Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 10:18 am BST

PDB ID	:	2WW8
Title	:	Structure of the pilus adhesin (RrgA) from Streptococcus pneumoniae
Authors	:	Izore, T.; Contreras-Martel, C.; El-Mortaji, L.; Manzano, C.; Terrasse, R.; Vernet, T.; Di-Guilmi, A.M.; Dessen, A.
Deposited on	:	2009-10-22
Resolution	:	1.90 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:

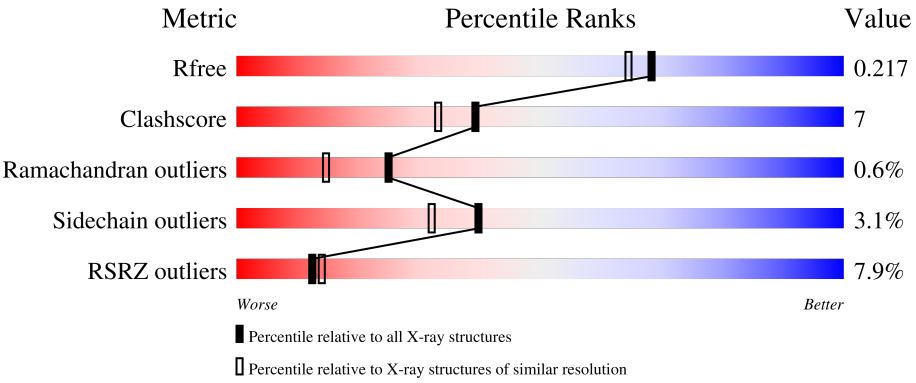
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	893	7% 76% 14% · 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7294 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 CELL WALL SURFACE ANCHOR FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	815	Total	C	N	O	S	0	7	0
			6453	4052	1094	1298	9			

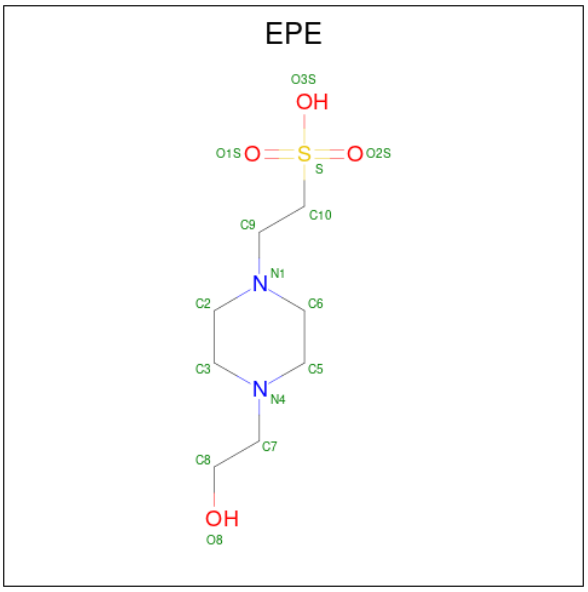
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- 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		
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

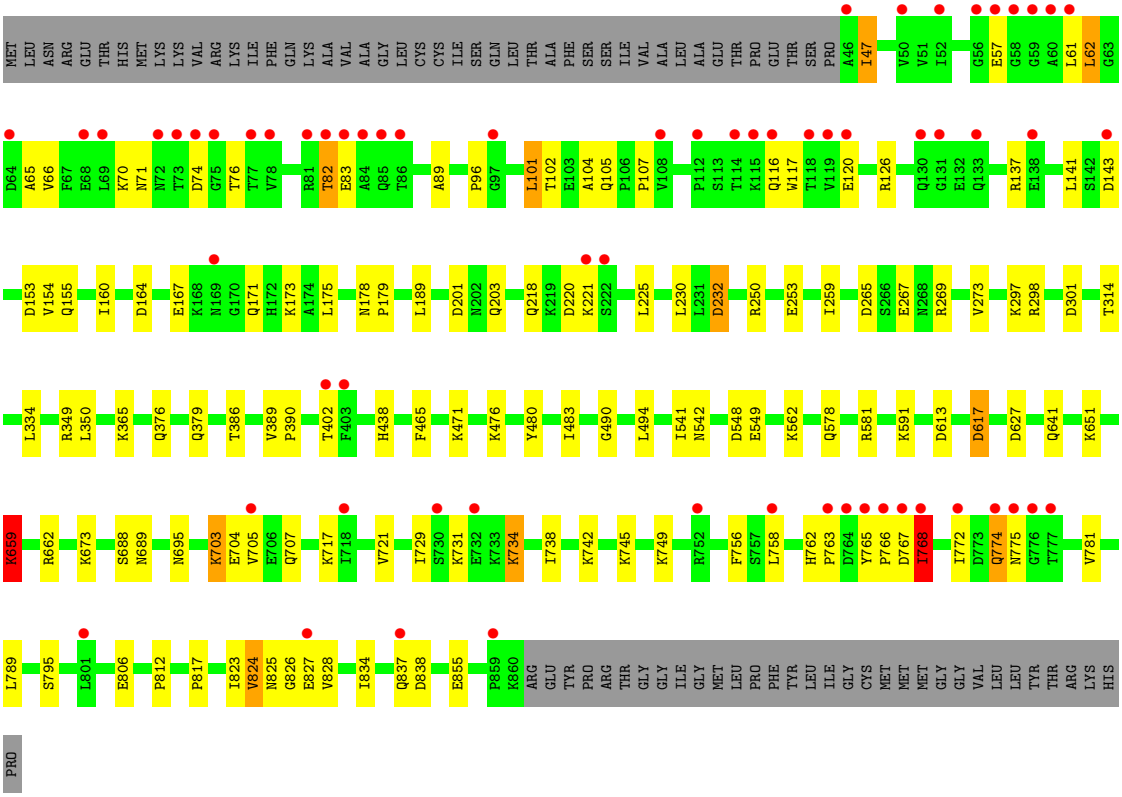
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	808	Total	O	0	0
			808	808		

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: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.08Å 82.70Å 299.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	149.07 – 1.90 19.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.7 (149.07-1.90) 93.9 (19.93-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.195 , 0.235 0.216 , 0.217	Depositor DCC
R_{free} test set	4761 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7294	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, CA, MG

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	0.73	0/6606	1.05	18/8965 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	A	298	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	703	LYS	CD-CE-NZ	8.01	130.12	111.70
1	A	662	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	A	153	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	301	ASP	CB-CG-OD1	6.79	124.42	118.30
1	A	659	LYS	CD-CE-NZ	6.78	127.30	111.70
1	A	232	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	265	ASP	CB-CG-OD1	5.68	123.42	118.30
1	A	476	LYS	CD-CE-NZ	-5.58	98.87	111.70
1	A	617	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	62	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	101	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	548	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	250	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	613	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	662	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	627	ASP	CB-CG-OD1	5.03	122.83	118.30

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	6453	0	6301	94	1
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	30	0	36	5	0
5	A	808	0	0	18	0
All	All	7294	0	6337	95	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 7.

All (95) 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:765:TYR:HB2	1:A:768:ILE:HG21	1.48	0.96
1:A:704:GLU:HG2	5:A:2595:HOH:O	1.69	0.92
1:A:71:ASN:HB3	1:A:74:ASP:OD1	1.75	0.87
1:A:143:ASP:HA	1:A:171:GLN:NE2	1.89	0.87
1:A:758:LEU:O	1:A:772:ILE:HD11	1.81	0.80
1:A:562:LYS:HE2	5:A:2554:HOH:O	1.86	0.75
1:A:738:ILE:HD12	1:A:828:VAL:HG11	1.68	0.74
1:A:673:LYS:HE3	5:A:2687:HOH:O	1.90	0.71
1:A:651:LYS:HE3	5:A:2662:HOH:O	1.90	0.71
1:A:102:THR:HG22	1:A:116:GLN:HG2	1.73	0.70
1:A:762:HIS:CD2	1:A:763:PRO:HD2	2.27	0.70
1:A:402:THR:HA	4:A:1100:EPE:C8	2.23	0.69
1:A:745:LYS:HD2	1:A:855:GLU:HG2	1.75	0.68
1:A:542:ASN:HA	1:A:549:GLU:OE1	1.92	0.68
1:A:102:THR:CG2	1:A:116:GLN:HE21	2.07	0.68
1:A:772:ILE:H	1:A:772:ILE:HD12	1.58	0.68
1:A:765:TYR:HB2	1:A:768:ILE:CG2	2.23	0.65
1:A:66:VAL:HG12	1:A:104:ALA:HB3	1.79	0.65
1:A:659:LYS:HE2	5:A:2192:HOH:O	1.96	0.64
1:A:66:VAL:HB	1:A:105:GLN:HG2	1.80	0.63
1:A:707:GLN:HG3	1:A:707:GLN:O	2.00	0.62
1:A:102:THR:HG21	1:A:116:GLN:HE21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:THR:HA	4:A:1100:EPE:H82	1.84	0.60
1:A:267:GLU:HG3	5:A:2218:HOH:O	2.02	0.60
1:A:772:ILE:HD12	1:A:772:ILE:N	2.16	0.59
1:A:465:PHE:HB2	1:A:494:LEU:HD21	1.84	0.59
1:A:765:TYR:CB	1:A:768:ILE:HG21	2.30	0.58
1:A:578:GLN:HE22	1:A:581:ARG:HE	1.51	0.57
1:A:143:ASP:HA	1:A:171:GLN:HE21	1.67	0.57
1:A:774:GLN:HE21	1:A:774:GLN:H	1.53	0.57
1:A:143:ASP:HA	1:A:171:GLN:HE22	1.68	0.57
1:A:749:LYS:HB3	5:A:2743:HOH:O	2.05	0.56
1:A:201:ASP:OD2	1:A:203:GLN:NE2	2.31	0.55
1:A:65:ALA:HB3	1:A:82:THR:CG2	2.38	0.54
1:A:62:LEU:HD23	1:A:107:PRO:HG2	1.89	0.54
1:A:734:LYS:HB2	1:A:734:LYS:NZ	2.22	0.54
1:A:734:LYS:HB2	1:A:734:LYS:HZ2	1.73	0.53
1:A:651:LYS:CE	5:A:2662:HOH:O	2.55	0.52
1:A:221:LYS:CD	5:A:2145:HOH:O	2.58	0.52
1:A:82:THR:HG22	1:A:89:ALA:HB2	1.91	0.51
1:A:591:LYS:NZ	5:A:2585:HOH:O	2.39	0.51
1:A:758:LEU:O	1:A:772:ILE:CD1	2.58	0.51
1:A:774:GLN:HE21	1:A:774:GLN:N	2.08	0.51
1:A:141:LEU:HD11	1:A:173:LYS:HG3	1.93	0.50
1:A:734:LYS:HD3	1:A:826:GLY:HA3	1.92	0.50
1:A:578:GLN:NE2	1:A:581:ARG:HE	2.11	0.49
1:A:164:ASP:HB3	5:A:2059:HOH:O	2.12	0.49
1:A:47:ILE:HG12	1:A:47:ILE:O	2.12	0.48
1:A:220:ASP:C	1:A:220:ASP:OD1	2.50	0.48
1:A:230:LEU:HD23	1:A:273:VAL:HB	1.95	0.47
1:A:734:LYS:HD2	1:A:825:ASN:O	2.14	0.47
1:A:402:THR:HG22	4:A:1100:EPE:O8	2.13	0.47
1:A:65:ALA:HB3	1:A:82:THR:HG23	1.97	0.46
1:A:349:ARG:NE	5:A:2323:HOH:O	2.40	0.46
1:A:781:VAL:HG23	1:A:789:LEU:CD2	2.46	0.46
1:A:334:LEU:HD23	1:A:334:LEU:C	2.36	0.46
1:A:117:TRP:CZ2	1:A:729:ILE:HD11	2.52	0.45
1:A:221:LYS:HD3	5:A:2145:HOH:O	2.15	0.45
1:A:259:ILE:HD13	1:A:334:LEU:CD2	2.47	0.45
4:A:1101:EPE:O8	4:A:1101:EPE:H31	2.16	0.45
1:A:232:ASP:HB3	1:A:386:THR:HA	1.99	0.45
1:A:742:LYS:HD3	1:A:756:PHE:CZ	2.51	0.45
1:A:823:ILE:HA	1:A:827:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD23	1:A:379:GLN:HB3	1.97	0.45
1:A:806:GLU:CD	1:A:812:PRO:HA	2.37	0.45
1:A:688:SER:O	1:A:689:ASN:HB2	2.16	0.44
1:A:47:ILE:HD11	1:A:688:SER:HB3	1.98	0.44
1:A:179:PRO:HB2	4:A:1101:EPE:O1S	2.17	0.44
1:A:65:ALA:HB3	1:A:82:THR:HG21	2.00	0.44
1:A:154:VAL:O	1:A:155:GLN:HB2	2.18	0.44
1:A:765:TYR:CB	1:A:768:ILE:CG2	2.94	0.43
1:A:817:PRO:HB2	1:A:834:ILE:HD12	1.99	0.43
1:A:659:LYS:HB3	1:A:659:LYS:HE3	1.81	0.43
1:A:297:LYS:HG3	1:A:480:TYR:CE1	2.54	0.43
1:A:837:GLN:O	1:A:838:ASP:HB2	2.19	0.43
1:A:218:GLN:HE21	1:A:225:LEU:HG	1.84	0.43
1:A:143:ASP:CA	1:A:171:GLN:NE2	2.71	0.43
1:A:141:LEU:HD23	1:A:721:VAL:HB	2.00	0.42
1:A:160:ILE:CG2	1:A:175:LEU:HB3	2.49	0.42
1:A:824:VAL:O	1:A:824:VAL:CG1	2.66	0.42
1:A:178:ASN:HA	1:A:179:PRO:HA	1.90	0.42
1:A:314:THR:HB	1:A:350:LEU:HD21	2.02	0.42
1:A:483:ILE:O	1:A:490:GLY:HA3	2.18	0.42
1:A:438:HIS:HD2	5:A:2246:HOH:O	2.02	0.42
1:A:365:LYS:HD3	1:A:365:LYS:HA	1.73	0.41
1:A:471:LYS:HE3	5:A:2264:HOH:O	2.20	0.41
1:A:189:LEU:C	1:A:189:LEU:HD12	2.41	0.41
1:A:253:GLU:HG2	5:A:2201:HOH:O	2.20	0.41
1:A:541:ILE:O	1:A:549:GLU:OE1	2.38	0.41
1:A:651:LYS:NZ	5:A:2662:HOH:O	2.54	0.41
1:A:703:LYS:HE3	5:A:2587:HOH:O	2.21	0.41
1:A:707:GLN:HE21	1:A:707:GLN:HB2	1.53	0.41
1:A:389:VAL:HB	1:A:390:PRO:HD2	2.02	0.41
1:A:765:TYR:HA	1:A:766:PRO:HD3	1.87	0.41
1:A:742:LYS:HD3	1:A:756:PHE:HZ	1.86	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:376:GLN:OE1	1:A:641:GLN:NE2[3_445]	2.08	0.12

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	820/893 (92%)	788 (96%)	27 (3%)	5 (1%)	25 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	768	ILE
1	A	76	THR
1	A	775	ASN
1	A	96	PRO

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	715/774 (92%)	693 (97%)	22 (3%)	40 32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	61	LEU
1	A	70	LYS
1	A	82	THR
1	A	83	GLU
1	A	101	LEU

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Mol	Chain	Res	Type
1	A	120	GLU
1	A	126	ARG
1	A	137	ARG
1	A	167	GLU
1	A	617	ASP
1	A	659	LYS
1	A	695	ASN
1	A	705	VAL
1	A	717	LYS
1	A	731	LYS
1	A	734	LYS
1	A	767	ASP
1	A	768	ILE
1	A	774	GLN
1	A	795	SER
1	A	824	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	171	GLN
1	A	438	HIS
1	A	707	GLN
1	A	708	ASN
1	A	762	HIS
1	A	774	GLN

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)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	EPE	A	1100	-	15,15,15	0.74	0	18,20,20	4.52	8 (44%)
4	EPE	A	1101	-	15,15,15	1.08	1 (6%)	18,20,20	2.62	7 (38%)

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	EPE	A	1100	-	-	5/9/19/19	0/1/1/1
4	EPE	A	1101	-	-	3/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	EPE	C10-S	3.64	1.82	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1100	EPE	O2S-S-C10	-14.64	89.28	106.92
4	A	1101	EPE	O2S-S-C10	7.46	115.90	106.92
4	A	1100	EPE	O1S-S-C10	7.35	115.76	106.92
4	A	1100	EPE	C6-N1-C2	5.79	121.87	108.83
4	A	1101	EPE	C6-N1-C2	5.01	120.12	108.83
4	A	1100	EPE	O3S-S-O2S	4.60	122.52	111.27
4	A	1100	EPE	O3S-S-O1S	-3.83	101.91	111.27
4	A	1101	EPE	C9-N1-C2	2.96	118.81	111.23
4	A	1101	EPE	C9-N1-C6	2.84	118.49	111.23
4	A	1100	EPE	O3S-S-C10	2.71	110.14	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1100	EPE	C6-C5-N4	-2.43	105.65	110.64
4	A	1100	EPE	C3-C2-N1	2.28	115.33	110.64
4	A	1101	EPE	O2S-S-O1S	-2.16	106.47	113.95
4	A	1101	EPE	C7-N4-C3	2.15	116.73	111.23
4	A	1101	EPE	C2-C3-N4	2.13	115.01	110.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	EPE	C8-C7-N4-C3
4	A	1100	EPE	N4-C7-C8-O8
4	A	1100	EPE	C9-C10-S-O3S
4	A	1100	EPE	C8-C7-N4-C5
4	A	1100	EPE	C8-C7-N4-C3
4	A	1100	EPE	C10-C9-N1-C2
4	A	1101	EPE	C10-C9-N1-C2
4	A	1101	EPE	C8-C7-N4-C5

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1100	EPE	3	0
4	A	1101	EPE	2	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	815/893 (91%)	0.33	64 (7%)	12	14	7, 17, 33, 50	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	GLN	7.9
1	A	765	TYR	7.6
1	A	58	GLY	7.2
1	A	46	ALA	6.1
1	A	73	THR	5.8
1	A	57	GLU	5.7
1	A	775	ASN	5.5
1	A	114	THR	5.3
1	A	84	ALA	5.1
1	A	56	GLY	4.8
1	A	86	THR	4.8
1	A	75	GLY	4.6
1	A	403	PHE	4.5
1	A	59	GLY	4.5
1	A	774	GLN	4.4
1	A	133	GLN	4.3
1	A	766	PRO	3.9
1	A	705	VAL	3.8
1	A	772	ILE	3.8
1	A	767	ASP	3.8
1	A	221	LYS	3.8
1	A	776	GLY	3.7
1	A	81	ARG	3.7
1	A	83	GLU	3.7
1	A	763	PRO	3.6
1	A	764	ASP	3.5
1	A	131	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	3.2
1	A	801	LEU	3.2
1	A	222	SER	3.0
1	A	768	ILE	2.9
1	A	732	GLU	2.9
1	A	718	ILE	2.9
1	A	143	ASP	2.9
1	A	116	GLN	2.9
1	A	77	THR	2.8
1	A	130	GLN	2.8
1	A	74	ASP	2.8
1	A	68	GLU	2.8
1	A	120	GLU	2.8
1	A	119	VAL	2.6
1	A	758	LEU	2.6
1	A	52	ILE	2.6
1	A	108	VAL	2.6
1	A	112	PRO	2.6
1	A	72	ASN	2.5
1	A	777	THR	2.5
1	A	118	THR	2.4
1	A	138	GLU	2.4
1	A	60	ALA	2.4
1	A	752	ARG	2.3
1	A	78	VAL	2.3
1	A	169	ASN	2.2
1	A	859	PRO	2.2
1	A	115	LYS	2.2
1	A	97	GLY	2.1
1	A	402	THR	2.1
1	A	50	VAL	2.1
1	A	82	THR	2.1
1	A	64	ASP	2.1
1	A	837	GLN	2.0
1	A	827	GLU	2.0
1	A	730	SER	2.0
1	A	69	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 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
4	EPE	A	1100	15/15	0.84	0.18	48,61,68,70	0
4	EPE	A	1101	15/15	0.90	0.33	48,79,89,91	0
2	MG	A	1000	1/1	0.98	0.11	21,21,21,21	0
3	CA	A	1002	1/1	0.98	0.06	37,37,37,37	0
3	CA	A	1001	1/1	1.00	0.10	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.