Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 01:52 AM EDT

PDB ID	:	3ZGI
Title	:	Crystal structure of the KRT10-binding region domain of the pneumococcal serine rich repeat protein PsrP
Authors	:	Schulte, T.; Loefling, J.; Mikaelsson, C.; Kikhney, A.; Hentrich, K.; Diamante, A.; Ebel, C.; Normark, S.; Svergun, D.; Henriques-Normark, B.; Achour, A.
Deposited on	:	2012-12-17
Resolution	:	2.25 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 (i) 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 (i)) were used in the production of this report:

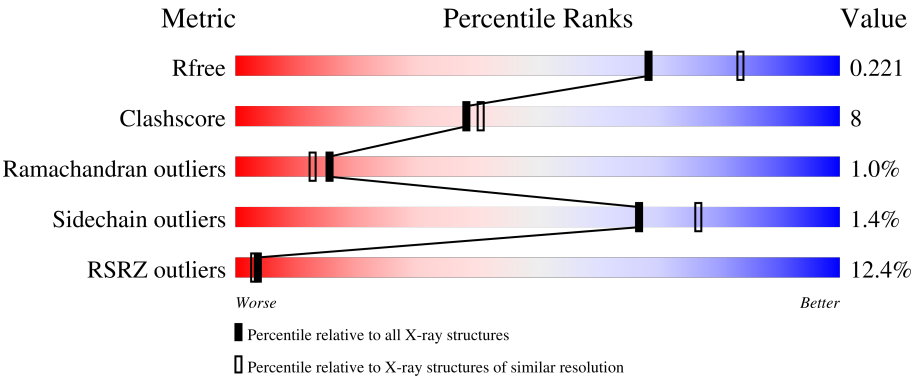
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	205	25% 63% 18% • 15%
1	B	205	3% 75% 10% 15%
1	C	205	2% 75% 10% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8064 atoms, of which 3893 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.

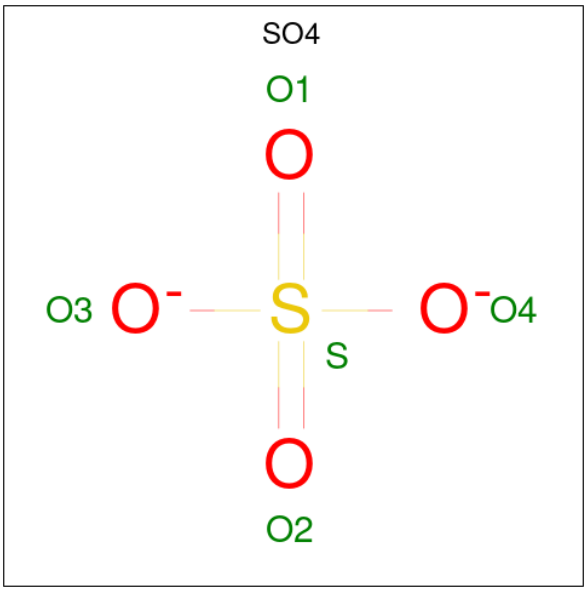
- Molecule 1 is a protein called CELL WALL SURFACE ANCHOR FAMILY PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	174	Total	C	H	N	O	Se	0	0	0
			2624	838	1295	219	268	4			
1	B	174	Total	C	H	N	O	Se	0	0	0
			2627	839	1296	220	268	4			
1	C	174	Total	C	H	N	O	Se	0	0	0
			2627	839	1296	220	268	4			

There are 18 discrepancies between the modelled and reference sequences:

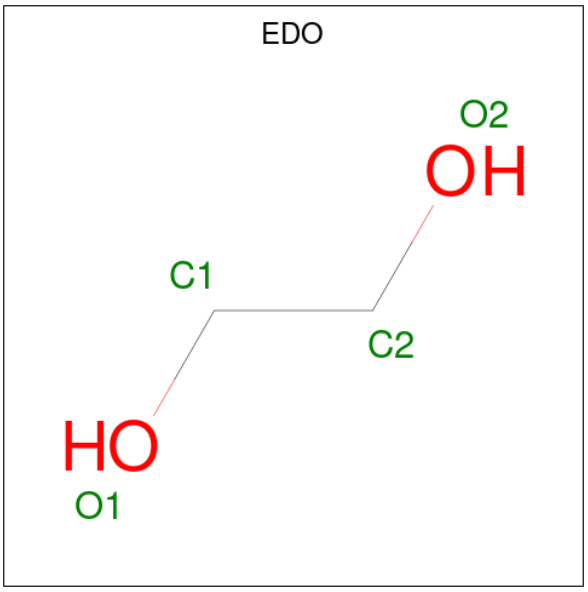
Chain	Residue	Modelled	Actual	Comment	Reference
A	181	HIS	-	expression tag	UNP Q97P71
A	182	HIS	-	expression tag	UNP Q97P71
A	183	HIS	-	expression tag	UNP Q97P71
A	184	HIS	-	expression tag	UNP Q97P71
A	185	HIS	-	expression tag	UNP Q97P71
A	186	HIS	-	expression tag	UNP Q97P71
B	181	HIS	-	expression tag	UNP Q97P71
B	182	HIS	-	expression tag	UNP Q97P71
B	183	HIS	-	expression tag	UNP Q97P71
B	184	HIS	-	expression tag	UNP Q97P71
B	185	HIS	-	expression tag	UNP Q97P71
B	186	HIS	-	expression tag	UNP Q97P71
C	181	HIS	-	expression tag	UNP Q97P71
C	182	HIS	-	expression tag	UNP Q97P71
C	183	HIS	-	expression tag	UNP Q97P71
C	184	HIS	-	expression tag	UNP Q97P71
C	185	HIS	-	expression tag	UNP Q97P71
C	186	HIS	-	expression tag	UNP Q97P71

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is water.

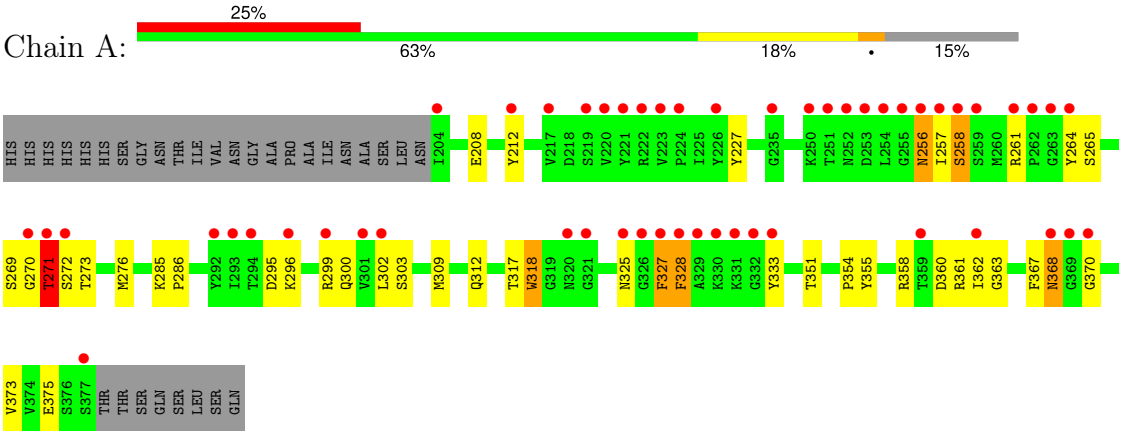
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	66	Total O 66 66	0	0
4	C	68	Total O 68 68	0	0

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.

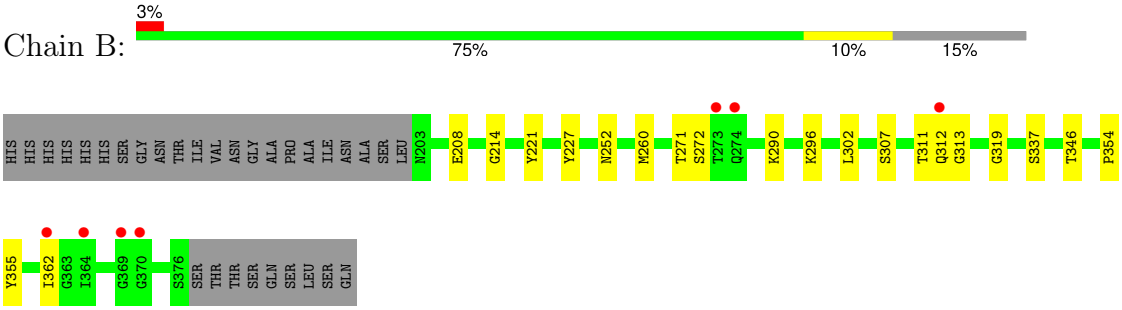
• Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN

Chain A:



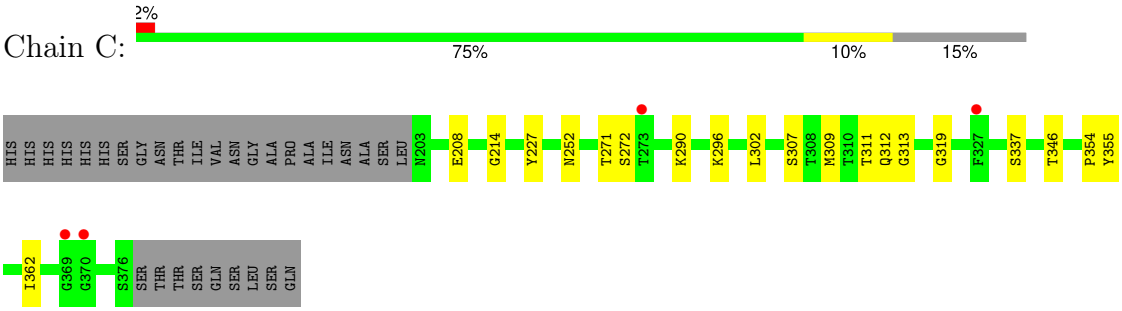
• Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN

Chain B:



• Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.58Å 105.58Å 120.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 2.25 48.35 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.35-2.25) 100.0 (48.35-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 2.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.186 , 0.214 0.191 , 0.221	Depositor DCC
R_{free} test set	1647 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8064	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9481e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, EDO

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	0.56	0/1354	0.96	7/1831 (0.4%)
1	B	0.48	0/1356	0.62	0/1834
1	C	0.54	0/1356	0.64	0/1834
All	All	0.53	0/4066	0.76	7/5499 (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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	261	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	261	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	318	TRP	C-N-CA	-6.79	108.04	122.30
1	A	261	ARG	CD-NE-CZ	5.99	131.98	123.60
1	A	299	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	299	ARG	CG-CD-NE	5.21	122.75	111.80
1	A	270	GLY	N-CA-C	-5.17	100.18	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	ASN	Peptide

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	1329	1295	1295	36	0
1	B	1331	1296	1296	14	0
1	C	1331	1296	1296	11	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	B	4	6	6	0	0
4	A	12	0	0	1	0
4	B	66	0	0	0	0
4	C	68	0	0	0	0
All	All	4171	3893	3893	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (60) 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:C:355:TYR:OH	1:C:362:ILE:O	1.90	0.89
1:A:367:PHE:O	1:A:368:ASN:HB2	1.75	0.85
1:A:256:ASN:HB3	1:A:257:ILE:HG23	1.56	0.85
1:A:257:ILE:O	1:A:258:SER:CB	2.31	0.78
1:B:355:TYR:OH	1:B:362:ILE:O	2.02	0.76
1:A:256:ASN:CB	1:A:257:ILE:HG23	2.20	0.71
1:A:273:THR:HG21	1:A:362:ILE:HD13	1.76	0.67
1:A:271:THR:O	1:A:317:THR:HG21	1.95	0.67
1:A:355:TYR:OH	1:A:362:ILE:O	2.13	0.66
1:A:257:ILE:O	1:A:258:SER:HB2	1.95	0.65
1:A:276:MSE:HG2	1:A:317:THR:HG23	1.79	0.64
1:A:368:ASN:CB	1:A:370:GLY:H	2.13	0.62
1:A:264:TYR:O	1:A:325:ASN:HA	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PHE:O	1:A:328:PHE:CG	2.58	0.56
1:B:302:LEU:C	1:B:302:LEU:HD12	2.25	0.56
1:A:212:TYR:OH	1:A:375:GLU:HG2	2.06	0.56
1:A:368:ASN:HB3	1:A:370:GLY:H	1.73	0.54
1:A:285:LYS:NZ	2:A:1380:SO4:O2	2.41	0.53
1:A:272:SER:CB	1:A:312:GLN:OE1	2.56	0.53
1:A:317:THR:HG22	1:A:318:TRP:H	1.74	0.53
1:A:212:TYR:OH	1:A:375:GLU:CG	2.57	0.53
1:C:214:GLY:HA3	1:C:227:TYR:CE2	2.45	0.52
1:C:302:LEU:C	1:C:302:LEU:HD12	2.29	0.52
1:B:271:THR:HG22	1:B:272:SER:H	1.76	0.51
1:A:368:ASN:HB2	1:A:370:GLY:H	1.75	0.50
1:B:227:TYR:CE2	1:B:354:PRO:HG3	2.46	0.50
1:C:271:THR:HG22	1:C:272:SER:H	1.76	0.50
1:A:325:ASN:OD1	1:A:327:PHE:O	2.28	0.50
1:B:311:THR:HG23	1:B:311:THR:O	2.12	0.50
1:A:208:GLU:OE1	4:A:2001:HOH:O	2.20	0.49
1:A:300:GLN:NE2	1:A:303:SER:HB3	2.28	0.49
1:A:265:SER:O	1:A:358:ARG:HA	2.13	0.49
1:B:290:LYS:O	1:B:337:SER:HA	2.13	0.48
1:A:227:TYR:CE2	1:A:354:PRO:HG3	2.49	0.47
1:B:214:GLY:HA3	1:B:227:TYR:CE2	2.50	0.47
1:A:257:ILE:O	1:A:258:SER:OG	2.31	0.47
1:A:367:PHE:O	1:A:368:ASN:CB	2.53	0.47
1:A:256:ASN:OD1	1:A:257:ILE:HG22	2.15	0.46
1:C:290:LYS:O	1:C:337:SER:HA	2.15	0.46
1:C:307:SER:HB3	1:C:319:GLY:O	2.16	0.46
1:A:360:ASP:O	1:A:361:ARG:HB3	2.16	0.45
1:A:286:PRO:HB2	1:A:309:MSE:HG2	1.98	0.45
1:A:295:ASP:HA	1:A:333:TYR:CD1	2.52	0.45
1:B:307:SER:HB3	1:B:319:GLY:O	2.17	0.45
1:A:302:LEU:C	1:A:302:LEU:HD12	2.38	0.44
1:C:311:THR:HG23	1:C:311:THR:O	2.17	0.44
1:B:252:ASN:O	1:B:296:LYS:CE	2.65	0.43
1:B:312:GLN:HA	1:B:313:GLY:HA2	1.78	0.42
1:A:351:THR:HA	1:A:373:VAL:O	2.18	0.42
1:B:208:GLU:OE2	1:C:208:GLU:OE2	2.38	0.42
1:C:227:TYR:CE2	1:C:354:PRO:HG3	2.54	0.42
1:C:252:ASN:O	1:C:296:LYS:HE2	2.19	0.42
1:B:221:TYR:CE1	1:B:260:MSE:HA	2.55	0.41
1:B:302:LEU:HD12	1:B:302:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:GLN:HA	1:C:313:GLY:HA2	1.73	0.41
1:A:362:ILE:HD12	1:A:363:GLY:N	2.35	0.41
1:B:252:ASN:O	1:B:296:LYS:HE2	2.21	0.41
1:A:317:THR:HG22	1:A:318:TRP:N	2.35	0.41
1:A:272:SER:HB3	1:A:312:GLN:OE1	2.21	0.41
1:A:272:SER:HA	1:A:312:GLN:OE1	2.21	0.41

There are no symmetry-related clashes.

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	172/205 (84%)	162 (94%)	5 (3%)	5 (3%)	4 2
1	B	172/205 (84%)	166 (96%)	6 (4%)	0	100 100
1	C	172/205 (84%)	166 (96%)	6 (4%)	0	100 100
All	All	516/615 (84%)	494 (96%)	17 (3%)	5 (1%)	15 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	A	328	PHE
1	A	271	THR
1	A	258	SER
1	A	327	PHE

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	147/169 (87%)	144 (98%)	3 (2%)	55	64
1	B	147/169 (87%)	146 (99%)	1 (1%)	84	90
1	C	147/169 (87%)	145 (99%)	2 (1%)	67	76
All	All	441/507 (87%)	435 (99%)	6 (1%)	67	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	SER
1	A	271	THR
1	A	296	LYS
1	B	346	THR
1	C	309	MSE
1	C	346	THR

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
2	SO4	C	1378	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	C	1379	-	4,4,4	0.26	0	6,6,6	0.12	0
3	EDO	B	1380	-	3,3,3	0.65	0	2,2,2	0.50	0
2	SO4	A	1380	-	4,4,4	0.22	0	6,6,6	0.14	0
2	SO4	A	1379	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	B	1379	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	B	1378	-	4,4,4	0.24	0	6,6,6	0.15	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
3	EDO	B	1380	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1380	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1380	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^{th} 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	170/205 (82%)	1.60	52 (30%) 0 0	41, 69, 123, 170	0
1	B	170/205 (82%)	0.28	7 (4%) 37 40	22, 34, 73, 134	0
1	C	170/205 (82%)	0.51	4 (2%) 59 62	18, 34, 74, 136	0
All	All	510/615 (82%)	0.80	63 (12%) 4 3	18, 44, 109, 170	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ILE	7.5
1	B	312	GLN	7.2
1	C	273	THR	6.8
1	A	330	LYS	6.8
1	C	370	GLY	6.7
1	A	369	GLY	6.7
1	A	327	PHE	6.4
1	A	222	ARG	5.9
1	A	259	SER	5.8
1	A	223	VAL	5.8
1	A	326	GLY	5.8
1	A	271	THR	5.6
1	A	329	ALA	5.3
1	A	362	ILE	4.9
1	A	254	LEU	4.8
1	A	261	ARG	4.6
1	A	256	ASN	4.5
1	B	369	GLY	4.5
1	A	220	VAL	4.4
1	A	253	ASP	4.4
1	A	262	PRO	4.1
1	C	369	GLY	4.0
1	A	255	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	272	SER	3.9
1	A	370	GLY	3.7
1	A	217	VAL	3.7
1	A	258	SER	3.7
1	A	263	GLY	3.7
1	A	332	GLY	3.5
1	A	328	PHE	3.5
1	A	221	TYR	3.4
1	A	377	SER	3.4
1	B	273	THR	3.3
1	B	370	GLY	3.3
1	A	368	ASN	3.3
1	B	364	ILE	3.2
1	A	301	VAL	3.1
1	A	320	ASN	3.1
1	A	302	LEU	3.1
1	A	270	GLY	3.1
1	A	321	GLY	3.1
1	A	204	ILE	3.0
1	A	219	SER	3.0
1	A	333	TYR	2.9
1	B	274	GLN	2.9
1	A	251	THR	2.8
1	A	325	ASN	2.8
1	A	296	LYS	2.8
1	A	299	ARG	2.7
1	A	226	TYR	2.5
1	A	235	GLY	2.4
1	A	212	TYR	2.4
1	A	293	ILE	2.4
1	A	252	ASN	2.4
1	A	359	THR	2.4
1	A	292	TYR	2.3
1	A	264	TYR	2.2
1	B	362	ILE	2.2
1	A	224	PRO	2.1
1	C	327	PHE	2.1
1	A	250	LYS	2.1
1	A	331	LYS	2.1
1	A	294	THR	2.1

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, 95^{th} 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
2	SO4	B	1379	5/5	0.56	0.19	89,101,108,110	0
2	SO4	C	1379	5/5	0.73	0.30	118,121,124,124	0
3	EDO	B	1380	4/4	0.75	0.33	43,52,59,60	0
2	SO4	A	1380	5/5	0.82	0.16	82,85,89,90	0
2	SO4	B	1378	5/5	0.91	0.13	81,89,96,99	0
2	SO4	C	1378	5/5	0.91	0.21	93,101,106,108	0
2	SO4	A	1379	5/5	0.97	0.19	75,79,81,84	5

6.5 Other polymers (i)

There are no such residues in this entry.