



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:38 PM UTC

PDB ID : 1LXT / pdb_00001lxt
Title : STRUCTURE OF PHOSPHOTRANSFERASE PHOSPHOGLUCOMUTASE
FROM RABBIT
Authors : Ray Junior, W.J.; Baranidharan, S.; Liu, Y.
Deposited on : 1996-07-28
Resolution : 2.70 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

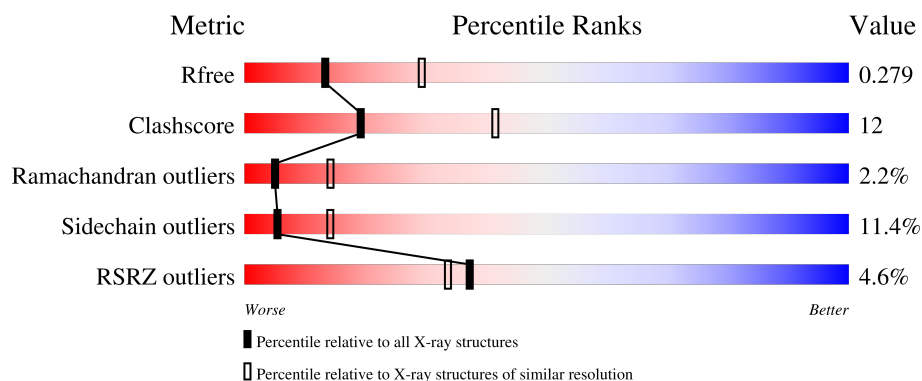
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	561	8% 48% 37% 13% .
1	B	561	% 50% 38% 11% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9060 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.

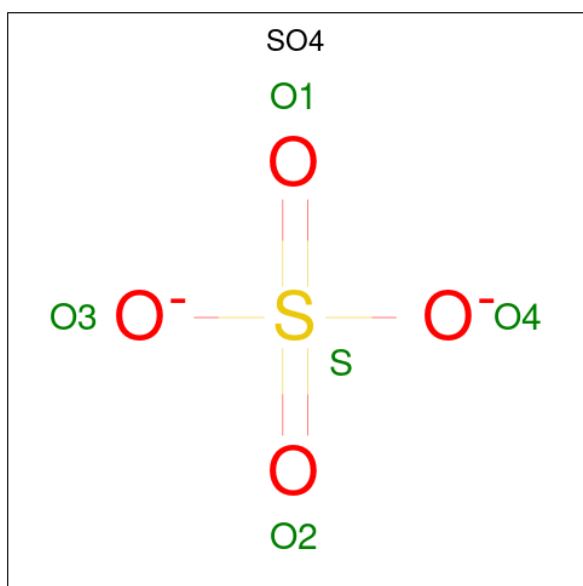
- Molecule 1 is a protein called PHOSPHOGLUCOMUTASE (DEPHOSPHO FORM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4329	2753	743	817	16			
1	B	561	Total	C	N	O	S	0	0	0
			4329	2753	743	817	16			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

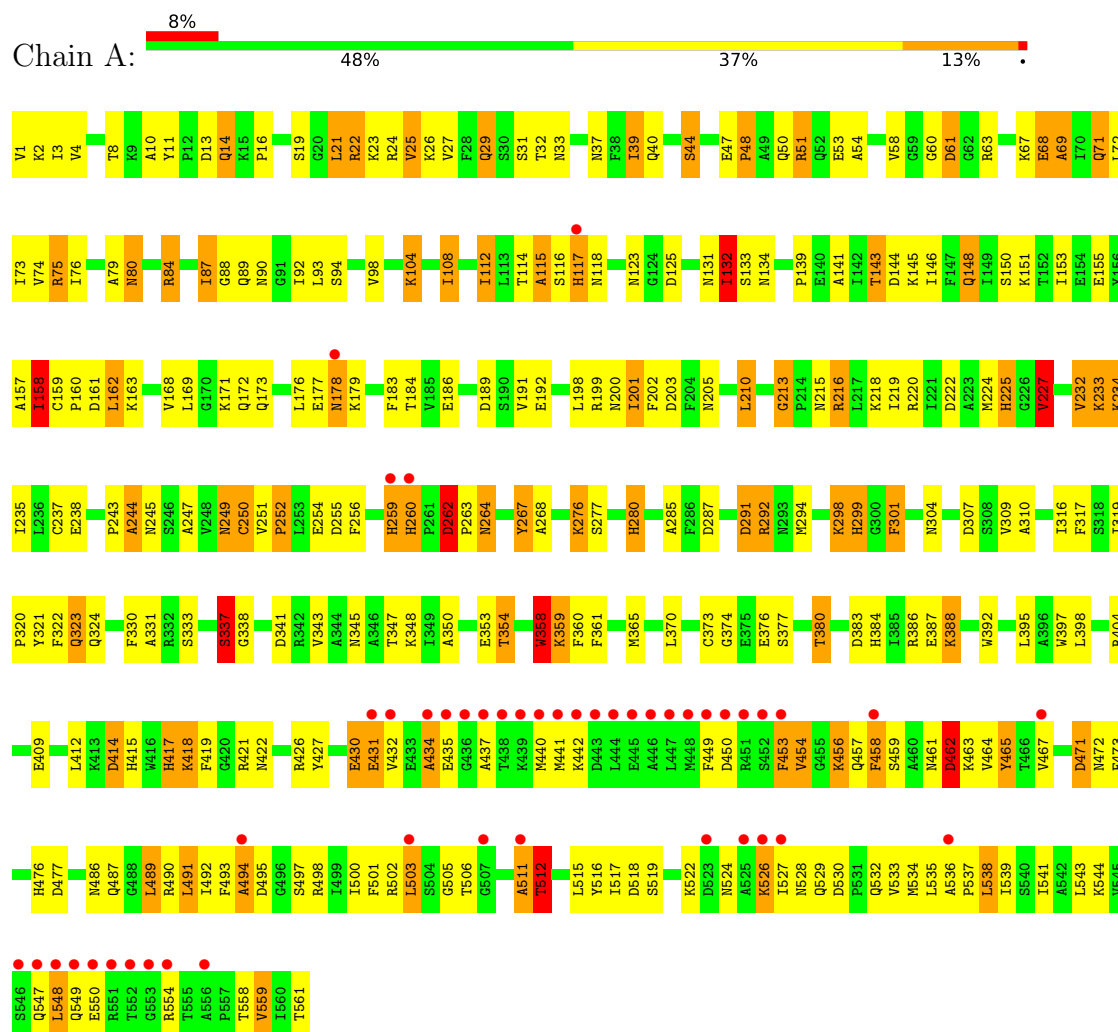
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	233	Total	O	0	0
			233	233		

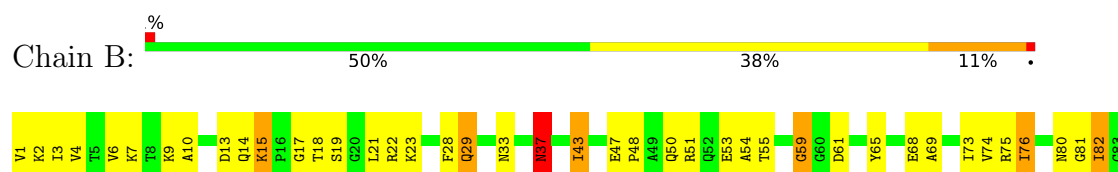
3 Residue-property plots

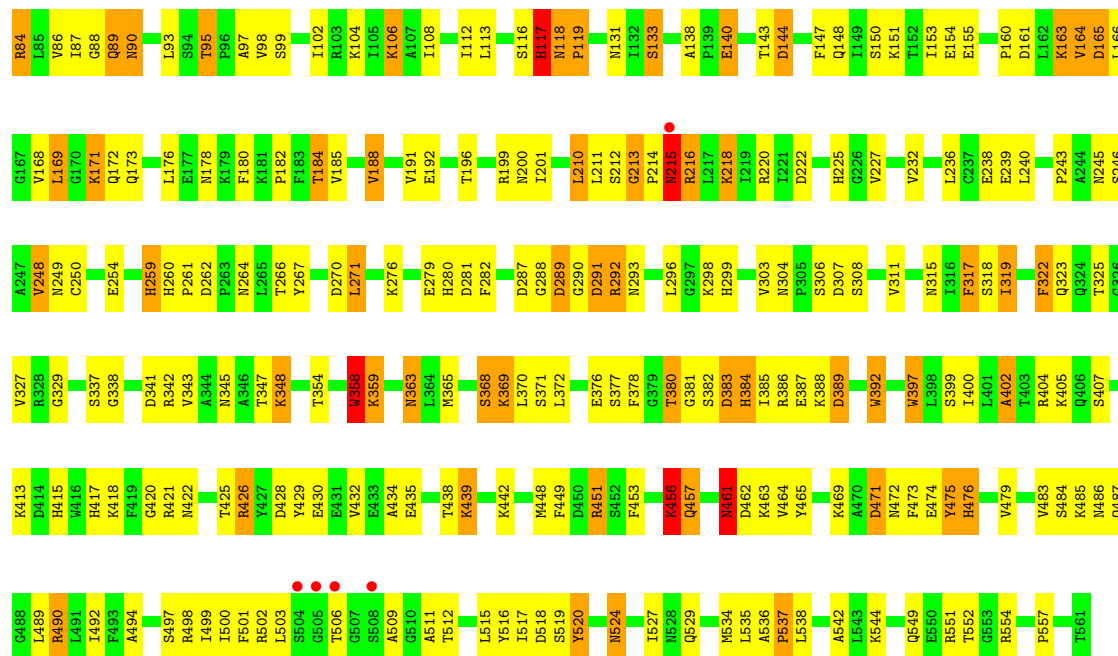
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: PHOSPHOGLUCOMUTASE (DEPHOSPHO FORM)



• Molecule 1: PHOSPHOGLUCOMUTASE (DEPHOSPHO FORM)





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.42Å 174.42Å 101.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.0 (6.00-2.70) 84.6 (6.00-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.69Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , 0.260 0.246 , 0.279	Depositor DCC
R_{free} test set	3815 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 100.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9060	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.08	13/4416 (0.3%)	2.16	210/5969 (3.5%)
1	B	1.16	21/4416 (0.5%)	2.18	187/5969 (3.1%)
All	All	1.12	34/8832 (0.4%)	2.17	397/11938 (3.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	HIS	CD2-NE2	-10.79	1.25	1.37
1	A	117	HIS	CD2-NE2	-10.09	1.26	1.37
1	B	117	HIS	CG-ND1	-7.33	1.30	1.38
1	A	225	HIS	CD2-NE2	-6.98	1.30	1.37
1	B	102	ILE	CA-CB	6.76	1.61	1.54
1	A	280	HIS	CD2-NE2	-6.72	1.30	1.37
1	B	74	VAL	CA-CB	6.70	1.61	1.54
1	B	415	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	260	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	476	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	500	ILE	CA-CB	6.36	1.62	1.54
1	B	417	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	384	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	74	VAL	CA-CB	6.26	1.60	1.54
1	A	415	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	201	ILE	CA-CB	6.10	1.62	1.54
1	B	225	HIS	CD2-NE2	-6.02	1.31	1.37
1	B	259	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	280	HIS	CD2-NE2	-5.95	1.31	1.37
1	B	557	PRO	CA-CB	-5.91	1.45	1.53
1	A	225	HIS	CG-ND1	-5.89	1.31	1.38
1	B	201	ILE	CA-CB	5.88	1.60	1.54
1	B	476	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	415	HIS	CG-ND1	-5.79	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	HIS	CD2-NE2	-5.70	1.31	1.37
1	B	260	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	299	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	259	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	417	HIS	CD2-NE2	-5.50	1.31	1.37
1	B	117	HIS	CB-CG	5.42	1.57	1.50
1	B	76	ILE	CA-CB	5.41	1.61	1.54
1	B	153	ILE	CA-CB	5.32	1.60	1.53
1	B	266	THR	CA-CB	5.12	1.61	1.53
1	B	384	HIS	CG-ND1	-5.07	1.32	1.38

All (397) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ASP	CA-CB-CG	14.09	126.69	112.60
1	A	527	ILE	N-CA-C	11.16	121.99	110.72
1	A	547	GLN	OE1-CD-NE2	-10.93	111.67	122.60
1	B	192	GLU	N-CA-C	10.84	124.11	111.11
1	B	168	VAL	N-CA-C	10.43	124.00	107.73
1	B	524	ASN	OD1-CG-ND2	-10.37	112.23	122.60
1	B	384	HIS	CA-CB-CG	10.05	123.85	113.80
1	B	13	ASP	N-CA-C	9.96	124.98	113.02
1	B	245	ASN	OD1-CG-ND2	-9.77	112.83	122.60
1	A	404	ARG	N-CA-C	9.75	123.13	111.82
1	B	215	ASN	OD1-CG-ND2	-9.65	112.95	122.60
1	B	434	ALA	N-CA-C	9.54	122.69	111.71
1	B	89	GLN	OE1-CD-NE2	-9.47	113.12	122.60
1	A	324	GLN	OE1-CD-NE2	-9.47	113.13	122.60
1	B	37	ASN	OD1-CG-ND2	-9.46	113.14	122.60
1	A	260	HIS	CB-CG-CD2	-9.31	119.09	131.20
1	A	168	VAL	N-CA-CB	-9.30	100.60	111.39
1	A	13	ASP	N-CA-C	9.30	124.18	113.02
1	B	289	ASP	N-CA-C	9.29	124.49	112.41
1	B	471	ASP	CA-CB-CG	9.23	121.83	112.60
1	B	29	GLN	N-CA-C	9.22	121.41	111.36
1	B	117	HIS	CA-CB-CG	9.22	123.02	113.80
1	A	383	ASP	CA-CB-CG	9.16	121.76	112.60
1	A	360	PHE	CA-CB-CG	-9.15	104.65	113.80
1	B	293	ASN	N-CA-C	9.09	124.29	108.75
1	B	29	GLN	OE1-CD-NE2	-9.06	113.54	122.60
1	A	492	ILE	N-CA-C	9.02	120.71	107.37
1	A	178	ASN	OD1-CG-ND2	-8.94	113.66	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ASP	CA-CB-CG	8.93	121.53	112.60
1	A	430	GLU	N-CA-C	8.92	122.48	110.35
1	B	188	VAL	N-CA-CB	-8.84	97.62	112.47
1	A	215	ASN	OD1-CG-ND2	-8.80	113.80	122.60
1	A	205	ASN	OD1-CG-ND2	-8.80	113.80	122.60
1	B	144	ASP	CA-CB-CG	8.71	121.31	112.60
1	A	8	THR	N-CA-C	8.65	123.76	109.06
1	B	487	GLN	OE1-CD-NE2	-8.60	114.00	122.60
1	A	322	PHE	CA-CB-CG	-8.58	105.22	113.80
1	B	486	ASN	CA-CB-CG	8.58	121.18	112.60
1	B	389	ASP	N-CA-C	8.54	122.57	107.80
1	A	529	GLN	OE1-CD-NE2	-8.53	114.07	122.60
1	B	404	ARG	N-CA-C	8.47	122.88	112.54
1	B	250	CYS	N-CA-C	8.41	124.63	113.20
1	A	191	VAL	N-CA-C	8.37	125.63	113.16
1	A	29	GLN	OE1-CD-NE2	-8.35	114.25	122.60
1	A	37	ASN	OD1-CG-ND2	-8.31	114.29	122.60
1	A	200	ASN	CA-CB-CG	-8.27	104.33	112.60
1	B	84	ARG	N-CA-C	8.22	122.97	109.24
1	A	219	ILE	N-CA-C	8.12	118.90	110.05
1	B	211	LEU	N-CA-C	8.08	123.14	113.28
1	A	421	ARG	N-CA-C	8.03	121.72	108.96
1	A	490	ARG	N-CA-C	8.03	122.00	109.07
1	A	532	GLN	OE1-CD-NE2	-7.96	114.64	122.60
1	A	153	ILE	N-CA-C	7.93	119.68	109.30
1	B	323	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	A	486	ASN	CA-CB-CG	7.89	120.49	112.60
1	B	289	ASP	N-CA-CB	-7.88	98.19	111.20
1	A	245	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	B	153	ILE	N-CA-C	7.81	118.93	107.37
1	A	457	GLN	OE1-CD-NE2	-7.76	114.83	122.60
1	A	453	PHE	CA-CB-CG	-7.74	106.06	113.80
1	A	220	ARG	CA-CB-CG	-7.71	98.67	114.10
1	B	292	ARG	N-CA-C	7.71	122.06	109.72
1	B	472	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	B	95	THR	CA-CB-OG1	-7.69	98.06	109.60
1	A	459	SER	N-CA-C	7.66	119.78	108.60
1	A	524	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	B	318	SER	N-CA-C	-7.65	103.84	113.02
1	A	458	PHE	CA-CB-CG	7.63	121.43	113.80
1	A	161	ASP	CA-CB-CG	7.62	120.22	112.60
1	B	345	ASN	OD1-CG-ND2	-7.61	114.99	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	ALA	N-CA-C	7.61	127.01	110.80
1	B	2	LYS	N-CA-C	7.61	121.54	110.28
1	B	430	GLU	N-CA-C	7.60	127.00	110.80
1	A	473	PHE	N-CA-C	7.60	121.41	110.24
1	B	216	ARG	N-CA-C	7.58	120.54	110.53
1	A	462	ASP	CA-CB-CG	7.54	120.14	112.60
1	A	132	ILE	N-CA-C	7.52	119.64	108.96
1	B	178	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	A	260	HIS	CA-CB-CG	7.51	121.31	113.80
1	B	76	ILE	N-CA-C	-7.48	103.56	110.82
1	A	123	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	A	260	HIS	CB-CG-ND1	7.47	133.91	122.70
1	A	254	GLU	N-CA-C	7.46	120.29	111.71
1	A	125	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	345	ASN	CA-CB-CG	-7.45	105.15	112.60
1	A	54	ALA	N-CA-C	7.44	121.57	109.59
1	B	4	VAL	N-CA-C	7.36	119.18	108.58
1	B	172	GLN	OE1-CD-NE2	-7.36	115.25	122.60
1	A	192	GLU	N-CA-C	7.35	119.99	111.02
1	B	168	VAL	N-CA-CB	-7.35	102.27	111.31
1	A	503	LEU	N-CA-C	7.34	121.29	108.52
1	A	548	LEU	N-CA-C	7.34	118.97	110.97
1	B	439	LYS	N-CA-C	-7.31	103.24	111.14
1	A	168	VAL	N-CA-C	7.28	118.97	107.98
1	A	123	ASN	CA-CB-CG	7.27	119.87	112.60
1	B	457	GLN	N-CA-C	7.26	120.48	110.24
1	A	414	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	476	HIS	CB-CG-CD2	-7.24	121.78	131.20
1	A	461	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	A	530	ASP	N-CA-C	7.24	118.84	109.64
1	B	200	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	A	264	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	B	51	ARG	N-CA-C	7.21	118.79	111.07
1	B	472	ASN	N-CA-C	-7.18	95.27	107.99
1	A	108	ILE	CA-CB-CG1	-7.16	98.22	110.40
1	A	528	ASN	N-CA-C	7.12	121.82	113.20
1	B	276	LYS	N-CA-C	7.12	119.04	111.28
1	B	527	ILE	N-CA-C	7.11	124.13	109.34
1	B	428	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	337	SER	N-CA-C	7.09	125.90	110.80
1	B	464	VAL	N-CA-C	7.05	118.02	107.51
1	A	172	GLN	OE1-CD-NE2	-7.01	115.59	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	LYS	N-CA-C	6.98	121.68	109.96
1	A	517	ILE	N-CA-C	6.95	118.33	107.28
1	A	259	HIS	N-CA-C	6.94	119.47	109.14
1	A	323	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	350	ALA	N-CA-C	6.89	119.96	110.24
1	B	384	HIS	CB-CG-CD2	-6.87	122.27	131.20
1	A	162	LEU	N-CA-C	6.86	120.18	109.96
1	B	498	ARG	NE-CZ-NH2	-6.85	113.03	119.20
1	A	249	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	B	465	TYR	N-CA-C	6.84	119.28	108.67
1	A	465	TYR	N-CA-C	6.82	120.38	108.52
1	A	238	GLU	N-CA-C	6.81	119.33	111.02
1	B	512	THR	N-CA-C	6.80	119.98	108.90
1	A	549	GLN	OE1-CD-NE2	-6.77	115.83	122.60
1	B	319	ILE	CA-C-N	6.77	126.28	119.24
1	B	319	ILE	C-N-CA	6.77	126.28	119.24
1	A	87	ILE	O-C-N	-6.75	115.54	123.03
1	A	80	ASN	CA-CB-CG	-6.75	105.86	112.60
1	B	524	ASN	CB-CG-ND2	6.73	126.50	116.40
1	B	171	LYS	N-CA-C	6.72	120.43	110.48
1	A	235	ILE	N-CA-C	6.69	116.79	110.30
1	A	450	ASP	N-CA-C	6.68	119.44	110.35
1	B	184	THR	N-CA-C	6.68	119.40	108.52
1	A	486	ASN	OD1-CG-ND2	-6.67	115.94	122.60
1	B	486	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	A	171	LYS	N-CA-C	6.63	120.30	109.76
1	B	358	TRP	N-CA-C	6.60	124.86	110.80
1	B	399	SER	CB-CA-C	-6.60	99.84	110.79
1	B	402	ALA	N-CA-C	-6.57	103.81	110.97
1	A	547	GLN	CG-CD-NE2	6.56	126.24	116.40
1	B	10	ALA	N-CA-C	6.56	118.77	110.24
1	B	345	ASN	CB-CG-ND2	6.56	126.23	116.40
1	B	323	GLN	CG-CD-NE2	6.53	126.20	116.40
1	A	422	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	A	277	SER	N-CA-C	6.50	119.20	111.33
1	A	262	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	322	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	317	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	487	GLN	N-CA-C	6.48	120.29	112.38
1	A	60	GLY	N-CA-C	6.47	120.76	111.12
1	B	65	TYR	O-C-N	-6.45	115.57	121.89
1	A	132	ILE	O-C-N	-6.45	116.20	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASN	CB-CG-ND2	6.42	126.04	116.40
1	A	434	ALA	N-CA-C	6.42	124.47	110.80
1	A	92	ILE	N-CA-C	6.41	117.31	109.30
1	A	131	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	A	417	HIS	CA-CB-CG	-6.41	107.39	113.80
1	B	317	PHE	CA-CB-CG	-6.41	107.39	113.80
1	A	117	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	B	90	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	B	387	GLU	O-C-N	-6.36	116.00	123.25
1	B	131	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	B	304	ASN	CA-CB-CG	-6.35	106.25	112.60
1	B	87	ILE	O-C-N	-6.35	115.98	123.03
1	A	348	LYS	CA-CB-CG	6.34	126.78	114.10
1	B	298	LYS	O-C-N	-6.33	115.02	122.81
1	B	245	ASN	CB-CG-ND2	6.33	125.90	116.40
1	B	289	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	430	GLU	O-C-N	-6.33	114.18	122.59
1	B	384	HIS	CB-CG-ND1	6.33	132.19	122.70
1	A	435	GLU	N-CA-C	6.32	118.98	111.33
1	A	203	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	526	LYS	N-CA-C	6.27	120.03	112.38
1	B	290	GLY	CA-C-O	-6.26	112.27	119.10
1	B	315	ASN	OD1-CG-ND2	-6.25	116.34	122.60
1	A	280	HIS	CB-CG-CD2	-6.22	123.12	131.20
1	A	227	VAL	N-CA-C	6.20	119.73	111.17
1	A	51	ARG	N-CA-C	6.19	118.03	111.28
1	A	205	ASN	CB-CG-ND2	6.18	125.67	116.40
1	B	99	SER	CA-C-N	6.18	128.47	120.44
1	B	99	SER	C-N-CA	6.18	128.47	120.44
1	A	276	LYS	N-CA-C	6.18	118.01	111.28
1	B	3	ILE	N-CA-CB	-6.17	106.07	112.06
1	A	376	GLU	CA-C-O	6.17	126.49	119.27
1	A	502	ARG	CA-C-O	6.17	126.99	120.33
1	A	330	PHE	O-C-N	-6.17	116.01	123.10
1	A	158	ILE	N-CA-C	6.16	117.99	108.44
1	B	475	TYR	O-C-N	-6.16	116.13	123.27
1	B	520	TYR	N-CA-C	6.16	118.67	109.25
1	B	442	LYS	N-CA-C	6.15	118.77	111.33
1	A	518	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	189	ASP	N-CA-C	-6.14	101.84	110.50
1	A	534	MET	N-CA-C	6.13	119.86	112.38
1	A	319	ILE	CA-C-N	6.12	125.61	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ILE	C-N-CA	6.12	125.61	119.24
1	B	75	ARG	N-CA-C	6.12	118.92	111.82
1	B	380	THR	O-C-N	-6.12	116.42	123.33
1	A	160	PRO	CA-C-N	6.11	128.47	120.28
1	A	160	PRO	C-N-CA	6.11	128.47	120.28
1	B	368	SER	N-CA-C	6.10	119.66	111.24
1	B	289	ASP	CA-C-O	6.08	127.30	119.95
1	A	251	VAL	CA-C-N	6.07	127.42	119.84
1	A	251	VAL	C-N-CA	6.07	127.42	119.84
1	A	354	THR	N-CA-C	6.04	117.97	108.55
1	B	407	SER	O-C-N	-6.04	115.91	122.79
1	A	148	GLN	OE1-CD-NE2	-6.01	116.58	122.60
1	A	14	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	B	118	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	324	GLN	CG-CD-NE2	5.99	125.38	116.40
1	B	173	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	B	29	GLN	CG-CD-NE2	5.97	125.35	116.40
1	B	509	ALA	N-CA-C	-5.96	104.69	111.07
1	B	86	VAL	O-C-N	-5.96	115.65	122.62
1	B	260	HIS	CB-CG-CD2	-5.96	123.46	131.20
1	B	249	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	A	31	SER	N-CA-C	5.95	118.47	108.23
1	A	216	ARG	N-CA-C	5.94	123.45	110.80
1	A	69	ALA	N-CA-C	-5.91	104.75	111.14
1	B	80	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	A	476	HIS	CB-CG-ND1	5.91	131.56	122.70
1	B	383	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	50	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	B	421	ARG	O-C-N	-5.87	116.35	123.16
1	B	95	THR	CA-CB-CG2	5.87	120.47	110.50
1	A	84	ARG	N-CA-C	5.86	118.77	108.75
1	A	472	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	A	232	VAL	CA-CB-CG1	5.84	120.33	110.40
1	A	511	ALA	N-CA-C	5.84	117.96	108.26
1	A	267	TYR	N-CA-C	5.84	118.59	111.82
1	A	397	TRP	CG-CD2-CE3	5.83	139.73	133.90
1	A	358	TRP	CA-CB-CG	-5.83	102.52	113.60
1	A	331	ALA	N-CA-C	5.83	117.38	108.52
1	B	299	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	B	191	VAL	N-CA-C	5.80	120.53	112.35
1	B	518	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	169	LEU	N-CA-C	5.79	118.22	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	B	254	GLU	N-CA-C	5.78	118.32	111.33
1	B	517	ILE	O-C-N	-5.77	116.35	123.10
1	B	22	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	B	22	ARG	NE-CZ-NH2	-5.75	114.03	119.20
1	A	104	LYS	N-CA-C	5.74	117.23	110.97
1	B	461	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	387	GLU	O-C-N	-5.74	117.08	123.04
1	A	192	GLU	CA-C-O	-5.72	114.78	121.07
1	B	240	LEU	N-CA-C	5.72	120.12	113.20
1	B	549	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	B	144	ASP	N-CA-C	-5.70	104.76	110.97
1	A	40	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	184	THR	N-CA-C	5.68	117.99	108.73
1	A	233	LYS	CB-CG-CD	-5.68	98.24	111.30
1	A	392	TRP	CE2-CD2-CG	-5.67	100.40	107.20
1	A	392	TRP	CG-CD2-CE3	5.67	139.57	133.90
1	B	363	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	298	LYS	O-C-N	-5.66	115.91	122.87
1	A	417	HIS	CB-CG-CD2	-5.66	123.85	131.20
1	A	244	ALA	N-CA-C	5.65	122.84	110.80
1	B	213	GLY	CA-C-N	5.65	125.77	119.32
1	B	213	GLY	C-N-CA	5.65	125.77	119.32
1	A	80	ASN	N-CA-C	5.62	119.62	112.87
1	A	464	VAL	CA-C-O	5.62	127.26	120.74
1	A	505	GLY	N-CA-C	5.62	120.23	112.37
1	B	463	LYS	CA-C-O	5.60	127.43	121.16
1	A	387	GLU	CB-CA-C	-5.59	100.70	111.78
1	B	490	ARG	N-CA-C	5.59	117.52	108.41
1	B	59	GLY	O-C-N	-5.58	118.57	123.76
1	A	94	SER	O-C-N	-5.57	116.23	122.75
1	B	81	GLY	N-CA-C	5.57	123.28	115.43
1	A	264	ASN	CA-CB-CG	5.56	118.16	112.60
1	B	155	GLU	N-CA-C	5.56	117.63	109.24
1	B	282	PHE	CA-C-N	5.54	126.01	122.18
1	B	282	PHE	C-N-CA	5.54	126.01	122.18
1	B	299	HIS	N-CA-C	5.54	119.86	113.38
1	A	108	ILE	CA-CB-CG2	5.53	119.90	110.50
1	A	44	SER	CA-CB-OG	-5.53	100.05	111.10
1	B	430	GLU	CA-C-O	-5.51	112.63	120.51
1	B	165	ASP	N-CA-C	-5.49	100.23	109.07
1	A	61	ASP	CA-CB-CG	5.48	118.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	B	270	ASP	CA-CB-CG	-5.48	107.12	112.60
1	A	67	LYS	N-CA-C	5.48	122.47	110.80
1	B	212	SER	N-CA-C	5.47	121.65	114.75
1	B	246	SER	N-CA-C	-5.47	105.74	112.90
1	A	213	GLY	CA-C-N	5.46	124.92	119.24
1	A	213	GLY	C-N-CA	5.46	124.92	119.24
1	A	421	ARG	O-C-N	-5.45	116.86	123.13
1	B	400	ILE	O-C-N	-5.45	116.22	121.83
1	B	303	VAL	CA-C-O	5.44	126.35	120.53
1	B	21	LEU	N-CA-C	5.44	118.20	107.98
1	A	528	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	4	VAL	O-C-N	-5.43	116.76	122.95
1	A	189	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	361	PHE	CA-C-N	5.43	126.12	119.99
1	A	361	PHE	C-N-CA	5.43	126.12	119.99
1	B	160	PRO	N-CA-C	5.43	122.57	113.78
1	A	454	VAL	O-C-N	-5.42	117.88	122.65
1	B	148	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	B	218	LYS	N-CA-C	5.42	117.07	108.67
1	A	11	TYR	N-CA-C	5.41	118.38	110.10
1	A	353	GLU	N-CA-C	-5.41	100.89	109.76
1	B	429	TYR	N-CA-C	-5.39	99.62	108.41
1	B	308	SER	O-C-N	-5.39	115.92	122.11
1	A	304	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	299	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	B	54	ALA	N-CA-C	5.38	118.83	110.17
1	B	345	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	164	VAL	N-CA-C	5.37	116.28	110.21
1	A	316	ILE	N-CA-CB	-5.36	101.49	110.65
1	B	422	ASN	CA-CB-CG	-5.35	107.25	112.60
1	B	529	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	A	550	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	549	GLN	CA-C-N	5.34	128.18	120.38
1	A	549	GLN	C-N-CA	5.34	128.18	120.38
1	A	358	TRP	N-CA-C	5.34	122.17	110.80
1	B	6	VAL	N-CA-C	5.34	115.99	108.36
1	A	172	GLN	CG-CD-NE2	5.32	124.38	116.40
1	A	506	THR	N-CA-C	5.32	117.75	108.76
1	B	260	HIS	CB-CG-ND1	5.32	130.68	122.70
1	B	61	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	323	GLN	O-C-N	-5.31	115.74	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	N-CA-C	5.30	117.81	111.71
1	A	354	THR	CA-CB-OG1	-5.30	101.66	109.60
1	A	554	ARG	N-CA-C	5.30	117.38	109.59
1	A	462	ASP	N-CA-CB	-5.29	101.55	110.49
1	B	50	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	B	169	LEU	CB-CA-C	-5.29	100.15	109.62
1	A	161	ASP	N-CA-C	5.28	117.04	111.28
1	A	518	ASP	O-C-N	-5.27	116.38	122.87
1	A	173	GLN	CG-CD-NE2	5.26	124.30	116.40
1	B	163	LYS	N-CA-C	5.26	116.91	107.80
1	A	115	ALA	N-CA-C	-5.26	106.62	112.57
1	A	169	LEU	N-CA-C	5.26	117.32	110.43
1	A	232	VAL	CA-CB-CG2	-5.26	101.46	110.40
1	A	155	GLU	N-CA-C	5.25	117.74	108.75
1	B	430	GLU	CA-CB-CG	-5.25	103.60	114.10
1	B	188	VAL	CA-CB-CG2	-5.25	101.48	110.40
1	B	307	ASP	N-CA-C	-5.23	105.49	111.14
1	A	114	THR	N-CA-C	5.23	117.95	108.69
1	A	73	ILE	CB-CA-C	-5.23	105.28	111.97
1	A	495	ASP	CA-C-O	5.22	125.81	119.38
1	A	39	ILE	CB-CG1-CD1	-5.22	102.83	113.80
1	A	92	ILE	CA-CB-CG1	-5.22	101.53	110.40
1	A	255	ASP	N-CA-CB	-5.22	102.59	111.20
1	B	463	LYS	N-CA-C	5.21	118.00	110.28
1	A	533	VAL	N-CA-C	-5.21	105.52	110.42
1	A	215	ASN	CB-CG-ND2	5.21	124.22	116.40
1	B	438	THR	CA-C-O	5.21	125.96	119.97
1	B	497	SER	O-C-N	-5.18	116.88	122.79
1	A	25	VAL	CG1-CB-CG2	-5.18	99.41	110.80
1	B	97	ALA	N-CA-C	-5.17	105.82	111.82
1	A	33	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	B	456	LYS	CA-CB-CG	5.15	124.41	114.10
1	A	512	THR	N-CA-C	5.15	117.94	109.76
1	A	487	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	A	125	ASP	N-CA-C	5.14	118.07	110.46
1	A	134	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	B	502	ARG	CG-CD-NE	-5.14	100.68	112.00
1	B	392	TRP	CB-CG-CD1	-5.14	119.19	126.90
1	B	392	TRP	CG-CD2-CE3	5.14	139.04	133.90
1	A	210	LEU	N-CA-C	5.14	116.88	111.28
1	B	420	GLY	O-C-N	-5.13	116.66	122.56
1	B	397	TRP	CG-CD2-CE3	5.13	139.03	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	VAL	N-CA-CB	-5.12	105.13	110.72
1	A	462	ASP	N-CA-C	5.12	121.70	110.80
1	B	59	GLY	N-CA-C	5.11	118.53	110.91
1	A	141	ALA	N-CA-C	5.11	117.52	111.33
1	B	498	ARG	CA-CB-CG	5.11	124.32	114.10
1	B	415	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	B	494	ALA	N-CA-C	5.11	118.61	112.38
1	B	47	GLU	CA-C-N	5.10	126.22	119.84
1	B	47	GLU	C-N-CA	5.10	126.22	119.84
1	A	250	CYS	N-CA-C	5.10	118.33	112.57
1	A	10	ALA	N-CA-C	5.10	121.66	110.80
1	B	290	GLY	N-CA-C	5.10	121.84	115.21
1	B	180	PHE	N-CA-C	5.09	118.59	112.38
1	B	392	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	B	434	ALA	O-C-N	-5.08	116.27	122.22
1	B	133	SER	N-CA-C	5.08	121.62	110.80
1	A	397	TRP	CB-CG-CD1	-5.08	119.29	126.90
1	B	287	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	173	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	188	VAL	N-CA-C	5.06	116.88	108.99
1	B	552	THR	CA-C-O	5.05	124.31	118.55
1	B	487	GLN	N-CA-C	5.05	119.29	113.18
1	A	202	PHE	N-CA-C	5.05	118.24	110.42
1	B	138	ALA	CA-C-N	5.04	125.05	120.21
1	B	138	ALA	C-N-CA	5.04	125.05	120.21
1	B	17	GLY	O-C-N	-5.04	116.77	122.91
1	B	303	VAL	N-CA-C	-5.03	100.51	107.80
1	A	384	HIS	CA-CB-CG	5.02	118.82	113.80
1	A	373	CYS	N-CA-C	5.02	116.87	108.99
1	B	50	GLN	N-CA-C	5.01	118.50	112.38
1	B	348	LYS	N-CA-C	5.01	121.47	110.80
1	A	477	ASP	CA-C-N	5.00	124.61	119.56
1	A	477	ASP	C-N-CA	5.00	124.61	119.56

There are no chirality outliers.

There are no planarity outliers.

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	4329	0	4332	105	0
1	B	4329	0	4332	98	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	157	0	0	6	0
4	B	233	0	0	12	0
All	All	9060	0	8664	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (203) 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:309:VAL:HG21	1:A:374:GLY:HA3	1.63	0.78
1:B:306:SER:HB3	1:B:337:SER:HB3	1.69	0.74
1:A:16:PRO:HB2	1:A:143:THR:HG22	1.68	0.74
1:A:292:ARG:HD3	1:A:377:SER:O	1.90	0.71
1:B:1:VAL:HG23	1:B:176:LEU:HD23	1.74	0.69
1:B:439:LYS:HD3	1:B:551:ARG:HD2	1.76	0.68
1:A:309:VAL:HG22	1:A:380:THR:HG23	1.74	0.68
1:B:448:MET:HA	1:B:453:PHE:CD2	2.29	0.67
1:A:14:GLN:HE21	1:A:150:SER:HB2	1.58	0.67
1:B:33:ASN:HB3	1:B:37:ASN:ND2	2.10	0.67
1:A:427:TYR:HB2	1:A:515:LEU:HB3	1.78	0.66
1:A:25:VAL:HG12	1:A:29:GLN:HE21	1.61	0.65
1:A:292:ARG:NH1	4:A:607:HOH:O	2.29	0.64
1:B:264:ASN:HD21	1:B:267:TYR:HD2	1.44	0.63
1:B:473:PHE:HD1	1:B:490:ARG:NH1	1.96	0.63
1:B:216:ARG:NH2	1:B:243:PRO:HG2	2.13	0.63
1:B:68:GLU:HB2	4:B:735:HOH:O	1.97	0.63
1:A:268:ALA:HB3	1:A:294:MET:HE1	1.81	0.62
1:B:18:THR:HG21	1:B:359:LYS:HD3	1.82	0.62
1:B:451:ARG:HD3	1:B:451:ARG:H	1.64	0.62
1:A:365:MET:HG3	1:A:370:LEU:HD23	1.83	0.61
1:B:104:LYS:NZ	4:B:568:HOH:O	2.35	0.60
1:B:216:ARG:HH21	1:B:243:PRO:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:HA	1:A:51:ARG:HD2	1.83	0.60
1:A:225:HIS:HD2	4:A:687:HOH:O	1.85	0.59
1:A:88:GLY:HA3	1:A:93:LEU:HD13	1.84	0.59
1:A:63:ARG:HB3	1:A:256:PHE:CE1	2.38	0.59
1:B:73:ILE:CD1	1:B:113:LEU:HD21	2.33	0.59
1:A:276:LYS:HA	1:A:299:HIS:O	2.03	0.58
1:A:441:MET:HE3	1:A:503:LEU:HB2	1.86	0.57
1:B:474:GLU:HG3	1:B:485:LYS:HG2	1.85	0.57
1:B:271:LEU:HD13	1:B:296:LEU:HD12	1.85	0.57
1:B:501:PHE:CE1	1:B:515:LEU:HD13	2.39	0.57
1:A:338:GLY:HA2	1:A:341:ASP:OD1	2.05	0.56
1:A:247:ALA:HB1	1:A:250:CYS:SG	2.45	0.56
1:A:427:TYR:HD2	1:A:515:LEU:HD23	1.71	0.56
1:B:14:GLN:HE21	1:B:150:SER:HB2	1.70	0.56
1:A:233:LYS:O	1:A:237:CYS:HB2	2.06	0.56
1:A:430:GLU:HA	1:A:512:THR:HG23	1.86	0.56
1:A:437:ALA:HB1	1:A:503:LEU:HD11	1.87	0.55
1:A:426:ARG:HG3	1:A:516:TYR:CD1	2.42	0.55
1:B:15:LYS:HG3	1:B:147:PHE:CD2	2.41	0.55
1:B:319:ILE:HB	1:B:322:PHE:HD2	1.72	0.54
1:A:359:LYS:HD3	1:A:359:LYS:H	1.72	0.54
1:B:519:SER:HB3	1:B:535:LEU:HD23	1.89	0.54
1:B:342:ARG:HD2	1:B:520:TYR:CE1	2.43	0.54
1:B:389:ASP:HB3	1:B:392:TRP:HB3	1.91	0.53
1:B:456:LYS:NZ	1:B:457:GLN:O	2.42	0.53
1:B:210:LEU:HG	1:B:402:ALA:HB2	1.90	0.53
1:B:432:VAL:HB	1:B:511:ALA:O	2.09	0.53
1:B:368:SER:HA	4:B:660:HOH:O	2.08	0.53
1:A:3:ILE:H	1:A:177:GLU:HG2	1.74	0.53
1:A:440:MET:SD	1:A:548:LEU:HA	2.48	0.53
1:A:14:GLN:HG2	1:A:21:LEU:HD21	1.91	0.52
1:B:73:ILE:HD12	1:B:113:LEU:HD21	1.91	0.52
1:B:259:HIS:HB2	4:B:620:HOH:O	2.09	0.52
1:B:317:PHE:CZ	1:B:327:VAL:HG23	2.45	0.52
1:B:426:ARG:HG3	1:B:516:TYR:CD1	2.44	0.52
1:B:117:HIS:CD2	1:B:262:ASP:HB2	2.44	0.52
1:A:201:ILE:HA	1:A:321:TYR:HB2	1.92	0.51
1:A:301:PHE:HE1	1:A:412:LEU:HD12	1.75	0.51
1:B:469:LYS:HB3	1:B:492:ILE:HB	1.93	0.51
1:B:448:MET:SD	1:B:489:LEU:HD13	2.52	0.50
1:A:489:LEU:HB2	1:A:501:PHE:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:MET:HE1	1:A:501:PHE:HB3	1.93	0.50
1:B:264:ASN:ND2	1:B:267:TYR:HD2	2.10	0.50
1:B:343:VAL:O	1:B:347:THR:HG22	2.12	0.49
1:A:143:THR:HA	1:A:146:ILE:HD12	1.94	0.49
1:A:358:TRP:CD1	1:A:388:LYS:HD3	2.47	0.49
1:B:384:HIS:CD2	1:B:385:ILE:HG12	2.47	0.49
1:A:441:MET:HG3	1:A:503:LEU:HD22	1.94	0.49
1:A:559:VAL:HG13	4:A:609:HOH:O	2.12	0.49
1:A:198:LEU:HD13	1:A:395:LEU:HD12	1.95	0.48
1:A:176:LEU:HD11	1:A:183:PHE:HB2	1.95	0.48
1:A:449:PHE:HE1	1:A:471:ASP:HA	1.78	0.48
1:B:383:ASP:HB2	4:B:669:HOH:O	2.12	0.48
1:A:537:PRO:O	1:A:541:ILE:HG13	2.14	0.48
1:A:395:LEU:HD23	1:A:398:LEU:HD12	1.95	0.48
1:A:536:ALA:HA	1:A:539:ILE:HD12	1.95	0.48
1:A:320:PRO:HA	1:A:323:GLN:HE21	1.79	0.48
1:A:497:SER:HB3	1:A:538:LEU:HD11	1.96	0.48
1:A:19:SER:O	1:A:22:ARG:NH2	2.46	0.48
1:A:333:SER:HA	1:A:354:THR:O	2.14	0.48
1:B:358:TRP:CH2	1:B:365:MET:SD	3.07	0.47
1:B:499:ILE:HD13	1:B:542:ALA:HB2	1.96	0.47
1:A:63:ARG:NH1	1:A:115:ALA:HB3	2.30	0.47
1:B:291:ASP:HB2	1:B:388:LYS:HB2	1.96	0.47
1:B:448:MET:HE1	1:B:489:LEU:HB3	1.95	0.47
1:A:89:GLN:O	1:A:90:ASN:HB2	2.15	0.47
1:B:451:ARG:HD3	1:B:451:ARG:N	2.29	0.47
1:B:413:LYS:NZ	4:B:794:HOH:O	2.48	0.47
1:B:23:LYS:HB2	1:B:28:PHE:CE2	2.49	0.47
1:B:338:GLY:HA2	1:B:341:ASP:OD1	2.15	0.47
1:A:24:ARG:HG3	1:A:27:VAL:HG23	1.97	0.47
1:B:544:LYS:HG2	4:B:778:HOH:O	2.14	0.47
1:A:491:LEU:O	1:A:498:ARG:HA	2.16	0.46
1:A:500:ILE:HB	1:A:516:TYR:HB2	1.97	0.46
1:A:432:VAL:HG22	1:A:511:ALA:O	2.15	0.46
1:B:363:ASN:HB3	1:B:479:VAL:HG11	1.97	0.46
1:A:39:ILE:HG22	1:A:76:ILE:HG21	1.98	0.46
1:A:68:GLU:HA	1:A:71:GLN:HB2	1.97	0.46
1:A:2:LYS:O	1:A:159:CYS:HA	2.16	0.46
1:A:76:ILE:O	1:A:80:ASN:HB2	2.16	0.46
1:A:84:ARG:HH21	1:A:186:GLU:CD	2.24	0.46
1:A:276:LYS:HA	1:A:299:HIS:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:THR:HA	1:B:84:ARG:O	2.15	0.46
1:A:80:ASN:ND2	1:A:157:ALA:HB3	2.31	0.46
1:A:280:HIS:O	1:A:298:LYS:HG3	2.16	0.46
1:B:365:MET:HG3	1:B:370:LEU:HD23	1.98	0.46
1:A:25:VAL:HG12	1:A:29:GLN:NE2	2.31	0.46
1:A:117:HIS:CD2	1:A:262:ASP:OD2	2.68	0.46
1:B:117:HIS:HB3	4:B:601:HOH:O	2.15	0.46
1:A:501:PHE:CZ	1:A:515:LEU:HD13	2.51	0.45
1:B:220:ARG:NH1	4:B:627:HOH:O	2.47	0.45
1:A:163:LYS:HD2	4:A:584:HOH:O	2.15	0.45
1:B:261:PRO:HB2	1:B:288:GLY:N	2.30	0.45
1:B:363:ASN:O	1:B:479:VAL:HG21	2.15	0.45
1:A:112:ILE:HD12	1:A:112:ILE:N	2.32	0.45
1:A:301:PHE:HE1	1:A:412:LEU:CD1	2.30	0.45
1:A:307:ASP:O	1:A:310:ALA:HB3	2.16	0.45
1:A:458:PHE:HB2	1:A:465:TYR:HB2	1.97	0.45
1:B:426:ARG:HG3	1:B:516:TYR:CE1	2.52	0.45
1:A:224:MET:HE3	1:A:285:ALA:HB1	1.98	0.45
1:B:425:THR:HG22	1:B:535:LEU:HD13	1.97	0.45
1:A:63:ARG:HB3	1:A:256:PHE:HE1	1.82	0.45
1:A:263:PRO:HD3	1:A:287:ASP:HB3	1.99	0.45
1:B:196:THR:O	1:B:199:ARG:HB2	2.17	0.45
1:A:280:HIS:H	1:A:280:HIS:CD2	2.35	0.44
1:A:536:ALA:HB3	1:A:537:PRO:HD3	1.98	0.44
1:B:214:PRO:HG2	1:B:215:ASN:OD1	2.17	0.44
1:B:222:ASP:HB2	1:B:271:LEU:HG	1.98	0.44
1:B:503:LEU:HG	1:B:506:THR:HA	1.98	0.44
1:A:264:ASN:HD21	1:A:267:TYR:HD2	1.65	0.44
1:A:58:VAL:HB	1:A:87:ILE:HG12	1.99	0.44
1:A:132:ILE:HD11	4:A:668:HOH:O	2.17	0.44
1:A:3:ILE:HG23	1:A:79:ALA:HB1	1.99	0.44
1:A:69:ALA:O	1:A:72:LEU:HB2	2.18	0.44
1:A:343:VAL:HA	1:A:419:PHE:CE1	2.53	0.44
1:B:140:GLU:O	1:B:144:ASP:HB2	2.18	0.44
1:B:490:ARG:HE	1:B:492:ILE:HD11	1.83	0.44
1:A:462:ASP:CG	1:A:526:LYS:HZ3	2.26	0.44
1:B:218:LYS:HZ1	1:B:279:GLU:CD	2.26	0.43
1:A:291:ASP:O	1:A:388:LYS:HE2	2.18	0.43
1:B:89:GLN:O	1:B:90:ASN:HB2	2.17	0.43
1:B:554:ARG:HD2	4:B:716:HOH:O	2.17	0.43
1:B:199:ARG:NH1	1:B:239:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD23	1:A:98:VAL:HG22	2.00	0.43
1:B:232:VAL:HG13	1:B:236:LEU:HD12	2.00	0.43
1:A:301:PHE:CE2	1:A:409:GLU:HG3	2.54	0.43
1:B:405:LYS:HA	4:B:757:HOH:O	2.19	0.43
1:B:118:ASN:HA	1:B:119:PRO:HD3	1.90	0.43
1:A:225:HIS:NE2	1:A:249:ASN:OD1	2.52	0.43
1:B:43:ILE:HG23	1:B:82:ILE:HD11	2.00	0.43
1:B:329:GLY:HA3	1:B:369:LYS:O	2.18	0.43
1:A:441:MET:SD	1:A:489:LEU:HG	2.59	0.42
1:A:519:SER:HB3	1:A:535:LEU:HD23	2.01	0.42
1:B:59:GLY:O	1:B:112:ILE:HA	2.19	0.42
1:B:106:LYS:NZ	4:B:741:HOH:O	2.51	0.42
1:A:453:PHE:O	1:A:456:LYS:NZ	2.52	0.42
1:A:71:GLN:HB3	1:A:75:ARG:NH1	2.35	0.42
1:B:354:THR:HG22	1:B:475:TYR:CZ	2.55	0.42
1:B:534:MET:HE3	1:B:534:MET:HB3	1.73	0.42
1:B:371:SER:O	1:B:382:SER:HA	2.18	0.42
1:B:171:LYS:HE3	1:B:184:THR:HG21	2.01	0.42
1:A:44:SER:HA	1:A:51:ARG:HH22	1.85	0.42
1:B:220:ARG:HH11	1:B:248:VAL:CG2	2.32	0.42
1:A:358:TRP:CH2	1:A:365:MET:SD	3.13	0.41
1:A:358:TRP:HH2	1:A:365:MET:SD	2.43	0.41
1:A:535:LEU:O	1:A:539:ILE:HG13	2.20	0.41
1:B:9:LYS:HB2	1:B:9:LYS:HE3	1.69	0.41
1:B:147:PHE:O	1:B:151:LYS:HG2	2.20	0.41
1:B:261:PRO:HB2	1:B:288:GLY:H	1.85	0.41
1:B:98:VAL:HG11	1:B:112:ILE:HG12	2.02	0.41
1:B:449:PHE:HE1	1:B:471:ASP:HA	1.85	0.41
1:B:476:HIS:CD2	1:B:483:VAL:HG22	2.55	0.41
1:B:199:ARG:NH1	1:B:239:GLU:OE1	2.51	0.41
1:A:63:ARG:CZ	1:A:115:ALA:HB3	2.50	0.41
1:A:465:TYR:HB3	1:A:493:PHE:CD1	2.56	0.41
1:A:21:LEU:HD11	1:A:23:LYS:HE3	2.03	0.41
1:B:164:VAL:HG12	1:B:165:ASP:N	2.35	0.41
1:B:164:VAL:HG21	1:B:185:VAL:HG21	2.02	0.41
1:B:292:ARG:HG2	1:B:378:PHE:O	2.20	0.41
1:B:292:ARG:HH11	1:B:292:ARG:HD3	1.65	0.41
1:A:44:SER:HA	1:A:51:ARG:NH2	2.36	0.41
1:A:61:ASP:HA	1:A:227:VAL:CG2	2.51	0.41
1:A:201:ILE:HG21	1:A:201:ILE:HD13	1.87	0.41
1:B:311:VAL:HG11	1:B:397:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HD2	1:B:520:TYR:HE1	1.85	0.41
1:B:536:ALA:HB3	1:B:537:PRO:HD3	2.02	0.41
1:A:76:ILE:HG13	1:A:158:ILE:HG13	2.03	0.41
1:B:347:THR:HG23	1:B:347:THR:O	2.21	0.41
1:B:359:LYS:H	1:B:359:LYS:HE2	1.85	0.41
1:B:554:ARG:HA	1:B:554:ARG:HD3	1.82	0.41
1:A:51:ARG:HD3	1:A:80:ASN:O	2.21	0.40
1:A:68:GLU:H	1:A:68:GLU:CD	2.29	0.40
1:B:88:GLY:HA3	1:B:93:LEU:HD13	2.03	0.40
1:A:104:LYS:NZ	4:A:593:HOH:O	2.54	0.40
1:A:259:HIS:CG	1:A:260:HIS:N	2.89	0.40
1:B:69:ALA:O	1:B:73:ILE:HG13	2.22	0.40
1:B:372:LEU:HD12	1:B:381:GLY:O	2.21	0.40
1:A:14:GLN:O	1:A:16:PRO:HD3	2.21	0.40
1:A:222:ASP:OD1	1:A:249:ASN:HB2	2.22	0.40
1:A:418:LYS:HE2	1:A:418:LYS:HB3	1.79	0.40

There are no symmetry-related clashes.

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	559/561 (100%)	499 (89%)	44 (8%)	16 (3%)	3	9
1	B	559/561 (100%)	505 (90%)	45 (8%)	9 (2%)	7	20
All	All	1118/1122 (100%)	1004 (90%)	89 (8%)	25 (2%)	5	14

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	301	PHE

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Mol	Chain	Res	Type
1	A	431	GLU
1	A	494	ALA
1	B	348	LYS
1	B	456	LYS
1	A	133	SER
1	A	213	GLY
1	A	244	ALA
1	A	434	ALA
1	A	467	VAL
1	B	133	SER
1	B	238	GLU
1	A	21	LEU
1	A	116	SER
1	A	337	SER
1	B	461	ASN
1	B	462	ASP
1	A	358	TRP
1	B	116	SER
1	A	234	LYS
1	A	252	PRO
1	B	119	PRO
1	A	53	GLU
1	B	213	GLY

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	462/462 (100%)	404 (87%)	58 (13%)	4	11
1	B	462/462 (100%)	415 (90%)	47 (10%)	7	18
All	All	924/924 (100%)	819 (89%)	105 (11%)	5	14

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	4	VAL
1	A	22	ARG
1	A	26	LYS
1	A	32	THR
1	A	47	GLU
1	A	48	PRO
1	A	68	GLU
1	A	108	ILE
1	A	112	ILE
1	A	118	ASN
1	A	132	ILE
1	A	139	PRO
1	A	143	THR
1	A	144	ASP
1	A	145	LYS
1	A	148	GLN
1	A	151	LYS
1	A	158	ILE
1	A	162	LEU
1	A	178	ASN
1	A	179	LYS
1	A	199	ARG
1	A	210	LEU
1	A	218	LYS
1	A	227	VAL
1	A	232	VAL
1	A	234	LYS
1	A	243	PRO
1	A	252	PRO
1	A	262	ASP
1	A	291	ASP
1	A	292	ARG
1	A	337	SER
1	A	347	THR
1	A	358	TRP
1	A	359	LYS
1	A	380	THR
1	A	386	ARG
1	A	388	LYS
1	A	414	ASP
1	A	417	HIS
1	A	418	LYS

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Mol	Chain	Res	Type
1	A	431	GLU
1	A	442	LYS
1	A	454	VAL
1	A	456	LYS
1	A	462	ASP
1	A	489	LEU
1	A	491	LEU
1	A	512	THR
1	A	522	LYS
1	A	538	LEU
1	A	543	LEU
1	A	544	LYS
1	A	558	THR
1	A	559	VAL
1	A	561	THR
1	B	7	LYS
1	B	15	LYS
1	B	19	SER
1	B	29	GLN
1	B	37	ASN
1	B	43	ILE
1	B	48	PRO
1	B	53	GLU
1	B	76	ILE
1	B	82	ILE
1	B	95	THR
1	B	106	LYS
1	B	108	ILE
1	B	117	HIS
1	B	140	GLU
1	B	143	THR
1	B	154	GLU
1	B	161	ASP
1	B	163	LYS
1	B	166	LEU
1	B	169	LEU
1	B	182	PRO
1	B	188	VAL
1	B	210	LEU
1	B	215	ASN
1	B	227	VAL
1	B	248	VAL

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Mol	Chain	Res	Type
1	B	271	LEU
1	B	281	ASP
1	B	289	ASP
1	B	325	THR
1	B	358	TRP
1	B	359	LYS
1	B	369	LYS
1	B	376	GLU
1	B	377	SER
1	B	380	THR
1	B	386	ARG
1	B	418	LYS
1	B	426	ARG
1	B	435	GLU
1	B	451	ARG
1	B	461	ASN
1	B	484	SER
1	B	524	ASN
1	B	537	PRO
1	B	538	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	GLN
1	A	117	HIS
1	A	172	GLN
1	A	173	GLN
1	A	178	ASN
1	A	249	ASN
1	A	280	HIS
1	A	323	GLN
1	A	345	ASN
1	A	384	HIS
1	A	422	ASN
1	A	472	ASN
1	B	14	GLN
1	B	37	ASN
1	B	89	GLN
1	B	324	GLN
1	B	476	HIS

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Mol	Chain	Res	Type
1	B	487	GLN
1	B	528	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	563	2	4,4,4	0.33	0	6,6,6	0.16	0
3	SO4	A	563	2	4,4,4	0.60	0	6,6,6	0.75	0

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	561/561 (100%)	0.28	47 (8%) 17 14	0, 37, 91, 98	0
1	B	561/561 (100%)	-0.33	5 (0%) 81 80	3, 24, 56, 84	0
All	All	1122/1122 (100%)	-0.02	52 (4%) 37 34	0, 29, 81, 98	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	ASP	9.0
1	A	437	ALA	7.8
1	A	436	GLY	7.7
1	A	438	THR	7.6
1	A	452	SER	7.5
1	A	448	MET	7.5
1	A	441	MET	7.3
1	A	440	MET	6.9
1	A	449	PHE	6.9
1	A	551	ARG	6.6
1	A	548	LEU	6.2
1	A	550	GLU	6.1
1	A	553	GLY	6.1
1	A	552	THR	5.9
1	A	431	GLU	5.4
1	A	526	LYS	4.9
1	A	549	GLN	4.7
1	A	442	LYS	4.2
1	B	508	SER	4.2
1	A	547	GLN	4.1
1	A	527	ILE	4.0
1	A	458	PHE	4.0
1	A	446	ALA	3.8
1	A	554	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	453	PHE	3.6
1	A	451	ARG	3.6
1	A	444	LEU	3.5
1	A	546	SER	3.4
1	A	525	ALA	3.4
1	A	511	ALA	3.4
1	A	507	GLY	3.3
1	B	506	THR	3.3
1	A	178	ASN	3.2
1	A	443	ASP	3.2
1	A	467	VAL	2.9
1	A	432	VAL	2.8
1	B	505	GLY	2.7
1	B	504	SER	2.7
1	A	523	ASP	2.6
1	A	434	ALA	2.5
1	A	556	ALA	2.4
1	A	259	HIS	2.3
1	A	445	GLU	2.3
1	A	260	HIS	2.2
1	A	536	ALA	2.2
1	A	494	ALA	2.1
1	A	447	LEU	2.1
1	A	503	LEU	2.1
1	A	435	GLU	2.1
1	A	439	LYS	2.1
1	B	215	ASN	2.0
1	A	117	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	563	5/5	0.79	0.23	82,82,83,84	0
3	SO4	A	563	5/5	0.86	0.19	76,76,77,77	0
2	CD	A	562	1/1	0.97	0.25	2,2,2,2	0
2	CD	B	562	1/1	0.98	0.23	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.