



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2017 – 04:42 PM EDT

PDB ID : 5NXH
Title : Crystal structure of the carboxy-terminal region of the bacteriophage T4 proximal long tail fibre protein gp34, residues 744-1289 at 2.9 Angstrom resolution
Authors : Namura, M.; van Raaij, M.J.; Kanamaru, S.
Deposited on : unknown
Resolution : 2.89 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

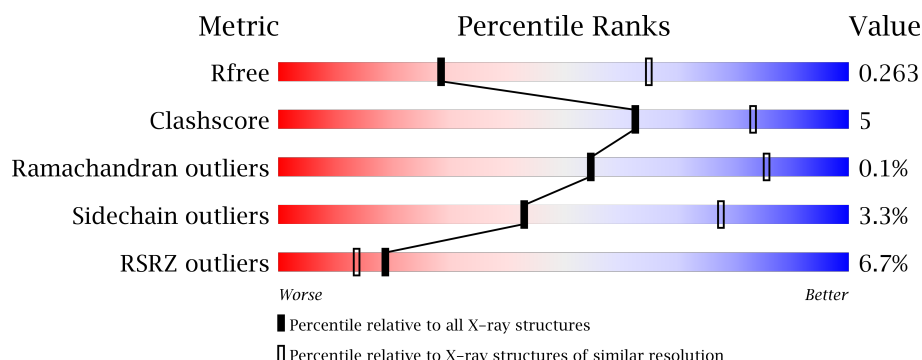
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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. 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	564	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>••</div> </div> </div>
1	B	564	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>••</div> </div> </div>
1	C	564	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12797 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	546	Total	C	N	O	S	0	0	0
			4147	2586	722	834	5			
1	B	546	Total	C	N	O	S	0	0	0
			4147	2586	722	834	5			
1	C	546	Total	C	N	O	S	0	0	0
			4147	2586	722	834	5			

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



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

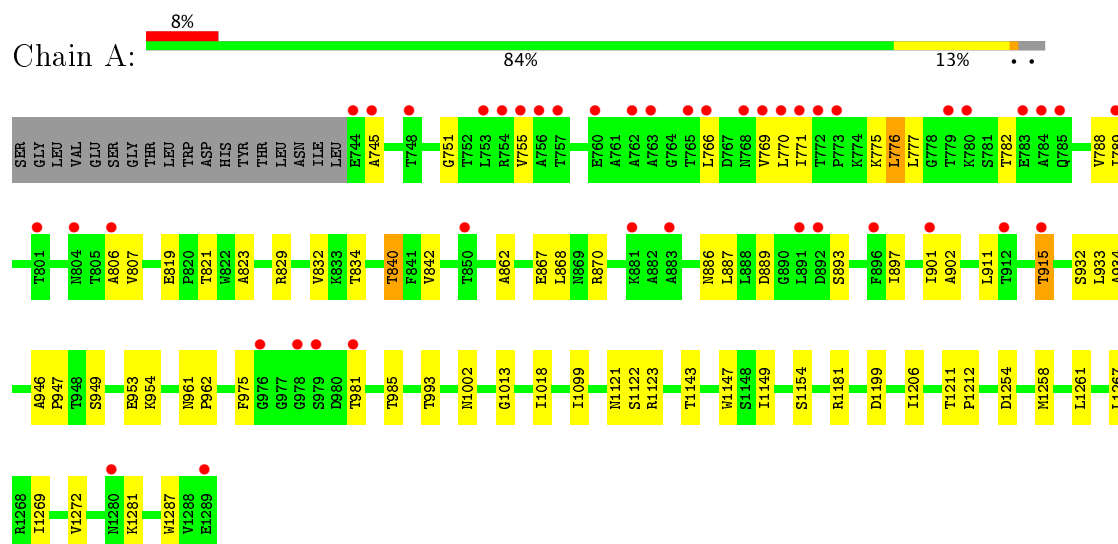
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total 105	O 105	0	0
3	B	126	Total 126	O 126	0	0
3	C	119	Total 119	O 119	0	0

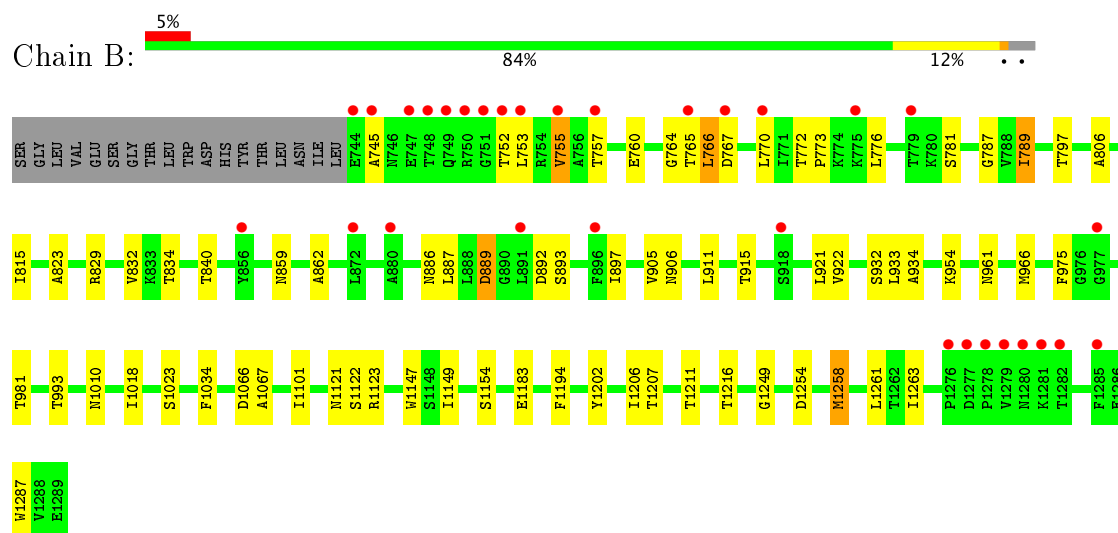
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

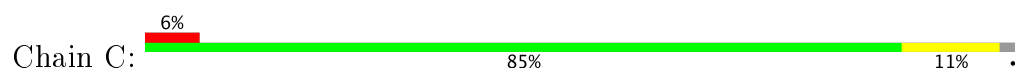
- Molecule 1: Long-tail fiber proximal subunit

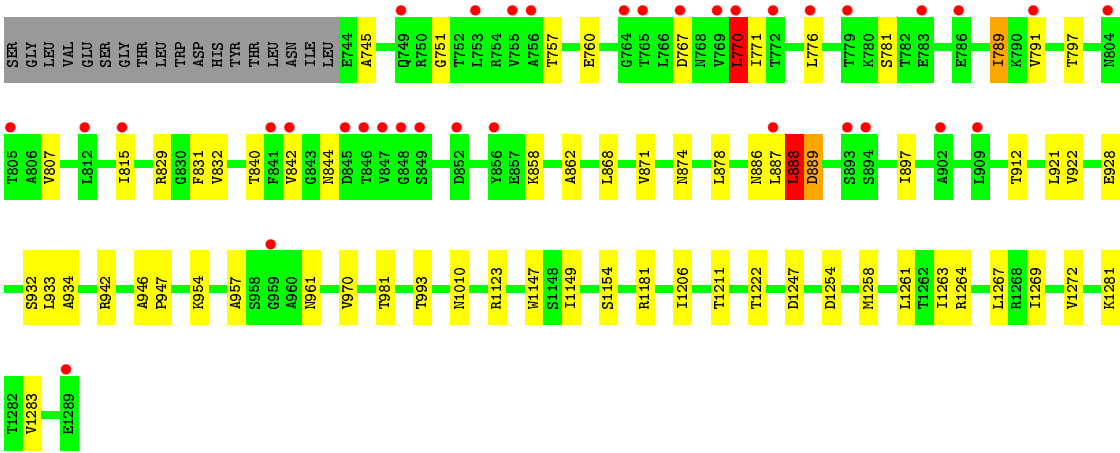


- Molecule 1: Long-tail fiber proximal subunit



- 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	107.30Å 76.13Å 139.87Å 90.00° 97.62° 90.00°	Depositor
Resolution (Å)	45.18 – 2.89 45.18 – 2.89	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.18-2.89) 96.5 (45.18-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.200 , 0.263 0.206 , 0.263	Depositor DCC
R_{free} test set	1911 reflections (4.07%)	DCC
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12797	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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

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	0.55	0/4227	0.76	3/5754 (0.1%)
1	B	0.55	0/4227	0.76	1/5754 (0.0%)
1	C	0.54	0/4227	0.76	4/5754 (0.1%)
All	All	0.55	0/12681	0.76	8/17262 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1199	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	1199	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	B	892	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	888	LEU	CB-CG-CD2	5.57	120.47	111.00
1	C	770	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	1181	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	1254	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	C	767	ASP	CB-CG-OD1	5.01	122.81	118.30

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	4147	0	4052	59	0
1	B	4147	0	4052	59	0
1	C	4147	0	4052	57	0
2	B	6	0	8	0	0
3	A	105	0	0	4	0
3	B	126	0	0	1	0
3	C	119	0	0	0	0
All	All	12797	0	12164	124	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 (124) 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:745:ALA:HB2	1:B:753:LEU:HD21	1.40	1.03
1:B:834:THR:HG21	1:C:858:LYS:O	1.74	0.85
1:A:776:LEU:HD13	1:A:777:LEU:HD23	1.65	0.78
1:B:1207:THR:O	1:B:1216:THR:HG23	1.85	0.77
1:A:789:ILE:CG2	1:B:789:ILE:HD11	2.18	0.72
1:A:775:LYS:NZ	1:B:767:ASP:OD1	2.23	0.72
1:B:1216:THR:HG21	1:C:1222:THR:OG1	1.92	0.69
1:A:819:GLU:OE2	1:A:821:THR:HG22	1.93	0.68
1:A:745:ALA:HB2	1:A:751:GLY:HA3	1.77	0.66
1:A:840:THR:HG21	1:A:867:GLU:HG3	1.77	0.66
1:A:766:LEU:HD13	1:A:769:VAL:HG21	1.78	0.65
1:A:823:ALA:HB2	1:B:829:ARG:NH1	2.13	0.63
1:A:897:ILE:HD12	1:C:897:ILE:HB	1.81	0.62
1:A:1013:GLY:N	1:B:1018:ILE:HD12	2.16	0.61
1:C:922:VAL:O	1:C:922:VAL:HG13	2.01	0.60
1:C:844:ASN:C	1:C:874:ASN:HD21	2.04	0.60
1:A:770:LEU:CD2	1:C:770:LEU:HD21	2.32	0.60
1:B:897:ILE:HB	1:C:897:ILE:HD12	1.86	0.57
1:A:1211:THR:HG22	1:A:1212:PRO:HD2	1.87	0.56
1:B:933:LEU:HD23	1:B:934:ALA:N	2.20	0.56
1:A:745:ALA:HB2	1:A:751:GLY:CA	2.35	0.55
1:A:782:THR:C	1:C:791:VAL:HG12	2.27	0.55
1:C:745:ALA:HB2	1:C:751:GLY:CA	2.37	0.55
1:C:933:LEU:HD23	1:C:934:ALA:N	2.22	0.55
1:B:765:THR:O	1:B:766:LEU:HG	2.07	0.55
1:C:1181:ARG:NH2	1:C:1247:ASP:OD2	2.40	0.54
1:A:1261:LEU:HD11	1:C:1258:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:886:ASN:O	1:C:887:LEU:HD12	2.08	0.54
1:B:797:THR:HG22	1:B:815:ILE:CD1	2.38	0.54
1:C:868:LEU:O	1:C:871:VAL:HG12	2.08	0.53
1:B:773:PRO:HA	1:C:771:ILE:HD11	1.91	0.53
1:B:1258:MET:HE2	1:C:1261:LEU:HD11	1.91	0.53
1:B:905:VAL:O	1:C:912:THR:HG22	2.09	0.53
1:A:933:LEU:HD23	1:A:934:ALA:N	2.23	0.52
1:B:752:THR:HG1	1:C:751:GLY:C	2.13	0.52
1:A:771:ILE:HD13	1:C:776:LEU:HD22	1.92	0.52
1:A:789:ILE:HG22	1:B:789:ILE:HD11	1.92	0.52
1:A:770:LEU:HD23	1:C:770:LEU:HD21	1.92	0.52
1:A:1143:THR:HG21	3:A:1345:HOH:O	2.10	0.52
1:B:781:SER:HB3	1:B:789:ILE:HG23	1.91	0.52
1:A:886:ASN:O	1:A:887:LEU:HD12	2.09	0.52
1:C:781:SER:HB3	1:C:789:ILE:HG23	1.92	0.52
1:C:921:LEU:HD23	1:C:922:VAL:N	2.26	0.51
1:B:1034:PHE:HB3	3:B:1409:HOH:O	2.11	0.51
1:B:772:THR:HG23	1:B:773:PRO:HD2	1.91	0.51
1:B:797:THR:HG22	1:B:815:ILE:HD12	1.93	0.51
1:C:745:ALA:HB2	1:C:751:GLY:HA3	1.93	0.51
1:B:921:LEU:HD23	1:B:922:VAL:N	2.25	0.51
1:C:797:THR:HG22	1:C:815:ILE:CD1	2.41	0.51
1:A:1206:ILE:HD12	1:A:1206:ILE:N	2.27	0.50
1:C:1206:ILE:N	1:C:1206:ILE:HD12	2.27	0.50
1:B:1206:ILE:N	1:B:1206:ILE:HD12	2.27	0.50
1:A:1287:TRP:CZ3	1:C:1281:LYS:HA	2.46	0.50
1:A:1258:MET:HE3	1:A:1261:LEU:HB2	1.94	0.50
1:B:789:ILE:CD1	1:C:789:ILE:HD11	2.42	0.49
1:B:893:SER:HB3	1:C:888:LEU:HD22	1.94	0.49
1:A:1211:THR:HG22	1:A:1212:PRO:CD	2.41	0.49
1:A:788:VAL:HG13	1:B:787:GLY:CA	2.43	0.49
1:A:829:ARG:HE	1:C:831:PHE:HB2	1.78	0.49
3:A:1353:HOH:O	1:B:1249:GLY:HA2	2.11	0.49
1:B:886:ASN:O	1:B:887:LEU:HD12	2.11	0.49
1:A:1267:LEU:HD11	1:C:1263:ILE:HD12	1.95	0.49
1:B:752:THR:OG1	1:C:751:GLY:C	2.51	0.48
1:A:1147:TRP:CZ3	1:A:1149:ILE:HD12	2.49	0.48
1:B:911:LEU:HD12	1:B:911:LEU:N	2.29	0.48
1:A:1143:THR:CG2	3:A:1345:HOH:O	2.62	0.47
1:B:1147:TRP:CZ3	1:B:1149:ILE:HD12	2.49	0.47
1:B:832:VAL:HG21	1:B:862:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:SER:HB2	1:B:889:ASP:HB2	1.97	0.47
1:B:1258:MET:CE	1:C:1261:LEU:HD11	2.44	0.47
1:B:906:ASN:HA	1:C:912:THR:HG22	1.97	0.47
1:B:789:ILE:HD12	1:B:806:ALA:HB2	1.97	0.46
1:C:844:ASN:O	1:C:874:ASN:ND2	2.32	0.46
1:B:752:THR:OG1	1:C:751:GLY:CA	2.63	0.46
1:A:777:LEU:HG	1:B:764:GLY:HA3	1.96	0.46
1:C:1147:TRP:CZ3	1:C:1149:ILE:HD12	2.50	0.46
1:A:834:THR:HG21	1:B:859:ASN:HA	1.98	0.46
1:C:832:VAL:HG21	1:C:862:ALA:HB2	1.96	0.46
1:A:832:VAL:HG21	1:A:862:ALA:HB2	1.96	0.45
1:A:901:ILE:HG22	1:A:902:ALA:N	2.31	0.45
1:A:1018:ILE:HA	1:B:1023:SER:OG	2.17	0.45
1:A:868:LEU:HD13	1:A:868:LEU:C	2.37	0.45
1:A:789:ILE:HG21	1:B:789:ILE:HD11	1.97	0.45
1:A:770:LEU:HD13	1:B:770:LEU:CD2	2.47	0.45
1:A:789:ILE:HD13	1:A:806:ALA:HB2	1.99	0.45
1:A:949:SER:HB3	3:A:1310:HOH:O	2.16	0.45
1:A:1272:VAL:HG11	1:C:1283:VAL:HG11	2.00	0.44
1:B:975:PHE:CD1	1:C:957:ALA:HB1	2.53	0.44
1:C:888:LEU:HD23	1:C:889:ASP:N	2.32	0.44
1:A:946:ALA:HB1	1:A:947:PRO:HD2	1.99	0.44
1:A:954:LYS:O	1:A:961:ASN:ND2	2.51	0.44
1:C:797:THR:HG22	1:C:815:ILE:HD12	2.00	0.43
1:C:954:LYS:O	1:C:961:ASN:ND2	2.51	0.43
1:A:776:LEU:CD1	1:A:777:LEU:HD23	2.44	0.43
1:B:1121:ASN:HA	1:B:1122:SER:HA	1.74	0.43
1:B:1216:THR:HG21	1:C:1222:THR:HG1	1.83	0.43
1:A:770:LEU:HD22	1:C:770:LEU:HD21	2.00	0.43
1:A:985:THR:HG22	1:B:966:MET:HE2	2.01	0.43
1:C:757:THR:HG22	1:C:760:GLU:OE1	2.19	0.43
1:B:954:LYS:O	1:B:961:ASN:ND2	2.51	0.43
1:A:953:GLU:OE1	1:C:942:ARG:HA	2.19	0.43
1:A:962:PRO:HG3	1:C:970:VAL:HG12	1.99	0.43
1:B:823:ALA:HB2	1:C:829:ARG:NH1	2.33	0.43
1:B:776:LEU:HD11	1:C:776:LEU:CD1	2.49	0.43
1:B:906:ASN:HA	1:C:912:THR:CG2	2.49	0.42
1:C:1269:ILE:O	1:C:1272:VAL:HG12	2.20	0.42
1:A:807:VAL:HG23	1:C:807:VAL:O	2.18	0.42
1:B:1263:ILE:HD12	1:C:1267:LEU:HD11	2.01	0.42
1:B:757:THR:HG22	1:B:760:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:ILE:HD12	1:B:1101:ILE:HG23	2.02	0.42
1:A:911:LEU:N	1:A:911:LEU:HD12	2.35	0.42
1:C:1258:MET:HE3	1:C:1261:LEU:HB2	2.01	0.41
1:A:1258:MET:HE2	1:B:1261:LEU:HD11	2.01	0.41
1:A:1121:ASN:HA	1:A:1122:SER:HA	1.71	0.41
1:B:1066:ASP:O	1:B:1067:ALA:HB3	2.20	0.41
1:A:1272:VAL:HG11	1:C:1283:VAL:CG1	2.50	0.41
1:B:789:ILE:HG13	1:C:789:ILE:HD11	2.03	0.41
1:B:1194:PHE:HB2	1:B:1202:TYR:CZ	2.57	0.41
1:A:1281:LYS:HA	1:B:1287:TRP:CZ3	2.56	0.41
1:C:946:ALA:HB1	1:C:947:PRO:HD2	2.03	0.41
1:A:911:LEU:HD23	1:A:915:THR:HB	2.03	0.40
1:B:755:VAL:HA	1:B:770:LEU:HB2	2.02	0.40
1:A:1269:ILE:O	1:A:1272:VAL:HG12	2.21	0.40
1:A:755:VAL:HA	1:A:770:LEU:HB2	2.03	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	544/564 (96%)	522 (96%)	22 (4%)	0	100	100
1	B	544/564 (96%)	521 (96%)	22 (4%)	1 (0%)	51	82
1	C	544/564 (96%)	519 (95%)	25 (5%)	0	100	100
All	All	1632/1692 (96%)	1562 (96%)	69 (4%)	1 (0%)	55	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	766	LEU

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	452/468 (97%)	438 (97%)	14 (3%)	45	79
1	B	452/468 (97%)	437 (97%)	15 (3%)	43	77
1	C	452/468 (97%)	436 (96%)	16 (4%)	41	75
All	All	1356/1404 (97%)	1311 (97%)	45 (3%)	43	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	776	LEU
1	A	840	THR
1	A	842	VAL
1	A	870	ARG
1	A	889	ASP
1	A	915	THR
1	A	932	SER
1	A	975	PHE
1	A	981	THR
1	A	993	THR
1	A	1002	ASN
1	A	1123	ARG
1	A	1154	SER
1	A	1254	ASP
1	B	755	VAL
1	B	789	ILE
1	B	840	THR
1	B	889	ASP
1	B	915	THR
1	B	932	SER
1	B	981	THR
1	B	993	THR
1	B	1010	ASN
1	B	1123	ARG
1	B	1154	SER
1	B	1183	GLU

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Mol	Chain	Res	Type
1	B	1211	THR
1	B	1254	ASP
1	B	1258	MET
1	C	770	LEU
1	C	789	ILE
1	C	840	THR
1	C	842	VAL
1	C	878	LEU
1	C	888	LEU
1	C	889	ASP
1	C	928	GLU
1	C	932	SER
1	C	981	THR
1	C	993	THR
1	C	1010	ASN
1	C	1123	ARG
1	C	1154	SER
1	C	1211	THR
1	C	1264	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	B	1301	-	5,5,5	0.24	0	5,5,5	0.35	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	1301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	546/564 (96%)	0.43	43 (7%) 13 10	25, 66, 117, 153	0
1	B	546/564 (96%)	0.36	31 (5%) 24 19	20, 62, 117, 176	0
1	C	546/564 (96%)	0.37	35 (6%) 20 15	23, 63, 120, 157	0
All	All	1638/1692 (96%)	0.39	109 (6%) 19 14	20, 64, 118, 176	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	770	LEU	8.5
1	A	784	ALA	5.8
1	A	769	VAL	5.1
1	B	753	LEU	5.1
1	C	847	VAL	4.9
1	A	779	THR	4.8
1	B	1282	THR	4.2
1	A	912	THR	4.1
1	A	755	VAL	4.0
1	B	755	VAL	3.9
1	B	1281	LYS	3.9
1	A	756	ALA	3.8
1	B	749	GLN	3.8
1	A	753	LEU	3.7
1	C	1289	GLU	3.7
1	C	756	ALA	3.6
1	A	754	ARG	3.6
1	A	762	ALA	3.5
1	B	748	THR	3.5
1	B	744	GLU	3.5
1	B	767	ASP	3.5
1	A	766	LEU	3.5
1	A	771	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	891	LEU	3.4
1	A	1289	GLU	3.3
1	B	896	PHE	3.3
1	B	1279	VAL	3.3
1	C	753	LEU	3.2
1	C	767	ASP	3.2
1	A	770	LEU	3.2
1	A	801	THR	3.2
1	C	749	GLN	3.2
1	B	747	GLU	3.2
1	A	783	GLU	3.1
1	A	768	ASN	3.1
1	A	978	GLY	3.1
1	C	755	VAL	3.1
1	A	744	GLU	3.1
1	C	779	THR	2.9
1	B	1277	ASP	2.9
1	B	775	LYS	2.8
1	A	760	GLU	2.8
1	A	1280	ASN	2.8
1	A	745	ALA	2.8
1	A	883	ALA	2.7
1	B	745	ALA	2.7
1	B	880	ALA	2.7
1	C	856	TYR	2.7
1	B	752	THR	2.7
1	A	757	THR	2.7
1	A	981	THR	2.7
1	B	751	GLY	2.6
1	C	776	LEU	2.6
1	A	979	SER	2.5
1	A	785	GLN	2.5
1	C	841	PHE	2.5
1	C	848	GLY	2.5
1	B	872	LEU	2.5
1	C	842	VAL	2.5
1	C	769	VAL	2.5
1	B	1280	ASN	2.5
1	C	772	THR	2.5
1	A	850	THR	2.4
1	A	806	ALA	2.4
1	B	750	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	901	ILE	2.4
1	A	896	PHE	2.4
1	C	887	LEU	2.4
1	A	789	ILE	2.4
1	B	1276	PRO	2.4
1	C	765	THR	2.4
1	A	891	LEU	2.4
1	C	815	ILE	2.4
1	C	791	VAL	2.3
1	A	773	PRO	2.3
1	A	892	ASP	2.3
1	A	765	THR	2.3
1	A	763	ALA	2.3
1	C	770	LEU	2.3
1	A	772	THR	2.3
1	B	918	SER	2.3
1	C	845	ASP	2.3
1	C	959	GLY	2.3
1	C	804	ASN	2.2
1	B	977	GLY	2.2
1	A	976	GLY	2.2
1	C	764	GLY	2.2
1	C	812	LEU	2.2
1	A	804	ASN	2.2
1	C	849	SER	2.2
1	A	748	THR	2.2
1	C	783	GLU	2.1
1	B	1285	PHE	2.1
1	B	1278	PRO	2.1
1	C	786	GLU	2.1
1	C	893	SER	2.1
1	B	779	THR	2.1
1	C	805	THR	2.1
1	B	765	THR	2.1
1	C	894	SER	2.1
1	A	915	THR	2.1
1	B	856	TYR	2.1
1	A	780	LYS	2.1
1	C	852	ASP	2.0
1	B	757	THR	2.0
1	C	846	THR	2.0
1	C	909	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	902	ALA	2.0
1	A	881	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	B	1301	6/6	0.90	0.32	-	50,60,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.