



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 08:19 AM BST

PDB ID : 5ZRY
Title : Crystal Structure of EphA6/Odin Complex
Authors : Wang, Y.; Shang, Y.; Li, J.; Chen, W.; Li, G.; Wan, J.; Liu, W.; Zhang, M.
Deposited on : 2018-04-25
Resolution : 1.30 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 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 : 2.13.1
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) : 2.13.1

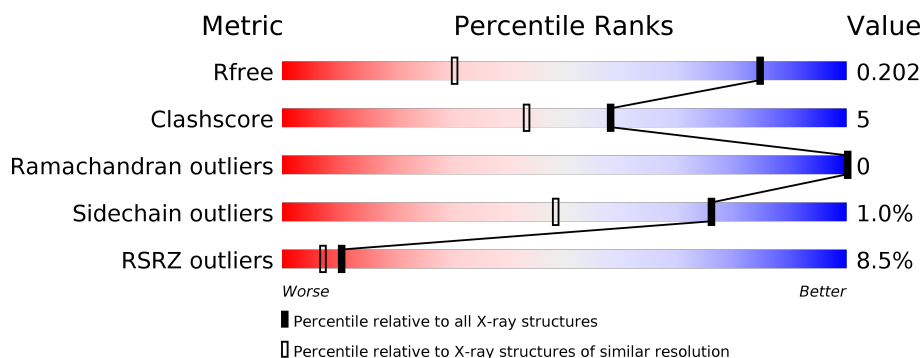
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	194	<div> <div>12%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	194	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>•</div> <div>17%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	204	-	-	X	X
3	GOL	B	202	-	-	X	X
5	TRS	B	203	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3188 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 Ankyrin repeat and SAM domain-containing protein 1A, Ephrin type-A receptor 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	16	0
			1397	900	235	254	8			
1	B	161	Total	C	N	O	S	0	11	0
			1348	861	234	245	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	-	expression tag	UNP P59672
A	3	GLY	-	expression tag	UNP P59672
A	4	ASP	-	expression tag	UNP P59672
A	5	ILE	-	expression tag	UNP P59672
A	6	HIS	-	expression tag	UNP P59672
A	7	MET	-	expression tag	UNP P59672
A	8	HIS	-	expression tag	UNP P59672
A	9	HIS	-	expression tag	UNP P59672
A	10	HIS	-	expression tag	UNP P59672
A	11	HIS	-	expression tag	UNP P59672
A	12	HIS	-	expression tag	UNP P59672
A	13	HIS	-	expression tag	UNP P59672
A	14	SER	-	expression tag	UNP P59672
A	15	SER	-	expression tag	UNP P59672
A	16	GLY	-	expression tag	UNP P59672
A	17	LEU	-	expression tag	UNP P59672
A	18	GLU	-	expression tag	UNP P59672
A	19	VAL	-	expression tag	UNP P59672
A	20	LEU	-	expression tag	UNP P59672
A	21	PHE	-	expression tag	UNP P59672
A	22	GLN	-	expression tag	UNP P59672
A	23	GLY	-	expression tag	UNP P59672
A	24	PRO	-	expression tag	UNP P59672
A	25	GLY	-	expression tag	UNP P59672

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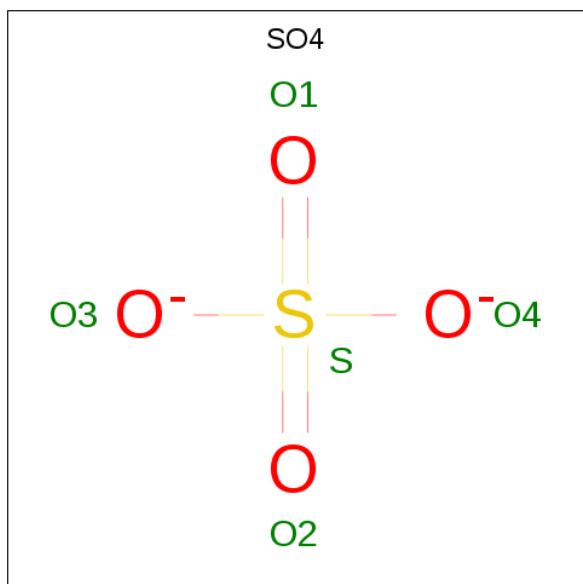
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	SER	-	expression tag	UNP P59672
A	100	PRO	-	linker	UNP P59672
A	101	SER	-	linker	UNP P59672
A	102	GLY	-	linker	UNP P59672
A	103	SER	-	linker	UNP P59672
A	104	SER	-	linker	UNP P59672
A	105	GLY	-	linker	UNP P59672
A	106	GLU	-	linker	UNP P59672
A	107	ASN	-	linker	UNP P59672
A	108	LEU	-	linker	UNP P59672
A	109	TYR	-	linker	UNP P59672
A	110	PHE	-	linker	UNP P59672
A	111	GLN	-	linker	UNP P59672
A	112	SER	-	linker	UNP P59672
A	113	GLY	-	linker	UNP P59672
A	114	SER	-	linker	UNP P59672
A	115	SER	-	linker	UNP P59672
A	116	GLY	-	linker	UNP P59672
B	2	GLU	-	expression tag	UNP P59672
B	3	GLY	-	expression tag	UNP P59672
B	4	ASP	-	expression tag	UNP P59672
B	5	ILE	-	expression tag	UNP P59672
B	6	HIS	-	expression tag	UNP P59672
B	7	MET	-	expression tag	UNP P59672
B	8	HIS	-	expression tag	UNP P59672
B	9	HIS	-	expression tag	UNP P59672
B	10	HIS	-	expression tag	UNP P59672
B	11	HIS	-	expression tag	UNP P59672
B	12	HIS	-	expression tag	UNP P59672
B	13	HIS	-	expression tag	UNP P59672
B	14	SER	-	expression tag	UNP P59672
B	15	SER	-	expression tag	UNP P59672
B	16	GLY	-	expression tag	UNP P59672
B	17	LEU	-	expression tag	UNP P59672
B	18	GLU	-	expression tag	UNP P59672
B	19	VAL	-	expression tag	UNP P59672
B	20	LEU	-	expression tag	UNP P59672
B	21	PHE	-	expression tag	UNP P59672
B	22	GLN	-	expression tag	UNP P59672
B	23	GLY	-	expression tag	UNP P59672
B	24	PRO	-	expression tag	UNP P59672
B	25	GLY	-	expression tag	UNP P59672

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	SER	-	expression tag	UNP P59672
B	100	PRO	-	linker	UNP P59672
B	101	SER	-	linker	UNP P59672
B	102	GLY	-	linker	UNP P59672
B	103	SER	-	linker	UNP P59672
B	104	SER	-	linker	UNP P59672
B	105	GLY	-	linker	UNP P59672
B	106	GLU	-	linker	UNP P59672
B	107	ASN	-	linker	UNP P59672
B	108	LEU	-	linker	UNP P59672
B	109	TYR	-	linker	UNP P59672
B	110	PHE	-	linker	UNP P59672
B	111	GLN	-	linker	UNP P59672
B	112	SER	-	linker	UNP P59672
B	113	GLY	-	linker	UNP P59672
B	114	SER	-	linker	UNP P59672
B	115	SER	-	linker	UNP P59672
B	116	GLY	-	linker	UNP P59672

- Molecule 2 is SULFATE ION (three-letter code: 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		

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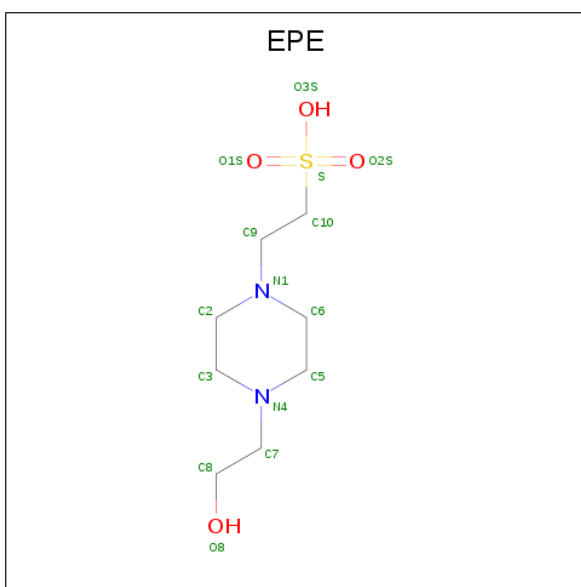
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



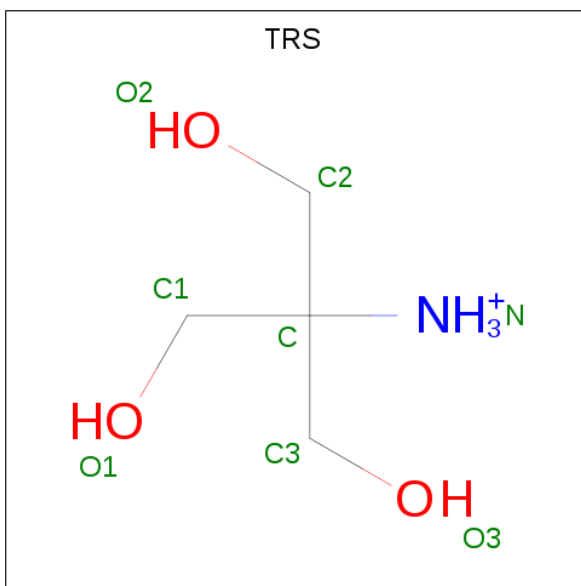
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

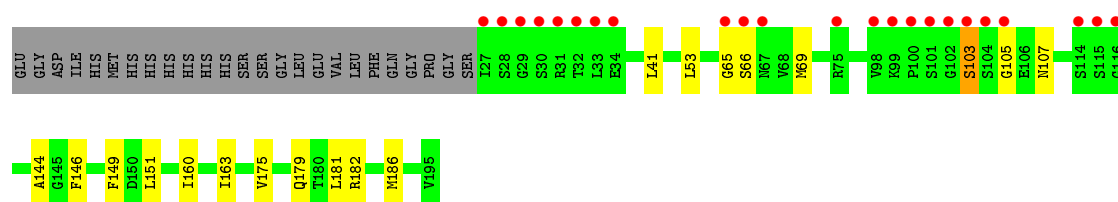
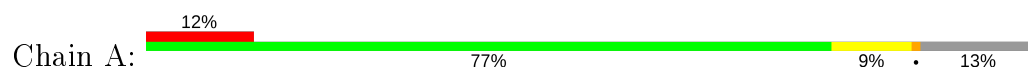
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	182	Total 182	O 182	0	0
6	B	201	Total 201	O 201	0	0

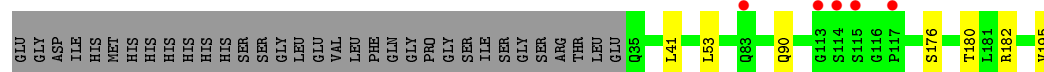
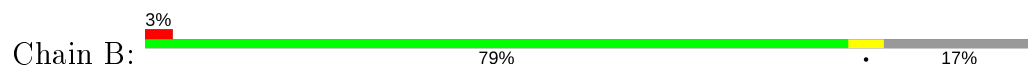
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ankyrin repeat and SAM domain-containing protein 1A,Ephrin type-A receptor 6



- Molecule 1: Ankyrin repeat and SAM domain-containing protein 1A,Ephrin type-A receptor 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.98Å 85.04Å 98.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.30 28.75 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-1.30) 97.7 (28.75-1.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.170 , 0.199 0.178 , 0.202	Depositor DCC
R_{free} test set	1947 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3188	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/1471	0.76	1/1979 (0.1%)
1	B	0.51	0/1404	0.75	2/1884 (0.1%)
All	All	0.51	0/2875	0.76	3/3863 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	69	MET	CG-SD-CE	-6.72	89.45	100.20
1	B	195	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	B	182	ARG	NE-CZ-NH1	5.39	123.00	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	GLY	Peptide

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	1397	0	1440	21	0
1	B	1348	0	1379	5	0
2	A	20	0	0	3	0
2	B	5	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	4	1
4	A	15	0	18	0	0
5	B	8	0	12	1	0
6	A	182	0	0	4	1
6	B	201	0	0	1	0
All	All	3188	0	2865	27	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 5.

The worst 5 of 27 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:107:ASN:ND2	6:A:301:HOH:O	1.82	1.09
1:B:176:SER:O	3:B:202:GOL:O2	1.77	1.02
1:A:179:GLN:HG2	2:A:204:SO4:O2	1.65	0.97
1:A:105:GLY:O	6:A:301:HOH:O	1.89	0.91
1:A:160[B]:ILE:HD12	1:A:175[B]:VAL:CG2	2.09	0.82

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)
3:B:202:GOL:C3	6:A:417:HOH:O[2_775]	2.15	0.05

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	183/194 (94%)	182 (100%)	1 (0%)	0	100	100
1	B	170/194 (88%)	168 (99%)	2 (1%)	0	100	100
All	All	353/388 (91%)	350 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	160/170 (94%)	158 (99%)	2 (1%)	69	35
1	B	153/170 (90%)	151 (99%)	2 (1%)	69	35
All	All	313/340 (92%)	309 (99%)	4 (1%)	76	35

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	103	SER
1	B	90[A]	GLN
1	B	90[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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$
4	EPE	A	206	-	15,15,15	2.15	1 (6%)	18,20,20	1.15	2 (11%)
2	SO4	A	203	-	4,4,4	0.33	0	6,6,6	0.23	0
3	GOL	A	205	-	5,5,5	0.31	0	5,5,5	0.71	0
2	SO4	A	204	-	4,4,4	0.36	0	6,6,6	0.38	0
2	SO4	A	201	-	4,4,4	1.67	1 (25%)	6,6,6	0.62	0
2	SO4	B	201	-	4,4,4	0.29	0	6,6,6	0.12	0
2	SO4	A	202	-	4,4,4	0.26	0	6,6,6	0.27	0
3	GOL	B	202	-	5,5,5	0.32	0	5,5,5	0.62	0
5	TRS	B	203	-	7,7,7	0.80	0	9,9,9	1.88	1 (11%)

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
3	GOL	B	202	-	-	3/4/4/4	-
4	EPE	A	206	-	-	1/9/19/19	0/1/1/1
3	GOL	A	205	-	-	2/4/4/4	-
5	TRS	B	203	-	-	9/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	206	EPE	C10-S	-7.97	1.66	1.77
2	A	201	SO4	O1-S	2.07	1.57	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	203	TRS	O1-C1-C	4.44	125.08	111.00
4	A	206	EPE	C7-N4-C3	-2.29	105.38	111.23
4	A	206	EPE	O3S-S-C10	2.09	109.15	105.77

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	GOL	O1-C1-C2-O2
3	B	202	GOL	O1-C1-C2-C3
5	B	203	TRS	N-C-C1-O1
5	B	203	TRS	C1-C-C2-O2
5	B	203	TRS	C3-C-C2-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	204	SO4	3	0
3	B	202	GOL	4	1
5	B	203	TRS	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	169/194 (87%)	0.60	23 (13%) 3 2	13, 21, 38, 47	6 (3%)
1	B	161/194 (82%)	0.17	5 (3%) 49 46	14, 21, 35, 50	1 (0%)
All	All	330/388 (85%)	0.39	28 (8%) 10 7	13, 21, 37, 50	7 (2%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	LEU	13.6
1	A	32	THR	8.7
1	A	27	ILE	8.5
1	A	30	SER	6.8
1	A	29	GLY	6.2

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 monosaccharides 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(\AA^2)	Q<0.9
3	GOL	B	202	6/6	0.56	0.42	47,50,54,55	0
2	SO4	A	204	5/5	0.80	0.41	40,42,43,45	0
5	TRS	B	203	8/8	0.82	0.20	26,36,39,39	0
2	SO4	A	203	5/5	0.84	0.18	46,47,50,52	5
4	EPE	A	206	15/15	0.88	0.11	29,32,43,44	5
2	SO4	B	201	5/5	0.88	0.13	56,59,61,62	5
3	GOL	A	205	6/6	0.91	0.19	24,45,51,57	0
2	SO4	A	201	5/5	0.96	0.11	68,73,76,78	0
2	SO4	A	202	5/5	0.97	0.10	29,31,34,35	5

6.5 Other polymers [i](#)

There are no such residues in this entry.