240:ILE:HG21	1:C:247:THR:HG23	1.64	0.80
1:A:208:VAL:O	1:A:210:PRO:HD3	1.82	0.80
1:B:208:VAL:O	1:B:210:PRO:HD3	1.82	0.80
1:A:74:LYS:HE2	1:B:266:GLU:CD	2.06	0.79
1:D:208:VAL:O	1:D:210:PRO:HD3	1.82	0.79
1:A:240:ILE:HG21	1:A:247:THR:HG23	1.64	0.79
1:A:266:GLU:CD	1:B:74:LYS:HE2	2.06	0.79
1:B:240:ILE:HG21	1:B:247:THR:CG2	2.11	0.79
1:D:240:ILE:HG21	1:D:247:THR:HG23	1.64	0.79
1:C:208:VAL:O	1:C:210:PRO:HD3	1.82	0.79
1:D:32:GLY:O	1:D:36:VAL:HG23	1.83	0.79
1:B:32:GLY:O	1:B:36:VAL:HG23	1.83	0.79
1:C:32:GLY:O	1:C:36:VAL:HG23	1.83	0.78
1:B:240:ILE:HG21	1:B:247:THR:HG23	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:O	1:A:36:VAL:HG23	1.83	0.78
1:A:136:ALA:HB1	1:A:251:ILE:HD11	1.67	0.77
1:C:199:PRO:O	1:C:199:PRO:HG2	1.85	0.77
1:A:189:ILE:CD1	1:A:233:VAL:HG11	2.15	0.77
1:D:136:ALA:HB1	1:D:251:ILE:HD11	1.67	0.77
1:B:136:ALA:HB1	1:B:251:ILE:HD11	1.67	0.77
1:A:279:LEU:HD12	1:A:303:GLU:OE1	1.85	0.76
1:B:279:LEU:HD12	1:B:303:GLU:OE1	1.85	0.76
1:B:313:ARG:HG2	1:B:313:ARG:NH1	2.00	0.76
1:C:183:GLN:HE22	4:C:6:FBP:C3	1.98	0.76
1:D:313:ARG:HG2	1:D:313:ARG:NH1	2.00	0.76
1:D:183:GLN:HE22	4:D:2:FBP:C3	1.98	0.76
1:B:189:ILE:CD1	1:B:233:VAL:HG11	2.15	0.76
1:C:214:LEU:CD1	1:C:215:VAL:N	2.45	0.76
1:D:189:ILE:CD1	1:D:233:VAL:HG11	2.15	0.76
1:A:160:GLY:HA3	1:A:273:SER:CB	2.16	0.76
1:A:199:PRO:HG2	1:A:199:PRO:O	1.85	0.76
1:C:189:ILE:CD1	1:C:233:VAL:HG11	2.15	0.76
1:C:313:ARG:HG2	1:C:313:ARG:NH1	2.00	0.76
1:C:160:GLY:HA3	1:C:273:SER:CB	2.16	0.76
1:C:240:ILE:CG2	1:C:247:THR:HG23	2.16	0.76
1:D:240:ILE:CG2	1:D:247:THR:HG23	2.16	0.76
1:C:279:LEU:HD12	1:C:303:GLU:OE1	1.85	0.76
1:B:160:GLY:HA3	1:B:273:SER:CB	2.16	0.75
1:D:199:PRO:O	1:D:199:PRO:HG2	1.85	0.75
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.00	0.75
1:B:214:LEU:CD1	1:B:215:VAL:N	2.45	0.75
1:B:240:ILE:CG2	1:B:247:THR:HG23	2.16	0.75
1:D:113:ASN:O	1:D:117:PHE:HB2	1.87	0.75
1:A:240:ILE:CG2	1:A:247:THR:HG23	2.16	0.75
1:B:199:PRO:O	1:B:199:PRO:HG2	1.85	0.75
1:B:226:LEU:C	1:B:228:ARG:H	1.95	0.75
1:B:243:LYS:NZ	1:B:243:LYS:HB3	2.02	0.75
1:D:160:GLY:HA3	1:D:273:SER:CB	2.16	0.75
1:A:113:ASN:O	1:A:117:PHE:HB2	1.87	0.74
1:A:214:LEU:CD1	1:A:215:VAL:N	2.45	0.74
1:A:215:VAL:O	1:A:216:GLU:HG2	1.87	0.74
1:B:215:VAL:O	1:B:216:GLU:HG2	1.87	0.74
1:B:113:ASN:O	1:B:117:PHE:HB2	1.87	0.74
1:C:226:LEU:C	1:C:228:ARG:H	1.95	0.74
1:D:279:LEU:HD12	1:D:303:GLU:OE1	1.85	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ALA:HB1	1:C:251:ILE:HD11	1.67	0.74
1:A:226:LEU:C	1:A:228:ARG:H	1.95	0.74
1:C:295:ARG:HG2	1:C:295:ARG:NH1	2.03	0.74
1:D:15:MET:HE1	1:D:18:ASN:CB	2.17	0.74
1:C:215:VAL:O	1:C:216:GLU:HG2	1.87	0.74
1:B:279:LEU:C	1:B:281:GLY:H	1.96	0.74
1:C:113:ASN:O	1:C:117:PHE:HB2	1.87	0.74
1:C:279:LEU:C	1:C:281:GLY:H	1.96	0.74
1:B:87:ARG:HG3	1:B:127:SER:O	1.88	0.74
1:C:15:MET:HE1	1:C:18:ASN:CB	2.17	0.74
1:D:243:LYS:HB3	1:D:243:LYS:NZ	2.02	0.74
1:D:215:VAL:O	1:D:216:GLU:HG2	1.87	0.74
1:A:87:ARG:HG3	1:A:127:SER:O	1.88	0.73
1:C:87:ARG:HG3	1:C:127:SER:O	1.88	0.73
1:D:295:ARG:HG2	1:D:295:ARG:NH1	2.03	0.73
1:A:279:LEU:C	1:A:281:GLY:H	1.96	0.73
1:C:243:LYS:NZ	1:C:243:LYS:HB3	2.02	0.73
1:C:183:GLN:NE2	1:C:183:GLN:HA	2.03	0.73
1:D:83:TYR:HD2	1:D:124:VAL:HG12	1.54	0.73
1:A:83:TYR:HD2	1:A:124:VAL:HG12	1.53	0.73
1:B:183:GLN:HA	1:B:183:GLN:NE2	2.03	0.73
1:C:83:TYR:HD2	1:C:124:VAL:HG12	1.54	0.73
1:D:226:LEU:C	1:D:228:ARG:H	1.95	0.73
1:D:15:MET:HE3	1:D:18:ASN:HB3	1.70	0.72
1:D:214:LEU:CD1	1:D:215:VAL:N	2.45	0.72
1:B:295:ARG:HG2	1:B:295:ARG:NH1	2.03	0.72
1:D:183:GLN:NE2	1:D:183:GLN:HA	2.03	0.72
1:A:243:LYS:NZ	1:A:243:LYS:HB3	2.02	0.72
1:B:83:TYR:HD2	1:B:124:VAL:HG12	1.54	0.72
1:B:15:MET:HE3	1:B:18:ASN:HB3	1.70	0.72
1:B:15:MET:HE1	1:B:18:ASN:CB	2.17	0.72
1:B:59:ILE:HG22	1:D:243:LYS:HD3	1.72	0.72
1:A:295:ARG:HG2	1:A:295:ARG:NH1	2.03	0.72
1:C:170:PHE:HA	1:C:233:VAL:CG2	2.20	0.72
1:A:15:MET:HE1	1:A:18:ASN:CB	2.17	0.71
1:A:15:MET:HE3	1:A:18:ASN:HB3	1.70	0.71
1:A:170:PHE:HA	1:A:233:VAL:CG2	2.20	0.71
1:A:183:GLN:HA	1:A:183:GLN:NE2	2.03	0.71
1:D:190:ILE:HD11	1:D:306:LEU:HD11	1.72	0.71
1:A:59:ILE:HG22	1:C:243:LYS:HD3	1.72	0.71
1:C:216:GLU:CG	1:C:217:SER:H	2.00	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:VAL:HG22	1:B:139:PRO:HG3	1.72	0.71
1:C:147:THR:O	1:C:151:SER:HB3	1.90	0.71
1:D:87:ARG:HG3	1:D:127:SER:O	1.88	0.71
1:B:170:PHE:HA	1:B:233:VAL:CG2	2.20	0.71
1:D:147:THR:O	1:D:151:SER:HB3	1.90	0.71
1:D:170:PHE:HA	1:D:233:VAL:CG2	2.20	0.71
1:A:190:ILE:HD11	1:A:306:LEU:HD11	1.73	0.71
1:B:147:THR:O	1:B:151:SER:HB3	1.91	0.71
1:B:243:LYS:HD3	1:D:59:ILE:HG22	1.72	0.71
1:C:15:MET:HE3	1:C:18:ASN:HB3	1.70	0.70
1:A:110:VAL:HG22	1:A:139:PRO:HG3	1.72	0.70
1:D:110:VAL:HG22	1:D:139:PRO:HG3	1.72	0.70
1:A:59:ILE:CG2	1:C:243:LYS:HD3	2.21	0.70
1:A:147:THR:O	1:A:151:SER:HB3	1.91	0.70
1:A:243:LYS:HD3	1:C:59:ILE:HG22	1.72	0.70
1:A:243:LYS:HD3	1:C:59:ILE:CG2	2.21	0.70
1:B:73:PRO:O	1:B:74:LYS:HB2	1.92	0.70
1:B:243:LYS:HD3	1:D:59:ILE:CG2	2.21	0.70
1:A:73:PRO:O	1:A:74:LYS:HB2	1.92	0.70
1:C:294:ASN:C	1:C:294:ASN:HD22	1.99	0.70
1:D:294:ASN:C	1:D:294:ASN:HD22	1.99	0.70
1:B:59:ILE:CG2	1:D:243:LYS:HD3	2.21	0.70
1:B:190:ILE:HD11	1:B:306:LEU:HD11	1.72	0.69
1:C:190:ILE:HD11	1:C:306:LEU:HD11	1.72	0.69
1:D:279:LEU:C	1:D:281:GLY:H	1.96	0.69
1:A:294:ASN:C	1:A:294:ASN:HD22	1.99	0.69
1:D:73:PRO:O	1:D:74:LYS:HB2	1.91	0.69
1:B:294:ASN:C	1:B:294:ASN:HD22	1.99	0.69
1:A:214:LEU:CD1	1:A:215:VAL:H	1.90	0.69
1:C:110:VAL:HG22	1:C:139:PRO:HG3	1.72	0.69
1:C:73:PRO:O	1:C:74:LYS:HB2	1.92	0.69
1:A:132:LEU:CD1	1:A:262:ILE:HD13	2.24	0.68
1:B:283:ARG:N	1:B:322:LYS:HZ2	1.92	0.68
1:C:132:LEU:CD1	1:C:262:ILE:HD13	2.24	0.68
1:D:132:LEU:CD1	1:D:262:ILE:HD13	2.24	0.68
1:A:215:VAL:C	1:A:216:GLU:CG	2.67	0.68
1:A:215:VAL:C	1:A:216:GLU:HG2	2.19	0.67
1:B:132:LEU:CD1	1:B:262:ILE:HD13	2.24	0.67
1:D:215:VAL:C	1:D:216:GLU:HG2	2.20	0.67
1:A:170:PHE:HA	1:A:233:VAL:HG21	1.77	0.67
1:C:215:VAL:C	1:C:216:GLU:CG	2.67	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:C	1:B:216:GLU:HG2	2.19	0.67
1:C:170:PHE:HA	1:C:233:VAL:HG21	1.77	0.67
1:D:170:PHE:HA	1:D:233:VAL:HG21	1.77	0.67
1:A:176:GLU:OE1	5:A:348:HOH:O	2.12	0.66
1:C:215:VAL:C	1:C:216:GLU:HG2	2.20	0.66
1:B:170:PHE:HA	1:B:233:VAL:HG21	1.77	0.66
1:A:61:ASP:OD1	1:C:244:LYS:HE3	1.96	0.66
1:B:61:ASP:OD1	1:D:244:LYS:HE3	1.96	0.65
1:A:244:LYS:HE3	1:C:61:ASP:OD1	1.96	0.65
1:D:214:LEU:CD1	1:D:215:VAL:H	1.91	0.65
1:B:215:VAL:C	1:B:216:GLU:CG	2.67	0.65
1:A:189:ILE:HD11	1:A:233:VAL:HG11	1.79	0.65
1:B:313:ARG:HH11	1:B:313:ARG:CG	2.05	0.65
1:D:215:VAL:C	1:D:216:GLU:CG	2.67	0.65
1:B:279:LEU:HD12	1:B:303:GLU:CD	2.22	0.65
1:C:279:LEU:HD12	1:C:303:GLU:CD	2.22	0.65
1:D:189:ILE:HD11	1:D:233:VAL:HG11	1.79	0.65
1:D:283:ARG:N	1:D:322:LYS:HZ2	1.94	0.65
1:B:244:LYS:HE3	1:D:61:ASP:OD1	1.96	0.64
1:A:272:VAL:O	1:A:288:GLY:HA2	1.97	0.64
1:C:272:VAL:O	1:C:288:GLY:HA2	1.96	0.64
1:A:107:LEU:CD1	1:A:328:ALA:HB2	2.28	0.64
1:B:189:ILE:HD11	1:B:233:VAL:HG11	1.79	0.64
1:B:206:ILE:HB	1:B:213:LYS:HE3	1.80	0.64
1:D:148:TRP:CH2	1:D:275:TYR:CE2	2.86	0.64
1:D:272:VAL:O	1:D:288:GLY:HA2	1.96	0.64
1:B:272:VAL:O	1:B:288:GLY:HA2	1.97	0.64
1:C:148:TRP:CH2	1:C:275:TYR:CE2	2.86	0.64
1:C:206:ILE:HB	1:C:213:LYS:HE3	1.80	0.64
1:A:148:TRP:CH2	1:A:275:TYR:CE2	2.86	0.64
1:A:279:LEU:HD12	1:A:303:GLU:CD	2.22	0.64
1:C:189:ILE:HD11	1:C:233:VAL:HG11	1.79	0.64
1:B:107:LEU:CD1	1:B:328:ALA:HB2	2.28	0.63
1:D:279:LEU:HD12	1:D:303:GLU:CD	2.22	0.63
1:D:107:LEU:CD1	1:D:328:ALA:HB2	2.28	0.63
1:A:313:ARG:NH1	1:A:313:ARG:CG	2.61	0.63
1:C:209:MET:HB3	1:C:213:LYS:HE2	1.81	0.63
1:D:87:ARG:O	1:D:88:ASP:CB	2.44	0.63
1:B:214:LEU:CD1	1:B:215:VAL:H	1.91	0.63
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.64	0.63
1:A:206:ILE:HB	1:A:213:LYS:HE3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:TRP:CH2	1:B:275:TYR:CE2	2.86	0.63
1:A:157:ARG:HG2	1:A:157:ARG:HH11	1.64	0.63
1:A:283:ARG:N	1:A:322:LYS:HZ2	1.93	0.63
1:A:296:ASN:OD1	1:B:15:MET:HG3	1.99	0.63
1:C:107:LEU:CD1	1:C:328:ALA:HB2	2.28	0.63
1:D:206:ILE:HB	1:D:213:LYS:HE3	1.80	0.63
1:D:216:GLU:CG	1:D:217:SER:H	2.00	0.63
1:C:296:ASN:OD1	1:D:15:MET:HG3	1.99	0.62
1:D:157:ARG:HG2	1:D:157:ARG:HH11	1.64	0.62
1:C:15:MET:HG3	1:D:296:ASN:OD1	1.99	0.62
1:B:209:MET:HB3	1:B:213:LYS:HE2	1.80	0.62
1:D:313:ARG:NH1	1:D:313:ARG:CG	2.61	0.62
1:B:279:LEU:C	1:B:281:GLY:N	2.57	0.62
1:B:313:ARG:NH1	1:B:313:ARG:CG	2.61	0.62
1:A:15:MET:HG3	1:B:296:ASN:OD1	1.99	0.62
1:A:59:ILE:HG22	1:C:243:LYS:CD	2.30	0.62
1:A:125:MET:HE2	1:A:125:MET:HA	1.82	0.62
1:B:289:VAL:HG11	1:B:301:VAL:HG13	1.82	0.62
1:B:59:ILE:HG22	1:D:243:LYS:CD	2.30	0.62
1:B:125:MET:HA	1:B:125:MET:HE2	1.82	0.62
1:B:157:ARG:HH11	1:B:157:ARG:HG2	1.64	0.62
1:A:251:ILE:HD12	3:A:1:NAD:C3N	2.30	0.62
1:A:289:VAL:HG11	1:A:301:VAL:HG13	1.82	0.62
1:B:251:ILE:HD12	3:B:5:NAD:C3N	2.30	0.62
1:A:279:LEU:C	1:A:281:GLY:N	2.57	0.61
1:C:289:VAL:HG11	1:C:301:VAL:HG13	1.82	0.61
1:A:98:ALA:HB2	1:A:112:LYS:HG2	1.83	0.61
1:C:251:ILE:HD12	3:C:9:NAD:C3N	2.30	0.61
1:A:29:GLY:HA3	3:A:1:NAD:H52A	1.83	0.61
1:B:243:LYS:CD	1:D:59:ILE:HG22	2.30	0.61
1:D:29:GLY:HA3	3:D:13:NAD:H52A	1.83	0.61
1:A:209:MET:HB3	1:A:213:LYS:HE2	1.81	0.61
1:A:243:LYS:CD	1:C:59:ILE:HG22	2.30	0.61
1:D:125:MET:HA	1:D:125:MET:HE2	1.82	0.61
1:D:251:ILE:HD12	3:D:13:NAD:C3N	2.30	0.61
1:D:209:MET:HB3	1:D:213:LYS:HE2	1.81	0.61
1:A:107:LEU:HB2	1:A:327:ARG:NH2	2.12	0.61
1:C:125:MET:HE2	1:C:125:MET:HA	1.83	0.61
1:C:279:LEU:C	1:C:281:GLY:N	2.57	0.61
1:D:174:LEU:O	1:D:177:TYR:HB3	2.01	0.61
1:D:289:VAL:HG11	1:D:301:VAL:HG13	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ALA:HB2	1:B:112:LYS:HG2	1.83	0.60
1:C:29:GLY:HA3	3:C:9:NAD:H52A	1.83	0.60
1:C:214:LEU:CD1	1:C:215:VAL:H	1.91	0.60
1:D:279:LEU:C	1:D:281:GLY:N	2.57	0.60
1:D:98:ALA:HB2	1:D:112:LYS:HG2	1.83	0.60
1:B:329:PHE:O	1:B:330:THR:C	2.44	0.60
1:A:174:LEU:O	1:A:177:TYR:HB3	2.02	0.60
1:C:54:ASN:C	1:C:54:ASN:HD22	2.09	0.60
1:B:174:LEU:O	1:B:177:TYR:HB3	2.01	0.60
1:C:174:LEU:O	1:C:177:TYR:HB3	2.01	0.60
1:A:54:ASN:C	1:A:54:ASN:HD22	2.09	0.59
1:B:29:GLY:HA3	3:B:5:NAD:H52A	1.83	0.59
1:A:329:PHE:O	1:A:330:THR:C	2.44	0.59
1:B:209:MET:HE1	1:C:305:GLU:CB	2.33	0.59
1:C:53:ALA:H	3:C:9:NAD:C2A	2.16	0.59
1:B:107:LEU:HB2	1:B:327:ARG:NH2	2.12	0.59
1:A:209:MET:HE1	1:D:305:GLU:CB	2.33	0.59
1:D:136:ALA:O	3:D:13:NAD:H2N	2.03	0.59
1:A:320:THR:O	1:A:324:VAL:HG23	2.03	0.59
1:C:98:ALA:HB2	1:C:112:LYS:HG2	1.83	0.59
1:C:319:ALA:O	1:C:323:SER:OG	2.20	0.59
1:D:107:LEU:HB2	1:D:327:ARG:NH2	2.12	0.59
1:D:329:PHE:O	1:D:330:THR:C	2.44	0.59
1:B:305:GLU:CB	1:C:209:MET:HE1	2.33	0.59
1:A:136:ALA:O	3:A:1:NAD:H2N	2.03	0.59
1:C:329:PHE:O	1:C:330:THR:C	2.44	0.59
1:D:53:ALA:H	3:D:13:NAD:C2A	2.16	0.59
1:A:53:ALA:H	3:A:1:NAD:C2A	2.15	0.59
1:B:35:TYR:O	1:B:38:ALA:HB3	2.03	0.58
1:C:136:ALA:O	3:C:9:NAD:H2N	2.03	0.58
1:A:125:MET:CE	1:A:129:PHE:HB3	2.33	0.58
1:A:132:LEU:HD12	1:A:262:ILE:HG21	1.85	0.58
1:B:53:ALA:H	3:B:5:NAD:C2A	2.15	0.58
1:B:129:PHE:CE2	1:B:133:PHE:CE1	2.92	0.58
1:C:283:ARG:N	1:C:322:LYS:HZ2	1.94	0.58
1:A:87:ARG:O	1:A:88:ASP:CB	2.44	0.58
1:A:132:LEU:HD12	1:A:262:ILE:HD13	1.86	0.58
1:A:305:GLU:CB	1:D:209:MET:HE1	2.33	0.58
1:C:125:MET:CE	1:C:129:PHE:HB3	2.33	0.58
1:B:132:LEU:HD12	1:B:262:ILE:HG21	1.85	0.58
1:D:320:THR:O	1:D:324:VAL:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:CE2	1:A:133:PHE:CE1	2.92	0.58
1:B:54:ASN:HD22	1:B:54:ASN:C	2.09	0.58
1:B:151:SER:HB2	1:B:153:LEU:HD12	1.85	0.58
1:B:320:THR:O	1:B:324:VAL:HG23	2.03	0.58
1:C:129:PHE:CE2	1:C:133:PHE:CE1	2.91	0.58
1:C:35:TYR:O	1:C:38:ALA:HB3	2.03	0.58
1:C:240:ILE:HG21	1:C:247:THR:HG22	1.85	0.58
1:C:320:THR:O	1:C:324:VAL:HG23	2.03	0.58
1:D:54:ASN:C	1:D:54:ASN:HD22	2.09	0.58
1:D:125:MET:CE	1:D:129:PHE:HB3	2.33	0.58
1:C:245:GLY:O	1:C:246:ALA:HB2	2.04	0.58
1:D:240:ILE:HG21	1:D:247:THR:HG22	1.86	0.58
1:B:136:ALA:O	3:B:5:NAD:H2N	2.03	0.58
1:D:129:PHE:CE2	1:D:133:PHE:CE1	2.92	0.58
1:D:132:LEU:HD12	1:D:262:ILE:HG21	1.85	0.58
1:B:132:LEU:HD12	1:B:262:ILE:HD13	1.86	0.58
1:B:169:ARG:HG2	1:D:67:HIS:CG	2.32	0.58
1:D:35:TYR:O	1:D:38:ALA:HB3	2.03	0.58
1:D:151:SER:HB2	1:D:153:LEU:HD12	1.85	0.58
1:A:35:TYR:O	1:A:38:ALA:HB3	2.03	0.57
1:B:216:GLU:CG	1:B:217:SER:H	2.00	0.57
1:B:125:MET:CE	1:B:129:PHE:HB3	2.33	0.57
1:B:245:GLY:O	1:B:246:ALA:HB2	2.04	0.57
1:C:15:MET:SD	1:C:16:LYS:N	2.73	0.57
1:C:151:SER:HB2	1:C:153:LEU:HD12	1.85	0.57
1:C:313:ARG:NH1	1:C:313:ARG:CG	2.61	0.57
1:A:319:ALA:O	1:A:323:SER:OG	2.20	0.57
1:D:132:LEU:HD12	1:D:262:ILE:HD13	1.86	0.57
2:B:7:SO4:O3	3:B:5:NAD:C4N	2.53	0.57
1:C:132:LEU:HD12	1:C:262:ILE:HG21	1.85	0.57
2:C:11:SO4:O3	3:C:9:NAD:C4N	2.53	0.57
1:A:151:SER:HB2	1:A:153:LEU:HD12	1.85	0.57
1:C:125:MET:HA	1:C:125:MET:CE	2.35	0.57
1:A:240:ILE:HG21	1:A:247:THR:HG22	1.86	0.57
1:B:125:MET:HA	1:B:125:MET:CE	2.35	0.57
1:D:200:VAL:HG21	1:D:304:ILE:HD11	1.87	0.56
1:B:319:ALA:O	1:B:323:SER:OG	2.20	0.56
1:C:117:PHE:HE1	1:C:137:THR:HG21	1.70	0.56
1:D:245:GLY:O	1:D:246:ALA:HB2	2.04	0.56
1:B:166:ASP:OD1	1:B:193:HIS:ND1	2.34	0.56
1:B:200:VAL:HG21	1:B:304:ILE:HD11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:HD12	1:C:262:ILE:HD13	1.86	0.56
1:D:117:PHE:HE1	1:D:137:THR:HG21	1.70	0.56
2:D:332:SO4:O3	3:D:13:NAD:C4N	2.53	0.56
1:D:166:ASP:OD1	1:D:193:HIS:ND1	2.34	0.56
1:A:42:GLN:OE1	1:A:44:ILE:HD11	2.06	0.56
1:A:215:VAL:O	1:A:216:GLU:CG	2.53	0.56
1:D:35:TYR:HA	1:D:252:ALA:HB1	1.87	0.56
1:A:216:GLU:CG	1:A:217:SER:H	2.00	0.56
1:A:245:GLY:O	1:A:246:ALA:HB2	2.04	0.56
1:B:240:ILE:HG21	1:B:247:THR:HG22	1.86	0.56
1:A:125:MET:HA	1:A:125:MET:CE	2.35	0.56
1:B:117:PHE:HE1	1:B:137:THR:HG21	1.70	0.56
1:A:199:PRO:O	1:A:199:PRO:CG	2.54	0.56
1:D:15:MET:SD	1:D:16:LYS:N	2.73	0.56
1:A:117:PHE:HE1	1:A:137:THR:HG21	1.70	0.56
1:A:267:ASN:ND2	1:A:299:ARG:NH2	2.54	0.56
1:B:190:ILE:HG12	1:B:200:VAL:CG2	2.36	0.56
1:A:200:VAL:HG21	1:A:304:ILE:HD11	1.87	0.55
1:C:42:GLN:OE1	1:C:44:ILE:HD11	2.06	0.55
1:C:98:ALA:HB3	1:C:113:ASN:OD1	2.06	0.55
1:C:107:LEU:HB2	1:C:327:ARG:NH2	2.12	0.55
1:D:125:MET:HA	1:D:125:MET:CE	2.35	0.55
1:A:190:ILE:HG12	1:A:200:VAL:CG2	2.36	0.55
2:A:3:SO4:O3	3:A:1:NAD:C4N	2.53	0.55
1:B:35:TYR:HA	1:B:252:ALA:HB1	1.87	0.55
1:A:35:TYR:HA	1:A:252:ALA:HB1	1.88	0.55
1:C:190:ILE:HG12	1:C:200:VAL:CG2	2.37	0.55
1:C:200:VAL:HG21	1:C:304:ILE:HD11	1.87	0.55
1:C:266:GLU:CG	1:D:74:LYS:HE2	2.36	0.55
1:D:160:GLY:CA	1:D:273:SER:HB3	2.32	0.55
1:D:215:VAL:O	1:D:216:GLU:CG	2.54	0.55
1:A:74:LYS:HE2	1:B:266:GLU:CG	2.36	0.55
1:B:15:MET:SD	1:B:16:LYS:N	2.73	0.55
1:B:42:GLN:OE1	1:B:44:ILE:HD11	2.06	0.55
1:B:98:ALA:HB1	1:B:112:LYS:HE3	1.89	0.55
1:B:295:ARG:NH1	1:B:295:ARG:CG	2.65	0.55
1:C:267:ASN:ND2	1:C:299:ARG:NH2	2.55	0.55
1:D:98:ALA:HB3	1:D:113:ASN:OD1	2.06	0.55
1:A:98:ALA:HB3	1:A:113:ASN:OD1	2.06	0.55
1:B:199:PRO:O	1:B:199:PRO:CG	2.54	0.55
1:D:42:GLN:OE1	1:D:44:ILE:HD11	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:CG	1:C:169:ARG:HG2	2.32	0.55
1:B:267:ASN:ND2	1:B:299:ARG:NH2	2.54	0.55
1:C:160:GLY:CA	1:C:273:SER:HB3	2.33	0.55
1:B:173:LEU:O	1:B:176:GLU:HB3	2.07	0.55
1:A:266:GLU:CG	1:B:74:LYS:HE2	2.36	0.55
1:B:98:ALA:HB3	1:B:113:ASN:OD1	2.06	0.55
1:C:316:HIS:C	1:C:316:HIS:CD2	2.85	0.55
1:A:198:LEU:N	1:A:198:LEU:HD23	2.22	0.55
1:B:110:VAL:O	1:B:114:ILE:HD12	2.07	0.55
1:C:98:ALA:HB1	1:C:112:LYS:HE3	1.89	0.55
1:D:190:ILE:HG12	1:D:200:VAL:CG2	2.36	0.55
1:A:111:ASP:O	1:A:115:ALA:HB2	2.07	0.55
1:A:214:LEU:HD12	1:A:214:LEU:C	2.18	0.55
1:C:35:TYR:HA	1:C:252:ALA:HB1	1.87	0.55
1:A:316:HIS:CD2	1:A:316:HIS:C	2.85	0.54
1:B:21:ALA:HB3	1:B:46:ASP:HB2	1.89	0.54
1:B:87:ARG:O	1:B:88:ASP:CB	2.44	0.54
1:B:111:ASP:O	1:B:115:ALA:HB2	2.07	0.54
1:C:74:LYS:HE2	1:D:266:GLU:CG	2.36	0.54
1:C:173:LEU:O	1:C:176:GLU:HB3	2.07	0.54
1:D:111:ASP:O	1:D:115:ALA:HB2	2.07	0.54
1:A:110:VAL:O	1:A:114:ILE:HD12	2.07	0.54
1:C:199:PRO:O	1:C:199:PRO:CG	2.54	0.54
1:D:173:LEU:O	1:D:176:GLU:HB3	2.07	0.54
1:B:316:HIS:C	1:B:316:HIS:CD2	2.85	0.54
1:C:111:ASP:O	1:C:115:ALA:HB2	2.07	0.54
1:C:132:LEU:HD23	1:C:157:ARG:HB3	1.90	0.54
1:D:267:ASN:ND2	1:D:299:ARG:NH2	2.55	0.54
1:B:283:ARG:HG2	1:B:283:ARG:O	2.08	0.54
1:D:21:ALA:HB3	1:D:46:ASP:HB2	1.90	0.54
1:B:167:THR:O	1:B:171:ARG:HG3	2.08	0.54
1:C:110:VAL:O	1:C:114:ILE:HD12	2.07	0.54
1:A:167:THR:O	1:A:171:ARG:HG3	2.08	0.54
1:D:316:HIS:C	1:D:316:HIS:CD2	2.85	0.54
1:D:319:ALA:O	1:D:323:SER:OG	2.20	0.54
1:C:166:ASP:OD1	1:C:193:HIS:ND1	2.34	0.54
1:D:98:ALA:HB1	1:D:112:LYS:HE3	1.89	0.54
1:A:173:LEU:O	1:A:176:GLU:HB3	2.07	0.54
1:C:83:TYR:C	1:C:85:ASP:H	2.16	0.54
1:D:83:TYR:C	1:D:85:ASP:N	2.66	0.54
1:B:198:LEU:HD23	1:B:198:LEU:N	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:O	1:B:216:GLU:CG	2.53	0.54
1:C:283:ARG:O	1:C:283:ARG:HG2	2.08	0.54
1:D:198:LEU:N	1:D:198:LEU:HD23	2.22	0.54
1:A:98:ALA:HB1	1:A:112:LYS:HE3	1.89	0.54
1:D:167:THR:O	1:D:171:ARG:HG3	2.08	0.54
1:C:21:ALA:HB3	1:C:46:ASP:HB2	1.89	0.53
1:C:83:TYR:CD2	1:C:124:VAL:HG12	2.41	0.53
1:C:132:LEU:HD13	1:C:262:ILE:HD13	1.90	0.53
1:A:21:ALA:HB3	1:A:46:ASP:HB2	1.89	0.53
1:A:132:LEU:HD13	1:A:262:ILE:HD13	1.90	0.53
1:A:204:ALA:O	1:A:211:ILE:HG13	2.09	0.53
1:D:83:TYR:CD2	1:D:124:VAL:HG12	2.41	0.53
1:D:321:LEU:C	1:D:323:SER:N	2.64	0.53
1:C:167:THR:O	1:C:171:ARG:HG3	2.08	0.53
1:C:215:VAL:O	1:C:216:GLU:CB	2.57	0.53
1:C:321:LEU:C	1:C:323:SER:N	2.64	0.53
1:D:110:VAL:O	1:D:114:ILE:HD12	2.07	0.53
1:D:132:LEU:HD23	1:D:157:ARG:HB3	1.90	0.53
1:D:132:LEU:HD13	1:D:262:ILE:HD13	1.90	0.53
1:D:178:PHE:O	1:D:179:SER:CB	2.54	0.53
1:A:83:TYR:C	1:A:85:ASP:N	2.66	0.53
1:C:68:GLY:O	1:C:71:PHE:HB2	2.09	0.53
1:D:154:PRO:HD2	1:D:157:ARG:HD3	1.91	0.53
1:D:199:PRO:O	1:D:199:PRO:CG	2.54	0.53
1:A:278:GLY:HA2	1:A:282:GLU:O	2.09	0.53
1:B:154:PRO:HD2	1:B:157:ARG:HD3	1.91	0.53
1:B:204:ALA:O	1:B:211:ILE:HG13	2.09	0.53
1:C:198:LEU:N	1:C:198:LEU:HD23	2.22	0.53
1:A:67:HIS:HB3	1:C:169:ARG:HG3	1.91	0.53
1:B:73:PRO:O	1:B:74:LYS:CB	2.57	0.53
1:B:294:ASN:C	1:B:294:ASN:ND2	2.67	0.53
1:C:204:ALA:O	1:C:211:ILE:HG13	2.09	0.53
1:C:73:PRO:O	1:C:74:LYS:CB	2.57	0.53
1:D:137:THR:HG22	1:D:143:LEU:CD1	2.39	0.53
1:D:283:ARG:O	1:D:283:ARG:HG2	2.08	0.53
1:A:132:LEU:HD23	1:A:157:ARG:HB3	1.89	0.53
1:A:169:ARG:HG3	1:C:67:HIS:HB3	1.91	0.53
1:A:283:ARG:O	1:A:283:ARG:HG2	2.08	0.53
1:B:83:TYR:C	1:B:85:ASP:H	2.16	0.53
1:B:132:LEU:HD13	1:B:262:ILE:HD13	1.90	0.53
1:B:321:LEU:C	1:B:323:SER:H	2.16	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PRO:HD2	1:C:157:ARG:HD3	1.91	0.53
1:D:202:SER:HA	1:D:218:LYS:HE2	1.91	0.53
1:D:321:LEU:C	1:D:323:SER:H	2.16	0.53
1:A:68:GLY:O	1:A:71:PHE:HB2	2.09	0.53
1:A:83:TYR:C	1:A:85:ASP:H	2.16	0.53
1:A:295:ARG:NH1	1:A:295:ARG:CG	2.65	0.53
1:B:68:GLY:O	1:B:71:PHE:HB2	2.09	0.53
1:D:215:VAL:O	1:D:216:GLU:CB	2.57	0.53
1:A:166:ASP:OD1	1:A:193:HIS:ND1	2.34	0.52
1:C:83:TYR:C	1:C:85:ASP:N	2.66	0.52
1:A:15:MET:SD	1:A:16:LYS:N	2.73	0.52
1:A:294:ASN:C	1:A:294:ASN:ND2	2.67	0.52
1:B:137:THR:HG22	1:B:143:LEU:CD1	2.39	0.52
1:C:137:THR:HG22	1:C:143:LEU:CD1	2.39	0.52
1:D:68:GLY:O	1:D:71:PHE:HB2	2.09	0.52
1:D:278:GLY:HA2	1:D:282:GLU:O	2.09	0.52
1:C:215:VAL:O	1:C:216:GLU:CG	2.54	0.52
1:C:295:ARG:HH11	1:C:295:ARG:CG	2.04	0.52
1:A:73:PRO:O	1:A:74:LYS:CB	2.57	0.52
1:B:132:LEU:HD23	1:B:157:ARG:HB3	1.90	0.52
1:D:204:ALA:O	1:D:211:ILE:HG13	2.09	0.52
1:A:148:TRP:CD1	1:A:153:LEU:O	2.63	0.52
1:C:202:SER:HA	1:C:218:LYS:HE2	1.92	0.52
1:A:154:PRO:HD2	1:A:157:ARG:HD3	1.91	0.52
1:B:278:GLY:HA2	1:B:282:GLU:O	2.09	0.52
1:D:83:TYR:C	1:D:85:ASP:H	2.16	0.52
1:D:148:TRP:CD1	1:D:153:LEU:O	2.63	0.52
1:A:215:VAL:O	1:A:216:GLU:CB	2.57	0.52
1:B:160:GLY:CA	1:B:273:SER:HB3	2.32	0.52
1:B:202:SER:HA	1:B:218:LYS:HE2	1.91	0.52
1:C:148:TRP:CD1	1:C:153:LEU:O	2.63	0.52
1:A:289:VAL:CG1	1:A:301:VAL:HG13	2.40	0.52
1:D:214:LEU:HD12	1:D:214:LEU:C	2.18	0.52
2:B:7:SO4:O3	3:B:5:NAD:O7N	2.28	0.52
1:A:94:ILE:HD11	1:A:133:PHE:CE2	2.45	0.51
1:A:137:THR:HG22	1:A:143:LEU:CD1	2.39	0.51
1:B:67:HIS:HB3	1:D:169:ARG:HG3	1.91	0.51
1:B:215:VAL:O	1:B:216:GLU:CB	2.57	0.51
1:C:278:GLY:HA2	1:C:282:GLU:O	2.09	0.51
1:D:125:MET:HE3	1:D:129:PHE:HB3	1.92	0.51
1:C:110:VAL:CG2	1:C:139:PRO:HG3	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:VAL:CG2	1:D:139:PRO:HG3	2.40	0.51
1:D:321:LEU:O	1:D:323:SER:N	2.44	0.51
1:A:160:GLY:CA	1:A:273:SER:HB3	2.32	0.51
1:A:321:LEU:C	1:A:323:SER:N	2.64	0.51
1:B:94:ILE:HD11	1:B:133:PHE:CE2	2.45	0.51
1:B:289:VAL:CG1	1:B:301:VAL:HG13	2.40	0.51
1:C:289:VAL:CG1	1:C:301:VAL:HG13	2.40	0.51
1:C:321:LEU:C	1:C:323:SER:H	2.16	0.51
1:D:295:ARG:NH1	1:D:295:ARG:CG	2.65	0.51
1:A:216:GLU:CG	1:A:217:SER:N	2.61	0.51
1:A:321:LEU:C	1:A:323:SER:H	2.16	0.51
1:B:142:ILE:HD11	1:B:324:VAL:HG11	1.93	0.51
1:C:94:ILE:HD11	1:C:133:PHE:CE2	2.45	0.51
1:C:189:ILE:HD13	1:C:233:VAL:HG11	1.93	0.51
1:C:265:ASN:HD22	1:C:295:ARG:H	1.58	0.51
1:C:321:LEU:O	1:C:323:SER:N	2.44	0.51
1:D:73:PRO:O	1:D:74:LYS:CB	2.57	0.51
1:D:265:ASN:HD22	1:D:295:ARG:H	1.58	0.51
1:A:125:MET:HE3	1:A:129:PHE:HD2	1.75	0.51
1:A:189:ILE:HD13	1:A:233:VAL:HG11	1.92	0.51
1:D:125:MET:HE3	1:D:129:PHE:HD2	1.75	0.51
1:D:189:ILE:HD13	1:D:233:VAL:HG11	1.93	0.51
1:A:202:SER:HA	1:A:218:LYS:HE2	1.91	0.51
2:A:3:SO4:O3	3:A:1:NAD:O7N	2.29	0.51
1:B:148:TRP:CD1	1:B:153:LEU:O	2.63	0.51
1:B:169:ARG:HG3	1:D:67:HIS:HB3	1.91	0.51
1:B:214:LEU:HD12	1:B:214:LEU:C	2.17	0.51
1:C:125:MET:HE3	1:C:129:PHE:HD2	1.75	0.51
1:C:294:ASN:C	1:C:294:ASN:ND2	2.67	0.51
1:D:94:ILE:HD11	1:D:133:PHE:CE2	2.45	0.51
1:D:243:LYS:HB3	1:D:243:LYS:HZ2	1.75	0.51
1:A:125:MET:HE3	1:A:129:PHE:HB3	1.92	0.51
1:A:321:LEU:O	1:A:323:SER:N	2.44	0.51
1:B:125:MET:HE3	1:B:129:PHE:HD2	1.75	0.51
1:B:279:LEU:CD1	1:B:303:GLU:HG3	2.41	0.51
1:B:321:LEU:O	1:B:323:SER:N	2.44	0.51
1:C:295:ARG:NH1	1:C:295:ARG:CG	2.65	0.51
1:A:125:MET:CE	1:A:129:PHE:HD2	2.24	0.51
1:A:157:ARG:HG2	1:A:157:ARG:NH1	2.26	0.51
1:A:169:ARG:HG2	1:C:67:HIS:CG	2.32	0.51
1:A:169:ARG:CG	1:C:67:HIS:HD2	2.12	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HH11	1:A:313:ARG:CG	2.05	0.51
1:B:265:ASN:HD22	1:B:295:ARG:H	1.58	0.51
1:D:94:ILE:HD11	1:D:133:PHE:CD2	2.45	0.51
1:D:157:ARG:HG2	1:D:157:ARG:NH1	2.25	0.51
1:B:107:LEU:HD13	1:B:328:ALA:HB2	1.93	0.51
1:B:125:MET:HE3	1:B:129:PHE:HB3	1.92	0.51
1:B:169:ARG:O	1:B:173:LEU:HG	2.11	0.51
1:C:63:MET:O	1:C:64:ASP:C	2.54	0.51
1:C:94:ILE:HD11	1:C:133:PHE:CD2	2.46	0.51
1:A:107:LEU:C	1:A:109:LEU:H	2.19	0.50
1:B:110:VAL:CG2	1:B:139:PRO:HG3	2.40	0.50
1:B:125:MET:CE	1:B:129:PHE:HD2	2.24	0.50
1:C:169:ARG:O	1:C:173:LEU:HG	2.11	0.50
2:C:11:SO4:O3	3:C:9:NAD:O7N	2.28	0.50
1:D:63:MET:O	1:D:64:ASP:C	2.54	0.50
1:D:279:LEU:CD1	1:D:303:GLU:HG3	2.41	0.50
1:D:289:VAL:CG1	1:D:301:VAL:HG13	2.40	0.50
1:C:107:LEU:C	1:C:109:LEU:H	2.19	0.50
1:C:125:MET:HE3	1:C:129:PHE:HB3	1.92	0.50
1:D:169:ARG:O	1:D:173:LEU:HG	2.11	0.50
1:A:63:MET:O	1:A:64:ASP:C	2.54	0.50
1:A:169:ARG:O	1:A:173:LEU:HG	2.11	0.50
1:A:178:PHE:O	1:A:179:SER:CB	2.54	0.50
1:A:265:ASN:HD22	1:A:295:ARG:H	1.58	0.50
1:B:189:ILE:HD13	1:B:233:VAL:HG11	1.92	0.50
1:B:284:ASP:H	1:B:322:LYS:HE3	1.77	0.50
1:C:279:LEU:CD1	1:C:303:GLU:HG3	2.41	0.50
1:B:94:ILE:HD11	1:B:133:PHE:CD2	2.45	0.50
1:A:94:ILE:HD11	1:A:133:PHE:CD2	2.45	0.50
1:A:259:THR:HG22	1:A:263:LEU:HD12	1.94	0.50
1:A:279:LEU:CD1	1:A:303:GLU:HG3	2.41	0.50
1:B:169:ARG:CG	1:D:67:HIS:HD2	2.12	0.50
1:C:142:ILE:HD11	1:C:324:VAL:HG11	1.93	0.50
1:C:259:THR:HG22	1:C:263:LEU:HD12	1.94	0.50
1:D:125:MET:CE	1:D:129:PHE:HD2	2.24	0.50
1:B:305:GLU:HB2	1:C:209:MET:HE1	1.93	0.50
1:B:321:LEU:C	1:B:323:SER:N	2.64	0.50
1:A:329:PHE:O	1:A:331:ARG:N	2.45	0.50
1:B:63:MET:O	1:B:64:ASP:C	2.54	0.50
1:C:284:ASP:H	1:C:322:LYS:HE3	1.76	0.50
1:A:107:LEU:HD13	1:A:328:ALA:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:HB2	1:D:209:MET:HE1	1.93	0.50
1:B:157:ARG:HG2	1:B:157:ARG:NH1	2.26	0.50
1:B:209:MET:HE1	1:C:305:GLU:HB2	1.93	0.50
1:B:67:HIS:CG	1:D:169:ARG:HG2	2.32	0.50
1:B:169:ARG:NH1	2:B:7:SO4:O2	2.38	0.50
1:C:125:MET:CE	1:C:129:PHE:HD2	2.24	0.50
1:D:259:THR:HG22	1:D:263:LEU:HD12	1.94	0.50
1:A:142:ILE:HD11	1:A:324:VAL:HG11	1.93	0.49
1:B:83:TYR:C	1:B:85:ASP:N	2.66	0.49
1:B:107:LEU:C	1:B:109:LEU:H	2.19	0.49
1:C:329:PHE:O	1:C:331:ARG:N	2.45	0.49
1:D:284:ASP:H	1:D:322:LYS:HE3	1.76	0.49
1:B:329:PHE:O	1:B:331:ARG:N	2.45	0.49
1:C:107:LEU:HD13	1:C:328:ALA:HB2	1.93	0.49
1:D:329:PHE:O	1:D:331:ARG:N	2.45	0.49
2:D:332:SO4:O3	3:D:13:NAD:O7N	2.28	0.49
1:A:110:VAL:CG2	1:A:139:PRO:HG3	2.40	0.49
1:A:209:MET:HE1	1:D:305:GLU:HB2	1.93	0.49
1:B:83:TYR:CD2	1:B:124:VAL:HG12	2.41	0.49
1:A:32:GLY:O	1:A:35:TYR:HB3	2.13	0.49
1:D:142:ILE:HD11	1:D:324:VAL:HG11	1.93	0.49
1:C:234:ARG:HG2	1:C:234:ARG:O	2.13	0.49
1:C:244:LYS:O	1:C:244:LYS:CG	2.55	0.49
1:D:107:LEU:HD13	1:D:328:ALA:HB2	1.93	0.49
1:B:243:LYS:HB3	1:B:243:LYS:HZ2	1.75	0.49
1:B:259:THR:HG22	1:B:263:LEU:HD12	1.94	0.49
1:D:196:THR:HG21	1:D:320:THR:HG21	1.95	0.49
1:B:32:GLY:O	1:B:35:TYR:HB3	2.13	0.49
1:B:234:ARG:O	1:B:234:ARG:HG2	2.13	0.49
1:D:107:LEU:C	1:D:109:LEU:H	2.19	0.49
1:A:174:LEU:HD23	1:A:229:ILE:HD12	1.95	0.49
1:A:205:TYR:HD2	1:A:210:PRO:HA	1.78	0.49
1:B:205:TYR:HD2	1:B:210:PRO:HA	1.78	0.49
1:C:226:LEU:C	1:C:228:ARG:N	2.64	0.49
1:D:205:TYR:HD2	1:D:210:PRO:HA	1.78	0.49
1:A:164:ILE:HG21	1:A:164:ILE:HD13	1.48	0.48
1:C:32:GLY:O	1:C:35:TYR:HB3	2.13	0.48
1:C:169:ARG:NH1	2:C:11:SO4:O2	2.38	0.48
1:C:214:LEU:HD12	1:C:214:LEU:C	2.17	0.48
1:C:157:ARG:HG2	1:C:157:ARG:NH1	2.25	0.48
1:D:32:GLY:O	1:D:35:TYR:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:HG21	1:A:304:ILE:CD1	2.44	0.48
1:A:226:LEU:C	1:A:228:ARG:N	2.63	0.48
1:D:174:LEU:HD23	1:D:229:ILE:HD12	1.95	0.48
1:A:234:ARG:O	1:A:234:ARG:HG2	2.13	0.48
1:A:284:ASP:H	1:A:322:LYS:HE3	1.77	0.48
1:D:145:TYR:O	1:D:148:TRP:HB3	2.13	0.48
1:D:328:ALA:O	1:D:329:PHE:CB	2.62	0.48
1:A:145:TYR:O	1:A:148:TRP:HB3	2.14	0.48
1:B:145:TYR:O	1:B:148:TRP:HB3	2.14	0.48
1:C:145:TYR:O	1:C:148:TRP:HB3	2.13	0.48
1:C:174:LEU:HD23	1:C:229:ILE:HD12	1.95	0.48
1:C:200:VAL:HG21	1:C:304:ILE:CD1	2.44	0.48
1:D:294:ASN:C	1:D:294:ASN:ND2	2.67	0.48
1:D:200:VAL:HG21	1:D:304:ILE:CD1	2.44	0.48
1:D:234:ARG:O	1:D:234:ARG:HG2	2.13	0.48
1:B:196:THR:HG21	1:B:320:THR:HG21	1.95	0.48
1:C:239:GLN:O	1:C:242:GLU:HG2	2.14	0.48
1:D:244:LYS:O	1:D:244:LYS:CG	2.55	0.48
1:A:253:MET:HE2	1:C:72:ALA:HB2	1.96	0.47
1:B:174:LEU:HD23	1:B:229:ILE:HD12	1.95	0.47
1:A:196:THR:HG21	1:A:320:THR:HG21	1.95	0.47
1:A:228:ARG:HH11	1:A:228:ARG:HD2	1.47	0.47
1:A:307:ASN:HB3	1:A:310:GLU:CD	2.39	0.47
1:B:200:VAL:HG21	1:B:304:ILE:CD1	2.43	0.47
1:B:203:GLN:HE22	1:B:305:GLU:H	1.62	0.47
1:C:307:ASN:HB3	1:C:310:GLU:CD	2.39	0.47
1:D:239:GLN:O	1:D:242:GLU:HG2	2.14	0.47
1:B:226:LEU:C	1:B:228:ARG:N	2.63	0.47
1:B:307:ASN:HB3	1:B:310:GLU:CD	2.39	0.47
1:B:328:ALA:O	1:B:329:PHE:CB	2.62	0.47
1:C:74:LYS:HE2	1:D:266:GLU:OE2	2.15	0.47
1:C:205:TYR:HD2	1:C:210:PRO:HA	1.78	0.47
1:C:279:LEU:HD12	1:C:303:GLU:HG3	1.97	0.47
1:C:178:PHE:O	1:C:179:SER:CB	2.54	0.47
1:B:164:ILE:HG21	1:B:164:ILE:HD13	1.48	0.47
1:A:279:LEU:HD12	1:A:303:GLU:HG3	1.97	0.47
1:B:72:ALA:HB2	1:D:253:MET:HE2	1.96	0.47
1:B:279:LEU:HD12	1:B:303:GLU:HG3	1.97	0.47
1:C:328:ALA:O	1:C:329:PHE:CB	2.62	0.47
1:D:155:HIS:CD2	1:D:275:TYR:HB3	2.50	0.47
1:B:239:GLN:O	1:B:242:GLU:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:MET:HE1	1:C:18:ASN:CA	2.44	0.47
1:C:86:CYS:O	1:C:127:SER:OG	2.31	0.47
1:D:15:MET:HE1	1:D:18:ASN:CA	2.44	0.47
1:A:155:HIS:CD2	1:A:275:TYR:HB3	2.50	0.47
1:A:328:ALA:O	1:A:329:PHE:CB	2.62	0.47
1:C:111:ASP:HB3	1:C:331:ARG:O	2.15	0.47
1:D:203:GLN:HE22	1:D:305:GLU:H	1.62	0.47
1:A:132:LEU:HD12	1:A:262:ILE:CG2	2.45	0.47
1:B:15:MET:HE1	1:B:18:ASN:CA	2.44	0.47
1:C:155:HIS:CD2	1:C:275:TYR:HB3	2.50	0.47
1:C:226:LEU:HA	1:C:229:ILE:HG13	1.97	0.47
1:D:226:LEU:C	1:D:228:ARG:N	2.64	0.47
1:D:307:ASN:HB3	1:D:310:GLU:CD	2.39	0.47
1:A:86:CYS:O	1:A:127:SER:OG	2.31	0.47
1:C:190:ILE:CD1	1:C:306:LEU:HD11	2.44	0.47
1:A:226:LEU:HA	1:A:229:ILE:HG13	1.97	0.46
1:B:67:HIS:HD2	1:D:169:ARG:CG	2.12	0.46
1:C:87:ARG:O	1:C:88:ASP:CB	2.44	0.46
1:B:305:GLU:HB3	1:C:209:MET:HE1	1.98	0.46
1:C:196:THR:HG21	1:C:320:THR:HG21	1.95	0.46
1:A:15:MET:HE1	1:A:18:ASN:CA	2.44	0.46
1:A:239:GLN:O	1:A:242:GLU:HG2	2.14	0.46
1:A:266:GLU:OE2	1:B:74:LYS:HE2	2.15	0.46
1:B:18:ASN:OD1	1:B:18:ASN:N	2.47	0.46
1:C:18:ASN:OD1	1:C:18:ASN:N	2.47	0.46
1:D:18:ASN:OD1	1:D:18:ASN:N	2.47	0.46
1:D:279:LEU:HD12	1:D:303:GLU:HG3	1.97	0.46
1:A:142:ILE:CD1	1:A:324:VAL:HG11	2.46	0.46
1:B:86:CYS:O	1:B:127:SER:OG	2.31	0.46
1:B:262:ILE:HD13	1:B:262:ILE:HG21	1.56	0.46
1:A:198:LEU:HD23	1:A:198:LEU:H	1.81	0.46
1:B:142:ILE:CD1	1:B:324:VAL:HG11	2.46	0.46
1:B:155:HIS:CD2	1:B:275:TYR:HB3	2.50	0.46
1:C:203:GLN:HE22	1:C:305:GLU:H	1.62	0.46
1:D:153:LEU:HA	1:D:154:PRO:HD3	1.81	0.46
1:D:198:LEU:HD23	1:D:198:LEU:H	1.81	0.46
1:A:86:CYS:HA	1:A:89:ALA:CB	2.46	0.46
1:A:169:ARG:NH1	2:A:3:SO4:O2	2.38	0.46
1:A:203:GLN:HE21	1:A:304:ILE:HB	1.81	0.46
1:A:209:MET:HE1	1:D:305:GLU:HB3	1.97	0.46
1:B:203:GLN:HE21	1:B:304:ILE:HB	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HA	1:B:229:ILE:HG13	1.97	0.46
1:C:142:ILE:CD1	1:C:324:VAL:HG11	2.46	0.46
1:C:203:GLN:HE21	1:C:304:ILE:HB	1.81	0.46
1:C:266:GLU:OE2	1:D:74:LYS:HE2	2.15	0.46
1:D:111:ASP:HB3	1:D:331:ARG:O	2.15	0.46
1:D:142:ILE:CD1	1:D:324:VAL:HG11	2.46	0.46
1:B:198:LEU:HD23	1:B:198:LEU:H	1.81	0.46
1:B:203:GLN:NE2	1:B:304:ILE:HB	2.31	0.46
1:C:132:LEU:HD12	1:C:262:ILE:CG2	2.45	0.46
1:D:160:GLY:CA	1:D:273:SER:CB	2.93	0.46
1:D:203:GLN:HE21	1:D:304:ILE:HB	1.81	0.46
1:A:82:ASP:HB3	1:A:83:TYR:H	1.34	0.46
1:A:83:TYR:CD2	1:A:124:VAL:HG12	2.40	0.46
1:A:262:ILE:HD13	1:A:262:ILE:HG21	1.57	0.46
1:B:59:ILE:HG13	1:B:79:TRP:CE2	2.51	0.46
1:B:190:ILE:CD1	1:B:306:LEU:HD11	2.44	0.46
1:C:203:GLN:NE2	1:C:304:ILE:HB	2.31	0.46
1:C:216:GLU:CG	1:C:217:SER:N	2.61	0.46
1:D:169:ARG:NH1	2:D:332:SO4:O2	2.38	0.46
1:A:72:ALA:HB2	1:C:253:MET:HE2	1.96	0.46
1:B:153:LEU:HA	1:B:154:PRO:HD3	1.81	0.46
1:B:209:MET:HB3	1:B:213:LYS:CE	2.46	0.46
1:B:269:ILE:HD13	1:B:269:ILE:HG21	1.70	0.46
1:D:86:CYS:HA	1:D:89:ALA:CB	2.46	0.46
1:A:74:LYS:HE2	1:B:266:GLU:OE2	2.15	0.45
1:B:111:ASP:HB3	1:B:331:ARG:O	2.15	0.45
1:B:132:LEU:HD12	1:B:262:ILE:CG2	2.45	0.45
1:B:178:PHE:O	1:B:179:SER:CB	2.54	0.45
1:B:253:MET:HE2	1:D:72:ALA:HB2	1.96	0.45
1:D:132:LEU:HD12	1:D:262:ILE:CG2	2.45	0.45
1:D:226:LEU:HA	1:D:229:ILE:HG13	1.97	0.45
1:A:18:ASN:OD1	1:A:18:ASN:N	2.47	0.45
1:A:59:ILE:HG13	1:A:79:TRP:CE2	2.51	0.45
1:A:203:GLN:HE22	1:A:305:GLU:H	1.62	0.45
1:C:86:CYS:HA	1:C:89:ALA:CB	2.46	0.45
1:A:293:ILE:O	1:A:294:ASN:HB3	2.17	0.45
1:C:59:ILE:HG13	1:C:79:TRP:CE2	2.51	0.45
1:A:111:ASP:HB3	1:A:331:ARG:O	2.15	0.45
1:B:15:MET:CE	1:B:18:ASN:CB	2.79	0.45
1:B:86:CYS:HA	1:B:89:ALA:CB	2.46	0.45
1:B:262:ILE:O	1:B:295:ARG:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ILE:HD13	1:B:302:ILE:HD13	1.99	0.45
1:D:262:ILE:O	1:D:295:ARG:HA	2.17	0.45
1:A:203:GLN:NE2	1:A:304:ILE:HB	2.31	0.45
1:A:243:LYS:HB2	1:C:56:SER:O	2.17	0.45
1:A:305:GLU:HB3	1:D:209:MET:HE1	1.98	0.45
1:B:37:PHE:HE2	1:D:34:SER:O	2.00	0.45
1:B:113:ASN:OD1	1:B:116:ILE:HD12	2.17	0.45
1:B:209:MET:HE1	1:C:305:GLU:HB3	1.97	0.45
1:C:262:ILE:O	1:C:295:ARG:HA	2.17	0.45
1:D:59:ILE:HG13	1:D:79:TRP:CE2	2.51	0.45
1:D:262:ILE:HD13	1:D:262:ILE:HG21	1.56	0.45
1:D:269:ILE:HD13	1:D:302:ILE:HD13	1.99	0.45
1:A:190:ILE:CD1	1:A:306:LEU:HD11	2.45	0.45
1:A:243:LYS:HB3	1:A:243:LYS:HZ2	1.77	0.45
1:A:262:ILE:O	1:A:295:ARG:HA	2.17	0.45
1:B:243:LYS:HB2	1:D:56:SER:O	2.17	0.45
1:C:113:ASN:OD1	1:C:116:ILE:HD12	2.17	0.45
1:C:244:LYS:HE2	1:C:248:TYR:CZ	2.52	0.45
1:C:284:ASP:N	1:C:322:LYS:NZ	2.65	0.45
1:D:203:GLN:NE2	1:D:304:ILE:HB	2.31	0.45
1:A:284:ASP:N	1:A:322:LYS:NZ	2.65	0.45
1:B:56:SER:O	1:D:243:LYS:HB2	2.17	0.45
1:C:241:ILE:O	1:C:245:GLY:N	2.49	0.45
1:D:209:MET:HB3	1:D:213:LYS:CE	2.46	0.45
1:D:216:GLU:CG	1:D:217:SER:N	2.61	0.45
1:D:293:ILE:O	1:D:294:ASN:HB3	2.17	0.45
1:A:37:PHE:HE2	1:C:34:SER:O	2.00	0.45
1:B:244:LYS:O	1:B:244:LYS:CG	2.55	0.45
1:B:283:ARG:H	1:B:322:LYS:NZ	2.03	0.45
1:C:209:MET:HB3	1:C:213:LYS:CE	2.46	0.45
1:A:269:ILE:HD13	1:A:302:ILE:HD13	1.99	0.45
1:C:198:LEU:HD23	1:C:198:LEU:H	1.81	0.45
1:C:293:ILE:O	1:C:294:ASN:HB3	2.17	0.45
1:D:39:LEU:HD22	1:D:44:ILE:HB	1.99	0.45
1:A:244:LYS:HE2	1:A:248:TYR:CZ	2.52	0.44
1:B:34:SER:O	1:D:37:PHE:HE2	2.00	0.44
1:B:244:LYS:HE2	1:B:248:TYR:CZ	2.52	0.44
1:D:113:ASN:OD1	1:D:116:ILE:HD12	2.17	0.44
1:A:39:LEU:HD22	1:A:44:ILE:HB	1.99	0.44
1:A:170:PHE:HD1	1:A:233:VAL:HG21	1.83	0.44
1:C:39:LEU:HD22	1:C:44:ILE:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LYS:HE2	1:D:248:TYR:CZ	2.52	0.44
1:A:56:SER:O	1:C:243:LYS:HB2	2.17	0.44
1:C:153:LEU:HA	1:C:154:PRO:HD3	1.81	0.44
1:C:269:ILE:HD13	1:C:302:ILE:HD13	1.99	0.44
1:C:294:ASN:HD22	1:C:295:ARG:N	2.15	0.44
1:D:164:ILE:HD13	1:D:164:ILE:HG21	1.48	0.44
1:A:113:ASN:OD1	1:A:116:ILE:HD12	2.17	0.44
1:B:39:LEU:HD22	1:B:44:ILE:HB	1.99	0.44
1:B:82:ASP:HB3	1:B:83:TYR:H	1.34	0.44
1:C:249:TYR:OH	5:C:385:HOH:O	2.16	0.44
1:A:63:MET:O	1:A:66:ASN:N	2.51	0.44
1:A:209:MET:HB3	1:A:213:LYS:CE	2.46	0.44
1:B:283:ARG:O	1:B:284:ASP:HB2	2.18	0.44
1:B:294:ASN:HD22	1:B:295:ARG:N	2.15	0.44
1:C:39:LEU:HD23	1:C:39:LEU:HA	1.72	0.44
1:C:254:GLY:O	1:C:258:VAL:HG23	2.18	0.44
1:D:284:ASP:N	1:D:322:LYS:NZ	2.65	0.44
1:B:63:MET:O	1:B:66:ASN:N	2.51	0.44
1:B:170:PHE:HD1	1:B:233:VAL:HG21	1.83	0.44
1:D:170:PHE:HD1	1:D:233:VAL:HG21	1.83	0.44
1:D:269:ILE:HD13	1:D:269:ILE:HG21	1.70	0.44
1:A:34:SER:O	1:C:37:PHE:HE2	2.00	0.44
1:A:125:MET:HE3	1:A:129:PHE:CD2	2.53	0.44
1:B:70:VAL:H	1:B:70:VAL:HG23	1.42	0.44
1:C:295:ARG:HG3	1:D:18:ASN:HD21	1.83	0.44
1:D:254:GLY:O	1:D:258:VAL:HG23	2.18	0.44
1:A:170:PHE:CD1	1:A:233:VAL:HG21	2.53	0.43
1:A:253:MET:HE1	1:C:41:ASN:OD1	2.18	0.43
1:C:63:MET:O	1:C:66:ASN:N	2.51	0.43
1:C:283:ARG:O	1:C:284:ASP:HB2	2.18	0.43
1:D:63:MET:O	1:D:66:ASN:N	2.51	0.43
1:A:171:ARG:HH11	1:A:171:ARG:HD3	1.56	0.43
1:A:244:LYS:O	1:A:244:LYS:CG	2.55	0.43
1:B:170:PHE:CD1	1:B:233:VAL:HG21	2.53	0.43
1:B:241:ILE:O	1:B:245:GLY:N	2.49	0.43
1:B:284:ASP:N	1:B:322:LYS:NZ	2.65	0.43
1:C:262:ILE:HD13	1:C:262:ILE:HG21	1.56	0.43
1:D:15:MET:CE	1:D:18:ASN:CB	2.78	0.43
1:D:190:ILE:CD1	1:D:306:LEU:HD11	2.44	0.43
1:B:293:ILE:O	1:B:294:ASN:HB3	2.17	0.43
1:C:201:TRP:NE1	1:C:227:GLU:OE1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:PHE:CD1	1:D:233:VAL:HG21	2.54	0.43
1:D:322:LYS:HA	1:D:325:LEU:HD12	2.01	0.43
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.59	0.43
1:A:241:ILE:O	1:A:245:GLY:N	2.49	0.43
1:A:283:ARG:O	1:A:284:ASP:HB2	2.18	0.43
1:B:253:MET:HE1	1:D:41:ASN:OD1	2.18	0.43
1:C:243:LYS:HB3	1:C:243:LYS:HZ2	1.78	0.43
1:A:41:ASN:OD1	1:C:253:MET:HE1	2.18	0.43
1:A:295:ARG:HG3	1:B:18:ASN:HD21	1.83	0.43
1:D:171:ARG:HH11	1:D:171:ARG:HD3	1.56	0.43
1:A:18:ASN:HD21	1:B:295:ARG:HG3	1.83	0.43
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.73	0.43
1:A:107:LEU:HD22	1:A:327:ARG:CG	2.49	0.43
1:B:107:LEU:HD22	1:B:327:ARG:CG	2.49	0.43
1:B:329:PHE:HB3	1:B:330:THR:H	1.58	0.43
1:C:109:LEU:HA	1:C:109:LEU:HD12	1.59	0.43
1:D:198:LEU:O	1:D:198:LEU:HG	2.18	0.43
1:A:31:VAL:HG22	1:A:251:ILE:CG2	2.48	0.43
1:A:196:THR:CG2	1:A:320:THR:HG21	2.49	0.43
1:D:283:ARG:O	1:D:284:ASP:HB2	2.18	0.43
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.60	0.43
1:B:196:THR:CG2	1:B:320:THR:HG21	2.49	0.43
1:C:160:GLY:CA	1:C:273:SER:CB	2.93	0.43
1:C:170:PHE:CD1	1:C:233:VAL:HG21	2.53	0.43
1:D:241:ILE:O	1:D:245:GLY:N	2.49	0.43
1:B:254:GLY:O	1:B:258:VAL:HG23	2.18	0.43
1:C:121:VAL:O	1:C:124:VAL:HG22	2.19	0.43
1:C:170:PHE:HD1	1:C:233:VAL:HG21	1.83	0.43
1:C:183:GLN:NE2	4:C:6:FBP:H4	2.33	0.43
1:A:322:LYS:HA	1:A:325:LEU:HD12	2.01	0.43
1:A:329:PHE:HB3	1:A:330:THR:H	1.58	0.43
1:B:39:LEU:HD23	1:B:39:LEU:HA	1.73	0.43
1:D:109:LEU:HD12	1:D:109:LEU:HA	1.59	0.43
1:A:260:ARG:HH11	1:A:260:ARG:HD2	1.15	0.42
1:B:121:VAL:O	1:B:124:VAL:HG22	2.19	0.42
1:C:138:ASN:OD1	3:C:9:NAD:C2N	2.67	0.42
1:C:196:THR:CG2	1:C:320:THR:HG21	2.49	0.42
1:D:31:VAL:HG22	1:D:251:ILE:CG2	2.49	0.42
1:A:138:ASN:OD1	3:A:1:NAD:C2N	2.68	0.42
1:A:198:LEU:HG	1:A:198:LEU:O	2.18	0.42
1:A:323:SER:C	1:A:325:LEU:N	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:GLN:NE2	4:D:2:FBP:H4	2.33	0.42
1:A:254:GLY:O	1:A:258:VAL:HG23	2.18	0.42
1:C:31:VAL:HG22	1:C:251:ILE:CG2	2.49	0.42
1:D:260:ARG:HH11	1:D:260:ARG:HD2	1.15	0.42
1:A:294:ASN:HD22	1:A:295:ARG:N	2.15	0.42
1:B:322:LYS:HA	1:B:325:LEU:HD12	2.01	0.42
1:B:31:VAL:HG22	1:B:251:ILE:CG2	2.49	0.42
1:B:201:TRP:NE1	1:B:227:GLU:OE1	2.51	0.42
1:C:322:LYS:HA	1:C:325:LEU:HD12	2.01	0.42
1:D:125:MET:HE3	1:D:129:PHE:CD2	2.53	0.42
1:B:129:PHE:HE2	1:B:133:PHE:CE1	2.37	0.42
1:B:267:ASN:H	1:B:294:ASN:HB3	1.85	0.42
1:C:328:ALA:O	1:C:329:PHE:HB2	2.20	0.42
1:B:41:ASN:OD1	1:D:253:MET:HE1	2.18	0.42
1:B:198:LEU:O	1:B:198:LEU:HG	2.18	0.42
1:C:156:GLU:O	1:C:298:ILE:N	2.50	0.42
1:C:198:LEU:HG	1:C:198:LEU:O	2.18	0.42
1:D:138:ASN:OD1	3:D:13:NAD:C2N	2.67	0.42
1:D:143:LEU:HD23	1:D:143:LEU:HA	1.93	0.42
1:A:124:VAL:CG2	1:A:133:PHE:HZ	2.32	0.42
1:B:328:ALA:O	1:B:329:PHE:HB2	2.20	0.42
1:B:138:ASN:OD1	3:B:5:NAD:C2N	2.68	0.42
1:C:18:ASN:HD21	1:D:295:ARG:HG3	1.83	0.42
1:C:192:GLU:HB3	1:C:196:THR:OG1	2.20	0.42
1:C:276:LEU:HG	1:C:287:ILE:HG22	2.02	0.42
1:D:121:VAL:O	1:D:124:VAL:HG22	2.19	0.42
1:D:283:ARG:H	1:D:322:LYS:NZ	2.03	0.42
1:D:294:ASN:HD22	1:D:295:ARG:N	2.15	0.42
1:A:121:VAL:O	1:A:124:VAL:HG22	2.19	0.42
1:A:267:ASN:H	1:A:294:ASN:HB3	1.85	0.42
1:B:253:MET:CE	1:D:72:ALA:HB2	2.50	0.42
1:C:124:VAL:CG2	1:C:133:PHE:HZ	2.33	0.42
1:C:165:LEU:HD21	1:C:169:ARG:NH2	2.35	0.42
1:D:201:TRP:NE1	1:D:227:GLU:OE1	2.52	0.42
1:D:323:SER:C	1:D:325:LEU:N	2.77	0.42
1:A:253:MET:CE	1:C:72:ALA:HB2	2.50	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.92	0.41
1:C:267:ASN:H	1:C:294:ASN:HB3	1.85	0.41
1:D:107:LEU:HD22	1:D:327:ARG:CG	2.49	0.41
1:D:124:VAL:CG2	1:D:133:PHE:HZ	2.33	0.41
1:D:165:LEU:HD21	1:D:169:ARG:NH2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TRP:NE1	1:A:227:GLU:OE1	2.52	0.41
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.93	0.41
1:B:125:MET:HE3	1:B:129:PHE:CD2	2.53	0.41
1:B:228:ARG:HH11	1:B:228:ARG:HD2	1.47	0.41
1:C:125:MET:HE3	1:C:129:PHE:CD2	2.53	0.41
1:C:276:LEU:HD21	1:C:289:VAL:HG21	2.03	0.41
1:A:15:MET:CE	1:A:18:ASN:CB	2.79	0.41
1:D:173:LEU:HA	1:D:173:LEU:HD23	1.61	0.41
1:D:196:THR:CG2	1:D:320:THR:HG21	2.49	0.41
1:A:72:ALA:HB2	1:C:253:MET:CE	2.50	0.41
1:A:156:GLU:O	1:A:298:ILE:N	2.50	0.41
1:C:227:GLU:OE1	1:C:227:GLU:HA	2.20	0.41
1:D:148:TRP:HD1	1:D:153:LEU:O	2.04	0.41
1:A:124:VAL:HG21	1:A:133:PHE:HZ	1.86	0.41
1:B:72:ALA:HB2	1:D:253:MET:CE	2.50	0.41
1:B:160:GLY:CA	1:B:273:SER:CB	2.93	0.41
1:B:165:LEU:HD21	1:B:169:ARG:NH2	2.35	0.41
1:C:276:LEU:HD23	1:C:276:LEU:HA	1.92	0.41
1:C:284:ASP:C	1:C:322:LYS:HE3	2.46	0.41
1:A:83:TYR:CD2	1:A:124:VAL:CG1	3.04	0.41
1:B:134:LEU:HD21	1:B:255:LEU:HD12	2.03	0.41
1:B:276:LEU:HG	1:B:287:ILE:HG22	2.02	0.41
1:B:323:SER:C	1:B:325:LEU:N	2.77	0.41
1:D:192:GLU:HB3	1:D:196:THR:OG1	2.20	0.41
1:D:276:LEU:HG	1:D:287:ILE:HG22	2.02	0.41
1:D:276:LEU:HD21	1:D:289:VAL:HG21	2.03	0.41
1:A:227:GLU:OE1	1:A:227:GLU:HA	2.20	0.41
1:D:267:ASN:H	1:D:294:ASN:HB3	1.85	0.41
1:D:328:ALA:O	1:D:329:PHE:HB2	2.20	0.41
2:D:332:SO4:O3	3:D:13:NAD:C7N	2.69	0.41
2:A:3:SO4:O3	3:A:1:NAD:C7N	2.69	0.41
1:B:124:VAL:CG2	1:B:133:PHE:HZ	2.32	0.41
2:B:7:SO4:O3	3:B:5:NAD:C7N	2.69	0.41
1:C:129:PHE:HE2	1:C:133:PHE:CE1	2.37	0.41
2:C:11:SO4:O3	3:C:9:NAD:C7N	2.69	0.41
1:D:39:LEU:HA	1:D:39:LEU:HD23	1.73	0.41
1:D:83:TYR:CD2	1:D:124:VAL:CG1	3.04	0.41
1:A:194:GLY:O	1:A:197:GLU:OE2	2.39	0.41
1:B:26:ILE:HG21	1:B:120:ILE:CG2	2.52	0.40
1:B:124:VAL:HG21	1:B:133:PHE:HZ	1.86	0.40
1:B:227:GLU:OE1	1:B:227:GLU:HA	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LEU:HD12	1:B:303:GLU:CG	2.51	0.40
1:B:284:ASP:C	1:B:322:LYS:HE3	2.46	0.40
1:C:83:TYR:CD2	1:C:124:VAL:CG1	3.04	0.40
1:D:54:ASN:C	1:D:54:ASN:ND2	2.79	0.40
1:A:192:GLU:HB3	1:A:196:THR:OG1	2.20	0.40
1:A:328:ALA:O	1:A:329:PHE:HB2	2.20	0.40
1:B:194:GLY:O	1:B:197:GLU:OE2	2.39	0.40
1:B:276:LEU:HD21	1:B:289:VAL:HG21	2.03	0.40
1:C:267:ASN:HA	1:C:293:ILE:O	2.21	0.40
1:C:279:LEU:HD12	1:C:303:GLU:CG	2.51	0.40
1:D:24:VAL:HG22	1:D:49:VAL:CG2	2.52	0.40
1:A:54:ASN:C	1:A:54:ASN:ND2	2.79	0.40
1:B:52:ASP:C	1:B:54:ASN:N	2.78	0.40
1:B:98:ALA:CB	1:B:113:ASN:OD1	2.70	0.40
1:B:169:ARG:CG	1:D:67:HIS:CG	3.01	0.40
1:C:173:LEU:HA	1:C:173:LEU:HD23	1.60	0.40
1:C:228:ARG:HH11	1:C:228:ARG:HD2	1.47	0.40
1:C:323:SER:C	1:C:325:LEU:N	2.77	0.40
1:D:276:LEU:HD23	1:D:276:LEU:HA	1.92	0.40
1:A:24:VAL:HG22	1:A:49:VAL:CG2	2.52	0.40
1:A:67:HIS:HD2	1:C:169:ARG:CG	2.12	0.40
1:A:165:LEU:HD21	1:A:169:ARG:NH2	2.36	0.40
1:A:269:ILE:HD13	1:A:269:ILE:HG21	1.70	0.40
1:C:26:ILE:HG21	1:C:120:ILE:CG2	2.52	0.40
1:C:329:PHE:HB3	1:C:330:THR:H	1.59	0.40
1:D:134:LEU:HD21	1:D:255:LEU:HD12	2.03	0.40
1:A:267:ASN:HA	1:A:293:ILE:O	2.21	0.40
1:A:284:ASP:C	1:A:322:LYS:HE3	2.46	0.40
1:B:24:VAL:HG22	1:B:49:VAL:CG2	2.52	0.40
1:D:279:LEU:HD12	1:D:303:GLU:CG	2.52	0.40

All (63) 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)
1:A:326:ALA:C	1:D:331:ARG:CB[6_665]	0.13	2.07
1:A:327:ARG:CB	1:D:330:THR:O[6_665]	0.27	1.93
1:A:324:VAL:N	1:D:330:THR:CG2[6_665]	0.54	1.66
1:A:325:LEU:C	1:D:331:ARG:NE[6_665]	0.77	1.43
1:B:107:LEU:CG	5:A:378:HOH:O[5_554]	0.77	1.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:HIS:CE1	1:D:316:HIS:NE2[6_655]	0.93	1.27
1:A:327:ARG:CB	1:D:330:THR:C[6_665]	1.03	1.17
1:A:327:ARG:N	1:D:331:ARG:CA[6_665]	1.05	1.15
1:A:323:SER:C	1:D:330:THR:CB[6_665]	1.06	1.14
1:A:325:LEU:O	1:D:331:ARG:NE[6_665]	1.10	1.10
1:A:325:LEU:C	1:D:331:ARG:CD[6_665]	1.17	1.03
1:C:316:HIS:NE2	1:D:316:HIS:CE1[6_655]	1.20	1.00
1:A:327:ARG:N	1:D:331:ARG:N[6_665]	1.21	0.99
1:A:323:SER:O	1:D:330:THR:CB[6_665]	1.24	0.96
1:A:325:LEU:O	1:D:331:ARG:CD[6_665]	1.24	0.96
1:A:326:ALA:O	1:D:331:ARG:CB[6_665]	1.31	0.89
1:A:326:ALA:N	1:D:331:ARG:CD[6_665]	1.33	0.87
1:A:326:ALA:N	1:D:331:ARG:CG[6_665]	1.34	0.86
1:A:327:ARG:CG	1:D:330:THR:O[6_665]	1.39	0.81
1:C:316:HIS:CE1	1:D:316:HIS:CE1[6_655]	1.39	0.81
1:C:316:HIS:NE2	1:D:316:HIS:NE2[6_655]	1.39	0.81
1:A:326:ALA:CA	1:D:331:ARG:CB[6_665]	1.40	0.80
1:A:327:ARG:N	1:D:331:ARG:CB[6_665]	1.40	0.80
1:A:111:ASP:OD2	1:D:118:ARG:NH2[6_665]	1.44	0.76
1:A:326:ALA:C	1:D:331:ARG:CA[6_665]	1.46	0.74
1:A:327:ARG:CA	1:D:330:THR:O[6_665]	1.48	0.72
1:A:323:SER:C	1:D:330:THR:CG2[6_665]	1.49	0.71
1:A:325:LEU:CB	1:D:331:ARG:NH2[6_665]	1.53	0.67
1:A:326:ALA:CA	1:D:331:ARG:CG[6_665]	1.53	0.67
1:C:235:ASP:OD2	1:D:235:ASP:OD2[6_655]	1.53	0.67
1:A:327:ARG:CA	1:D:331:ARG:CA[6_665]	1.55	0.65
1:A:326:ALA:C	1:D:331:ARG:CG[6_665]	1.57	0.63
1:A:325:LEU:CA	1:D:331:ARG:NE[6_665]	1.59	0.61
1:A:326:ALA:CA	1:D:331:ARG:CD[6_665]	1.61	0.59
1:A:324:VAL:N	1:D:330:THR:CB[6_665]	1.64	0.56
1:A:327:ARG:CA	1:D:331:ARG:N[6_665]	1.67	0.53
1:A:327:ARG:CA	1:D:330:THR:C[6_665]	1.68	0.52
1:A:324:VAL:CA	1:D:330:THR:CG2[6_665]	1.69	0.51
1:B:107:LEU:CD1	5:A:378:HOH:O[5_554]	1.69	0.51
1:A:325:LEU:C	1:D:331:ARG:CG[6_665]	1.77	0.43
1:A:327:ARG:N	1:D:331:ARG:CG[6_665]	1.78	0.42
1:A:323:SER:C	1:D:330:THR:OG1[6_665]	1.88	0.32
1:A:326:ALA:N	1:D:331:ARG:NE[6_665]	1.88	0.32
1:A:323:SER:CA	1:D:330:THR:OG1[6_665]	1.89	0.31
1:A:323:SER:CB	1:D:330:THR:OG1[6_665]	1.94	0.26
1:A:323:SER:O	1:D:331:ARG:N[6_665]	1.95	0.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:CB	5:A:378:HOH:O[5_554]	1.95	0.25
1:A:325:LEU:CG	1:D:331:ARG:NH2[6_665]	1.96	0.24
1:A:325:LEU:CB	1:D:331:ARG:CZ[6_665]	1.98	0.22
1:A:326:ALA:O	1:D:331:ARG:CA[6_665]	2.01	0.19
1:A:325:LEU:CD2	1:D:331:ARG:NH2[6_665]	2.04	0.16
1:C:316:HIS:CD2	1:D:316:HIS:CE1[6_655]	2.04	0.16
1:C:320:THR:OG1	1:D:316:HIS:ND1[6_655]	2.04	0.16
1:A:325:LEU:O	1:D:331:ARG:CZ[6_665]	2.05	0.15
1:C:316:HIS:CE1	1:D:316:HIS:CD2[6_655]	2.05	0.15
1:A:323:SER:O	1:D:330:THR:OG1[6_665]	2.07	0.13
1:B:107:LEU:CD2	5:A:378:HOH:O[5_554]	2.07	0.13
1:A:325:LEU:C	1:D:331:ARG:CZ[6_665]	2.08	0.12
1:A:327:ARG:N	1:D:330:THR:C[6_665]	2.12	0.08
1:A:327:ARG:CB	1:D:331:ARG:N[6_665]	2.13	0.07
1:C:316:HIS:ND1	1:D:316:HIS:CE1[6_655]	2.13	0.07
1:C:316:HIS:ND1	1:D:320:THR:OG1[6_655]	2.16	0.04
1:A:323:SER:O	1:D:330:THR:CA[6_665]	2.17	0.03

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	293/317 (92%)	235 (80%)	40 (14%)	18 (6%)	1	7
1	B	293/317 (92%)	235 (80%)	40 (14%)	18 (6%)	1	7
1	C	293/317 (92%)	235 (80%)	40 (14%)	18 (6%)	1	7
1	D	293/317 (92%)	235 (80%)	40 (14%)	18 (6%)	1	7
All	All	1172/1268 (92%)	940 (80%)	160 (14%)	72 (6%)	1	7

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	88	ASP
1	A	217	SER
1	A	328	ALA
1	A	329	PHE
1	B	74	LYS
1	B	88	ASP
1	B	217	SER
1	B	328	ALA
1	B	329	PHE
1	C	74	LYS
1	C	88	ASP
1	C	217	SER
1	C	328	ALA
1	C	329	PHE
1	D	74	LYS
1	D	88	ASP
1	D	217	SER
1	D	328	ALA
1	D	329	PHE
1	A	69	LYS
1	A	75	PRO
1	A	216	GLU
1	A	330	THR
1	B	69	LYS
1	B	75	PRO
1	B	216	GLU
1	B	330	THR
1	C	69	LYS
1	C	75	PRO
1	C	216	GLU
1	C	330	THR
1	D	69	LYS
1	D	75	PRO
1	D	216	GLU
1	D	330	THR
1	A	18	ASN
1	A	87	ARG
1	B	18	ASN
1	B	87	ARG
1	C	18	ASN
1	C	87	ARG
1	D	18	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	87	ARG
1	A	73	PRO
1	B	73	PRO
1	C	73	PRO
1	D	73	PRO
1	A	70	VAL
1	A	172	PHE
1	A	246	ALA
1	A	284	ASP
1	B	70	VAL
1	B	172	PHE
1	B	246	ALA
1	B	284	ASP
1	C	70	VAL
1	C	172	PHE
1	C	246	ALA
1	C	284	ASP
1	D	70	VAL
1	D	172	PHE
1	D	246	ALA
1	D	284	ASP
1	A	19	GLY
1	A	180	VAL
1	B	19	GLY
1	B	180	VAL
1	C	19	GLY
1	C	180	VAL
1	D	19	GLY
1	D	180	VAL

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	243/255 (95%)	204 (84%)	39 (16%)	2	12
1	B	243/255 (95%)	204 (84%)	39 (16%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	225/255 (88%)	187 (83%)	38 (17%)	2	11
1	D	171/255 (67%)	141 (82%)	30 (18%)	2	10
All	All	882/1020 (86%)	736 (83%)	146 (17%)	2	12

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	18	ASN
1	A	25	VAL
1	A	26	ILE
1	A	31	VAL
1	A	54	ASN
1	A	56	SER
1	A	59	ILE
1	A	69	LYS
1	A	88	ASP
1	A	91	LEU
1	A	111	ASP
1	A	119	SER
1	A	125	MET
1	A	147	THR
1	A	161	SER
1	A	183	GLN
1	A	199	PRO
1	A	202	SER
1	A	210	PRO
1	A	211	ILE
1	A	214	LEU
1	A	227	GLU
1	A	229	ILE
1	A	233	VAL
1	A	243	LYS
1	A	244	LYS
1	A	247	THR
1	A	251	ILE
1	A	257	ARG
1	A	271	THR
1	A	273	SER
1	A	287	ILE
1	A	289	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	293	ILE
1	A	294	ASN
1	A	302	ILE
1	A	320	THR
1	A	330	THR
1	B	15	MET
1	B	18	ASN
1	B	25	VAL
1	B	26	ILE
1	B	31	VAL
1	B	54	ASN
1	B	56	SER
1	B	59	ILE
1	B	69	LYS
1	B	88	ASP
1	B	91	LEU
1	B	111	ASP
1	B	119	SER
1	B	125	MET
1	B	147	THR
1	B	161	SER
1	B	183	GLN
1	B	199	PRO
1	B	202	SER
1	B	210	PRO
1	B	211	ILE
1	B	214	LEU
1	B	227	GLU
1	B	229	ILE
1	B	233	VAL
1	B	243	LYS
1	B	244	LYS
1	B	247	THR
1	B	251	ILE
1	B	257	ARG
1	B	271	THR
1	B	273	SER
1	B	287	ILE
1	B	289	VAL
1	B	293	ILE
1	B	294	ASN
1	B	302	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	320	THR
1	B	330	THR
1	C	15	MET
1	C	18	ASN
1	C	25	VAL
1	C	26	ILE
1	C	31	VAL
1	C	54	ASN
1	C	56	SER
1	C	59	ILE
1	C	69	LYS
1	C	88	ASP
1	C	91	LEU
1	C	111	ASP
1	C	119	SER
1	C	125	MET
1	C	147	THR
1	C	161	SER
1	C	183	GLN
1	C	199	PRO
1	C	202	SER
1	C	210	PRO
1	C	211	ILE
1	C	214	LEU
1	C	227	GLU
1	C	229	ILE
1	C	233	VAL
1	C	243	LYS
1	C	244	LYS
1	C	247	THR
1	C	251	ILE
1	C	257	ARG
1	C	271	THR
1	C	273	SER
1	C	287	ILE
1	C	289	VAL
1	C	293	ILE
1	C	294	ASN
1	C	320	THR
1	C	330	THR
1	D	15	MET
1	D	18	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	25	VAL
1	D	26	ILE
1	D	31	VAL
1	D	147	THR
1	D	161	SER
1	D	183	GLN
1	D	199	PRO
1	D	202	SER
1	D	210	PRO
1	D	211	ILE
1	D	214	LEU
1	D	227	GLU
1	D	229	ILE
1	D	233	VAL
1	D	243	LYS
1	D	244	LYS
1	D	247	THR
1	D	251	ILE
1	D	257	ARG
1	D	271	THR
1	D	273	SER
1	D	287	ILE
1	D	289	VAL
1	D	293	ILE
1	D	294	ASN
1	D	302	ILE
1	D	320	THR
1	D	330	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	67	HIS
1	A	155	HIS
1	A	183	GLN
1	A	203	GLN
1	A	232	ASN
1	A	239	GLN
1	A	264	HIS
1	A	265	ASN
1	A	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	294	ASN
1	A	307	ASN
1	B	54	ASN
1	B	67	HIS
1	B	155	HIS
1	B	183	GLN
1	B	203	GLN
1	B	232	ASN
1	B	239	GLN
1	B	264	HIS
1	B	265	ASN
1	B	267	ASN
1	B	294	ASN
1	B	307	ASN
1	B	316	HIS
1	C	54	ASN
1	C	67	HIS
1	C	155	HIS
1	C	183	GLN
1	C	203	GLN
1	C	232	ASN
1	C	239	GLN
1	C	294	ASN
1	C	316	HIS
1	D	155	HIS
1	D	183	GLN
1	D	203	GLN
1	D	232	ASN
1	D	239	GLN
1	D	264	HIS
1	D	265	ASN
1	D	267	ASN
1	D	294	ASN
1	D	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

14 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	B	8	-	4,4,4	0.98	0	6,6,6	0.21	0
3	NAD	B	5	-	46,48,48	1.39	5 (10%)	64,73,73	2.22	14 (21%)
3	NAD	D	13	-	46,48,48	1.39	5 (10%)	64,73,73	2.22	14 (21%)
3	NAD	C	9	-	46,48,48	1.39	5 (10%)	64,73,73	2.22	14 (21%)
2	SO4	C	11	-	4,4,4	0.82	0	6,6,6	0.57	0
2	SO4	B	7	-	4,4,4	0.81	0	6,6,6	0.57	0
2	SO4	D	332	-	4,4,4	0.82	0	6,6,6	0.57	0
3	NAD	A	1	-	46,48,48	1.39	6 (13%)	64,73,73	2.22	14 (21%)
2	SO4	D	333	-	4,4,4	0.98	0	6,6,6	0.22	0
4	FBP	C	6	-	18,20,20	0.79	0	21,32,32	0.95	1 (4%)
2	SO4	A	4	-	4,4,4	0.97	0	6,6,6	0.21	0
2	SO4	C	12	-	4,4,4	0.97	0	6,6,6	0.22	0
2	SO4	A	3	-	4,4,4	0.81	0	6,6,6	0.57	0
4	FBP	D	2	-	18,20,20	0.78	0	21,32,32	0.95	1 (4%)

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
3	NAD	B	5	-	-	10/30/62/62	0/5/5/5
3	NAD	D	13	-	-	10/30/62/62	0/5/5/5
3	NAD	C	9	-	-	10/30/62/62	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	1	-	-	10/30/62/62	0/5/5/5
4	FBP	C	6	-	-	6/13/32/32	0/1/1/1
4	FBP	D	2	-	-	6/13/32/32	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	13	NAD	C3N-C7N	3.59	1.55	1.50
3	C	9	NAD	C3N-C7N	3.56	1.55	1.50
3	A	1	NAD	C3N-C7N	3.49	1.55	1.50
3	B	5	NAD	C3N-C7N	3.48	1.55	1.50
3	B	5	NAD	C2A-N1A	3.46	1.40	1.33
3	A	1	NAD	C2A-N1A	3.44	1.40	1.33
3	D	13	NAD	O4D-C4D	3.44	1.52	1.45
3	D	13	NAD	C2A-N1A	3.43	1.40	1.33
3	C	9	NAD	O4D-C4D	3.42	1.52	1.45
3	B	5	NAD	O4D-C4D	3.41	1.52	1.45
3	A	1	NAD	O4D-C4D	3.40	1.52	1.45
3	C	9	NAD	C2A-N1A	3.39	1.39	1.33
3	A	1	NAD	C6N-N1N	2.90	1.41	1.35
3	B	5	NAD	C6N-N1N	2.89	1.41	1.35
3	C	9	NAD	C6N-N1N	2.89	1.41	1.35
3	D	13	NAD	C6N-N1N	2.87	1.41	1.35
3	A	1	NAD	PN-O3	-2.46	1.56	1.59
3	D	13	NAD	PN-O3	-2.34	1.57	1.59
3	B	5	NAD	PN-O3	-2.32	1.57	1.59
3	C	9	NAD	PN-O3	-2.32	1.57	1.59
3	A	1	NAD	C2N-C3N	-2.00	1.35	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	NAD	C4D-O4D-C1D	-8.68	101.97	109.92
3	B	5	NAD	C4D-O4D-C1D	-8.62	102.03	109.92
3	D	13	NAD	C4D-O4D-C1D	-8.60	102.05	109.92
3	C	9	NAD	C4D-O4D-C1D	-8.58	102.06	109.92
3	C	9	NAD	C5N-C4N-C3N	-7.31	113.18	120.36
3	D	13	NAD	C5N-C4N-C3N	-7.29	113.20	120.36
3	B	5	NAD	C5N-C4N-C3N	-7.28	113.21	120.36
3	A	1	NAD	C5N-C4N-C3N	-7.27	113.22	120.36
3	C	9	NAD	C6N-C5N-C4N	6.30	128.53	119.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	13	NAD	C6N-C5N-C4N	6.29	128.51	119.45
3	B	5	NAD	C6N-C5N-C4N	6.28	128.49	119.45
3	A	1	NAD	C6N-C5N-C4N	6.25	128.46	119.45
3	D	13	NAD	C5N-C6N-N1N	-5.41	113.00	120.38
3	C	9	NAD	C5N-C6N-N1N	-5.40	113.02	120.38
3	B	5	NAD	C5N-C6N-N1N	-5.39	113.04	120.38
3	A	1	NAD	C5N-C6N-N1N	-5.36	113.07	120.38
3	B	5	NAD	O4B-C1B-C2B	-3.78	98.52	106.62
3	A	1	NAD	O4B-C1B-C2B	-3.77	98.55	106.62
3	C	9	NAD	O4B-C1B-C2B	-3.75	98.59	106.62
3	D	13	NAD	O4B-C1B-C2B	-3.74	98.61	106.62
3	C	9	NAD	C4N-C3N-C7N	-3.54	111.41	121.06
3	D	13	NAD	C4N-C3N-C7N	-3.54	111.41	121.06
3	A	1	NAD	C4N-C3N-C7N	-3.54	111.43	121.06
3	B	5	NAD	C4N-C3N-C7N	-3.53	111.45	121.06
3	D	13	NAD	C4B-O4B-C1B	-3.39	101.99	109.47
3	B	5	NAD	C4B-O4B-C1B	-3.36	102.06	109.47
3	C	9	NAD	C4B-O4B-C1B	-3.35	102.06	109.47
3	A	1	NAD	C4B-O4B-C1B	-3.35	102.08	109.47
3	C	9	NAD	C2N-C3N-C4N	3.30	122.10	118.26
3	B	5	NAD	C2N-C3N-C4N	3.27	122.07	118.26
3	D	13	NAD	C2N-C3N-C4N	3.27	122.06	118.26
3	A	1	NAD	C2N-C3N-C4N	3.27	122.06	118.26
3	B	5	NAD	O2A-PA-O3	3.06	115.55	107.27
3	D	13	NAD	O2A-PA-O3	3.06	115.55	107.27
3	A	1	NAD	O2A-PA-O3	3.05	115.53	107.27
3	C	9	NAD	O2A-PA-O3	3.05	115.53	107.27
3	A	1	NAD	O4B-C1B-N9A	-2.75	102.81	108.09
3	D	13	NAD	O4B-C1B-N9A	-2.74	102.83	108.09
3	B	5	NAD	O4B-C1B-N9A	-2.73	102.84	108.09
3	C	9	NAD	O4B-C1B-N9A	-2.73	102.85	108.09
3	A	1	NAD	O4D-C4D-C5D	-2.49	101.34	109.33
3	B	5	NAD	O4D-C4D-C5D	-2.49	101.37	109.33
3	D	13	NAD	O4D-C4D-C5D	-2.48	101.40	109.33
3	C	9	NAD	O4D-C4D-C5D	-2.47	101.41	109.33
3	B	5	NAD	O2D-C2D-C3D	2.44	119.63	111.82
3	C	9	NAD	O2D-C2D-C3D	2.43	119.62	111.82
3	D	13	NAD	O2D-C2D-C3D	2.43	119.59	111.82
3	A	1	NAD	O2D-C2D-C3D	2.42	119.58	111.82
3	D	13	NAD	C2N-C3N-C7N	2.34	126.22	119.46
3	A	1	NAD	C2N-C3N-C7N	2.34	126.22	119.46
3	C	9	NAD	C2N-C3N-C7N	2.33	126.19	119.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	NAD	C2N-C3N-C7N	2.33	126.19	119.46
3	C	9	NAD	C5B-C4B-C3B	2.10	122.76	115.21
3	A	1	NAD	C5B-C4B-C3B	2.09	122.73	115.21
3	D	13	NAD	C5B-C4B-C3B	2.09	122.72	115.21
3	B	5	NAD	C5B-C4B-C3B	2.08	122.70	115.21
4	D	2	FBP	O2P-P1-O1P	2.05	118.81	110.83
4	C	6	FBP	O2P-P1-O1P	2.04	118.80	110.83

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAD	C5D-O5D-PN-O3
3	A	1	NAD	C5D-O5D-PN-O1N
3	A	1	NAD	C5D-O5D-PN-O2N
3	A	1	NAD	O4D-C1D-N1N-C6N
3	B	5	NAD	C5D-O5D-PN-O3
3	B	5	NAD	C5D-O5D-PN-O1N
3	B	5	NAD	C5D-O5D-PN-O2N
3	B	5	NAD	O4D-C1D-N1N-C6N
3	C	9	NAD	C5D-O5D-PN-O3
3	C	9	NAD	C5D-O5D-PN-O1N
3	C	9	NAD	C5D-O5D-PN-O2N
3	C	9	NAD	O4D-C1D-N1N-C6N
3	D	13	NAD	C5D-O5D-PN-O3
3	D	13	NAD	C5D-O5D-PN-O1N
3	D	13	NAD	C5D-O5D-PN-O2N
3	D	13	NAD	O4D-C1D-N1N-C6N
4	C	6	FBP	C1-O1-P1-O2P
4	C	6	FBP	C1-O1-P1-O3P
4	C	6	FBP	O1-C1-C2-C3
4	C	6	FBP	O1-C1-C2-O5
4	D	2	FBP	C1-O1-P1-O2P
4	D	2	FBP	C1-O1-P1-O3P
4	D	2	FBP	O1-C1-C2-C3
4	D	2	FBP	O1-C1-C2-O5
3	A	1	NAD	O4D-C4D-C5D-O5D
3	B	5	NAD	O4D-C4D-C5D-O5D
3	C	9	NAD	O4D-C4D-C5D-O5D
3	D	13	NAD	O4D-C4D-C5D-O5D
3	A	1	NAD	C3D-C4D-C5D-O5D
3	B	5	NAD	C3D-C4D-C5D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1	NAD	O4B-C4B-C5B-O5B
3	B	5	NAD	O4B-C4B-C5B-O5B
3	C	9	NAD	O4B-C4B-C5B-O5B
3	C	9	NAD	C3D-C4D-C5D-O5D
3	D	13	NAD	O4B-C4B-C5B-O5B
3	D	13	NAD	C3D-C4D-C5D-O5D
4	C	6	FBP	C1-O1-P1-O1P
4	D	2	FBP	C1-O1-P1-O1P
4	C	6	FBP	O1-C1-C2-O2
4	D	2	FBP	O1-C1-C2-O2
3	A	1	NAD	PN-O3-PA-O2A
3	B	5	NAD	PN-O3-PA-O2A
3	C	9	NAD	PN-O3-PA-O2A
3	D	13	NAD	PN-O3-PA-O2A
3	A	1	NAD	O4D-C1D-N1N-C2N
3	B	5	NAD	O4D-C1D-N1N-C2N
3	C	9	NAD	O4D-C1D-N1N-C2N
3	D	13	NAD	O4D-C1D-N1N-C2N
3	A	1	NAD	PN-O3-PA-O1A
3	B	5	NAD	PN-O3-PA-O1A
3	C	9	NAD	PN-O3-PA-O1A
3	D	13	NAD	PN-O3-PA-O1A

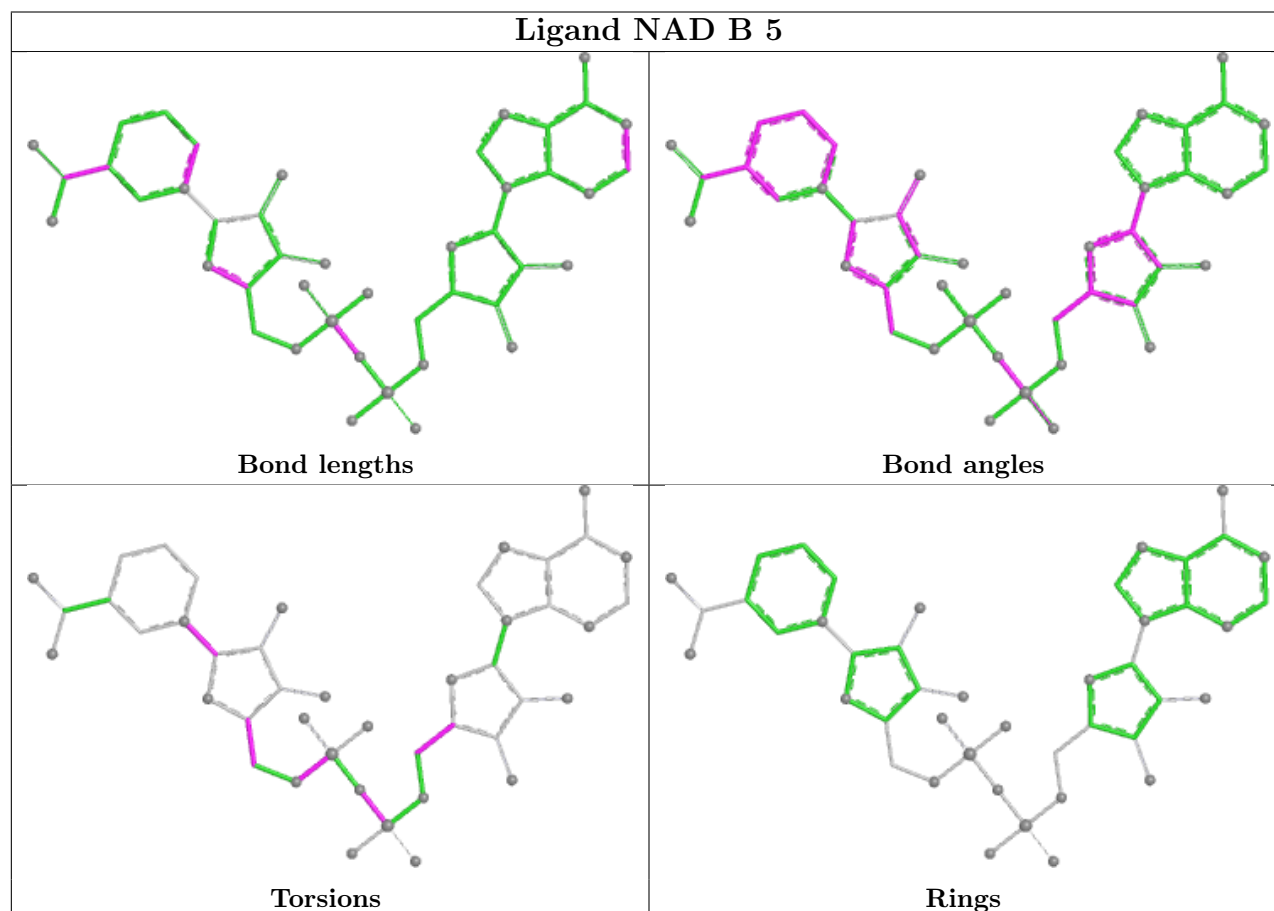
There are no ring outliers.

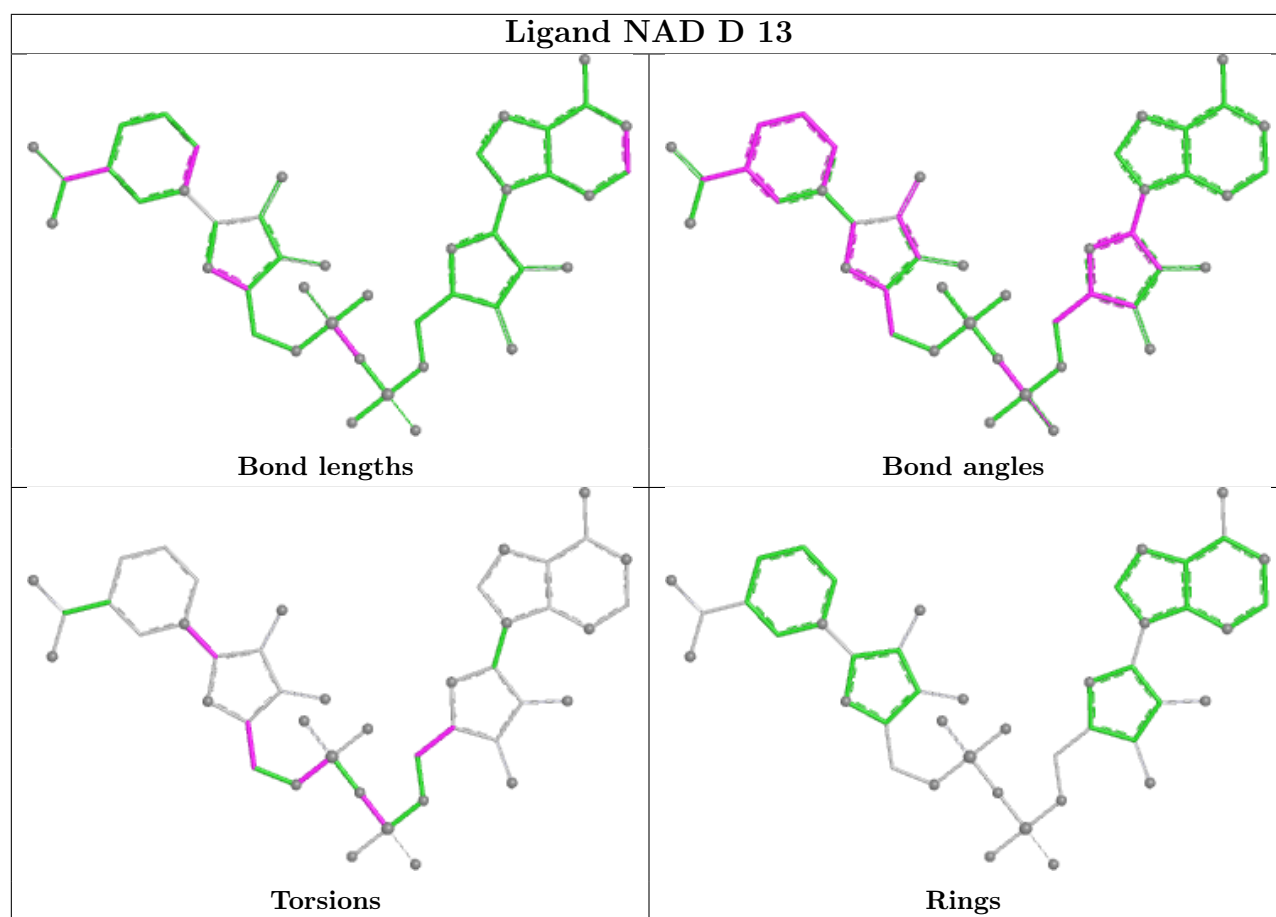
10 monomers are involved in 42 short contacts:

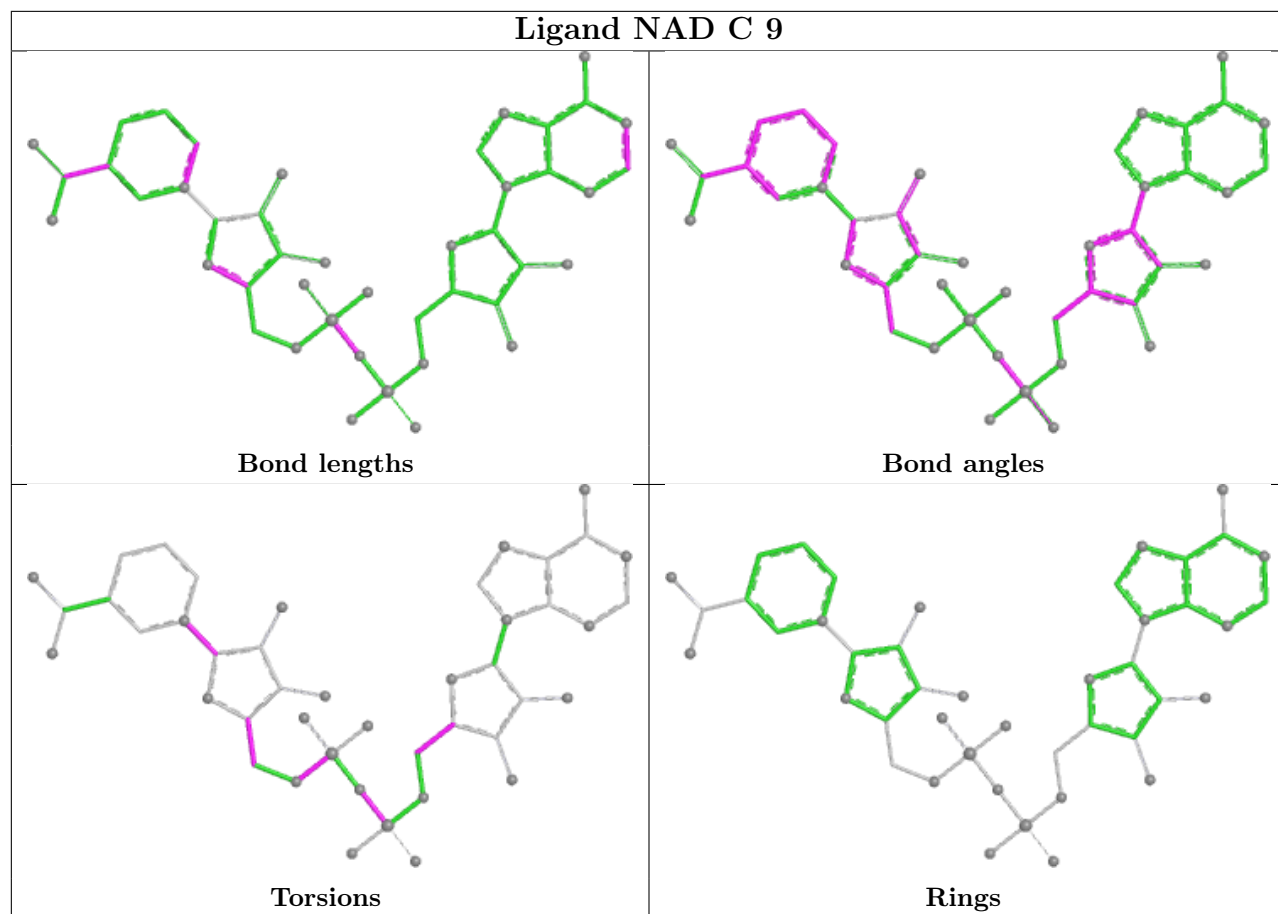
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5	NAD	8	0
3	D	13	NAD	8	0
3	C	9	NAD	8	0
2	C	11	SO4	4	0
2	B	7	SO4	4	0
2	D	332	SO4	4	0
3	A	1	NAD	8	0
4	C	6	FBP	3	0
2	A	3	SO4	4	0
4	D	2	FBP	3	0

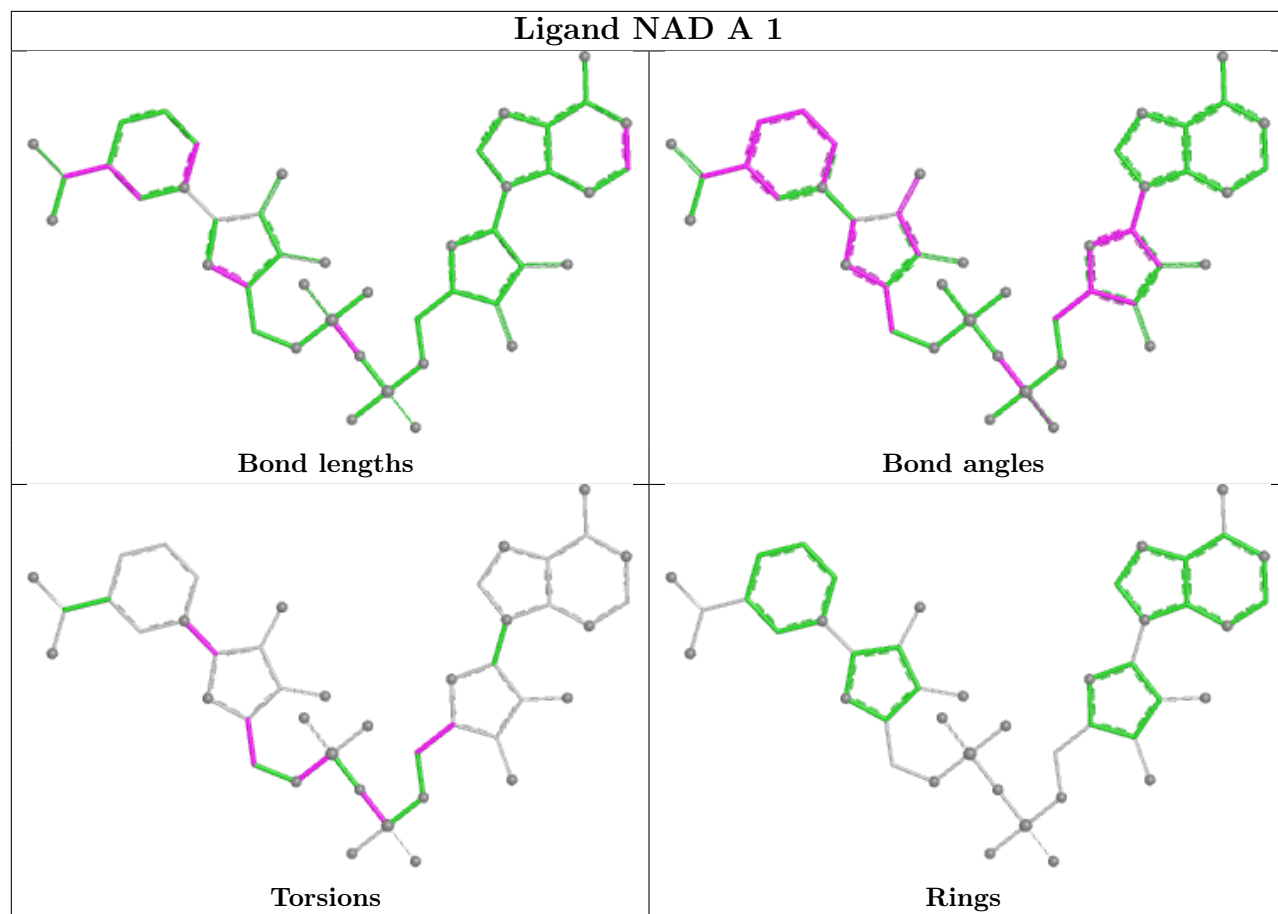
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

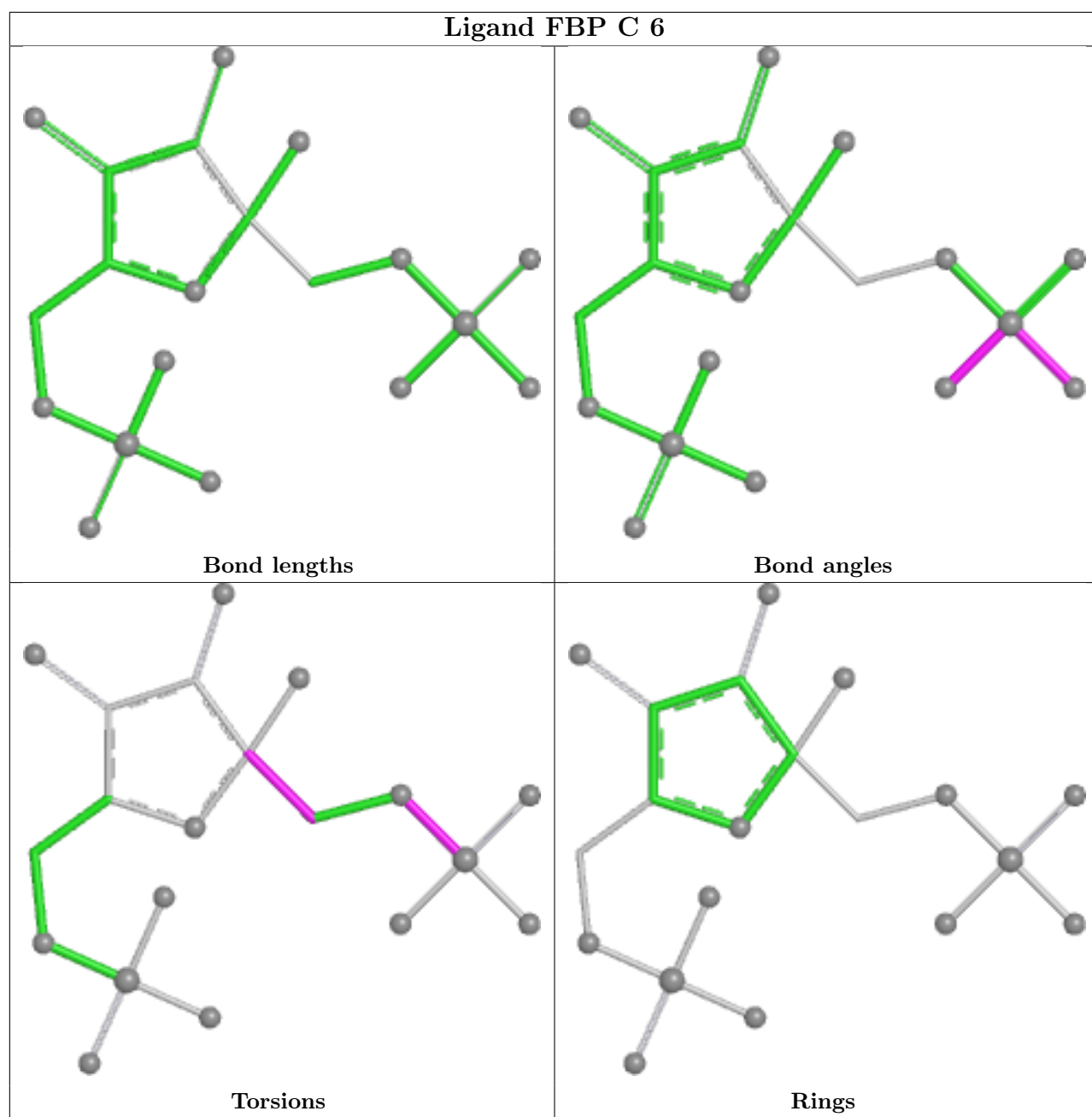
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

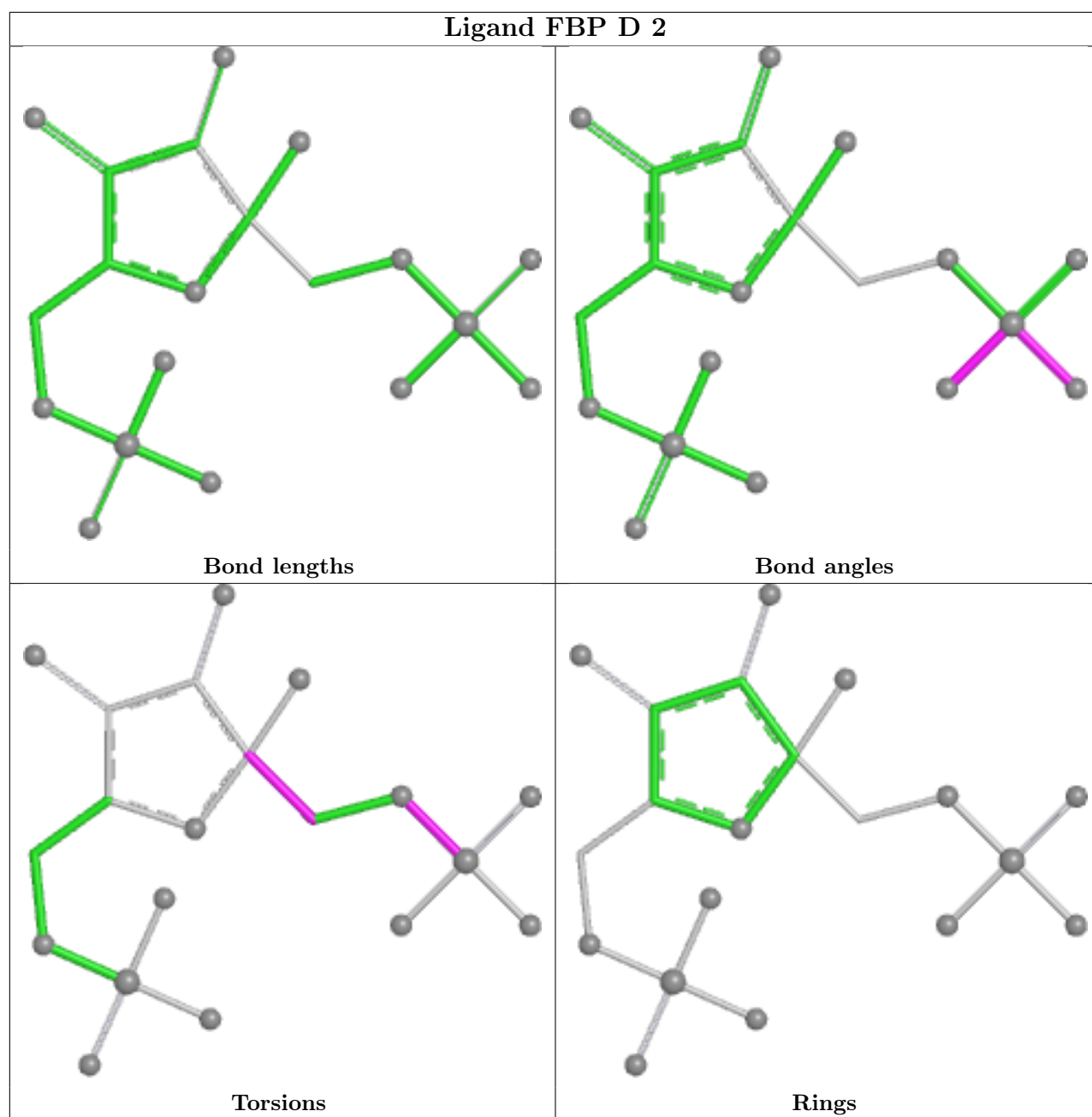












5.7 Other polymers [i](#)

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.