Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 03:39 PM EDT

PDB ID	:	6R6K
Title	:	Structure of a FpvC mutant from pseudomonas aeruginosa
Authors	:	Morera, S.; Vigouroux, A.
Deposited on	:	2019-03-27
Resolution	:	2.10 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 (1)) were used in the production of this report:

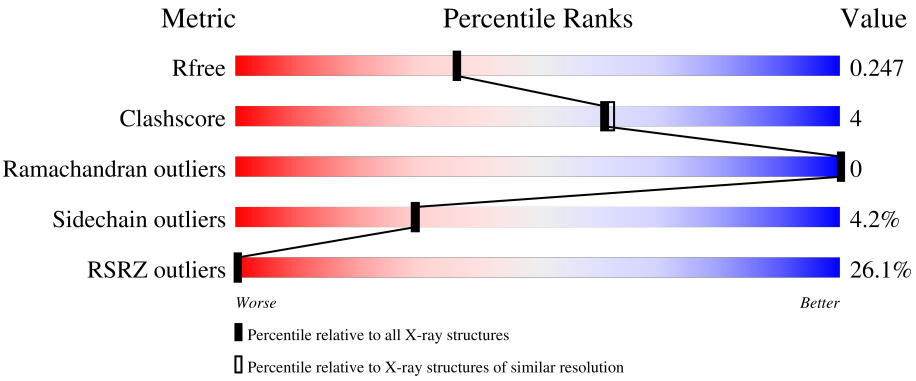
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	294	2% 84% 8% • 6%
1	B	294	46% 84% 7% • 7%

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
4	GOL	A	430	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4482 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 ABC transporter substrate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2088	1326	362	397	3			
1	B	273	Total	C	N	O	S	0	0	0
			2063	1309	356	395	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP A0A3G3N2S3
A	77	GLY	HIS	conflict	UNP A0A3G3N2S3
A	102	GLY	HIS	conflict	UNP A0A3G3N2S3
A	147	GLY	HIS	conflict	UNP A0A3G3N2S3
A	213	GLY	HIS	conflict	UNP A0A3G3N2S3
A	235	GLY	HIS	conflict	UNP A0A3G3N2S3
A	286	GLY	HIS	conflict	UNP A0A3G3N2S3
A	318	GLU	-	expression tag	UNP A0A3G3N2S3
A	319	ASN	-	expression tag	UNP A0A3G3N2S3
A	320	LEU	-	expression tag	UNP A0A3G3N2S3
A	321	TYR	-	expression tag	UNP A0A3G3N2S3
A	322	PHE	-	expression tag	UNP A0A3G3N2S3
A	323	GLN	-	expression tag	UNP A0A3G3N2S3
A	324	GLY	-	expression tag	UNP A0A3G3N2S3
A	325	HIS	-	expression tag	UNP A0A3G3N2S3
A	326	HIS	-	expression tag	UNP A0A3G3N2S3
A	327	HIS	-	expression tag	UNP A0A3G3N2S3
A	328	HIS	-	expression tag	UNP A0A3G3N2S3
A	329	HIS	-	expression tag	UNP A0A3G3N2S3
A	330	HIS	-	expression tag	UNP A0A3G3N2S3
B	37	MET	-	initiating methionine	UNP A0A3G3N2S3
B	77	GLY	HIS	conflict	UNP A0A3G3N2S3
B	102	GLY	HIS	conflict	UNP A0A3G3N2S3
B	147	GLY	HIS	conflict	UNP A0A3G3N2S3
B	213	GLY	HIS	conflict	UNP A0A3G3N2S3

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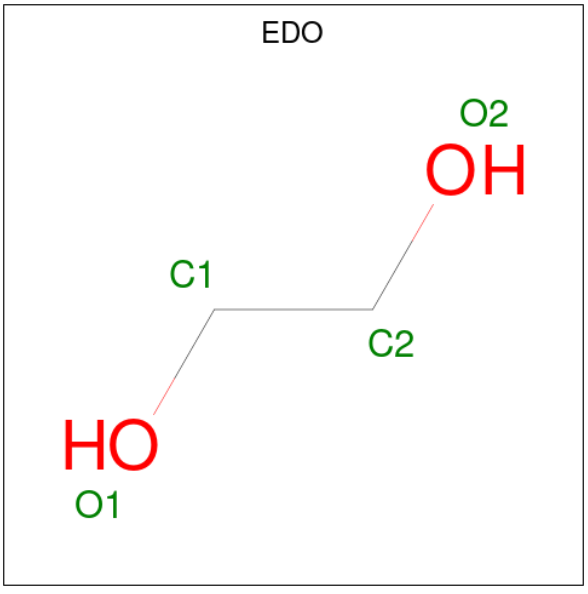
Chain	Residue	Modelled	Actual	Comment	Reference
B	235	GLY	HIS	conflict	UNP A0A3G3N2S3
B	286	GLY	HIS	conflict	UNP A0A3G3N2S3
B	318	GLU	-	expression tag	UNP A0A3G3N2S3
B	319	ASN	-	expression tag	UNP A0A3G3N2S3
B	320	LEU	-	expression tag	UNP A0A3G3N2S3
B	321	TYR	-	expression tag	UNP A0A3G3N2S3
B	322	PHE	-	expression tag	UNP A0A3G3N2S3
B	323	GLN	-	expression tag	UNP A0A3G3N2S3
B	324	GLY	-	expression tag	UNP A0A3G3N2S3
B	325	HIS	-	expression tag	UNP A0A3G3N2S3
B	326	HIS	-	expression tag	UNP A0A3G3N2S3
B	327	HIS	-	expression tag	UNP A0A3G3N2S3
B	328	HIS	-	expression tag	UNP A0A3G3N2S3
B	329	HIS	-	expression tag	UNP A0A3G3N2S3
B	330	HIS	-	expression tag	UNP A0A3G3N2S3

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

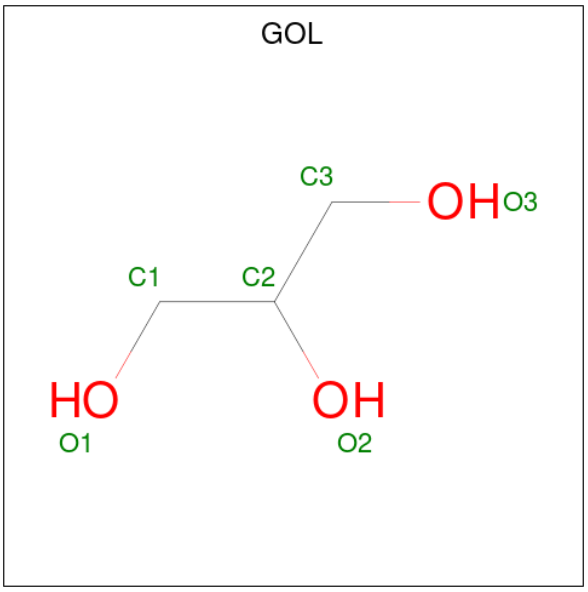
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Na 6 6	0	0

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



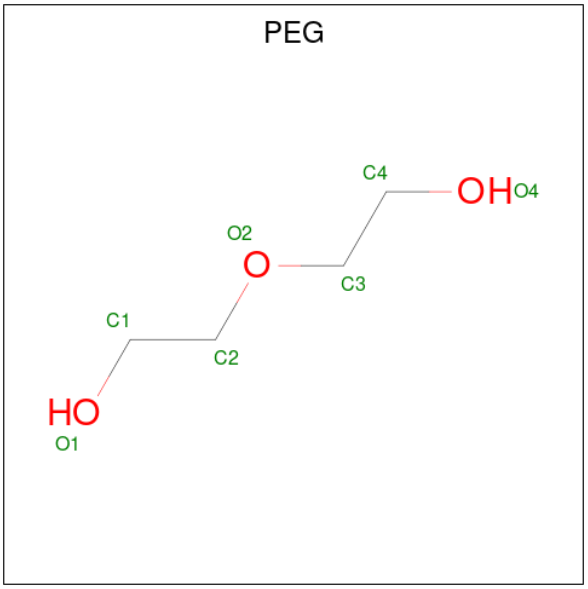
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

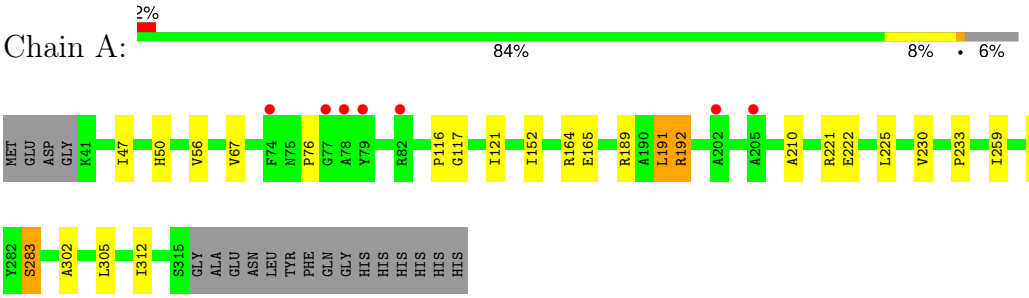
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	152	Total O 152 152	0	0
6	B	24	Total O 24 24	0	0

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.

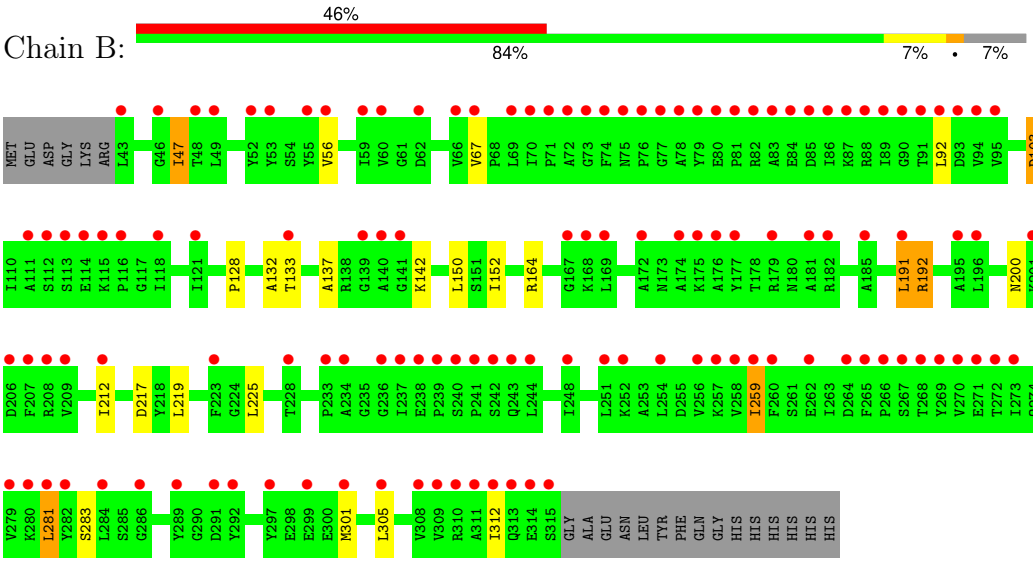
• Molecule 1: ABC transporter substrate-binding protein

Chain A:



• Molecule 1: ABC transporter substrate-binding protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.27Å 53.56Å 84.39Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	43.74 – 2.10 43.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	67.8 (43.74-2.10) 67.8 (43.74-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.194 , 0.234 0.201 , 0.247	Depositor DCC
R_{free} test set	1396 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 76.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4482	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: GOL, PEG, NA, 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	0.54	0/2126	0.70	0/2883
1	B	0.47	0/2098	0.68	0/2847
All	All	0.51	0/4224	0.69	0/5730

There are no bond length outliers.

There are no bond angle outliers.

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	2088	0	2140	25	0
1	B	2063	0	2103	14	0
2	A	6	0	0	0	0
3	A	80	0	120	9	0
3	B	4	0	6	0	0
4	A	30	0	40	4	0
5	A	35	0	50	4	0
6	A	152	0	0	1	0
6	B	24	0	0	0	0
All	All	4482	0	4459	39	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 4.

All (39) 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:117:GLY:H	5:A:434:PEG:H11	1.12	1.14
1:A:121:ILE:HA	3:A:419:EDO:H11	1.59	0.85
1:A:50:HIS:ND1	4:A:430:GOL:H12	1.93	0.84
1:A:67:VAL:HG13	5:A:433:PEG:H11	1.60	0.82
1:A:117:GLY:N	5:A:434:PEG:H11	1.92	0.82
1:A:47[B]:ILE:HD11	1:A:56:VAL:HG21	1.64	0.78
1:B:47:ILE:HD11	1:B:56:VAL:HG21	1.66	0.77
1:A:76:PRO:HD3	4:A:430:GOL:H32	1.75	0.68
1:A:283:SER:HB2	3:A:426:EDO:H22	1.75	0.66
1:A:281:LEU:HD23	3:A:426:EDO:H21	1.78	0.64
1:A:165:GLU:HG3	3:A:419:EDO:H12	1.79	0.64
1:B:225:LEU:HD21	1:B:312:ILE:HD11	1.85	0.59
1:A:233:PRO:HB3	1:A:263:ILE:HD11	1.84	0.59
1:A:50:HIS:ND1	4:A:430:GOL:C1	2.64	0.58
1:A:225:LEU:HD21	1:A:312:ILE:HD11	1.86	0.58
1:A:270:VAL:HG21	3:A:426:EDO:H12	1.86	0.58
1:A:189:ARG:HH22	3:A:413:EDO:H22	1.71	0.55
1:B:67:VAL:HB	1:B:92:LEU:HD21	1.92	0.52
3:A:413:EDO:H11	6:A:527:HOH:O	2.09	0.52
1:B:137:ALA:O	1:B:142:LYS:HB2	2.11	0.51
1:A:47[B]:ILE:HD11	1:A:56:VAL:CG2	2.38	0.50
1:B:152:ILE:HG21	1:B:192:ARG:HB2	1.94	0.50
1:B:47:ILE:HD11	1:B:56:VAL:CG2	2.40	0.50
1:A:152:ILE:HG21	1:A:192:ARG:HB2	1.95	0.49
1:B:103:ASP:HB2	1:B:105:PHE:HE1	1.79	0.47
1:A:116:PRO:HG2	5:A:434:PEG:H41	1.96	0.47
1:A:116:PRO:HB2	3:A:411:EDO:H12	1.96	0.46
1:B:150:LEU:O	1:B:219:LEU:HB2	2.16	0.46
1:A:221:ARG:NH2	1:B:128:PRO:HG3	2.31	0.45
1:B:191:LEU:HD22	1:B:305:LEU:HD12	1.99	0.45
1:B:301:MET:O	1:B:305:LEU:HG	2.18	0.44
1:A:191:LEU:HD22	1:A:305:LEU:HD12	1.99	0.44
1:A:210:ALA:HB3	1:A:259:ILE:HG13	1.99	0.44
1:A:191:LEU:HD21	1:A:302:ALA:HA	2.00	0.43
1:B:259:ILE:HG23	1:B:281:LEU:HA	2.00	0.43
1:A:50:HIS:H	4:A:430:GOL:H11	1.84	0.43
1:A:222:GLU:HA	3:A:410:EDO:H21	2.01	0.42
1:B:132:ALA:HB1	1:B:137:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ILE:HG13	1:B:259:ILE:HD11	2.03	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	274/294 (93%)	266 (97%)	8 (3%)	0	100	100
1	B	271/294 (92%)	260 (96%)	11 (4%)	0	100	100
All	All	545/588 (93%)	526 (96%)	19 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	217/231 (94%)	211 (97%)	6 (3%)	43	47
1	B	214/231 (93%)	202 (94%)	12 (6%)	21	18
All	All	431/462 (93%)	413 (96%)	18 (4%)	30	30

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	191	LEU
1	A	192	ARG
1	A	230	VAL
1	A	281	LEU
1	A	283	SER
1	B	47	ILE
1	B	103	ASP
1	B	105	PHE
1	B	133	THR
1	B	164	ARG
1	B	191	LEU
1	B	192	ARG
1	B	200	ASN
1	B	217	ASP
1	B	259	ILE
1	B	281	LEU
1	B	283	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	158	GLN
1	B	75	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
3	EDO	A	409	-	3,3,3	0.54	0	2,2,2	0.36	0
3	EDO	A	407	-	3,3,3	0.42	0	2,2,2	0.50	0
3	EDO	A	420	-	3,3,3	0.56	0	2,2,2	0.38	0
3	EDO	A	408	-	3,3,3	0.61	0	2,2,2	0.12	0
3	EDO	A	419	2	3,3,3	0.39	0	2,2,2	0.46	0
3	EDO	A	410	-	3,3,3	0.49	0	2,2,2	0.51	0
3	EDO	A	417	-	3,3,3	0.62	0	2,2,2	0.34	0
4	GOL	A	430	-	5,5,5	0.10	0	5,5,5	0.50	0
3	EDO	A	422	-	3,3,3	0.53	0	2,2,2	0.37	0
3	EDO	A	416	-	3,3,3	0.57	0	2,2,2	0.29	0
3	EDO	A	424	-	3,3,3	0.66	0	2,2,2	0.11	0
4	GOL	A	431	-	5,5,5	0.21	0	5,5,5	0.41	0
3	EDO	A	411	-	3,3,3	0.52	0	2,2,2	0.39	0
3	EDO	A	426	-	3,3,3	0.52	0	2,2,2	0.07	0
3	EDO	A	412	-	3,3,3	0.50	0	2,2,2	0.52	0
3	EDO	A	413	-	3,3,3	0.80	0	2,2,2	0.23	0
4	GOL	A	428	-	5,5,5	0.17	0	5,5,5	0.30	0
5	PEG	A	432	-	6,6,6	0.30	0	5,5,5	0.18	0
3	EDO	A	423	-	3,3,3	0.68	0	2,2,2	0.28	0
5	PEG	A	434	-	6,6,6	0.33	0	5,5,5	0.21	0
4	GOL	A	427	-	5,5,5	0.13	0	5,5,5	0.25	0
3	EDO	A	425	-	3,3,3	0.64	0	2,2,2	0.31	0
3	EDO	B	401	-	3,3,3	0.60	0	2,2,2	0.38	0
5	PEG	A	436	-	6,6,6	0.16	0	5,5,5	0.04	0
5	PEG	A	435	-	6,6,6	0.29	0	5,5,5	0.20	0
3	EDO	A	415	-	3,3,3	0.62	0	2,2,2	0.26	0
3	EDO	A	418	-	3,3,3	0.57	0	2,2,2	0.34	0
4	GOL	A	429	-	5,5,5	0.07	0	5,5,5	0.52	0
3	EDO	A	414	-	3,3,3	0.44	0	2,2,2	0.49	0
5	PEG	A	433	-	6,6,6	0.30	0	5,5,5	0.30	0
3	EDO	A	421	-	3,3,3	0.65	0	2,2,2	0.13	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	A	409	-	-	0/1/1/1	-
3	EDO	A	407	-	-	0/1/1/1	-
3	EDO	A	420	-	-	0/1/1/1	-
3	EDO	A	408	-	-	0/1/1/1	-
3	EDO	A	419	2	-	1/1/1/1	-
3	EDO	A	410	-	-	1/1/1/1	-
3	EDO	A	417	-	-	0/1/1/1	-
4	GOL	A	430	-	-	0/4/4/4	-
3	EDO	A	422	-	-	0/1/1/1	-
3	EDO	A	416	-	-	0/1/1/1	-
3	EDO	A	424	-	-	0/1/1/1	-
4	GOL	A	431	-	-	3/4/4/4	-
3	EDO	A	411	-	-	1/1/1/1	-
3	EDO	A	426	-	-	1/1/1/1	-
3	EDO	A	412	-	-	1/1/1/1	-
3	EDO	A	413	-	-	0/1/1/1	-
4	GOL	A	428	-	-	0/4/4/4	-
5	PEG	A	432	-	-	1/4/4/4	-
3	EDO	A	423	-	-	1/1/1/1	-
5	PEG	A	434	-	-	3/4/4/4	-
4	GOL	A	427	-	-	0/4/4/4	-
3	EDO	A	425	-	-	1/1/1/1	-
3	EDO	B	401	-	-	0/1/1/1	-
5	PEG	A	436	-	-	3/4/4/4	-
5	PEG	A	435	-	-	2/4/4/4	-
3	EDO	A	415	-	-	1/1/1/1	-
3	EDO	A	418	-	-	1/1/1/1	-
4	GOL	A	429	-	-	0/4/4/4	-
3	EDO	A	414	-	-	1/1/1/1	-
5	PEG	A	433	-	-	0/4/4/4	-
3	EDO	A	421	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	431	GOL	O1-C1-C2-C3
3	A	425	EDO	O1-C1-C2-O2
5	A	436	PEG	O2-C3-C4-O4
3	A	410	EDO	O1-C1-C2-O2
5	A	436	PEG	C4-C3-O2-C2
5	A	436	PEG	C1-C2-O2-C3
5	A	432	PEG	C1-C2-O2-C3
4	A	431	GOL	O1-C1-C2-O2
5	A	434	PEG	O2-C3-C4-O4
3	A	414	EDO	O1-C1-C2-O2
5	A	435	PEG	C4-C3-O2-C2
3	A	419	EDO	O1-C1-C2-O2
3	A	423	EDO	O1-C1-C2-O2
4	A	431	GOL	C1-C2-C3-O3
3	A	426	EDO	O1-C1-C2-O2
5	A	434	PEG	O1-C1-C2-O2
5	A	435	PEG	C1-C2-O2-C3
3	A	411	EDO	O1-C1-C2-O2
3	A	412	EDO	O1-C1-C2-O2
3	A	415	EDO	O1-C1-C2-O2
3	A	418	EDO	O1-C1-C2-O2
5	A	434	PEG	C1-C2-O2-C3

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	419	EDO	2	0
3	A	410	EDO	1	0
4	A	430	GOL	4	0
3	A	411	EDO	1	0
3	A	426	EDO	3	0
3	A	413	EDO	2	0
5	A	434	PEG	3	0
5	A	433	PEG	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	275/294 (93%)	0.33	7 (2%) 57 62	21, 41, 91, 123	0
1	B	273/294 (92%)	2.73	136 (49%) 0 0	59, 131, 171, 190	0
All	All	548/588 (93%)	1.53	143 (26%) 0 0	21, 88, 162, 190	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	PHE	17.7
1	B	289	TYR	12.4
1	B	77	GLY	11.5
1	B	72	ALA	11.4
1	B	248	ILE	11.1
1	B	89	ILE	9.3
1	B	81	PRO	9.2
1	B	257	LYS	9.2
1	B	233	PRO	8.8
1	A	77	GLY	8.7
1	B	312	ILE	8.6
1	B	82	ARG	7.9
1	B	279	VAL	7.7
1	B	71	PRO	7.6
1	B	202	ALA	7.6
1	B	73	GLY	7.5
1	B	79	TYR	7.3
1	B	90	GLY	7.2
1	B	205	ALA	7.1
1	B	114	GLU	6.7
1	B	237	ILE	6.7
1	B	258	VAL	6.6
1	B	266	PRO	6.6
1	B	111	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	75	ASN	6.4
1	B	53	TYR	6.2
1	B	203	PRO	6.2
1	B	308	VAL	6.1
1	B	78	ALA	6.0
1	B	282	TYR	6.0
1	B	244	LEU	6.0
1	B	251	LEU	5.9
1	B	254	LEU	5.9
1	B	84	GLU	5.8
1	B	83	ALA	5.8
1	B	206	ASP	5.7
1	B	256	VAL	5.7
1	B	172	ALA	5.6
1	B	70	ILE	5.5
1	B	259	ILE	5.4
1	B	66	VAL	5.3
1	B	76	PRO	5.2
1	B	281	LEU	5.0
1	B	315	SER	5.0
1	B	212	ILE	5.0
1	B	264	ASP	5.0
1	B	268	THR	5.0
1	B	86	ILE	4.9
1	B	239	PRO	4.9
1	B	109	MET	4.9
1	B	223	PHE	4.8
1	B	241	PRO	4.8
1	B	297	TYR	4.8
1	B	80	GLU	4.7
1	B	236	GLY	4.7
1	B	113	SER	4.6
1	B	207	PHE	4.6
1	B	139	GLY	4.5
1	B	92	LEU	4.5
1	B	91	THR	4.5
1	B	69	LEU	4.5
1	B	196	LEU	4.5
1	B	240	SER	4.4
1	B	271	GLU	4.4
1	B	280	LYS	4.3
1	B	273	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	275	ARG	4.3
1	B	118	ILE	4.2
1	B	277	SER	4.2
1	B	174	ALA	4.2
1	B	310	ARG	4.1
1	B	176	ALA	4.0
1	B	94	VAL	4.0
1	A	74	PHE	4.0
1	B	181	ALA	3.9
1	B	242	SER	3.9
1	B	267	SER	3.8
1	B	208	ARG	3.8
1	B	286	GLY	3.7
1	B	95	VAL	3.7
1	B	278	GLY	3.7
1	B	87	LYS	3.7
1	B	59	ILE	3.7
1	B	67	VAL	3.6
1	B	201	LYS	3.6
1	B	48	THR	3.6
1	B	313	GLN	3.5
1	B	185	ALA	3.4
1	B	85	ASP	3.4
1	A	82	ARG	3.4
1	B	43	LEU	3.3
1	B	204	ALA	3.3
1	A	202	ALA	3.3
1	B	260	PHE	3.2
1	A	78	ALA	3.2
1	B	314	GLU	3.1
1	B	141	GLY	3.1
1	B	234	ALA	3.1
1	B	195	ALA	3.1
1	B	292	TYR	3.0
1	B	49	LEU	3.0
1	B	88	ARG	3.0
1	B	116	PRO	3.0
1	B	46	GLY	2.9
1	B	60	VAL	2.9
1	B	272	THR	2.9
1	B	112	SER	2.8
1	B	301	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	115	LYS	2.7
1	B	228	THR	2.7
1	B	191	LEU	2.7
1	B	140	ALA	2.6
1	B	311	ALA	2.6
1	B	269	TYR	2.6
1	B	133	THR	2.5
1	B	169	LEU	2.5
1	B	167	GLY	2.5
1	B	305	LEU	2.5
1	B	309	VAL	2.5
1	B	265	PHE	2.5
1	B	209	VAL	2.4
1	B	62	ASP	2.4
1	B	179	ARG	2.4
1	B	270	VAL	2.4
1	A	205	ALA	2.4
1	B	55	TYR	2.4
1	B	291	ASP	2.3
1	B	252	LYS	2.3
1	B	238	GLU	2.3
1	B	93	ASP	2.3
1	A	79	TYR	2.3
1	B	175	LYS	2.3
1	B	177	TYR	2.2
1	B	168	LYS	2.2
1	B	52	TYR	2.2
1	B	105	PHE	2.2
1	B	284	LEU	2.1
1	B	243	GLN	2.1
1	B	262	GLU	2.1
1	B	299	GLU	2.1
1	B	182	ARG	2.1
1	B	56	VAL	2.1
1	B	121	ILE	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
5	PEG	A	432	7/7	0.61	0.19	82,85,86,87	0
3	EDO	A	424	4/4	0.68	0.25	80,81,81,82	0
5	PEG	A	433	7/7	0.69	0.22	76,77,79,80	0
5	PEG	A	435	7/7	0.72	0.21	57,61,63,65	0
3	EDO	A	416	4/4	0.77	0.24	69,70,70,71	0
3	EDO	A	420	4/4	0.77	0.23	89,90,90,91	0
3	EDO	A	415	4/4	0.77	0.15	73,74,75,77	0
3	EDO	A	421	4/4	0.78	0.17	73,75,75,75	0
2	NA	A	405	1/1	0.79	0.39	75,75,75,75	0
3	EDO	A	418	4/4	0.79	0.28	47,53,57,58	0
3	EDO	A	413	4/4	0.81	0.19	47,49,50,50	0
3	EDO	A	408	4/4	0.81	0.15	73,73,74,74	0
2	NA	A	401	1/1	0.83	0.31	71,71,71,71	0
3	EDO	A	409	4/4	0.83	0.24	51,54,58,59	0
3	EDO	A	414	4/4	0.84	0.15	71,71,72,72	0
3	EDO	A	417	4/4	0.84	0.24	60,65,69,70	0
3	EDO	A	412	4/4	0.84	0.25	58,63,66,69	0
3	EDO	A	425	4/4	0.86	0.18	54,57,59,59	0
5	PEG	A	436	7/7	0.86	0.17	78,80,81,83	0
3	EDO	A	410	4/4	0.88	0.22	60,61,62,62	0
3	EDO	B	401	4/4	0.88	0.23	60,61,62,62	0
3	EDO	A	411	4/4	0.88	0.34	55,57,60,62	0
3	EDO	A	422	4/4	0.89	0.17	71,72,72,72	0
2	NA	A	402	1/1	0.90	0.27	78,78,78,78	0
4	GOL	A	430	6/6	0.90	0.17	49,58,58,59	0
3	EDO	A	426	4/4	0.90	0.27	46,47,48,48	0
4	GOL	A	429	6/6	0.91	0.16	77,78,80,81	0
2	NA	A	406	1/1	0.91	0.21	64,64,64,64	0
3	EDO	A	423	4/4	0.91	0.23	59,62,64,65	0
4	GOL	A	431	6/6	0.92	0.19	40,45,51,61	0
3	EDO	A	419	4/4	0.93	0.19	45,46,49,52	0
2	NA	A	404	1/1	0.94	0.27	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	A	434	7/7	0.95	0.15	29,34,42,45	0
4	GOL	A	428	6/6	0.96	0.14	46,47,50,55	0
2	NA	A	403	1/1	0.96	0.09	67,67,67,67	0
4	GOL	A	427	6/6	0.96	0.14	42,47,48,49	0
3	EDO	A	407	4/4	0.97	0.16	57,59,62,64	0

6.5 Other polymers

There are no such residues in this entry.