



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:41 PM UTC

PDB ID : 6R6K / pdb_00006r6k
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 ⓘ 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

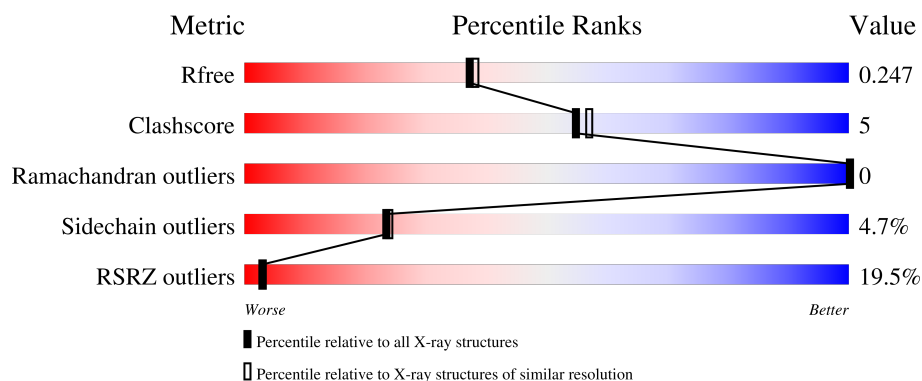
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	294	
1	B	294	

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

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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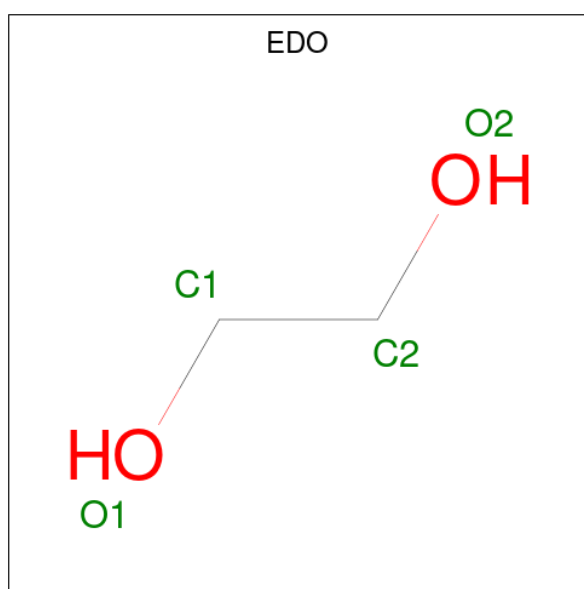
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Chain	Residue	Modelled	Actual	Comment	Reference
B	235	GLY	HIS	conflict	UNP A0A3G3N2S3
B	286	GLY	HIS	conflict	UNP A0A3G3N2S3
B	318	GLU	-	expression tag	UNP A0A3G3N2S3
B	319	ASN	-	expression tag	UNP A0A3G3N2S3
B	320	LEU	-	expression tag	UNP A0A3G3N2S3
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 (CCD ID: NA) (formula: Na).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



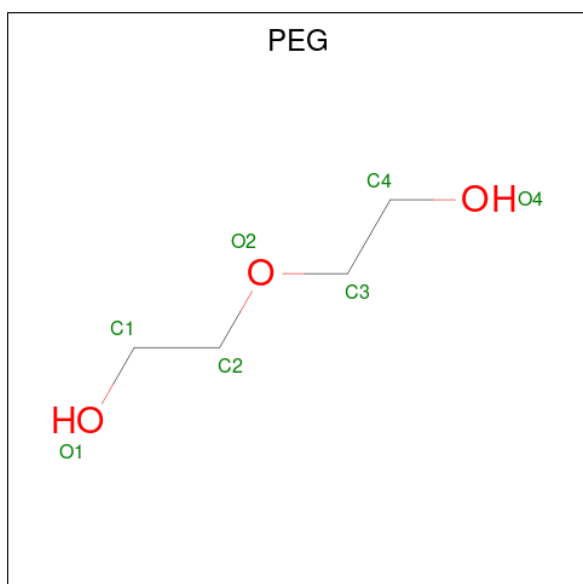
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

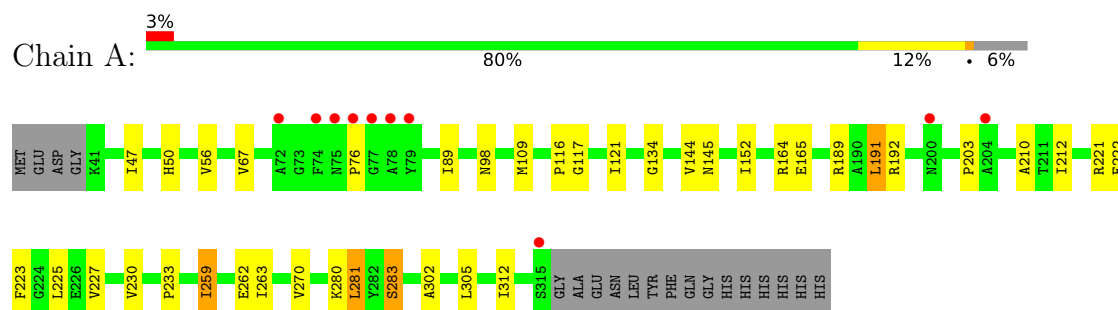
- Molecule 6 is water.

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

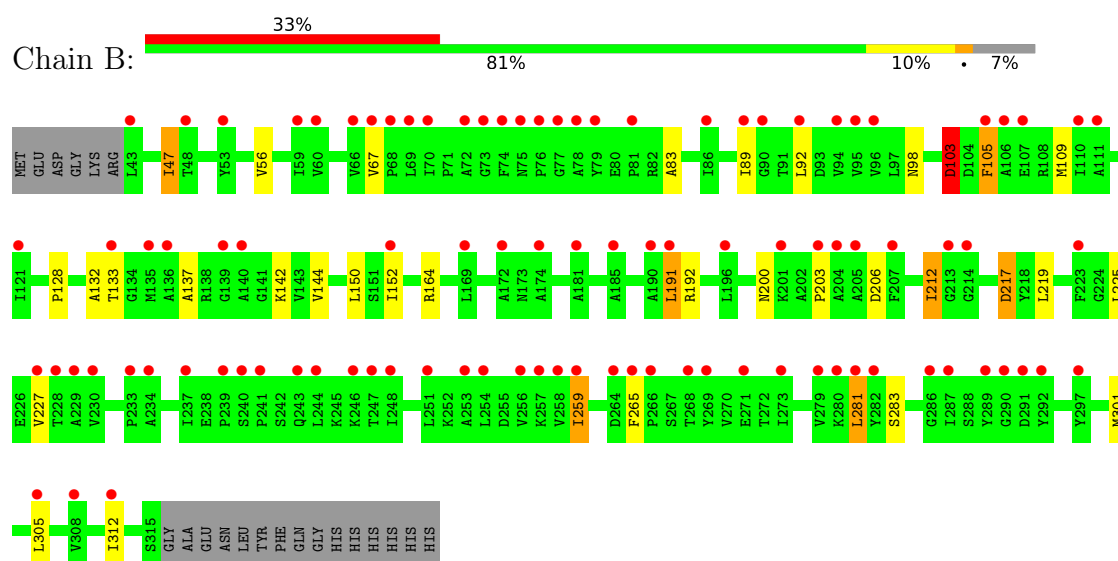
3 Residue-property plots

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



- Molecule 1: ABC transporter substrate-binding protein



4 Data and refinement statistics

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) 67.9 (43.74-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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: EDO, NA, GOL, PEG

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	0.92	1/2126 (0.0%)	1.40	10/2883 (0.3%)
1	B	0.84	0/2098	1.40	12/2847 (0.4%)
All	All	0.88	1/4224 (0.0%)	1.40	22/5730 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ASN	CA-C	5.81	1.59	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASN	N-CA-C	-9.18	101.22	111.14
1	B	98	ASN	N-CA-C	-8.64	101.81	111.14
1	B	103	ASP	CA-CB-CG	8.52	121.11	112.60
1	A	227	VAL	CA-C-N	7.18	129.78	120.44
1	A	227	VAL	C-N-CA	7.18	129.78	120.44
1	B	227	VAL	CA-C-N	6.91	129.42	120.44
1	B	227	VAL	C-N-CA	6.91	129.42	120.44
1	B	217	ASP	N-CA-C	6.01	117.83	111.28
1	A	223	PHE	CA-CB-CG	-5.84	107.96	113.80
1	B	212	ILE	N-CA-C	-5.59	99.18	107.51
1	A	212	ILE	N-CA-C	-5.54	99.17	107.37
1	B	203	PRO	CA-C-N	5.48	128.38	120.38
1	B	203	PRO	C-N-CA	5.48	128.38	120.38
1	A	134	GLY	CA-C-N	5.35	127.77	120.54
1	A	134	GLY	C-N-CA	5.35	127.77	120.54
1	A	203	PRO	CA-C-N	5.32	128.14	120.38
1	A	203	PRO	C-N-CA	5.32	128.14	120.38
1	B	265	PHE	CA-CB-CG	5.24	119.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ALA	CA-C-N	5.03	127.02	120.28
1	B	83	ALA	C-N-CA	5.03	127.02	120.28
1	A	262	GLU	N-CA-C	-5.01	106.00	111.82
1	B	206	ASP	CA-CB-CG	5.01	117.61	112.60

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	26	0
1	B	2063	0	2103	16	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	42	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 5.

All (42) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:219:LEU:HD12	1:B:301:MET:HE1	1.94	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:A:89:ILE:HD11	1:A:109:MET:HE2	1.99	0.44
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:B:89:ILE:HD11	1:B:109:MET:HE2	2.01	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
1:B:212:ILE:HG13	1:B:259:ILE:HD11	2.03	0.41

There are no symmetry-related clashes.

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	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

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%)	209 (96%)	8 (4%)	30	33
1	B	214/231 (93%)	202 (94%)	12 (6%)	19	18
All	All	431/462 (93%)	411 (95%)	20 (5%)	23	25

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	VAL
1	A	164	ARG
1	A	191	LEU
1	A	230	VAL
1	A	259	ILE
1	A	280	LYS
1	A	281	LEU
1	A	283	SER

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Mol	Chain	Res	Type
1	B	47	ILE
1	B	103	ASP
1	B	105	PHE
1	B	133	THR
1	B	144	VAL
1	B	164	ARG
1	B	191	LEU
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	124	ASN
1	A	158	GLN
1	A	200	ASN
1	B	98	ASN
1	B	124	ASN
1	B	200	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 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	$\# Z > 2$
4	GOL	A	430	-	5,5,5	0.10	0	5,5,5	0.50	0
3	EDO	A	414	-	3,3,3	0.44	0	2,2,2	0.49	0
3	EDO	A	412	-	3,3,3	0.50	0	2,2,2	0.52	0
5	PEG	A	433	-	6,6,6	0.30	0	5,5,5	0.30	0
5	PEG	A	434	-	6,6,6	0.33	0	5,5,5	0.21	0
3	EDO	A	413	-	3,3,3	0.80	0	2,2,2	0.23	0
3	EDO	A	408	-	3,3,3	0.61	0	2,2,2	0.12	0
3	EDO	A	426	-	3,3,3	0.52	0	2,2,2	0.07	0
3	EDO	A	425	-	3,3,3	0.64	0	2,2,2	0.31	0
4	GOL	A	428	-	5,5,5	0.17	0	5,5,5	0.30	0
3	EDO	A	421	-	3,3,3	0.65	0	2,2,2	0.13	0
3	EDO	A	417	-	3,3,3	0.62	0	2,2,2	0.34	0
3	EDO	A	419	2	3,3,3	0.39	0	2,2,2	0.46	0
3	EDO	A	422	-	3,3,3	0.53	0	2,2,2	0.37	0
3	EDO	A	418	-	3,3,3	0.57	0	2,2,2	0.34	0
3	EDO	A	409	-	3,3,3	0.54	0	2,2,2	0.36	0
4	GOL	A	429	-	5,5,5	0.07	0	5,5,5	0.52	0
5	PEG	A	432	-	6,6,6	0.30	0	5,5,5	0.18	0
3	EDO	B	401	-	3,3,3	0.60	0	2,2,2	0.38	0
3	EDO	A	416	-	3,3,3	0.57	0	2,2,2	0.29	0
5	PEG	A	436	-	6,6,6	0.16	0	5,5,5	0.04	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
5	PEG	A	435	-	6,6,6	0.29	0	5,5,5	0.20	0
3	EDO	A	424	-	3,3,3	0.66	0	2,2,2	0.11	0
4	GOL	A	427	-	5,5,5	0.13	0	5,5,5	0.25	0
3	EDO	A	411	-	3,3,3	0.52	0	2,2,2	0.39	0
3	EDO	A	423	-	3,3,3	0.68	0	2,2,2	0.28	0
3	EDO	A	415	-	3,3,3	0.62	0	2,2,2	0.26	0
4	GOL	A	431	-	5,5,5	0.21	0	5,5,5	0.41	0
3	EDO	A	410	-	3,3,3	0.49	0	2,2,2	0.51	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	430	-	-	0/4/4/4	-
3	EDO	A	414	-	-	1/1/1/1	-
3	EDO	A	412	-	-	1/1/1/1	-
5	PEG	A	433	-	-	0/4/4/4	-
5	PEG	A	434	-	-	3/4/4/4	-
3	EDO	A	413	-	-	0/1/1/1	-
3	EDO	A	408	-	-	0/1/1/1	-
3	EDO	A	426	-	-	1/1/1/1	-
3	EDO	A	425	-	-	1/1/1/1	-
4	GOL	A	428	-	-	0/4/4/4	-
3	EDO	A	421	-	-	0/1/1/1	-
3	EDO	A	417	-	-	0/1/1/1	-
3	EDO	A	419	2	-	1/1/1/1	-
3	EDO	A	422	-	-	0/1/1/1	-
3	EDO	A	418	-	-	1/1/1/1	-
3	EDO	A	409	-	-	0/1/1/1	-
4	GOL	A	429	-	-	0/4/4/4	-
5	PEG	A	432	-	-	1/4/4/4	-
3	EDO	B	401	-	-	0/1/1/1	-
3	EDO	A	416	-	-	0/1/1/1	-
5	PEG	A	436	-	-	3/4/4/4	-
3	EDO	A	407	-	-	0/1/1/1	-
3	EDO	A	420	-	-	0/1/1/1	-
5	PEG	A	435	-	-	2/4/4/4	-
3	EDO	A	424	-	-	0/1/1/1	-
4	GOL	A	427	-	-	0/4/4/4	-
3	EDO	A	411	-	-	1/1/1/1	-
3	EDO	A	423	-	-	1/1/1/1	-
3	EDO	A	415	-	-	1/1/1/1	-
4	GOL	A	431	-	-	3/4/4/4	-
3	EDO	A	410	-	-	1/1/1/1	-

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

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Mol	Chain	Res	Type	Atoms
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
4	A	430	GOL	4	0
5	A	433	PEG	1	0
5	A	434	PEG	3	0
3	A	413	EDO	2	0
3	A	426	EDO	3	0
3	A	419	EDO	2	0
3	A	411	EDO	1	0
3	A	410	EDO	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

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, 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	275/294 (93%)	-0.07	10 (3%) 46 48	15, 41, 91, 123	1 (0%)
1	B	273/294 (92%)	1.75	97 (35%) 1 1	59, 131, 171, 190	0
All	All	548/588 (93%)	0.84	107 (19%) 3 3	15, 88, 162, 190	1 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	TYR	6.4
1	B	244	LEU	5.5
1	A	77	GLY	4.9
1	B	281	LEU	4.9
1	B	70	ILE	4.6
1	B	72	ALA	4.5
1	B	312	ILE	4.3
1	B	74	PHE	4.2
1	B	76	PRO	4.1
1	B	205	ALA	4.0
1	B	237	ILE	3.9
1	B	230	VAL	3.8
1	B	66	VAL	3.8
1	B	264	ASP	3.6
1	B	234	ALA	3.6
1	B	73	GLY	3.6
1	B	140	ALA	3.5
1	B	53	TYR	3.5
1	B	133	THR	3.4
1	B	90	GLY	3.4
1	B	111	ALA	3.4
1	A	76	PRO	3.4
1	B	69	LEU	3.3
1	B	268	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	3.3
1	B	279	VAL	3.2
1	B	172	ALA	3.2
1	B	228	THR	3.1
1	B	77	GLY	3.1
1	B	233	PRO	3.1
1	B	181	ALA	3.1
1	B	259	ILE	3.1
1	B	292	TYR	3.0
1	B	203	PRO	3.0
1	B	139	GLY	3.0
1	B	227	VAL	2.9
1	B	241	PRO	2.9
1	B	95	VAL	2.9
1	A	79	TYR	2.9
1	B	79	TYR	2.9
1	B	290	GLY	2.9
1	B	273	ILE	2.8
1	B	223	PHE	2.8
1	B	251	LEU	2.8
1	A	74	PHE	2.8
1	A	78	ALA	2.8
1	B	169	LEU	2.8
1	B	254	LEU	2.8
1	B	190	ALA	2.7
1	B	229	ALA	2.7
1	B	196	LEU	2.7
1	B	297	TYR	2.7
1	B	239	PRO	2.7
1	B	43	LEU	2.6
1	B	266	PRO	2.6
1	B	286	GLY	2.6
1	B	248	ILE	2.6
1	B	67	VAL	2.5
1	B	247	THR	2.5
1	A	204	ALA	2.5
1	B	305	LEU	2.5
1	B	89	ILE	2.5
1	B	105	PHE	2.5
1	B	78	ALA	2.4
1	B	92	LEU	2.4
1	B	107	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	60	VAL	2.4
1	B	94	VAL	2.4
1	B	48	THR	2.4
1	B	174	ALA	2.4
1	B	75	ASN	2.4
1	B	308	VAL	2.4
1	B	253	ALA	2.3
1	B	135	MET	2.3
1	B	185	ALA	2.3
1	B	68	PRO	2.3
1	B	136	ALA	2.3
1	B	269	TYR	2.3
1	B	243	GLN	2.2
1	A	200	ASN	2.2
1	B	291	ASP	2.2
1	B	106	ALA	2.2
1	B	214	GLY	2.2
1	B	240	SER	2.2
1	B	121	ILE	2.2
1	B	257	LYS	2.2
1	B	271	GLU	2.2
1	B	280	LYS	2.2
1	A	75	ASN	2.2
1	B	287	ILE	2.2
1	B	282	TYR	2.2
1	B	246	LYS	2.2
1	B	86	ILE	2.1
1	B	96	VAL	2.1
1	B	256	VAL	2.1
1	B	110	ILE	2.1
1	B	207	PHE	2.1
1	B	265	PHE	2.1
1	A	315	SER	2.1
1	B	81	PRO	2.1
1	B	258	VAL	2.1
1	B	204	ALA	2.1
1	B	201	LYS	2.0
1	B	59	ILE	2.0
1	B	152	ILE	2.0
1	B	191	LEU	2.0
1	B	213	GLY	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 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
3	EDO	A	420	4/4	0.64	0.19	89,90,90,91	0
4	GOL	A	429	6/6	0.74	0.16	77,78,80,81	0
5	PEG	A	432	7/7	0.74	0.19	82,85,86,87	0
3	EDO	A	417	4/4	0.76	0.20	60,65,69,70	0
5	PEG	A	433	7/7	0.77	0.18	76,77,79,80	0
5	PEG	A	435	7/7	0.78	0.18	57,61,63,65	0
3	EDO	A	416	4/4	0.79	0.20	69,70,70,71	0
3	EDO	A	415	4/4	0.80	0.19	73,74,75,77	0
3	EDO	A	412	4/4	0.80	0.20	58,63,66,69	0
3	EDO	B	401	4/4	0.82	0.12	60,61,62,62	0
4	GOL	A	430	6/6	0.83	0.16	49,58,58,59	0
3	EDO	A	421	4/4	0.83	0.14	73,75,75,75	0
3	EDO	A	410	4/4	0.83	0.20	60,61,62,62	0
2	NA	A	405	1/1	0.83	0.22	75,75,75,75	0
3	EDO	A	425	4/4	0.84	0.16	54,57,59,59	0
2	NA	A	402	1/1	0.85	0.20	78,78,78,78	0
3	EDO	A	414	4/4	0.86	0.15	71,71,72,72	0
3	EDO	A	411	4/4	0.86	0.23	55,57,60,62	0
3	EDO	A	424	4/4	0.86	0.18	80,81,81,82	0
2	NA	A	401	1/1	0.86	0.17	71,71,71,71	0
3	EDO	A	413	4/4	0.86	0.23	47,49,50,50	0
5	PEG	A	436	7/7	0.87	0.15	78,80,81,83	0
3	EDO	A	423	4/4	0.89	0.18	59,62,64,65	0
3	EDO	A	426	4/4	0.90	0.20	46,47,48,48	0
3	EDO	A	409	4/4	0.90	0.16	51,54,58,59	0
3	EDO	A	418	4/4	0.90	0.19	47,53,57,58	0
3	EDO	A	422	4/4	0.90	0.14	71,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	408	4/4	0.91	0.13	73,73,74,74	0
2	NA	A	403	1/1	0.91	0.10	67,67,67,67	0
3	EDO	A	407	4/4	0.91	0.12	57,59,62,64	0
4	GOL	A	431	6/6	0.91	0.12	40,45,51,61	0
4	GOL	A	428	6/6	0.93	0.09	46,47,50,55	0
2	NA	A	406	1/1	0.93	0.18	64,64,64,64	0
3	EDO	A	419	4/4	0.93	0.13	45,46,49,52	0
4	GOL	A	427	6/6	0.93	0.11	42,47,48,49	0
2	NA	A	404	1/1	0.94	0.16	69,69,69,69	0
5	PEG	A	434	7/7	0.95	0.14	29,34,42,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.