Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 07:59 PM EST

PDB ID	:	1D8H
Title	:	X-RAY CRYSTAL STRUCTURE OF YEAST RNA TRIPHOSPHATASE IN COMPLEX WITH SULFATE AND MANGANESE IONS.
Authors	:	Lima, C.D.; Wang, L.K.; Shuman, S.
Deposited on	:	1999-10-24
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

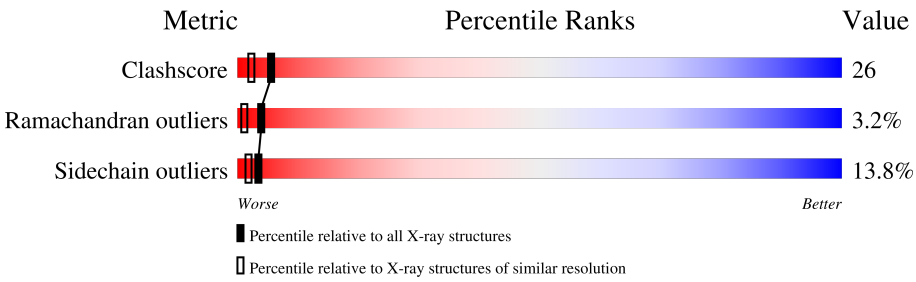
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	311	27% 39% 21% 6% 7%
1	B	311	27% 36% 23% 6% 7%
1	C	311	23% 39% 22% 8% 7%

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
3	SO4	C	603	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7626 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 mRNA TRIPHOSPHATASE CET1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2313	1470	395	443	5	0	0	0
1	B	288	2313	1470	395	443	5	0	0	0
1	C	288	2313	1470	395	443	5	0	0	0

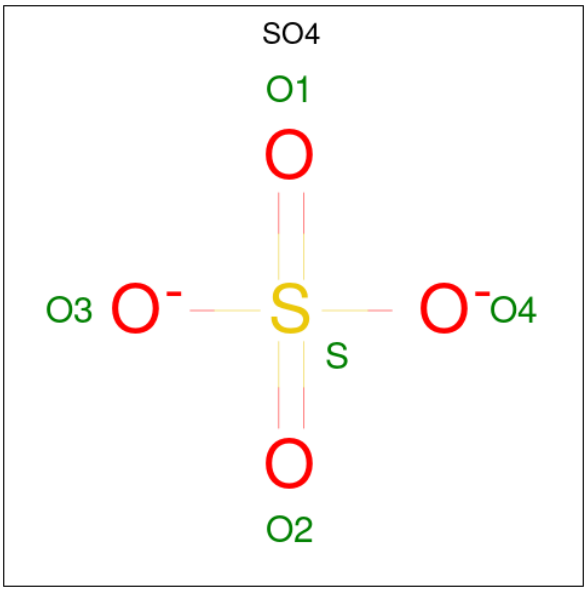
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	ARG	LYS	conflict	UNP O13297
B	242	ARG	LYS	conflict	UNP O13297
C	242	ARG	LYS	conflict	UNP O13297

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	222	Total O 222 222	0	0
4	B	226	Total O 226 226	0	0
4	C	221	Total O 221 221	0	0

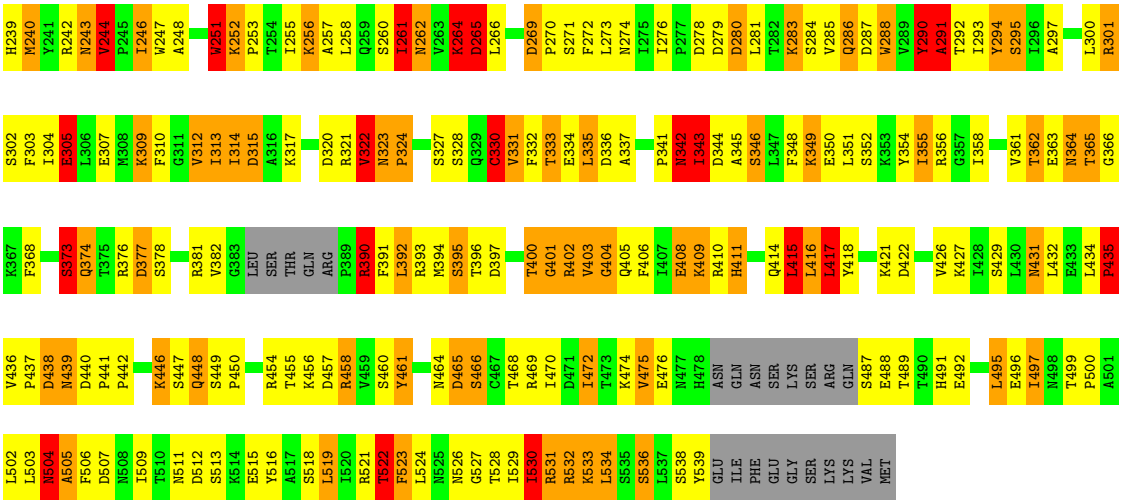
3 Residue-property plots (i)

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.

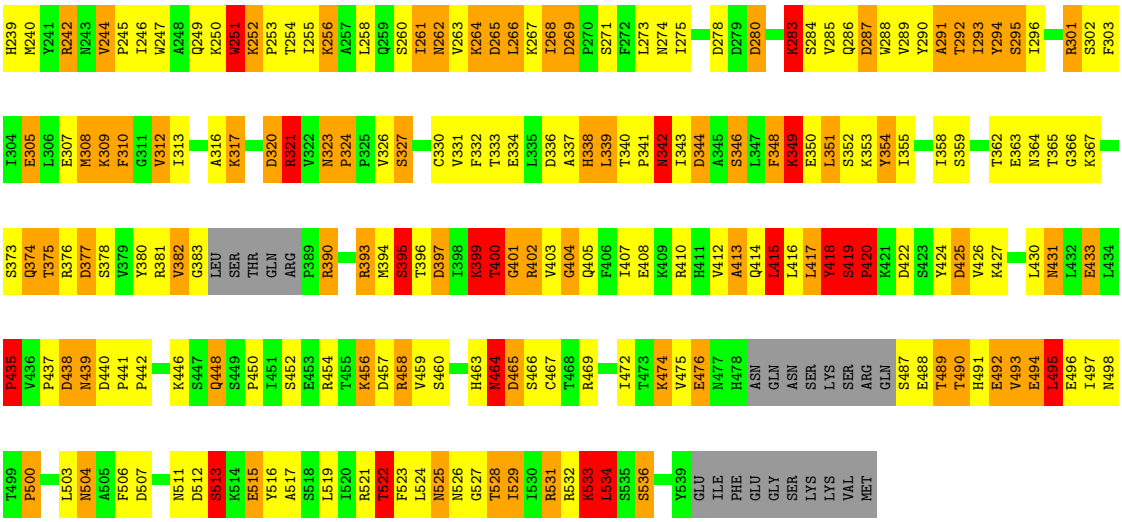
• Molecule 1: mRNA TRIPHOSPHATASE CET1

Chain A: 27% 39% 21% 6% 7%



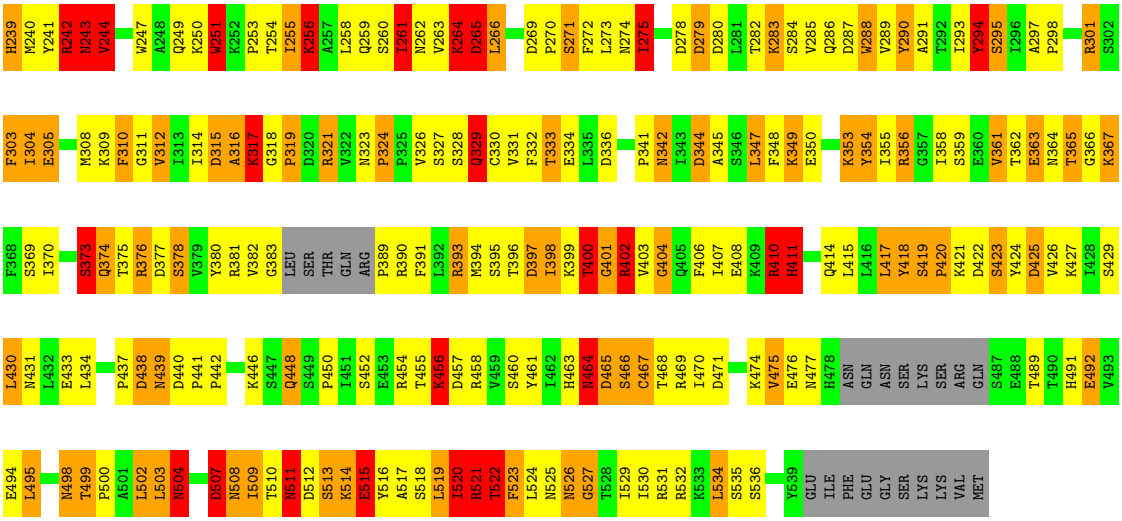
• Molecule 1: mRNA TRIPHOSPHATASE CET1

Chain B: 27% 36% 23% 6% 7%



- Molecule 1: mRNA TRIPHOSPHATASE CET1

Chain C: 23% 39% 22% 8% 7%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.44Å 118.72Å 85.14Å 90.00° 108.06° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00	Depositor
% Data completeness (in resolution range)	88.1 (25.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7626	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, SO4

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	1.66	28/2360 (1.2%)	3.02	221/3199 (6.9%)
1	B	1.60	28/2360 (1.2%)	2.95	237/3199 (7.4%)
1	C	1.57	24/2360 (1.0%)	3.07	233/3199 (7.3%)
All	All	1.61	80/7080 (1.1%)	3.02	691/9597 (7.2%)

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	1	29
1	B	0	26
1	C	0	29
All	All	1	84

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	SER	CA-CB	10.79	1.69	1.52
1	A	321	ARG	CZ-NH1	10.26	1.46	1.33
1	C	327	SER	CA-CB	9.87	1.67	1.52
1	B	288	TRP	CD2-CE2	-9.27	1.30	1.41
1	A	302	SER	CA-CB	8.84	1.66	1.52
1	B	271	SER	CA-CB	8.61	1.65	1.52
1	B	413	ALA	CA-CB	8.55	1.70	1.52
1	B	531	ARG	CZ-NH1	8.17	1.43	1.33
1	C	301	ARG	CZ-NH2	8.10	1.43	1.33
1	A	284	SER	CB-OG	8.09	1.52	1.42
1	C	327	SER	CB-OG	-8.02	1.31	1.42
1	A	327	SER	CA-CB	7.50	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	SER	CA-CB	7.42	1.64	1.52
1	A	527	GLY	CA-C	7.26	1.63	1.51
1	C	284	SER	CA-CB	7.08	1.63	1.52
1	C	536	SER	CB-OG	6.92	1.51	1.42
1	C	328	SER	CB-OG	6.74	1.51	1.42
1	C	305	GLU	CD-OE1	6.69	1.33	1.25
1	A	292	THR	CB-OG1	6.67	1.56	1.43
1	A	531	ARG	NE-CZ	-6.66	1.24	1.33
1	B	424	TYR	N-CA	6.65	1.59	1.46
1	C	418	TYR	CB-CG	6.57	1.61	1.51
1	A	350	GLU	CD-OE1	6.54	1.32	1.25
1	C	324	PRO	N-CD	6.54	1.57	1.47
1	A	305	GLU	CB-CG	6.49	1.64	1.52
1	A	301	ARG	CZ-NH2	6.49	1.41	1.33
1	C	527	GLY	CA-C	6.37	1.62	1.51
1	B	324	PRO	CA-C	6.32	1.65	1.52
1	B	522	THR	N-CA	-6.28	1.33	1.46
1	A	304	ILE	N-CA	6.13	1.58	1.46
1	B	324	PRO	C-N	-6.11	1.22	1.34
1	A	538	SER	CB-OG	6.06	1.50	1.42
1	A	305	GLU	CA-C	6.01	1.68	1.52
1	A	305	GLU	CD-OE1	-5.97	1.19	1.25
1	A	297	ALA	N-CA	5.96	1.58	1.46
1	B	341	PRO	N-CD	5.96	1.56	1.47
1	A	271	SER	CA-CB	5.94	1.61	1.52
1	A	536	SER	C-O	5.92	1.34	1.23
1	B	295	SER	C-N	-5.90	1.20	1.34
1	B	323	ASN	CB-CG	5.90	1.64	1.51
1	C	419	SER	CB-OG	5.89	1.50	1.42
1	A	307	GLU	CD-OE1	5.86	1.32	1.25
1	C	503	LEU	N-CA	5.81	1.57	1.46
1	B	292	THR	N-CA	-5.80	1.34	1.46
1	A	323	ASN	N-CA	5.79	1.57	1.46
1	C	297	ALA	N-CA	5.75	1.57	1.46
1	C	350	GLU	CD-OE2	5.74	1.31	1.25
1	A	330	CYS	CB-SG	-5.70	1.72	1.81
1	B	302	SER	CB-OG	5.68	1.49	1.42
1	B	323	ASN	CG-ND2	-5.65	1.18	1.32
1	A	332	PHE	CE2-CZ	5.64	1.48	1.37
1	B	326	VAL	CA-CB	5.62	1.66	1.54
1	C	323	ASN	C-O	5.62	1.34	1.23
1	C	288	TRP	N-CA	-5.55	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	318	GLY	N-CA	-5.53	1.37	1.46
1	B	327	SER	N-CA	-5.49	1.35	1.46
1	B	291	ALA	N-CA	-5.47	1.35	1.46
1	B	293	ILE	CA-CB	-5.45	1.42	1.54
1	B	424	TYR	CG-CD2	-5.39	1.32	1.39
1	A	307	GLU	CA-CB	-5.34	1.42	1.53
1	B	305	GLU	N-CA	5.33	1.57	1.46
1	A	460	SER	CA-CB	5.33	1.60	1.52
1	B	313	ILE	CA-CB	5.30	1.67	1.54
1	B	332	PHE	CG-CD2	5.29	1.46	1.38
1	C	418	TYR	N-CA	5.29	1.56	1.46
1	A	524	LEU	CA-C	5.29	1.66	1.52
1	B	289	VAL	CB-CG2	5.28	1.64	1.52
1	B	321	ARG	CZ-NH1	5.23	1.39	1.33
1	C	332	PHE	CG-CD1	5.22	1.46	1.38
1	C	321	ARG	CZ-NH1	5.13	1.39	1.33
1	C	525	ASN	CB-CG	-5.11	1.39	1.51
1	A	303	PHE	CA-C	5.09	1.66	1.52
1	C	294	TYR	CA-CB	-5.08	1.42	1.53
1	C	328	SER	N-CA	5.08	1.56	1.46
1	B	419	SER	CA-CB	5.08	1.60	1.52
1	B	242	ARG	CZ-NH1	5.06	1.39	1.33
1	B	466	SER	CB-OG	-5.04	1.35	1.42
1	A	418	TYR	CE1-CZ	5.04	1.45	1.38
1	A	350	GLU	CD-OE2	5.04	1.31	1.25
1	A	429	SER	CB-OG	-5.02	1.35	1.42

All (691) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	301	ARG	NE-CZ-NH1	43.95	142.27	120.30
1	A	532	ARG	NE-CZ-NH1	29.98	135.29	120.30
1	B	531	ARG	NE-CZ-NH2	27.91	134.26	120.30
1	A	532	ARG	NE-CZ-NH2	-25.79	107.41	120.30
1	A	242	ARG	NE-CZ-NH2	-25.72	107.44	120.30
1	B	532	ARG	NE-CZ-NH2	-25.54	107.53	120.30
1	C	397	ASP	CB-CG-OD1	-24.87	95.92	118.30
1	A	531	ARG	NE-CZ-NH2	23.66	132.13	120.30
1	C	469	ARG	NE-CZ-NH2	-20.15	110.23	120.30
1	C	321	ARG	NE-CZ-NH2	20.02	130.31	120.30
1	C	321	ARG	NE-CZ-NH1	-20.00	110.30	120.30
1	B	458	ARG	NE-CZ-NH2	19.98	130.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	279	ASP	CB-CG-OD1	19.67	136.00	118.30
1	A	242	ARG	NH1-CZ-NH2	19.49	140.84	119.40
1	A	531	ARG	CD-NE-CZ	19.08	150.31	123.60
1	A	305	GLU	OE1-CD-OE2	-18.47	101.13	123.30
1	B	377	ASP	CB-CG-OD1	18.15	134.63	118.30
1	B	425	ASP	CB-CG-OD2	18.09	134.58	118.30
1	C	461	TYR	CB-CG-CD2	17.75	131.65	121.00
1	A	321	ARG	NE-CZ-NH2	17.62	129.11	120.30
1	A	242	ARG	NE-CZ-NH1	-17.56	111.52	120.30
1	B	397	ASP	CB-CG-OD1	-17.55	102.50	118.30
1	A	458	ARG	NE-CZ-NH2	17.33	128.97	120.30
1	A	376	ARG	NE-CZ-NH1	17.31	128.96	120.30
1	C	461	TYR	CB-CG-CD1	-17.19	110.69	121.00
1	A	397	ASP	CB-CG-OD1	-16.56	103.39	118.30
1	C	287	ASP	CB-CG-OD2	15.79	132.51	118.30
1	C	425	ASP	CB-CG-OD2	-15.22	104.60	118.30
1	B	521	ARG	NE-CZ-NH2	-15.07	112.76	120.30
1	A	321	ARG	NE-CZ-NH1	-14.90	112.85	120.30
1	B	496	GLU	OE1-CD-OE2	-14.76	105.59	123.30
1	A	469	ARG	NE-CZ-NH1	-14.73	112.94	120.30
1	B	531	ARG	NE-CZ-NH1	-14.45	113.07	120.30
1	C	422	ASP	CB-CG-OD1	-14.43	105.31	118.30
1	C	465	ASP	CB-CG-OD2	14.39	131.25	118.30
1	B	344	ASP	CB-CG-OD1	-14.27	105.46	118.30
1	C	532	ARG	NE-CZ-NH1	-14.08	113.26	120.30
1	B	458	ARG	NE-CZ-NH1	-13.97	113.32	120.30
1	C	301	ARG	NH1-CZ-NH2	-13.75	104.28	119.40
1	C	301	ARG	NE-CZ-NH2	-13.70	113.45	120.30
1	C	469	ARG	NH1-CZ-NH2	13.59	134.34	119.40
1	A	307	GLU	OE1-CD-OE2	13.32	139.29	123.30
1	B	349	LYS	CB-CG-CD	13.31	146.22	111.60
1	B	531	ARG	CD-NE-CZ	13.29	142.21	123.60
1	B	469	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	C	458	ARG	NE-CZ-NH2	13.10	126.85	120.30
1	C	242	ARG	CD-NE-CZ	13.00	141.80	123.60
1	A	504	ASN	OD1-CG-ND2	12.90	151.58	121.90
1	B	418	TYR	CB-CG-CD2	12.64	128.59	121.00
1	B	301	ARG	NE-CZ-NH2	-12.64	113.98	120.30
1	B	349	LYS	CA-CB-CG	12.56	141.04	113.40
1	B	474	LYS	CA-CB-CG	12.54	140.99	113.40
1	B	458	ARG	CD-NE-CZ	12.38	140.93	123.60
1	A	350	GLU	CA-CB-CG	12.33	140.52	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	TRP	N-CA-CB	12.19	132.55	110.60
1	C	334	GLU	CA-CB-CG	12.07	139.96	113.40
1	C	516	TYR	CB-CG-CD2	-12.06	113.77	121.00
1	A	454	ARG	NE-CZ-NH2	12.00	126.30	120.30
1	B	532	ARG	NH1-CZ-NH2	11.90	132.49	119.40
1	A	531	ARG	NH1-CZ-NH2	-11.88	106.33	119.40
1	A	305	GLU	CG-CD-OE1	11.76	141.81	118.30
1	C	532	ARG	NE-CZ-NH2	11.69	126.15	120.30
1	C	377	ASP	CB-CG-OD1	11.66	128.80	118.30
1	B	425	ASP	CB-CG-OD1	-11.63	107.83	118.30
1	B	422	ASP	CB-CG-OD2	11.57	128.71	118.30
1	B	506	PHE	CB-CG-CD1	11.54	128.88	120.80
1	B	422	ASP	CB-CG-OD1	-11.54	107.92	118.30
1	C	315	ASP	CB-CG-OD2	-11.52	107.93	118.30
1	B	354	TYR	CB-CG-CD2	-11.51	114.10	121.00
1	C	464	ASN	OD1-CG-ND2	11.51	148.36	121.90
1	C	310	PHE	CB-CG-CD2	11.44	128.81	120.80
1	B	251	TRP	N-CA-CB	11.40	131.13	110.60
1	C	471	ASP	CB-CG-OD1	-11.29	108.14	118.30
1	B	244	VAL	CA-CB-CG1	11.26	127.79	110.90
1	A	390	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	C	278	ASP	CB-CG-OD2	-11.23	108.19	118.30
1	B	288	TRP	CE2-CD2-CE3	11.21	132.15	118.70
1	A	504	ASN	N-CA-CB	-11.21	90.43	110.60
1	C	377	ASP	CB-CG-OD2	-11.19	108.23	118.30
1	C	317	LYS	C-N-CA	11.08	145.56	122.30
1	A	284	SER	N-CA-CB	11.07	127.11	110.50
1	B	288	TRP	NE1-CE2-CD2	10.89	118.19	107.30
1	A	408	GLU	OE1-CD-OE2	-10.83	110.30	123.30
1	A	303	PHE	O-C-N	10.81	140.00	122.70
1	A	377	ASP	CB-CG-OD2	10.73	127.96	118.30
1	A	356	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	B	390	ARG	NE-CZ-NH2	10.63	125.61	120.30
1	A	458	ARG	NE-CZ-NH1	-10.61	115.00	120.30
1	B	397	ASP	N-CA-CB	10.56	129.60	110.60
1	A	521	ARG	CD-NE-CZ	10.48	138.28	123.60
1	A	539	TYR	CB-CG-CD2	-10.43	114.74	121.00
1	C	410	ARG	NE-CZ-NH2	-10.41	115.10	120.30
1	C	289	VAL	CG1-CB-CG2	-10.36	94.32	110.90
1	C	494	GLU	OE1-CD-OE2	-10.36	110.86	123.30
1	A	376	ARG	CD-NE-CZ	10.23	137.92	123.60
1	A	287	ASP	CB-CG-OD2	10.22	127.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	469	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	B	278	ASP	CB-CG-OD1	10.11	127.39	118.30
1	A	461	TYR	CB-CG-CD1	9.94	126.96	121.00
1	A	291	ALA	N-CA-CB	9.91	123.97	110.10
1	B	516	TYR	CB-CG-CD2	-9.79	115.13	121.00
1	C	469	ARG	NE-CZ-NH1	-9.76	115.42	120.30
1	B	506	PHE	CG-CD1-CE1	9.76	131.53	120.80
1	C	356	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	C	415	LEU	CB-CA-C	-9.71	91.75	110.20
1	B	522	THR	N-CA-CB	9.68	128.70	110.30
1	B	290	TYR	CB-CG-CD1	-9.68	115.19	121.00
1	C	316	ALA	CB-CA-C	9.67	124.61	110.10
1	C	316	ALA	N-CA-CB	-9.65	96.59	110.10
1	C	285	VAL	CA-CB-CG1	9.61	125.31	110.90
1	B	309	LYS	CD-CE-NZ	-9.60	89.63	111.70
1	C	495	LEU	CB-CG-CD2	-9.58	94.72	111.00
1	B	334	GLU	OE1-CD-OE2	-9.56	111.83	123.30
1	B	275	ILE	CB-CG1-CD1	9.56	140.66	113.90
1	B	454	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	A	342	ASN	CB-CG-ND2	9.50	139.49	116.70
1	C	397	ASP	OD1-CG-OD2	9.42	141.20	123.30
1	A	522	THR	CA-CB-CG2	9.38	125.54	112.40
1	B	349	LYS	CB-CA-C	9.30	128.99	110.40
1	C	356	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	A	536	SER	CA-C-N	9.29	137.64	117.20
1	C	458	ARG	CD-NE-CZ	9.24	136.54	123.60
1	C	331	VAL	CA-CB-CG2	-9.23	97.05	110.90
1	B	288	TRP	CE2-CD2-CG	-9.23	99.92	107.30
1	C	531	ARG	O-C-N	9.23	137.46	122.70
1	A	336	ASP	CB-CG-OD1	9.22	126.60	118.30
1	C	251	TRP	N-CA-CB	9.22	127.19	110.60
1	C	402	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	C	271	SER	CB-CA-C	-9.19	92.64	110.10
1	C	421	LYS	N-CA-CB	9.18	127.12	110.60
1	A	240	MET	CA-CB-CG	9.12	128.80	113.30
1	B	303	PHE	CB-CG-CD1	-9.10	114.43	120.80
1	A	244	VAL	CA-CB-CG2	9.08	124.52	110.90
1	C	294	TYR	CB-CG-CD1	-9.08	115.55	121.00
1	B	288	TRP	CD2-CE2-CZ2	-9.04	111.45	122.30
1	B	246	ILE	CA-CB-CG2	-9.02	92.87	110.90
1	C	329	GLN	CG-CD-OE1	-9.01	103.58	121.60
1	A	244	VAL	CA-CB-CG1	8.96	124.34	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	ASP	CB-CG-OD1	-8.89	110.30	118.30
1	C	280	ASP	N-CA-CB	8.87	126.57	110.60
1	B	504	ASN	CA-CB-CG	-8.87	93.90	113.40
1	C	334	GLU	N-CA-CB	8.85	126.53	110.60
1	C	319	PRO	N-CA-CB	-8.84	92.69	103.30
1	A	350	GLU	OE1-CD-OE2	-8.84	112.69	123.30
1	A	417	LEU	CB-CG-CD2	8.84	126.02	111.00
1	C	410	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	A	287	ASP	OD1-CG-OD2	-8.79	106.59	123.30
1	C	315	ASP	CB-CG-OD1	8.77	126.19	118.30
1	C	393	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	B	465	ASP	CB-CG-OD1	-8.74	110.43	118.30
1	C	415	LEU	N-CA-CB	8.73	127.86	110.40
1	C	516	TYR	CB-CG-CD1	8.72	126.23	121.00
1	B	433	GLU	CG-CD-OE2	8.67	135.64	118.30
1	C	404	GLY	N-CA-C	8.67	134.78	113.10
1	A	523	PHE	CD1-CE1-CZ	8.65	130.49	120.10
1	B	301	ARG	NH1-CZ-NH2	8.64	128.91	119.40
1	C	336	ASP	CB-CG-OD1	8.62	126.06	118.30
1	A	504	ASN	CA-CB-CG	-8.62	94.44	113.40
1	A	469	ARG	NH1-CZ-NH2	8.59	128.85	119.40
1	C	465	ASP	CB-CG-OD1	-8.51	110.64	118.30
1	B	393	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	B	350	GLU	OE1-CD-OE2	-8.46	113.15	123.30
1	B	404	GLY	N-CA-C	8.44	134.21	113.10
1	A	404	GLY	N-CA-C	8.43	134.18	113.10
1	C	464	ASN	CA-CB-CG	-8.43	94.86	113.40
1	A	310	PHE	CB-CG-CD1	8.43	126.70	120.80
1	A	345	ALA	CB-CA-C	-8.42	97.47	110.10
1	A	406	PHE	CB-CG-CD1	8.40	126.68	120.80
1	C	424	TYR	CG-CD1-CE1	-8.40	114.58	121.30
1	B	316	ALA	CB-CA-C	8.38	122.68	110.10
1	B	415	LEU	CB-CG-CD2	8.38	125.24	111.00
1	A	461	TYR	CB-CG-CD2	-8.37	115.98	121.00
1	A	287	ASP	CB-CG-OD1	8.33	125.79	118.30
1	B	525	ASN	O-C-N	-8.31	109.40	122.70
1	A	432	LEU	O-C-N	8.31	135.99	122.70
1	C	419	SER	N-CA-CB	-8.31	98.04	110.50
1	B	521	ARG	CD-NE-CZ	8.30	135.22	123.60
1	C	402	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	C	278	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	377	ASP	OD1-CG-OD2	-8.29	107.55	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	425	ASP	CA-CB-CG	8.28	131.62	113.40
1	B	454	ARG	CG-CD-NE	8.25	129.13	111.80
1	A	434	LEU	CB-CG-CD2	8.24	125.01	111.00
1	A	332	PHE	CB-CG-CD2	8.19	126.53	120.80
1	B	321	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	B	420	PRO	O-C-N	-8.17	109.63	122.70
1	B	426	VAL	N-CA-CB	8.16	129.45	111.50
1	A	279	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	A	507	ASP	CB-CG-OD2	8.09	125.58	118.30
1	C	464	ASN	CB-CG-OD1	-8.08	105.45	121.60
1	A	281	LEU	CB-CG-CD2	-8.05	97.32	111.00
1	A	410	ARG	NE-CZ-NH2	8.05	124.32	120.30
1	A	422	ASP	CB-CG-OD1	8.05	125.54	118.30
1	B	354	TYR	CB-CG-CD1	8.04	125.83	121.00
1	B	418	TYR	CG-CD2-CE2	8.04	127.73	121.30
1	A	530	ILE	O-C-N	-8.03	109.85	122.70
1	B	288	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	C	410	ARG	O-C-N	-7.97	109.94	122.70
1	C	458	ARG	C-N-CA	7.97	141.63	121.70
1	A	349	LYS	CA-CB-CG	7.96	130.92	113.40
1	A	354	TYR	CG-CD2-CE2	-7.96	114.93	121.30
1	A	393	ARG	CD-NE-CZ	7.96	134.74	123.60
1	A	342	ASN	OD1-CG-ND2	-7.93	103.66	121.90
1	C	376	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	B	377	ASP	OD1-CG-OD2	-7.91	108.28	123.30
1	A	397	ASP	OD1-CG-OD2	7.89	138.28	123.30
1	B	414	GLN	O-C-N	7.88	135.31	122.70
1	C	457	ASP	CA-CB-CG	7.86	130.69	113.40
1	B	344	ASP	CB-CG-OD2	7.86	125.37	118.30
1	B	412	VAL	CA-CB-CG2	-7.85	99.12	110.90
1	C	303	PHE	N-CA-CB	-7.82	96.52	110.60
1	C	295	SER	O-C-N	-7.79	110.23	122.70
1	B	490	THR	O-C-N	7.74	135.09	122.70
1	C	457	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	C	290	TYR	CG-CD1-CE1	-7.72	115.12	121.30
1	C	502	LEU	CB-CG-CD1	7.72	124.13	111.00
1	B	307	GLU	O-C-N	7.70	135.03	122.70
1	B	433	GLU	OE1-CD-OE2	-7.70	114.06	123.30
1	B	288	TRP	CE3-CZ3-CH2	-7.69	112.74	121.20
1	A	397	ASP	N-CA-CB	7.69	124.45	110.60
1	B	531	ARG	CB-CG-CD	7.69	131.60	111.60
1	C	331	VAL	CA-CB-CG1	-7.68	99.37	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	534	LEU	N-CA-CB	7.68	125.76	110.40
1	B	308	MET	O-C-N	7.68	134.98	122.70
1	A	536	SER	CB-CA-C	7.67	124.68	110.10
1	B	495	LEU	CB-CG-CD1	-7.66	97.98	111.00
1	A	322	VAL	CA-CB-CG2	7.64	122.36	110.90
1	A	454	ARG	CA-CB-CG	7.63	130.20	113.40
1	C	427	LYS	CD-CE-NZ	-7.63	94.14	111.70
1	C	519	LEU	CA-CB-CG	7.63	132.85	115.30
1	B	504	ASN	OD1-CG-ND2	7.62	139.42	121.90
1	A	431	ASN	CB-CA-C	-7.61	95.18	110.40
1	A	400	THR	CA-C-N	7.59	131.38	116.20
1	A	431	ASN	CA-CB-CG	-7.59	96.70	113.40
1	A	400	THR	CA-CB-CG2	7.53	122.94	112.40
1	B	532	ARG	CD-NE-CZ	-7.53	113.06	123.60
1	A	521	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	504	ASN	CB-CG-ND2	-7.49	98.72	116.70
1	C	367	LYS	CD-CE-NZ	7.49	128.93	111.70
1	B	294	TYR	CD1-CE1-CZ	-7.49	113.06	119.80
1	A	346	SER	CB-CA-C	7.48	124.31	110.10
1	C	328	SER	CB-CA-C	7.47	124.29	110.10
1	A	432	LEU	C-N-CA	-7.46	103.05	121.70
1	C	463	HIS	CA-C-O	7.46	135.76	120.10
1	A	251	TRP	CB-CA-C	-7.43	95.54	110.40
1	A	350	GLU	CG-CD-OE1	7.41	133.12	118.30
1	C	353	LYS	CB-CA-C	7.41	125.21	110.40
1	B	399	LYS	CA-CB-CG	7.38	129.64	113.40
1	C	265	ASP	CB-CA-C	7.38	125.16	110.40
1	C	515	GLU	OE1-CD-OE2	-7.38	114.45	123.30
1	A	312	VAL	CA-CB-CG1	7.37	121.96	110.90
1	A	281	LEU	O-C-N	-7.36	110.93	122.70
1	B	454	ARG	CD-NE-CZ	7.35	133.89	123.60
1	C	456	LYS	CB-CG-CD	7.33	130.65	111.60
1	C	287	ASP	OD1-CG-OD2	-7.32	109.38	123.30
1	C	492	GLU	OE1-CD-OE2	7.30	132.06	123.30
1	A	290	TYR	CB-CG-CD1	-7.30	116.62	121.00
1	A	516	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	A	403	VAL	CA-CB-CG1	7.28	121.82	110.90
1	B	531	ARG	CA-CB-CG	7.28	129.42	113.40
1	B	431	ASN	OD1-CG-ND2	7.28	138.64	121.90
1	B	522	THR	OG1-CB-CG2	7.25	126.69	110.00
1	C	525	ASN	CB-CG-OD1	7.25	136.10	121.60
1	A	300	LEU	CB-CG-CD2	7.23	123.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	354	TYR	CZ-CE2-CD2	7.22	126.30	119.80
1	C	425	ASP	OD1-CG-OD2	7.21	137.00	123.30
1	B	332	PHE	CZ-CE2-CD2	7.18	128.72	120.10
1	B	534	LEU	CA-CB-CG	7.17	131.79	115.30
1	A	418	TYR	CG-CD1-CE1	7.17	127.03	121.30
1	A	310	PHE	O-C-N	-7.17	111.02	123.20
1	A	538	SER	CB-CA-C	7.16	123.70	110.10
1	B	496	GLU	CG-CD-OE1	7.15	132.60	118.30
1	A	497	ILE	CB-CG1-CD1	-7.11	93.99	113.90
1	A	393	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	B	290	TYR	CB-CG-CD2	7.10	125.26	121.00
1	B	242	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	415	LEU	CA-CB-CG	7.05	131.53	115.30
1	C	499	THR	O-C-N	-7.05	107.71	121.10
1	A	512	ASP	CB-CG-OD1	-7.04	111.96	118.30
1	C	349	LYS	CA-CB-CG	7.04	128.89	113.40
1	A	247	TRP	CH2-CZ2-CE2	-7.03	110.37	117.40
1	C	504	ASN	CB-CA-C	-7.03	96.35	110.40
1	B	402	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	C	399	LYS	CA-CB-CG	7.02	128.84	113.40
1	B	467	CYS	CA-CB-SG	7.01	126.62	114.00
1	A	532	ARG	CD-NE-CZ	-7.00	113.79	123.60
1	C	457	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C	434	LEU	CB-CG-CD2	6.97	122.85	111.00
1	C	291	ALA	O-C-N	-6.96	111.57	122.70
1	A	344	ASP	CB-CG-OD1	-6.95	112.04	118.30
1	B	349	LYS	N-CA-CB	-6.94	98.10	110.60
1	C	495	LEU	CB-CA-C	-6.94	97.02	110.20
1	C	395	SER	N-CA-CB	-6.94	100.09	110.50
1	A	524	LEU	O-C-N	6.93	133.79	122.70
1	A	288	TRP	CD1-NE1-CE2	-6.91	102.78	109.00
1	B	498	ASN	N-CA-CB	-6.91	98.17	110.60
1	C	420	PRO	CB-CA-C	-6.91	94.73	112.00
1	B	316	ALA	N-CA-CB	-6.89	100.45	110.10
1	B	353	LYS	N-CA-CB	-6.89	98.20	110.60
1	A	272	PHE	CB-CG-CD2	6.89	125.62	120.80
1	B	288	TRP	CG-CD2-CE3	-6.88	127.71	133.90
1	B	494	GLU	CB-CA-C	-6.88	96.64	110.40
1	B	416	LEU	CB-CG-CD2	-6.87	99.31	111.00
1	C	499	THR	CA-C-O	6.87	134.53	120.10
1	B	375	THR	CA-CB-CG2	6.87	122.01	112.40
1	B	321	ARG	CB-CA-C	6.87	124.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	312	VAL	O-C-N	-6.84	111.76	122.70
1	B	280	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	539	TYR	CB-CG-CD1	6.83	125.10	121.00
1	C	249	GLN	CG-CD-NE2	6.83	133.08	116.70
1	A	313	ILE	CB-CG1-CD1	6.80	132.95	113.90
1	B	511	ASN	N-CA-CB	-6.80	98.37	110.60
1	A	377	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	523	PHE	CB-CG-CD1	6.79	125.55	120.80
1	A	536	SER	CA-C-O	-6.76	105.90	120.10
1	B	294	TYR	CB-CG-CD1	-6.75	116.95	121.00
1	C	519	LEU	O-C-N	6.74	133.49	122.70
1	C	305	GLU	CA-CB-CG	6.74	128.23	113.40
1	C	468	THR	O-C-N	-6.74	111.92	122.70
1	C	242	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	492	GLU	CG-CD-OE1	-6.72	104.86	118.30
1	A	435	PRO	CA-C-N	6.71	131.97	117.20
1	C	495	LEU	N-CA-CB	6.71	123.82	110.40
1	B	246	ILE	CA-C-N	6.71	131.95	117.20
1	C	520	ILE	C-N-CA	6.70	138.46	121.70
1	A	270	PRO	N-CD-CG	-6.70	93.15	103.20
1	A	342	ASN	CA-CB-CG	-6.70	98.67	113.40
1	B	288	TRP	CD1-NE1-CE2	-6.68	102.99	109.00
1	C	244	VAL	CG1-CB-CG2	6.67	121.57	110.90
1	C	279	ASP	OD1-CG-OD2	-6.67	110.63	123.30
1	C	521	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	242	ARG	CD-NE-CZ	-6.65	114.29	123.60
1	A	516	TYR	CZ-CE2-CD2	-6.64	113.83	119.80
1	B	244	VAL	CA-CB-CG2	6.63	120.85	110.90
1	B	427	LYS	CA-CB-CG	6.59	127.91	113.40
1	B	381	ARG	CD-NE-CZ	6.59	132.83	123.60
1	C	494	GLU	O-C-N	-6.59	112.16	122.70
1	A	454	ARG	NH1-CZ-NH2	-6.58	112.16	119.40
1	A	435	PRO	O-C-N	-6.58	112.17	122.70
1	B	492	GLU	OE1-CD-OE2	-6.57	115.42	123.30
1	A	294	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	536	SER	O-C-N	-6.57	112.19	122.70
1	C	294	TYR	CD1-CG-CD2	6.55	125.11	117.90
1	C	525	ASN	OD1-CG-ND2	-6.55	106.83	121.90
1	C	312	VAL	CG1-CB-CG2	6.54	121.37	110.90
1	C	422	ASP	C-N-CA	-6.54	105.34	121.70
1	B	415	LEU	N-CA-CB	-6.54	97.31	110.40
1	A	248	ALA	CB-CA-C	-6.53	100.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	GLN	N-CA-CB	6.53	122.35	110.60
1	A	373	SER	N-CA-CB	-6.53	100.71	110.50
1	B	287	ASP	CA-CB-CG	-6.53	99.04	113.40
1	A	302	SER	CA-C-O	-6.52	106.40	120.10
1	A	470	ILE	CA-C-N	6.50	131.50	117.20
1	B	459	VAL	C-N-CA	6.49	137.92	121.70
1	C	536	SER	CA-C-N	6.49	131.47	117.20
1	C	427	LYS	CB-CG-CD	6.48	128.44	111.60
1	B	507	ASP	CB-CG-OD2	6.46	124.12	118.30
1	C	407	ILE	CA-CB-CG2	6.46	123.82	110.90
1	C	293	ILE	C-N-CA	6.46	137.85	121.70
1	B	531	ARG	NH1-CZ-NH2	-6.45	112.30	119.40
1	A	274	ASN	O-C-N	-6.45	112.38	122.70
1	C	256	LYS	CA-CB-CG	6.45	127.59	113.40
1	A	454	ARG	CD-NE-CZ	6.44	132.62	123.60
1	C	286	GLN	C-N-CA	6.44	137.81	121.70
1	A	393	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	B	424	TYR	N-CA-CB	-6.43	99.02	110.60
1	B	496	GLU	CB-CA-C	-6.43	97.55	110.40
1	C	504	ASN	OD1-CG-ND2	6.42	136.66	121.90
1	C	531	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	526	ASN	CA-CB-CG	-6.41	99.30	113.40
1	A	334	GLU	N-CA-C	-6.39	93.75	111.00
1	C	241	TYR	C-N-CA	6.39	137.68	121.70
1	A	458	ARG	CD-NE-CZ	6.39	132.54	123.60
1	B	301	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	B	274	ASN	O-C-N	-6.37	112.50	122.70
1	B	310	PHE	O-C-N	-6.37	112.36	123.20
1	A	303	PHE	C-N-CA	-6.36	105.79	121.70
1	C	345	ALA	N-CA-CB	6.36	119.00	110.10
1	A	538	SER	N-CA-CB	-6.35	100.97	110.50
1	B	395	SER	CB-CA-C	6.34	122.14	110.10
1	B	504	ASN	CB-CG-ND2	-6.33	101.50	116.70
1	C	280	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	395	SER	CB-CA-C	6.33	122.13	110.10
1	A	465	ASP	N-CA-CB	-6.31	99.25	110.60
1	A	470	ILE	CA-C-O	-6.30	106.87	120.10
1	A	290	TYR	CD1-CG-CD2	6.30	124.83	117.90
1	B	417	LEU	CB-CG-CD1	6.30	121.70	111.00
1	B	460	SER	CA-CB-OG	-6.29	94.22	111.20
1	C	511	ASN	N-CA-CB	-6.28	99.29	110.60
1	B	331	VAL	O-C-N	-6.28	112.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	430	LEU	O-C-N	-6.27	112.67	122.70
1	C	334	GLU	CG-CD-OE2	-6.25	105.80	118.30
1	C	411	HIS	O-C-N	-6.24	112.72	122.70
1	B	349	LYS	CG-CD-CE	6.24	130.62	111.90
1	A	522	THR	N-CA-CB	6.23	122.14	110.30
1	B	492	GLU	CA-C-N	-6.22	103.51	117.20
1	A	391	PHE	CB-CG-CD2	6.21	125.15	120.80
1	A	435	PRO	CB-CA-C	-6.21	96.47	112.00
1	A	317	LYS	CA-C-O	6.21	133.14	120.10
1	A	466	SER	O-C-N	-6.20	112.78	122.70
1	A	538	SER	C-N-CA	6.19	137.18	121.70
1	C	317	LYS	O-C-N	-6.19	112.68	123.20
1	C	278	ASP	N-CA-CB	-6.19	99.47	110.60
1	C	244	VAL	CA-CB-CG2	6.18	120.17	110.90
1	C	254	THR	CA-CB-OG1	-6.18	96.01	109.00
1	B	323	ASN	OD1-CG-ND2	6.18	136.12	121.90
1	B	376	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	304	ILE	CA-C-N	-6.16	103.64	117.20
1	A	294	TYR	CB-CG-CD1	6.16	124.69	121.00
1	A	396	THR	CA-CB-CG2	-6.16	103.78	112.40
1	A	457	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	242	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	391	PHE	CB-CG-CD1	-6.14	116.50	120.80
1	C	329	GLN	OE1-CD-NE2	6.14	136.02	121.90
1	C	417	LEU	O-C-N	6.14	132.52	122.70
1	B	512	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	376	ARG	CD-NE-CZ	6.12	132.16	123.60
1	A	454	ARG	CG-CD-NE	6.11	124.62	111.80
1	C	522	THR	CA-CB-CG2	6.11	120.95	112.40
1	C	410	ARG	C-N-CA	6.10	136.96	121.70
1	B	303	PHE	O-C-N	6.09	132.45	122.70
1	B	242	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	A	302	SER	CA-C-N	6.06	130.52	117.20
1	A	317	LYS	C-N-CA	6.04	134.99	122.30
1	B	283	LYS	CD-CE-NZ	-6.04	97.80	111.70
1	C	284	SER	N-CA-CB	6.04	119.55	110.50
1	C	251	TRP	CB-CA-C	-6.03	98.33	110.40
1	B	339	LEU	CB-CG-CD2	6.03	121.24	111.00
1	B	454	ARG	CA-CB-CG	6.03	126.66	113.40
1	A	504	ASN	CB-CG-OD1	-6.02	109.56	121.60
1	B	327	SER	CB-CA-C	-6.02	98.66	110.10
1	A	465	ASP	CB-CG-OD1	6.02	123.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	285	VAL	CA-CB-CG2	-6.02	101.88	110.90
1	C	433	GLU	O-C-N	6.01	132.32	122.70
1	B	506	PHE	CD1-CE1-CZ	-6.00	112.90	120.10
1	A	279	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	406	PHE	CG-CD1-CE1	5.99	127.39	120.80
1	B	396	THR	CA-C-N	5.99	130.37	117.20
1	A	505	ALA	O-C-N	5.98	132.26	122.70
1	C	373	SER	N-CA-CB	-5.97	101.54	110.50
1	C	305	GLU	OE1-CD-OE2	-5.97	116.13	123.30
1	C	363	GLU	CA-CB-CG	5.97	126.53	113.40
1	B	419	SER	N-CA-CB	-5.97	101.55	110.50
1	B	288	TRP	CZ3-CH2-CZ2	5.95	128.74	121.60
1	B	459	VAL	CA-CB-CG2	-5.95	101.97	110.90
1	C	424	TYR	CD1-CE1-CZ	5.94	125.14	119.80
1	B	431	ASN	CB-CA-C	-5.94	98.53	110.40
1	B	271	SER	CB-CA-C	-5.93	98.83	110.10
1	B	310	PHE	CB-CG-CD1	5.92	124.94	120.80
1	B	397	ASP	OD1-CG-OD2	5.92	134.54	123.30
1	A	376	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	332	PHE	C-N-CA	5.89	136.43	121.70
1	C	289	VAL	O-C-N	5.88	132.12	122.70
1	A	242	ARG	CG-CD-NE	-5.88	99.45	111.80
1	C	347	LEU	N-CA-CB	-5.88	98.64	110.40
1	A	278	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	411	HIS	CA-CB-CG	-5.88	103.61	113.60
1	A	418	TYR	CB-CG-CD2	5.88	124.53	121.00
1	A	335	LEU	N-CA-CB	-5.87	98.66	110.40
1	A	327	SER	CA-CB-OG	-5.85	95.40	111.20
1	B	251	TRP	CB-CA-C	-5.85	98.70	110.40
1	B	513	SER	CB-CA-C	-5.83	99.01	110.10
1	C	534	LEU	CB-CG-CD1	5.83	120.91	111.00
1	A	321	ARG	O-C-N	-5.83	113.37	122.70
1	B	258	LEU	CA-C-O	5.82	132.32	120.10
1	B	308	MET	CG-SD-CE	5.81	109.49	100.20
1	C	312	VAL	N-CA-CB	-5.81	98.72	111.50
1	C	327	SER	N-CA-CB	-5.81	101.79	110.50
1	B	313	ILE	CG1-CB-CG2	5.81	124.17	111.40
1	A	293	ILE	CA-CB-CG1	-5.79	100.00	111.00
1	B	531	ARG	O-C-N	5.79	131.96	122.70
1	B	247	TRP	CE3-CZ3-CH2	-5.78	114.84	121.20
1	C	353	LYS	N-CA-CB	-5.78	100.19	110.60
1	B	321	ARG	O-C-N	-5.78	113.45	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303	PHE	CA-C-N	-5.77	104.51	117.20
1	A	400	THR	OG1-CB-CG2	-5.77	96.73	110.00
1	A	265	ASP	N-CA-CB	5.76	120.98	110.60
1	C	507	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	285	VAL	O-C-N	5.76	131.91	122.70
1	B	393	ARG	CD-NE-CZ	-5.76	115.54	123.60
1	B	251	TRP	O-C-N	5.75	131.91	122.70
1	C	526	ASN	CB-CG-OD1	5.75	133.11	121.60
1	C	529	ILE	CA-CB-CG1	-5.75	100.06	111.00
1	C	512	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	417	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	242	ARG	CB-CA-C	-5.74	98.92	110.40
1	A	492	GLU	CA-C-O	5.74	132.15	120.10
1	A	401	GLY	N-CA-C	5.74	127.44	113.10
1	B	310	PHE	CA-C-O	5.73	132.13	120.10
1	A	496	GLU	CB-CA-C	-5.71	98.98	110.40
1	B	435	PRO	O-C-N	-5.67	113.62	122.70
1	C	508	ASN	CA-CB-CG	-5.67	100.92	113.40
1	B	286	GLN	O-C-N	5.67	131.77	122.70
1	C	327	SER	CB-CA-C	-5.67	99.34	110.10
1	B	252	LYS	N-CA-CB	5.66	120.79	110.60
1	B	332	PHE	CG-CD2-CE2	-5.66	114.57	120.80
1	A	533	LYS	O-C-N	-5.66	113.65	122.70
1	A	272	PHE	CB-CG-CD1	-5.65	116.84	120.80
1	B	526	ASN	CA-C-N	-5.64	104.91	116.20
1	A	468	THR	CA-CB-CG2	-5.63	104.52	112.40
1	C	395	SER	O-C-N	-5.63	113.69	122.70
1	A	285	VAL	CA-C-O	-5.62	108.29	120.10
1	C	425	ASP	N-CA-CB	-5.62	100.48	110.60
1	A	283	LYS	N-CA-CB	5.61	120.70	110.60
1	A	401	GLY	C-N-CA	5.60	135.71	121.70
1	C	255	ILE	CA-CB-CG2	5.60	122.11	110.90
1	C	275	ILE	N-CA-CB	5.60	123.67	110.80
1	B	285	VAL	C-N-CA	5.59	135.68	121.70
1	B	424	TYR	CG-CD1-CE1	-5.59	116.83	121.30
1	C	508	ASN	OD1-CG-ND2	5.59	134.76	121.90
1	A	297	ALA	N-CA-CB	-5.59	102.28	110.10
1	C	400	THR	N-CA-CB	5.58	120.89	110.30
1	A	246	ILE	CA-CB-CG1	-5.57	100.41	111.00
1	B	324	PRO	N-CA-CB	-5.57	96.47	102.60
1	A	295	SER	CA-CB-OG	5.57	126.23	111.20
1	B	291	ALA	CB-CA-C	5.56	118.45	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	348	PHE	N-CA-CB	-5.56	100.59	110.60
1	B	493	VAL	CB-CA-C	-5.56	100.84	111.40
1	B	342	ASN	CB-CA-C	-5.55	99.31	110.40
1	C	429	SER	CA-C-N	-5.54	105.01	117.20
1	C	463	HIS	N-CA-CB	5.53	120.56	110.60
1	C	298	PRO	N-CA-CB	5.53	109.94	103.30
1	C	399	LYS	CD-CE-NZ	5.53	124.42	111.70
1	A	411	HIS	CA-CB-CG	-5.53	104.21	113.60
1	A	247	TRP	CE3-CZ3-CH2	-5.52	115.12	121.20
1	B	268	ILE	CG1-CB-CG2	-5.52	99.25	111.40
1	B	273	LEU	N-CA-CB	5.52	121.44	110.40
1	B	312	VAL	N-CA-CB	-5.51	99.37	111.50
1	B	338	HIS	N-CA-CB	-5.51	100.68	110.60
1	B	351	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	B	246	ILE	CA-CB-CG1	-5.51	100.53	111.00
1	A	312	VAL	N-CA-CB	-5.51	99.38	111.50
1	C	503	LEU	O-C-N	-5.50	113.90	122.70
1	B	494	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	A	343	ILE	O-C-N	-5.50	113.90	122.70
1	B	414	GLN	C-N-CA	-5.50	107.95	121.70
1	B	536	SER	O-C-N	-5.50	113.90	122.70
1	C	511	ASN	CB-CA-C	5.50	121.39	110.40
1	B	289	VAL	CA-CB-CG1	5.49	119.14	110.90
1	C	310	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	A	313	ILE	C-N-CA	5.49	135.42	121.70
1	B	344	ASP	CA-C-O	5.49	131.62	120.10
1	B	426	VAL	CB-CA-C	-5.48	100.98	111.40
1	C	279	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	C	310	PHE	C-N-CA	-5.47	110.81	122.30
1	B	488	GLU	OE1-CD-OE2	-5.47	116.74	123.30
1	A	330	CYS	N-CA-CB	-5.47	100.76	110.60
1	B	492	GLU	CG-CD-OE1	5.47	129.23	118.30
1	A	519	LEU	CA-C-O	5.46	131.57	120.10
1	A	272	PHE	CD1-CE1-CZ	5.46	126.65	120.10
1	A	350	GLU	CB-CA-C	5.45	121.31	110.40
1	B	293	ILE	C-N-CA	5.45	135.32	121.70
1	B	293	ILE	CA-CB-CG2	5.45	121.80	110.90
1	C	247	TRP	CE3-CZ3-CH2	-5.44	115.21	121.20
1	C	294	TYR	CG-CD2-CE2	-5.43	116.95	121.30
1	A	285	VAL	C-N-CA	5.43	135.28	121.70
1	A	374	GLN	CG-CD-OE1	-5.43	110.74	121.60
1	B	506	PHE	CB-CG-CD2	-5.43	117.00	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	250	LYS	CA-CB-CG	5.42	125.33	113.40
1	B	320	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	424	TYR	CA-CB-CG	-5.41	103.11	113.40
1	A	410	ARG	CD-NE-CZ	5.41	131.17	123.60
1	B	521	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	401	GLY	C-N-CA	5.39	135.19	121.70
1	C	240	MET	CA-CB-CG	5.39	122.46	113.30
1	B	292	THR	CA-C-O	-5.38	108.80	120.10
1	A	345	ALA	O-C-N	-5.38	114.09	122.70
1	A	257	ALA	N-CA-CB	-5.38	102.57	110.10
1	B	308	MET	CA-C-N	-5.38	105.37	117.20
1	C	319	PRO	O-C-N	-5.37	114.10	122.70
1	C	531	ARG	CD-NE-CZ	5.37	131.12	123.60
1	C	344	ASP	N-CA-CB	-5.37	100.93	110.60
1	A	526	ASN	OD1-CG-ND2	-5.37	109.55	121.90
1	C	514	LYS	CB-CG-CD	5.37	125.55	111.60
1	A	333	THR	O-C-N	-5.36	114.12	122.70
1	B	424	TYR	CZ-CE2-CD2	-5.36	114.97	119.80
1	C	336	ASP	OD1-CG-OD2	-5.36	113.11	123.30
1	A	530	ILE	N-CA-CB	5.35	123.11	110.80
1	B	310	PHE	CG-CD1-CE1	5.35	126.68	120.80
1	A	507	ASP	OD1-CG-OD2	-5.34	113.15	123.30
1	A	472	ILE	O-C-N	-5.34	114.16	122.70
1	C	334	GLU	CB-CG-CD	-5.34	99.78	114.20
1	C	317	LYS	CA-C-O	5.33	131.30	120.10
1	C	393	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	315	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	406	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	B	400	THR	N-CA-CB	5.33	120.43	110.30
1	C	494	GLU	CB-CG-CD	5.32	128.57	114.20
1	C	294	TYR	CA-CB-CG	5.32	123.50	113.40
1	B	418	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	C	294	TYR	N-CA-CB	5.31	120.16	110.60
1	C	461	TYR	OH-CZ-CE2	5.31	134.43	120.10
1	B	524	LEU	N-CA-CB	5.30	121.01	110.40
1	C	430	LEU	C-N-CA	5.30	134.96	121.70
1	B	427	LYS	CD-CE-NZ	-5.30	99.51	111.70
1	A	392	LEU	CB-CA-C	5.30	120.26	110.20
1	C	504	ASN	CB-CG-OD1	-5.30	111.00	121.60
1	A	523	PHE	CG-CD1-CE1	-5.29	114.97	120.80
1	A	492	GLU	O-C-N	-5.29	114.23	122.70
1	B	516	TYR	CG-CD1-CE1	-5.29	117.07	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	314	ILE	CA-CB-CG2	5.29	121.47	110.90
1	B	498	ASN	CA-CB-CG	-5.29	101.77	113.40
1	A	524	LEU	CA-C-O	-5.29	109.00	120.10
1	A	401	GLY	O-C-N	-5.28	114.26	122.70
1	C	331	VAL	O-C-N	-5.27	114.27	122.70
1	C	269	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	C	463	HIS	CA-C-N	-5.25	105.65	117.20
1	B	493	VAL	CA-CB-CG2	-5.25	103.03	110.90
1	B	401	GLY	C-N-CA	5.24	134.81	121.70
1	B	246	ILE	CA-C-O	-5.23	109.11	120.10
1	B	528	THR	N-CA-CB	-5.23	100.36	110.30
1	B	465	ASP	OD1-CG-OD2	5.23	133.24	123.30
1	A	376	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	B	348	PHE	CD1-CE1-CZ	-5.22	113.84	120.10
1	C	326	VAL	CA-C-O	5.22	131.06	120.10
1	C	458	ARG	NH1-CZ-NH2	-5.21	113.66	119.40
1	C	470	ILE	CA-C-O	-5.21	109.15	120.10
1	A	283	LYS	CA-C-O	-5.21	109.16	120.10
1	C	326	VAL	CA-CB-CG1	5.21	118.72	110.90
1	B	533	LYS	N-CA-CB	5.21	119.97	110.60
1	B	504	ASN	N-CA-CB	-5.21	101.23	110.60
1	A	345	ALA	CA-C-O	5.20	131.03	120.10
1	B	401	GLY	N-CA-C	5.20	126.09	113.10
1	C	266	LEU	CA-C-O	5.20	131.01	120.10
1	C	513	SER	CB-CA-C	-5.19	100.23	110.10
1	A	323	ASN	CB-CG-OD1	-5.19	111.22	121.60
1	C	536	SER	CA-CB-OG	-5.19	97.19	111.20
1	B	309	LYS	CA-CB-CG	5.18	124.80	113.40
1	B	424	TYR	CG-CD2-CE2	5.17	125.44	121.30
1	B	359	SER	N-CA-CB	5.17	118.25	110.50
1	C	520	ILE	CA-C-O	5.17	130.95	120.10
1	C	401	GLY	N-CA-C	5.17	126.02	113.10
1	A	355	ILE	CB-CG1-CD1	-5.16	99.44	113.90
1	B	317	LYS	CA-CB-CG	-5.16	102.04	113.40
1	B	280	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	C	422	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	516	TYR	CB-CG-CD2	5.15	124.09	121.00
1	B	342	ASN	O-C-N	5.15	130.94	122.70
1	B	344	ASP	O-C-N	-5.15	114.45	122.70
1	C	492	GLU	CA-CB-CG	-5.15	102.06	113.40
1	C	423	SER	CA-CB-OG	-5.15	97.30	111.20
1	C	381	ARG	NE-CZ-NH1	-5.15	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	317	LYS	C-N-CA	5.14	133.09	122.30
1	A	416	LEU	CA-CB-CG	-5.14	103.48	115.30
1	C	498	ASN	CA-C-N	5.13	128.48	117.20
1	C	433	GLU	CA-C-N	-5.12	105.93	117.20
1	A	409	LYS	CD-CE-NZ	5.12	123.48	111.70
1	B	366	GLY	CA-C-O	-5.12	111.38	120.60
1	B	307	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	C	333	THR	CA-CB-CG2	5.11	119.56	112.40
1	B	340	THR	CA-C-O	5.11	130.83	120.10
1	A	346	SER	CA-CB-OG	-5.11	97.41	111.20
1	B	397	ASP	CB-CG-OD2	5.11	122.89	118.30
1	C	424	TYR	CZ-CE2-CD2	-5.10	115.21	119.80
1	B	464	ASN	CA-CB-CG	-5.10	102.19	113.40
1	B	358	ILE	CA-CB-CG1	5.09	120.67	111.00
1	B	242	ARG	O-C-N	-5.09	114.56	122.70
1	B	275	ILE	O-C-N	5.09	130.84	122.70
1	B	286	GLN	CB-CA-C	5.09	120.58	110.40
1	C	264	LYS	N-CA-CB	-5.09	101.44	110.60
1	A	528	THR	CA-CB-OG1	-5.09	98.32	109.00
1	B	376	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	C	396	THR	C-N-CA	-5.09	108.98	121.70
1	B	353	LYS	CB-CA-C	5.08	120.57	110.40
1	A	244	VAL	N-CA-CB	5.08	122.69	111.50
1	B	407	ILE	CB-CA-C	-5.08	101.44	111.60
1	C	293	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	B	456	LYS	CB-CG-CD	5.08	124.80	111.60
1	C	272	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	B	525	ASN	CA-C-N	5.07	128.35	117.20
1	B	515	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	B	500	PRO	O-C-N	-5.06	114.60	122.70
1	A	240	MET	CB-CA-C	5.06	120.52	110.40
1	A	465	ASP	CB-CA-C	5.06	120.51	110.40
1	C	470	ILE	CA-C-N	5.05	128.32	117.20
1	A	529	ILE	CA-C-N	-5.05	106.10	117.20
1	B	337	ALA	N-CA-CB	5.04	117.16	110.10
1	A	495	LEU	N-CA-CB	5.03	120.46	110.40
1	B	463	HIS	CA-CB-CG	-5.03	105.05	113.60
1	C	249	GLN	O-C-N	-5.03	114.66	122.70
1	A	258	LEU	N-CA-CB	5.02	120.44	110.40
1	B	492	GLU	CA-C-O	5.02	130.64	120.10
1	B	376	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	B	418	TYR	CD1-CG-CD2	-5.02	112.38	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	355	ILE	CB-CG1-CD1	-5.02	99.86	113.90
1	A	331	VAL	CA-CB-CG2	5.01	118.42	110.90
1	C	282	THR	CA-CB-CG2	-5.01	105.38	112.40
1	C	467	CYS	O-C-N	5.01	130.72	122.70
1	C	275	ILE	CB-CA-C	-5.01	101.58	111.60
1	C	239	HIS	CA-C-O	5.00	130.61	120.10
1	C	242	ARG	NH1-CZ-NH2	5.00	124.90	119.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	522	THR	CB

All (84) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ILE	Mainchain
1	A	269	ASP	Mainchain
1	A	276	ILE	Mainchain
1	A	280	ASP	Mainchain
1	A	286	GLN	Mainchain
1	A	290	TYR	Mainchain
1	A	291	ALA	Mainchain
1	A	295	SER	Mainchain
1	A	305	GLU	Mainchain
1	A	314	ILE	Mainchain
1	A	322	VAL	Mainchain
1	A	324	PRO	Mainchain
1	A	328	SER	Mainchain
1	A	330	CYS	Mainchain
1	A	331	VAL	Mainchain
1	A	335	LEU	Mainchain
1	A	342	ASN	Mainchain
1	A	343	ILE	Mainchain
1	A	414	GLN	Mainchain
1	A	415	LEU	Mainchain
1	A	417	LEU	Mainchain
1	A	435	PRO	Mainchain
1	A	466	SER	Mainchain
1	A	495	LEU	Mainchain
1	A	506	PHE	Mainchain
1	A	530	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	532	ARG	Mainchain
1	A	533	LYS	Mainchain
1	A	536	SER	Mainchain
1	B	269	ASP	Mainchain
1	B	283	LYS	Mainchain
1	B	291	ALA	Mainchain
1	B	292	THR	Mainchain
1	B	293	ILE	Mainchain
1	B	296	ILE	Mainchain
1	B	312	VAL	Mainchain
1	B	321	ARG	Mainchain
1	B	323	ASN	Mainchain
1	B	336	ASP	Mainchain
1	B	339	LEU	Mainchain
1	B	343	ILE	Mainchain
1	B	413	ALA	Mainchain
1	B	418	TYR	Mainchain
1	B	419	SER	Mainchain
1	B	420	PRO	Mainchain
1	B	435	PRO	Mainchain
1	B	493	VAL	Mainchain
1	B	495	LEU	Mainchain
1	B	523	PHE	Mainchain
1	B	525	ASN	Mainchain
1	B	527	GLY	Mainchain
1	B	529	ILE	Mainchain
1	B	533	LYS	Mainchain
1	B	534	LEU	Mainchain
1	B	536	SER	Mainchain
1	C	243	ASN	Mainchain
1	C	244	VAL	Mainchain
1	C	255	ILE	Mainchain
1	C	283	LYS	Mainchain
1	C	288	TRP	Mainchain
1	C	290	TYR	Mainchain
1	C	294	TYR	Mainchain
1	C	303	PHE	Mainchain
1	C	304	ILE	Mainchain
1	C	321	ARG	Mainchain
1	C	324	PRO	Mainchain
1	C	329	GLN	Mainchain
1	C	330	CYS	Mainchain

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Mol	Chain	Res	Type	Group
1	C	354	TYR	Mainchain
1	C	359	SER	Mainchain
1	C	411	HIS	Mainchain
1	C	417	LEU	Mainchain
1	C	419	SER	Mainchain
1	C	420	PRO	Mainchain
1	C	423	SER	Mainchain
1	C	430	LEU	Mainchain
1	C	466	SER	Mainchain
1	C	503	LEU	Mainchain
1	C	507	ASP	Mainchain
1	C	515	GLU	Mainchain
1	C	520	ILE	Mainchain
1	C	521	ARG	Mainchain
1	C	524	LEU	Mainchain
1	C	535	SER	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	2313	0	2318	112	0
1	B	2313	0	2315	128	0
1	C	2313	0	2316	129	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	2	0
4	A	222	0	0	24	2
4	B	226	0	0	47	3
4	C	221	0	0	36	1
All	All	7626	0	6949	359	4

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 26.

All (359) 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:C:239:HIS:N	4:C:675:HOH:O	1.91	1.02
1:C:403:VAL:HG21	1:C:446:LYS:HE2	1.48	0.95
1:C:264:LYS:O	1:C:266:LEU:HG	1.73	0.89
1:C:502:LEU:HA	1:C:519:LEU:HD21	1.57	0.87
1:C:256:LYS:HB2	4:C:793:HOH:O	1.75	0.87
1:B:375:THR:HG22	4:B:761:HOH:O	1.75	0.86
1:A:464:ASN:HB3	4:A:707:HOH:O	1.75	0.86
1:B:383:GLY:HA3	4:B:800:HOH:O	1.77	0.85
1:C:448:GLN:HE21	1:C:448:GLN:HA	1.40	0.85
1:C:398:ILE:HA	4:C:714:HOH:O	1.77	0.84
1:C:242:ARG:NH1	4:C:606:HOH:O	2.05	0.83
1:B:252:LYS:HE2	4:B:611:HOH:O	1.78	0.83
1:B:342:ASN:HD22	1:B:491:HIS:H	1.27	0.82
1:C:522:THR:HG22	4:C:645:HOH:O	1.80	0.81
1:C:382:VAL:HG23	1:C:383:GLY:H	1.45	0.81
1:A:363:GLU:HG2	1:A:364:ASN:ND2	1.96	0.81
1:A:362:THR:O	1:A:365:THR:HG22	1.82	0.80
1:A:256:LYS:NZ	1:A:256:LYS:HA	1.97	0.79
1:A:313:ILE:HG22	4:A:792:HOH:O	1.82	0.79
1:B:349:LYS:HG3	4:B:632:HOH:O	1.82	0.79
1:A:435:PRO:O	4:A:821:HOH:O	2.01	0.78
1:B:321:ARG:O	4:B:642:HOH:O	2.00	0.78
1:C:342:ASN:ND2	1:C:491:HIS:H	1.81	0.77
1:A:363:GLU:HG3	4:A:729:HOH:O	1.85	0.77
1:B:464:ASN:HB2	4:B:720:HOH:O	1.84	0.77
1:B:342:ASN:ND2	1:B:491:HIS:H	1.83	0.77
1:B:448:GLN:HE21	1:B:448:GLN:HA	1.49	0.76
1:B:497:ILE:HD11	1:B:519:LEU:HG	1.68	0.76
1:B:374:GLN:HB3	4:B:743:HOH:O	1.86	0.76
1:C:464:ASN:HB2	4:C:657:HOH:O	1.87	0.75
1:A:500:PRO:O	1:A:504:ASN:HB2	1.88	0.74
1:C:499:THR:HB	1:C:500:PRO:HD3	1.70	0.74
1:B:476:GLU:OE1	1:B:489:THR:HG23	1.89	0.72
1:A:239:HIS:N	4:A:714:HOH:O	2.21	0.72
1:B:403:VAL:HG21	1:B:446:LYS:HE2	1.70	0.72
1:B:240:MET:SD	4:B:808:HOH:O	2.46	0.72
1:B:397:ASP:HB3	4:B:761:HOH:O	1.87	0.72
1:C:517:ALA:O	1:C:521:ARG:HG3	1.89	0.72
1:C:507:ASP:O	4:C:698:HOH:O	2.06	0.72
1:B:363:GLU:HG2	1:B:364:ASN:ND2	2.04	0.71
1:B:435:PRO:O	4:B:741:HOH:O	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:SER:O	1:C:522:THR:HG23	1.91	0.70
1:B:242:ARG:HD2	4:B:625:HOH:O	1.89	0.70
1:C:317:LYS:HE2	4:C:786:HOH:O	1.90	0.70
1:C:342:ASN:HD22	1:C:491:HIS:H	1.35	0.70
1:A:256:LYS:HA	1:A:256:LYS:HZ3	1.54	0.69
1:B:362:THR:O	1:B:365:THR:HG22	1.92	0.69
1:B:244:VAL:HG13	1:B:294:TYR:CZ	2.27	0.69
1:B:441:PRO:HD2	1:B:442:PRO:HD2	1.75	0.68
1:C:253:PRO:HD2	4:C:748:HOH:O	1.94	0.68
1:A:301:ARG:O	1:A:503:LEU:HD11	1.93	0.68
1:A:448:GLN:HA	1:A:448:GLN:HE21	1.58	0.68
1:B:377:ASP:OD1	1:B:395:SER:HB2	1.94	0.67
1:B:333:THR:O	1:B:333:THR:OG1	2.06	0.67
1:A:246:ILE:HG12	1:A:291:ALA:HB1	1.77	0.67
1:B:491:HIS:ND1	4:B:719:HOH:O	2.27	0.67
1:A:366:GLY:HA2	4:A:782:HOH:O	1.94	0.67
1:A:476:GLU:HG3	1:A:487:SER:OG	1.95	0.67
1:A:402:ARG:HG2	4:C:822:HOH:O	1.95	0.66
1:B:305:GLU:OE1	1:B:431:ASN:ND2	2.27	0.66
1:C:242:ARG:HD2	4:C:606:HOH:O	1.94	0.66
1:A:349:LYS:HD3	1:C:362:THR:HG22	1.76	0.66
1:B:344:ASP:HA	4:B:670:HOH:O	1.96	0.66
1:B:415:LEU:HD23	4:B:747:HOH:O	1.95	0.66
1:C:344:ASP:HB3	1:C:347:LEU:HB2	1.78	0.66
1:C:441:PRO:CD	1:C:442:PRO:HD2	2.25	0.66
1:B:402:ARG:HA	4:B:737:HOH:O	1.96	0.66
1:A:400:THR:O	1:A:402:ARG:N	2.28	0.65
1:B:441:PRO:CD	1:B:442:PRO:HD2	2.25	0.65
1:C:382:VAL:HG23	1:C:383:GLY:N	2.10	0.65
1:C:499:THR:HB	1:C:500:PRO:CD	2.27	0.65
1:C:502:LEU:HA	1:C:519:LEU:CD2	2.26	0.65
1:A:405:GLN:HB3	4:A:667:HOH:O	1.96	0.65
1:B:367:LYS:HE2	1:B:465:ASP:OD1	1.97	0.64
4:A:777:HOH:O	1:B:267:LYS:HB2	1.97	0.64
1:C:448:GLN:HA	1:C:448:GLN:NE2	2.09	0.64
1:B:448:GLN:HA	1:B:448:GLN:NE2	2.12	0.63
1:B:239:HIS:N	4:B:665:HOH:O	2.30	0.63
1:B:320:ASP:HB2	4:B:666:HOH:O	1.97	0.63
1:B:346:SER:HB3	1:B:349:LYS:HE3	1.80	0.63
1:B:365:THR:HG23	4:B:823:HOH:O	1.99	0.63
1:C:391:PHE:HA	4:C:792:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:GLU:HG2	1:C:410:ARG:HD3	1.81	0.62
1:C:315:ASP:HB2	4:C:732:HOH:O	1.98	0.62
1:B:433:GLU:O	4:B:778:HOH:O	2.16	0.62
1:C:498:ASN:OD1	1:C:500:PRO:HG2	2.00	0.61
1:A:363:GLU:HG2	1:A:364:ASN:HD22	1.62	0.61
1:A:417:LEU:HB2	1:A:426:VAL:HG23	1.82	0.61
1:B:348:PHE:CE1	1:B:472:ILE:HG23	2.36	0.61
1:A:253:PRO:HD2	4:A:622:HOH:O	2.00	0.61
1:A:273:LEU:HD12	1:B:529:ILE:HD13	1.81	0.61
1:A:441:PRO:HB2	1:A:442:PRO:HD3	1.83	0.61
1:A:465:ASP:OD1	4:A:614:HOH:O	2.16	0.60
1:B:348:PHE:CZ	1:B:472:ILE:HG23	2.37	0.60
1:A:348:PHE:CD1	1:A:491:HIS:HB3	2.37	0.60
1:A:522:THR:HG22	4:A:674:HOH:O	2.01	0.60
1:B:283:LYS:HE3	4:B:803:HOH:O	2.00	0.60
1:C:400:THR:O	1:C:402:ARG:N	2.29	0.60
1:A:251:TRP:NE1	4:A:735:HOH:O	2.32	0.60
1:B:393:ARG:NH2	1:B:405:GLN:OE1	2.34	0.59
1:C:495:LEU:HD11	1:C:530:ILE:HG13	1.84	0.59
1:C:262:ASN:CB	4:C:820:HOH:O	2.50	0.59
1:B:437:PRO:O	1:B:439:ASN:N	2.36	0.59
1:C:441:PRO:HD2	1:C:442:PRO:HD2	1.85	0.59
1:A:382:VAL:HG21	1:A:390:ARG:HG3	1.85	0.58
1:B:408:GLU:OE1	1:B:410:ARG:HD3	2.03	0.58
1:B:338:HIS:HB2	4:B:631:HOH:O	2.03	0.58
1:A:491:HIS:ND1	4:A:704:HOH:O	2.32	0.58
1:C:258:LEU:O	1:C:275:ILE:HG22	2.03	0.58
1:C:364:ASN:HB3	4:C:799:HOH:O	2.02	0.58
1:C:370:ILE:HG13	4:C:728:HOH:O	2.02	0.58
1:C:365:THR:HB	4:C:691:HOH:O	2.02	0.58
1:B:351:LEU:HD22	1:B:534:LEU:CD1	2.33	0.58
1:B:382:VAL:HG23	4:B:706:HOH:O	2.03	0.57
1:B:475:VAL:HG13	1:B:490:THR:OG1	2.04	0.57
1:C:283:LYS:HG2	4:C:622:HOH:O	2.04	0.57
1:C:394:MET:SD	1:C:403:VAL:HG11	2.44	0.57
1:B:256:LYS:HA	1:B:256:LYS:CE	2.35	0.57
1:A:264:LYS:O	1:A:265:ASP:C	2.43	0.56
1:A:436:VAL:HA	4:A:821:HOH:O	2.05	0.56
1:A:283:LYS:NZ	4:A:619:HOH:O	2.38	0.56
1:B:351:LEU:HD22	1:B:534:LEU:HD13	1.85	0.56
1:A:464:ASN:HA	4:A:723:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HG	1:B:355:ILE:HD11	1.88	0.56
1:C:408:GLU:CG	1:C:410:ARG:HD3	2.35	0.56
1:B:494:GLU:OE2	4:B:641:HOH:O	2.17	0.56
1:B:500:PRO:O	1:B:504:ASN:HB2	2.06	0.56
1:C:362:THR:HA	1:C:365:THR:HG22	1.88	0.56
1:A:377:ASP:OD1	1:A:395:SER:HB2	2.06	0.56
1:C:361:VAL:HG12	1:C:364:ASN:H	1.69	0.56
1:C:403:VAL:HG12	1:C:403:VAL:O	2.06	0.55
1:A:261:ILE:HG22	1:A:262:ASN:H	1.70	0.55
1:C:362:THR:HA	1:C:365:THR:CG2	2.37	0.55
1:A:373:SER:HB3	4:A:670:HOH:O	2.06	0.55
1:C:362:THR:O	1:C:365:THR:HG23	2.06	0.55
1:A:448:GLN:HA	1:A:448:GLN:NE2	2.22	0.55
1:C:526:ASN:O	1:C:530:ILE:HG12	2.06	0.55
1:A:348:PHE:HE2	1:A:474:LYS:HE2	1.72	0.55
1:C:520:ILE:O	1:C:523:PHE:HB3	2.08	0.54
1:A:240:MET:HB3	4:A:728:HOH:O	2.07	0.54
1:A:437:PRO:O	1:A:439:ASN:N	2.41	0.54
1:B:255:ILE:HA	1:B:513:SER:OG	2.08	0.54
1:C:329:GLN:HA	1:C:418:TYR:O	2.08	0.54
1:A:355:ILE:HD13	1:A:472:ILE:HD11	1.89	0.53
1:B:494:GLU:OE1	4:B:745:HOH:O	2.19	0.53
1:C:394:MET:SD	1:C:403:VAL:CG1	2.97	0.53
1:C:266:LEU:HD22	4:C:721:HOH:O	2.08	0.53
1:C:274:ASN:ND2	4:C:670:HOH:O	2.40	0.53
1:C:508:ASN:ND2	1:C:511:ASN:OD1	2.40	0.53
1:A:309:LYS:HG3	1:A:341:PRO:HG3	1.90	0.53
1:A:392:LEU:HD22	1:A:436:VAL:HG22	1.90	0.53
1:B:441:PRO:N	1:B:442:PRO:HD2	2.24	0.53
1:B:344:ASP:OD2	1:B:346:SER:N	2.42	0.53
1:B:363:GLU:HG2	1:B:364:ASN:HD22	1.72	0.52
1:C:437:PRO:O	1:C:439:ASN:N	2.42	0.52
1:C:441:PRO:N	1:C:442:PRO:HD2	2.25	0.52
1:C:273:LEU:O	1:C:274:ASN:C	2.47	0.52
1:B:256:LYS:HA	1:B:256:LYS:HE2	1.92	0.52
1:A:382:VAL:HG22	1:A:390:ARG:O	2.10	0.52
1:A:497:ILE:HD12	1:A:523:PHE:HB2	1.92	0.52
1:A:522:THR:CG2	4:A:674:HOH:O	2.57	0.52
1:C:391:PHE:HD2	4:C:792:HOH:O	1.92	0.52
1:A:251:TRP:HA	1:A:251:TRP:CE3	2.45	0.52
1:A:382:VAL:CG2	1:A:390:ARG:HG3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:TRP:HA	1:C:251:TRP:CE3	2.45	0.52
1:A:305:GLU:OE2	1:A:409:LYS:NZ	2.44	0.51
1:B:399:LYS:O	1:B:400:THR:HG23	2.10	0.51
1:B:244:VAL:HG22	1:B:249:GLN:HG3	1.91	0.51
1:C:305:GLU:OE1	1:C:431:ASN:ND2	2.41	0.51
1:C:448:GLN:O	1:C:450:PRO:HD3	2.09	0.51
1:A:505:ALA:CB	1:A:515:GLU:HG2	2.40	0.51
1:B:528:THR:HA	1:B:531:ARG:NH2	2.26	0.51
1:A:421:LYS:NZ	1:B:284:SER:OG	2.41	0.51
1:A:244:VAL:HG13	1:A:294:TYR:CZ	2.45	0.51
1:C:348:PHE:CD1	1:C:491:HIS:HB3	2.46	0.51
1:C:373:SER:HB3	4:C:723:HOH:O	2.10	0.51
1:C:263:VAL:O	1:C:264:LYS:C	2.50	0.50
1:C:310:PHE:CD2	1:C:426:VAL:HG12	2.45	0.50
1:A:522:THR:HG21	1:B:269:ASP:O	2.11	0.50
1:C:367:LYS:HD2	4:C:705:HOH:O	2.10	0.50
1:A:489:THR:HG21	1:C:366:GLY:HA3	1.93	0.50
1:B:354:TYR:CD2	1:B:533:LYS:HG2	2.45	0.50
1:B:402:ARG:CA	4:B:737:HOH:O	2.58	0.50
1:B:403:VAL:HG12	1:B:403:VAL:O	2.12	0.50
1:A:441:PRO:CB	1:A:442:PRO:HD3	2.42	0.50
1:C:251:TRP:HA	1:C:251:TRP:HE3	1.77	0.49
1:A:497:ILE:HD12	1:A:523:PHE:CG	2.47	0.49
1:C:264:LYS:HD3	1:C:266:LEU:HD21	1.93	0.49
1:B:351:LEU:HG	1:B:355:ILE:CD1	2.43	0.49
1:C:309:LYS:CD	1:C:341:PRO:HG3	2.42	0.49
1:B:287:ASP:OD2	4:B:770:HOH:O	2.20	0.49
1:B:390:ARG:NH1	1:B:408:GLU:OE2	2.45	0.49
1:C:242:ARG:CD	4:C:606:HOH:O	2.58	0.49
1:A:390:ARG:HD2	1:A:408:GLU:OE1	2.13	0.49
1:B:264:LYS:O	1:B:265:ASP:C	2.50	0.49
1:C:389:PRO:N	4:C:666:HOH:O	2.46	0.49
1:C:264:LYS:O	1:C:265:ASP:C	2.51	0.49
1:A:269:ASP:OD2	1:B:367:LYS:NZ	2.45	0.49
1:A:499:THR:HB	1:A:500:PRO:HD3	1.93	0.49
1:A:503:LEU:HD23	1:A:503:LEU:HA	1.66	0.49
1:A:252:LYS:HG3	4:A:622:HOH:O	2.13	0.48
1:A:264:LYS:O	1:A:266:LEU:N	2.46	0.48
1:C:410:ARG:HA	1:C:410:ARG:HH21	1.78	0.48
1:A:349:LYS:CD	1:C:362:THR:HG22	2.41	0.48
1:A:392:LEU:HD23	1:A:408:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:SER:CB	1:B:349:LYS:HE3	2.42	0.48
1:C:460:SER:HA	4:C:803:HOH:O	2.14	0.48
1:C:311:GLY:O	1:C:425:ASP:N	2.43	0.48
1:C:356:ARG:O	1:C:356:ARG:HG3	2.14	0.48
1:B:264:LYS:O	1:B:266:LEU:N	2.47	0.48
1:B:251:TRP:HA	1:B:251:TRP:CE3	2.48	0.48
1:B:457:ASP:OD1	4:B:626:HOH:O	2.20	0.47
1:C:455:THR:O	1:C:475:VAL:HA	2.14	0.47
1:A:290:TYR:CD2	1:A:290:TYR:C	2.86	0.47
1:A:305:GLU:CD	1:A:409:LYS:HZ1	2.16	0.47
1:C:239:HIS:O	1:C:301:ARG:NH1	2.36	0.47
1:A:437:PRO:O	1:A:438:ASP:C	2.52	0.47
1:C:316:ALA:HB3	4:C:743:HOH:O	2.14	0.47
1:A:309:LYS:HD3	1:A:341:PRO:HG2	1.96	0.47
1:C:361:VAL:HG12	1:C:364:ASN:N	2.30	0.47
1:B:320:ASP:N	4:B:666:HOH:O	2.09	0.47
1:B:348:PHE:CZ	1:B:472:ILE:CG2	2.97	0.47
1:B:346:SER:HB3	1:B:349:LYS:CE	2.43	0.47
1:B:448:GLN:O	1:B:450:PRO:HD3	2.15	0.47
1:C:390:ARG:NH1	1:C:408:GLU:OE2	2.43	0.47
1:A:448:GLN:O	1:A:450:PRO:HD3	2.15	0.47
1:A:348:PHE:CE2	1:A:474:LYS:HE2	2.49	0.46
1:C:499:THR:N	1:C:500:PRO:HD2	2.30	0.46
1:C:475:VAL:HG13	1:C:492:GLU:OE1	2.15	0.46
1:C:374:GLN:O	1:C:397:ASP:HB2	2.15	0.46
1:C:402:ARG:NE	4:C:690:HOH:O	2.43	0.46
1:A:382:VAL:HG11	1:A:392:LEU:HD11	1.98	0.46
1:B:492:GLU:OE2	4:B:729:HOH:O	2.21	0.46
1:B:352:SER:OG	1:B:472:ILE:HG21	2.15	0.46
1:B:373:SER:OG	4:B:657:HOH:O	2.21	0.46
1:C:256:LYS:NZ	4:C:788:HOH:O	2.42	0.46
1:C:502:LEU:CA	1:C:519:LEU:HD21	2.37	0.46
1:A:441:PRO:CB	1:A:442:PRO:CD	2.94	0.45
1:C:244:VAL:HG13	1:C:294:TYR:CZ	2.51	0.45
1:B:394:MET:HB2	1:B:394:MET:HE2	1.76	0.45
1:C:406:PHE:HB3	4:C:789:HOH:O	2.15	0.45
1:C:454:ARG:CZ	1:C:475:VAL:HG21	2.47	0.45
1:B:252:LYS:NZ	4:B:697:HOH:O	2.26	0.45
1:C:530:ILE:HD13	4:C:781:HOH:O	2.15	0.45
1:A:243:ASN:HD22	1:A:243:ASN:N	2.14	0.45
1:A:333:THR:HG22	4:A:696:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:SER:N	1:C:394:MET:O	2.38	0.45
1:A:436:VAL:HG13	1:A:437:PRO:HD2	1.98	0.45
1:A:456:LYS:NZ	1:A:458:ARG:NH2	2.65	0.45
1:A:502:LEU:HA	1:A:519:LEU:CD2	2.46	0.45
1:B:474:LYS:HB2	1:B:474:LYS:HE3	1.54	0.45
1:B:400:THR:O	1:B:402:ARG:N	2.47	0.45
1:A:365:THR:O	4:A:782:HOH:O	2.21	0.44
1:B:475:VAL:CG1	1:B:490:THR:OG1	2.65	0.44
1:C:309:LYS:HD3	1:C:341:PRO:HG3	1.99	0.44
1:B:251:TRP:HA	1:B:251:TRP:HE3	1.82	0.44
1:B:310:PHE:HE2	1:B:531:ARG:HB2	1.82	0.44
1:B:263:VAL:O	1:B:264:LYS:C	2.54	0.44
1:C:317:LYS:NZ	1:C:317:LYS:HB3	2.32	0.44
1:C:393:ARG:NH2	3:C:603:SO4:O4	2.48	0.44
1:A:381:ARG:HH11	1:A:381:ARG:HD3	1.64	0.44
1:A:438:ASP:O	1:A:440:ASP:N	2.50	0.44
1:C:383:GLY:O	1:C:389:PRO:HG3	2.18	0.44
1:A:288:TRP:CD2	1:A:415:LEU:HG	2.52	0.44
1:A:403:VAL:HG21	1:A:446:LYS:HE3	2.00	0.44
1:C:244:VAL:O	1:C:295:SER:HA	2.18	0.44
1:A:330:CYS:HB3	1:B:330:CYS:HB3	2.00	0.44
1:C:518:SER:O	1:C:522:THR:CG2	2.64	0.44
1:C:256:LYS:NZ	1:C:256:LYS:HA	2.33	0.43
1:C:367:LYS:HE2	1:C:465:ASP:OD1	2.18	0.43
1:C:504:ASN:ND2	4:C:764:HOH:O	2.51	0.43
1:A:243:ASN:HD22	1:A:243:ASN:H	1.67	0.43
1:C:394:MET:CG	1:C:403:VAL:HG13	2.48	0.43
1:A:342:ASN:ND2	1:A:491:HIS:H	2.16	0.43
1:A:355:ILE:HD13	1:A:472:ILE:CD1	2.47	0.43
1:B:438:ASP:O	1:B:440:ASP:N	2.51	0.43
1:B:522:THR:HG22	4:B:769:HOH:O	2.18	0.43
1:A:441:PRO:CD	1:A:442:PRO:HD2	2.49	0.43
1:B:253:PRO:HG2	4:B:649:HOH:O	2.17	0.43
1:C:266:LEU:HB2	4:C:819:HOH:O	2.18	0.43
1:A:411:HIS:HA	1:A:431:ASN:OD1	2.18	0.43
1:B:252:LYS:HG2	4:B:649:HOH:O	2.19	0.43
1:B:403:VAL:O	1:B:403:VAL:CG1	2.66	0.43
1:C:514:LYS:O	1:C:515:GLU:C	2.56	0.43
1:A:518:SER:O	1:A:522:THR:HG23	2.19	0.43
1:A:351:LEU:HD11	1:A:355:ILE:HD11	2.01	0.43
1:A:390:ARG:HB3	1:A:408:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:HIS:HA	1:B:294:TYR:CE1	2.54	0.43
1:B:402:ARG:HG2	4:B:737:HOH:O	2.19	0.43
1:C:344:ASP:HB3	1:C:347:LEU:HD12	1.99	0.43
1:C:342:ASN:HA	1:C:491:HIS:O	2.19	0.43
1:B:283:LYS:NZ	4:B:740:HOH:O	2.51	0.42
1:B:440:ASP:HA	1:B:441:PRO:HD3	1.87	0.42
1:B:458:ARG:HG2	4:B:728:HOH:O	2.18	0.42
1:C:354:TYR:O	1:C:358:ILE:HG12	2.19	0.42
1:A:530:ILE:HA	1:A:530:ILE:HD13	1.73	0.42
1:A:522:THR:CG2	1:B:268:ILE:HD13	2.49	0.42
1:C:239:HIS:HA	1:C:294:TYR:CE1	2.54	0.42
1:C:382:VAL:CG2	1:C:383:GLY:N	2.82	0.42
1:B:253:PRO:HD2	4:B:649:HOH:O	2.19	0.42
1:C:265:ASP:OD1	1:C:265:ASP:N	2.52	0.42
1:C:333:THR:HG22	4:C:638:HOH:O	2.20	0.42
1:A:358:ILE:O	1:A:364:ASN:OD1	2.36	0.42
1:B:380:TYR:CE2	1:B:450:PRO:HG3	2.54	0.42
1:A:333:THR:HG21	1:B:327:SER:OG	2.20	0.42
1:C:243:ASN:HA	1:C:294:TYR:O	2.19	0.42
1:C:398:ILE:N	4:C:618:HOH:O	2.52	0.42
1:A:441:PRO:HB2	1:A:442:PRO:CD	2.50	0.42
1:B:305:GLU:OE2	4:B:713:HOH:O	2.21	0.42
1:B:515:GLU:OE1	4:B:712:HOH:O	2.22	0.42
1:B:399:LYS:HB3	4:B:727:HOH:O	2.19	0.42
1:C:438:ASP:O	1:C:440:ASP:N	2.53	0.42
1:A:323:ASN:N	1:A:324:PRO:CD	2.83	0.41
1:B:245:PRO:HD3	4:B:633:HOH:O	2.19	0.41
1:B:301:ARG:O	1:B:503:LEU:HD11	2.20	0.41
1:C:376:ARG:HB2	1:C:398:ILE:HD11	2.01	0.41
1:C:382:VAL:HG22	1:C:390:ARG:O	2.20	0.41
1:C:259:GLN:O	1:C:261:ILE:HG13	2.20	0.41
1:B:261:ILE:HG22	1:B:262:ASN:H	1.85	0.41
1:C:414:GLN:NE2	4:C:800:HOH:O	2.32	0.41
1:C:456:LYS:HE3	3:C:603:SO4:O1	2.21	0.41
1:A:361:VAL:HG12	1:A:363:GLU:HB3	2.02	0.41
1:A:315:ASP:HA	1:A:337:ALA:HA	2.02	0.41
1:A:322:VAL:HG11	4:A:792:HOH:O	2.20	0.41
1:A:427:LYS:HG2	4:A:774:HOH:O	2.21	0.41
1:A:441:PRO:N	1:A:442:PRO:HD2	2.35	0.41
1:A:455:THR:O	1:A:475:VAL:HA	2.20	0.41
1:C:310:PHE:CE2	1:C:426:VAL:CG1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:PHE:CE1	1:A:472:ILE:HG23	2.55	0.41
1:B:503:LEU:HD23	1:B:503:LEU:HA	1.63	0.41
1:A:411:HIS:ND1	1:A:431:ASN:OD1	2.52	0.41
1:A:416:LEU:H	1:A:416:LEU:HG	1.73	0.41
1:A:505:ALA:HB2	1:A:515:GLU:HG2	2.03	0.41
1:B:250:LYS:HD2	4:B:714:HOH:O	2.21	0.41
1:B:261:ILE:H	1:B:261:ILE:HG13	1.60	0.41
1:B:374:GLN:O	1:B:397:ASP:HB2	2.21	0.41
1:C:261:ILE:HG13	1:C:261:ILE:H	1.72	0.41
1:C:308:MET:SD	1:C:527:GLY:HA3	2.60	0.41
1:C:466:SER:O	1:C:467:CYS:C	2.59	0.41
1:C:509:ILE:CG2	1:C:510:THR:N	2.83	0.41
1:A:239:HIS:HA	1:A:294:TYR:CE1	2.56	0.41
1:A:312:VAL:HG12	1:A:314:ILE:HD11	2.03	0.41
1:A:394:MET:HE2	1:A:394:MET:HB2	1.72	0.41
1:B:308:MET:O	1:B:494:GLU:HA	2.21	0.41
1:B:430:LEU:HD23	1:B:430:LEU:C	2.42	0.41
1:C:353:LYS:O	1:C:354:TYR:C	2.58	0.41
1:C:380:TYR:CE2	1:C:450:PRO:HG3	2.56	0.41
1:B:244:VAL:O	1:B:295:SER:HA	2.21	0.40
1:B:254:THR:HG21	4:B:826:HOH:O	2.21	0.40
1:B:252:LYS:HB2	1:B:252:LYS:HE3	1.89	0.40
1:B:342:ASN:ND2	1:B:490:THR:HA	2.36	0.40
1:B:255:ILE:HG22	1:B:517:ALA:HB2	2.03	0.40
1:B:317:LYS:NZ	4:B:804:HOH:O	2.40	0.40
1:A:368:PHE:CD2	1:A:461:TYR:HB3	2.56	0.40
1:B:487:SER:HA	4:B:760:HOH:O	2.21	0.40
1:B:494:GLU:CD	4:B:641:HOH:O	2.58	0.40
1:B:418:TYR:CZ	1:B:420:PRO:HB3	2.56	0.40
1:B:419:SER:HB2	1:B:425:ASP:HA	2.02	0.40
1:C:441:PRO:HB2	1:C:442:PRO:CD	2.52	0.40

All (4) 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)
4:A:730:HOH:O	4:B:656:HOH:O[2_556]	2.06	0.14
4:A:682:HOH:O	4:C:773:HOH:O[4_557]	2.12	0.08
4:B:684:HOH:O	4:B:747:HOH:O[2_556]	2.17	0.03
4:B:678:HOH:O	4:B:747:HOH:O[2_556]	2.18	0.02

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	282/311 (91%)	253 (90%)	19 (7%)	10 (4%)	3 1
1	B	282/311 (91%)	247 (88%)	27 (10%)	8 (3%)	5 1
1	C	282/311 (91%)	252 (89%)	21 (7%)	9 (3%)	4 1
All	All	846/933 (91%)	752 (89%)	67 (8%)	27 (3%)	4 1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	LYS
1	A	401	GLY
1	A	404	GLY
1	A	438	ASP
1	B	400	THR
1	B	401	GLY
1	B	404	GLY
1	B	438	ASP
1	B	439	ASN
1	C	400	THR
1	C	401	GLY
1	C	404	GLY
1	C	438	ASP
1	A	439	ASN
1	B	264	LYS
1	B	265	ASP
1	C	265	ASP
1	C	439	ASN
1	A	262	ASN
1	A	265	ASP
1	B	262	ASN
1	C	411	HIS
1	C	264	LYS
1	A	342	ASN

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Mol	Chain	Res	Type
1	A	446	LYS
1	C	261	ILE
1	A	261	ILE

5.3.2 Protein sidechains (i)

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	265/291 (91%)	229 (86%)	36 (14%)	3 2
1	B	265/291 (91%)	236 (89%)	29 (11%)	6 3
1	C	265/291 (91%)	220 (83%)	45 (17%)	2 1
All	All	795/873 (91%)	685 (86%)	110 (14%)	3 2

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	A	244	VAL
1	A	251	TRP
1	A	252	LYS
1	A	256	LYS
1	A	260	SER
1	A	261	ILE
1	A	264	LYS
1	A	265	ASP
1	A	280	ASP
1	A	309	LYS
1	A	342	ASN
1	A	343	ILE
1	A	346	SER
1	A	352	SER
1	A	362	THR
1	A	364	ASN
1	A	365	THR
1	A	373	SER

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Mol	Chain	Res	Type
1	A	374	GLN
1	A	378	SER
1	A	390	ARG
1	A	402	ARG
1	A	417	LEU
1	A	447	SER
1	A	448	GLN
1	A	449	SER
1	A	475	VAL
1	A	488	GLU
1	A	504	ASN
1	A	509	ILE
1	A	511	ASN
1	A	513	SER
1	A	522	THR
1	A	531	ARG
1	A	534	LEU
1	B	251	TRP
1	B	256	LYS
1	B	260	SER
1	B	261	ILE
1	B	266	LEU
1	B	280	ASP
1	B	309	LYS
1	B	324	PRO
1	B	342	ASN
1	B	346	SER
1	B	349	LYS
1	B	374	GLN
1	B	378	SER
1	B	382	VAL
1	B	395	SER
1	B	399	LYS
1	B	400	THR
1	B	415	LEU
1	B	417	LEU
1	B	448	GLN
1	B	452	SER
1	B	456	LYS
1	B	464	ASN
1	B	476	GLU
1	B	489	THR

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Mol	Chain	Res	Type
1	B	495	LEU
1	B	513	SER
1	B	522	THR
1	B	534	LEU
1	C	242	ARG
1	C	243	ASN
1	C	244	VAL
1	C	251	TRP
1	C	256	LYS
1	C	260	SER
1	C	261	ILE
1	C	264	LYS
1	C	265	ASP
1	C	270	PRO
1	C	271	SER
1	C	275	ILE
1	C	279	ASP
1	C	312	VAL
1	C	317	LYS
1	C	319	PRO
1	C	342	ASN
1	C	349	LYS
1	C	361	VAL
1	C	363	GLU
1	C	365	THR
1	C	369	SER
1	C	373	SER
1	C	374	GLN
1	C	375	THR
1	C	378	SER
1	C	398	ILE
1	C	400	THR
1	C	402	ARG
1	C	410	ARG
1	C	448	GLN
1	C	452	SER
1	C	456	LYS
1	C	464	ASN
1	C	474	LYS
1	C	475	VAL
1	C	476	GLU
1	C	477	ASN

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Mol	Chain	Res	Type
1	C	489	THR
1	C	504	ASN
1	C	509	ILE
1	C	511	ASN
1	C	513	SER
1	C	522	THR
1	C	534	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	A	342	ASN
1	A	364	ASN
1	A	448	GLN
1	A	508	ASN
1	B	323	ASN
1	B	342	ASN
1	B	448	GLN
1	B	477	ASN
1	B	508	ASN
1	C	274	ASN
1	C	338	HIS
1	C	342	ASN
1	C	364	ASN
1	C	448	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	601	-	4,4,4	0.77	0	6,6,6	2.67	2 (33%)
3	SO4	B	602	-	4,4,4	0.80	0	6,6,6	2.05	3 (50%)
3	SO4	C	603	-	4,4,4	0.79	0	6,6,6	1.52	1 (16%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	SO4	O4-S-O1	5.41	137.56	109.31
3	C	603	SO4	O3-S-O1	3.21	126.08	109.31
3	B	602	SO4	O4-S-O1	3.14	125.70	109.31
3	A	601	SO4	O4-S-O3	-2.92	96.61	109.06
3	B	602	SO4	O4-S-O3	-2.59	97.99	109.06
3	B	602	SO4	O3-S-O1	2.06	120.05	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.