



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:42 AM BST

PDB ID : 5NXF
Title : Crystal structure of the carboxy-terminal region of the bacteriophage T4 proximal long tail fibre protein gp34, residues 795 to 1289, at 1.9 Angstrom.
Authors : Namura, M.; van Raaij, M.J.; Kanamaru, S.
Deposited on : 2017-05-10
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

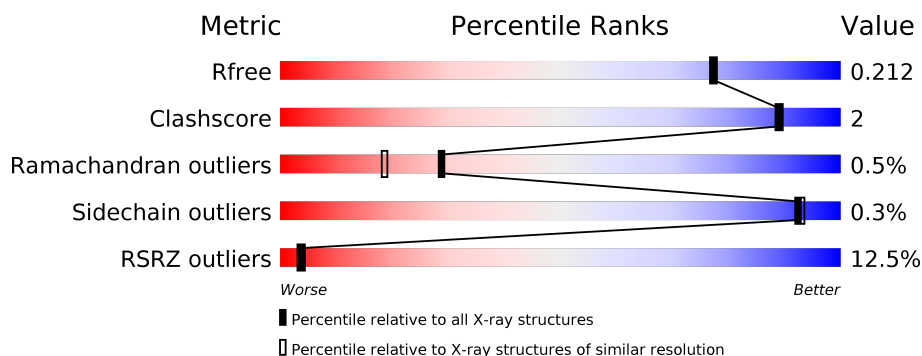
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 on 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	509	<div> <div>10%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> </div>
1	B	509	<div> <div>13%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> </div>
1	C	509	<div> <div>13%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>

2 Entry composition [i](#)

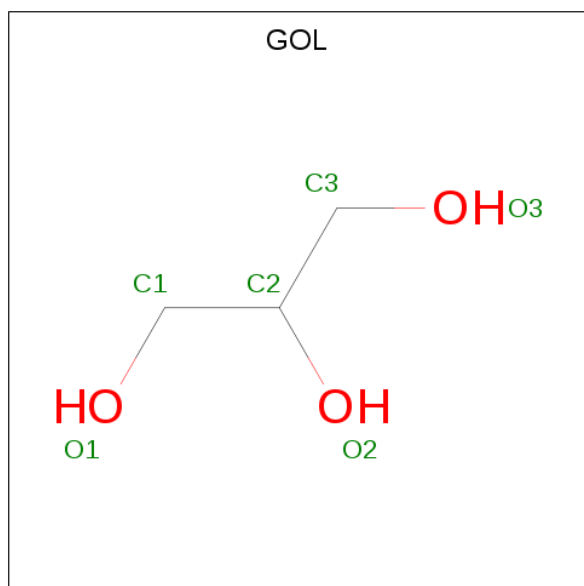
There are 7 unique types of molecules in this entry. The entry contains 13250 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Long-tail fiber proximal subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	Se	0	0	0
			3773	2357	655	756	5			
1	B	494	Total	C	N	O	Se	0	0	0
			3763	2352	654	752	5			
1	C	494	Total	C	N	O	Se	0	0	0
			3763	2352	654	752	5			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



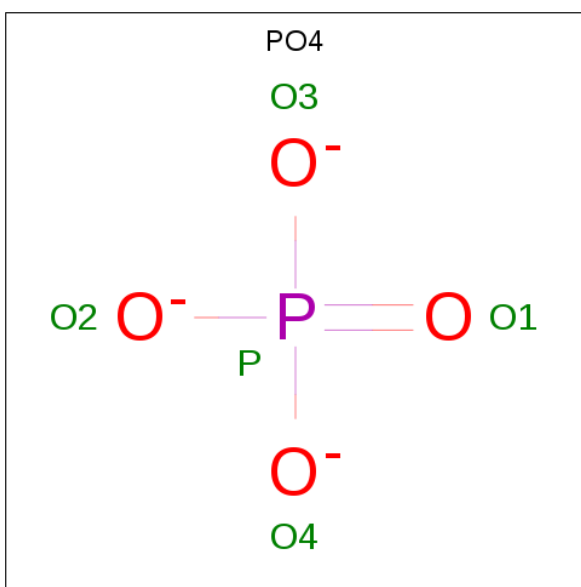
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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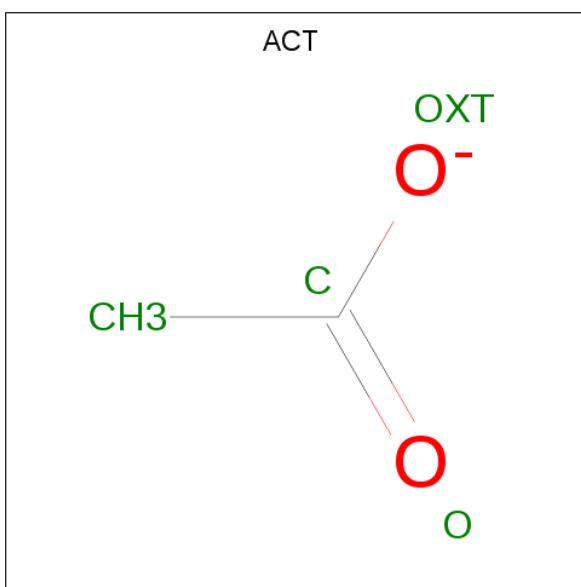
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

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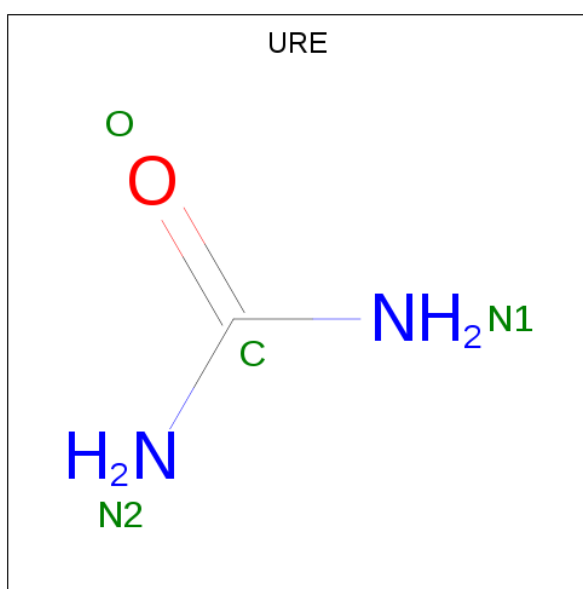
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is UREA (three-letter code: URE) (formula: CH₄N₂O).

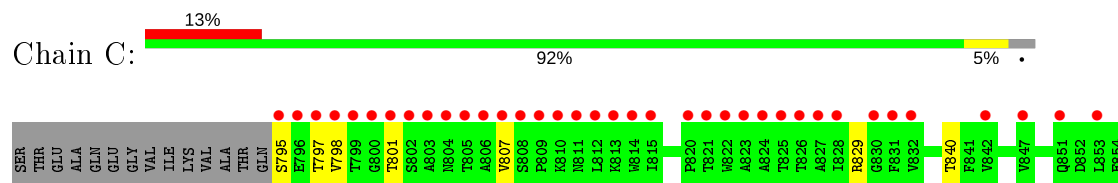
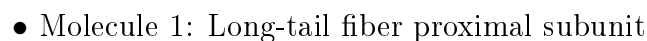
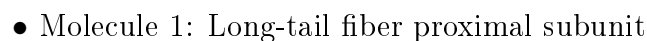


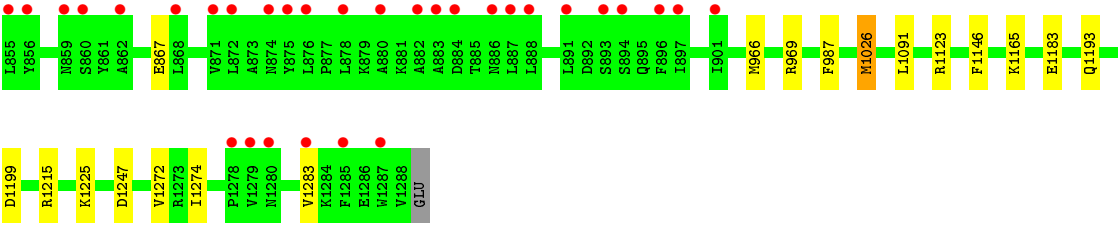
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			4	1	2	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	626	Total	O	0	0
			626	626		
7	B	576	Total	O	0	0
			576	576		
7	C	619	Total	O	0	0
			619	619		

- Molecule 1: Long-tail fiber proximal subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.11Å 75.94Å 149.13Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	46.12 – 1.90 46.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.12-1.90) 99.0 (46.12-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.171 , 0.208 0.182 , 0.212	Depositor DCC
R_{free} test set	1957 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13250	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: URE, PO4, ACT, NA, GOL

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	0.58	0/3847	0.75	3/5230 (0.1%)
1	B	0.59	0/3837	0.74	5/5218 (0.1%)
1	C	0.58	0/3837	0.72	4/5218 (0.1%)
All	All	0.58	0/11521	0.74	12/15666 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1166	MSE	CG-SE-CE	-7.38	82.67	98.90
1	B	1026	MSE	CG-SE-CE	-5.96	85.79	98.90
1	A	1181	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	1166	MSE	CG-SE-CE	-5.57	86.64	98.90
1	B	1150	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	1215	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	1215	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	969	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	1247	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	1088	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	1088	ARG	NE-CZ-NH1	5.03	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1026	MSE	CG-SE-CE	-5.03	87.84	98.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	796	GLU	Peptide
1	B	796	GLU	Peptide

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	3773	0	3659	17	0
1	B	3763	0	3653	19	0
1	C	3763	0	3653	16	0
2	A	18	0	24	0	0
2	B	30	0	40	0	0
2	C	54	0	72	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	8	0	6	1	0
5	A	1	0	0	0	0
6	C	4	0	4	1	0
7	A	626	0	0	1	0
7	B	576	0	0	0	0
7	C	619	0	0	1	0
All	All	13250	0	11111	43	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 2.

All (43) 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:798:VAL:HG21	1:B:811:ASN:HB3	1.72	0.71
1:A:1267:LEU:HD23	1:A:1274:ILE:HD12	1.76	0.66
1:A:1034:PHE:CZ	1:C:1026:MSE:HE1	2.30	0.65
1:A:1026:MSE:HE1	1:B:1034:PHE:CZ	2.35	0.60
1:C:798:VAL:HG21	1:C:807:VAL:HG13	1.87	0.57
1:B:1166:MSE:HE3	1:B:1179:LEU:HB3	1.87	0.56
1:A:1263:ILE:HD12	1:B:1267:LEU:HD11	1.87	0.56
1:C:795:SER:O	1:C:798:VAL:HG23	2.07	0.55
1:C:840:THR:HG21	1:C:867:GLU:HB3	1.89	0.55
2:C:1304:GOL:O2	6:C:1311:URE:N1	2.42	0.53
1:A:1263:ILE:HD13	1:A:1267:LEU:HB2	1.90	0.53
1:A:1206:ILE:N	1:A:1206:ILE:HD12	2.25	0.51
1:B:852:ASP:HB3	1:B:855:LEU:HD13	1.92	0.50
1:A:966:MSE:SE	1:C:987:PHE:HB2	2.63	0.49
4:A:1305:ACT:H1	7:A:1871:HOH:O	2.13	0.49
1:C:1199:ASP:OD1	1:C:1225:LYS:HD3	2.14	0.48
1:A:1280:ASN:HB2	1:A:1282:THR:HG22	1.97	0.47
1:B:831:PHE:HB2	1:C:829:ARG:HE	1.80	0.47
1:C:1091:LEU:C	1:C:1091:LEU:HD12	2.36	0.47
1:A:840:THR:HG21	1:A:867:GLU:HB3	1.97	0.46
1:C:1274:ILE:CG2	1:C:1283:VAL:HG11	2.46	0.46
1:C:795:SER:HB3	1:C:797:THR:HG22	1.98	0.45
1:A:1281:LYS:HA	1:B:1287:TRP:CZ3	2.51	0.45
1:A:1049:ALA:O	1:A:1064:ARG:HA	2.17	0.45
1:B:798:VAL:CG1	1:B:807:VAL:HG22	2.47	0.45
1:B:809:PRO:HG3	1:C:798:VAL:HG22	1.99	0.44
1:B:1166:MSE:CE	1:B:1242:PRO:HD2	2.47	0.44
1:A:1066:ASP:O	1:A:1067:ALA:HB3	2.18	0.44
1:B:1283:VAL:HG13	1:C:1272:VAL:HG11	2.00	0.44
1:B:844:ASN:OD1	1:B:847:VAL:HG22	2.17	0.43
1:A:1146:PHE:HA	1:A:1193:GLN:O	2.19	0.43
1:A:1271:ASN:ND2	1:A:1288:VAL:O	2.51	0.43
1:B:987:PHE:HB2	1:C:966:MSE:SE	2.69	0.43
1:B:1206:ILE:HD12	1:B:1206:ILE:N	2.35	0.42
1:C:1146:PHE:HA	1:C:1193:GLN:O	2.19	0.42
1:B:1166:MSE:HE1	1:B:1242:PRO:HD2	2.02	0.42
1:B:981:THR:O	1:B:1003:LYS:HE2	2.20	0.42
1:C:1165:LYS:HD3	1:C:1183:GLU:HG2	2.01	0.41
1:A:987:PHE:HB2	1:B:966:MSE:SE	2.70	0.41
1:A:990:GLY:HA3	1:A:995:HIS:HA	2.03	0.41
1:B:798:VAL:HG12	1:B:807:VAL:HG22	2.02	0.41
1:A:868:LEU:HD22	1:B:863:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:969:ARG:NH1	7:C:1423:HOH:O	2.53	0.40

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	493/509 (97%)	480 (97%)	10 (2%)	3 (1%)	25	15
1	B	492/509 (97%)	472 (96%)	17 (4%)	3 (1%)	25	15
1	C	492/509 (97%)	476 (97%)	15 (3%)	1 (0%)	47	38
All	All	1477/1527 (97%)	1428 (97%)	42 (3%)	7 (0%)	29	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	803	ALA
1	B	802	SER
1	B	1067	ALA
1	A	1067	ALA
1	C	801	THR
1	B	837	GLY
1	A	1018	ILE

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	412/418 (99%)	411 (100%)	1 (0%)	93	94
1	B	411/418 (98%)	409 (100%)	2 (0%)	88	89
1	C	411/418 (98%)	410 (100%)	1 (0%)	93	94
All	All	1234/1254 (98%)	1230 (100%)	4 (0%)	92	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1123	ARG
1	B	1123	ARG
1	B	1157	TYR
1	C	1123	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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
2	GOL	C	1301	-	5,5,5	0.35	0	5,5,5	0.20	0
2	GOL	A	1301	-	5,5,5	0.42	0	5,5,5	0.44	0
6	URE	C	1311	-	3,3,3	0.49	0	3,3,3	0.48	0
3	PO4	B	1306	-	4,4,4	0.98	0	6,6,6	0.95	0
2	GOL	C	1303	-	5,5,5	0.22	0	5,5,5	0.40	0
2	GOL	C	1307	-	5,5,5	0.20	0	5,5,5	0.51	0
2	GOL	C	1305	-	5,5,5	0.28	0	5,5,5	0.48	0
2	GOL	A	1302	-	5,5,5	0.27	0	5,5,5	0.39	0
2	GOL	C	1302	-	5,5,5	0.19	0	5,5,5	0.38	0
2	GOL	C	1309	-	5,5,5	0.24	0	5,5,5	0.30	0
2	GOL	C	1304	-	5,5,5	0.26	0	5,5,5	0.26	0
2	GOL	B	1304	-	5,5,5	0.53	0	5,5,5	0.61	0
3	PO4	A	1304	-	4,4,4	1.63	1 (25%)	6,6,6	1.14	0
4	ACT	A	1306	-	1,3,3	1.21	0	0,3,3	0.00	-
2	GOL	B	1302	-	5,5,5	0.39	0	5,5,5	0.61	0
2	GOL	C	1306	-	5,5,5	0.33	0	5,5,5	0.70	0
2	GOL	B	1301	-	5,5,5	0.20	0	5,5,5	0.36	0
3	PO4	C	1310	-	4,4,4	1.50	1 (25%)	6,6,6	0.68	0
2	GOL	C	1308	-	5,5,5	0.23	0	5,5,5	0.45	0
2	GOL	B	1303	-	5,5,5	0.23	0	5,5,5	0.68	0
4	ACT	A	1305	-	1,3,3	0.24	0	0,3,3	0.00	-
2	GOL	A	1303	-	5,5,5	0.36	0	5,5,5	0.37	0
2	GOL	B	1305	-	5,5,5	0.68	0	5,5,5	0.43	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
2	GOL	B	1303	-	-	0/4/4/4	-
2	GOL	C	1301	-	-	0/4/4/4	-
2	GOL	A	1301	-	-	0/4/4/4	-
2	GOL	C	1305	-	-	2/4/4/4	-
2	GOL	A	1302	-	-	0/4/4/4	-
2	GOL	C	1302	-	-	2/4/4/4	-
2	GOL	B	1302	-	-	0/4/4/4	-
2	GOL	C	1306	-	-	2/4/4/4	-
2	GOL	B	1301	-	-	0/4/4/4	-
2	GOL	A	1303	-	-	0/4/4/4	-
2	GOL	B	1305	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	1303	-	-	2/4/4/4	-
2	GOL	C	1308	-	-	3/4/4/4	-
2	GOL	C	1307	-	-	4/4/4/4	-
2	GOL	C	1309	-	-	0/4/4/4	-
2	GOL	C	1304	-	-	0/4/4/4	-
2	GOL	B	1304	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1310	PO4	P-O1	2.23	1.56	1.50
3	A	1304	PO4	P-O4	-2.21	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1303	GOL	C1-C2-C3-O3
2	C	1307	GOL	O1-C1-C2-O2
2	C	1307	GOL	O1-C1-C2-C3
2	B	1304	GOL	O1-C1-C2-C3
2	C	1306	GOL	O1-C1-C2-C3
2	C	1308	GOL	O1-C1-C2-O2
2	C	1307	GOL	C1-C2-C3-O3
2	C	1305	GOL	C1-C2-C3-O3
2	C	1302	GOL	C1-C2-C3-O3
2	C	1308	GOL	O1-C1-C2-C3
2	C	1307	GOL	O2-C2-C3-O3
2	B	1304	GOL	O1-C1-C2-O2
2	C	1306	GOL	O1-C1-C2-O2
2	C	1303	GOL	O2-C2-C3-O3
2	C	1305	GOL	O2-C2-C3-O3
2	C	1308	GOL	C1-C2-C3-O3
2	C	1302	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1311	URE	1	0
2	C	1304	GOL	1	0
4	A	1305	ACT	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, 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	490/509 (96%)	0.43	52 (10%) 6 7	7, 17, 59, 91	0
1	B	489/509 (96%)	0.52	64 (13%) 3 3	8, 18, 65, 105	0
1	C	489/509 (96%)	0.50	68 (13%) 2 3	8, 17, 61, 111	0
All	All	1468/1527 (96%)	0.48	184 (12%) 3 4	7, 17, 63, 111	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	803	ALA	10.9
1	B	803	ALA	8.7
1	B	822	TRP	8.3
1	C	804	ASN	8.1
1	B	801	THR	7.8
1	B	806	ALA	7.8
1	A	801	THR	7.8
1	A	805	THR	7.4
1	C	801	THR	7.3
1	A	807	VAL	7.3
1	A	806	ALA	7.1
1	C	799	THR	6.6
1	B	812	LEU	6.6
1	C	805	THR	6.5
1	B	804	ASN	6.4
1	C	806	ALA	6.4
1	C	815	ILE	6.2
1	C	807	VAL	6.0
1	C	797	THR	5.9
1	A	811	ASN	5.8
1	A	815	ILE	5.8
1	B	1279	VAL	5.8
1	C	1279	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	804	ASN	5.5
1	A	814	TRP	5.5
1	C	823	ALA	5.4
1	C	800	GLY	5.3
1	A	803	ALA	5.1
1	C	795	SER	5.0
1	B	814	TRP	4.9
1	B	823	ALA	4.8
1	B	802	SER	4.7
1	A	795	SER	4.7
1	A	799	THR	4.7
1	B	883	ALA	4.7
1	C	862	ALA	4.6
1	B	800	GLY	4.6
1	B	807	VAL	4.6
1	B	828	ILE	4.5
1	C	802	SER	4.5
1	A	816	ALA	4.5
1	A	809	PRO	4.3
1	B	795	SER	4.3
1	C	812	LEU	4.3
1	A	798	VAL	4.2
1	A	802	SER	4.2
1	C	798	VAL	4.2
1	A	813	LYS	4.2
1	A	1279	VAL	4.1
1	B	896	PHE	4.1
1	B	841	PHE	4.1
1	C	880	ALA	4.1
1	C	871	VAL	4.0
1	B	1282	THR	4.0
1	C	824	ALA	4.0
1	B	1280	ASN	3.9
1	C	808	SER	3.9
1	B	1278	PRO	3.9
1	B	861	TYR	3.8
1	B	805	THR	3.8
1	B	871	VAL	3.8
1	C	814	TRP	3.8
1	C	822	TRP	3.8
1	B	870	ARG	3.8
1	B	824	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	896	PHE	3.7
1	A	797	THR	3.7
1	C	811	ASN	3.6
1	B	820	PRO	3.6
1	B	811	ASN	3.6
1	A	831	PHE	3.5
1	A	875	TYR	3.5
1	C	859	ASN	3.5
1	C	1285	PHE	3.5
1	A	800	GLY	3.5
1	A	812	LEU	3.5
1	B	825	THR	3.5
1	A	822	TRP	3.4
1	C	809	PRO	3.4
1	B	809	PRO	3.4
1	A	832	VAL	3.4
1	B	853	LEU	3.4
1	A	808	SER	3.3
1	C	847	VAL	3.3
1	C	796	GLU	3.3
1	C	810	LYS	3.3
1	A	868	LEU	3.3
1	B	810	LYS	3.3
1	A	896	PHE	3.2
1	B	797	THR	3.2
1	B	827	ALA	3.2
1	C	891	LEU	3.2
1	C	813	LYS	3.2
1	C	883	ALA	3.2
1	B	815	ILE	3.1
1	B	890	GLY	3.1
1	A	893	SER	3.1
1	C	882	ALA	3.1
1	C	821	THR	3.1
1	C	827	ALA	3.1
1	B	855	LEU	3.0
1	B	863	VAL	3.0
1	A	841	PHE	3.0
1	B	842	VAL	3.0
1	B	860	SER	3.0
1	C	1283	VAL	3.0
1	B	1285	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	878	LEU	2.9
1	C	831	PHE	2.9
1	C	826	THR	2.9
1	C	832	VAL	2.9
1	B	816	ALA	2.9
1	A	1278	PRO	2.9
1	C	820	PRO	2.8
1	C	830	GLY	2.8
1	C	825	THR	2.8
1	B	838	SER	2.8
1	C	897	ILE	2.8
1	A	856	TYR	2.8
1	C	893	SER	2.8
1	C	851	GLN	2.8
1	B	1281	LYS	2.7
1	B	876	LEU	2.7
1	A	821	THR	2.7
1	B	837	GLY	2.7
1	A	824	ALA	2.7
1	A	891	LEU	2.7
1	C	878	LEU	2.7
1	A	860	SER	2.7
1	B	1277	ASP	2.6
1	C	853	LEU	2.6
1	B	894	SER	2.6
1	B	873	ALA	2.6
1	B	831	PHE	2.6
1	C	828	ILE	2.6
1	B	844	ASN	2.6
1	A	882	ALA	2.6
1	B	893	SER	2.6
1	A	834	THR	2.6
1	A	1280	ASN	2.6
1	A	861	TYR	2.5
1	B	888	LEU	2.5
1	C	1278	PRO	2.5
1	A	865	PRO	2.5
1	B	798	VAL	2.5
1	C	855	LEU	2.5
1	C	842	VAL	2.4
1	C	872	LEU	2.4
1	C	875	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	874	ASN	2.4
1	C	887	LEU	2.4
1	B	847	VAL	2.4
1	A	1281	LYS	2.4
1	B	850	THR	2.3
1	A	895	GLN	2.3
1	A	880	ALA	2.3
1	A	1282	THR	2.3
1	C	886	ASN	2.3
1	A	826	THR	2.3
1	C	868	LEU	2.3
1	A	847	VAL	2.3
1	B	808	SER	2.3
1	C	894	SER	2.3
1	A	887	LEU	2.3
1	B	796	GLU	2.2
1	B	1283	VAL	2.2
1	A	820	PRO	2.2
1	A	835	SER	2.2
1	A	884	ASP	2.2
1	C	888	LEU	2.2
1	C	860	SER	2.2
1	B	891	LEU	2.2
1	C	876	LEU	2.1
1	B	799	THR	2.1
1	C	856	TYR	2.1
1	B	839	ILE	2.1
1	B	866	TYR	2.1
1	C	884	ASP	2.1
1	C	1280	ASN	2.1
1	B	874	ASN	2.1
1	A	864	SER	2.0
1	B	858	LYS	2.0
1	C	1287	TRP	2.0
1	C	901	ILE	2.0

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 monosaccharides 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(\AA^2)	Q<0.9
2	GOL	C	1304	6/6	0.75	0.31	47,56,59,61	0
2	GOL	C	1305	6/6	0.77	0.22	51,53,53,55	0
2	GOL	B	1305	6/6	0.77	0.20	27,40,41,42	0
4	ACT	A	1305	4/4	0.79	0.18	44,45,47,48	0
2	GOL	A	1302	6/6	0.79	0.26	43,45,48,52	0
6	URE	C	1311	4/4	0.80	0.12	36,39,41,44	0
2	GOL	C	1302	6/6	0.81	0.20	48,54,56,60	0
2	GOL	C	1303	6/6	0.84	0.23	33,45,46,46	0
2	GOL	C	1308	6/6	0.84	0.16	43,46,47,48	0
2	GOL	B	1304	6/6	0.86	0.15	36,39,39,41	0
2	GOL	C	1306	6/6	0.88	0.18	30,36,37,45	0
5	NA	A	1307	1/1	0.89	0.22	41,41,41,41	0
2	GOL	C	1307	6/6	0.89	0.24	30,37,39,45	0
4	ACT	A	1306	4/4	0.94	0.11	28,33,33,33	0
2	GOL	A	1301	6/6	0.94	0.10	20,23,23,25	0
2	GOL	A	1303	6/6	0.95	0.13	21,27,31,34	0
2	GOL	C	1309	6/6	0.95	0.09	23,27,30,31	0
2	GOL	B	1302	6/6	0.96	0.08	19,22,24,24	0
2	GOL	C	1301	6/6	0.96	0.08	21,24,24,24	0
2	GOL	B	1303	6/6	0.96	0.10	20,24,27,29	0
2	GOL	B	1301	6/6	0.97	0.12	18,18,20,21	0
3	PO4	B	1306	5/5	0.97	0.10	18,21,22,26	0
3	PO4	C	1310	5/5	0.98	0.10	20,20,23,25	0
3	PO4	A	1304	5/5	0.99	0.09	15,17,17,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.