



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:55 PM UTC

PDB ID : 5NXF / pdb_00005nxf
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 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

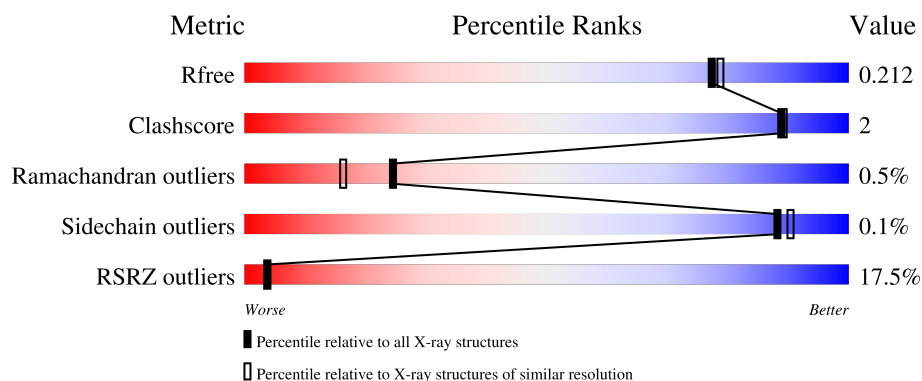
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	15% 92% 6% .
1	B	509	19% 92% 5% .
1	C	509	17% 93% . .

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 (CCD ID: 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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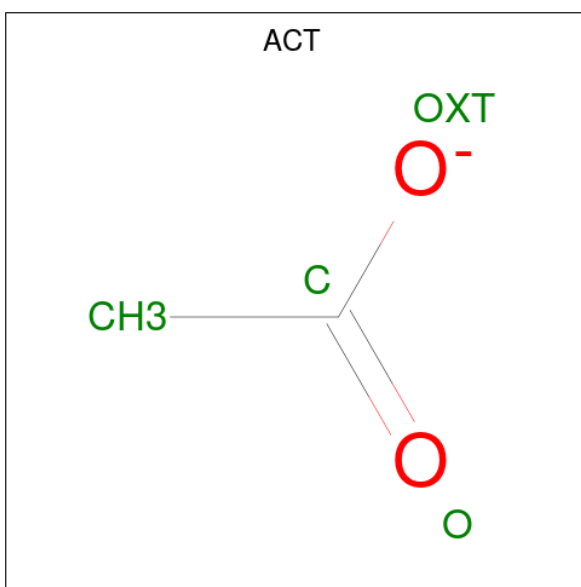
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	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 (CCD ID: 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 (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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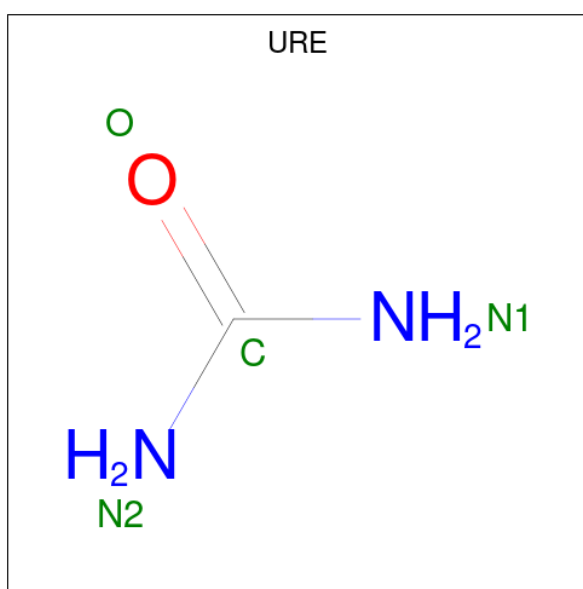
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is UREA (CCD ID: URE) (formula: CH₄N₂O).

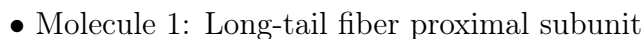
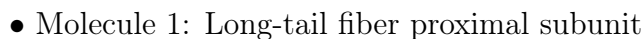


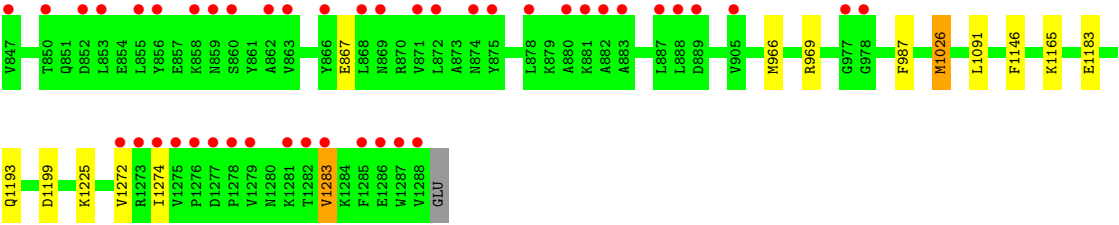
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			4	1	2	1		

- 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) 99.4 (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 (1.20%)	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)	0.37 , 58.5	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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.76	1/3847 (0.0%)	0.84	1/5230 (0.0%)
1	B	0.76	0/3837	0.83	2/5218 (0.0%)
1	C	0.76	0/3837	0.83	1/5218 (0.0%)
All	All	0.76	1/11521 (0.0%)	0.84	4/15666 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	925	SER	CA-C	5.07	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1166	MSE	CG-SE-CE	-7.39	82.67	98.92
1	B	1026	MSE	CG-SE-CE	-5.97	85.79	98.92
1	B	1166	MSE	CG-SE-CE	-5.58	86.64	98.92
1	C	1026	MSE	CG-SE-CE	-5.04	87.84	98.92

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:1206:ILE:N	2.25	0.51
1:C:1091:LEU:C	1:C:1091:LEU:HD12	2.36	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: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
1:C:969:ARG:NH1	7:C:1423:HOH:O	2.53	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	493/509 (97%)	480 (97%)	10 (2%)	3 (1%)	21	13
1	B	492/509 (97%)	472 (96%)	17 (4%)	3 (1%)	21	13
1	C	492/509 (97%)	476 (97%)	15 (3%)	1 (0%)	43	36
All	All	1477/1527 (97%)	1428 (97%)	42 (3%)	7 (0%)	24	16

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

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%)	412 (100%)	0	100	100
1	B	411/418 (98%)	411 (100%)	0	100	100
1	C	411/418 (98%)	410 (100%)	1 (0%)	87	90
All	All	1234/1254 (98%)	1233 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1283	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	804	ASN
1	A	851	GLN
1	A	974	GLN
1	A	1121	ASN
1	A	1228	ASN
1	B	886	ASN
1	B	1027	ASN
1	B	1127	GLN
1	C	811	ASN
1	C	859	ASN
1	C	869	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 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	1304	-	5,5,5	0.26	0	5,5,5	0.30	0
3	PO4	B	1306	-	4,4,4	1.01	0	6,6,6	0.98	0
4	ACT	A	1305	-	3,3,3	0.79	0	3,3,3	1.14	0
6	URE	C	1311	-	3,3,3	0.51	0	3,3,3	0.52	0
2	GOL	C	1302	-	5,5,5	0.19	0	5,5,5	0.43	0
2	GOL	C	1307	-	5,5,5	0.20	0	5,5,5	0.53	0
2	GOL	C	1309	-	5,5,5	0.23	0	5,5,5	0.34	0
2	GOL	B	1305	-	5,5,5	0.70	0	5,5,5	0.44	0
2	GOL	A	1303	-	5,5,5	0.37	0	5,5,5	0.41	0
2	GOL	C	1305	-	5,5,5	0.28	0	5,5,5	0.51	0
2	GOL	C	1306	-	5,5,5	0.34	0	5,5,5	0.74	0
2	GOL	A	1302	-	5,5,5	0.27	0	5,5,5	0.41	0
3	PO4	C	1310	-	4,4,4	1.56	1 (25%)	6,6,6	0.71	0
2	GOL	C	1301	-	5,5,5	0.35	0	5,5,5	0.23	0
2	GOL	B	1303	-	5,5,5	0.23	0	5,5,5	0.73	0
4	ACT	A	1306	-	3,3,3	0.68	0	3,3,3	0.82	0
2	GOL	B	1301	-	5,5,5	0.20	0	5,5,5	0.41	0
2	GOL	B	1302	-	5,5,5	0.40	0	5,5,5	0.64	0
2	GOL	C	1308	-	5,5,5	0.23	0	5,5,5	0.50	0
2	GOL	C	1303	-	5,5,5	0.22	0	5,5,5	0.44	0
2	GOL	B	1304	-	5,5,5	0.54	0	5,5,5	0.63	0
3	PO4	A	1304	-	4,4,4	1.71	1 (25%)	6,6,6	1.19	0
2	GOL	A	1301	-	5,5,5	0.43	0	5,5,5	0.46	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	C	1304	-	-	0/4/4/4	-
2	GOL	A	1303	-	-	0/4/4/4	-
2	GOL	C	1308	-	-	2/4/4/4	-
2	GOL	C	1301	-	-	0/4/4/4	-
2	GOL	C	1305	-	-	2/4/4/4	-
2	GOL	B	1303	-	-	0/4/4/4	-
2	GOL	C	1303	-	-	2/4/4/4	-
2	GOL	C	1306	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1301	-	-	0/4/4/4	-
2	GOL	B	1304	-	-	2/4/4/4	-
2	GOL	A	1302	-	-	0/4/4/4	-
2	GOL	C	1302	-	-	2/4/4/4	-
2	GOL	C	1307	-	-	4/4/4/4	-
2	GOL	C	1309	-	-	0/4/4/4	-
2	GOL	B	1305	-	-	0/4/4/4	-
2	GOL	A	1301	-	-	0/4/4/4	-
2	GOL	B	1302	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1310	PO4	P-O1	2.35	1.56	1.50
3	A	1304	PO4	P-O4	-2.30	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1304	GOL	O1-C1-C2-C3
2	C	1303	GOL	C1-C2-C3-O3
2	C	1306	GOL	O1-C1-C2-C3
2	C	1307	GOL	O1-C1-C2-O2
2	C	1307	GOL	O1-C1-C2-C3
2	C	1308	GOL	O1-C1-C2-O2
2	C	1302	GOL	C1-C2-C3-O3
2	C	1305	GOL	C1-C2-C3-O3
2	C	1307	GOL	C1-C2-C3-O3
2	C	1308	GOL	O1-C1-C2-C3
2	B	1304	GOL	O1-C1-C2-O2
2	C	1306	GOL	O1-C1-C2-O2
2	C	1307	GOL	O2-C2-C3-O3
2	C	1303	GOL	O2-C2-C3-O3
2	C	1305	GOL	O2-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
2	C	1304	GOL	1	0
4	A	1305	ACT	1	0
6	C	1311	URE	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%)	0.37	77 (15%) 5 5	7, 17, 59, 91	0
1	B	489/509 (96%)	0.49	95 (19%) 3 3	8, 18, 65, 105	0
1	C	489/509 (96%)	0.38	85 (17%) 4 4	8, 17, 61, 111	0
All	All	1468/1527 (96%)	0.42	257 (17%) 4 4	7, 17, 63, 111	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	803	ALA	8.7
1	B	822	TRP	7.9
1	A	801	THR	7.7
1	C	798	VAL	7.2
1	B	798	VAL	6.9
1	C	807	VAL	6.9
1	C	801	THR	6.7
1	B	823	ALA	6.5
1	A	815	ILE	6.4
1	B	853	LEU	6.3
1	C	815	ILE	6.3
1	B	801	THR	6.3
1	A	816	ALA	6.2
1	A	807	VAL	6.2
1	A	814	TRP	6.0
1	A	806	ALA	6.0
1	C	823	ALA	6.0
1	B	814	TRP	6.0
1	B	795	SER	5.7
1	B	807	VAL	5.7
1	C	824	ALA	5.6
1	B	811	ASN	5.6
1	B	803	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	797	THR	5.5
1	C	799	THR	5.4
1	B	861	TYR	5.4
1	B	812	LEU	5.4
1	B	842	VAL	5.3
1	C	806	ALA	5.3
1	C	797	THR	5.2
1	B	827	ALA	5.2
1	B	806	ALA	5.1
1	A	797	THR	5.1
1	A	800	GLY	5.1
1	B	828	ILE	5.1
1	B	800	GLY	5.0
1	A	803	ALA	4.9
1	B	815	ILE	4.9
1	B	1283	VAL	4.8
1	B	816	ALA	4.8
1	A	799	THR	4.8
1	C	804	ASN	4.7
1	B	839	ILE	4.7
1	A	795	SER	4.7
1	B	855	LEU	4.7
1	B	799	THR	4.6
1	B	824	ALA	4.6
1	A	832	VAL	4.6
1	B	1279	VAL	4.6
1	A	831	PHE	4.5
1	B	831	PHE	4.5
1	B	841	PHE	4.4
1	A	812	LEU	4.4
1	A	802	SER	4.4
1	C	800	GLY	4.4
1	B	860	SER	4.3
1	C	814	TRP	4.3
1	A	813	LYS	4.3
1	A	823	ALA	4.3
1	C	1285	PHE	4.2
1	B	858	LYS	4.2
1	B	856	TYR	4.1
1	B	820	PRO	4.1
1	B	805	THR	4.1
1	C	1283	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	862	ALA	4.1
1	B	1288	VAL	4.0
1	C	831	PHE	4.0
1	C	805	THR	4.0
1	C	802	SER	4.0
1	B	870	ARG	4.0
1	C	828	ILE	4.0
1	B	796	GLU	4.0
1	B	871	VAL	4.0
1	B	1287	TRP	3.9
1	A	822	TRP	3.9
1	C	829	ARG	3.9
1	C	809	PRO	3.9
1	A	811	ASN	3.9
1	A	861	TYR	3.9
1	B	1278	PRO	3.9
1	C	832	VAL	3.9
1	C	1279	VAL	3.9
1	A	805	THR	3.8
1	A	862	ALA	3.8
1	B	1282	THR	3.8
1	C	1287	TRP	3.8
1	A	847	VAL	3.8
1	B	802	SER	3.8
1	B	804	ASN	3.8
1	C	822	TRP	3.8
1	B	883	ALA	3.7
1	B	1285	PHE	3.7
1	C	830	GLY	3.7
1	C	816	ALA	3.7
1	C	837	GLY	3.7
1	C	860	SER	3.7
1	A	865	PRO	3.6
1	C	825	THR	3.6
1	C	871	VAL	3.6
1	C	813	LYS	3.6
1	A	866	TYR	3.6
1	B	850	THR	3.5
1	B	847	VAL	3.5
1	B	863	VAL	3.5
1	A	841	PHE	3.5
1	A	804	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	875	TYR	3.5
1	B	832	VAL	3.5
1	A	1285	PHE	3.5
1	C	1278	PRO	3.5
1	B	878	LEU	3.5
1	B	826	THR	3.4
1	A	839	ILE	3.4
1	A	798	VAL	3.4
1	A	837	GLY	3.4
1	A	808	SER	3.4
1	A	856	TYR	3.4
1	B	810	LYS	3.4
1	B	1281	LYS	3.4
1	C	1288	VAL	3.4
1	A	853	LEU	3.4
1	A	835	SER	3.3
1	A	860	SER	3.3
1	B	809	PRO	3.3
1	A	864	SER	3.2
1	C	827	ALA	3.2
1	A	871	VAL	3.2
1	A	1279	VAL	3.2
1	C	812	LEU	3.2
1	B	835	SER	3.2
1	B	873	ALA	3.2
1	A	820	PRO	3.2
1	C	855	LEU	3.2
1	A	834	THR	3.1
1	C	856	TYR	3.1
1	A	842	VAL	3.1
1	C	795	SER	3.1
1	B	849	SER	3.1
1	C	826	THR	3.1
1	A	868	LEU	3.0
1	A	796	GLU	3.0
1	B	837	GLY	3.0
1	C	820	PRO	3.0
1	A	848	GLY	3.0
1	B	840	THR	2.9
1	C	883	ALA	2.9
1	B	808	SER	2.9
1	B	825	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	1282	THR	2.9
1	B	1276	PRO	2.9
1	C	842	VAL	2.9
1	A	828	ILE	2.9
1	B	859	ASN	2.8
1	B	1280	ASN	2.8
1	B	866	TYR	2.8
1	A	1281	LYS	2.8
1	C	859	ASN	2.8
1	C	977	GLY	2.8
1	C	846	THR	2.8
1	B	875	TYR	2.8
1	A	824	ALA	2.8
1	A	887	LEU	2.8
1	C	811	ASN	2.7
1	C	841	PHE	2.7
1	C	868	LEU	2.7
1	C	808	SER	2.7
1	B	848	GLY	2.7
1	B	817	GLN	2.7
1	A	840	THR	2.7
1	A	855	LEU	2.7
1	B	1275	VAL	2.7
1	C	882	ALA	2.6
1	B	829	ARG	2.6
1	B	838	SER	2.6
1	C	880	ALA	2.6
1	C	866	TYR	2.6
1	A	821	THR	2.6
1	B	821	THR	2.6
1	C	874	ASN	2.6
1	A	863	VAL	2.6
1	B	844	ASN	2.6
1	A	1273	ARG	2.6
1	A	843	GLY	2.6
1	A	1278	PRO	2.5
1	A	851	GLN	2.5
1	A	878	LEU	2.5
1	C	878	LEU	2.5
1	B	862	ALA	2.5
1	A	825	THR	2.5
1	C	1273	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1277	ASP	2.5
1	C	858	LYS	2.5
1	A	1283	VAL	2.5
1	B	857	GLU	2.4
1	B	864	SER	2.4
1	C	839	ILE	2.4
1	C	1274	ILE	2.4
1	A	809	PRO	2.4
1	C	853	LEU	2.4
1	C	872	LEU	2.4
1	C	887	LEU	2.4
1	C	888	LEU	2.4
1	B	834	THR	2.4
1	A	880	ALA	2.4
1	C	1276	PRO	2.4
1	C	1275	VAL	2.4
1	B	896	PHE	2.4
1	B	854	GLU	2.4
1	A	1280	ASN	2.4
1	B	818	SER	2.4
1	B	887	LEU	2.3
1	B	833	LYS	2.3
1	C	810	LYS	2.3
1	C	905	VAL	2.3
1	B	1277	ASP	2.3
1	B	869	ASN	2.3
1	A	901	ILE	2.3
1	B	843	GLY	2.3
1	B	890	GLY	2.3
1	C	847	VAL	2.3
1	A	846	THR	2.3
1	C	875	TYR	2.3
1	C	1281	LYS	2.3
1	C	838	SER	2.3
1	C	850	THR	2.3
1	A	873	ALA	2.2
1	A	810	LYS	2.2
1	B	852	ASP	2.2
1	C	833	LYS	2.2
1	B	1273	ARG	2.2
1	B	868	LEU	2.2
1	A	827	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	796	GLU	2.2
1	B	874	ASN	2.1
1	B	865	PRO	2.1
1	A	1289	GLU	2.1
1	B	1271	ASN	2.1
1	C	869	ASN	2.1
1	B	851	GLN	2.1
1	C	1272	VAL	2.1
1	A	869	ASN	2.1
1	A	872	LEU	2.1
1	B	886	ASN	2.1
1	A	838	SER	2.1
1	B	836	SER	2.1
1	C	1286	GLU	2.1
1	C	863	VAL	2.1
1	C	889	ASP	2.1
1	A	896	PHE	2.0
1	A	1286	GLU	2.0
1	A	1282	THR	2.0
1	B	830	GLY	2.0
1	C	852	ASP	2.0
1	C	881	LYS	2.0
1	C	978	GLY	2.0
1	A	1288	VAL	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
2	GOL	C	1305	6/6	0.73	0.20	51,53,53,55	0
2	GOL	C	1304	6/6	0.80	0.21	47,56,59,61	0
2	GOL	A	1302	6/6	0.81	0.22	43,45,48,52	0
2	GOL	C	1302	6/6	0.84	0.20	48,54,56,60	0
4	ACT	A	1305	4/4	0.84	0.18	44,45,47,48	0
6	URE	C	1311	4/4	0.85	0.11	36,39,41,44	0
2	GOL	B	1305	6/6	0.86	0.16	27,40,41,42	0
2	GOL	C	1303	6/6	0.86	0.16	33,45,46,46	0
2	GOL	B	1304	6/6	0.87	0.14	36,39,39,41	0
2	GOL	C	1306	6/6	0.88	0.16	30,36,37,45	0
2	GOL	C	1308	6/6	0.88	0.16	43,46,47,48	0
5	NA	A	1307	1/1	0.89	0.10	41,41,41,41	0
2	GOL	C	1307	6/6	0.90	0.13	30,37,39,45	0
4	ACT	A	1306	4/4	0.91	0.10	28,33,33,33	0
2	GOL	A	1303	6/6	0.93	0.09	21,27,31,34	0
2	GOL	A	1301	6/6	0.93	0.08	20,23,23,25	0
2	GOL	B	1303	6/6	0.94	0.07	20,24,27,29	0
2	GOL	C	1309	6/6	0.95	0.08	23,27,30,31	0
2	GOL	C	1301	6/6	0.96	0.06	21,24,24,24	0
2	GOL	B	1302	6/6	0.96	0.07	19,22,24,24	0
2	GOL	B	1301	6/6	0.96	0.06	18,18,20,21	0
3	PO4	C	1310	5/5	0.96	0.11	20,20,23,25	0
3	PO4	B	1306	5/5	0.97	0.09	18,21,22,26	0
3	PO4	A	1304	5/5	0.98	0.06	15,17,17,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.