



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:10 PM UTC

PDB ID : 5TNU / pdb_00005tnu
Title : S. tokodaii XPB II crystal structure at 3.0 Angstrom resolution
Authors : DuPrez, K.T.; Hilario, E.; Wang, I.; Fan, L.
Deposited on : 2016-10-14
Resolution : 3.05 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)	:	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

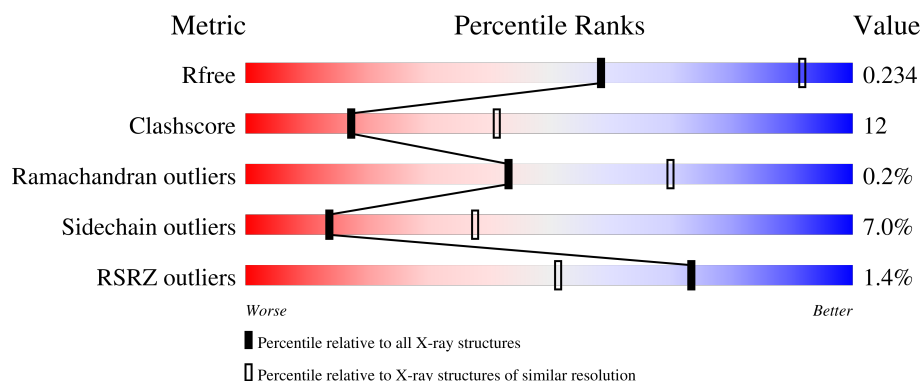
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	459	67% 27% • •
1	B	459	2% 71% 18% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6642 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 DNA-dependent ATPase XPBII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3448	2229	578	636	5			
1	B	411	Total	C	N	O	S	0	1	0
			2956	1897	499	556	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q970I2
A	-18	GLY	-	expression tag	UNP Q970I2
A	-17	SER	-	expression tag	UNP Q970I2
A	-16	SER	-	expression tag	UNP Q970I2
A	-15	HIS	-	expression tag	UNP Q970I2
A	-14	HIS	-	expression tag	UNP Q970I2
A	-13	HIS	-	expression tag	UNP Q970I2
A	-12	HIS	-	expression tag	UNP Q970I2
A	-11	HIS	-	expression tag	UNP Q970I2
A	-10	HIS	-	expression tag	UNP Q970I2
A	-9	SER	-	expression tag	UNP Q970I2
A	-8	SER	-	expression tag	UNP Q970I2
A	-7	GLY	-	expression tag	UNP Q970I2
A	-6	LEU	-	expression tag	UNP Q970I2
A	-5	VAL	-	expression tag	UNP Q970I2
A	-4	PRO	-	expression tag	UNP Q970I2
A	-3	ARG	-	expression tag	UNP Q970I2
A	-2	GLY	-	expression tag	UNP Q970I2
A	-1	SER	-	expression tag	UNP Q970I2
A	0	HIS	-	expression tag	UNP Q970I2
B	-19	MET	-	initiating methionine	UNP Q970I2
B	-18	GLY	-	expression tag	UNP Q970I2
B	-17	SER	-	expression tag	UNP Q970I2
B	-16	SER	-	expression tag	UNP Q970I2
B	-15	HIS	-	expression tag	UNP Q970I2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q970I2
B	-13	HIS	-	expression tag	UNP Q970I2
B	-12	HIS	-	expression tag	UNP Q970I2
B	-11	HIS	-	expression tag	UNP Q970I2
B	-10	HIS	-	expression tag	UNP Q970I2
B	-9	SER	-	expression tag	UNP Q970I2
B	-8	SER	-	expression tag	UNP Q970I2
B	-7	GLY	-	expression tag	UNP Q970I2
B	-6	LEU	-	expression tag	UNP Q970I2
B	-5	VAL	-	expression tag	UNP Q970I2
B	-4	PRO	-	expression tag	UNP Q970I2
B	-3	ARG	-	expression tag	UNP Q970I2
B	-2	GLY	-	expression tag	UNP Q970I2
B	-1	SER	-	expression tag	UNP Q970I2
B	0	HIS	-	expression tag	UNP Q970I2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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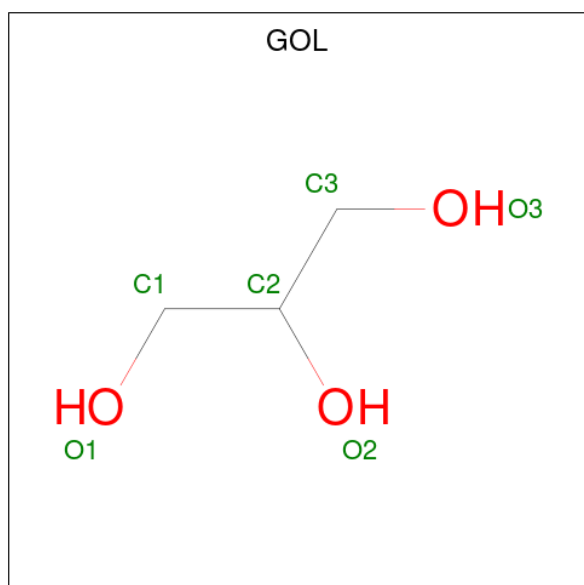
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Cl 5 5	0	0
3	B	2	Total Cl 2 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		
5	B	58	Total	O	0	0
			58	58		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	160.92Å 160.92Å 122.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.05 29.88 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.88-3.05) 99.8 (29.88-3.05)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.196 , 0.226 0.201 , 0.234	Depositor DCC
R_{free} test set	1562 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 94.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6642	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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, CL, GOL

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	0.70	0/3514	0.92	4/4750 (0.1%)
1	B	0.68	0/3011	0.89	2/4089 (0.0%)
All	All	0.69	0/6525	0.91	6/8839 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	VAL	CB-CA-C	-5.89	104.32	112.04
1	B	179	LEU	CA-C-N	-5.85	113.72	120.04
1	B	179	LEU	C-N-CA	-5.85	113.72	120.04
1	A	179	LEU	CA-C-N	-5.74	113.84	120.04
1	A	179	LEU	C-N-CA	-5.74	113.84	120.04
1	A	298	TRP	N-CA-C	-5.01	105.70	111.07

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	3448	0	3417	104	1
1	B	2956	0	2703	53	1
2	A	35	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	0	2	0
3	A	5	0	0	1	0
3	B	2	0	0	0	0
4	A	36	0	48	2	0
4	B	6	0	8	0	0
5	A	71	0	0	11	0
5	B	58	0	0	6	0
All	All	6642	0	6176	158	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 12.

All (158) 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:388:ALA:O	1:A:411:LEU:O	1.76	1.01
1:A:307:ASN:O	1:A:336:MET:HE2	1.71	0.90
1:B:40:ARG:HD3	5:B:623:HOH:O	1.75	0.85
1:A:253:ARG:HD3	5:A:621:HOH:O	1.79	0.83
1:B:329:VAL:HA	1:B:392:ILE:O	1.81	0.81
1:B:208:GLY:O	1:B:211:GLU:HG3	1.81	0.80
1:A:144:ASP:OD1	1:A:160:ARG:NH2	2.15	0.79
1:B:2:VAL:HG11	1:B:43:PHE:HE2	1.47	0.78
1:A:25:GLU:HG3	5:A:658:HOH:O	1.85	0.77
1:B:40:ARG:CD	5:B:623:HOH:O	2.31	0.77
1:B:82:LYS:HE2	5:B:638:HOH:O	1.86	0.74
1:B:40:ARG:HB3	5:B:623:HOH:O	1.88	0.73
1:A:415:ASP:CB	5:A:644:HOH:O	2.36	0.73
1:A:349:VAL:O	1:A:375:ALA:HA	1.88	0.72
1:B:205:ARG:NH2	1:B:207:ASP:OD2	2.23	0.72
1:B:42:TYR:HD1	1:B:43:PHE:HD1	1.37	0.71
1:A:331:THR:O	1:A:376:SER:HA	1.90	0.70
1:A:436:ARG:NH1	3:A:510:CL:CL	2.62	0.70
1:B:144:ASP:OD1	1:B:160:ARG:NH1	2.26	0.69
1:A:237:TYR:HB3	5:A:644:HOH:O	1.92	0.68
1:B:85:ARG:HG3	1:B:217:VAL:O	1.94	0.68
1:A:387:ASP:HA	1:A:410:ILE:O	1.94	0.67
1:A:85:ARG:HG3	1:A:217:VAL:O	1.94	0.67
1:A:225:SER:HB2	1:A:227:GLU:OE1	1.93	0.67
1:A:244:VAL:HG12	1:A:314:LYS:HG3	1.78	0.66
1:B:63:ILE:O	2:B:505:SO4:O3	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASN:CB	1:A:371:ARG:CB	2.74	0.65
1:A:341:SER:HB2	1:A:348:VAL:CG1	2.27	0.65
1:A:5:ARG:HG2	1:A:12:LEU:HB2	1.78	0.64
1:B:40:ARG:CG	5:B:623:HOH:O	2.45	0.64
1:A:315:LEU:HD23	1:A:315:LEU:O	1.98	0.63
1:B:329:VAL:O	1:B:374:VAL:CB	2.47	0.63
1:A:207:ASP:OD2	1:A:209:LYS:HD2	1.99	0.62
1:B:2:VAL:HG11	1:B:43:PHE:CE2	2.33	0.61
1:B:17:ALA:HB2	1:B:43:PHE:CE1	2.35	0.61
1:B:42:TYR:HD1	1:B:43:PHE:CD1	2.19	0.61
1:A:412:ARG:CB	1:A:415:ASP:CB	2.80	0.60
1:A:329:VAL:HG23	1:A:374:VAL:CB	2.31	0.59
1:A:204:GLU:HA	1:A:210:HIS:ND1	2.18	0.58
1:A:327:ILE:HG12	1:A:390:LEU:HB3	1.84	0.58
1:A:395:GLY:HA3	1:A:397:TYR:CE2	2.38	0.58
1:B:191:PHE:O	1:B:196:ARG:NH2	2.36	0.58
1:B:204:GLU:HA	1:B:210:HIS:ND1	2.19	0.58
1:A:393:VAL:HG13	1:A:422:GLU:CB	2.34	0.58
1:B:282:VAL:O	1:B:283:LYS:HG2	2.04	0.58
1:B:96:LYS:HE3	2:B:501:SO4:O1	2.04	0.57
1:B:207:ASP:OD2	1:B:209:LYS:HD2	2.04	0.57
1:B:111:THR:HG22	1:B:170:LEU:HD23	1.87	0.57
1:A:329:VAL:HG23	1:A:374:VAL:HG23	1.87	0.56
1:A:331:THR:O	1:A:376:SER:CA	2.53	0.56
1:B:42:TYR:CD1	1:B:43:PHE:HD1	2.19	0.56
1:A:24:ASP:OD1	1:A:24:ASP:N	2.35	0.56
1:A:347:PRO:HG2	1:A:373:ILE:HG12	1.85	0.56
1:A:329:VAL:HG12	1:A:392:ILE:HB	1.87	0.56
1:B:350:THR:HA	1:B:375:ALA:HB1	1.88	0.56
1:B:40:ARG:CB	5:B:623:HOH:O	2.52	0.56
1:A:412:ARG:CB	1:A:415:ASP:CA	2.84	0.55
1:B:71:ASP:OD1	1:B:233:TYR:CE2	2.61	0.54
1:A:329:VAL:HG23	1:A:374:VAL:HB	1.90	0.54
1:A:372:VAL:O	1:A:373:ILE:HG13	2.07	0.54
1:B:109:VAL:O	1:B:111:THR:HG23	2.08	0.53
1:B:385:VAL:N	1:B:386:PRO:HD2	2.23	0.53
1:A:227:GLU:HG2	1:A:234:ILE:HG22	1.91	0.53
1:A:261:LEU:HD22	1:A:298:TRP:HB2	1.91	0.53
1:B:31:ALA:HB1	1:B:35:LYS:HD2	1.89	0.53
1:B:91:PRO:HB3	1:B:226:VAL:HG22	1.91	0.53
1:A:329:VAL:CG2	1:A:374:VAL:HB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ILE:HD11	1:A:146:LEU:HD13	1.92	0.52
4:A:518:GOL:H2	5:A:649:HOH:O	2.10	0.52
1:A:196:ARG:HD2	5:A:619:HOH:O	2.09	0.52
1:A:223:ARG:O	1:A:224:LYS:HG2	2.10	0.52
1:A:237:TYR:HB2	1:A:418:ALA:O	2.10	0.51
1:A:393:VAL:HG13	1:A:422:GLU:HB2	1.93	0.51
1:B:42:TYR:CD1	1:B:43:PHE:CD1	2.98	0.51
1:B:393:VAL:HG22	1:B:421:ILE:O	2.11	0.51
1:A:259:LYS:HE2	1:A:263:ASP:OD1	2.11	0.50
1:A:359:GLU:O	1:A:363:GLN:HG2	2.12	0.50
1:A:324:ASN:O	1:A:371:ARG:CB	2.60	0.50
1:A:390:LEU:HD12	1:A:391:ALA:H	1.77	0.50
1:A:326:LYS:O	1:A:388:ALA:HB1	2.12	0.49
1:A:328:ILE:HG21	1:A:330:PHE:CZ	2.48	0.49
1:B:339:ARG:O	1:B:343:THR:N	2.45	0.49
1:A:312:ILE:HG12	1:A:340:ILE:HG12	1.94	0.49
1:B:213:TYR:HB2	1:B:214:PRO:HD3	1.95	0.49
1:B:31:ALA:CB	1:B:35:LYS:HD2	2.44	0.48
1:B:139:ILE:HD11	1:B:146:LEU:HD13	1.95	0.48
1:A:312:ILE:HG12	1:A:340:ILE:CG1	2.44	0.48
1:B:24:ASP:O	1:B:27:LYS:HE3	2.13	0.48
1:A:108:LYS:HE2	4:A:513:GOL:H31	1.96	0.48
1:A:329:VAL:HG23	1:A:374:VAL:CG2	2.44	0.48
1:A:139:ILE:HB	1:A:152:ILE:HG13	1.97	0.47
1:A:349:VAL:O	1:A:375:ALA:CA	2.59	0.47
1:A:26:LEU:C	1:A:27:LYS:HG3	2.39	0.47
1:A:274:ASN:HB3	1:A:277:ASP:HB2	1.97	0.47
1:A:328:ILE:CG2	1:A:330:PHE:CZ	2.97	0.47
1:A:349:VAL:O	1:A:375:ALA:CB	2.63	0.47
1:A:432:ARG:NH1	2:A:506:SO4:O1	2.48	0.47
1:A:328:ILE:HD11	1:A:365:PHE:CE2	2.50	0.47
1:A:130:LYS:HD3	1:A:131:TYR:CZ	2.50	0.46
1:A:411:LEU:HD11	1:A:419:LEU:O	2.14	0.46
1:A:327:ILE:O	1:A:365:PHE:CZ	2.68	0.46
1:A:391:ALA:HB3	1:A:420:LEU:CD2	2.46	0.46
1:B:130:LYS:HD3	1:B:131:TYR:CZ	2.51	0.46
1:B:121:ILE:HD11	1:B:153:THR:HG23	1.98	0.46
1:A:363:GLN:OE1	1:A:366:ARG:NE	2.49	0.46
1:A:351:TYR:CD1	1:A:351:TYR:C	2.94	0.45
1:A:379:PHE:CE1	1:A:382:GLY:HA3	2.51	0.45
1:B:325:GLU:C	1:B:388:ALA:HB1	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG13	1:A:423:ILE:CG2	2.47	0.45
1:A:320:GLN:O	1:A:323:LYS:HD2	2.16	0.45
1:A:331:THR:HG21	1:A:336:MET:HB3	1.99	0.45
1:A:439:GLU:O	1:A:439:GLU:HG3	2.17	0.45
1:A:326:LYS:HZ1	1:A:366:ARG:HA	1.83	0.44
1:A:160:ARG:HA	5:A:640:HOH:O	2.18	0.44
1:A:311:LYS:NZ	1:A:430:ASP:OD2	2.47	0.44
1:B:196:ARG:NH1	1:B:216:LEU:O	2.51	0.44
1:A:349:VAL:CB	1:A:375:ALA:HB2	2.48	0.44
1:B:160:ARG:HH21	1:B:163:GLU:CD	2.25	0.44
1:A:41:LYS:HG3	5:A:641:HOH:O	2.17	0.43
1:A:274:ASN:OD1	1:A:276:ASP:N	2.47	0.43
1:A:209:LYS:NZ	5:A:606:HOH:O	2.51	0.43
1:A:265:LEU:HD22	1:A:270:LEU:HB2	1.99	0.43
1:A:407:LEU:O	1:A:411:LEU:N	2.43	0.43
1:B:286:ALA:N	1:B:290:GLU:OE1	2.51	0.43
1:A:238:LYS:HB3	1:A:419:LEU:HD13	2.00	0.43
1:B:139:ILE:HB	1:B:152:ILE:HG13	2.01	0.43
1:A:127:ARG:NH1	2:A:502:SO4:O4	2.49	0.43
1:A:253:ARG:CD	5:A:621:HOH:O	2.54	0.42
1:A:125:LYS:HD2	5:A:638:HOH:O	2.19	0.42
1:B:387:ASP:O	1:B:410:ILE:CB	2.67	0.42
1:A:236:LYS:HE2	1:A:415:ASP:CB	2.49	0.42
1:A:115:VAL:O	1:A:153:THR:HA	2.20	0.42
1:A:121:ILE:HD11	1:A:153:THR:HG23	2.00	0.42
1:B:351:TYR:O	1:B:352:LYS:CB	2.68	0.42
1:B:115:VAL:O	1:B:153:THR:HA	2.20	0.42
1:A:158:TYR:HA	1:A:187:MET:HG3	2.02	0.41
1:A:245:SER:O	1:A:310:SER:OG	2.35	0.41
1:A:274:ASN:OD1	1:A:275:LEU:N	2.53	0.41
1:A:1:MET:HA	1:A:49:GLU:O	2.19	0.41
1:A:237:TYR:HE2	1:A:408:GLY:HA2	1.86	0.41
1:B:229:LEU:H	1:B:229:LEU:HD13	1.85	0.41
1:B:327:ILE:O	1:B:372:VAL:HA	2.21	0.41
1:A:341:SER:CB	1:A:348:VAL:CG1	2.98	0.41
1:A:394:MET:SD	1:A:423:ILE:HD13	2.61	0.41
1:B:223:ARG:O	1:B:224:LYS:HD2	2.21	0.41
1:A:327:ILE:O	1:A:365:PHE:HZ	2.04	0.41
1:A:379:PHE:CD1	1:A:382:GLY:HA3	2.56	0.41
1:A:26:LEU:O	1:A:27:LYS:HG3	2.21	0.40
1:A:64:LYS:NZ	2:A:504:SO4:O1	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:N	1:A:180:PRO:CD	2.84	0.40
1:B:292:ARG:O	1:B:296:LEU:CB	2.69	0.40
1:A:351:TYR:CD1	1:A:351:TYR:O	2.74	0.40
1:A:309:GLN:O	1:A:312:ILE:N	2.53	0.40
1:A:341:SER:HB2	1:A:348:VAL:HG13	2.03	0.40
1:A:412:ARG:CB	1:A:415:ASP:HA	2.50	0.40
1:A:433:LEU:HA	1:A:436:ARG:HB2	2.03	0.40
1:B:160:ARG:NH2	1:B:163:GLU:OE2	2.54	0.40
1:A:341:SER:HB2	1:A:348:VAL:HG12	2.01	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)
1:A:56:ASP:OD2	1:B:167:LYS:NZ[4_555]	2.10	0.10

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	439/459 (96%)	428 (98%)	11 (2%)	0	100	100
1	B	406/459 (88%)	369 (91%)	35 (9%)	2 (0%)	24	52
All	All	845/918 (92%)	797 (94%)	46 (5%)	2 (0%)	43	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	378	VAL
1	B	304	ILE

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	343/401 (86%)	314 (92%)	29 (8%)	10	31
1	B	257/401 (64%)	244 (95%)	13 (5%)	21	48
All	All	600/802 (75%)	558 (93%)	42 (7%)	14	38

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	5	ARG
1	A	13	SER
1	A	21	LYS
1	A	24	ASP
1	A	97	THR
1	A	133	ASP
1	A	160	ARG
1	A	215	ILE
1	A	220	ILE
1	A	228	GLU
1	A	242	LEU
1	A	273	GLN
1	A	316	ARG
1	A	318	ILE
1	A	320	GLN
1	A	323	LYS
1	A	325	GLU
1	A	336	MET
1	A	350	THR
1	A	351	TYR
1	A	353	THR
1	A	355	LYS
1	A	379	PHE
1	A	393	VAL
1	A	416	LYS
1	A	420	LEU

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Mol	Chain	Res	Type
1	A	437	ARG
1	A	439	GLU
1	B	13	SER
1	B	23	SER
1	B	25	GLU
1	B	41	LYS
1	B	133	ASP
1	B	145	SER
1	B	160	ARG
1	B	220	ILE
1	B	229	LEU
1	B	265	LEU
1	B	267	SER
1	B	281	LEU
1	B	290	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	248	ASN
1	A	303	ASN
1	B	129	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 7 are monoatomic - leaving 19 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	$\# Z > 2$
2	SO4	B	502	-	4,4,4	0.50	0	6,6,6	0.28	0
4	GOL	B	508	-	5,5,5	0.51	0	5,5,5	0.45	0
4	GOL	A	515	-	5,5,5	0.55	0	5,5,5	0.64	0
4	GOL	A	517	-	5,5,5	0.55	0	5,5,5	0.41	0
2	SO4	A	505	-	4,4,4	0.52	0	6,6,6	0.24	0
2	SO4	B	505	-	4,4,4	0.60	0	6,6,6	0.40	0
2	SO4	A	504	-	4,4,4	0.56	0	6,6,6	0.48	0
4	GOL	A	518	-	5,5,5	0.67	0	5,5,5	0.49	0
2	SO4	B	501	-	4,4,4	0.43	0	6,6,6	0.42	0
2	SO4	B	503	-	4,4,4	0.53	0	6,6,6	0.26	0
2	SO4	A	507	-	4,4,4	0.52	0	6,6,6	0.32	0
4	GOL	A	514	-	5,5,5	0.39	0	5,5,5	0.29	0
2	SO4	A	501	-	4,4,4	0.43	0	6,6,6	0.35	0
4	GOL	A	516	-	5,5,5	0.44	0	5,5,5	0.33	0
2	SO4	A	502	-	4,4,4	0.46	0	6,6,6	0.44	0
2	SO4	A	503	-	4,4,4	0.55	0	6,6,6	0.33	0
4	GOL	A	513	-	5,5,5	0.42	0	5,5,5	0.39	0
2	SO4	A	506	-	4,4,4	0.51	0	6,6,6	0.75	0
2	SO4	B	504	-	4,4,4	0.56	0	6,6,6	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	518	-	-	1/4/4/4	-
4	GOL	A	513	-	-	0/4/4/4	-
4	GOL	B	508	-	-	4/4/4/4	-
4	GOL	A	515	-	-	4/4/4/4	-
4	GOL	A	514	-	-	2/4/4/4	-
4	GOL	A	517	-	-	4/4/4/4	-
4	GOL	A	516	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	515	GOL	O1-C1-C2-C3
4	A	515	GOL	C1-C2-C3-O3
4	A	516	GOL	O1-C1-C2-C3
4	A	516	GOL	C1-C2-C3-O3
4	A	517	GOL	C1-C2-C3-O3
4	B	508	GOL	C1-C2-C3-O3
4	A	514	GOL	O1-C1-C2-C3
4	A	517	GOL	O1-C1-C2-C3
4	A	518	GOL	C1-C2-C3-O3
4	B	508	GOL	O1-C1-C2-C3
4	A	516	GOL	O1-C1-C2-O2
4	A	516	GOL	O2-C2-C3-O3
4	A	517	GOL	O2-C2-C3-O3
4	B	508	GOL	O1-C1-C2-O2
4	B	508	GOL	O2-C2-C3-O3
4	A	514	GOL	O1-C1-C2-O2
4	A	515	GOL	O2-C2-C3-O3
4	A	515	GOL	O1-C1-C2-O2
4	A	517	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	SO4	1	0
2	A	504	SO4	1	0
4	A	518	GOL	1	0
2	B	501	SO4	1	0
2	A	502	SO4	1	0
4	A	513	GOL	1	0
2	A	506	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	441/459 (96%)	-0.22	4 (0%)	81 61	25, 79, 156, 205	0
1	B	411/459 (89%)	0.04	8 (1%)	66 43	27, 98, 232, 271	1 (0%)
All	All	852/918 (92%)	-0.09	12 (1%)	73 51	25, 86, 222, 271	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	ASN	3.2
1	A	419	LEU	3.0
1	B	392	ILE	2.8
1	B	337	ALA	2.8
1	B	394	MET	2.5
1	A	386	PRO	2.4
1	B	282	VAL	2.4
1	A	345	LEU	2.2
1	B	387	ASP	2.1
1	A	384	ASP	2.1
1	B	354	ASP	2.1
1	B	284	LEU	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 ⓘ

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
4	GOL	A	516	6/6	0.76	0.14	127,139,149,150	0
4	GOL	A	518	6/6	0.79	0.11	70,79,86,96	0
3	CL	B	506	1/1	0.83	0.11	103,103,103,103	0
4	GOL	A	517	6/6	0.85	0.18	57,100,112,128	0
2	SO4	B	504	5/5	0.87	0.19	88,121,142,157	0
4	GOL	A	515	6/6	0.88	0.16	82,127,135,164	0
3	CL	A	509	1/1	0.92	0.08	82,82,82,82	0
3	CL	A	510	1/1	0.92	0.07	85,85,85,85	0
3	CL	A	511	1/1	0.92	0.09	83,83,83,83	0
2	SO4	B	502	5/5	0.92	0.19	81,111,139,148	0
2	SO4	A	507	5/5	0.93	0.11	90,93,115,138	0
2	SO4	A	505	5/5	0.94	0.23	66,93,112,122	0
2	SO4	A	504	5/5	0.95	0.20	48,89,107,108	0
4	GOL	A	514	6/6	0.95	0.15	88,102,143,164	0
3	CL	A	512	1/1	0.95	0.10	71,71,71,71	0
4	GOL	B	508	6/6	0.95	0.28	66,83,93,104	0
2	SO4	A	501	5/5	0.96	0.07	49,61,77,122	0
2	SO4	A	503	5/5	0.96	0.09	71,74,94,96	0
4	GOL	A	513	6/6	0.96	0.08	44,55,59,59	0
2	SO4	B	503	5/5	0.97	0.13	79,115,128,136	0
2	SO4	A	502	5/5	0.97	0.06	59,64,102,105	0
2	SO4	B	505	5/5	0.97	0.19	72,81,90,96	0
2	SO4	B	501	5/5	0.97	0.07	49,72,93,134	0
2	SO4	A	506	5/5	0.97	0.09	57,68,103,107	0
3	CL	B	507	1/1	0.98	0.04	81,81,81,81	0
3	CL	A	508	1/1	0.98	0.08	62,62,62,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.