



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:48 am BST

PDB ID : 5TNU  
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](mailto: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

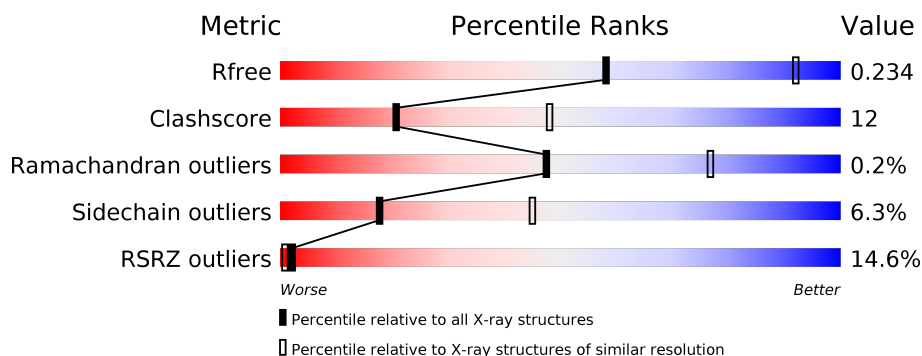
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	459	

## 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:

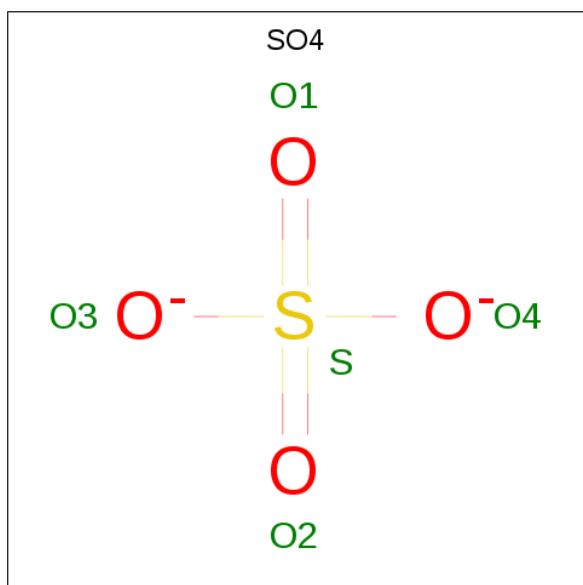
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q970I2
A	-18	GLY	-	expression tag	UNP Q970I2
A	-17	SER	-	expression tag	UNP Q970I2
A	-16	SER	-	expression tag	UNP Q970I2
A	-15	HIS	-	expression tag	UNP Q970I2
A	-14	HIS	-	expression tag	UNP Q970I2
A	-13	HIS	-	expression 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

*Continued on next page...*

Continued from previous page...

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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

Continued on next page...

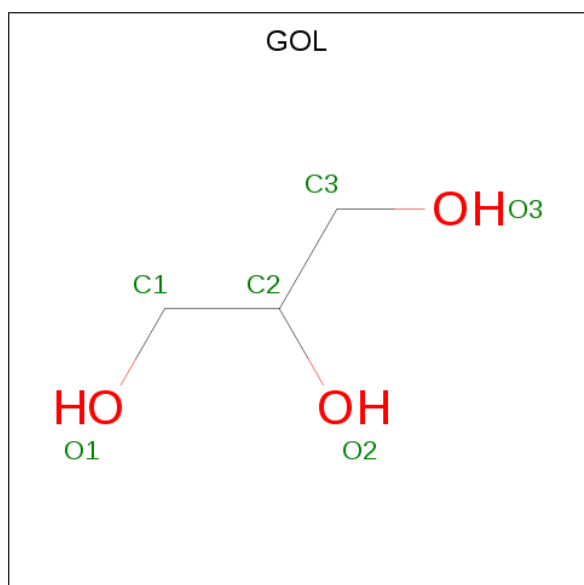
Continued from previous page...

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



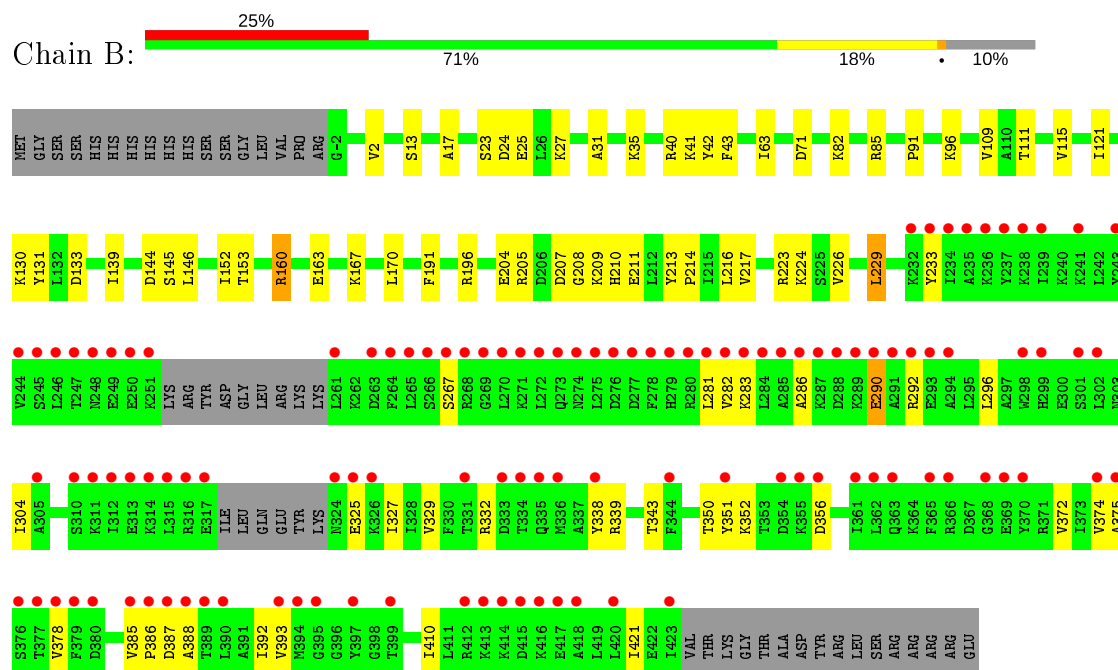
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- 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		



- Molecule 1: DNA-dependent ATPase XPBII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 100.0 (29.88-3.05)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	70.6	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 91.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.53	0/3514	0.69	0/4750
1	B	0.49	0/3011	0.66	1/4089 (0.0%)
All	All	0.51	0/6525	0.67	1/8839 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ARG	NE-CZ-NH2	6.54	123.57	120.30

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	3448	0	3417	103	1
1	B	2956	0	2703	52	1
2	A	35	0	0	2	0
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	71	0	0	11	0
5	B	58	0	0	6	0
All	All	6642	0	6176	156	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 (156) 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: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:225:SER:HB2	1:A:227:GLU:OE1	1.93	0.67
1:A:85:ARG:HG3	1:A:217:VAL:O	1.94	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
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:O	1:A:315:LEU:HD23	1.98	0.63
1:B:329:VAL:O	1:B:374:VAL:CB	2.47	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ASP:OD2	1:A:209:LYS:HD2	1.99	0.62
1:B:17:ALA:HB2	1:B:43:PHE:CE1	2.35	0.61
1:B:2:VAL:HG11	1:B:43:PHE:CE2	2.33	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:B:42:TYR:CD1	1:B:43:PHE:HD1	2.19	0.56
1:A:331:THR:O	1:A:376:SER:CA	2.53	0.56
1:A:24:ASP:N	1:A:24:ASP:OD1	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:VAL:HG22	1:B:421:ILE:O	2.11	0.51
1:B:42:TYR:CD1	1:B:43:PHE:CD1	2.98	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:A:307:ASN:O	1:A:336:MET:HE2	2.13	0.48
1:B:31:ALA:CB	1:B:35:LYS:HD2	2.44	0.48
1:A:311:LYS:NZ	1:A:394:MET:O	2.45	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:329:VAL:HG23	1:A:374:VAL:CG2	2.44	0.48
1:A:108:LYS:HE2	4:A:513:GOL:H31	1.96	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: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:379:PHE:CE1	1:A:382:GLY:HA3	2.51	0.45
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:B:196:ARG:NH1	1:B:216:LEU:O	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:CB	1:A:375:ALA:HB2	2.48	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:307:ASN:O	1:A:336:MET:CE	2.66	0.42
1:A:253:ARG:CD	5:A:621:HOH:O	2.54	0.42
1:A:26:LEU:C	1:A:27:LYS:HG3	2.39	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: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:HD13	1:B:229:LEU:H	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:351:TYR:CD1	1:A:351:TYR:C	2.94	0.41
1:A:379:PHE:CD1	1:A:382:GLY:HA3	2.56	0.41
1:A:179:LEU:N	1:A:180:PRO:CD	2.84	0.40
1:A:26:LEU:O	1:A:27:LYS:HG3	2.21	0.40
1:B:292:ARG:O	1:B:296:LEU:CB	2.69	0.40
1:A:351:TYR:O	1:A:351:TYR:CD1	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:C	1:B:388:ALA:HB1	2.41	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 [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	439/459 (96%)	428 (98%)	11 (2%)	0	100	100
1	B	406/459 (88%)	369 (91%)	35 (9%)	2 (0%)	29	60
All	All	845/918 (92%)	797 (94%)	46 (5%)	2 (0%)	47	77

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/401 (86%)	318 (93%)	25 (7%)	14	40
1	B	257/401 (64%)	244 (95%)	13 (5%)	24	53
All	All	600/802 (75%)	562 (94%)	38 (6%)	18	45

All (38) 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	24	ASP
1	A	97	THR
1	A	133	ASP
1	A	220	ILE
1	A	253	ARG
1	A	273	GLN
1	A	278	PHE
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	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	229	LEU
1	B	267	SER
1	B	281	LEU
1	B	290	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	332	ARG
1	B	338	TYR
1	B	356	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	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 carbohydrates 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	A	506	-	4,4,4	0.42	0	6,6,6	0.75	0
4	GOL	A	518	-	5,5,5	0.64	0	5,5,5	0.47	0
4	GOL	A	517	-	5,5,5	0.53	0	5,5,5	0.39	0
2	SO4	A	502	-	4,4,4	0.36	0	6,6,6	0.47	0
4	GOL	A	514	-	5,5,5	0.38	0	5,5,5	0.29	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	513	-	5,5,5	0.42	0	5,5,5	0.39	0
2	SO4	A	505	-	4,4,4	0.43	0	6,6,6	0.25	0
2	SO4	B	505	-	4,4,4	0.52	0	6,6,6	0.40	0
2	SO4	A	501	-	4,4,4	0.33	0	6,6,6	0.36	0
2	SO4	B	501	-	4,4,4	0.33	0	6,6,6	0.39	0
2	SO4	A	507	-	4,4,4	0.43	0	6,6,6	0.37	0
4	GOL	A	515	-	5,5,5	0.53	0	5,5,5	0.61	0
2	SO4	B	502	-	4,4,4	0.41	0	6,6,6	0.28	0
4	GOL	B	508	-	5,5,5	0.50	0	5,5,5	0.43	0
2	SO4	B	503	-	4,4,4	0.44	0	6,6,6	0.25	0
4	GOL	A	516	-	5,5,5	0.42	0	5,5,5	0.33	0
2	SO4	A	503	-	4,4,4	0.46	0	6,6,6	0.36	0
2	SO4	A	504	-	4,4,4	0.47	0	6,6,6	0.45	0
2	SO4	B	504	-	4,4,4	0.48	0	6,6,6	0.29	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	517	-	-	4/4/4/4	-
4	GOL	A	514	-	-	2/4/4/4	-
4	GOL	A	513	-	-	0/4/4/4	-
4	GOL	A	515	-	-	4/4/4/4	-
4	GOL	B	508	-	-	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	517	GOL	C1-C2-C3-O3
4	B	508	GOL	C1-C2-C3-O3
4	A	516	GOL	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

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

There are no ring outliers.

6 monomers are involved in 6 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	441/459 (96%)	-0.35	11 (2%) 57 32	25, 79, 156, 205	0
1	B	411/459 (89%)	1.00	113 (27%) 0 0	27, 98, 232, 271	0
All	All	852/918 (92%)	0.30	124 (14%) 2 1	25, 86, 222, 271	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	ASN	11.9
1	B	237	TYR	9.8
1	B	376	SER	9.0
1	B	334	THR	8.3
1	B	414	LYS	8.2
1	B	285	ALA	8.2
1	B	377	THR	7.6
1	B	415	ASP	7.3
1	B	282	VAL	7.1
1	B	280	ARG	7.1
1	B	288	ASP	6.7
1	B	264	PHE	6.4
1	B	333	ASP	6.4
1	B	273	GLN	5.7
1	B	243	TYR	5.7
1	B	276	ASP	5.6
1	B	245	SER	5.6
1	B	313	GLU	5.5
1	B	251	LYS	5.4
1	B	269	GLY	5.3
1	B	248	ASN	5.3
1	B	388	ALA	5.3
1	B	335	GLN	5.1
1	B	378	VAL	5.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	416	LYS	4.9
1	B	301	SER	4.8
1	B	266	SER	4.8
1	B	270	LEU	4.8
1	B	281	LEU	4.8
1	B	361	ILE	4.8
1	B	271	LYS	4.8
1	B	351	TYR	4.8
1	B	394	MET	4.8
1	B	289	LYS	4.7
1	B	336	MET	4.7
1	B	312	ILE	4.7
1	B	387	ASP	4.7
1	B	390	LEU	4.7
1	B	247	THR	4.6
1	B	265	LEU	4.6
1	B	423	ILE	4.6
1	B	395	GLY	4.5
1	B	369	GLU	4.5
1	B	249	GLU	4.4
1	B	283	LYS	4.4
1	B	389	THR	4.4
1	B	250	GLU	4.3
1	B	279	HIS	4.3
1	B	287	LYS	4.3
1	B	236	LYS	4.2
1	B	418	ALA	4.2
1	B	417	GLU	4.2
1	B	365	PHE	4.2
1	B	325	GLU	4.1
1	B	380	ASP	4.1
1	B	244	VAL	4.0
1	B	310	SER	3.9
1	B	284	LEU	3.7
1	B	274	ASN	3.7
1	B	261	LEU	3.6
1	B	413	LYS	3.6
1	B	397	TYR	3.5
1	B	299	HIS	3.5
1	B	354	ASP	3.4
1	B	379	PHE	3.4
1	B	246	LEU	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	272	LEU	3.4
1	B	286	ALA	3.3
1	B	356	ASP	3.3
1	B	234	ILE	3.3
1	B	267	SER	3.2
1	B	344	PHE	3.2
1	B	290	GLU	3.1
1	B	368	GLY	3.1
1	B	275	LEU	3.1
1	B	311	LYS	3.1
1	A	380	ASP	3.0
1	B	277	ASP	3.0
1	B	239	ILE	3.0
1	B	235	ALA	3.0
1	B	366	ARG	3.0
1	B	363	GLN	3.0
1	B	238	LYS	3.0
1	B	241	LYS	2.9
1	B	362	LEU	2.9
1	B	370	TYR	2.8
1	B	338	TYR	2.8
1	B	291	ALA	2.8
1	A	418	ALA	2.7
1	B	393	VAL	2.7
1	B	232	LYS	2.7
1	B	315	LEU	2.7
1	B	293	GLU	2.7
1	B	412	ARG	2.7
1	B	233	TYR	2.7
1	B	314	LYS	2.6
1	B	298	TRP	2.6
1	A	320	GLN	2.5
1	B	326	LYS	2.5
1	B	355	LYS	2.5
1	A	383	VAL	2.5
1	B	278	PHE	2.5
1	B	374	VAL	2.5
1	B	292	ARG	2.4
1	B	386	PRO	2.4
1	A	382	GLY	2.4
1	B	316	ARG	2.3
1	B	420	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	368	GLY	2.3
1	B	331	THR	2.3
1	B	375	ALA	2.2
1	B	399	THR	2.2
1	B	317	GLU	2.2
1	A	384	ASP	2.2
1	B	385	VAL	2.2
1	B	263	ASP	2.1
1	A	367	ASP	2.1
1	B	305	ALA	2.1
1	A	419	LEU	2.1
1	B	268	ARG	2.1
1	A	381	GLU	2.1
1	A	353	THR	2.0
1	B	294	ALA	2.0
1	B	302	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	A	515	6/6	0.76	0.27	82,127,135,164	0
3	CL	A	511	1/1	0.83	0.18	83,83,83,83	0
4	GOL	A	514	6/6	0.84	0.34	88,102,143,164	0
3	CL	B	506	1/1	0.84	0.18	103,103,103,103	0
4	GOL	A	516	6/6	0.85	0.20	127,139,149,150	0
4	GOL	A	518	6/6	0.86	0.18	70,79,86,96	0
2	SO4	B	504	5/5	0.89	0.21	88,121,142,157	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	517	6/6	0.90	0.33	57,100,112,128	0
2	SO4	B	502	5/5	0.91	0.21	81,111,139,148	0
4	GOL	B	508	6/6	0.92	0.59	66,83,93,104	0
3	CL	B	507	1/1	0.92	0.10	81,81,81,81	0
3	CL	A	510	1/1	0.93	0.09	85,85,85,85	0
2	SO4	A	503	5/5	0.93	0.18	71,74,94,96	0
3	CL	A	512	1/1	0.93	0.14	71,71,71,71	0
3	CL	A	509	1/1	0.94	0.17	82,82,82,82	0
2	SO4	A	507	5/5	0.95	0.15	90,93,115,138	0
2	SO4	A	504	5/5	0.95	0.19	48,89,107,108	0
2	SO4	B	503	5/5	0.96	0.17	79,115,128,136	0
2	SO4	A	506	5/5	0.96	0.15	57,68,103,107	0
2	SO4	B	505	5/5	0.97	0.17	72,81,90,96	0
3	CL	A	508	1/1	0.97	0.15	62,62,62,62	0
2	SO4	A	501	5/5	0.97	0.26	49,61,77,122	0
2	SO4	B	501	5/5	0.97	0.18	49,72,93,134	0
2	SO4	A	502	5/5	0.97	0.20	59,64,102,105	0
2	SO4	A	505	5/5	0.97	0.24	66,93,112,122	0
4	GOL	A	513	6/6	0.98	0.18	44,55,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.