



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 07:08 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 wwPDB X-ray Structure Validation Summary 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

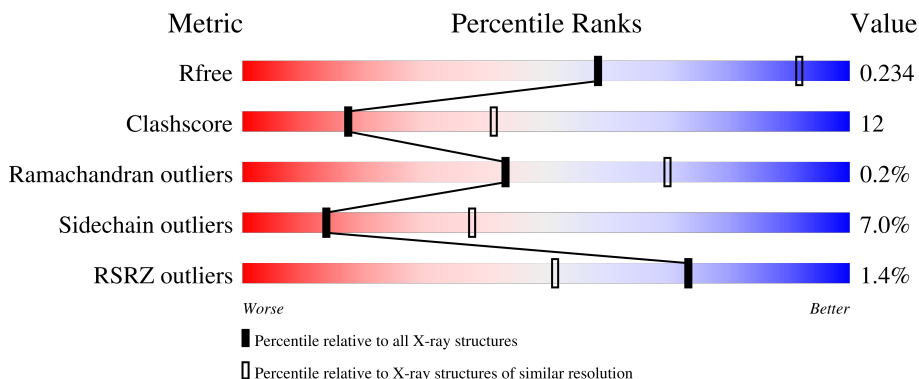
1 Overall quality at a glance

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	 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

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 (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		

Continued on next page...

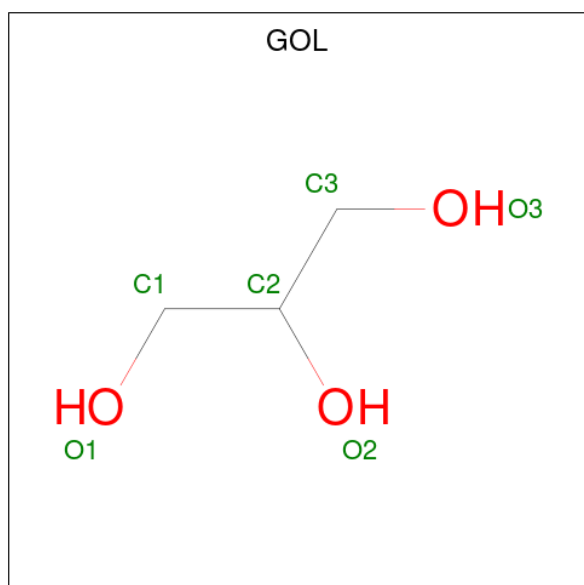
Continued from previous page...

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	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

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

- 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		

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.

Chain A:

Chain B:

2% 71% 18% 10%

Residue	Category
MET	Grey
GLY	Grey
SER	Grey
L132	Green
L133	Green
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
SER	Grey
SER	Grey
GLY	Grey
LEU	Grey
VAL	Grey
PRO	Grey
ARG	Grey
G-2	Green
V2	Green
S13	Green
A17	Green
S23	Green
D24	Green
E25	Green
L26	Green
K27	Green
A31	Green
K35	Green
R40	Green
K41	Green
V42	Green
F43	Green
I63	Green
D71	Green
K82	Green
R85	Green
P91	Green
K96	Green
V109	Green
A110	Green
T111	Green
V115	Green
I121	Green
K130	Green
Y131	Green
L132	Green
D133	Green
I139	Green
D144	Green
S145	Green
L146	Green
I152	Green
T153	Green
R160	Orange
E163	Green
K167	Green
L170	Green
L179	Green
F191	Green
R196	Green
E204	Green
R205	Green
D206	Green
G208	Green
K209	Green
H210	Green
E211	Green
L212	Green
Y213	Green
P214	Green
I215	Green
L216	Green
V217	Green
I220	Green
R223	Green
K224	Green
S225	Green
V226	Green
L229	Orange
Y233	Green
K251	Green
LYS	Grey
ARG	Grey
TYR	Grey
GLY	Grey
LEU	Grey
ARG	Grey
L261	Green
L265	Green
S266	Green
S267	Green
L281	Green
V282	Green
K283	Green
L284	Green
A285	Green
A286	Green
E290	Orange
A291	Green
T292	Green
L296	Green
I304	Green
E317	Green
ILE	Green
LEU	Green
GLN	Green
GLU	Green
TYR	Grey
LYS	Green
N324	Green
E325	Green
K326	Green
I327	Green
I328	Green
V329	Green
A337	Green
Y338	Green
R339	Green
T343	Green
T350	Green
Y351	Green
K352	Green
T353	Green
D354	Green
V372	Green
I373	Green
V374	Green
A375	Green
V378	Green
V385	Green
P386	Green
D387	Red
A388	Green
I392	Red
V393	Green
M394	Red
I410	Green
I421	Green
E422	Green
I423	Green
VAL	Green
THR	Green
LYS	Green
GLY	Green
THR	Green
ALA	Green
ASP	Green
TYR	Green
ARG	Green
LEU	Green
SER	Green
ARG	Green
ARG	Green
ARG	Green
GLU	Green

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.

The worst 5 of 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

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
2	B	25	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	GLU
1	B	160	ARG
1	B	13	SER
1	B	41	LYS
1	B	229	LEU

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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.

5 of 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

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 [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 [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%)

The worst 5 of 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

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($\text{\AA}^2$)	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 [i](#)

There are no such residues in this entry.