



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:51 AM UTC

PDB ID : 8UQU / pdb_00008uqu
Title : Crystal Structure of N-terminal Domain of Fic Family Protein from Bordetella bronchiseptica
Authors : Minasov, G.; Shuvalova, L.; Brunzelle, J.S.; Kiryukhina, O.; Satchell, K.J.F.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2023-10-24
Resolution : 2.95 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

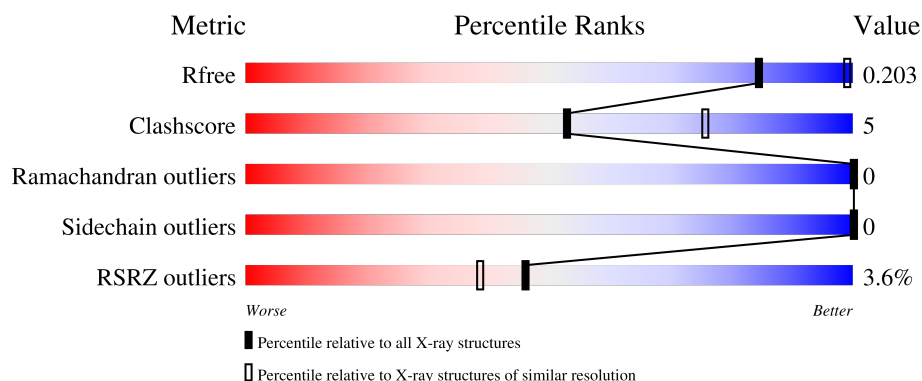
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	366	2% 60% 7% 33%
1	B	366	2% 60% 8% 32%
1	C	366	4% 58% 11% 31%

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
6	EDO	A	406	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6252 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 Fido domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1969	1258	340	363	8			
1	B	250	Total	C	N	O	S	0	0	0
			2004	1277	351	368	8			
1	C	253	Total	C	N	O	S	0	0	0
			2027	1293	355	371	8			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP A0A0H3LJJ5
A	-16	HIS	-	expression tag	UNP A0A0H3LJJ5
A	-15	HIS	-	expression tag	UNP A0A0H3LJJ5
A	-14	HIS	-	expression tag	UNP A0A0H3LJJ5
A	-13	HIS	-	expression tag	UNP A0A0H3LJJ5
A	-12	HIS	-	expression tag	UNP A0A0H3LJJ5
A	-11	HIS	-	expression tag	UNP A0A0H3LJJ5
A	-10	SER	-	expression tag	UNP A0A0H3LJJ5
A	-9	SER	-	expression tag	UNP A0A0H3LJJ5
A	-8	GLY	-	expression tag	UNP A0A0H3LJJ5
A	-7	ARG	-	expression tag	UNP A0A0H3LJJ5
A	-6	GLU	-	expression tag	UNP A0A0H3LJJ5
A	-5	ASN	-	expression tag	UNP A0A0H3LJJ5
A	-4	LEU	-	expression tag	UNP A0A0H3LJJ5
A	-3	TYR	-	expression tag	UNP A0A0H3LJJ5
A	-2	PHE	-	expression tag	UNP A0A0H3LJJ5
A	-1	GLN	-	expression tag	UNP A0A0H3LJJ5
A	0	GLY	-	expression tag	UNP A0A0H3LJJ5
B	-17	MET	-	expression tag	UNP A0A0H3LJJ5
B	-16	HIS	-	expression tag	UNP A0A0H3LJJ5
B	-15	HIS	-	expression tag	UNP A0A0H3LJJ5
B	-14	HIS	-	expression tag	UNP A0A0H3LJJ5
B	-13	HIS	-	expression tag	UNP A0A0H3LJJ5

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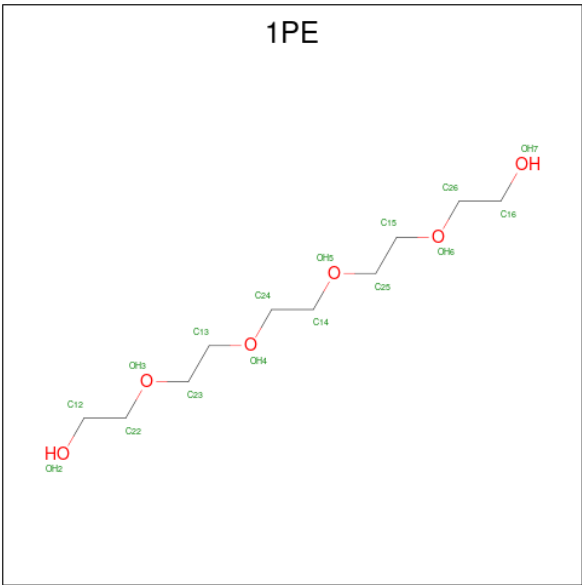
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A0H3LJJ5
B	-11	HIS	-	expression tag	UNP A0A0H3LJJ5
B	-10	SER	-	expression tag	UNP A0A0H3LJJ5
B	-9	SER	-	expression tag	UNP A0A0H3LJJ5
B	-8	GLY	-	expression tag	UNP A0A0H3LJJ5
B	-7	ARG	-	expression tag	UNP A0A0H3LJJ5
B	-6	GLU	-	expression tag	UNP A0A0H3LJJ5
B	-5	ASN	-	expression tag	UNP A0A0H3LJJ5
B	-4	LEU	-	expression tag	UNP A0A0H3LJJ5
B	-3	TYR	-	expression tag	UNP A0A0H3LJJ5
B	-2	PHE	-	expression tag	UNP A0A0H3LJJ5
B	-1	GLN	-	expression tag	UNP A0A0H3LJJ5
B	0	GLY	-	expression tag	UNP A0A0H3LJJ5
C	-17	MET	-	expression tag	UNP A0A0H3LJJ5
C	-16	HIS	-	expression tag	UNP A0A0H3LJJ5
C	-15	HIS	-	expression tag	UNP A0A0H3LJJ5
C	-14	HIS	-	expression tag	UNP A0A0H3LJJ5
C	-13	HIS	-	expression tag	UNP A0A0H3LJJ5
C	-12	HIS	-	expression tag	UNP A0A0H3LJJ5
C	-11	HIS	-	expression tag	UNP A0A0H3LJJ5
C	-10	SER	-	expression tag	UNP A0A0H3LJJ5
C	-9	SER	-	expression tag	UNP A0A0H3LJJ5
C	-8	GLY	-	expression tag	UNP A0A0H3LJJ5
C	-7	ARG	-	expression tag	UNP A0A0H3LJJ5
C	-6	GLU	-	expression tag	UNP A0A0H3LJJ5
C	-5	ASN	-	expression tag	UNP A0A0H3LJJ5
C	-4	LEU	-	expression tag	UNP A0A0H3LJJ5
C	-3	TYR	-	expression tag	UNP A0A0H3LJJ5
C	-2	PHE	-	expression tag	UNP A0A0H3LJJ5
C	-1	GLN	-	expression tag	UNP A0A0H3LJJ5
C	0	GLY	-	expression tag	UNP A0A0H3LJJ5

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

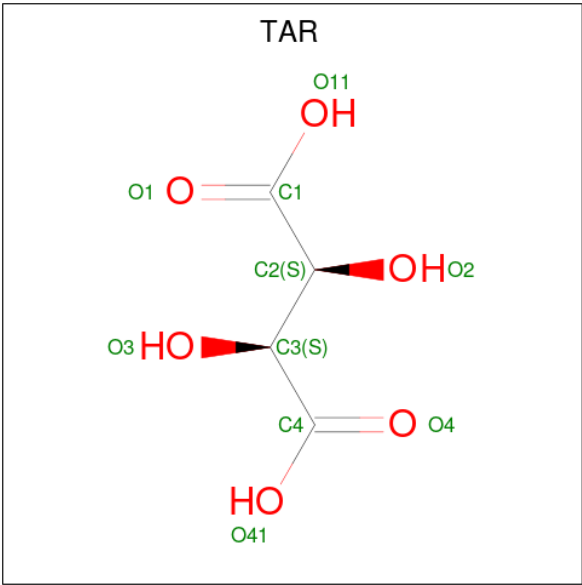
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: C₄H₆O₆).



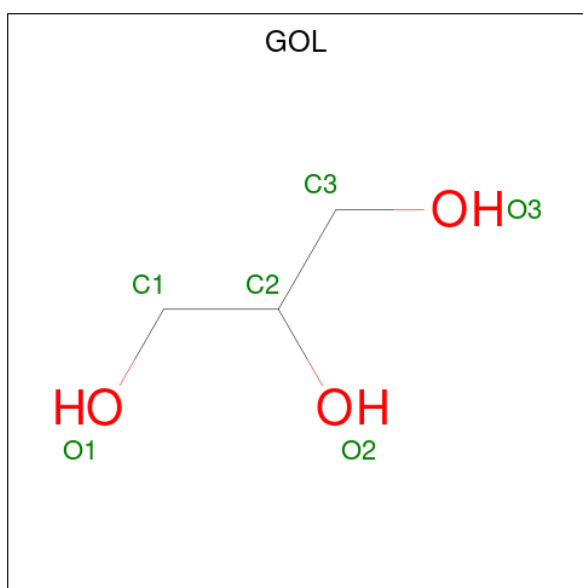
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	A	1	Total	C	O	0	0
			10	4	6		
4	B	1	Total	C	O	0	0
			10	4	6		

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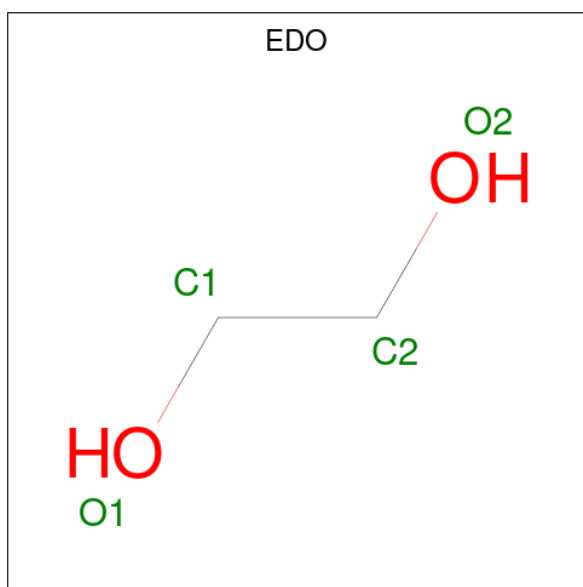
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	4	6		
4	B	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

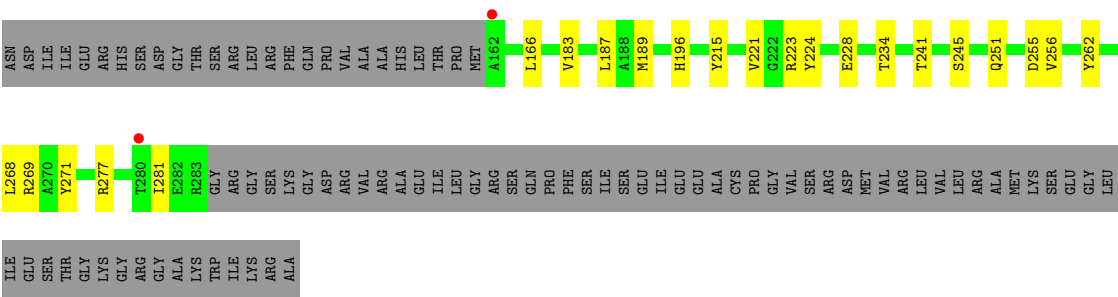
- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	40	Total	O	0	0
			40	40		
7	B	39	Total	O	0	0
			39	39		
7	C	36	Total	O	0	0
			36	36		



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.97Å 149.97Å 371.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.95 29.91 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-2.95) 99.8 (29.91-2.95)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.178 , 0.207 0.177 , 0.203	Depositor DCC
R_{free} test set	2699 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6252	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: 1PE, GOL, NA, TAR, 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	0.98	0/2015	1.30	1/2732 (0.0%)
1	B	0.99	0/2050	1.28	0/2777
1	C	0.99	0/2075	1.29	3/2812 (0.1%)
All	All	0.99	0/6140	1.29	4/8321 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	VAL	N-CA-C	-5.59	106.75	111.56
1	A	183	VAL	N-CA-C	-5.53	106.81	111.56
1	C	32	GLN	CB-CA-C	-5.50	102.25	110.88
1	C	196	HIS	CB-CA-C	5.26	114.93	111.20

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	1969	0	1944	19	0
1	B	2004	0	1981	19	0
1	C	2027	0	1999	25	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	22	0	0
4	A	20	0	8	0	0
4	B	30	0	12	0	0
4	C	30	0	12	0	0
5	A	6	0	8	0	0
5	C	6	0	8	0	0
6	A	8	0	12	0	0
6	B	20	0	30	0	0
7	A	40	0	0	1	0
7	B	39	0	0	0	0
7	C	36	0	0	0	0
All	All	6252	0	6036	61	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 (61) 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:B:189:MET:HA	1:B:189:MET:HE2	1.71	0.72
1:C:189:MET:HA	1:C:189:MET:HE2	1.75	0.69
1:A:189:MET:HA	1:A:189:MET:HE2	1.76	0.67
1:C:1:MET:HG2	1:C:166:LEU:HA	1.79	0.65
1:B:58:SER:HB2	1:B:228:GLU:HG2	1.80	0.64
1:C:58:SER:HB2	1:C:228:GLU:HG2	1.81	0.62
1:C:34:LEU:C	1:C:34:LEU:HD23	2.25	0.61
1:A:58:SER:HB2	1:A:228:GLU:HG2	1.81	0.61
1:B:29:GLN:HB2	1:B:219:TYR:CE1	2.36	0.60
1:C:215:TYR:OH	1:C:223:ARG:HB2	2.06	0.55
1:B:165:ASP:O	1:B:166:LEU:C	2.50	0.54
1:B:83:ASN:O	1:B:87:GLN:HG3	2.07	0.54
1:A:23:ARG:NH2	1:A:27:GLU:OE1	2.38	0.54
1:A:277:ARG:HB2	7:A:521:HOH:O	2.09	0.52
1:C:43:LEU:HB3	1:C:224:TYR:CE1	2.45	0.51
1:C:34:LEU:HD21	1:C:38:GLN:NE2	2.26	0.51
1:C:84:ARG:HG3	1:C:124:MET:HE1	1.91	0.51
1:A:83:ASN:O	1:A:87:GLN:HG3	2.11	0.51
1:A:189:MET:HE2	1:A:189:MET:CA	2.41	0.51
1:B:1:MET:HE3	1:B:165:ASP:HB2	1.94	0.49
1:B:56:GLU:HB2	1:B:71:LEU:HD21	1.95	0.49
1:C:29:GLN:O	1:C:29:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:HG21	1:B:269:ARG:NH2	2.27	0.49
1:C:187:LEU:HD22	1:C:256:VAL:HG11	1.94	0.48
1:A:21:THR:HG23	1:A:268:LEU:HD11	1.95	0.48
1:B:187:LEU:HD22	1:B:256:VAL:HG11	1.96	0.48
1:A:121:TYR:HD1	1:A:124:MET:HG3	1.78	0.48
1:A:36:ALA:O	1:A:40:PRO:HD3	2.14	0.48
1:A:277:ARG:O	1:A:277:ARG:HG3	2.13	0.47
1:B:108:PHE:HB2	1:B:213:LEU:HD21	1.96	0.47
1:C:241:THR:HG21	1:C:262:TYR:HB2	1.96	0.47
1:C:23:ARG:NH2	1:C:27:GLU:OE1	2.49	0.46
1:C:28:TYR:HB3	1:C:271:TYR:CD1	2.51	0.46
1:A:113:VAL:HG11	1:A:163:MET:HE2	1.99	0.45
1:B:110:GLU:OE2	1:B:164:ALA:HA	2.16	0.45
1:A:23:ARG:HD3	1:B:180:ASP:OD2	2.16	0.45
1:A:221:VAL:HB	1:A:271:TYR:CE1	2.52	0.45
1:B:189:MET:HE2	1:B:189:MET:CA	2.42	0.45
1:C:21:THR:HG23	1:C:268:LEU:HD11	1.99	0.45
1:B:14:PHE:HA	1:B:18:GLN:OE1	2.17	0.45
1:A:28:TYR:CD1	1:A:271:TYR:HB3	2.52	0.44
1:C:223:ARG:HD2	1:C:224:TYR:CZ	2.53	0.44
1:C:234:THR:HG21	1:C:269:ARG:NH2	2.32	0.44
1:A:185:VAL:HG22	1:A:213:LEU:HB3	1.99	0.44
1:B:2:HIS:HB3	1:B:252:GLY:HA2	1.99	0.43
1:C:277:ARG:O	1:C:281:ILE:HG13	2.19	0.43
1:C:221:VAL:HB	1:C:271:TYR:CE1	2.54	0.42
1:C:1:MET:SD	1:C:1:MET:N	2.76	0.42
1:C:36:ALA:HA	1:C:43:LEU:HD11	2.01	0.42
1:A:51:VAL:HG12	1:A:75:VAL:CG1	2.49	0.42
1:A:183:VAL:O	1:A:187:LEU:HG	2.20	0.41
1:C:245:SER:HA	1:C:255:ASP:O	2.20	0.41
1:B:53:GLU:OE2	1:B:229:ARG:NE	2.52	0.41
1:A:26:GLY:O	1:B:27:GLU:HA	2.20	0.41
1:B:61:LEU:HD21	1:B:232:GLU:HA	2.02	0.41
1:B:29:GLN:CD	1:B:29:GLN:C	2.89	0.41
1:C:34:LEU:HD23	1:C:35:TYR:N	2.36	0.41
1:C:189:MET:HE2	1:C:189:MET:CA	2.46	0.40
1:A:268:LEU:O	1:A:272:ARG:HD3	2.22	0.40
1:C:90:ALA:O	1:C:93:ARG:HB3	2.22	0.40
1:C:251:GLN:OE1	1:C:251:GLN:N	2.52	0.40

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	242/366 (66%)	235 (97%)	7 (3%)	0	100	100
1	B	246/366 (67%)	230 (94%)	16 (6%)	0	100	100
1	C	249/366 (68%)	241 (97%)	8 (3%)	0	100	100
All	All	737/1098 (67%)	706 (96%)	31 (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	206/303 (68%)	206 (100%)	0	100	100
1	B	209/303 (69%)	209 (100%)	0	100	100
1	C	210/303 (69%)	210 (100%)	0	100	100
All	All	625/909 (69%)	625 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	117	HIS
1	B	117	HIS
1	B	176	GLN

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Mol	Chain	Res	Type
1	B	250	HIS
1	C	2	HIS
1	C	38	GLN
1	C	78	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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	TAR	B	401	-	9,9,9	1.05	0	12,12,12	0.95	0
5	GOL	A	405	-	5,5,5	0.10	0	5,5,5	0.26	0
4	TAR	B	403	-	9,9,9	0.99	0	12,12,12	0.94	0
4	TAR	A	404	-	9,9,9	1.05	0	12,12,12	0.89	0
6	EDO	A	407	-	3,3,3	0.08	0	2,2,2	0.07	0
6	EDO	B	405	-	3,3,3	0.10	0	2,2,2	0.15	0
6	EDO	B	408	-	3,3,3	0.16	0	2,2,2	0.40	0
6	EDO	B	404	-	3,3,3	0.22	0	2,2,2	0.25	0
6	EDO	B	406	-	3,3,3	0.09	0	2,2,2	0.13	0
4	TAR	C	401	-	9,9,9	1.04	0	12,12,12	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TAR	A	403	-	9,9,9	1.06	0	12,12,12	0.91	0
5	GOL	C	404	-	5,5,5	0.09	0	5,5,5	0.28	0
6	EDO	B	407	-	3,3,3	0.07	0	2,2,2	0.12	0
4	TAR	C	402	-	9,9,9	1.00	0	12,12,12	0.95	0
6	EDO	A	406	-	3,3,3	0.06	0	2,2,2	0.06	0
4	TAR	B	402	-	9,9,9	1.07	0	12,12,12	0.90	0
4	TAR	C	403	-	9,9,9	1.01	0	12,12,12	0.94	0
3	1PE	A	402	2	15,15,15	0.22	0	14,14,14	0.10	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	TAR	B	401	-	-	6/12/12/12	-
5	GOL	A	405	-	-	2/4/4/4	-
4	TAR	B	403	-	-	10/12/12/12	-
4	TAR	A	404	-	-	8/12/12/12	-
6	EDO	A	407	-	-	1/1/1/1	-
6	EDO	B	405	-	-	0/1/1/1	-
6	EDO	B	408	-	-	1/1/1/1	-
6	EDO	B	404	-	-	1/1/1/1	-
6	EDO	B	406	-	-	0/1/1/1	-
4	TAR	C	401	-	-	4/12/12/12	-
4	TAR	A	403	-	-	10/12/12/12	-
5	GOL	C	404	-	-	0/4/4/4	-
6	EDO	B	407	-	-	0/1/1/1	-
4	TAR	C	402	-	-	2/12/12/12	-
6	EDO	A	406	-	-	1/1/1/1	-
4	TAR	B	402	-	-	6/12/12/12	-
4	TAR	C	403	-	-	7/12/12/12	-
3	1PE	A	402	2	-	2/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	TAR	C1-C2-C3-O3
4	A	403	TAR	O2-C2-C3-O3
4	A	403	TAR	O2-C2-C3-C4
4	B	401	TAR	C1-C2-C3-O3
4	B	401	TAR	C1-C2-C3-C4
4	B	401	TAR	O2-C2-C3-O3
4	B	401	TAR	O2-C2-C3-C4
4	B	402	TAR	C1-C2-C3-O3
4	B	402	TAR	O2-C2-C3-O3
4	B	402	TAR	O2-C2-C3-C4
4	A	403	TAR	C1-C2-C3-C4
4	B	402	TAR	C1-C2-C3-C4
4	A	404	TAR	O3-C3-C4-O4
4	A	404	TAR	O3-C3-C4-O41
4	B	402	TAR	O3-C3-C4-O4
4	B	402	TAR	O3-C3-C4-O41
4	B	403	TAR	O1-C1-C2-O2
4	B	403	TAR	O11-C1-C2-O2
4	B	403	TAR	O3-C3-C4-O4
4	B	403	TAR	O3-C3-C4-O41
4	C	402	TAR	O1-C1-C2-O2
4	C	402	TAR	O11-C1-C2-O2
4	A	403	TAR	C2-C3-C4-O4
4	A	403	TAR	C2-C3-C4-O41
4	A	404	TAR	O1-C1-C2-C3
4	A	404	TAR	O11-C1-C2-C3
4	A	403	TAR	O3-C3-C4-O4
4	A	403	TAR	O3-C3-C4-O41
4	B	401	TAR	O1-C1-C2-O2
4	B	401	TAR	O11-C1-C2-O2
4	C	403	TAR	O3-C3-C4-O4
4	C	403	TAR	O3-C3-C4-O41
4	A	403	TAR	O1-C1-C2-O2
4	A	403	TAR	O11-C1-C2-O2
4	A	404	TAR	O1-C1-C2-O2
4	A	404	TAR	O11-C1-C2-O2
4	C	401	TAR	O1-C1-C2-C3
4	C	401	TAR	O11-C1-C2-C3
5	A	405	GOL	O1-C1-C2-C3
4	B	403	TAR	O1-C1-C2-C3
5	A	405	GOL	O1-C1-C2-O2
4	B	403	TAR	C1-C2-C3-O3
4	B	403	TAR	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	B	403	TAR	O11-C1-C2-C3
4	C	403	TAR	O2-C2-C3-O3
4	C	403	TAR	C1-C2-C3-O3
4	C	403	TAR	O2-C2-C3-C4
4	A	404	TAR	C2-C3-C4-O4
6	B	408	EDO	O1-C1-C2-O2
4	A	404	TAR	C2-C3-C4-O41
4	C	403	TAR	C1-C2-C3-C4
4	B	403	TAR	C1-C2-C3-C4
4	C	401	TAR	O1-C1-C2-O2
4	B	403	TAR	O2-C2-C3-O3
3	A	402	1PE	C14-C24-OH4-C13
6	A	406	EDO	O1-C1-C2-O2
6	A	407	EDO	O1-C1-C2-O2
6	B	404	EDO	O1-C1-C2-O2
3	A	402	1PE	OH2-C12-C22-OH3
4	C	401	TAR	O11-C1-C2-O2
4	C	403	TAR	O11-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	246/366 (67%)	-0.39	6 (2%) 59 51	60, 75, 113, 162	0
1	B	250/366 (68%)	-0.28	8 (3%) 50 43	58, 82, 125, 166	0
1	C	253/366 (69%)	-0.24	13 (5%) 33 28	57, 76, 142, 173	0
All	All	749/1098 (68%)	-0.30	27 (3%) 46 38	57, 77, 128, 173	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	TRP	6.9
1	C	127	ALA	6.4
1	C	128	GLY	4.7
1	C	162	ALA	4.7
1	B	162	ALA	4.1
1	A	281	ILE	3.8
1	A	279	GLY	3.5
1	C	35	TYR	3.0
1	C	280	THR	3.0
1	A	162	ALA	2.8
1	B	283	ARG	2.8
1	C	37	ALA	2.8
1	C	1	MET	2.7
1	C	30	GLY	2.7
1	B	281	ILE	2.6
1	C	130	ARG	2.6
1	C	36	ALA	2.6
1	B	44	LYS	2.6
1	B	285	ARG	2.5
1	B	282	GLU	2.5
1	A	125	PRO	2.4
1	C	129	GLY	2.3
1	C	72	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	165	ASP	2.2
1	B	32	GLN	2.2
1	B	1	MET	2.1
1	A	280	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
4	TAR	B	403	10/10	0.67	0.13	123,136,153,158	0
4	TAR	A	403	10/10	0.69	0.21	113,134,144,145	0
6	EDO	B	408	4/4	0.70	0.33	109,112,112,119	0
4	TAR	C	402	10/10	0.71	0.15	109,143,156,163	0
4	TAR	B	402	10/10	0.77	0.14	103,133,155,159	0
6	EDO	A	406	4/4	0.79	0.41	97,100,100,102	0
6	EDO	A	407	4/4	0.83	0.28	109,114,116,119	0
5	GOL	C	404	6/6	0.83	0.20	125,131,138,142	0
6	EDO	B	406	4/4	0.84	0.27	100,106,110,112	0
4	TAR	C	401	10/10	0.84	0.12	95,111,121,140	0
6	EDO	B	407	4/4	0.85	0.20	105,112,115,116	0
6	EDO	B	405	4/4	0.86	0.36	88,95,98,100	0
6	EDO	B	404	4/4	0.88	0.21	71,78,82,85	0
4	TAR	B	401	10/10	0.89	0.13	94,121,139,147	0
4	TAR	A	404	10/10	0.91	0.19	108,130,151,160	0
4	TAR	C	403	10/10	0.94	0.10	92,112,125,133	0
5	GOL	A	405	6/6	0.94	0.17	107,113,117,118	0
3	1PE	A	402	16/16	0.96	0.11	83,92,103,107	0
2	NA	A	401	1/1	0.99	0.03	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.