



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:04 AM EDT

PDB ID : 1MIO / pdb_00001mio
Title : X-RAY CRYSTAL STRUCTURE OF THE NITROGENASE
MOLYBDENUM-IRON PROTEIN FROM CLOSTRIDIUM PASTEURIANUM AT 3.0 ANGSTROMS RESOLUTION
Authors : Kim, J.; Woo, D.; Rees, D.C.
Deposited on : 1993-03-24
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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

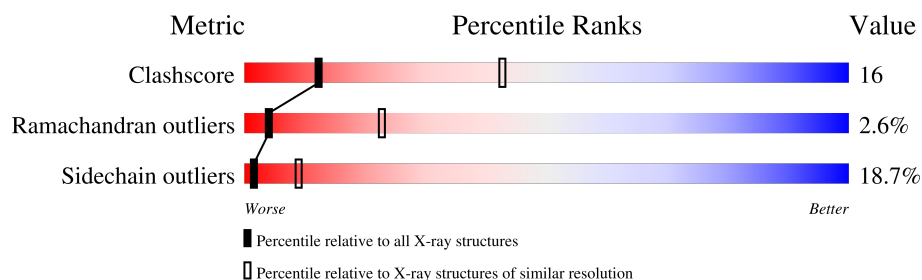
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	533	
1	C	533	
2	B	458	
2	D	458	

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
5	CFM	B	496	-	-	X	-
5	CFM	D	496	-	-	X	-
6	CLP	B	498	-	-	X	-
6	CLP	D	498	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15269 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 NITROGENASE MOLYBDENUM IRON PROTEIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4074	2588	682	777	27			
1	C	525	Total	C	N	O	S	0	0	0
			4077	2589	683	778	27			

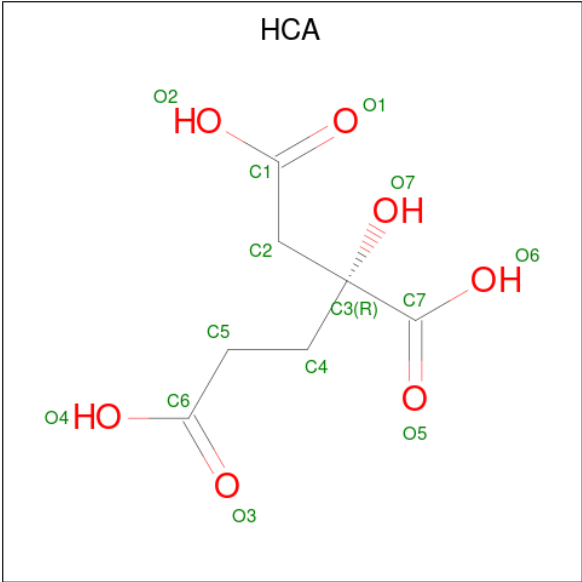
- Molecule 2 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	457	Total	C	N	O	S	0	0	0
			3511	2231	579	681	20			
2	D	457	Total	C	N	O	S	0	0	0
			3511	2231	579	681	20			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

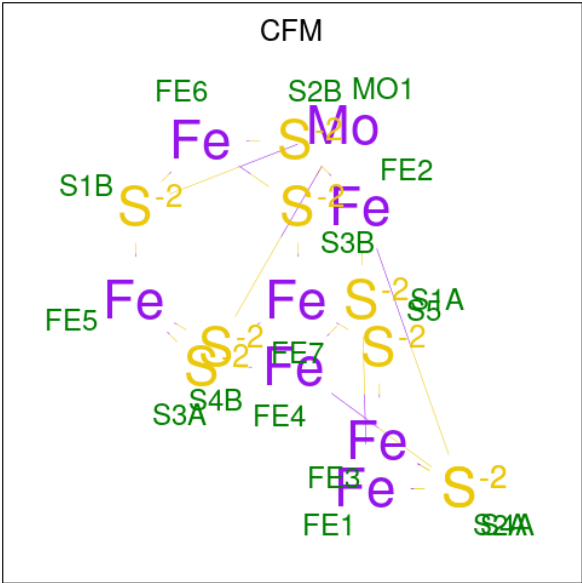
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇).



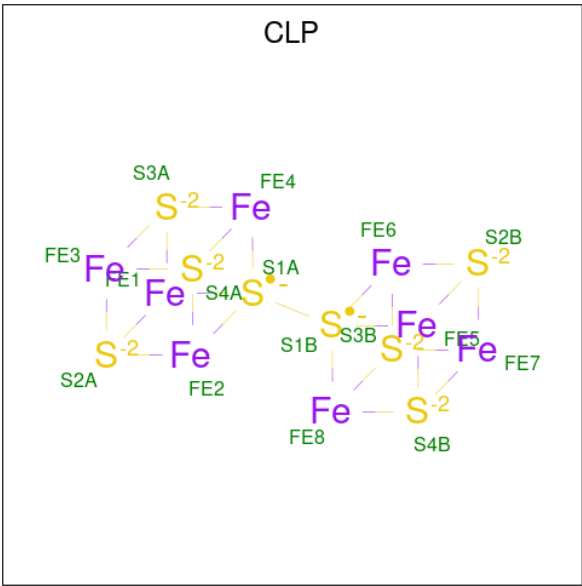
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			14	7	7		
4	D	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe₇MoS₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	D	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is FE-S CLUSTER (CCD ID: CLP) (formula: Fe₈S₈).



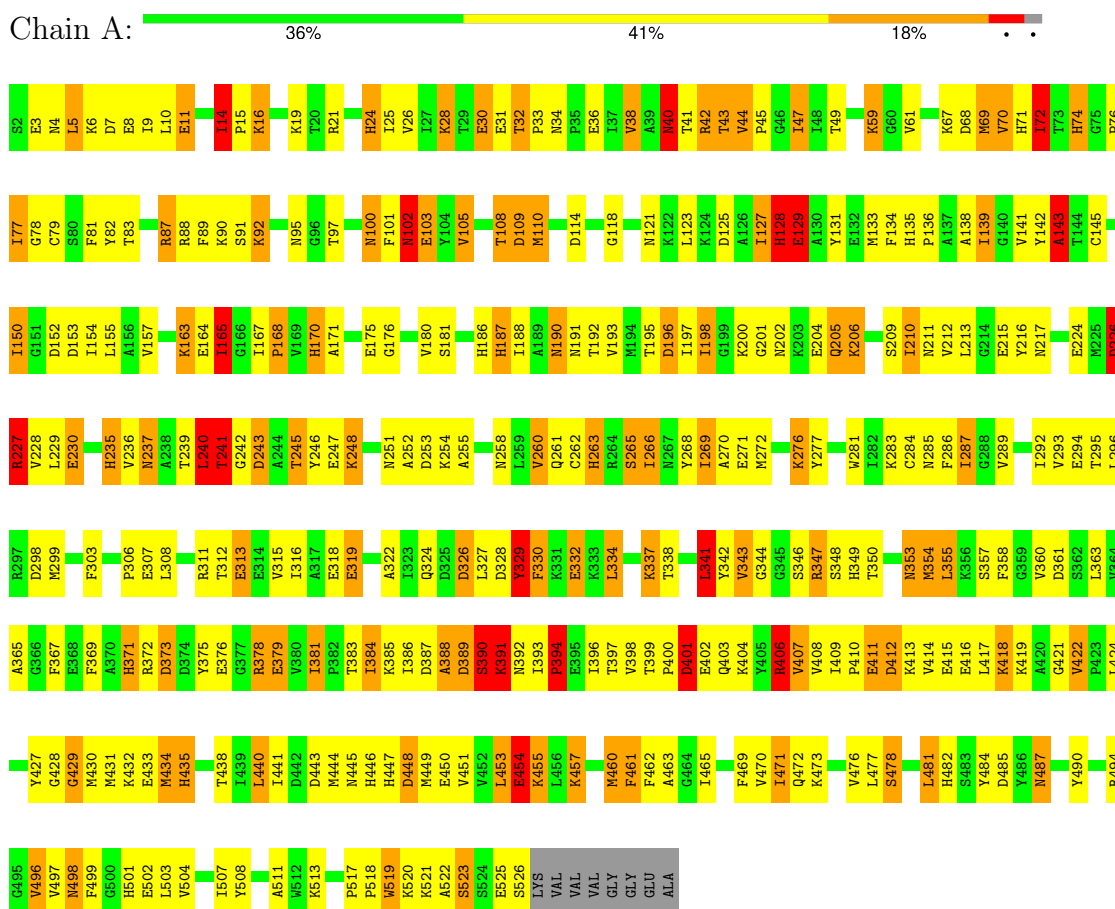
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			16	8	8		
6	D	1	Total	Fe	S	0	0
			16	8	8		

3 Residue-property plots

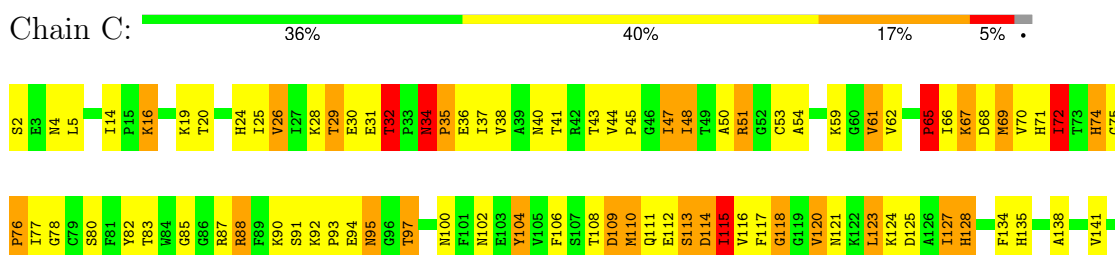
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

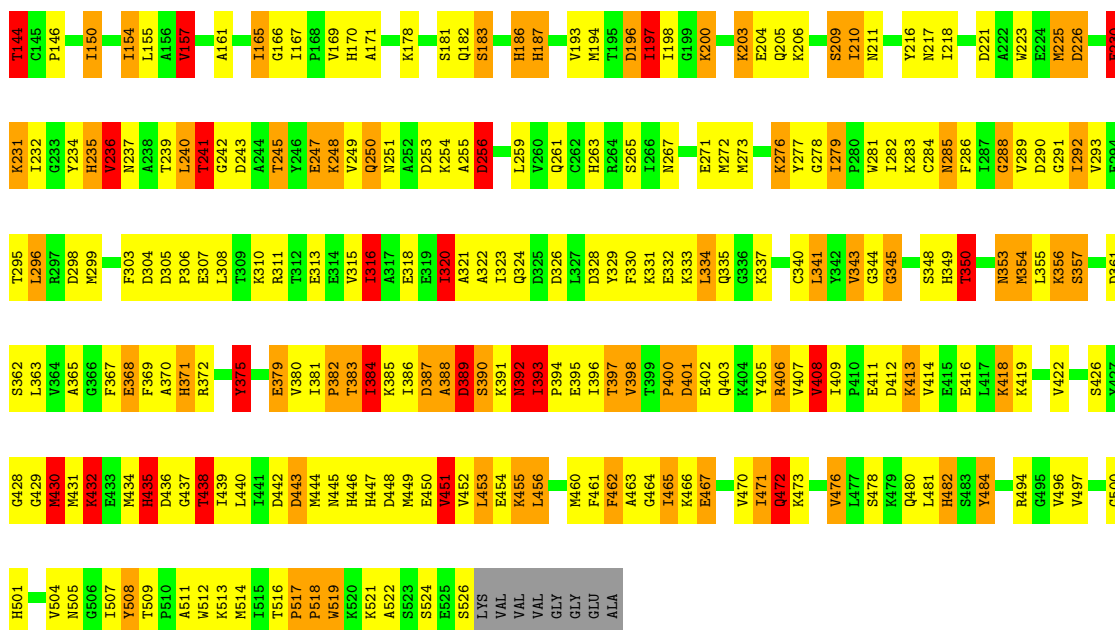
Note EDS was not executed.

- Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN (ALPHA CHAIN)



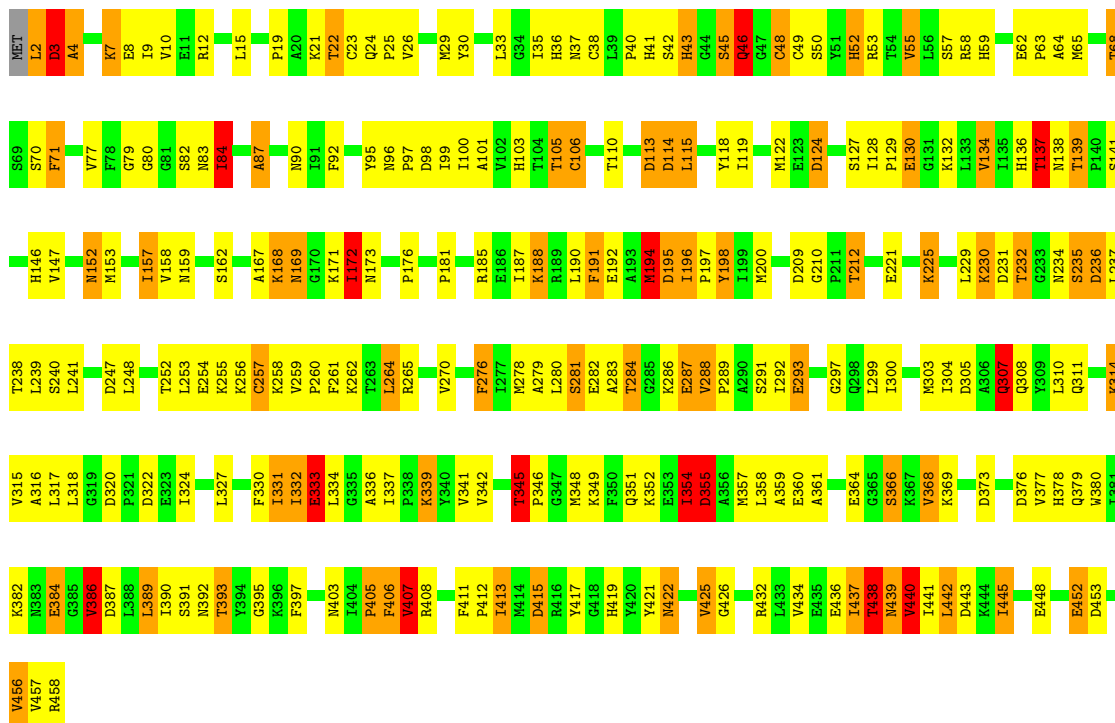
- Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN (ALPHA CHAIN)





• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN)

Chain B: 44% 38% 14%



• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN)

Chain D: 44% 40% 13%

E455	V370	R296	K217	H146	F78	MET
V456	D373	L299	M218	V147	G81	L2
V457		I300	E221	F150	S82	D3
R458	D376	D301		A151	N83	A4
	V377	L302	T224	N152	I84	E8
	H378	M303	E227	M153	K85	I9
	Q379	I304	D228	V154	T86	V10
	W380	D305	L229		A87	E11
		A306	E227	I157	V88	R12
	V386	Q307	K230	V158	K89	
	D387	Q308	D231	N159	N90	L15
	L388		T232	Y160	I91	R16
	L389	Q311	G233	F92	F92	I17
	I390	V315	N234	L161	S93	N18
	S391	A316	S235	S162	L94	
	N392	L317	L239	E163	Y95	T22
	T393	L318	S240	N164	N96	
		G319	L241	T165	P97	P25
	K396	D320		K168	D98	
	A399	P321	A245	M169	D99	P25
	R400	D322	S246	N199	I100	A28
	E401	E323	D247	I172		M29
E402		I324	L248	N173	H103	Y30
N403		I325	G249	I175	T104	G34
I404		A326	A250	P176	T105	I35
F406		L327		G177	C106	H36
F407		S328	L253	F178	S108	N37
V407		K329	E254		C38	
R408			K255	P181	L39	L39
F409		E333	K256	A182	P40	P40
G410		L394	C257	D183	H41	H41
F411		I337	K258	M184	S42	S42
			V259	R185	H43	H43
H419		P338	P260		S45	S45
Y420		K339	F261	K188	Q46	Q46
Y421		Y340	K262	R189		
N422		V341	T263	L190	HS2	HS2
		V342	L264	F191	R53	R53
Y427		T343	R265	E192	T54	T54
K428		G344	T266	A193	V55	V55
		T345	P267	M194	L56	L56
I431		P346	L268	D195	S57	S57
			G269		R58	R58
E436		K349	V270	Y198	H59	H59
I437		F350		I199	F60	F60
T438		Q351	E275	M200	K61	K61
N439			F276	F201	L133	L133
V440			I277	P202	V134	V134
				D203	I135	I135
				T204	H136	H136
D443		D355	E282		T137	T137
E448		A356			N138	N138
G449		M357	K286	L208	T139	T139
T450		L358	E287	D209	P140	P140
E451				G210	S141	S141
E452		G365	S291	P211	Y142	Y142
D453		S366	L292	T212	V143	V143
F454		K367	E293		G144	G144
		V368			S145	S145
		K369		Y216		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.96Å 151.30Å 121.90Å 90.00° 110.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15269	wwPDB-VP
Average B, all atoms (Å ²)	8.0	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: CLP, CFM, HCA, CA

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	1.29	34/4163 (0.8%)	2.38	237/5629 (4.2%)
1	C	1.33	47/4166 (1.1%)	2.34	241/5631 (4.3%)
2	B	1.21	23/3582 (0.6%)	2.24	184/4845 (3.8%)
2	D	1.24	26/3582 (0.7%)	2.27	190/4845 (3.9%)
All	All	1.27	130/15493 (0.8%)	2.31	852/20950 (4.1%)

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	2
1	C	0	5
2	B	0	2
2	D	0	4
All	All	0	13

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	ILE	CA-CB	10.01	1.68	1.54
2	D	43	HIS	CD2-NE2	-9.05	1.27	1.37
1	C	236	VAL	CA-CB	8.71	1.63	1.53
1	C	186	HIS	CD2-NE2	-8.68	1.28	1.37
1	C	407	VAL	CA-CB	8.51	1.64	1.53
1	C	451	VAL	CA-CB	8.45	1.67	1.54
2	B	134	VAL	CA-CB	8.37	1.64	1.54
1	A	186	HIS	CD2-NE2	-8.01	1.29	1.37
1	A	71	HIS	CD2-NE2	-7.93	1.29	1.37
1	A	349	HIS	CD2-NE2	-7.92	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	HIS	CD2-NE2	-7.92	1.29	1.37
2	B	407	VAL	CA-CB	7.92	1.64	1.54
2	B	146	HIS	CD2-NE2	-7.90	1.29	1.37
2	B	354	ILE	CA-CB	7.78	1.63	1.54
2	D	345	THR	CA-CB	7.72	1.66	1.53
1	C	435	HIS	CA-CB	7.68	1.64	1.53
1	A	446	HIS	CD2-NE2	-7.65	1.29	1.37
2	D	146	HIS	CD2-NE2	-7.60	1.29	1.37
1	C	408	VAL	CA-CB	7.58	1.64	1.54
2	B	437	ILE	CA-CB	7.56	1.65	1.54
1	C	71	HIS	CD2-NE2	-7.54	1.29	1.37
1	C	157	VAL	CA-CB	7.53	1.63	1.54
1	C	47	ILE	CA-CB	7.52	1.64	1.54
2	D	378	HIS	CD2-NE2	-7.48	1.29	1.37
2	B	103	HIS	CD2-NE2	-7.46	1.29	1.37
1	A	38	VAL	CA-CB	7.43	1.63	1.54
2	D	41	HIS	CD2-NE2	-7.42	1.29	1.37
1	A	74	HIS	CD2-NE2	-7.39	1.29	1.37
2	D	52	HIS	CD2-NE2	-7.26	1.29	1.37
2	B	172	ILE	CA-CB	7.25	1.65	1.54
1	C	393	ILE	CA-CB	7.25	1.63	1.54
1	C	447	HIS	CD2-NE2	-7.20	1.29	1.37
1	C	392	ASN	CA-CB	7.15	1.62	1.52
1	C	349	HIS	CD2-NE2	-7.10	1.30	1.37
1	C	187	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	72	ILE	CA-CB	7.06	1.62	1.54
1	C	72	ILE	CA-CB	7.06	1.63	1.54
2	B	10	VAL	CA-CB	7.03	1.62	1.53
1	C	74	HIS	CD2-NE2	-7.02	1.30	1.37
2	D	158	VAL	CA-CB	6.98	1.63	1.54
2	B	43	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	407	VAL	CA-CB	6.91	1.61	1.53
2	D	268	ILE	CA-CB	6.87	1.62	1.54
2	B	36	HIS	CD2-NE2	-6.84	1.30	1.37
1	C	263	HIS	CD2-NE2	-6.81	1.30	1.37
2	B	158	VAL	CA-CB	6.80	1.62	1.54
2	D	36	HIS	CD2-NE2	-6.79	1.30	1.37
1	C	446	HIS	CD2-NE2	-6.77	1.30	1.37
2	B	59	HIS	CD2-NE2	-6.73	1.30	1.37
2	D	59	HIS	CD2-NE2	-6.73	1.30	1.37
2	B	378	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	128	HIS	CD2-NE2	-6.66	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	316	ILE	CA-CB	6.59	1.61	1.54
1	A	349	HIS	CG-ND1	-6.57	1.31	1.38
1	A	170	HIS	CD2-NE2	-6.56	1.30	1.37
2	B	419	HIS	CD2-NE2	-6.56	1.30	1.37
2	B	52	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	135	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	150	ILE	CA-CB	6.42	1.61	1.54
2	B	136	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	447	HIS	CD2-NE2	-6.31	1.30	1.37
1	C	235	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	70	VAL	CA-CB	6.28	1.61	1.54
1	C	135	HIS	CD2-NE2	-6.26	1.30	1.37
1	C	371	HIS	CD2-NE2	-6.26	1.30	1.37
2	D	130	GLU	CA-CB	6.24	1.62	1.53
1	C	435	HIS	CB-CG	6.22	1.58	1.50
2	D	419	HIS	CD2-NE2	-6.21	1.31	1.37
2	B	41	HIS	CD2-NE2	-6.19	1.31	1.37
2	D	136	HIS	CD2-NE2	-6.13	1.31	1.37
1	C	167	ILE	CA-CB	6.04	1.61	1.54
2	D	52	HIS	CG-ND1	-5.98	1.31	1.38
1	A	263	HIS	CD2-NE2	-5.96	1.31	1.37
2	D	103	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	187	HIS	CD2-NE2	-5.95	1.31	1.37
2	D	141	SER	CA-CB	-5.93	1.43	1.53
1	C	279	ILE	CA-CB	5.91	1.61	1.54
1	A	482	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	316	ILE	CA-CB	5.87	1.60	1.54
2	D	354	ILE	CA-CB	5.86	1.61	1.54
1	C	482	HIS	CD2-NE2	-5.86	1.31	1.37
1	C	186	HIS	CG-ND1	-5.84	1.31	1.38
2	D	378	HIS	CG-ND1	-5.83	1.31	1.38
2	D	165	THR	CA-CB	5.82	1.61	1.53
1	A	435	HIS	CD2-NE2	-5.82	1.31	1.37
2	D	43	HIS	CG-ND1	-5.80	1.31	1.38
1	C	465	ILE	CA-CB	5.76	1.61	1.55
1	A	501	HIS	CD2-NE2	-5.73	1.31	1.37
1	C	127	ILE	CA-CB	5.73	1.60	1.54
1	A	71	HIS	CG-ND1	-5.68	1.32	1.38
1	C	320	ILE	CA-CB	5.67	1.62	1.54
2	B	195	ASP	CA-CB	5.65	1.61	1.54
1	A	266	ILE	CA-CB	5.62	1.62	1.54
1	C	170	HIS	CD2-NE2	-5.61	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	516	THR	CA-CB	5.60	1.61	1.53
1	A	465	ILE	CA-CB	5.59	1.60	1.54
1	C	349	HIS	CG-ND1	-5.59	1.32	1.38
1	C	71	HIS	CG-ND1	-5.57	1.32	1.38
1	A	235	HIS	CD2-NE2	-5.54	1.31	1.37
2	D	41	HIS	CG-ND1	-5.54	1.32	1.38
1	A	312	THR	CA-CB	5.53	1.61	1.53
1	A	83	THR	CA-CB	5.50	1.60	1.53
1	C	446	HIS	CG-ND1	-5.47	1.32	1.38
2	B	146	HIS	CG-ND1	-5.47	1.32	1.38
2	B	77	VAL	CA-CB	5.46	1.61	1.54
1	C	476	VAL	CA-CB	5.43	1.64	1.55
1	C	61	VAL	CA-CB	5.38	1.61	1.54
2	D	337	ILE	CA-CB	5.37	1.58	1.54
1	C	24	HIS	CD2-NE2	-5.37	1.31	1.37
1	A	157	VAL	CA-CB	5.36	1.60	1.54
2	D	124	ASP	CA-CB	5.36	1.61	1.53
1	A	371	HIS	CD2-NE2	-5.34	1.31	1.37
1	C	375	TYR	CA-CB	-5.34	1.46	1.53
1	C	150	ILE	CA-CB	5.32	1.61	1.54
1	C	128	HIS	CD2-NE2	-5.31	1.32	1.37
1	C	62	VAL	CA-CB	5.28	1.62	1.54
1	C	463	ALA	CA-C	5.25	1.54	1.52
2	B	445	ILE	CA-CB	5.24	1.61	1.54
1	A	386	ILE	CA-CB	5.23	1.62	1.55
2	D	36	HIS	CG-ND1	-5.23	1.32	1.38
1	A	269	ILE	CA-CB	5.21	1.60	1.54
1	A	24	HIS	CG-ND1	-5.19	1.32	1.38
1	C	235	HIS	CG-ND1	-5.14	1.32	1.38
1	C	501	HIS	CD2-NE2	-5.12	1.32	1.37
2	D	143	VAL	CA-CB	5.11	1.61	1.54
1	C	187	HIS	CG-ND1	-5.10	1.32	1.38
2	B	345	THR	CA-CB	5.09	1.61	1.52
2	B	36	HIS	CG-ND1	-5.08	1.32	1.38
2	D	59	HIS	CB-CG	5.02	1.57	1.50
1	A	204	GLU	CA-CB	5.01	1.59	1.52

All (852) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	443	ASP	CA-CB-CG	20.04	132.64	112.60
2	D	124	ASP	CA-CB-CG	18.36	130.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ASN	CA-CB-CG	15.65	128.25	112.60
1	A	390	SER	N-CA-C	15.30	143.38	110.80
1	A	240	LEU	O-C-N	14.92	140.83	122.63
1	A	240	LEU	CA-C-N	12.97	146.31	121.54
1	A	240	LEU	C-N-CA	12.97	146.31	121.54
1	C	40	ASN	N-CA-C	12.53	128.19	111.28
1	A	386	ILE	N-CA-C	12.44	128.00	108.85
1	C	305	ASP	N-CA-C	12.11	128.42	110.14
1	C	411	GLU	N-CA-C	12.01	129.10	111.81
1	C	95	ASN	CA-CB-CG	11.99	124.59	112.60
1	C	392	ASN	CA-CB-CG	11.91	124.51	112.60
2	B	422	ASN	CA-CB-CG	11.79	124.39	112.60
2	D	203	ASP	CA-CB-CG	11.74	124.34	112.60
1	A	521	LYS	N-CA-C	-11.50	95.26	108.49
1	A	142	TYR	N-CA-C	11.37	127.54	112.88
1	C	392	ASN	N-CA-C	-11.33	88.84	108.56
2	B	453	ASP	CA-CB-CG	11.30	123.90	112.60
1	C	387	ASP	N-CA-C	-11.19	94.67	111.34
2	D	141	SER	N-CA-C	11.18	126.06	111.75
1	A	243	ASP	CA-CB-CG	11.17	123.77	112.60
2	B	169	ASN	OD1-CG-ND2	-11.12	111.48	122.60
1	C	435	HIS	CA-CB-CG	11.11	124.91	113.80
1	C	240	LEU	O-C-N	11.10	136.86	122.43
1	C	353	ASN	CA-CB-CG	10.99	123.59	112.60
2	B	392	ASN	OD1-CG-ND2	-10.73	111.87	122.60
2	B	195	ASP	CA-CB-CG	10.69	123.29	112.60
2	D	403	ASN	CA-CB-CG	10.66	123.26	112.60
1	A	376	GLU	N-CA-C	10.64	126.25	113.28
1	A	24	HIS	CA-CB-CG	-10.59	103.21	113.80
2	B	440	VAL	N-CA-CB	-10.54	97.30	110.47
1	A	40	ASN	OD1-CG-ND2	-10.42	112.18	122.60
1	A	329	TYR	N-CA-C	-10.30	99.23	112.93
1	A	7	ASP	CA-CB-CG	10.26	122.86	112.60
1	A	353	ASN	CA-CB-CG	10.18	122.78	112.60
1	C	256	ASP	CA-CB-CG	10.16	122.76	112.60
1	C	240	LEU	CA-C-N	10.13	140.89	121.54
1	C	240	LEU	C-N-CA	10.13	140.89	121.54
2	D	299	LEU	N-CA-C	-10.05	99.14	111.40
1	A	391	LYS	N-CA-C	10.00	126.79	107.98
2	B	236	ASP	CA-CB-CG	10.00	122.60	112.60
2	D	69	SER	N-CA-C	-10.00	93.50	109.39
1	C	51	ARG	CA-CB-CG	9.98	134.06	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	392	ASN	OD1-CG-ND2	-9.98	112.62	122.60
2	D	71	PHE	CA-CB-CG	9.88	123.68	113.80
2	D	234	ASN	CA-CB-CG	9.84	122.44	112.60
1	C	47	ILE	N-CA-C	-9.82	96.00	109.55
1	A	389	ASP	N-CA-C	-9.76	90.01	110.80
1	A	408	VAL	N-CA-C	-9.71	101.91	110.74
2	D	221	GLU	N-CA-C	9.69	125.17	113.16
1	C	226	ASP	CA-CB-CG	9.60	122.20	112.60
1	A	109	ASP	CA-CB-CG	9.56	122.16	112.60
2	B	3	ASP	N-CA-C	9.51	131.05	110.80
1	A	266	ILE	CB-CG1-CD1	-9.49	93.86	113.80
1	A	108	THR	N-CA-C	-9.48	91.99	108.20
2	D	90	ASN	CA-CB-CG	-9.24	103.36	112.60
1	A	40	ASN	CA-CB-CG	9.24	121.84	112.60
2	B	345	THR	CB-CA-C	9.20	122.62	109.38
1	A	521	LYS	O-C-N	-9.06	116.31	123.11
1	C	253	ASP	CA-CB-CG	8.97	121.58	112.60
2	D	3	ASP	N-CA-C	8.97	129.90	110.80
1	A	11	GLU	N-CA-C	8.96	122.02	111.71
1	C	196	ASP	CA-CB-CG	8.95	121.55	112.60
2	D	453	ASP	CA-CB-CG	8.95	121.55	112.60
2	B	37	ASN	CA-CB-CG	8.93	121.53	112.60
1	A	128	HIS	CB-CG-CD2	-8.89	119.65	131.20
1	A	390	SER	N-CA-CB	-8.83	95.56	110.49
1	A	285	ASN	OD1-CG-ND2	-8.83	113.77	122.60
1	A	390	SER	CA-CB-OG	8.80	128.71	111.10
1	C	68	ASP	CA-CB-CG	8.73	121.33	112.60
1	A	100	ASN	OD1-CG-ND2	-8.73	113.87	122.60
1	A	498	ASN	OD1-CG-ND2	-8.71	113.89	122.60
1	A	454	GLU	CB-CG-CD	8.68	127.35	112.60
1	A	239	THR	N-CA-C	-8.65	95.14	109.07
1	C	245	THR	CA-CB-OG1	-8.65	96.63	109.60
1	C	67	LYS	N-CA-C	8.64	121.84	111.82
1	C	36	GLU	CA-CB-CG	8.63	131.35	114.10
1	C	401	ASP	CA-CB-CG	-8.58	104.02	112.60
2	D	114	ASP	CA-CB-CG	8.57	121.17	112.60
1	C	77	ILE	N-CA-C	8.56	119.37	110.72
1	A	67	LYS	N-CA-C	8.51	123.22	113.01
2	B	270	VAL	N-CA-C	8.51	118.55	110.30
2	B	84	ILE	CB-CA-C	-8.48	100.51	112.22
1	A	186	HIS	CB-CG-CD2	-8.43	120.25	131.20
1	A	198	ILE	N-CA-C	8.40	126.80	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	457	VAL	N-CA-C	-8.39	96.03	108.12
2	B	71	PHE	CA-CB-CG	8.39	122.19	113.80
1	A	14	ILE	N-CA-CB	-8.38	100.87	110.17
1	C	387	ASP	CA-CB-CG	8.36	120.96	112.60
1	A	14	ILE	CB-CA-C	8.35	120.29	110.68
1	A	435	HIS	CB-CG-CD2	-8.31	120.39	131.20
2	B	386	VAL	N-CA-CB	-8.27	98.58	112.47
2	D	387	ASP	CA-CB-CG	8.27	120.86	112.60
1	A	210	ILE	N-CA-CB	-8.26	102.92	112.34
1	A	334	LEU	N-CA-C	8.26	123.54	113.38
1	A	443	ASP	CA-CB-CG	8.25	120.85	112.60
2	D	78	PHE	CA-CB-CG	8.23	122.03	113.80
1	A	435	HIS	CA-CB-CG	8.22	122.02	113.80
1	A	227	ARG	CA-CB-CG	8.21	130.53	114.10
2	B	443	ASP	CA-CB-CG	8.22	120.82	112.60
2	B	352	LYS	N-CA-C	8.18	119.83	111.07
1	A	129	GLU	N-CA-C	-8.15	93.45	110.80
1	C	51	ARG	N-CA-CB	-8.11	98.66	110.26
2	D	357	MET	N-CA-C	-8.09	102.42	113.18
1	C	371	HIS	CA-CB-CG	8.05	121.85	113.80
1	C	451	VAL	N-CA-C	-8.04	103.06	111.58
1	A	373	ASP	CA-CB-CG	7.99	120.59	112.60
2	D	439	ASN	CA-CB-CG	7.96	120.56	112.60
2	D	357	MET	CA-CB-CG	7.92	129.95	114.10
1	A	143	ALA	N-CA-C	7.92	127.67	110.80
1	C	466	LYS	O-C-N	7.91	130.32	122.09
1	C	237	ASN	OD1-CG-ND2	-7.90	114.70	122.60
2	D	275	GLU	CB-CG-CD	7.88	126.00	112.60
2	B	221	GLU	N-CA-C	7.87	120.95	111.82
2	B	386	VAL	CB-CA-C	7.87	122.23	110.90
1	C	292	ILE	CA-C-O	-7.86	112.83	121.17
1	A	121	ASN	CB-CG-ND2	7.86	128.19	116.40
2	D	301	ASP	CA-CB-CG	7.85	120.45	112.60
2	D	96	ASN	CA-CB-CG	7.84	120.44	112.60
2	B	259	VAL	N-CA-C	-7.84	98.28	107.61
1	A	389	ASP	CA-CB-CG	7.83	120.43	112.60
2	B	124	ASP	CA-CB-CG	7.80	120.40	112.60
2	B	403	ASN	OD1-CG-ND2	-7.80	114.80	122.60
1	C	265	SER	CA-CB-OG	7.78	126.67	111.10
1	C	371	HIS	CB-CG-CD2	-7.77	121.10	131.20
2	B	373	ASP	CA-CB-CG	7.77	120.37	112.60
1	A	210	ILE	O-C-N	-7.76	115.47	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	ASP	CA-C-N	7.75	127.46	119.56
1	C	305	ASP	C-N-CA	7.75	127.46	119.56
1	C	109	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	40	ASN	CB-CG-ND2	7.73	127.99	116.40
1	C	328	ASP	CA-CB-CG	7.72	120.32	112.60
1	C	285	ASN	OD1-CG-ND2	-7.67	114.93	122.60
2	B	138	ASN	OD1-CG-ND2	-7.66	114.94	122.60
2	D	201	PHE	CA-CB-CG	7.65	121.45	113.80
1	C	442	ASP	CA-C-N	7.65	133.24	122.46
1	C	442	ASP	C-N-CA	7.65	133.24	122.46
1	C	438	THR	N-CA-CB	-7.63	98.03	111.08
1	A	226	ASP	CA-CB-CG	7.58	120.18	112.60
1	C	186	HIS	CB-CG-CD2	-7.57	121.36	131.20
1	A	347	ARG	N-CA-C	7.53	120.44	111.33
2	B	2	LEU	CD1-CG-CD2	-7.53	94.24	110.80
1	C	371	HIS	CB-CG-ND1	7.52	133.98	122.70
1	A	108	THR	CA-C-O	-7.51	112.73	120.54
1	C	307	GLU	N-CA-C	-7.50	103.04	111.14
2	D	169	ASN	N-CA-C	-7.48	99.45	110.52
1	C	412	ASP	N-CA-C	-7.47	103.24	112.88
1	C	247	GLU	CB-CG-CD	7.46	125.29	112.60
1	A	371	HIS	CB-CG-CD2	-7.46	121.50	131.20
2	D	402	GLU	N-CA-C	-7.45	95.45	108.20
1	A	89	PHE	CA-CB-CG	7.44	121.24	113.80
1	A	47	ILE	N-CA-C	-7.44	97.44	108.45
2	B	209	ASP	N-CA-C	-7.42	96.84	109.24
1	A	102	ASN	OD1-CG-ND2	-7.42	115.19	122.60
1	C	134	PHE	O-C-N	-7.41	114.54	123.29
1	A	153	ASP	CA-C-O	7.40	128.62	120.92
1	A	110	MET	O-C-N	7.40	131.59	122.86
2	D	121	GLN	OE1-CD-NE2	-7.39	115.21	122.60
2	B	448	GLU	CA-CB-CG	7.37	128.85	114.10
2	D	113	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	196	ASP	CA-CB-CG	7.37	119.97	112.60
2	B	322	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	397	THR	N-CA-CB	-7.37	97.94	111.13
1	C	456	LEU	N-CA-C	7.37	122.36	113.23
2	D	64	ALA	N-CA-C	-7.36	97.74	109.59
1	A	270	ALA	O-C-N	7.35	129.73	122.09
1	A	268	TYR	N-CA-C	-7.34	103.36	111.36
1	C	482	HIS	CA-CB-CG	7.33	121.14	113.80
1	A	24	HIS	CB-CG-CD2	-7.33	121.67	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	130	GLU	CB-CG-CD	7.33	125.05	112.60
1	A	330	PHE	CA-CB-CG	7.31	121.11	113.80
2	B	46	GLN	N-CA-C	7.31	118.89	111.07
2	B	392	ASN	CA-CB-CG	7.30	119.90	112.60
2	D	454	PHE	CA-CB-CG	7.29	121.09	113.80
1	A	70	VAL	N-CA-C	-7.28	97.09	108.23
1	C	121	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	A	241	THR	CA-C-O	-7.27	110.12	120.51
1	C	509	THR	CA-C-N	7.25	126.78	119.24
1	C	509	THR	C-N-CA	7.25	126.78	119.24
1	A	347	ARG	CA-CB-CG	-7.24	99.61	114.10
1	A	88	ARG	N-CA-C	7.24	122.23	111.81
1	A	204	GLU	CB-CG-CD	7.24	124.90	112.60
1	A	139	ILE	O-C-N	-7.22	115.47	122.98
2	D	376	ASP	CA-CB-CG	7.21	119.81	112.60
1	C	243	ASP	N-CA-C	-7.18	101.82	110.44
1	C	303	PHE	N-CA-C	-7.17	100.87	110.55
2	B	124	ASP	N-CA-C	-7.16	103.21	112.23
1	A	361	ASP	CA-CB-CG	7.15	119.75	112.60
2	D	98	ASP	N-CA-C	-7.15	103.22	112.23
2	D	159	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	C	48	ILE	N-CA-CB	-7.13	103.53	111.66
1	C	470	VAL	N-CA-C	-7.12	103.92	110.82
1	C	290	ASP	CA-CB-CG	7.12	119.72	112.60
2	D	71	PHE	N-CA-C	7.11	120.80	110.42
1	C	245	THR	CA-CB-CG2	7.11	122.58	110.50
1	C	51	ARG	N-CA-C	7.09	119.72	110.43
1	C	95	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	A	33	PRO	N-CA-C	-7.07	100.09	111.19
2	B	157	ILE	CA-C-O	-7.05	113.61	120.95
2	B	134	VAL	N-CA-C	-7.05	98.24	108.11
2	B	307	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	C	134	PHE	N-CA-C	-7.04	97.73	109.07
1	C	435	HIS	CB-CG-ND1	7.04	133.26	122.70
1	A	498	ASN	CB-CG-ND2	7.04	126.96	116.40
2	D	208	LEU	N-CA-C	7.04	121.82	112.25
2	D	4	ALA	N-CA-C	7.02	125.75	110.80
1	A	237	ASN	OD1-CG-ND2	-7.01	115.59	122.60
2	D	392	ASN	CA-CB-CG	7.00	119.60	112.60
1	A	135	HIS	CB-CG-CD2	-6.99	122.11	131.20
1	A	445	ASN	CA-CB-CG	6.99	119.59	112.60
2	D	135	ILE	O-C-N	-6.99	115.49	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	ASN	CA-C-N	6.99	128.57	119.84
1	C	34	ASN	C-N-CA	6.99	128.57	119.84
2	B	7	LYS	N-CA-C	-6.98	102.88	111.40
1	C	237	ASN	CB-CG-ND2	6.98	126.87	116.40
1	C	67	LYS	N-CA-CB	-6.97	99.47	110.28
2	D	154	VAL	N-CA-CB	-6.96	101.07	110.54
2	D	130	GLU	CA-CB-CG	6.95	128.00	114.10
2	B	139	THR	N-CA-CB	-6.95	98.53	111.24
2	B	310	LEU	N-CA-C	6.95	119.70	111.71
1	C	397	THR	O-C-N	6.95	131.75	123.27
2	D	133	LEU	N-CA-C	6.95	119.42	108.79
1	C	357	SER	CA-CB-OG	6.94	124.98	111.10
2	B	147	VAL	CA-C-N	6.94	129.58	120.28
2	B	147	VAL	C-N-CA	6.94	129.58	120.28
1	C	504	VAL	CA-C-N	6.93	129.90	120.54
1	C	504	VAL	C-N-CA	6.93	129.90	120.54
2	D	128	ILE	N-CA-C	-6.93	100.18	107.60
1	A	384	ILE	CB-CA-C	-6.93	101.50	111.34
2	D	83	ASN	N-CA-C	6.92	118.47	111.07
1	C	157	VAL	N-CA-C	-6.92	103.78	110.42
1	C	30	GLU	O-C-N	6.91	129.44	122.12
2	D	59	HIS	CB-CG-ND1	6.90	133.06	122.70
1	A	342	TYR	N-CA-C	-6.90	97.03	108.34
1	C	110	MET	O-C-N	6.89	131.35	122.87
2	D	282	GLU	CB-CG-CD	6.89	124.31	112.60
1	C	390	SER	CA-CB-OG	6.88	124.87	111.10
1	A	415	GLU	N-CA-C	-6.88	103.70	111.07
2	D	161	LEU	N-CA-C	6.88	122.34	113.88
1	C	221	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	237	ASN	CA-CB-CG	6.84	119.44	112.60
1	A	202	ASN	CA-CB-CG	6.84	119.44	112.60
2	B	169	ASN	CB-CG-ND2	6.84	126.66	116.40
2	B	283	ALA	CA-C-O	-6.83	113.64	120.82
1	C	385	LYS	CA-CB-CG	-6.83	100.44	114.10
2	B	8	GLU	CB-CG-CD	6.82	124.20	112.60
2	D	247	ASP	N-CA-C	6.82	121.83	112.90
1	A	72	ILE	CA-C-O	6.81	127.82	120.53
2	B	439	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	C	397	THR	CA-C-N	6.81	131.51	122.93
1	C	397	THR	C-N-CA	6.81	131.51	122.93
1	A	324	GLN	N-CA-C	6.80	118.49	111.14
2	D	212	THR	N-CA-C	-6.79	98.17	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	A	401	ASP	N-CA-C	6.79	121.15	113.01
2	B	257	CYS	CA-C-O	-6.78	113.05	120.30
2	B	98	ASP	CA-CB-CG	6.78	119.38	112.60
2	B	230	LYS	CA-CB-CG	6.78	127.66	114.10
2	D	96	ASN	CA-C-O	6.77	125.05	119.36
1	A	367	PHE	CA-CB-CG	6.76	120.56	113.80
2	D	403	ASN	CB-CG-ND2	6.75	126.53	116.40
2	B	376	ASP	CA-C-O	-6.75	113.91	121.00
1	C	271	GLU	N-CA-C	6.74	118.42	111.14
1	A	10	LEU	N-CA-C	6.74	118.62	111.28
2	B	345	THR	N-CA-CB	-6.74	101.41	110.23
1	A	422	VAL	N-CA-C	-6.73	101.62	108.96
2	D	307	GLN	N-CA-C	6.72	119.47	111.33
2	D	443	ASP	CA-CB-CG	6.72	119.32	112.60
2	D	437	ILE	N-CA-C	-6.72	104.31	110.82
1	A	424	LEU	N-CA-C	-6.71	98.28	108.96
1	C	432	LYS	N-CA-C	6.71	119.45	111.33
1	A	388	ALA	N-CA-C	-6.69	104.15	112.72
2	D	22	THR	CA-CB-OG1	-6.69	99.57	109.60
1	C	436	ASP	CA-CB-CG	-6.69	105.91	112.60
1	A	69	MET	N-CA-C	-6.69	99.02	109.72
1	C	14	ILE	CA-C-N	6.68	126.63	119.28
1	C	14	ILE	C-N-CA	6.68	126.63	119.28
2	B	4	ALA	N-CA-C	6.66	124.98	110.80
2	D	192	GLU	CB-CG-CD	-6.66	101.28	112.60
1	A	165	ILE	CA-CB-CG1	-6.65	99.09	110.40
2	B	29	MET	O-C-N	6.65	129.28	122.09
2	D	300	ILE	CA-C-O	-6.64	114.04	120.95
2	D	370	VAL	N-CA-C	-6.61	98.82	108.87
2	D	192	GLU	N-CA-CB	-6.61	100.38	110.16
1	C	61	VAL	O-C-N	-6.61	114.31	122.57
1	A	447	HIS	CB-CG-CD2	-6.60	122.62	131.20
2	D	100	ILE	CB-CA-C	-6.60	102.98	110.96
1	C	437	GLY	CA-C-O	6.58	127.58	119.88
1	C	125	ASP	CA-CB-CG	6.58	119.18	112.60
1	C	372	ARG	N-CA-C	6.57	118.44	111.28
1	A	397	THR	CB-CA-C	6.57	122.71	109.38
2	B	439	ASN	CA-C-N	6.57	129.79	120.53
2	B	439	ASN	C-N-CA	6.57	129.79	120.53
2	D	43	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	C	135	HIS	CB-CG-CD2	-6.56	122.68	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	HIS	CB-CG-ND1	6.55	132.53	122.70
1	A	448	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	30	GLU	N-CA-C	6.53	124.71	110.80
1	A	265	SER	CA-C-O	-6.53	114.03	120.89
2	D	184	MET	N-CA-C	-6.53	104.09	111.14
2	D	351	GLN	CA-CB-CG	6.52	127.15	114.10
1	C	65	PRO	N-CA-C	6.52	125.90	112.47
2	B	136	HIS	CA-CB-CG	6.52	120.32	113.80
1	A	198	ILE	O-C-N	-6.51	114.44	122.57
1	C	279	ILE	CA-C-N	6.50	126.26	119.76
1	C	279	ILE	C-N-CA	6.50	126.26	119.76
1	C	226	ASP	N-CA-CB	-6.50	100.21	110.22
2	D	322	ASP	N-CA-C	6.49	118.36	111.28
2	D	201	PHE	O-C-N	-6.49	117.27	121.88
1	A	125	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	392	ASN	N-CA-C	-6.48	102.67	110.44
1	A	38	VAL	N-CA-CB	6.47	117.77	110.72
1	C	169	VAL	O-C-N	-6.47	116.07	122.99
1	A	418	LYS	N-CA-C	-6.45	104.10	112.68
1	A	465	ILE	N-CA-C	6.45	117.13	110.36
2	B	436	GLU	CB-CG-CD	6.44	123.55	112.60
2	B	159	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	A	128	HIS	O-C-N	6.43	132.39	122.87
1	C	384	ILE	N-CA-C	6.43	117.56	108.17
2	B	438	THR	N-CA-C	-6.43	104.19	111.14
1	C	241	THR	O-C-N	-6.43	114.04	122.59
1	C	243	ASP	CA-CB-CG	6.43	119.03	112.60
2	B	55	VAL	CB-CA-C	-6.42	102.20	112.16
2	B	84	ILE	N-CA-CB	6.42	120.21	110.58
2	D	324	ILE	CA-C-O	-6.41	114.05	120.85
2	D	343	THR	N-CA-CB	6.41	122.61	111.00
2	B	265	ARG	CB-CG-CD	-6.41	96.56	111.30
1	C	463	ALA	O-C-N	-6.41	116.09	120.83
1	A	412	ASP	CA-CB-CG	6.40	119.00	112.60
2	D	265	ARG	N-CA-C	-6.39	101.07	110.52
1	A	79	CYS	CA-CB-SG	-6.38	99.72	114.40
1	A	77	ILE	N-CA-C	6.38	119.03	111.05
2	D	224	THR	O-C-N	-6.38	115.77	123.16
1	A	435	HIS	CB-CG-ND1	6.36	132.24	122.70
2	D	260	PRO	O-C-N	-6.36	115.24	123.06
1	A	190	ASN	OD1-CG-ND2	-6.36	116.24	122.60
2	D	387	ASP	N-CA-C	6.35	121.11	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	231	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	253	ASP	CA-CB-CG	6.34	118.94	112.60
2	B	457	VAL	N-CA-C	-6.34	99.15	108.97
2	B	2	LEU	CB-CA-C	6.32	122.11	110.10
1	C	157	VAL	CA-C-O	-6.32	114.47	121.17
2	B	384	GLU	CA-CB-CG	6.30	126.70	114.10
1	A	44	VAL	N-CA-CB	-6.30	104.22	110.08
2	D	78	PHE	N-CA-C	6.29	120.30	111.30
2	B	210	GLY	CA-C-N	6.27	127.68	119.84
2	B	210	GLY	C-N-CA	6.27	127.68	119.84
1	A	187	HIS	CB-CG-ND1	6.27	132.11	122.70
1	A	357	SER	CA-CB-OG	6.27	123.63	111.10
2	D	343	THR	CB-CA-C	-6.27	96.94	109.35
1	A	520	LYS	CA-C-N	6.26	131.02	120.81
1	A	520	LYS	C-N-CA	6.26	131.02	120.81
2	B	152	ASN	OD1-CG-ND2	-6.25	116.35	122.60
2	B	83	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	C	182	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	C	480	GLN	CA-CB-CG	6.24	126.58	114.10
1	C	241	THR	N-CA-C	6.24	124.08	110.80
2	D	199	ILE	N-CA-C	-6.23	98.50	107.78
2	D	380	TRP	CG-CD2-CE3	6.23	140.13	133.90
2	B	345	THR	CA-C-N	6.23	127.62	119.84
2	B	345	THR	C-N-CA	6.23	127.62	119.84
2	B	59	HIS	CA-CB-CG	6.22	120.02	113.80
1	C	239	THR	N-CA-C	-6.21	99.14	109.46
2	D	191	PHE	CA-C-O	6.21	127.35	120.82
1	A	24	HIS	CB-CG-ND1	6.21	132.02	122.70
2	D	245	ALA	N-CA-C	6.21	121.52	113.88
1	C	283	LYS	N-CA-C	-6.20	99.16	109.46
1	A	211	ASN	CA-CB-CG	6.20	118.80	112.60
1	A	237	ASN	CB-CG-ND2	6.20	125.70	116.40
1	C	61	VAL	N-CA-C	6.20	122.23	109.34
2	B	257	CYS	O-C-N	-6.20	116.08	123.27
1	C	4	ASN	N-CA-C	6.18	118.10	111.36
2	B	90	ASN	CB-CG-ND2	-6.18	107.14	116.40
2	D	122	MET	CB-CA-C	-6.17	100.18	110.68
2	D	439	ASN	CB-CG-ND2	6.17	125.65	116.40
1	A	525	GLU	CA-C-N	6.16	132.78	121.70
1	A	525	GLU	C-N-CA	6.16	132.78	121.70
2	D	190	LEU	CA-C-N	6.16	128.44	120.44
2	D	190	LEU	C-N-CA	6.16	128.44	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	355	ASP	CA-CB-CG	6.15	118.75	112.60
1	C	292	ILE	CB-CA-C	-6.13	104.13	111.97
1	C	265	SER	CA-C-O	-6.12	112.40	119.14
1	C	344	GLY	N-CA-C	-6.12	105.44	112.79
2	B	113	ASP	N-CA-C	6.12	118.42	108.63
2	D	448	GLU	N-CA-C	6.12	119.94	112.23
2	B	287	GLU	CB-CG-CD	6.11	122.99	112.60
1	A	434	MET	N-CA-CB	-6.11	101.37	110.17
2	B	79	GLY	CA-C-O	6.10	128.07	122.39
2	D	182	ALA	N-CA-C	6.10	118.73	111.71
2	D	22	THR	CA-CB-CG2	6.10	120.87	110.50
2	B	92	PHE	N-CA-C	6.09	118.00	111.36
1	C	343	VAL	O-C-N	-6.09	114.96	122.57
2	B	359	ALA	N-CA-C	-6.08	104.28	111.03
1	C	43	THR	N-CA-C	-6.08	101.48	110.48
2	D	409	PHE	CA-CB-CG	6.08	119.88	113.80
1	C	422	VAL	CA-C-N	6.07	127.43	119.84
1	C	422	VAL	C-N-CA	6.07	127.43	119.84
1	C	127	ILE	N-CA-C	-6.06	104.72	110.42
1	A	187	HIS	CA-C-N	6.06	128.42	120.60
1	A	187	HIS	C-N-CA	6.06	128.42	120.60
2	B	320	ASP	N-CA-C	6.06	118.65	110.29
2	B	422	ASN	CB-CG-ND2	6.05	125.48	116.40
2	B	7	LYS	CG-CD-CE	6.05	125.22	111.30
2	D	59	HIS	CB-CG-CD2	-6.05	123.34	131.20
1	A	411	GLU	CA-C-N	6.04	129.20	120.38
1	A	411	GLU	C-N-CA	6.04	129.20	120.38
1	A	71	HIS	CB-CG-CD2	-6.04	123.35	131.20
2	B	43	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	A	38	VAL	CA-CB-CG2	6.03	120.65	110.40
2	D	261	PHE	CA-C-O	-6.03	114.41	121.46
1	C	448	ASP	CA-CB-CG	6.03	118.63	112.60
2	D	296	ARG	CA-CB-CG	6.03	126.16	114.10
2	B	191	PHE	CB-CA-C	-6.02	100.79	110.79
1	C	443	ASP	CA-C-O	6.02	129.08	122.03
2	D	3	ASP	N-CA-CB	-6.02	100.31	110.49
2	B	137	THR	OG1-CB-CG2	6.02	121.34	109.30
1	C	211	ASN	CA-C-O	-6.01	113.87	120.36
2	D	266	THR	O-C-N	-6.01	116.45	121.38
2	D	403	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	A	525	GLU	CA-C-O	6.01	125.62	119.97
2	D	311	GLN	CG-CD-NE2	6.01	125.41	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	HIS	CB-CG-CD2	-6.00	123.39	131.20
1	C	38	VAL	CA-C-O	6.00	127.08	120.48
1	A	186	HIS	CA-CB-CG	6.00	119.80	113.80
2	B	194	MET	N-CA-C	5.99	120.59	113.28
1	C	496	VAL	N-CA-CB	-5.98	101.36	111.23
2	D	127	SER	CA-CB-OG	5.98	123.06	111.10
1	C	237	ASN	CA-CB-CG	5.98	118.58	112.60
1	C	445	ASN	CA-CB-CG	5.98	118.58	112.60
2	D	121	GLN	CG-CD-NE2	5.98	125.37	116.40
2	B	240	SER	CA-CB-OG	5.97	123.04	111.10
2	B	46	GLN	CA-CB-CG	5.96	126.02	114.10
2	B	333	GLU	CA-CB-CG	5.96	126.01	114.10
1	A	100	ASN	CB-CG-ND2	5.95	125.33	116.40
1	A	434	MET	CA-CB-CG	5.95	126.00	114.10
2	B	376	ASP	CA-CB-CG	5.95	118.55	112.60
2	D	401	GLU	N-CA-CB	-5.95	101.33	110.13
2	B	46	GLN	N-CA-CB	-5.94	101.39	110.01
1	A	188	ILE	N-CA-C	5.94	116.60	110.36
1	A	4	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	A	195	THR	N-CA-CB	-5.93	101.41	110.01
2	D	349	LYS	CA-C-O	-5.93	114.22	120.63
2	B	270	VAL	N-CA-CB	-5.92	104.16	110.62
1	C	353	ASN	O-C-N	5.92	128.39	122.12
1	C	435	HIS	CB-CG-CD2	-5.92	123.51	131.20
2	B	58	ARG	CB-CG-CD	-5.91	97.71	111.30
2	B	236	ASP	N-CA-C	5.91	118.67	111.82
1	A	440	LEU	N-CA-C	-5.90	100.17	109.50
2	B	305	ASP	CA-CB-CG	5.90	118.50	112.60
2	D	163	GLU	N-CA-C	5.90	118.72	108.76
1	A	92	LYS	CA-CB-CG	5.89	125.89	114.10
1	A	471	ILE	O-C-N	-5.88	116.06	121.94
1	A	226	ASP	CA-C-O	-5.88	114.32	120.55
1	A	263	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	C	413	LYS	N-CA-C	-5.87	104.96	111.36
1	C	482	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	C	100	ASN	OD1-CG-ND2	-5.87	116.73	122.60
2	B	422	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	C	467	GLU	N-CA-C	5.86	119.62	112.23
1	A	245	THR	N-CA-C	-5.86	101.81	110.48
2	D	99	ILE	N-CA-C	5.86	116.55	108.12
2	B	387	ASP	CA-CB-CG	5.85	118.45	112.60
2	B	59	HIS	CB-CG-CD2	-5.85	123.59	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ILE	CA-CB-CG2	5.85	120.44	110.50
2	B	281	SER	N-CA-C	5.85	117.34	110.97
2	B	384	GLU	CA-C-O	5.85	127.11	119.98
2	B	425	VAL	N-CA-CB	-5.84	101.86	111.44
2	B	9	ILE	N-CA-C	5.84	117.25	109.37
2	B	128	ILE	N-CA-C	-5.83	101.78	107.55
1	A	522	ALA	O-C-N	5.82	129.73	122.63
1	A	313	GLU	CB-CG-CD	5.82	122.50	112.60
2	D	136	HIS	CB-CG-CD2	-5.82	123.64	131.20
2	B	127	SER	N-CA-C	5.81	119.56	112.23
1	C	50	ALA	CA-C-N	5.81	130.68	120.87
1	C	50	ALA	C-N-CA	5.81	130.68	120.87
2	D	334	LEU	N-CA-C	5.80	118.55	111.82
2	B	366	SER	N-CA-C	5.80	119.36	110.20
1	A	285	ASN	CB-CG-ND2	5.79	125.09	116.40
1	A	508	TYR	N-CA-CB	-5.79	102.57	110.56
1	C	335	GLN	OE1-CD-NE2	-5.79	116.81	122.60
2	D	173	ASN	CA-CB-CG	5.79	118.39	112.60
1	A	186	HIS	CB-CG-ND1	5.79	131.38	122.70
1	A	447	HIS	CB-CG-ND1	5.79	131.38	122.70
1	C	76	PRO	O-C-N	-5.78	115.77	122.71
2	B	257	CYS	N-CA-C	-5.78	98.99	108.41
1	A	163	LYS	CA-CB-CG	5.77	125.64	114.10
2	D	369	LYS	CA-C-O	5.77	126.36	120.24
2	B	29	MET	CA-C-N	5.76	128.79	120.79
2	B	29	MET	C-N-CA	5.76	128.79	120.79
1	C	183	SER	CA-C-N	5.76	129.06	120.31
1	C	183	SER	C-N-CA	5.76	129.06	120.31
1	A	198	ILE	CA-C-O	-5.75	113.59	120.78
1	A	258	ASN	CA-CB-CG	5.75	118.35	112.60
1	C	16	LYS	CA-CB-CG	5.75	125.60	114.10
2	B	393	THR	O-C-N	-5.75	115.50	122.22
2	D	452	GLU	CA-C-O	5.75	126.44	119.31
2	D	37	ASN	CA-CB-CG	5.75	118.34	112.60
2	B	212	THR	CA-CB-OG1	-5.74	100.99	109.60
1	C	100	ASN	CB-CG-ND2	5.74	125.01	116.40
1	A	520	LYS	CA-C-O	5.74	129.35	122.41
2	D	136	HIS	CA-CB-CG	5.74	119.54	113.80
2	D	305	ASP	CA-CB-CG	5.74	118.34	112.60
1	C	16	LYS	N-CA-CB	-5.73	101.67	110.16
1	C	97	THR	CA-CB-OG1	-5.73	101.01	109.60
1	C	276	LYS	CB-CG-CD	-5.72	98.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316	ILE	N-CA-C	-5.72	104.75	110.30
1	C	428	GLY	N-CA-C	-5.72	99.63	113.18
1	C	125	ASP	CA-C-O	-5.71	115.00	121.00
2	D	124	ASP	N-CA-CB	5.71	118.45	109.94
1	C	170	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	C	114	ASP	CA-CB-CG	5.71	118.31	112.60
2	B	152	ASN	CB-CG-ND2	5.71	124.96	116.40
1	C	95	ASN	CB-CG-ND2	5.71	124.96	116.40
1	C	305	ASP	CA-CB-CG	5.70	118.30	112.60
2	B	440	VAL	CA-CB-CG2	-5.70	100.71	110.40
2	D	147	VAL	N-CA-C	-5.69	104.97	110.72
2	B	95	TYR	CA-C-N	5.68	128.97	122.83
2	B	95	TYR	C-N-CA	5.68	128.97	122.83
1	A	386	ILE	CA-C-N	5.68	132.38	121.54
1	A	386	ILE	C-N-CA	5.68	132.38	121.54
1	A	261	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	A	341	LEU	O-C-N	-5.67	116.68	123.31
1	A	332	GLU	CA-C-O	5.67	126.75	120.63
2	B	139	THR	O-C-N	-5.67	116.26	121.42
2	B	415	ASP	CB-CA-C	-5.66	98.05	109.55
1	C	340	CYS	O-C-N	-5.66	115.83	123.19
2	B	172	ILE	N-CA-C	-5.66	100.28	108.89
2	D	308	GLN	CG-CD-NE2	5.65	124.88	116.40
1	A	68	ASP	CA-CB-CG	5.65	118.25	112.60
2	B	2	LEU	N-CA-C	-5.65	95.19	111.00
1	C	230	GLU	CA-C-N	5.64	129.63	120.60
1	C	230	GLU	C-N-CA	5.64	129.63	120.60
2	D	123	GLU	CA-C-N	5.64	128.16	120.54
2	D	123	GLU	C-N-CA	5.64	128.16	120.54
1	A	170	HIS	CA-CB-CG	5.64	119.44	113.80
2	B	106	CYS	CB-CA-C	-5.64	100.20	110.63
1	A	379	GLU	N-CA-C	5.64	118.15	111.33
2	B	440	VAL	CB-CA-C	5.64	119.42	112.04
2	B	212	THR	CA-CB-CG2	5.63	120.08	110.50
1	C	293	VAL	O-C-N	5.62	127.33	121.87
2	D	210	GLY	CA-C-N	5.62	126.06	119.99
2	D	210	GLY	C-N-CA	5.62	126.06	119.99
1	A	526	SER	N-CA-C	-5.62	95.27	111.00
1	A	337	LYS	CA-C-N	5.61	131.01	122.65
1	A	337	LYS	C-N-CA	5.61	131.01	122.65
2	D	210	GLY	O-C-N	5.61	127.38	121.77
1	C	88	ARG	N-CA-C	5.61	118.39	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	VAL	N-CA-CB	-5.61	105.05	112.34
1	C	365	ALA	O-C-N	-5.60	117.38	123.26
2	B	354	ILE	N-CA-C	-5.60	105.45	113.07
1	C	112	GLU	O-C-N	-5.60	116.18	122.12
1	C	167	ILE	N-CA-C	-5.60	96.79	108.88
1	A	215	GLU	CB-CG-CD	5.59	122.10	112.60
1	C	231	LYS	CA-CB-CG	5.59	125.28	114.10
1	A	153	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	288	GLY	CA-C-O	-5.59	117.38	122.24
2	D	138	ASN	CA-CB-CG	5.59	118.19	112.60
1	C	388	ALA	N-CA-C	5.58	122.69	110.80
1	C	472	GLN	CA-C-N	5.58	128.79	120.31
1	C	472	GLN	C-N-CA	5.58	128.79	120.31
2	B	29	MET	CG-SD-CE	-5.57	88.64	100.90
1	A	433	GLU	CA-C-N	5.57	129.68	120.94
1	A	433	GLU	C-N-CA	5.57	129.68	120.94
2	B	3	ASP	CA-C-N	5.56	132.17	121.54
2	B	3	ASP	C-N-CA	5.56	132.17	121.54
1	C	35	PRO	N-CA-C	5.56	123.93	112.47
2	D	70	SER	N-CA-C	5.56	122.65	110.80
2	D	337	ILE	CA-C-N	5.56	126.79	119.84
2	D	337	ILE	C-N-CA	5.56	126.79	119.84
1	C	466	LYS	CA-C-N	5.56	130.13	120.68
1	C	466	LYS	C-N-CA	5.56	130.13	120.68
1	C	248	LYS	CB-CG-CD	-5.55	98.54	111.30
2	D	154	VAL	CA-CB-CG2	-5.55	100.97	110.40
2	D	3	ASP	CA-C-N	5.54	132.13	121.54
2	D	3	ASP	C-N-CA	5.54	132.13	121.54
1	A	74	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	A	103	GLU	N-CA-C	5.54	119.03	112.72
1	C	334	LEU	N-CA-C	5.54	120.92	113.72
1	A	168	PRO	O-C-N	-5.54	115.17	122.64
2	D	104	THR	N-CA-CB	-5.53	102.19	110.60
2	D	154	VAL	CA-CB-CG1	5.53	119.80	110.40
1	A	372	ARG	N-CA-C	5.53	117.31	111.28
2	B	2	LEU	CA-C-O	5.53	130.19	120.80
2	B	225	LYS	CA-CB-CG	-5.52	103.06	114.10
1	A	328	ASP	CA-CB-CG	5.52	118.12	112.60
2	D	406	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	519	TRP	O-C-N	-5.51	115.71	122.11
1	C	144	THR	N-CA-CB	-5.51	102.37	110.85
1	C	221	ASP	CB-CA-C	-5.51	99.46	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	438	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	470	VAL	N-CA-C	-5.50	105.25	110.42
2	D	333	GLU	CA-CB-CG	5.50	125.11	114.10
1	C	438	THR	CB-CA-C	5.50	120.17	109.33
1	C	419	LYS	CA-CB-CG	5.50	125.11	114.10
2	D	452	GLU	N-CA-CB	-5.50	101.43	110.40
1	A	217	ASN	N-CA-C	5.50	118.70	111.28
1	A	187	HIS	CB-CG-CD2	-5.50	124.06	131.20
1	A	212	VAL	N-CA-C	-5.50	100.56	108.53
1	C	356	LYS	CA-CB-CG	5.49	125.07	114.10
1	A	403	GLN	CB-CG-CD	5.48	121.92	112.60
1	C	54	ALA	CA-C-N	5.48	128.38	120.38
1	C	54	ALA	C-N-CA	5.48	128.38	120.38
2	D	303	MET	O-C-N	5.48	127.93	122.12
1	A	186	HIS	N-CA-CB	5.48	118.77	110.28
1	A	371	HIS	CB-CG-ND1	5.48	130.92	122.70
2	B	122	MET	O-C-N	-5.48	115.31	122.59
2	B	136	HIS	CB-CG-CD2	-5.47	124.08	131.20
1	C	234	TYR	N-CA-C	-5.47	101.62	110.32
1	A	281	TRP	CG-CD2-CE3	5.47	139.37	133.90
1	C	505	ASN	OD1-CG-ND2	-5.47	117.13	122.60
2	B	307	GLN	CA-CB-CG	5.47	125.03	114.10
1	C	217	ASN	CA-CB-CG	5.46	118.06	112.60
2	B	2	LEU	CA-C-N	5.46	131.97	121.54
2	B	2	LEU	C-N-CA	5.46	131.97	121.54
1	A	478	SER	N-CA-C	-5.46	99.53	108.76
2	B	188	LYS	CB-CG-CD	5.46	123.85	111.30
2	B	442	LEU	CA-C-N	5.46	127.53	120.44
2	B	442	LEU	C-N-CA	5.46	127.53	120.44
2	D	77	VAL	N-CA-C	-5.45	106.87	111.56
1	A	31	GLU	N-CA-C	-5.45	105.34	111.28
2	B	425	VAL	CB-CA-C	5.45	118.89	110.50
2	D	84	ILE	CB-CA-C	-5.45	103.43	112.26
1	C	69	MET	CA-CB-CG	5.45	125.00	114.10
2	D	37	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	186	HIS	CB-CA-C	-5.44	100.22	110.67
2	B	378	HIS	CA-CB-CG	5.44	119.24	113.80
1	A	105	VAL	CB-CA-C	5.44	116.61	110.41
2	B	284	THR	N-CA-C	5.43	119.91	113.28
1	C	263	HIS	CB-CG-CD2	-5.43	124.14	131.20
2	B	308	GLN	CA-C-O	5.43	126.49	120.63
1	A	3	GLU	CA-C-O	5.43	128.27	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	GLN	O-C-N	-5.43	116.52	122.38
2	D	103	HIS	CB-CG-CD2	-5.42	124.15	131.20
2	B	232	THR	N-CA-C	-5.41	106.52	113.01
2	D	36	HIS	CB-CG-CD2	-5.41	124.17	131.20
2	D	365	GLY	N-CA-C	-5.41	108.55	115.42
2	D	422	ASN	CB-CA-C	-5.41	102.66	109.31
2	B	30	TYR	CA-C-N	5.40	127.78	120.38
2	B	30	TYR	C-N-CA	5.40	127.78	120.38
2	B	426	GLY	O-C-N	5.40	127.36	122.88
2	D	45	SER	CA-C-O	5.39	127.80	121.87
2	B	139	THR	CA-CB-CG2	5.39	119.67	110.50
2	D	154	VAL	CB-CA-C	5.39	119.42	112.14
1	A	430	MET	CG-SD-CE	-5.39	89.04	100.90
1	C	186	HIS	CB-CG-ND1	5.38	130.77	122.70
1	A	490	TYR	CA-C-O	5.37	125.27	119.15
2	D	124	ASP	CB-CA-C	-5.37	102.22	110.81
2	D	83	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	C	350	THR	N-CA-C	5.37	117.13	111.28
2	B	355	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	152	ASP	CB-CA-C	-5.36	102.22	110.26
1	A	228	VAL	CB-CA-C	-5.36	105.00	112.02
2	D	93	SER	N-CA-C	5.36	116.80	111.07
2	B	110	THR	N-CA-C	-5.35	105.11	111.69
2	D	123	GLU	CA-C-O	-5.35	115.39	120.90
1	C	368	GLU	CA-C-O	-5.35	113.05	119.15
1	A	496	VAL	O-C-N	5.35	127.34	121.83
1	A	97	THR	N-CA-C	-5.35	98.58	107.99
2	B	380	TRP	CG-CD2-CE3	5.35	139.25	133.90
2	D	90	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	C	70	VAL	N-CA-C	-5.34	102.62	109.30
1	C	102	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	206	LYS	N-CA-C	5.34	117.99	110.14
1	C	285	ASN	CB-CG-ND2	5.34	124.41	116.40
2	D	163	GLU	CA-C-N	-5.34	114.56	122.41
2	D	163	GLU	C-N-CA	-5.34	114.56	122.41
2	D	453	ASP	N-CA-CB	-5.34	102.38	110.92
1	A	271	GLU	CA-CB-CG	5.33	124.77	114.10
1	A	473	LYS	N-CA-C	-5.33	105.51	112.23
2	D	71	PHE	CB-CA-C	-5.33	102.30	109.71
2	D	262	LYS	CA-CB-CG	5.33	124.76	114.10
2	D	276	PHE	O-C-N	-5.33	116.48	122.03
2	B	234	ASN	CA-CB-CG	5.32	117.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	PHE	N-CA-C	-5.32	105.17	110.97
2	B	169	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	384	ILE	N-CA-CB	5.31	117.53	110.26
2	D	15	LEU	N-CA-C	-5.31	100.52	108.96
2	B	41	HIS	CA-CB-CG	5.31	119.11	113.80
1	C	465	ILE	N-CA-C	5.31	116.71	111.67
2	D	61	LYS	CG-CD-CE	5.30	123.50	111.30
1	A	79	CYS	N-CA-C	5.30	117.81	111.71
1	C	340	CYS	N-CA-C	-5.30	101.24	109.72
1	A	303	PHE	CB-CA-C	-5.30	104.23	112.07
1	C	30	GLU	CB-CG-CD	5.29	121.60	112.60
1	C	111	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	D	94	LEU	N-CA-C	5.29	119.81	112.45
2	B	194	MET	CA-CB-CG	-5.29	103.52	114.10
2	D	113	ASP	N-CA-C	5.29	117.36	109.59
1	C	517	PRO	N-CA-C	5.29	117.15	110.70
2	D	70	SER	N-CA-CB	-5.29	101.56	110.49
1	A	25	ILE	N-CA-C	-5.29	100.87	108.53
1	A	59	LYS	CB-CG-CD	5.29	123.45	111.30
1	C	26	VAL	O-C-N	-5.29	117.47	123.18
1	C	225	MET	N-CA-C	-5.29	105.43	111.14
2	D	12	ARG	O-C-N	5.29	130.10	123.23
2	D	114	ASP	N-CA-CB	-5.28	104.09	110.53
1	C	321	ALA	N-CA-C	5.28	117.03	111.28
1	A	441	ILE	N-CA-CB	-5.27	102.53	111.23
2	B	37	ASN	OD1-CG-ND2	-5.27	117.33	122.60
2	D	123	GLU	N-CA-CB	-5.27	102.34	109.98
2	B	247	ASP	N-CA-C	5.27	117.03	111.28
1	A	5	LEU	N-CA-C	-5.27	105.45	111.14
2	B	36	HIS	CB-CG-CD2	-5.27	124.36	131.20
1	A	236	VAL	O-C-N	-5.26	116.87	122.61
2	B	440	VAL	CA-CB-CG1	5.26	119.35	110.40
2	D	69	SER	CA-C-O	-5.26	116.06	122.64
2	B	48	CYS	CB-CA-C	-5.26	102.87	110.96
1	C	218	ILE	N-CA-C	-5.25	101.02	108.58
2	D	327	LEU	O-C-N	-5.25	116.56	122.12
1	C	102	ASN	N-CA-C	5.24	119.16	112.34
2	B	419	HIS	CA-CB-CG	5.24	119.04	113.80
2	D	57	SER	CA-C-N	5.24	127.25	120.44
2	D	57	SER	C-N-CA	5.24	127.25	120.44
1	A	406	ARG	N-CA-C	5.24	117.22	108.99
2	B	139	THR	CA-CB-OG1	-5.24	101.75	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	377	VAL	CG1-CB-CG2	-5.24	99.28	110.80
1	C	447	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	C	462	PHE	N-CA-C	5.24	117.73	107.57
1	C	281	TRP	CG-CD1-NE1	-5.23	103.40	110.20
2	D	345	THR	CB-CA-C	5.23	117.64	109.42
2	B	96	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	127	ILE	N-CA-CB	-5.23	103.43	110.54
1	A	433	GLU	CA-C-O	5.23	124.89	119.14
2	B	314	LYS	O-C-N	-5.22	116.50	122.93
1	A	34	ASN	N-CA-C	5.22	123.72	112.23
1	C	217	ASN	OD1-CG-ND2	-5.22	117.38	122.60
2	B	411	PHE	N-CA-C	-5.22	101.50	109.64
2	D	16	ARG	NE-CZ-NH1	5.22	126.72	121.50
2	D	159	ASN	CB-CG-ND2	5.22	124.23	116.40
1	C	123	LEU	N-CA-C	-5.22	105.03	111.40
1	C	393	ILE	N-CA-C	-5.22	97.61	108.88
1	C	371	HIS	O-C-N	-5.21	116.58	122.68
1	C	337	LYS	CA-CB-CG	-5.21	103.68	114.10
1	C	389	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	298	ASP	CB-CA-C	-5.21	102.71	110.88
2	D	169	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	C	32	THR	CA-C-N	5.20	126.34	119.84
1	C	32	THR	C-N-CA	5.20	126.34	119.84
1	C	519	TRP	CE2-CD2-CG	-5.20	100.96	107.20
2	D	128	ILE	CA-C-N	5.20	126.34	119.84
2	D	128	ILE	C-N-CA	5.20	126.34	119.84
1	A	386	ILE	O-C-N	5.20	128.49	123.03
1	A	142	TYR	O-C-N	-5.19	116.07	122.25
2	D	121	GLN	CA-C-O	-5.19	115.55	121.00
2	D	393	THR	CA-C-O	-5.19	113.09	120.51
1	C	313	GLU	N-CA-C	5.19	116.93	111.28
2	D	142	TYR	N-CA-CB	-5.19	103.40	110.56
1	A	384	ILE	CA-CB-CG2	-5.18	101.69	110.50
2	B	320	ASP	CA-C-O	-5.18	115.93	120.60
1	C	251	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	108	THR	CA-CB-OG1	5.18	117.37	109.60
1	A	224	GLU	CB-CG-CD	5.18	121.40	112.60
2	B	168	LYS	O-C-N	5.18	129.10	123.04
2	D	188	LYS	CA-CB-CG	-5.18	103.75	114.10
1	C	245	THR	N-CA-CB	-5.17	102.42	110.29
1	C	354	MET	CG-SD-CE	-5.17	89.52	100.90
1	A	32	THR	O-C-N	-5.17	115.37	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	VAL	O-C-N	-5.17	117.06	122.95
1	A	28	LYS	N-CA-C	-5.17	100.81	109.24
1	C	182	GLN	CG-CD-NE2	5.16	124.14	116.40
1	C	324	GLN	N-CA-C	5.16	121.79	110.80
2	B	64	ALA	N-CA-C	-5.15	98.85	108.02
2	D	181	PRO	CA-C-N	5.15	127.70	120.28
2	D	181	PRO	C-N-CA	5.15	127.70	120.28
2	B	52	HIS	CB-CG-CD2	-5.15	124.50	131.20
1	C	267	ASN	CA-C-N	5.15	127.61	120.29
1	C	267	ASN	C-N-CA	5.15	127.61	120.29
1	C	318	GLU	CA-CB-CG	5.15	124.41	114.10
1	C	430	MET	N-CA-C	5.15	117.68	111.40
1	A	105	VAL	CA-CB-CG2	-5.15	101.65	110.40
1	A	152	ASP	N-CA-CB	5.15	117.64	109.71
1	A	210	ILE	CA-CB-CG1	-5.15	101.65	110.40
1	A	501	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	C	135	HIS	CB-CG-ND1	5.14	130.41	122.70
1	A	92	LYS	CA-C-N	5.14	125.14	119.90
1	A	92	LYS	C-N-CA	5.14	125.14	119.90
2	B	52	HIS	CB-CG-ND1	5.14	130.41	122.70
1	C	454	GLU	N-CA-C	5.14	116.96	111.36
1	C	505	ASN	CB-CG-ND2	5.14	124.11	116.40
1	A	145	CYS	N-CA-C	5.13	121.16	109.81
1	C	291	GLY	O-C-N	5.13	127.21	122.13
1	C	97	THR	N-CA-CB	-5.13	100.00	109.18
1	C	324	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	413	LYS	CA-CB-CG	5.12	124.35	114.10
2	D	122	MET	CB-CG-SD	-5.12	97.36	112.70
2	B	448	GLU	CB-CG-CD	5.11	121.29	112.60
2	B	196	ILE	N-CA-CB	-5.11	105.33	110.08
2	D	136	HIS	CB-CG-ND1	5.11	130.36	122.70
1	C	200	LYS	N-CA-C	-5.11	102.30	109.96
2	B	136	HIS	N-CA-C	5.11	116.83	108.76
1	C	121	ASN	N-CA-C	-5.11	105.80	112.23
2	D	157	ILE	CA-C-O	-5.10	114.74	120.25
2	B	421	TYR	CA-CB-CG	5.10	123.08	113.90
2	B	139	THR	CB-CA-C	5.10	118.92	110.87
1	C	401	ASP	N-CA-CB	5.10	117.63	110.24
2	D	402	GLU	CA-C-O	-5.09	115.25	120.54
2	B	231	ASP	CA-C-O	5.09	125.58	119.43
1	A	247	GLU	CB-CG-CD	5.08	121.24	112.60
1	C	71	HIS	CB-CG-CD2	-5.08	124.59	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ALA	CA-C-O	5.08	125.63	119.38
2	B	276	PHE	CA-C-N	5.08	127.15	120.60
2	B	276	PHE	C-N-CA	5.08	127.15	120.60
1	A	281	TRP	CA-CB-CG	5.07	123.24	113.60
1	C	30	GLU	CA-C-O	5.07	125.93	120.55
1	C	226	ASP	CB-CA-C	5.07	120.02	110.63
2	D	307	GLN	CA-CB-CG	5.07	124.25	114.10
2	B	26	VAL	CB-CA-C	-5.07	105.22	112.22
2	B	265	ARG	N-CA-C	5.07	116.65	110.41
2	D	122	MET	N-CA-CB	5.07	117.67	110.06
1	C	209	SER	CA-CB-OG	5.07	121.23	111.10
2	B	406	PHE	CA-CB-CG	5.06	118.86	113.80
1	C	397	THR	CA-CB-OG1	-5.06	102.00	109.60
2	D	334	LEU	O-C-N	5.05	128.49	122.27
1	C	322	ALA	CA-C-N	5.05	129.03	120.64
1	C	322	ALA	C-N-CA	5.05	129.03	120.64
1	A	428	GLY	N-CA-C	-5.05	101.39	111.34
2	D	146	HIS	N-CA-C	5.05	121.56	110.80
1	C	450	GLU	O-C-N	-5.05	116.31	122.22
1	A	446	HIS	CB-CG-CD2	-5.04	124.64	131.20
2	D	67	SER	CA-C-O	-5.04	115.56	121.46
2	D	455	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	211	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	C	115	ILE	N-CA-CB	-5.04	101.42	110.95
1	A	461	PHE	N-CA-C	-5.04	99.46	108.13
2	B	413	ILE	CB-CG1-CD1	-5.03	103.23	113.80
2	B	100	ILE	N-CA-C	-5.03	101.07	108.11
1	A	204	GLU	CA-CB-CG	5.03	124.15	114.10
1	A	4	ASN	CB-CG-ND2	5.03	123.94	116.40
2	B	288	VAL	CA-C-N	5.03	125.47	120.14
2	B	288	VAL	C-N-CA	5.03	125.47	120.14
2	B	438	THR	CA-C-O	-5.03	115.52	120.70
1	C	178	LYS	CA-CB-CG	-5.03	104.05	114.10
1	C	471	ILE	N-CA-CB	-5.03	104.67	110.55
1	A	519	TRP	CE2-CD2-CG	-5.02	101.17	107.20
1	C	141	VAL	N-CA-CB	-5.02	104.96	110.99
2	D	95	TYR	O-C-N	-5.02	117.72	123.40
2	D	411	PHE	N-CA-C	-5.02	98.76	108.45
1	C	512	TRP	CE2-CD2-CG	-5.02	101.18	107.20
2	D	404	ILE	O-C-N	-5.02	116.90	121.41
2	B	293	GLU	CB-CA-C	-5.01	102.16	110.68
1	C	59	LYS	N-CA-C	-5.01	105.29	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	GLU	N-CA-C	-5.01	107.22	113.38
1	A	95	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	66	ILE	CA-C-N	5.01	127.92	120.31
1	C	66	ILE	C-N-CA	5.01	127.92	120.31
2	B	114	ASP	CA-CB-CG	5.01	117.61	112.60
2	D	451	GLU	CA-CB-CG	5.01	124.11	114.10
2	D	173	ASN	CB-CA-C	-5.00	101.27	109.53
2	B	87	ALA	CA-C-O	-5.00	115.25	120.55
1	C	438	THR	N-CA-C	-5.00	101.72	109.72
2	D	402	GLU	O-C-N	-5.00	117.10	123.05

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ILE	Peptide
1	A	240	LEU	Mainchain
2	B	198	TYR	Sidechain
2	B	337	ILE	Peptide
1	C	104	TYR	Sidechain
1	C	216	TYR	Sidechain
1	C	32	THR	Peptide
1	C	375	TYR	Sidechain
1	C	508	TYR	Sidechain
2	D	115	LEU	Peptide
2	D	216	TYR	Sidechain
2	D	30	TYR	Sidechain
2	D	420	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	0	3992	144	0
1	C	4077	0	3999	159	0
2	B	3511	0	3495	104	0
2	D	3511	0	3495	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	14	0	6	0	0
4	D	14	0	6	2	0
5	B	17	0	0	4	0
5	D	17	0	0	4	0
6	B	16	0	0	4	0
6	D	16	0	0	5	0
All	All	15269	0	14993	469	0

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 16.

All (469) 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)
6:B:498:CLP:S1A	6:B:498:CLP:S1B	2.30	1.28
6:D:498:CLP:S1A	6:D:498:CLP:S1B	2.33	1.26
1:C:345:GLY:HA3	5:D:496:CFM:S1A	2.01	0.99
1:C:197:ILE:HD11	1:C:249:VAL:HB	1.43	0.99
2:D:162:SER:HB3	2:D:257:CYS:SG	2.06	0.96
1:A:43:THR:HG21	1:A:49:THR:HG21	1.58	0.86
2:D:325:ILE:HD11	2:D:350:PHE:HA	1.59	0.83
1:A:191:ASN:HD22	1:A:396:ILE:CG2	1.93	0.82
1:A:391:LYS:HE3	1:A:393:ILE:HB	1.66	0.77
1:C:76:PRO:HB2	6:D:498:CLP:S2B	2.24	0.77
2:B:452:GLU:HG2	1:C:92:LYS:HB3	1.66	0.77
1:A:229:LEU:HD21	1:A:299:MET:HE1	1.68	0.76
1:A:76:PRO:HB2	6:B:498:CLP:S2B	2.25	0.76
1:C:72:ILE:HD11	1:C:108:THR:HG23	1.66	0.76
1:A:213:LEU:HB3	1:A:266:ILE:HD11	1.68	0.76
2:B:278:MET:HA	2:B:278:MET:HE2	1.67	0.76
1:C:187:HIS:ND1	1:C:391:LYS:HB2	2.02	0.75
1:C:369:PHE:HZ	5:D:496:CFM:S1A	2.10	0.73
1:A:388:ALA:H	1:A:390:SER:HB3	1.53	0.73
1:C:48:ILE:HD11	2:D:218:MET:CE	2.18	0.73
1:C:2:SER:N	1:C:29:THR:HG1	1.87	0.72
2:B:330:PHE:HA	2:B:333:GLU:HG2	1.72	0.71
2:B:332:ILE:HD11	2:B:358:LEU:HD12	1.73	0.71
2:D:318:LEU:HD11	2:D:377:VAL:HG11	1.72	0.71
2:B:278:MET:HE1	1:C:519:TRP:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ILE:HD12	1:C:497:VAL:HG11	1.72	0.71
1:C:193:VAL:HA	1:C:197:ILE:HG23	1.71	0.70
2:B:354:ILE:HD11	2:B:368:VAL:HB	1.72	0.70
2:D:145:SER:OG	2:D:345:THR:HB	1.91	0.70
1:A:450:GLU:O	1:A:454:GLU:HG2	1.92	0.69
1:C:232:ILE:HG12	1:C:315:VAL:HG11	1.75	0.69
2:B:297:GLY:HA3	2:D:211:PRO:HB3	1.75	0.68
1:A:191:ASN:ND2	1:A:396:ILE:CG2	2.55	0.68
2:B:129:PRO:HG2	2:B:132:LYS:HG3	1.75	0.68
2:D:69:SER:HB3	2:D:83:ASN:HB3	1.74	0.68
1:A:87:ARG:NH1	5:B:496:CFM:S5	2.67	0.67
2:B:278:MET:HE3	1:C:519:TRP:HE3	1.59	0.67
2:D:325:ILE:HA	2:D:354:ILE:HD11	1.76	0.67
2:B:169:ASN:OD1	2:B:235:SER:HA	1.95	0.67
1:C:28:LYS:HB3	1:C:438:THR:HG22	1.75	0.67
2:B:299:LEU:HG	2:B:303:MET:HE2	1.75	0.66
1:C:74:HIS:O	1:C:144:THR:HB	1.95	0.66
2:B:176:PRO:HA	2:B:241:LEU:HD12	1.78	0.66
1:A:431:MET:HE2	1:A:440:LEU:HD22	1.78	0.66
1:A:431:MET:HG2	1:A:440:LEU:HD21	1.78	0.66
2:D:81:GLY:O	2:D:85:LYS:HG2	1.96	0.66
1:A:190:ASN:OD1	1:A:269:ILE:HG12	1.95	0.65
1:C:65:PRO:HB2	1:C:241:THR:HB	1.78	0.65
1:C:93:PRO:HB2	1:C:97:THR:O	1.95	0.65
2:B:137:THR:HG21	2:B:152:ASN:O	1.96	0.65
1:A:343:VAL:HG21	1:A:481:LEU:HD23	1.76	0.65
1:C:144:THR:HG22	1:C:146:PRO:HD2	1.78	0.65
1:C:154:ILE:HD12	1:C:171:ALA:HB1	1.79	0.65
1:C:48:ILE:HD11	2:D:218:MET:HE1	1.76	0.65
1:A:460:MET:HE3	1:A:503:LEU:HD11	1.77	0.65
1:C:75:GLY:HA2	1:C:110:MET:HE2	1.79	0.65
1:C:389:ASP:HA	1:C:392:ASN:OD1	1.97	0.64
1:C:261:GLN:HE22	1:C:286:PHE:H	1.44	0.64
1:C:431:MET:HA	1:C:434:MET:HE3	1.80	0.64
1:A:191:ASN:HD22	1:A:396:ILE:HG21	1.62	0.64
1:C:209:SER:HB3	1:C:255:ALA:HA	1.80	0.63
1:C:471:ILE:HB	1:C:478:SER:HB2	1.80	0.63
2:D:319:GLY:O	2:D:343:THR:HG22	1.98	0.63
1:C:209:SER:O	1:C:256:ASP:HB2	1.99	0.63
1:C:482:HIS:CE1	4:D:494:HCA:H51	2.34	0.63
1:A:180:VAL:HG13	1:A:390:SER:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:CD1	2:D:218:MET:HE1	2.29	0.62
2:D:39:LEU:HG	2:D:218:MET:HE2	1.81	0.62
1:C:48:ILE:CD1	2:D:218:MET:CE	2.76	0.62
2:D:138:ASN:O	2:D:140:PRO:HD3	1.99	0.62
1:A:276:LYS:HA	1:A:400:PRO:HA	1.82	0.62
2:B:57:SER:HA	2:B:62:GLU:O	2.01	0.61
1:C:353:ASN:HA	1:C:356:LYS:HE3	1.83	0.61
2:B:254:GLU:O	2:B:258:LYS:HA	2.01	0.61
2:B:45:SER:HB2	6:B:498:CLP:S2A	2.41	0.61
1:C:259:LEU:HD21	1:C:299:MET:SD	2.41	0.60
1:A:378:ARG:HG3	1:A:427:TYR:HB3	1.83	0.60
2:B:241:LEU:HD23	2:B:264:LEU:HD13	1.82	0.60
1:A:133:MET:HE1	2:B:12:ARG:HD3	1.83	0.60
2:B:84:ILE:HD11	2:B:118:TYR:CD2	2.37	0.60
1:C:369:PHE:CZ	5:D:496:CFM:S1A	2.94	0.60
1:C:375:TYR:HB3	1:C:431:MET:HE3	1.84	0.59
1:C:123:LEU:HD23	1:C:157:VAL:HG21	1.83	0.59
2:D:254:GLU:O	2:D:258:LYS:HA	2.03	0.59
1:A:469:PHE:HB3	2:B:63:PRO:HD3	1.84	0.59
2:D:189:ARG:NH2	2:D:428:LYS:HG3	2.17	0.59
1:A:272:MET:SD	1:A:396:ILE:CG2	2.90	0.58
1:C:465:ILE:HG21	2:D:54:THR:HG23	1.84	0.58
2:B:281:SER:HB3	1:C:526:SER:C	2.29	0.58
1:C:65:PRO:HB3	1:C:242:GLY:H	1.69	0.58
1:C:114:ASP:O	1:C:118:GLY:HA2	2.03	0.58
1:C:381:ILE:HA	1:C:384:ILE:HD12	1.86	0.58
1:A:326:ASP:HA	1:A:329:TYR:HB3	1.86	0.57
1:C:51:ARG:HG2	2:D:46:GLN:HE22	1.67	0.57
1:A:42:ARG:N	1:A:388:ALA:HB1	2.19	0.57
2:B:24:GLN:HB3	2:B:139:THR:HG23	1.84	0.57
1:C:434:MET:HB3	1:C:438:THR:HG21	1.86	0.57
1:A:401:ASP:HB3	1:A:404:LYS:H	1.68	0.57
1:C:316:ILE:O	1:C:320:ILE:HG22	2.05	0.57
1:A:511:ALA:HB3	2:D:304:ILE:HG13	1.87	0.57
1:C:78:GLY:O	1:C:82:TYR:HD2	1.88	0.57
2:B:441:ILE:O	2:B:445:ILE:HG23	2.04	0.57
1:A:191:ASN:ND2	1:A:396:ILE:HG22	2.18	0.57
1:C:104:TYR:HA	2:D:18:ASN:HD21	1.70	0.57
1:C:183:SER:HA	1:C:186:HIS:HD1	1.69	0.57
1:A:347:ARG:HA	1:A:350:THR:OG1	2.05	0.57
1:C:118:GLY:HA2	1:C:150:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLY:HA2	1:C:110:MET:CE	2.34	0.56
1:A:229:LEU:CD2	1:A:299:MET:HE1	2.34	0.56
1:A:378:ARG:HH12	1:A:381:ILE:HD12	1.69	0.56
2:B:351:GLN:O	2:B:355:ASP:HB2	2.05	0.56
1:C:273:MET:HE2	1:C:279:ILE:HD12	1.86	0.56
1:A:190:ASN:HD21	1:A:266:ILE:HG22	1.70	0.56
2:B:456:VAL:HG11	1:C:85:GLY:HA3	1.88	0.56
2:B:314:LYS:HB3	2:B:339:LYS:HG3	1.87	0.56
2:D:253:LEU:HD22	2:D:259:VAL:HB	1.88	0.56
1:A:298:ASP:HB3	1:A:422:VAL:HG13	1.87	0.56
1:C:226:ASP:O	1:C:230:GLU:HB2	2.06	0.56
1:C:511:ALA:HA	1:C:514:MET:HG2	1.87	0.56
1:A:170:HIS:HE1	1:A:246:TYR:OH	1.89	0.56
2:B:405:PRO:HB3	2:B:440:VAL:HG13	1.87	0.56
2:B:171:LYS:HG2	2:B:197:PRO:HB2	1.87	0.55
1:A:284:CYS:HB2	1:A:295:THR:HG23	1.88	0.55
2:B:35:ILE:HD12	2:B:229:LEU:HD11	1.89	0.55
2:B:417:TYR:HB2	2:D:438:THR:HG21	1.87	0.55
2:D:389:LEU:HD23	2:D:399:ALA:HB2	1.89	0.55
1:A:327:LEU:HA	1:A:330:PHE:CD2	2.41	0.55
1:C:409:ILE:O	1:C:413:LYS:HE2	2.06	0.55
1:C:482:HIS:ND1	4:D:494:HCA:H51	2.21	0.55
2:D:390:ILE:HG12	2:D:407:VAL:HB	1.88	0.55
1:C:203:LYS:O	1:C:254:LYS:HG2	2.07	0.55
2:D:34:GLY:HA3	2:D:202:PRO:HB3	1.88	0.55
2:B:43:HIS:CE1	2:B:84:ILE:HG12	2.42	0.55
2:B:252:THR:HG22	2:B:256:LYS:NZ	2.22	0.55
2:B:278:MET:CE	1:C:519:TRP:HB3	2.37	0.55
1:C:311:ARG:O	1:C:315:VAL:HG12	2.07	0.55
2:B:40:PRO:HG2	2:B:65:MET:O	2.07	0.54
1:C:183:SER:HB2	1:C:369:PHE:HD1	1.72	0.54
1:C:210:ILE:HG13	1:C:259:LEU:HD11	1.89	0.54
2:B:194:MET:HB3	2:B:196:ILE:HD12	1.89	0.54
2:B:300:ILE:HD13	2:B:303:MET:HE3	1.89	0.54
1:C:383:THR:O	1:C:384:ILE:HG13	2.07	0.54
1:C:245:THR:HG22	1:C:247:GLU:HB2	1.89	0.54
1:C:432:LYS:NZ	1:C:432:LYS:HB3	2.23	0.54
2:D:393:THR:O	2:D:396:LYS:HG2	2.08	0.54
1:A:141:VAL:HB	1:A:171:ALA:HA	1.88	0.54
2:B:239:LEU:HD23	2:B:262:LYS:HB3	1.89	0.54
2:D:137:THR:HG23	2:D:139:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:ASN:O	2:D:373:ASP:HB2	2.09	0.53
1:A:77:ILE:HG21	2:B:21:LYS:HE2	1.90	0.53
1:A:276:LYS:HD3	1:A:399:THR:O	2.08	0.53
2:D:321:PRO:HG3	2:D:343:THR:HG21	1.90	0.53
1:A:289:VAL:HG23	1:A:496:VAL:HG21	1.90	0.53
1:A:365:ALA:O	1:A:440:LEU:HA	2.09	0.53
1:C:48:ILE:HD11	2:D:218:MET:HE3	1.90	0.53
1:A:260:VAL:HG12	1:A:283:LYS:HD2	1.91	0.52
1:A:499:PHE:CE1	1:A:503:LEU:HD22	2.45	0.52
1:C:277:TYR:HB2	1:C:279:ILE:HG13	1.91	0.52
2:B:153:MET:O	2:B:157:ILE:HG13	2.10	0.52
2:D:317:LEU:HD23	2:D:327:LEU:HD13	1.92	0.52
1:A:289:VAL:O	1:A:293:VAL:HG13	2.10	0.52
2:D:25:PRO:HG3	6:D:498:CLP:S3B	2.49	0.52
1:A:74:HIS:HD2	1:A:108:THR:OG1	1.92	0.52
2:D:41:HIS:HE1	2:D:87:ALA:HB1	1.74	0.52
1:C:194:MET:HE1	1:C:273:MET:HG3	1.92	0.52
1:C:209:SER:HA	1:C:235:HIS:O	2.10	0.52
1:C:48:ILE:CD1	2:D:218:MET:HE3	2.40	0.51
1:C:278:GLY:HA3	1:C:406:ARG:O	2.09	0.51
1:A:209:SER:HB3	1:A:255:ALA:HA	1.91	0.51
2:B:238:THR:O	2:B:261:PHE:HA	2.10	0.51
1:C:210:ILE:HG22	1:C:236:VAL:HB	1.93	0.51
2:B:452:GLU:HB3	1:C:91:SER:O	2.10	0.51
1:A:272:MET:SD	1:A:396:ILE:HG21	2.51	0.51
2:B:348:MET:O	2:B:351:GLN:HB3	2.11	0.51
1:C:434:MET:HE1	1:C:440:LEU:HD21	1.91	0.51
1:A:131:TYR:HB2	1:A:139:ILE:HD11	1.93	0.51
2:B:35:ILE:HD11	2:B:157:ILE:HD13	1.93	0.51
2:B:173:ASN:HB2	2:B:238:THR:HG23	1.93	0.51
2:D:38:CYS:HA	2:D:99:ILE:HG23	1.93	0.51
1:A:14:ILE:HG23	1:A:16:LYS:HD3	1.91	0.51
1:C:461:PHE:O	1:C:478:SER:HA	2.11	0.51
1:A:451:VAL:O	1:A:455:LYS:HB2	2.11	0.51
1:A:108:THR:HG21	1:A:123:LEU:HA	1.92	0.51
1:A:216:TYR:CE2	5:B:496:CFM:S2A	3.04	0.51
2:B:71:PHE:CZ	2:B:80:GLY:HA3	2.46	0.51
2:B:300:ILE:HD13	2:B:303:MET:CE	2.40	0.51
1:A:61:VAL:HG13	1:A:87:ARG:HH12	1.76	0.50
2:B:48:CYS:SG	2:B:105:THR:HG21	2.50	0.50
1:C:90:LYS:HB3	1:C:223:TRP:CH2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LYS:O	1:C:405:TYR:HD1	1.93	0.50
1:C:464:GLY:H	1:C:467:GLU:HG3	1.76	0.50
2:D:317:LEU:HD23	2:D:327:LEU:CD1	2.41	0.50
1:A:209:SER:HA	1:A:235:HIS:O	2.11	0.50
2:B:187:ILE:O	2:B:191:PHE:HD2	1.94	0.50
1:A:16:LYS:H	1:A:16:LYS:HD2	1.76	0.50
1:A:180:VAL:HG11	1:A:388:ALA:HB3	1.93	0.50
1:A:248:LYS:NZ	1:A:248:LYS:HB3	2.26	0.50
2:B:276:PHE:O	2:B:280:LEU:HD12	2.11	0.50
2:D:97:PRO:HG2	2:D:100:ILE:HD13	1.94	0.50
1:C:106:PHE:HD1	2:D:17:ILE:HG12	1.76	0.50
1:C:462:PHE:HB3	1:C:481:LEU:HG	1.94	0.50
2:B:49:CYS:O	2:B:53:ARG:HG3	2.11	0.50
2:B:68:THR:HB	2:B:70:SER:H	1.76	0.50
1:C:430:MET:HG2	1:C:434:MET:HE2	1.94	0.50
1:A:201:GLY:HA3	1:A:251:ASN:ND2	2.27	0.50
1:C:53:CYS:HB3	6:D:498:CLP:S2A	2.52	0.50
1:A:262:CYS:SG	1:A:265:SER:OG	2.69	0.50
1:C:113:SER:HA	1:C:116:VAL:HG22	1.93	0.50
2:D:119:ILE:HA	2:D:122:MET:SD	2.52	0.49
1:A:205:GLN:HG3	1:A:254:LYS:O	2.12	0.49
1:A:334:LEU:HG	1:A:504:VAL:HG12	1.93	0.49
1:C:431:MET:HE2	1:C:440:LEU:HD22	1.93	0.49
2:D:169:ASN:OD1	2:D:235:SER:HA	2.12	0.49
2:B:141:SER:HB3	6:B:498:CLP:S3B	2.52	0.49
2:D:436:GLU:O	2:D:440:VAL:HG13	2.12	0.49
2:B:194:MET:O	2:B:195:ASP:HB3	2.12	0.49
1:A:519:TRP:HZ2	2:D:293:GLU:HG2	1.77	0.49
1:A:409:ILE:HG22	1:A:410:PRO:O	2.12	0.49
1:A:15:PRO:O	1:A:19:LYS:HD2	2.13	0.49
1:C:272:MET:HB3	1:C:398:VAL:HG11	1.94	0.49
1:C:306:PRO:O	1:C:310:LYS:HB2	2.13	0.48
1:C:210:ILE:HG22	1:C:236:VAL:HA	1.95	0.48
1:C:449:MET:O	1:C:453:LEU:HB2	2.13	0.48
1:A:143:ALA:HB2	1:A:154:ILE:HD13	1.94	0.48
1:A:378:ARG:NH1	1:A:381:ILE:HD12	2.28	0.48
2:D:85:LYS:NZ	2:D:121:GLN:HE21	2.11	0.48
2:D:135:ILE:HG21	2:D:157:ILE:HG22	1.95	0.48
1:A:444:MET:HG3	1:A:448:ASP:HB2	1.95	0.48
1:C:187:HIS:CE1	1:C:391:LYS:HB2	2.49	0.48
1:A:292:ILE:O	1:A:296:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ILE:O	2:B:198:TYR:HA	2.13	0.48
1:A:14:ILE:HD12	1:A:14:ILE:HA	1.75	0.48
2:B:23:CYS:HB2	2:B:141:SER:HB2	1.95	0.48
2:B:97:PRO:HB2	2:B:99:ILE:O	2.13	0.48
2:B:330:PHE:O	2:B:334:LEU:HG	2.13	0.48
1:C:435:HIS:O	1:C:438:THR:HB	2.14	0.48
2:D:296:ARG:HG3	2:D:296:ARG:HH11	1.78	0.48
1:C:414:VAL:O	1:C:418:LYS:HD2	2.13	0.48
2:D:358:LEU:HD13	2:D:366:SER:HB2	1.96	0.48
2:B:408:ARG:HB3	2:B:413:ILE:HG12	1.96	0.48
1:C:277:TYR:HA	1:C:405:TYR:HA	1.96	0.48
1:A:5:LEU:O	1:A:9:ILE:HG13	2.14	0.47
2:B:237:LEU:HA	2:B:260:PRO:HG2	1.96	0.47
1:C:379:GLU:O	1:C:382:PRO:HD2	2.14	0.47
1:C:341:LEU:HD12	1:C:348:SER:O	2.14	0.47
1:A:100:ASN:OD1	1:A:102:ASN:HB3	2.14	0.47
1:A:226:ASP:O	1:A:230:GLU:HB2	2.14	0.47
2:B:169:ASN:HD21	2:B:235:SER:HB3	1.78	0.47
1:C:494:ARG:O	1:C:497:VAL:HG22	2.14	0.47
2:B:239:LEU:HB3	2:B:264:LEU:HD11	1.96	0.47
2:B:393:THR:OG1	2:B:413:ILE:HA	2.14	0.47
1:C:451:VAL:O	1:C:455:LYS:HB2	2.15	0.47
2:D:109:GLU:HG3	2:D:140:PRO:HA	1.96	0.47
1:C:90:LYS:HB3	1:C:223:TRP:CZ3	2.49	0.47
1:C:128:HIS:ND1	1:C:165:ILE:HD13	2.29	0.47
1:A:315:VAL:HA	1:A:318:GLU:HG2	1.97	0.47
1:A:444:MET:HE3	1:A:449:MET:HB2	1.96	0.47
2:D:69:SER:O	2:D:71:PHE:N	2.48	0.47
2:D:194:MET:HE2	2:D:286:LYS:HB3	1.97	0.47
1:C:401:ASP:O	1:C:405:TYR:HB2	2.14	0.47
1:A:378:ARG:O	1:A:381:ILE:HB	2.14	0.47
1:C:197:ILE:HD12	1:C:250:GLN:HG3	1.97	0.47
1:C:181:SER:OG	1:C:369:PHE:HB2	2.15	0.47
2:D:38:CYS:HA	2:D:99:ILE:O	2.15	0.47
2:B:300:ILE:HA	2:B:303:MET:HE3	1.95	0.46
2:B:354:ILE:HD11	2:B:368:VAL:CB	2.45	0.46
1:A:286:PHE:CE1	1:A:295:THR:HG21	2.51	0.46
2:B:434:VAL:O	2:B:438:THR:HB	2.14	0.46
2:D:427:TYR:O	2:D:431:ILE:HG13	2.15	0.46
1:C:116:VAL:HG23	1:C:117:PHE:CD2	2.50	0.46
2:D:175:ILE:HB	2:D:246:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:HIS:CE1	1:A:38:VAL:HG23	2.50	0.46
1:A:213:LEU:HB3	1:A:266:ILE:CD1	2.41	0.46
2:B:307:GLN:O	2:B:311:GLN:HG2	2.16	0.46
1:C:51:ARG:HD2	1:C:368:GLU:O	2.16	0.46
1:C:444:MET:HE2	1:C:449:MET:HB3	1.97	0.46
2:D:303:MET:HE3	2:D:334:LEU:HD23	1.96	0.46
1:A:187:HIS:CE1	1:A:394:PRO:O	2.68	0.46
1:A:519:TRP:HA	1:A:523:SER:O	2.15	0.46
1:C:363:LEU:HD13	1:C:456:LEU:HD23	1.98	0.46
2:D:240:SER:HB2	2:D:263:THR:HG23	1.98	0.46
2:D:255:LYS:HA	2:D:258:LYS:NZ	2.31	0.46
1:A:307:GLU:O	1:A:311:ARG:HG3	2.15	0.46
2:B:49:CYS:HB2	2:B:68:THR:HG23	1.98	0.46
2:B:84:ILE:HD11	2:B:118:TYR:HD2	1.79	0.46
2:B:397:PHE:HZ	2:D:456:VAL:HG12	1.80	0.46
2:D:41:HIS:CE1	2:D:87:ALA:HB1	2.51	0.46
2:D:88:VAL:HG21	2:D:122:MET:HE3	1.96	0.46
1:A:434:MET:SD	1:A:438:THR:HG21	2.57	0.45
1:C:276:LYS:HG2	1:C:401:ASP:HB2	1.98	0.45
2:D:345:THR:HA	2:D:346:PRO:HD3	1.72	0.45
2:D:391:SER:HB3	2:D:406:PHE:HE1	1.80	0.45
1:A:263:HIS:HB2	1:A:283:LYS:HE2	1.98	0.45
1:A:369:PHE:HZ	5:B:496:CFM:S1A	2.39	0.45
1:C:284:CYS:HB2	1:C:295:THR:HG23	1.99	0.45
1:A:375:TYR:O	1:A:431:MET:HG3	2.17	0.45
1:C:452:VAL:O	1:C:456:LEU:HB2	2.15	0.45
2:D:402:GLU:O	2:D:404:ILE:HG13	2.17	0.45
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.73	0.45
2:B:316:ALA:HB2	2:B:386:VAL:HG11	1.98	0.45
1:C:120:VAL:HG12	1:C:157:VAL:HG11	1.96	0.45
2:D:224:THR:HB	2:D:229:LEU:HD11	1.97	0.45
1:A:344:GLY:HA3	5:B:496:CFM:S1B	2.57	0.45
1:C:88:ARG:NH1	1:C:484:TYR:HB2	2.32	0.45
1:C:106:PHE:CD1	2:D:17:ILE:HG12	2.52	0.45
1:C:278:GLY:O	1:C:408:VAL:HG13	2.17	0.45
1:C:308:LEU:HA	1:C:311:ARG:HG2	1.98	0.45
1:A:341:LEU:O	1:A:365:ALA:HA	2.17	0.45
1:A:457:LYS:HE3	1:A:457:LYS:HB2	1.83	0.45
1:A:216:TYR:CD1	1:A:241:THR:OG1	2.70	0.45
2:B:389:LEU:O	2:B:406:PHE:HA	2.17	0.45
1:C:198:ILE:HG21	1:C:273:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HG2	1:A:476:VAL:O	2.16	0.45
1:C:414:VAL:O	1:C:418:LYS:HB2	2.16	0.45
1:A:101:PHE:CZ	1:A:134:PHE:HB3	2.52	0.44
1:A:287:ILE:HG23	1:A:354:MET:HE2	1.99	0.44
1:A:453:LEU:HD11	1:A:471:ILE:HG23	1.99	0.44
1:A:517:PRO:HA	1:A:518:PRO:HD3	1.84	0.44
2:B:43:HIS:HE1	2:B:80:GLY:O	2.01	0.44
1:A:277:TYR:O	1:A:406:ARG:HD2	2.17	0.44
1:A:472:GLN:HE21	1:A:477:LEU:HA	1.83	0.44
1:C:67:LYS:HZ1	1:C:94:GLU:HG2	1.82	0.44
1:C:517:PRO:HA	1:C:518:PRO:HD2	1.66	0.44
2:B:38:CYS:SG	2:B:101:ALA:HB2	2.58	0.44
1:C:53:CYS:CB	6:D:498:CLP:S2A	3.06	0.44
1:C:354:MET:O	1:C:357:SER:HB2	2.17	0.44
1:C:256:ASP:O	1:C:408:VAL:HG21	2.18	0.44
1:C:393:ILE:HG23	1:C:394:PRO:HD2	1.98	0.44
2:B:339:LYS:HA	2:B:339:LYS:HD2	1.73	0.44
2:B:315:VAL:HG21	2:B:331:ILE:HG21	2.00	0.44
2:D:88:VAL:HA	2:D:91:ILE:HD12	1.98	0.44
2:D:315:VAL:HG13	2:D:388:LEU:HB3	1.98	0.44
2:B:341:VAL:O	2:B:368:VAL:HA	2.18	0.44
1:A:78:GLY:HA3	2:B:23:CYS:SG	2.58	0.44
1:A:81:PHE:CG	2:B:22:THR:HG23	2.52	0.44
1:A:81:PHE:CD2	2:B:22:THR:HG23	2.53	0.44
1:A:343:VAL:HG12	1:A:344:GLY:H	1.83	0.44
1:A:401:ASP:O	1:A:402:GLU:HB2	2.18	0.44
2:B:331:ILE:HG22	2:B:336:ALA:HB3	2.00	0.44
1:A:330:PHE:CZ	1:A:497:VAL:HA	2.52	0.43
1:C:289:VAL:HA	1:C:292:ILE:HD12	2.00	0.43
1:A:82:TYR:CZ	2:B:22:THR:HG21	2.53	0.43
2:D:42:SER:HB2	2:D:68:THR:HG23	2.01	0.43
2:D:176:PRO:HG3	2:D:184:MET:HG2	2.01	0.43
1:A:191:ASN:ND2	1:A:396:ILE:CB	2.81	0.43
2:B:119:ILE:HD12	2:B:134:VAL:HG23	2.00	0.43
2:B:255:LYS:HD3	2:B:255:LYS:HA	1.81	0.43
2:B:293:GLU:CD	1:C:519:TRP:HE1	2.26	0.43
2:B:332:ILE:CD1	2:B:357:MET:HG2	2.49	0.43
1:C:326:ASP:O	1:C:329:TYR:HB3	2.18	0.43
2:D:52:HIS:O	2:D:55:VAL:HG12	2.17	0.43
2:D:96:ASN:HA	2:D:97:PRO:HD3	1.72	0.43
1:A:181:SER:HB2	1:A:369:PHE:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HA	1:A:240:LEU:HB2	2.01	0.43
1:A:338:THR:HG23	1:A:363:LEU:HG	2.00	0.43
1:A:410:PRO:O	1:A:412:ASP:N	2.51	0.43
2:B:284:THR:OG1	2:B:286:LYS:HG2	2.19	0.43
2:B:379:GLN:O	2:B:382:LYS:HB2	2.18	0.43
1:C:334:LEU:HD11	1:C:507:ILE:HD12	1.99	0.43
1:A:69:MET:HG2	1:A:138:ALA:HB3	2.01	0.43
1:A:163:LYS:HE3	1:A:163:LYS:HB2	1.75	0.43
2:B:25:PRO:HB2	2:B:52:HIS:CE1	2.53	0.43
1:C:472:GLN:HA	1:C:476:VAL:O	2.19	0.43
1:A:193:VAL:HA	1:A:197:ILE:HD12	1.99	0.43
1:A:513:LYS:HD2	1:A:513:LYS:N	2.33	0.43
1:C:146:PRO:O	1:C:150:ILE:HG12	2.18	0.43
1:C:65:PRO:CB	1:C:241:THR:HB	2.47	0.43
1:C:69:MET:HG2	1:C:138:ALA:HB3	1.99	0.43
2:D:316:ALA:HB2	2:D:386:VAL:HG11	1.99	0.43
1:A:103:GLU:H	1:A:103:GLU:HG2	1.67	0.43
1:A:205:GLN:HG2	1:A:206:LYS:N	2.33	0.43
1:C:292:ILE:HG22	1:C:296:LEU:HD23	2.00	0.43
1:A:26:VAL:HG11	1:A:36:GLU:O	2.19	0.43
1:A:227:ARG:HG3	1:A:227:ARG:HH11	1.83	0.43
2:B:130:GLU:CD	2:B:130:GLU:H	2.26	0.43
2:B:390:ILE:HA	2:B:407:VAL:O	2.18	0.43
1:C:205:GLN:HG2	1:C:206:LYS:N	2.33	0.43
2:D:88:VAL:HG21	2:D:122:MET:CE	2.48	0.43
1:A:355:LEU:O	1:A:358:PHE:HB2	2.19	0.42
2:B:237:LEU:HG	2:B:238:THR:N	2.32	0.42
2:B:342:VAL:HG22	2:B:369:LYS:HB3	2.01	0.42
1:C:333:LYS:HB2	1:C:334:LEU:HD13	2.01	0.42
1:A:131:TYR:CD1	1:A:167:ILE:HD12	2.54	0.42
1:A:449:MET:O	1:A:453:LEU:HB2	2.19	0.42
1:C:88:ARG:HH12	1:C:484:TYR:HB2	1.84	0.42
1:C:330:PHE:HE2	1:C:497:VAL:HA	1.84	0.42
1:A:91:SER:O	2:D:452:GLU:HB2	2.19	0.42
1:A:461:PHE:O	1:A:478:SER:HA	2.19	0.42
2:B:115:LEU:O	2:B:119:ILE:HG12	2.19	0.42
1:C:391:LYS:HA	1:C:393:ILE:HB	2.01	0.42
1:A:337:LYS:HE2	1:A:507:ILE:HG21	2.02	0.42
1:C:225:MET:HE2	1:C:286:PHE:HB2	2.01	0.42
1:A:296:LEU:HA	1:A:299:MET:HE3	2.02	0.42
2:B:276:PHE:O	2:B:279:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:THR:C	1:C:34:ASN:H	2.27	0.42
1:C:210:ILE:HG13	1:C:259:LEU:CD1	2.50	0.42
2:D:367:LYS:HD3	2:D:368:VAL:N	2.35	0.42
1:A:14:ILE:HG23	1:A:16:LYS:CD	2.49	0.42
1:A:131:TYR:HA	1:A:136:PRO:HD3	2.02	0.42
1:C:511:ALA:HA	1:C:514:MET:CG	2.49	0.42
2:D:176:PRO:HD2	2:D:201:PHE:O	2.20	0.42
2:D:115:LEU:HD23	2:D:115:LEU:H	1.84	0.42
2:B:288:VAL:HA	2:B:289:PRO:HD3	1.80	0.42
1:C:330:PHE:CE2	1:C:500:GLY:HA3	2.54	0.42
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.79	0.42
1:A:358:PHE:HE2	1:A:499:PHE:CE1	2.38	0.42
1:C:245:THR:HB	1:C:248:LYS:HB2	2.02	0.42
2:D:195:ASP:O	2:D:286:LYS:NZ	2.53	0.42
2:D:87:ALA:O	2:D:91:ILE:HG13	2.20	0.41
1:A:484:TYR:O	1:A:487:ASN:ND2	2.53	0.41
2:B:345:THR:HA	2:B:346:PRO:HD2	1.66	0.41
2:B:391:SER:OG	2:B:395:GLY:HA3	2.19	0.41
1:C:127:ILE:HG21	1:C:161:ALA:HB1	2.02	0.41
1:C:288:GLY:O	1:C:292:ILE:HG13	2.20	0.41
1:C:331:LYS:HG2	1:C:357:SER:O	2.20	0.41
1:A:319:GLU:O	1:A:322:ALA:HB3	2.20	0.41
2:B:46:GLN:HA	2:B:68:THR:HG21	2.01	0.41
1:C:37:ILE:HB	1:C:431:MET:HE1	2.01	0.41
2:D:194:MET:O	2:D:286:LYS:HG2	2.20	0.41
1:A:131:TYR:CD2	1:A:165:ILE:HG12	2.55	0.41
1:C:76:PRO:HG2	2:D:106:CYS:SG	2.60	0.41
1:A:216:TYR:HA	1:A:242:GLY:H	1.85	0.41
1:C:115:ILE:HG22	1:C:116:VAL:HG13	2.02	0.41
1:C:333:LYS:HB3	1:C:508:TYR:HE2	1.84	0.41
2:B:162:SER:OG	2:B:253:LEU:HD13	2.20	0.41
2:D:95:TYR:HB3	2:D:218:MET:SD	2.61	0.41
2:D:137:THR:OG1	2:D:152:ASN:HB3	2.20	0.41
2:D:204:THR:CG2	2:D:208:LEU:HB2	2.51	0.41
2:D:233:GLY:HA2	2:D:257:CYS:SG	2.60	0.41
1:A:70:VAL:HG12	1:A:72:ILE:HG22	2.03	0.41
1:A:343:VAL:CG2	1:A:481:LEU:HD23	2.47	0.41
1:C:75:GLY:HA3	1:C:144:THR:HG21	2.02	0.41
1:C:87:ARG:NH1	5:D:496:CFM:S5	2.94	0.41
2:D:28:ALA:HB2	2:D:139:THR:HG21	2.02	0.41
1:A:61:VAL:HG13	1:A:87:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:O	1:A:118:GLY:N	2.51	0.41
1:A:193:VAL:HG13	1:A:269:ILE:HD11	2.03	0.41
1:A:393:ILE:HA	1:A:394:PRO:HD2	1.94	0.41
1:A:462:PHE:HB3	1:A:481:LEU:HD22	2.02	0.41
1:C:330:PHE:CE2	1:C:497:VAL:HA	2.55	0.41
1:C:461:PHE:HB3	1:C:471:ILE:HG21	2.02	0.41
2:D:65:MET:HE3	2:D:216:TYR:OH	2.19	0.41
2:D:239:LEU:HD22	2:D:264:LEU:HD21	2.03	0.41
2:D:250:ALA:HB1	2:D:261:PHE:CD2	2.55	0.41
2:D:450:THR:HB	2:D:453:ASP:HB3	2.03	0.41
1:A:128:HIS:CG	1:A:165:ILE:HD11	2.56	0.41
2:B:181:PRO:O	2:B:185:ARG:HG3	2.21	0.41
2:B:232:THR:HG22	2:B:253:LEU:HD21	2.03	0.41
1:C:5:LEU:HD23	1:C:439:ILE:HG12	2.02	0.41
1:C:431:MET:CE	1:C:440:LEU:HD22	2.50	0.41
2:D:172:ILE:O	2:D:198:TYR:HA	2.21	0.41
2:B:438:THR:HG22	2:B:439:ASN:ND2	2.36	0.41
1:C:74:HIS:HA	1:C:108:THR:OG1	2.21	0.41
1:C:154:ILE:O	1:C:157:VAL:HG22	2.21	0.41
2:D:150:PHE:CD2	2:D:178:PHE:HD1	2.39	0.41
2:D:181:PRO:O	2:D:185:ARG:HG3	2.20	0.41
1:C:261:GLN:HE22	1:C:286:PHE:N	2.13	0.40
2:B:176:PRO:HB3	2:B:200:MET:HE2	2.03	0.40
2:D:168:LYS:HA	2:D:234:ASN:O	2.21	0.40
1:A:45:PRO:O	2:B:87:ALA:HA	2.20	0.40
1:A:427:TYR:CZ	1:A:429:GLY:HA2	2.56	0.40
1:A:40:ASN:O	1:A:388:ALA:HB2	2.20	0.40
1:A:216:TYR:HD1	1:A:241:THR:OG1	2.04	0.40
1:A:308:LEU:HD23	1:A:311:ARG:NH1	2.36	0.40
1:C:259:LEU:HB3	1:C:284:CYS:SG	2.62	0.40
1:C:391:LYS:C	1:C:393:ILE:N	2.79	0.40
2:D:188:LYS:HD2	2:D:198:TYR:HE2	1.85	0.40
1:C:285:ASN:OD1	1:C:350:THR:HG22	2.22	0.40
1:C:367:PHE:CD2	1:C:370:ALA:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	523/533 (98%)	447 (86%)	58 (11%)	18 (3%)	3	17
1	C	523/533 (98%)	452 (86%)	51 (10%)	20 (4%)	2	15
2	B	455/458 (99%)	414 (91%)	35 (8%)	6 (1%)	9	38
2	D	455/458 (99%)	411 (90%)	37 (8%)	7 (2%)	8	35
All	All	1956/1982 (99%)	1724 (88%)	181 (9%)	51 (3%)	4	23

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	143	ALA
1	A	241	THR
1	A	387	ASP
1	A	411	GLU
1	A	523	SER
2	B	3	ASP
2	B	361	ALA
1	C	34	ASN
1	C	241	THR
1	C	345	GLY
1	C	429	GLY
2	D	4	ALA
2	D	70	SER
1	A	176	GLY
1	A	205	GLN
1	A	390	SER
1	C	388	ALA
1	C	524	SER
1	A	129	GLU
1	A	168	PRO
1	A	346	SER

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Mol	Chain	Res	Type
1	A	394	PRO
1	A	463	ALA
2	B	4	ALA
2	B	114	ASP
1	C	203	LYS
1	C	402	GLU
1	C	484	TYR
2	D	129	PRO
1	A	429	GLY
1	C	35	PRO
1	C	109	ASP
1	C	389	ASP
1	C	521	LYS
1	C	522	ALA
2	D	115	LEU
2	D	451	GLU
1	C	390	SER
1	C	400	PRO
1	A	419	LYS
2	B	167	ALA
1	C	118	GLY
1	A	306	PRO
1	C	65	PRO
1	A	421	GLY
2	D	91	ILE
2	D	270	VAL
1	C	166	GLY
1	C	518	PRO
2	B	412	PRO

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	434/446 (97%)	344 (79%)	90 (21%)	1 7
1	C	435/446 (98%)	353 (81%)	82 (19%)	1 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	383/384 (100%)	309 (81%)	74 (19%)	1	8
2	D	383/384 (100%)	323 (84%)	60 (16%)	2	13
All	All	1635/1660 (98%)	1329 (81%)	306 (19%)	1	9

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	8	GLU
1	A	11	GLU
1	A	14	ILE
1	A	16	LYS
1	A	21	ARG
1	A	28	LYS
1	A	32	THR
1	A	40	ASN
1	A	41	THR
1	A	42	ARG
1	A	43	THR
1	A	47	ILE
1	A	59	LYS
1	A	72	ILE
1	A	87	ARG
1	A	90	LYS
1	A	92	LYS
1	A	102	ASN
1	A	105	VAL
1	A	109	ASP
1	A	110	MET
1	A	127	ILE
1	A	128	HIS
1	A	129	GLU
1	A	150	ILE
1	A	155	LEU
1	A	164	GLU
1	A	165	ILE
1	A	175	GLU
1	A	192	THR
1	A	196	ASP
1	A	198	ILE
1	A	200	LYS

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Mol	Chain	Res	Type
1	A	210	ILE
1	A	226	ASP
1	A	227	ARG
1	A	230	GLU
1	A	237	ASN
1	A	240	LEU
1	A	243	ASP
1	A	245	THR
1	A	248	LYS
1	A	260	VAL
1	A	276	LYS
1	A	287	ILE
1	A	294	GLU
1	A	313	GLU
1	A	319	GLU
1	A	326	ASP
1	A	329	TYR
1	A	332	GLU
1	A	341	LEU
1	A	343	VAL
1	A	348	SER
1	A	353	ASN
1	A	354	MET
1	A	355	LEU
1	A	371	HIS
1	A	373	ASP
1	A	378	ARG
1	A	379	GLU
1	A	381	ILE
1	A	383	THR
1	A	384	ILE
1	A	385	LYS
1	A	389	ASP
1	A	391	LYS
1	A	394	PRO
1	A	398	VAL
1	A	401	ASP
1	A	406	ARG
1	A	407	VAL
1	A	414	VAL
1	A	416	GLU
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	418	LYS
1	A	432	LYS
1	A	435	HIS
1	A	453	LEU
1	A	454	GLU
1	A	455	LYS
1	A	457	LYS
1	A	460	MET
1	A	481	LEU
1	A	485	ASP
1	A	487	ASN
1	A	494	ARG
1	A	498	ASN
1	A	502	GLU
2	B	2	LEU
2	B	3	ASP
2	B	7	LYS
2	B	15	LEU
2	B	19	PRO
2	B	22	THR
2	B	33	LEU
2	B	42	SER
2	B	45	SER
2	B	46	GLN
2	B	50	SER
2	B	55	VAL
2	B	68	THR
2	B	82	SER
2	B	84	ILE
2	B	105	THR
2	B	106	CYS
2	B	113	ASP
2	B	115	LEU
2	B	124	ASP
2	B	130	GLU
2	B	137	THR
2	B	168	LYS
2	B	172	ILE
2	B	188	LYS
2	B	190	LEU
2	B	192	GLU
2	B	194	MET

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Mol	Chain	Res	Type
2	B	212	THR
2	B	225	LYS
2	B	230	LYS
2	B	235	SER
2	B	236	ASP
2	B	248	LEU
2	B	257	CYS
2	B	264	LEU
2	B	282	GLU
2	B	287	GLU
2	B	291	SER
2	B	292	ILE
2	B	304	ILE
2	B	307	GLN
2	B	317	LEU
2	B	318	LEU
2	B	324	ILE
2	B	327	LEU
2	B	331	ILE
2	B	332	ILE
2	B	333	GLU
2	B	339	LYS
2	B	345	THR
2	B	349	LYS
2	B	354	ILE
2	B	355	ASP
2	B	360	GLU
2	B	364	GLU
2	B	366	SER
2	B	368	VAL
2	B	384	GLU
2	B	386	VAL
2	B	389	LEU
2	B	405	PRO
2	B	407	VAL
2	B	415	ASP
2	B	422	ASN
2	B	425	VAL
2	B	432	ARG
2	B	437	ILE
2	B	438	THR
2	B	440	VAL

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Mol	Chain	Res	Type
2	B	442	LEU
2	B	452	GLU
2	B	456	VAL
2	B	458	ARG
1	C	16	LYS
1	C	19	LYS
1	C	20	THR
1	C	25	ILE
1	C	26	VAL
1	C	29	THR
1	C	31	GLU
1	C	41	THR
1	C	44	VAL
1	C	45	PRO
1	C	47	ILE
1	C	61	VAL
1	C	65	PRO
1	C	72	ILE
1	C	80	SER
1	C	83	THR
1	C	95	ASN
1	C	113	SER
1	C	115	ILE
1	C	120	VAL
1	C	124	LYS
1	C	144	THR
1	C	154	ILE
1	C	155	LEU
1	C	157	VAL
1	C	165	ILE
1	C	196	ASP
1	C	197	ILE
1	C	200	LYS
1	C	204	GLU
1	C	210	ILE
1	C	230	GLU
1	C	231	LYS
1	C	236	VAL
1	C	240	LEU
1	C	250	GLN
1	C	256	ASP
1	C	282	ILE

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Mol	Chain	Res	Type
1	C	296	LEU
1	C	304	ASP
1	C	316	ILE
1	C	320	ILE
1	C	332	GLU
1	C	341	LEU
1	C	343	VAL
1	C	350	THR
1	C	355	LEU
1	C	361	ASP
1	C	362	SER
1	C	371	HIS
1	C	379	GLU
1	C	380	VAL
1	C	382	PRO
1	C	383	THR
1	C	384	ILE
1	C	386	ILE
1	C	387	ASP
1	C	392	ASN
1	C	393	ILE
1	C	395	GLU
1	C	396	ILE
1	C	397	THR
1	C	398	VAL
1	C	400	PRO
1	C	403	GLN
1	C	406	ARG
1	C	408	VAL
1	C	416	GLU
1	C	418	LYS
1	C	426	SER
1	C	430	MET
1	C	432	LYS
1	C	435	HIS
1	C	438	THR
1	C	443	ASP
1	C	451	VAL
1	C	453	LEU
1	C	455	LYS
1	C	460	MET
1	C	472	GLN

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Mol	Chain	Res	Type
1	C	473	LYS
1	C	513	LYS
2	D	8	GLU
2	D	10	VAL
2	D	39	LEU
2	D	46	GLN
2	D	56	LEU
2	D	68	THR
2	D	72	THR
2	D	78	PHE
2	D	82	SER
2	D	84	ILE
2	D	86	THR
2	D	95	TYR
2	D	96	ASN
2	D	108	SER
2	D	115	LEU
2	D	120	SER
2	D	122	MET
2	D	130	GLU
2	D	133	LEU
2	D	143	VAL
2	D	154	VAL
2	D	159	ASN
2	D	190	LEU
2	D	202	PRO
2	D	212	THR
2	D	217	LYS
2	D	224	THR
2	D	227	GLU
2	D	229	LEU
2	D	240	SER
2	D	241	LEU
2	D	248	LEU
2	D	255	LYS
2	D	264	LEU
2	D	277	ILE
2	D	287	GLU
2	D	291	SER
2	D	304	ILE
2	D	307	GLN
2	D	308	GLN

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Mol	Chain	Res	Type
2	D	311	GLN
2	D	327	LEU
2	D	329	LYS
2	D	339	LYS
2	D	341	VAL
2	D	342	VAL
2	D	343	THR
2	D	345	THR
2	D	351	GLN
2	D	377	VAL
2	D	386	VAL
2	D	400	ARG
2	D	402	GLU
2	D	403	ASN
2	D	420	TYR
2	D	438	THR
2	D	448	GLU
2	D	450	THR
2	D	451	GLU
2	D	456	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	74	HIS
1	A	170	HIS
1	A	190	ASN
1	A	191	ASN
1	A	202	ASN
1	A	285	ASN
1	A	353	ASN
1	A	392	ASN
1	A	445	ASN
1	A	472	GLN
1	A	498	ASN
1	A	501	HIS
2	B	41	HIS
2	B	96	ASN
2	B	121	GLN
2	B	307	GLN
2	B	308	GLN

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Mol	Chain	Res	Type
2	B	439	ASN
1	C	121	ASN
1	C	237	ASN
1	C	261	GLN
1	C	267	ASN
1	C	353	ASN
1	C	445	ASN
1	C	447	HIS
1	C	472	GLN
1	C	487	ASN
2	D	18	ASN
2	D	37	ASN
2	D	96	ASN
2	D	121	GLN
2	D	298	GLN
2	D	378	HIS
2	D	379	GLN
2	D	403	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CFM	D	496	4,1	0,24,24	-	-	-		
5	CFM	B	496	4,1	0,24,24	-	-	-		
6	CLP	D	498	1,2	0,25,25	-	-	-		
6	CLP	B	498	1,2	0,25,25	-	-	-		
4	HCA	D	494	5	13,13,13	2.38	4 (30%)	15,18,18	2.34	6 (40%)
4	HCA	B	494	5	13,13,13	2.38	4 (30%)	15,18,18	1.87	3 (20%)

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
6	CLP	D	498	1,2	-	-	0/12/10/10
4	HCA	D	494	5	-	6/17/17/17	-
4	HCA	B	494	5	-	10/17/17/17	-
6	CLP	B	498	1,2	-	-	0/12/10/10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	494	HCA	O5-C7	7.05	1.44	1.22
4	D	494	HCA	O5-C7	6.72	1.43	1.22
4	B	494	HCA	O3-C6	2.84	1.31	1.22
4	D	494	HCA	O1-C1	2.67	1.30	1.22
4	D	494	HCA	O3-C6	2.62	1.30	1.22
4	B	494	HCA	O6-C7	-2.54	1.21	1.30
4	B	494	HCA	O1-C1	2.52	1.30	1.22
4	D	494	HCA	O6-C7	-2.25	1.22	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	494	HCA	O6-C7-C3	5.39	123.49	113.14
4	B	494	HCA	O6-C7-C3	4.53	121.84	113.14
4	D	494	HCA	O2-C1-O1	-3.24	115.00	123.33
4	D	494	HCA	O4-C6-C5	3.14	123.92	114.00
4	D	494	HCA	O3-C6-C5	-2.82	114.16	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	494	HCA	O5-C7-C3	-2.53	117.19	122.09
4	B	494	HCA	O2-C1-O1	-2.38	117.21	123.33
4	D	494	HCA	C4-C5-C6	2.33	118.16	112.77
4	D	494	HCA	O5-C7-C3	-2.22	117.79	122.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	494	HCA	C1-C2-C3-C4
4	B	494	HCA	C1-C2-C3-C7
4	B	494	HCA	C1-C2-C3-O7
4	B	494	HCA	C2-C3-C4-C5
4	B	494	HCA	C7-C3-C4-C5
4	B	494	HCA	O7-C3-C4-C5
4	B	494	HCA	C3-C4-C5-C6
4	D	494	HCA	C2-C3-C4-C5
4	D	494	HCA	C7-C3-C4-C5
4	D	494	HCA	O7-C3-C4-C5
4	D	494	HCA	C3-C4-C5-C6
4	D	494	HCA	C4-C5-C6-O3
4	D	494	HCA	C4-C5-C6-O4
4	B	494	HCA	C4-C5-C6-O3
4	B	494	HCA	O1-C1-C2-C3
4	B	494	HCA	C4-C5-C6-O4

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	496	CFM	4	0
5	B	496	CFM	4	0
6	D	498	CLP	5	0
6	B	498	CLP	4	0
4	D	494	HCA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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.