



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:57 AM UTC

PDB ID : 1D8I / pdb_00001d8i
Title : X-RAY CRYSTAL STRUCTURE OF YEAST RNA TRIPHOSPHATASE IN COMPLEX WITH A SULFATE ION.
Authors : Lima, C.D.; Wang, L.K.; Shuman, S.
Deposited on : 1999-10-24
Resolution : 2.05 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)	:	2.49

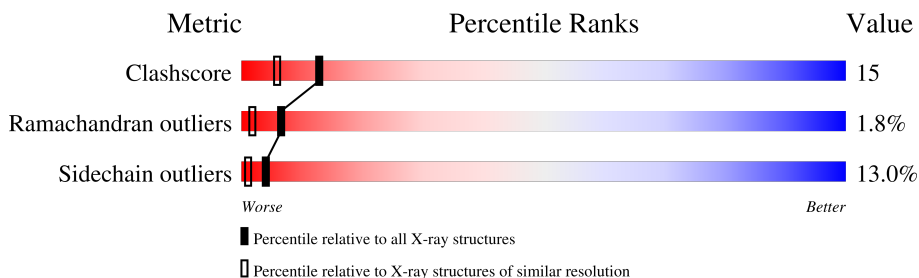
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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	311	
1	B	311	
1	C	311	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7329 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.

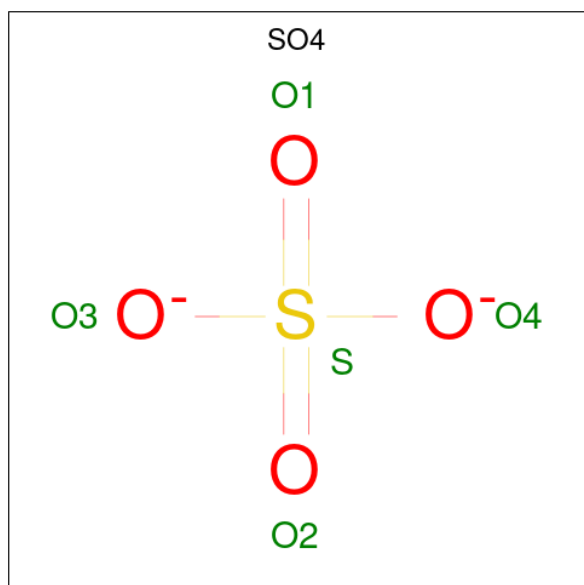
- Molecule 1 is a protein called MRNA TRIPHOSPHATASE CET1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2295	1457	393	440	5			
1	B	288	Total	C	N	O	S	0	0	0
			2295	1457	393	440	5			
1	C	288	Total	C	N	O	S	0	0	0
			2295	1457	393	440	5			

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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

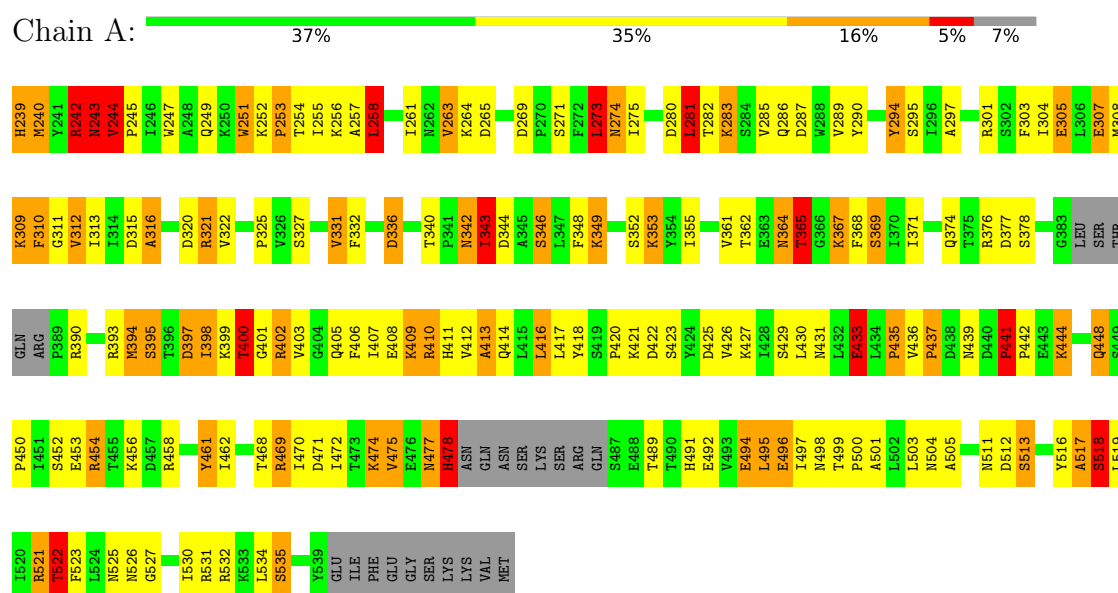
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	121	Total O 121 121	0	0
3	B	134	Total O 134 134	0	0
3	C	159	Total O 159 159	0	0

3 Residue-property plots

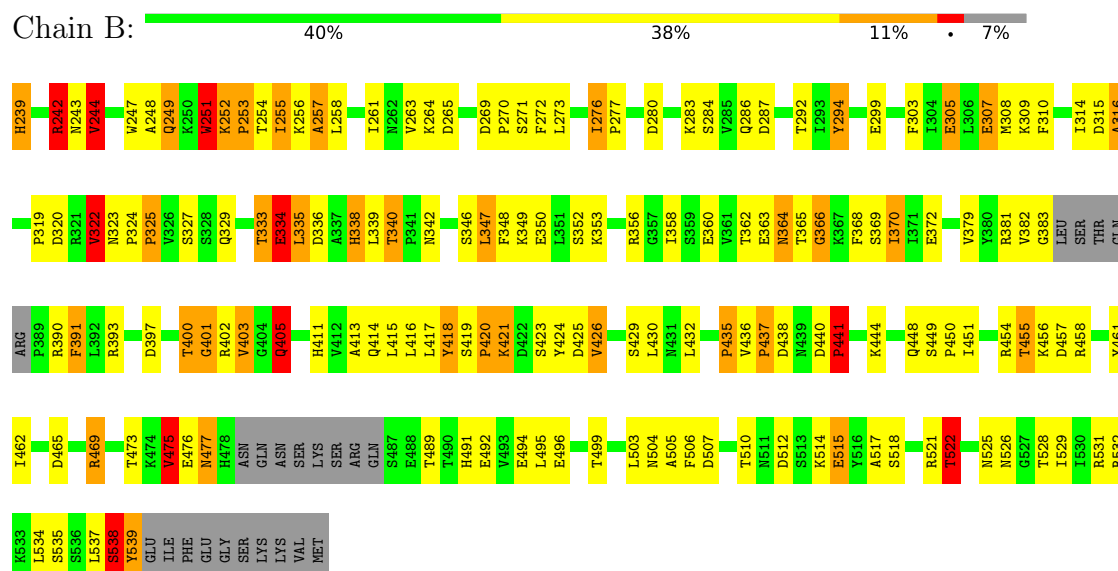
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

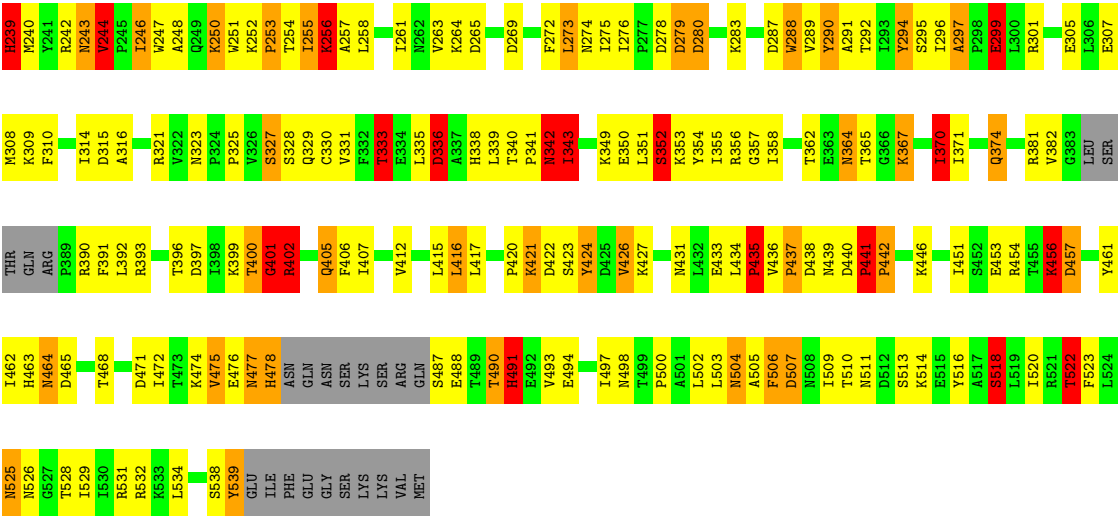
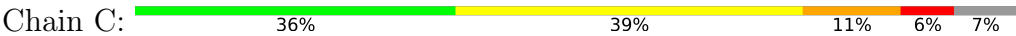
• Molecule 1: MRNA TRIPHOSPHATASE CET1



• Molecule 1: MRNA TRIPHOSPHATASE CET1



● Molecule 1: MRNA TRIPHOSPHATASE CET1



4 Data and refinement statistics

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	121.36Å 116.09Å 82.31Å 90.00° 110.25° 90.00°	Depositor
Resolution (Å)	25.00 – 2.05	Depositor
% Data completeness (in resolution range)	82.2 (25.00-2.05)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7329	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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: 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	1.34	9/2342 (0.4%)	2.59	178/3178 (5.6%)
1	B	1.25	8/2342 (0.3%)	2.35	126/3178 (4.0%)
1	C	1.30	15/2342 (0.6%)	2.56	172/3178 (5.4%)
All	All	1.30	32/7026 (0.5%)	2.50	476/9534 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	B	0	15
1	C	0	19
All	All	0	52

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	PHE	N-CA	-16.86	1.25	1.46
1	A	331	VAL	CA-C	-8.70	1.43	1.52
1	C	247	TRP	NE1-CE2	-7.90	1.28	1.37
1	B	333	THR	C-N	-7.87	1.23	1.33
1	C	325	PRO	N-CA	-7.09	1.42	1.47
1	A	311	GLY	N-CA	7.00	1.53	1.45
1	C	331	VAL	C-O	6.97	1.32	1.24
1	B	324	PRO	CA-C	6.84	1.58	1.52
1	A	331	VAL	C-N	6.74	1.42	1.33
1	C	244	VAL	CA-CB	-6.42	1.49	1.54
1	C	327	SER	N-CA	-6.34	1.39	1.46
1	A	282	THR	CA-CB	6.25	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	419	SER	C-N	-6.12	1.27	1.34
1	C	325	PRO	CA-CB	6.05	1.57	1.53
1	B	276	ILE	CA-CB	-6.04	1.49	1.54
1	B	247	TRP	NE1-CE2	-5.82	1.31	1.37
1	B	325	PRO	C-N	-5.65	1.26	1.33
1	C	327	SER	C-N	-5.61	1.26	1.33
1	B	366	GLY	N-CA	5.48	1.52	1.45
1	C	328	SER	C-O	5.45	1.30	1.23
1	A	525	ASN	C-O	-5.42	1.17	1.24
1	C	292	THR	N-CA	-5.41	1.40	1.46
1	C	297	ALA	N-CA	5.41	1.52	1.45
1	B	324	PRO	N-CD	5.40	1.55	1.47
1	A	531	ARG	C-N	-5.34	1.27	1.33
1	C	500	PRO	CA-C	-5.32	1.44	1.52
1	A	462	ILE	N-CA	-5.21	1.39	1.46
1	A	332	PHE	CA-C	5.10	1.58	1.52
1	C	502	LEU	CB-CG	5.10	1.63	1.53
1	C	416	LEU	C-O	5.08	1.30	1.24
1	C	532	ARG	CD-NE	5.04	1.53	1.46
1	C	330	CYS	N-CA	-5.03	1.39	1.45

All (476) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	439	ASN	CA-CB-CG	34.04	146.64	112.60
1	A	477	ASN	CA-CB-CG	18.28	130.88	112.60
1	A	331	VAL	O-C-N	-17.39	103.71	122.67
1	C	526	ASN	OD1-CG-ND2	-16.43	106.17	122.60
1	A	471	ASP	CA-CB-CG	15.27	127.87	112.60
1	A	512	ASP	CA-CB-CG	13.46	126.06	112.60
1	A	342	ASN	OD1-CG-ND2	-12.97	109.63	122.60
1	C	288	TRP	CG-CD2-CE3	-12.72	121.17	133.90
1	B	414	GLN	OE1-CD-NE2	-12.54	110.06	122.60
1	B	531	ARG	NE-CZ-NH2	11.75	129.78	119.20
1	B	457	ASP	CA-CB-CG	11.74	124.34	112.60
1	A	321	ARG	NE-CZ-NH1	-11.60	109.90	121.50
1	A	364	ASN	CA-CB-CG	11.48	124.08	112.60
1	A	331	VAL	CA-C-N	11.27	138.83	123.05
1	A	331	VAL	C-N-CA	11.27	138.83	123.05
1	A	517	ALA	CA-C-O	-11.00	108.76	120.42
1	A	321	ARG	NE-CZ-NH2	11.00	129.10	119.20
1	C	327	SER	CA-C-O	-10.94	108.13	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	ARG	NE-CZ-NH2	10.33	128.50	119.20
1	C	422	ASP	CA-CB-CG	-10.32	102.28	112.60
1	C	528	THR	CA-CB-OG1	-10.25	94.23	109.60
1	C	526	ASN	CB-CG-ND2	10.17	131.65	116.40
1	B	521	ARG	NE-CZ-NH1	-10.15	111.35	121.50
1	A	411	HIS	CA-CB-CG	-10.14	103.66	113.80
1	A	454	ARG	CD-NE-CZ	10.14	138.59	124.40
1	B	242	ARG	CD-NE-CZ	10.04	138.46	124.40
1	C	477	ASN	CA-CB-CG	10.04	122.64	112.60
1	A	247	TRP	CZ3-CH2-CZ2	9.95	134.44	121.50
1	C	244	VAL	CA-CB-CG2	9.92	127.27	110.40
1	C	283	LYS	CA-C-O	-9.72	110.25	120.55
1	C	288	TRP	CE2-CD2-CE3	9.70	128.50	118.80
1	B	521	ARG	NH1-CZ-NH2	9.69	131.90	119.30
1	A	331	VAL	CB-CA-C	9.62	125.67	111.33
1	A	247	TRP	CH2-CZ2-CE2	-9.50	105.15	117.50
1	A	458	ARG	NE-CZ-NH1	-9.48	112.02	121.50
1	B	364	ASN	OD1-CG-ND2	9.46	132.06	122.60
1	B	477	ASN	OD1-CG-ND2	-9.44	113.16	122.60
1	B	477	ASN	CA-CB-CG	9.41	122.01	112.60
1	A	397	ASP	CA-CB-CG	9.34	121.94	112.60
1	B	323	ASN	OD1-CG-ND2	-9.28	113.32	122.60
1	A	305	GLU	CA-CB-CG	9.19	132.48	114.10
1	A	376	ARG	CD-NE-CZ	9.19	137.26	124.40
1	B	314	ILE	CB-CG1-CD1	9.17	133.06	113.80
1	C	525	ASN	CA-C-O	9.05	130.59	120.90
1	C	457	ASP	CA-CB-CG	8.97	121.58	112.60
1	C	364	ASN	N-CA-CB	8.90	124.44	111.54
1	C	491	HIS	CA-C-O	-8.74	111.45	120.54
1	C	498	ASN	OD1-CG-ND2	8.74	131.34	122.60
1	B	401	GLY	CA-C-N	8.62	133.82	121.50
1	B	401	GLY	C-N-CA	8.62	133.82	121.50
1	A	423	SER	CA-C-O	8.57	129.38	119.18
1	A	320	ASP	CA-CB-CG	-8.56	104.04	112.60
1	A	287	ASP	CA-CB-CG	-8.55	104.05	112.60
1	A	531	ARG	CA-C-N	8.52	131.52	120.44
1	A	531	ARG	C-N-CA	8.52	131.52	120.44
1	A	285	VAL	CA-CB-CG2	-8.51	95.93	110.40
1	C	497	ILE	CB-CG1-CD1	-8.48	95.99	113.80
1	C	246	ILE	N-CA-CB	-8.48	99.87	110.47
1	A	494	GLU	CB-CG-CD	8.46	126.97	112.60
1	C	274	ASN	CA-CB-CG	-8.41	104.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	ALA	CA-C-O	-8.37	111.94	120.90
1	B	465	ASP	CA-CB-CG	-8.34	104.26	112.60
1	C	269	ASP	CA-CB-CG	8.32	120.92	112.60
1	C	504	ASN	OD1-CG-ND2	8.27	130.87	122.60
1	B	477	ASN	CB-CG-ND2	8.22	128.73	116.40
1	C	477	ASN	OD1-CG-ND2	-8.21	114.39	122.60
1	A	492	GLU	CA-C-O	8.17	129.53	120.70
1	A	368	PHE	CA-CB-CG	8.15	121.95	113.80
1	C	525	ASN	O-C-N	-8.14	113.62	122.09
1	A	522	THR	CA-CB-OG1	8.12	121.79	109.60
1	A	426	VAL	N-CA-CB	8.10	124.73	111.44
1	C	374	GLN	N-CA-CB	8.09	123.27	110.65
1	A	521	ARG	CD-NE-CZ	-8.05	113.13	124.40
1	B	539	TYR	CB-CA-C	8.02	125.33	110.10
1	A	423	SER	O-C-N	-8.01	111.04	122.41
1	B	272	PHE	CA-CB-CG	7.99	121.79	113.80
1	B	286	GLN	CA-C-N	7.97	131.75	120.28
1	B	286	GLN	C-N-CA	7.97	131.75	120.28
1	A	531	ARG	NE-CZ-NH1	-7.95	113.55	121.50
1	B	333	THR	CA-CB-OG1	-7.95	97.68	109.60
1	C	343	ILE	CA-CB-CG2	7.93	123.98	110.50
1	B	327	SER	CA-C-O	-7.93	110.59	119.78
1	C	358	ILE	O-C-N	-7.92	114.19	121.87
1	B	425	ASP	CA-C-O	7.91	131.39	121.82
1	C	523	PHE	CA-CB-CG	7.84	121.64	113.80
1	A	532	ARG	N-CA-CB	7.79	121.31	110.01
1	C	401	GLY	CA-C-N	7.79	133.17	122.19
1	C	401	GLY	C-N-CA	7.79	133.17	122.19
1	C	253	PRO	CA-C-O	-7.76	112.49	121.34
1	A	474	LYS	O-C-N	-7.76	113.82	123.05
1	B	458	ARG	NE-CZ-NH1	-7.74	113.76	121.50
1	A	504	ASN	CA-CB-CG	-7.69	104.91	112.60
1	C	299	GLU	O-C-N	-7.69	113.44	122.20
1	A	433	GLU	O-C-N	-7.66	114.52	122.64
1	C	441	PRO	CB-CA-C	7.65	120.25	110.92
1	C	342	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	B	492	GLU	O-C-N	-7.63	114.29	123.29
1	C	283	LYS	N-CA-CB	7.58	121.26	110.12
1	C	336	ASP	O-C-N	-7.56	112.53	122.59
1	C	478	HIS	CA-CB-CG	7.55	121.35	113.80
1	C	336	ASP	CA-CB-CG	7.55	120.15	112.60
1	B	310	PHE	CA-CB-CG	-7.55	106.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	ARG	CD-NE-CZ	-7.53	113.86	124.40
1	A	532	ARG	CA-C-O	-7.50	112.95	120.82
1	A	349	LYS	CA-C-O	-7.49	112.48	120.42
1	A	412	VAL	N-CA-C	-7.45	105.40	111.81
1	C	494	GLU	CB-CG-CD	7.44	125.25	112.60
1	A	414	GLN	CA-C-N	-7.43	112.16	122.93
1	A	414	GLN	C-N-CA	-7.43	112.16	122.93
1	A	532	ARG	O-C-N	7.42	129.72	122.07
1	C	381	ARG	CA-C-O	-7.41	112.36	120.43
1	C	463	HIS	CA-CB-CG	-7.40	106.40	113.80
1	C	342	ASN	CB-CG-ND2	7.39	127.49	116.40
1	B	528	THR	CA-CB-OG1	-7.39	98.51	109.60
1	C	364	ASN	CA-C-O	7.39	129.25	120.53
1	A	518	SER	CA-CB-OG	-7.38	96.35	111.10
1	C	343	ILE	N-CA-CB	-7.36	100.11	112.47
1	A	426	VAL	CA-C-N	-7.35	112.85	123.00
1	A	426	VAL	C-N-CA	-7.35	112.85	123.00
1	A	393	ARG	CA-C-N	-7.34	111.92	122.94
1	A	393	ARG	C-N-CA	-7.34	111.92	122.94
1	A	369	SER	CB-CA-C	7.27	123.75	109.35
1	C	272	PHE	CA-CB-CG	7.26	121.06	113.80
1	A	369	SER	CA-CB-OG	7.26	125.61	111.10
1	C	397	ASP	CA-C-O	-7.22	112.69	120.92
1	A	521	ARG	N-CA-CB	7.18	120.64	109.94
1	B	514	LYS	CA-C-O	-7.14	112.98	120.55
1	A	327	SER	CB-CA-C	-7.12	94.97	110.41
1	A	274	ASN	CA-CB-CG	-7.11	105.49	112.60
1	C	427	LYS	CA-C-O	7.09	128.01	120.36
1	C	349	LYS	CD-CE-NZ	7.08	134.57	111.90
1	A	365	THR	CB-CA-C	7.06	124.75	109.99
1	B	334	GLU	O-C-N	-7.03	115.04	123.27
1	A	496	GLU	CA-CB-CG	6.99	128.09	114.10
1	B	316	ALA	CA-C-N	-6.98	112.59	123.13
1	B	316	ALA	C-N-CA	-6.98	112.59	123.13
1	A	281	LEU	CA-C-O	-6.98	111.94	119.97
1	C	476	GLU	CA-C-O	-6.98	112.99	120.46
1	A	310	PHE	CA-CB-CG	-6.92	106.88	113.80
1	A	301	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	C	289	VAL	N-CA-C	-6.89	103.80	110.42
1	C	297	ALA	O-C-N	-6.89	115.73	121.38
1	B	531	ARG	NE-CZ-NH1	-6.88	114.62	121.50
1	C	493	VAL	CA-C-O	-6.88	113.24	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ASP	CB-CA-C	6.86	121.11	109.53
1	C	283	LYS	CB-CA-C	-6.82	99.47	110.79
1	A	343	ILE	N-CA-CB	-6.81	99.18	111.92
1	B	418	TYR	CA-C-N	-6.81	113.65	122.98
1	B	418	TYR	C-N-CA	-6.81	113.65	122.98
1	C	370	ILE	CA-C-O	-6.80	113.26	120.53
1	C	329	GLN	CG-CD-OE1	-6.79	107.21	120.80
1	C	341	PRO	CA-C-O	-6.79	114.14	121.27
1	A	271	SER	CA-C-O	-6.78	114.19	121.38
1	C	475	VAL	CA-C-O	6.76	128.58	120.67
1	A	512	ASP	CA-C-N	6.72	130.19	120.38
1	A	512	ASP	C-N-CA	6.72	130.19	120.38
1	B	323	ASN	CB-CG-ND2	6.70	126.45	116.40
1	A	414	GLN	OE1-CD-NE2	6.69	129.29	122.60
1	C	353	LYS	CA-C-O	6.69	127.52	120.42
1	C	292	THR	O-C-N	-6.68	115.19	122.07
1	A	395	SER	N-CA-CB	-6.67	100.09	110.57
1	A	410	ARG	CA-C-N	6.67	130.85	121.24
1	A	410	ARG	C-N-CA	6.67	130.85	121.24
1	A	527	GLY	CA-C-O	6.67	128.21	121.00
1	C	522	THR	CA-CB-OG1	6.66	119.59	109.60
1	A	376	ARG	CA-C-O	-6.64	113.20	120.30
1	C	518	SER	CA-CB-OG	-6.60	97.90	111.10
1	C	464	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	B	458	ARG	NH1-CZ-NH2	6.58	127.85	119.30
1	B	333	THR	CA-CB-CG2	6.57	121.66	110.50
1	B	532	ARG	NE-CZ-NH1	-6.55	114.95	121.50
1	B	435	PRO	O-C-N	-6.54	115.77	123.10
1	A	325	PRO	O-C-N	-6.54	114.07	122.44
1	C	288	TRP	CD2-CE3-CZ3	-6.54	110.10	118.60
1	A	398	ILE	CB-CA-C	-6.53	101.68	112.26
1	B	458	ARG	N-CA-CB	-6.53	99.49	111.37
1	B	248	ALA	CA-C-O	-6.52	111.72	119.35
1	C	239	HIS	N-CA-CB	6.52	121.59	110.50
1	C	465	ASP	CA-CB-CG	6.52	119.12	112.60
1	C	310	PHE	CB-CG-CD2	6.51	131.77	120.70
1	A	368	PHE	CA-C-O	-6.50	113.81	121.16
1	B	340	THR	CB-CA-C	-6.50	102.44	109.85
1	A	444	LYS	CA-C-O	-6.50	114.01	120.70
1	C	295	SER	CA-C-O	-6.49	111.26	119.31
1	B	284	SER	CA-CB-OG	-6.49	98.13	111.10
1	C	532	ARG	NE-CZ-NH2	-6.47	113.38	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	435	PRO	O-C-N	-6.47	115.86	123.10
1	C	244	VAL	CB-CA-C	6.45	116.39	110.13
1	A	461	TYR	CA-C-N	6.44	131.14	122.90
1	A	461	TYR	C-N-CA	6.44	131.14	122.90
1	C	407	ILE	O-C-N	6.44	130.18	123.04
1	C	321	ARG	CA-C-O	-6.40	114.16	121.07
1	A	311	GLY	CA-C-O	-6.40	115.98	121.04
1	A	365	THR	CA-C-O	-6.39	111.38	119.31
1	B	368	PHE	CA-C-O	6.39	128.38	121.16
1	A	513	SER	CA-CB-OG	-6.39	98.33	111.10
1	A	303	PHE	CA-C-O	6.38	127.03	119.56
1	B	414	GLN	CG-CD-NE2	6.38	125.97	116.40
1	A	405	GLN	OE1-CD-NE2	6.35	128.95	122.60
1	B	239	HIS	N-CA-CB	6.32	121.24	110.50
1	B	273	LEU	N-CA-C	-6.32	104.84	113.30
1	A	412	VAL	CA-C-N	-6.30	111.02	121.80
1	A	412	VAL	C-N-CA	-6.30	111.02	121.80
1	A	305	GLU	CB-CA-C	6.29	120.61	110.16
1	A	283	LYS	CA-C-O	-6.29	113.88	120.55
1	A	377	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	522	THR	CA-CB-CG2	6.28	121.18	110.50
1	A	312	VAL	N-CA-CB	-6.28	101.15	111.44
1	B	347	LEU	CA-C-N	6.26	128.59	120.44
1	B	347	LEU	C-N-CA	6.26	128.59	120.44
1	A	253	PRO	CA-C-O	-6.24	114.23	121.34
1	C	291	ALA	O-C-N	-6.24	115.65	122.07
1	C	504	ASN	CA-CB-CG	-6.23	106.37	112.60
1	B	403	VAL	CB-CA-C	6.22	118.36	111.08
1	C	356	ARG	CA-C-O	6.21	127.13	120.55
1	B	334	GLU	CA-C-O	6.21	126.82	120.24
1	B	379	VAL	N-CA-CB	-6.20	103.96	111.21
1	C	454	ARG	CD-NE-CZ	6.19	133.06	124.40
1	B	338	HIS	CA-C-O	-6.18	114.58	121.51
1	B	476	GLU	CA-C-O	6.16	126.87	120.40
1	B	283	LYS	N-CA-CB	6.14	119.15	110.12
1	C	427	LYS	O-C-N	-6.13	116.01	123.30
1	C	528	THR	OG1-CB-CG2	-6.13	97.05	109.30
1	B	277	PRO	CA-C-O	-6.12	114.46	121.56
1	C	456	LYS	CB-CG-CD	6.12	125.37	111.30
1	B	538	SER	CA-C-N	6.10	132.69	121.70
1	B	538	SER	C-N-CA	6.10	132.69	121.70
1	A	342	ASN	CB-CG-ND2	6.10	125.55	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	ARG	O-C-N	-6.09	115.79	122.07
1	C	464	ASN	CA-C-O	-6.09	113.22	120.10
1	A	371	ILE	CA-C-O	-6.08	114.07	120.39
1	A	251	TRP	CA-CB-CG	6.08	125.14	113.60
1	A	461	TYR	CB-CG-CD1	6.08	129.91	120.80
1	C	351	LEU	CA-C-O	-6.07	113.50	120.24
1	A	521	ARG	CB-CA-C	-6.07	101.10	110.81
1	A	400	THR	N-CA-CB	-6.07	101.81	110.79
1	A	332	PHE	N-CA-CB	6.07	120.07	110.55
1	C	498	ASN	CA-CB-CG	-6.06	106.54	112.60
1	B	248	ALA	N-CA-CB	-6.03	101.56	110.49
1	B	294	TYR	CA-C-O	-6.03	113.03	119.97
1	C	273	LEU	O-C-N	-6.03	114.94	122.24
1	A	242	ARG	CA-CB-CG	6.03	126.15	114.10
1	B	249	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	C	248	ALA	CA-C-O	-6.01	112.32	119.35
1	C	353	LYS	O-C-N	-6.00	115.31	122.15
1	C	507	ASP	O-C-N	-5.99	115.21	122.22
1	A	496	GLU	CB-CG-CD	-5.99	102.42	112.60
1	B	512	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	538	SER	N-CA-CB	5.97	117.81	110.53
1	C	243	ASN	CA-C-N	5.96	128.52	123.33
1	C	243	ASN	C-N-CA	5.96	128.52	123.33
1	A	342	ASN	CA-CB-CG	-5.94	106.66	112.60
1	B	469	ARG	N-CA-CB	-5.94	100.50	110.83
1	B	521	ARG	CG-CD-NE	-5.92	98.99	112.00
1	B	333	THR	CB-CA-C	-5.90	103.39	111.95
1	B	475	VAL	CA-CB-CG1	5.90	120.43	110.40
1	C	247	TRP	CD1-NE1-CE2	5.90	119.52	108.90
1	A	521	ARG	CA-C-N	-5.89	111.92	120.29
1	A	521	ARG	C-N-CA	-5.89	111.92	120.29
1	A	478	HIS	CA-CB-CG	5.89	119.69	113.80
1	C	296	ILE	N-CA-CB	-5.89	102.44	110.56
1	C	239	HIS	CA-CB-CG	5.88	119.68	113.80
1	B	308	MET	O-C-N	-5.87	116.34	123.27
1	A	311	GLY	O-C-N	-5.87	118.93	123.80
1	A	422	ASP	CA-C-N	-5.86	111.16	122.06
1	A	422	ASP	C-N-CA	-5.86	111.16	122.06
1	A	282	THR	CA-CB-OG1	-5.85	100.82	109.60
1	A	239	HIS	N-CA-CB	-5.84	100.56	110.50
1	A	501	ALA	CA-C-O	-5.84	114.35	120.55
1	A	336	ASP	CA-CB-CG	5.83	118.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	SER	O-C-N	5.82	130.12	123.48
1	B	334	GLU	CB-CA-C	5.82	119.45	110.14
1	C	424	TYR	CA-CB-CG	-5.82	103.42	113.90
1	A	282	THR	N-CA-C	5.81	117.70	111.36
1	A	332	PHE	CA-C-O	-5.80	113.94	120.32
1	C	365	THR	CA-C-N	-5.79	110.05	121.41
1	C	365	THR	C-N-CA	-5.79	110.05	121.41
1	C	279	ASP	N-CA-CB	5.79	119.25	110.45
1	C	423	SER	O-C-N	-5.78	114.48	122.46
1	B	489	THR	CA-C-O	-5.78	114.28	120.92
1	C	531	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	A	325	PRO	CA-C-O	5.76	125.57	121.31
1	B	489	THR	CA-CB-OG1	-5.76	100.96	109.60
1	B	507	ASP	O-C-N	-5.76	116.02	122.12
1	A	519	LEU	CA-C-O	5.76	126.63	120.70
1	B	529	ILE	CB-CG1-CD1	-5.75	101.73	113.80
1	B	405	GLN	N-CA-CB	-5.74	101.05	110.52
1	A	290	TYR	CA-C-O	-5.74	114.47	120.55
1	B	525	ASN	CB-CA-C	-5.74	101.27	110.79
1	C	329	GLN	CG-CD-NE2	5.74	125.00	116.40
1	B	462	ILE	N-CA-CB	5.73	117.53	111.00
1	B	532	ARG	CA-CB-CG	-5.73	102.65	114.10
1	B	411	HIS	CA-CB-CG	-5.72	108.08	113.80
1	C	323	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	365	THR	CA-C-N	-5.72	107.02	122.46
1	B	365	THR	C-N-CA	-5.72	107.02	122.46
1	A	283	LYS	N-CA-CB	5.72	118.52	110.12
1	C	243	ASN	O-C-N	-5.71	116.62	123.31
1	C	343	ILE	O-C-N	-5.71	116.86	122.97
1	B	441	PRO	N-CA-C	5.70	117.65	110.70
1	C	331	VAL	CA-CB-CG1	-5.70	100.72	110.40
1	A	503	LEU	N-CA-CB	5.68	119.09	110.28
1	A	441	PRO	CB-CA-C	5.67	117.84	110.92
1	C	310	PHE	O-C-N	-5.66	116.59	123.10
1	A	313	ILE	O-C-N	-5.65	116.54	122.81
1	C	352	SER	CB-CA-C	5.65	121.52	110.67
1	C	518	SER	N-CA-CB	-5.64	101.20	110.40
1	C	358	ILE	CA-C-O	5.64	126.82	120.95
1	A	282	THR	CB-CA-C	-5.64	101.26	110.85
1	A	431	ASN	CA-CB-CG	-5.64	106.96	112.60
1	B	335	LEU	CA-C-N	-5.63	114.56	123.91
1	B	335	LEU	C-N-CA	-5.63	114.56	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	MET	CB-CA-C	5.63	120.12	109.37
1	C	391	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	425	ASP	CB-CG-OD2	5.61	131.30	118.40
1	C	255	ILE	CA-C-O	-5.61	114.47	120.59
1	A	426	VAL	O-C-N	5.61	129.10	123.10
1	B	292	THR	CA-C-O	-5.60	114.61	120.55
1	A	410	ARG	CD-NE-CZ	5.59	132.22	124.40
1	A	367	LYS	N-CA-C	5.58	119.27	112.23
1	A	422	ASP	CB-CA-C	5.58	120.49	109.66
1	B	435	PRO	CB-CA-C	5.58	118.21	111.46
1	B	420	PRO	O-C-N	-5.57	114.73	122.37
1	C	468	THR	OG1-CB-CG2	-5.57	98.16	109.30
1	B	425	ASP	O-C-N	-5.55	115.32	122.20
1	C	294	TYR	O-C-N	-5.54	115.74	122.22
1	A	458	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	C	520	ILE	CB-CG1-CD1	5.53	125.42	113.80
1	A	251	TRP	N-CA-CB	5.53	118.41	110.06
1	A	406	PHE	CA-C-N	-5.53	115.51	123.03
1	A	406	PHE	C-N-CA	-5.53	115.51	123.03
1	A	243	ASN	N-CA-CB	5.52	119.88	110.71
1	B	535	SER	N-CA-CB	5.52	118.24	110.12
1	B	358	ILE	CB-CA-C	-5.52	104.69	112.14
1	B	499	THR	CA-CB-OG1	-5.51	101.33	109.60
1	C	357	GLY	N-CA-C	-5.50	106.11	112.50
1	A	517	ALA	CA-C-N	-5.50	112.42	122.38
1	A	517	ALA	C-N-CA	-5.50	112.42	122.38
1	B	257	ALA	CA-C-O	-5.50	115.82	121.87
1	C	352	SER	N-CA-CB	-5.49	101.77	110.28
1	A	407	ILE	CA-CB-CG2	5.48	119.82	110.50
1	A	263	VAL	CB-CA-C	-5.48	102.30	111.29
1	C	439	ASN	CB-CA-C	-5.47	102.28	110.16
1	C	280	ASP	CA-C-N	5.47	127.61	120.28
1	C	280	ASP	C-N-CA	5.47	127.61	120.28
1	C	272	PHE	CA-C-O	-5.47	111.94	119.05
1	B	329	GLN	CB-CG-CD	5.47	121.89	112.60
1	A	435	PRO	O-C-N	-5.46	116.99	123.10
1	B	432	LEU	CA-C-O	-5.46	114.47	120.36
1	B	506	PHE	CA-C-O	-5.44	115.10	120.82
1	A	470	ILE	CB-CA-C	-5.44	103.53	110.98
1	B	255	ILE	CB-CA-C	5.43	118.91	111.31
1	B	391	PHE	CA-CB-CG	-5.42	108.38	113.80
1	C	490	THR	CA-C-O	-5.42	114.10	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	ASN	CA-C-O	5.41	126.16	120.42
1	A	295	SER	CA-C-N	-5.41	115.18	122.91
1	A	295	SER	C-N-CA	-5.41	115.18	122.91
1	C	431	ASN	CA-C-N	-5.41	115.09	122.93
1	C	431	ASN	C-N-CA	-5.41	115.09	122.93
1	A	304	ILE	CA-C-O	5.40	127.20	121.04
1	B	518	SER	CA-CB-OG	-5.39	100.32	111.10
1	B	320	ASP	CA-CB-CG	-5.38	107.22	112.60
1	C	474	LYS	CA-C-N	-5.37	115.64	123.06
1	C	474	LYS	C-N-CA	-5.37	115.64	123.06
1	C	405	GLN	CB-CG-CD	-5.37	103.47	112.60
1	B	462	ILE	CA-C-O	-5.37	114.37	120.65
1	B	429	SER	CA-C-O	5.36	126.49	120.70
1	C	290	TYR	CA-C-O	-5.36	115.20	120.82
1	C	283	LYS	O-C-N	5.35	127.79	122.12
1	A	474	LYS	N-CA-CB	-5.35	101.55	110.37
1	A	316	ALA	CA-C-O	-5.34	115.21	120.82
1	C	310	PHE	CA-CB-CG	-5.34	108.46	113.80
1	C	412	VAL	N-CA-C	-5.33	107.23	111.81
1	A	522	THR	N-CA-CB	5.33	118.05	110.16
1	A	409	LYS	O-C-N	-5.33	117.01	123.13
1	A	331	VAL	N-CA-CB	-5.32	103.76	110.31
1	A	352	SER	CA-C-O	5.32	126.19	120.55
1	C	325	PRO	CA-C-O	5.31	125.24	121.31
1	C	532	ARG	NH1-CZ-NH2	5.31	126.20	119.30
1	A	239	HIS	CA-C-O	5.31	129.82	120.80
1	A	244	VAL	CA-CB-CG2	5.30	119.42	110.40
1	B	305	GLU	CA-C-N	5.30	130.81	123.07
1	B	305	GLU	C-N-CA	5.30	130.81	123.07
1	A	489	THR	CA-C-O	-5.30	114.65	120.69
1	C	254	THR	N-CA-CB	5.30	118.16	109.95
1	B	251	TRP	CA-C-O	5.29	126.72	120.69
1	C	314	ILE	CB-CG1-CD1	5.29	124.91	113.80
1	C	356	ARG	CA-C-N	5.29	125.81	119.94
1	C	356	ARG	C-N-CA	5.29	125.81	119.94
1	B	458	ARG	N-CA-C	5.27	117.83	109.50
1	A	346	SER	CA-CB-OG	-5.27	100.56	111.10
1	C	514	LYS	CA-C-O	-5.27	113.91	119.97
1	B	418	TYR	O-C-N	5.26	129.41	122.93
1	C	243	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	307	GLU	CA-C-O	-5.25	114.96	121.11
1	C	278	ASP	CA-CB-CG	-5.25	107.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	THR	CB-CA-C	-5.25	103.87	109.85
1	A	517	ALA	N-CA-CB	5.25	117.92	110.16
1	C	522	THR	N-CA-CB	5.25	118.30	110.22
1	B	368	PHE	O-C-N	-5.24	116.55	123.16
1	A	413	ALA	CA-C-O	-5.24	115.83	121.38
1	C	400	THR	CA-C-O	-5.24	112.42	121.53
1	C	354	TYR	N-CA-CB	5.23	117.59	110.01
1	B	253	PRO	CB-CA-C	5.22	117.81	110.98
1	A	469	ARG	CD-NE-CZ	5.21	131.70	124.40
1	A	462	ILE	N-CA-CB	5.21	117.31	111.21
1	A	340	THR	CB-CA-C	-5.21	104.16	110.15
1	B	244	VAL	CA-CB-CG1	5.21	119.25	110.40
1	B	305	GLU	CA-CB-CG	5.21	124.51	114.10
1	C	504	ASN	N-CA-CB	-5.21	102.46	110.16
1	C	522	THR	CA-C-O	-5.20	114.22	120.10
1	C	421	LYS	CG-CD-CE	5.20	123.26	111.30
1	B	269	ASP	CA-C-N	5.20	124.70	119.19
1	B	269	ASP	C-N-CA	5.20	124.70	119.19
1	A	257	ALA	CA-C-O	-5.20	116.04	121.55
1	A	492	GLU	O-C-N	-5.19	116.48	123.23
1	A	498	ASN	O-C-N	-5.19	116.42	122.96
1	A	301	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	C	477	ASN	CB-CG-OD1	5.19	131.18	120.80
1	A	523	PHE	N-CA-CB	-5.18	102.22	109.94
1	A	444	LYS	N-CA-C	5.18	116.74	111.14
1	B	255	ILE	N-CA-CB	-5.18	104.94	111.41
1	C	333	THR	CB-CA-C	-5.18	103.51	111.74
1	C	506	PHE	CA-C-O	-5.18	115.37	120.70
1	B	269	ASP	CA-CB-CG	5.17	117.78	112.60
1	A	273	LEU	O-C-N	-5.17	115.87	122.34
1	C	297	ALA	CA-C-N	5.17	126.31	119.84
1	C	297	ALA	C-N-CA	5.17	126.31	119.84
1	B	271	SER	CB-CA-C	-5.17	101.54	111.78
1	A	309	LYS	CA-C-O	-5.16	115.12	120.70
1	C	396	THR	CB-CA-C	-5.16	101.60	110.16
1	B	249	GLN	CA-C-O	-5.15	115.18	121.05
1	B	397	ASP	CB-CA-C	-5.15	101.65	109.89
1	A	517	ALA	O-C-N	5.15	128.02	122.15
1	C	500	PRO	CA-C-N	-5.14	112.49	120.31
1	C	500	PRO	C-N-CA	-5.14	112.49	120.31
1	C	405	GLN	CA-CB-CG	5.14	124.38	114.10
1	A	281	LEU	CA-C-N	-5.13	113.00	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	LEU	C-N-CA	-5.13	113.00	120.29
1	A	519	LEU	N-CA-C	-5.13	105.59	111.14
1	A	535	SER	CA-CB-OG	-5.13	100.84	111.10
1	C	315	ASP	N-CA-CB	5.13	118.41	110.46
1	C	287	ASP	CB-CA-C	-5.12	102.81	110.90
1	C	273	LEU	CA-C-N	5.12	129.41	122.19
1	C	273	LEU	C-N-CA	5.12	129.41	122.19
1	C	330	CYS	CA-C-O	-5.12	115.81	121.33
1	C	529	ILE	O-C-N	-5.11	116.90	121.91
1	A	289	VAL	CA-C-O	-5.11	115.44	120.85
1	C	364	ASN	OD1-CG-ND2	5.11	127.70	122.60
1	A	269	ASP	N-CA-C	-5.10	103.16	109.64
1	A	416	LEU	O-C-N	-5.09	116.99	123.05
1	C	329	GLN	OE1-CD-NE2	5.09	127.69	122.60
1	B	284	SER	O-C-N	5.09	127.31	122.07
1	B	469	ARG	CA-C-N	5.09	129.50	123.19
1	B	469	ARG	C-N-CA	5.09	129.50	123.19
1	B	537	LEU	CA-C-N	5.08	129.57	122.05
1	B	537	LEU	C-N-CA	5.08	129.57	122.05
1	C	256	LYS	N-CA-CB	5.08	118.58	110.46
1	B	526	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	C	464	ASN	CA-CB-CG	-5.07	107.53	112.60
1	C	471	ASP	N-CA-CB	5.07	119.20	110.68
1	C	314	ILE	O-C-N	-5.06	117.72	123.18
1	B	538	SER	CB-CA-C	-5.05	104.54	112.12
1	C	525	ASN	CB-CA-C	-5.05	102.73	110.81
1	A	258	LEU	CB-CA-C	-5.05	102.89	110.16
1	C	247	TRP	CG-CD1-NE1	-5.04	103.64	110.20
1	B	303	PHE	CA-CB-CG	-5.04	108.76	113.80
1	A	423	SER	CB-CA-C	5.04	119.39	109.72
1	C	402	ARG	CA-CB-CG	5.04	124.17	114.10
1	A	361	VAL	CB-CA-C	5.03	119.80	111.59
1	C	365	THR	CA-CB-OG1	-5.03	102.05	109.60
1	C	416	LEU	CA-C-N	-5.03	116.30	122.84
1	C	416	LEU	C-N-CA	-5.03	116.30	122.84
1	C	301	ARG	CA-CB-CG	-5.03	104.05	114.10
1	C	247	TRP	CB-CG-CD1	5.00	134.41	126.90
1	C	274	ASN	OD1-CG-ND2	5.00	127.60	122.60

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	MET	Mainchain
1	A	242	ARG	Mainchain
1	A	243	ASN	Mainchain
1	A	273	LEU	Mainchain
1	A	294	TYR	Mainchain
1	A	297	ALA	Mainchain
1	A	365	THR	Mainchain
1	A	369	SER	Mainchain
1	A	374	GLN	Mainchain
1	A	400	THR	Mainchain
1	A	413	ALA	Mainchain
1	A	416	LEU	Mainchain
1	A	433	GLU	Mainchain
1	A	435	PRO	Mainchain
1	A	474	LYS	Mainchain
1	A	477	ASN	Mainchain
1	A	518	SER	Mainchain
1	A	535	SER	Mainchain
1	B	287	ASP	Mainchain
1	B	319	PRO	Mainchain
1	B	322	VAL	Mainchain
1	B	325	PRO	Mainchain
1	B	334	GLU	Mainchain
1	B	338	HIS	Mainchain
1	B	364	ASN	Mainchain
1	B	366	GLY	Mainchain
1	B	372	GLU	Mainchain
1	B	413	ALA	Mainchain
1	B	415	LEU	Mainchain
1	B	416	LEU	Mainchain
1	B	421	LYS	Mainchain
1	B	435	PRO	Mainchain
1	B	538	SER	Mainchain
1	C	239	HIS	Mainchain
1	C	273	LEU	Mainchain
1	C	297	ALA	Mainchain
1	C	299	GLU	Mainchain
1	C	327	SER	Mainchain
1	C	333	THR	Mainchain
1	C	335	LEU	Mainchain
1	C	352	SER	Mainchain
1	C	362	THR	Mainchain
1	C	416	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	C	420	PRO	Mainchain
1	C	421	LYS	Mainchain
1	C	433	GLU	Mainchain
1	C	435	PRO	Mainchain
1	C	477	ASN	Mainchain
1	C	490	THR	Mainchain
1	C	491	HIS	Mainchain
1	C	503	LEU	Mainchain
1	C	518	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	2295	0	2274	77	0
1	B	2295	0	2274	68	0
1	C	2295	0	2274	66	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	121	0	0	19	0
3	B	134	0	0	16	1
3	C	159	0	0	9	1
All	All	7329	0	6822	208	1

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 15.

All (208) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PRO:HB2	1:A:442:PRO:HD3	1.47	0.94
1:C:441:PRO:HB2	1:C:442:PRO:HD3	1.51	0.91
1:C:441:PRO:HB2	1:C:442:PRO:CD	2.04	0.86
1:C:538:SER:O	1:C:539:TYR:HB3	1.74	0.85
1:A:263:VAL:HA	3:A:701:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:THR:HG22	3:B:615:HOH:O	1.79	0.83
1:C:316:ALA:HB2	1:C:336:ASP:HB3	1.60	0.83
1:A:263:VAL:CA	3:A:701:HOH:O	2.27	0.82
1:B:265:ASP:HA	3:B:707:HOH:O	1.81	0.81
1:A:421:LYS:HE2	3:A:691:HOH:O	1.82	0.78
1:A:400:THR:O	1:A:402:ARG:N	2.18	0.77
1:B:381:ARG:HG2	1:B:391:PHE:CE2	2.21	0.76
1:C:256:LYS:HE3	1:C:257:ALA:H	1.51	0.76
1:B:400:THR:O	1:B:402:ARG:N	2.19	0.75
1:A:448:GLN:HE21	1:A:448:GLN:HA	1.50	0.75
1:C:256:LYS:HA	1:C:256:LYS:NZ	2.01	0.74
1:C:400:THR:O	1:C:402:ARG:N	2.21	0.73
1:C:393:ARG:HH21	1:C:405:GLN:NE2	1.87	0.72
1:A:244:VAL:HG22	1:A:249:GLN:HG3	1.72	0.71
1:C:393:ARG:HH21	1:C:405:GLN:HE22	1.40	0.69
1:C:522:THR:HG22	3:C:625:HOH:O	1.93	0.69
1:C:364:ASN:ND2	3:C:607:HOH:O	2.27	0.68
1:A:441:PRO:CB	1:A:442:PRO:HD3	2.24	0.68
1:A:398:ILE:HG23	1:A:399:LYS:HG3	1.75	0.68
1:A:500:PRO:HA	3:A:721:HOH:O	1.93	0.67
1:C:251:TRP:CZ2	1:C:253:PRO:HA	2.31	0.66
1:C:342:ASN:ND2	1:C:491:HIS:H	1.93	0.66
1:B:360:GLU:HG3	3:B:717:HOH:O	1.96	0.66
1:A:518:SER:O	1:A:522:THR:HG23	1.95	0.66
1:A:448:GLN:HA	1:A:448:GLN:NE2	2.12	0.65
1:B:340:THR:O	3:B:690:HOH:O	2.13	0.65
1:B:309:LYS:HG2	1:B:494:GLU:HG2	1.79	0.65
1:C:342:ASN:HD22	1:C:491:HIS:H	1.42	0.65
1:A:398:ILE:HG23	1:A:399:LYS:N	2.12	0.63
1:A:436:VAL:HG13	1:A:437:PRO:HD2	1.79	0.63
1:A:522:THR:HG22	3:A:619:HOH:O	1.99	0.63
1:B:417:LEU:HB2	1:B:426:VAL:HG22	1.81	0.63
1:C:251:TRP:CH2	1:C:510:THR:HG22	2.33	0.63
1:A:454:ARG:NH1	1:A:475:VAL:HG21	2.14	0.63
1:A:442:PRO:HA	3:A:654:HOH:O	1.98	0.62
1:C:364:ASN:HB3	3:C:607:HOH:O	1.99	0.62
1:C:441:PRO:CB	1:C:442:PRO:CD	2.77	0.62
1:C:513:SER:HB3	3:C:645:HOH:O	2.00	0.62
1:B:255:ILE:CG2	1:B:517:ALA:HB2	2.29	0.62
1:B:251:TRP:CZ2	1:B:253:PRO:HB3	2.35	0.62
1:C:256:LYS:HA	1:C:256:LYS:HZ1	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:THR:HG22	3:B:650:HOH:O	2.00	0.61
1:B:335:LEU:O	1:B:336:ASP:HB2	2.00	0.61
1:C:250:LYS:NZ	3:C:710:HOH:O	2.33	0.60
1:A:316:ALA:HB2	1:A:336:ASP:HB2	1.84	0.60
1:A:461:TYR:OH	3:A:631:HOH:O	2.17	0.58
1:B:348:PHE:CD1	1:B:491:HIS:HB3	2.38	0.58
1:B:264:LYS:O	1:B:265:ASP:C	2.45	0.58
1:B:491:HIS:HE1	3:B:679:HOH:O	1.86	0.58
1:C:355:ILE:HD12	1:C:472:ILE:HD11	1.86	0.58
1:C:393:ARG:NH2	1:C:405:GLN:HE22	2.00	0.58
1:B:333:THR:O	1:B:333:THR:OG1	2.18	0.57
1:A:244:VAL:HG22	1:A:249:GLN:CG	2.34	0.57
1:B:242:ARG:HG3	3:B:623:HOH:O	2.05	0.57
1:A:403:VAL:HG21	3:A:708:HOH:O	2.04	0.57
1:C:308:MET:HE2	1:C:426:VAL:HG11	1.86	0.57
1:A:342:ASN:ND2	1:A:491:HIS:H	2.03	0.57
1:B:251:TRP:N	3:B:620:HOH:O	2.32	0.57
1:A:264:LYS:O	1:A:265:ASP:C	2.48	0.56
1:A:364:ASN:HB3	3:A:648:HOH:O	2.06	0.56
1:A:441:PRO:HB2	1:A:442:PRO:CD	2.28	0.56
1:C:264:LYS:O	1:C:265:ASP:C	2.50	0.55
1:C:342:ASN:O	1:C:343:ILE:HD12	2.06	0.55
1:C:343:ILE:HG13	1:C:424:TYR:CZ	2.41	0.55
1:B:257:ALA:HB1	1:B:276:ILE:O	2.06	0.55
1:A:253:PRO:O	3:A:673:HOH:O	2.19	0.54
1:B:356:ARG:HH12	1:B:370:ILE:HG21	1.73	0.54
1:B:477:ASN:HB3	3:B:641:HOH:O	2.08	0.53
1:C:257:ALA:HB1	1:C:276:ILE:O	2.08	0.53
1:B:255:ILE:HG23	1:B:517:ALA:HB2	1.91	0.53
1:C:252:LYS:HG2	1:C:253:PRO:HD2	1.91	0.53
1:B:307:GLU:OE2	1:B:496:GLU:HB2	2.08	0.53
1:C:316:ALA:HB2	1:C:336:ASP:CB	2.36	0.53
1:B:393:ARG:HH21	1:B:405:GLN:NE2	2.07	0.53
1:B:455:THR:HG22	3:B:651:HOH:O	2.09	0.52
1:B:270:PRO:O	1:C:522:THR:HB	2.10	0.52
1:C:371:ILE:HG23	3:C:693:HOH:O	2.10	0.52
1:A:394:MET:HE2	3:A:708:HOH:O	2.09	0.52
1:A:242:ARG:NH1	3:A:609:HOH:O	2.42	0.51
1:A:252:LYS:HG2	3:A:673:HOH:O	2.11	0.51
1:A:362:THR:HG22	1:B:346:SER:OG	2.10	0.51
1:A:355:ILE:CD1	1:A:472:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:HD21	1:A:331:VAL:HG23	1.93	0.51
1:A:495:LEU:HD11	1:A:530:ILE:HG13	1.91	0.51
1:B:244:VAL:HG13	1:B:294:TYR:CZ	2.44	0.51
1:A:342:ASN:HD22	1:A:491:HIS:H	1.57	0.51
1:A:263:VAL:O	1:A:264:LYS:C	2.53	0.50
1:A:283:LYS:HG2	3:A:665:HOH:O	2.11	0.50
1:B:421:LYS:HG2	3:B:723:HOH:O	2.11	0.50
1:A:355:ILE:HD12	1:A:472:ILE:HD11	1.92	0.50
1:A:390:ARG:HD2	1:A:408:GLU:OE2	2.11	0.50
1:B:382:VAL:HG22	1:B:390:ARG:H	1.76	0.50
1:B:382:VAL:CG2	1:B:390:ARG:H	2.25	0.50
1:B:504:ASN:ND2	1:B:515:GLU:OE1	2.42	0.50
1:C:244:VAL:HG13	1:C:294:TYR:CZ	2.47	0.50
1:A:468:THR:HG21	1:A:495:LEU:HD23	1.94	0.49
1:C:308:MET:HG3	1:C:426:VAL:HG13	1.93	0.49
1:A:505:ALA:HB1	1:A:516:TYR:HA	1.93	0.49
1:C:364:ASN:CB	3:C:607:HOH:O	2.60	0.49
1:C:374:GLN:HG3	1:C:457:ASP:HA	1.94	0.49
1:A:439:ASN:OD1	1:A:444:LYS:HD3	2.13	0.49
1:B:382:VAL:HG21	1:B:390:ARG:HB2	1.94	0.49
1:A:518:SER:HB3	3:A:624:HOH:O	2.11	0.49
1:A:258:LEU:HD22	1:A:521:ARG:NH1	2.28	0.49
1:C:240:MET:SD	1:C:507:ASP:HB3	2.53	0.48
1:A:441:PRO:CB	1:A:442:PRO:CD	2.89	0.48
1:C:288:TRP:CD2	1:C:415:LEU:HG	2.48	0.48
1:C:436:VAL:HA	1:C:437:PRO:HD3	1.72	0.48
1:C:382:VAL:HG22	1:C:390:ARG:HB2	1.96	0.48
1:B:369:SER:HB3	3:B:680:HOH:O	2.12	0.48
1:A:398:ILE:CG2	1:A:399:LYS:N	2.76	0.48
1:C:242:ARG:HG2	1:C:242:ARG:HH11	1.79	0.48
1:B:381:ARG:HG3	1:B:451:ILE:HG21	1.96	0.48
1:C:263:VAL:O	1:C:264:LYS:C	2.56	0.48
1:B:342:ASN:HD22	1:B:491:HIS:H	1.61	0.48
1:B:454:ARG:CZ	1:B:475:VAL:HG21	2.44	0.48
1:A:281:LEU:CD2	1:A:331:VAL:HG23	2.44	0.47
1:C:255:ILE:HG13	1:C:513:SER:OG	2.13	0.47
1:B:538:SER:O	1:B:539:TYR:HB2	2.15	0.47
1:C:333:THR:O	1:C:333:THR:OG1	2.24	0.47
1:C:538:SER:O	1:C:539:TYR:CB	2.53	0.47
1:B:473:THR:HG22	1:B:475:VAL:HG12	1.96	0.47
1:C:518:SER:O	1:C:522:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASP:OD2	1:A:346:SER:HB3	2.15	0.46
1:C:406:PHE:CE1	1:C:436:VAL:HG11	2.49	0.46
1:B:449:SER:HA	1:B:450:PRO:HD3	1.81	0.46
1:B:244:VAL:HG22	1:B:249:GLN:HG3	1.97	0.46
1:B:393:ARG:NH2	1:B:405:GLN:HE22	2.14	0.46
1:A:365:THR:OG1	1:B:349:LYS:HD2	2.16	0.46
1:B:421:LYS:HE3	3:B:723:HOH:O	2.16	0.46
1:A:468:THR:HG22	1:A:469:ARG:N	2.30	0.46
1:C:364:ASN:HB2	1:C:367:LYS:HB2	1.98	0.46
1:A:305:GLU:OE2	1:A:307:GLU:HG3	2.17	0.45
1:C:338:HIS:CD2	3:C:656:HOH:O	2.68	0.45
1:B:315:ASP:HB3	1:B:322:VAL:HG12	1.98	0.45
1:C:239:HIS:HA	1:C:294:TYR:CE1	2.52	0.45
1:A:263:VAL:CB	3:A:701:HOH:O	2.61	0.45
1:B:242:ARG:HD2	3:B:634:HOH:O	2.16	0.45
1:B:370:ILE:HG13	1:B:461:TYR:CE2	2.51	0.45
1:B:448:GLN:HE21	1:B:449:SER:H	1.63	0.45
1:C:382:VAL:CG2	1:C:390:ARG:HB2	2.46	0.45
1:C:505:ALA:HB1	1:C:516:TYR:HA	1.97	0.45
1:A:448:GLN:HE21	1:A:448:GLN:CA	2.23	0.45
1:B:347:LEU:HD12	1:B:424:TYR:HE1	1.80	0.45
1:A:398:ILE:CG2	1:A:399:LYS:HG3	2.45	0.44
1:A:499:THR:O	1:A:500:PRO:C	2.60	0.44
1:B:263:VAL:O	1:B:264:LYS:C	2.59	0.44
1:A:239:HIS:N	3:A:627:HOH:O	2.49	0.44
1:A:244:VAL:HG13	1:A:294:TYR:CZ	2.52	0.44
1:B:316:ALA:HB2	1:B:336:ASP:CB	2.47	0.44
1:A:353:LYS:HE2	1:A:353:LYS:HB3	1.53	0.44
1:B:382:VAL:HG23	1:B:383:GLY:N	2.33	0.44
1:A:307:GLU:HG2	1:A:496:GLU:HG3	1.99	0.44
1:B:418:TYR:CZ	1:B:420:PRO:HB3	2.53	0.44
1:A:239:HIS:HD2	1:A:240:MET:HG3	1.82	0.44
1:A:242:ARG:HD2	3:A:609:HOH:O	2.17	0.44
1:B:505:ALA:CB	1:B:515:GLU:HG2	2.47	0.43
1:C:437:PRO:HB2	1:C:438:ASP:H	1.60	0.43
1:B:503:LEU:HD23	1:B:503:LEU:HA	1.67	0.43
1:B:239:HIS:HA	1:B:294:TYR:CE1	2.53	0.43
1:A:315:ASP:HB3	1:A:322:VAL:HG12	2.01	0.43
1:B:315:ASP:HB3	1:B:322:VAL:CG1	2.48	0.43
1:A:309:LYS:HE2	1:A:494:GLU:OE1	2.19	0.43
1:A:255:ILE:HD12	1:A:286:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD21	3:A:624:HOH:O	2.19	0.43
1:B:239:HIS:HE1	1:B:510:THR:HG23	1.83	0.43
1:C:307:GLU:HG2	1:C:309:LYS:HE3	2.01	0.43
1:A:378:SER:HB3	1:A:450:PRO:HB3	2.00	0.42
1:B:239:HIS:CE1	1:B:510:THR:HG23	2.54	0.42
1:B:339:LEU:C	1:B:339:LEU:HD23	2.44	0.42
1:C:370:ILE:HD12	1:C:461:TYR:CD2	2.55	0.42
1:A:244:VAL:HA	1:A:245:PRO:HD3	1.93	0.42
1:B:437:PRO:HB2	1:B:438:ASP:H	1.74	0.42
1:A:255:ILE:HG23	1:A:517:ALA:HB2	2.00	0.42
1:B:382:VAL:CG2	1:B:390:ARG:HB2	2.49	0.42
1:C:434:LEU:HA	1:C:435:PRO:HD3	1.86	0.42
1:B:342:ASN:ND2	1:B:491:HIS:H	2.18	0.42
1:C:256:LYS:CE	1:C:257:ALA:H	2.27	0.41
1:C:522:THR:O	1:C:525:ASN:HB2	2.20	0.41
1:C:440:ASP:HA	1:C:441:PRO:HD3	1.90	0.41
1:A:273:LEU:HB2	1:A:275:ILE:HG12	2.03	0.41
1:C:456:LYS:HB2	1:C:456:LYS:NZ	2.35	0.41
1:C:400:THR:O	1:C:401:GLY:C	2.62	0.41
1:A:310:PHE:HB3	1:A:343:ILE:HD11	2.02	0.41
1:B:252:LYS:NZ	3:B:658:HOH:O	2.53	0.41
1:B:436:VAL:HA	1:B:437:PRO:HD3	1.77	0.41
1:C:239:HIS:N	3:C:633:HOH:O	2.54	0.41
1:C:251:TRP:HH2	1:C:510:THR:HG22	1.84	0.41
1:C:299:GLU:H	1:C:299:GLU:CD	2.28	0.41
1:A:418:TYR:CE2	1:A:420:PRO:HB3	2.56	0.41
1:B:242:ARG:NE	3:B:623:HOH:O	2.41	0.41
1:B:299:GLU:H	1:B:299:GLU:CD	2.29	0.41
1:A:348:PHE:CE1	1:A:472:ILE:HG23	2.56	0.41
1:A:499:THR:HB	1:A:500:PRO:CD	2.51	0.41
1:A:305:GLU:HG2	1:A:433:GLU:OE1	2.21	0.40
1:A:312:VAL:CG1	1:A:321:ARG:HB2	2.51	0.40
1:C:339:LEU:HD23	1:C:339:LEU:C	2.46	0.40
1:C:506:PHE:O	1:C:509:ILE:HG22	2.21	0.40
1:A:305:GLU:OE1	1:A:409:LYS:NZ	2.49	0.40
1:A:308:MET:HA	1:A:427:LYS:O	2.21	0.40
1:A:453:GLU:HB2	1:A:478:HIS:HD2	1.87	0.40
1:B:440:ASP:HA	1:B:441:PRO:HD3	1.95	0.40
1:C:290:TYR:CD2	1:C:290:TYR:C	2.98	0.40

All (1) 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)
3:B:723:HOH:O	3:C:662:HOH:O[2_657]	2.13	0.07

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%)	260 (92%)	18 (6%)	4 (1%)	9	3
1	B	282/311 (91%)	264 (94%)	13 (5%)	5 (2%)	6	2
1	C	282/311 (91%)	260 (92%)	16 (6%)	6 (2%)	5	1
All	All	846/933 (91%)	784 (93%)	47 (6%)	15 (2%)	6	2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	GLY
1	A	437	PRO
1	B	401	GLY
1	B	437	PRO
1	C	401	GLY
1	C	441	PRO
1	A	441	PRO
1	C	437	PRO
1	B	261	ILE
1	C	336	ASP
1	B	441	PRO
1	C	342	ASN
1	A	261	ILE
1	C	261	ILE
1	B	322	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/291 (89%)	227 (88%)	32 (12%)	4	1
1	B	259/291 (89%)	226 (87%)	33 (13%)	4	1
1	C	259/291 (89%)	223 (86%)	36 (14%)	3	1
All	All	777/873 (89%)	676 (87%)	101 (13%)	4	1

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	ARG
1	A	243	ASN
1	A	244	VAL
1	A	251	TRP
1	A	254	THR
1	A	256	LYS
1	A	258	LEU
1	A	274	ASN
1	A	280	ASP
1	A	281	LEU
1	A	343	ILE
1	A	349	LYS
1	A	353	LYS
1	A	367	LYS
1	A	395	SER
1	A	397	ASP
1	A	400	THR
1	A	402	ARG
1	A	410	ARG
1	A	417	LEU
1	A	429	SER
1	A	430	LEU
1	A	448	GLN
1	A	456	LYS
1	A	475	VAL
1	A	478	HIS

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Mol	Chain	Res	Type
1	A	495	LEU
1	A	497	ILE
1	A	511	ASN
1	A	513	SER
1	A	522	THR
1	A	534	LEU
1	B	242	ARG
1	B	243	ASN
1	B	244	VAL
1	B	251	TRP
1	B	252	LYS
1	B	254	THR
1	B	256	LYS
1	B	258	LEU
1	B	280	ASP
1	B	305	GLU
1	B	307	GLU
1	B	334	GLU
1	B	350	GLU
1	B	352	SER
1	B	353	LYS
1	B	362	THR
1	B	363	GLU
1	B	370	ILE
1	B	400	THR
1	B	403	VAL
1	B	405	GLN
1	B	423	SER
1	B	426	VAL
1	B	430	LEU
1	B	444	LYS
1	B	455	THR
1	B	456	LYS
1	B	469	ARG
1	B	475	VAL
1	B	495	LEU
1	B	515	GLU
1	B	522	THR
1	B	534	LEU
1	C	243	ASN
1	C	244	VAL
1	C	246	ILE

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Mol	Chain	Res	Type
1	C	250	LYS
1	C	256	LYS
1	C	258	LEU
1	C	275	ILE
1	C	279	ASP
1	C	280	ASP
1	C	305	GLU
1	C	343	ILE
1	C	350	GLU
1	C	352	SER
1	C	367	LYS
1	C	370	ILE
1	C	392	LEU
1	C	399	LYS
1	C	402	ARG
1	C	417	LEU
1	C	426	VAL
1	C	442	PRO
1	C	446	LYS
1	C	451	ILE
1	C	453	GLU
1	C	456	LYS
1	C	462	ILE
1	C	464	ASN
1	C	475	VAL
1	C	478	HIS
1	C	487	SER
1	C	488	GLU
1	C	504	ASN
1	C	511	ASN
1	C	522	THR
1	C	534	LEU
1	C	539	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	A	342	ASN
1	A	448	GLN
1	A	478	HIS
1	A	508	ASN

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Mol	Chain	Res	Type
1	A	511	ASN
1	B	239	HIS
1	B	243	ASN
1	B	342	ASN
1	B	364	ASN
1	B	405	GLN
1	B	411	HIS
1	B	448	GLN
1	B	464	ASN
1	B	491	HIS
1	B	508	ASN
1	B	511	ASN
1	C	243	ASN
1	C	338	HIS
1	C	342	ASN
1	C	374	GLN
1	C	405	GLN
1	C	411	HIS
1	C	491	HIS
1	C	508	ASN
1	C	511	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	606	-	4,4,4	0.48	0	6,6,6	0.62	0
2	SO4	B	605	-	4,4,4	0.99	0	6,6,6	1.27	1 (16%)
2	SO4	C	603	-	4,4,4	0.64	0	6,6,6	0.40	0
2	SO4	B	602	-	4,4,4	0.70	0	6,6,6	0.28	0
2	SO4	A	604	-	4,4,4	0.69	0	6,6,6	1.06	0
2	SO4	A	601	-	4,4,4	0.70	0	6,6,6	0.21	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	605	SO4	O4-S-O2	2.37	121.92	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.