



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:25 am BST

PDB ID : 1LXT
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

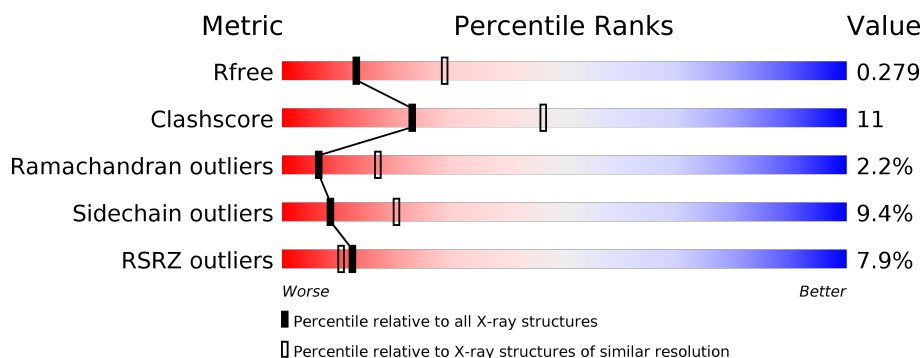
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on 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	<div> <div>14%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>7%</div> </div> </div>
1	B	561	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>5%</div> </div> </div>

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 (three-letter code: CD) (formula: Cd).

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

- Molecule 3 is SULFATE ION (three-letter code: 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		

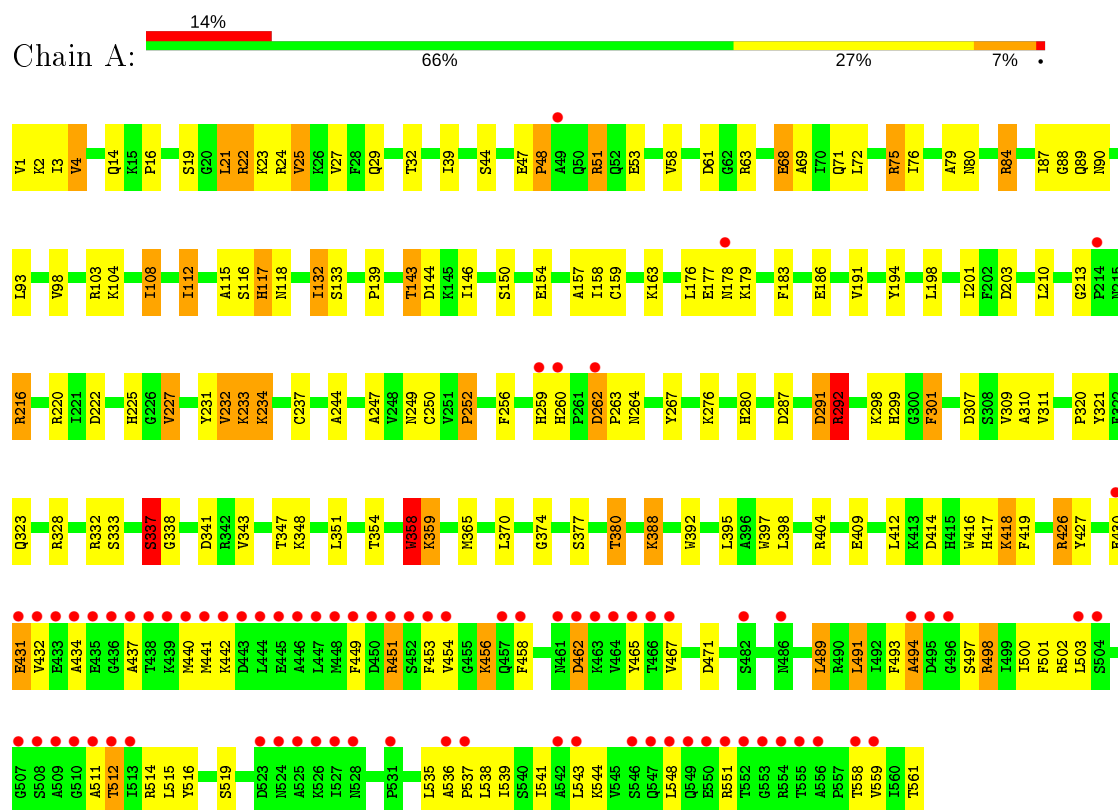
- Molecule 4 is water.

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

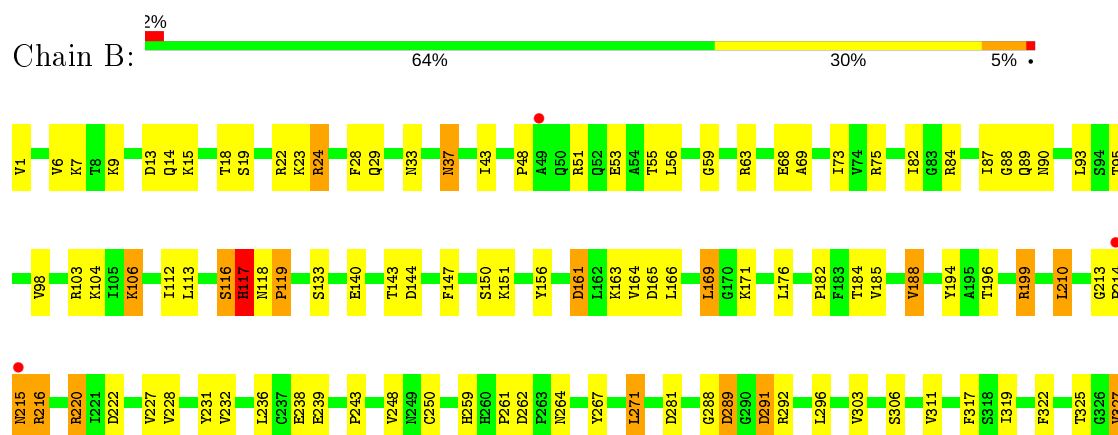
3 Residue-property plots

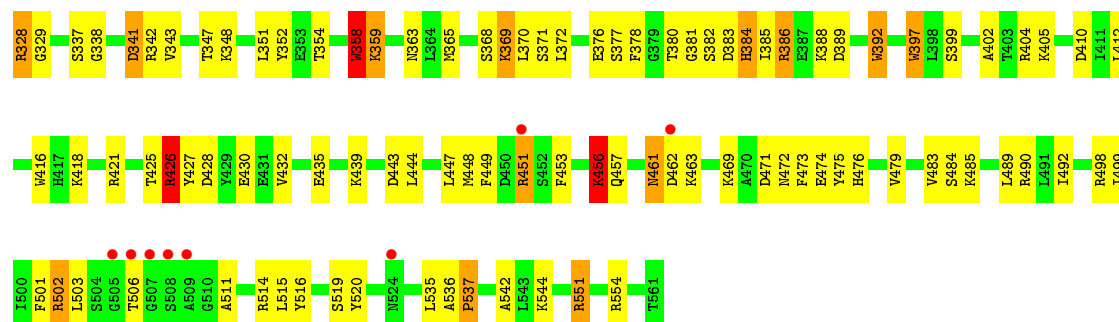
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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) 93.7 (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)	0.27 , 103.6	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	0.89	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	0.83	2/4416 (0.0%)	1.64	53/5969 (0.9%)
1	B	0.88	1/4416 (0.0%)	1.74	84/5969 (1.4%)
All	All	0.85	3/8832 (0.0%)	1.69	137/11938 (1.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	HIS	CD2-NE2	-5.44	1.25	1.38
1	A	292	ARG	CZ-NH1	-5.35	1.26	1.33
1	A	117	HIS	CD2-NE2	-5.09	1.26	1.38

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	ARG	NE-CZ-NH2	-14.53	113.03	120.30
1	B	22	ARG	NE-CZ-NH1	13.90	127.25	120.30
1	B	22	ARG	NE-CZ-NH2	-12.55	114.03	120.30
1	B	498	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	B	502	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	B	404	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	B	386	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	A	392	TRP	CE2-CD2-CG	-8.63	100.40	107.30
1	A	332	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	332	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	551	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	404	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	63	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	451	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	A	392	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	B	392	TRP	CD1-CG-CD2	7.99	112.69	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	TRP	CD1-CG-CD2	7.91	112.62	106.30
1	B	51	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	B	392	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	498	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	358	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	292	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	B	397	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	B	386	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	B	51	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	397	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	B	397	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	404	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	358	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	B	156	TYR	CB-CG-CD2	-7.26	116.64	121.00
1	B	24	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	B	430	GLU	CA-C-N	7.25	133.14	117.20
1	B	231	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	A	25	VAL	CG1-CB-CG2	-7.18	99.41	110.90
1	A	231	TYR	CB-CG-CD2	-7.07	116.75	121.00
1	A	51	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	498	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	194	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	A	210	LEU	CA-CB-CG	7.03	131.48	115.30
1	A	416	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	A	397	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	A	358	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	B	426	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	289	ASP	N-CA-CB	-6.89	98.19	110.60
1	A	216	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	108	ILE	CA-CB-CG1	-6.72	98.22	111.00
1	A	220	ARG	CA-CB-CG	-6.70	98.67	113.40
1	B	514	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	194	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	B	421	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	416	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	A	416	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	B	502	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	A	397	TRP	CG-CD2-CE3	6.48	139.73	133.90
1	A	358	TRP	CD1-CG-CD2	6.45	111.46	106.30
1	A	328	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	289	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	421	ARG	NE-CZ-NH2	-6.33	117.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	VAL	N-CA-CB	-6.31	97.62	111.50
1	A	392	TRP	CG-CD2-CE3	6.30	139.57	133.90
1	A	232	VAL	CA-CB-CG2	-6.29	101.46	110.90
1	A	232	VAL	CA-CB-CG1	6.29	120.33	110.90
1	A	84	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	188	VAL	CA-CB-CG2	-6.28	101.48	110.90
1	A	502	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	348	LYS	CA-CB-CG	6.08	126.78	113.40
1	A	426	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	216	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	291	ASP	CA-CB-CG	6.04	126.69	113.40
1	B	384	HIS	CA-CB-CG	6.03	123.85	113.60
1	B	392	TRP	CB-CG-CD1	-6.01	119.19	127.00
1	A	397	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	A	494	ALA	N-CA-C	5.93	127.01	111.00
1	B	430	GLU	N-CA-C	5.92	127.00	111.00
1	A	358	TRP	CA-CB-CG	-5.88	102.52	113.70
1	A	103	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	472	ASN	N-CA-C	-5.83	95.27	111.00
1	A	514	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	220	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	103	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	291	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	116	SER	CA-C-N	5.77	129.90	117.20
1	B	95	THR	CA-CB-CG2	5.76	120.47	112.40
1	A	451	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	428	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	351	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	B	392	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	B	397	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	B	24	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	328	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	169	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	392	TRP	CB-CG-CD1	-5.63	119.67	127.00
1	B	404	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	4	VAL	CA-CB-CG2	-5.63	102.45	110.90
1	B	444	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	B	551	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	87	ILE	CA-C-N	5.56	127.31	116.20
1	B	117	HIS	CA-CB-CG	5.54	123.02	113.60
1	B	352	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	A	337	SER	N-CA-C	5.52	125.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	VAL	CA-CB-CG2	-5.50	102.66	110.90
1	B	199	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	412	LEU	CA-CB-CG	-5.44	102.79	115.30
1	B	444	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	191	VAL	N-CA-C	5.42	125.63	111.00
1	B	351	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	399	SER	CB-CA-C	-5.40	99.84	110.10
1	B	216	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	341	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	430	GLU	O-C-N	-5.33	114.18	122.70
1	A	551	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	502	ARG	CG-CD-NE	-5.29	100.68	111.80
1	B	169	LEU	CB-CA-C	-5.29	100.15	110.20
1	B	228	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	A	232	VAL	CG1-CB-CG2	-5.28	102.46	110.90
1	B	291	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	75	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	327	VAL	CG1-CB-CG2	-5.26	102.49	110.90
1	B	427	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	B	397	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	B	161	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	95	THR	CA-CB-OG1	-5.21	98.06	109.00
1	B	328	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	210	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	13	ASP	N-CA-C	5.18	124.98	111.00
1	B	447	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	203	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	233	LYS	CB-CG-CD	-5.14	98.24	111.60
1	B	358	TRP	N-CA-C	5.13	124.86	111.00
1	B	426	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	56	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	303	VAL	CA-CB-CG2	-5.10	103.25	110.90
1	A	311	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	A	75	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	250	CYS	N-CA-C	5.05	124.63	111.00
1	A	462	ASP	N-CA-CB	-5.03	101.55	110.60
1	B	456	LYS	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4329	0	4332	101	0
1	B	4329	0	4332	96	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	197	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 11.

All (197) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:448:MET:HE1	1:B:489:LEU:HB3	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:HIS:CD2	1:A:262:ASP:OD2	2.68	0.46
1:A:25:VAL:HG12	1:A:29:GLN:NE2	2.31	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:307:ASP:O	1:A:310:ALA:HB3	2.16	0.45
1:A:301:PHE:HE1	1:A:412:LEU:CD1	2.30	0.45
1:A:458:PHE:HB2	1:A:465:TYR:HB2	1.97	0.45
1:B:463:LYS:NZ	4:B:702:HOH:O	2.49	0.45
1:B:426:ARG:HG3	1:B:516:TYR:CE1	2.52	0.45
1:B:425:THR:HG22	1:B:535:LEU:HD13	1.97	0.45
1:A:263:PRO:HD3	1:A:287:ASP:HB3	1.99	0.45
1:A:63:ARG:HB3	1:A:256:PHE:HE1	1.82	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:132:ILE:HD11	4:A:668:HOH:O	2.17	0.44
1:A:58:VAL:HB	1:A:87:ILE:HG12	1.99	0.44
1:A:343:VAL:HA	1:A:419:PHE:CE1	2.53	0.44
1:A:69:ALA:O	1:A:72:LEU:HB2	2.18	0.44
1:A:3:ILE:HG23	1:A:79:ALA:HB1	1.99	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:291:ASP:O	1:A:388:LYS:HE2	2.18	0.43
1:B:554:ARG:HD2	4:B:716:HOH:O	2.17	0.43
1:B:89:GLN:O	1:B:90:ASN:HB2	2.17	0.43
1:B:199:ARG:NH1	1:B:239:GLU:OE2	2.51	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:329:GLY:HA3	1:B:369:LYS:O	2.18	0.43
1:B:43:ILE:HG23	1:B:82:ILE:HD11	2.00	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:106:LYS:NZ	4:B:741:HOH:O	2.51	0.42
1:B:59:GLY:O	1:B:112:ILE:HA	2.19	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: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:147:PHE:O	1:B:151:LYS:HG2	2.20	0.41
1:B:9:LYS:HB2	1:B:9:LYS:HE3	1.69	0.41
1:B:261:PRO:HB2	1:B:288:GLY:H	1.85	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:98:VAL:HG11	1:B:112:ILE:HG12	2.02	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:453:PHE:O	1:A:456:LYS:NZ	2.52	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:A:276:LYS:HA	1:A:299:HIS:C	2.41	0.41
1:A:84:ARG:HH21	1:A:186:GLU:CD	2.24	0.41
1:B:164:VAL:HG12	1:B:165:ASP:N	2.35	0.41
1:A:456:LYS:HB3	1:A:456:LYS:HZ3	1.86	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:HD3	1:B:292:ARG:HH11	1.65	0.41
1:A:61:ASP:HA	1:A:227:VAL:CG2	2.51	0.41
1:A:44:SER:HA	1:A:51:ARG:NH2	2.36	0.41
1:B:311:VAL:HG11	1:B:397:TRP:CH2	2.55	0.41
1:B:342:ARG:HD2	1:B:520:TYR:HE1	1.85	0.41
1:A:201:ILE:HD13	1:A:201:ILE:HG21	1.87	0.41
1:B:536:ALA:HB3	1:B:537:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:B:359:LYS:H	1.85	0.41
1:B:554:ARG:HD3	1:B:554:ARG:HA	1.82	0.41
1:A:51:ARG:HD3	1:A:80:ASN:O	2.21	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:372:LEU:HD12	1:B:381:GLY:O	2.21	0.40
1:B:69:ALA:O	1:B:73:ILE:HG13	2.22	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
1:A:441:MET:HE2	1:A:503:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	559/561 (100%)	499 (89%)	44 (8%)	16 (3%)	4	10
1	B	559/561 (100%)	505 (90%)	45 (8%)	9 (2%)	9	24
All	All	1118/1122 (100%)	1004 (90%)	89 (8%)	25 (2%)	6	17

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	301	PHE
1	A	431	GLU
1	A	494	ALA

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Mol	Chain	Res	Type
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%)	416 (90%)	46 (10%)	7	18
1	B	462/462 (100%)	421 (91%)	41 (9%)	9	22
All	All	924/924 (100%)	837 (91%)	87 (9%)	8	20

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	4	VAL

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Mol	Chain	Res	Type
1	A	22	ARG
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	154	GLU
1	A	178	ASN
1	A	179	LYS
1	A	227	VAL
1	A	232	VAL
1	A	234	LYS
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	388	LYS
1	A	414	ASP
1	A	417	HIS
1	A	418	LYS
1	A	431	GLU
1	A	442	LYS
1	A	451	ARG
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	543	LEU
1	A	544	LYS

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Mol	Chain	Res	Type
1	A	558	THR
1	A	561	THR
1	B	7	LYS
1	B	19	SER
1	B	24	ARG
1	B	29	GLN
1	B	37	ASN
1	B	48	PRO
1	B	53	GLU
1	B	106	LYS
1	B	117	HIS
1	B	143	THR
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	215	ASN
1	B	220	ARG
1	B	227	VAL
1	B	271	LEU
1	B	281	ASP
1	B	289	ASP
1	B	325	THR
1	B	328	ARG
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	410	ASP
1	B	418	LYS
1	B	426	ARG
1	B	435	GLU
1	B	443	ASP
1	B	451	ARG
1	B	461	ASN
1	B	484	SER
1	B	502	ARG

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Mol	Chain	Res	Type
1	B	537	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	249	ASN
1	A	280	HIS
1	A	323	GLN
1	A	324	GLN
1	A	363	ASN
1	A	384	HIS
1	A	472	ASN
1	B	14	GLN
1	B	476	HIS

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 carbohydrates 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	0.46	0	6,6,6	0.17	0
3	SO4	A	563	2	4,4,4	0.71	0	6,6,6	0.76	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%)	0.56	78 (13%) 2 2	0, 37, 91, 98	0
1	B	561/561 (100%)	-0.31	11 (1%) 65 67	3, 24, 56, 84	0
All	All	1122/1122 (100%)	0.13	89 (7%) 12 10	0, 29, 81, 98	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	ALA	8.6
1	A	511	ALA	8.1
1	A	510	GLY	6.7
1	A	448	MET	6.6
1	A	452	SER	6.3
1	A	432	VAL	6.2
1	A	436	GLY	6.1
1	A	447	LEU	6.0
1	A	437	ALA	5.9
1	A	440	MET	5.9
1	A	450	ASP	5.9
1	A	438	THR	5.7
1	A	556	ALA	5.5
1	A	441	MET	5.5
1	A	444	LEU	5.5
1	A	449	PHE	5.5
1	A	525	ALA	5.4
1	B	508	SER	5.3
1	A	552	THR	5.2
1	A	524	ASN	5.2
1	A	442	LYS	5.1
1	A	434	ALA	5.1
1	A	464	VAL	4.9
1	A	553	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	431	GLU	4.8
1	A	453	PHE	4.7
1	A	178	ASN	4.7
1	A	543	LEU	4.7
1	A	548	LEU	4.6
1	A	551	ARG	4.6
1	A	507	GLY	4.5
1	A	546	SER	4.5
1	A	467	VAL	4.5
1	A	547	GLN	4.5
1	A	458	PHE	4.3
1	A	549	GLN	4.3
1	A	462	ASP	4.2
1	B	506	THR	4.2
1	A	554	ARG	4.1
1	A	503	LEU	4.0
1	A	558	THR	3.9
1	A	527	ILE	3.9
1	A	550	GLU	3.8
1	A	435	GLU	3.8
1	A	463	LYS	3.7
1	A	259	HIS	3.7
1	A	494	ALA	3.7
1	B	509	ALA	3.7
1	A	461	ASN	3.6
1	A	439	LYS	3.6
1	A	523	ASP	3.6
1	A	443	ASP	3.5
1	A	433	GLU	3.5
1	A	512	THR	3.4
1	A	508	SER	3.4
1	A	454	VAL	3.4
1	A	526	LYS	3.3
1	A	495	ASP	3.3
1	A	465	TYR	3.2
1	A	466	THR	3.1
1	A	445	GLU	3.0
1	A	457	GLN	2.9
1	A	451	ARG	2.9
1	A	504	SER	2.7
1	A	509	ALA	2.7
1	A	260	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	555	THR	2.7
1	B	507	GLY	2.6
1	B	462	ASP	2.5
1	B	451	ARG	2.5
1	A	513	ILE	2.5
1	A	536	ALA	2.4
1	B	49	ALA	2.4
1	A	482	SER	2.4
1	B	215	ASN	2.4
1	A	430	GLU	2.4
1	A	528	ASN	2.4
1	A	559	VAL	2.4
1	A	531	PRO	2.3
1	B	505	GLY	2.3
1	A	496	GLY	2.3
1	A	542	ALA	2.2
1	A	486	ASN	2.2
1	B	524	ASN	2.1
1	A	214	PRO	2.1
1	A	49	ALA	2.1
1	A	537	PRO	2.1
1	A	262	ASP	2.1
1	B	214	PRO	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 carbohydrates 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	B	563	5/5	0.85	0.31	82,82,83,84	0
3	SO4	A	563	5/5	0.88	0.30	76,76,77,77	0
2	CD	B	562	1/1	0.99	0.26	2,2,2,2	0
2	CD	A	562	1/1	0.99	0.27	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.