



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:44 pm BST

PDB ID : 5CWU
Title : Crystal structure of Chaetomium thermophilum Nup188 TAIL domain
Authors : Stuwe, T.; Bley, C.J.; Thierbach, K.; Petrovic, S.; Schilbach, S.; Mayo, D.J.; Perriches, T.; Rundlet, E.J.; Jeon, Y.E.; Collins, L.N.; Lin, D.H.; Paduch, M.; Koide, A.; Lu, V.; Fischer, J.; Hurt, E.; Koide, S.; Kossiakoff, A.A.; Hoelz, A.
Deposited on : 2015-07-28
Resolution : 3.35 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 : 2.11
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) : 2.11

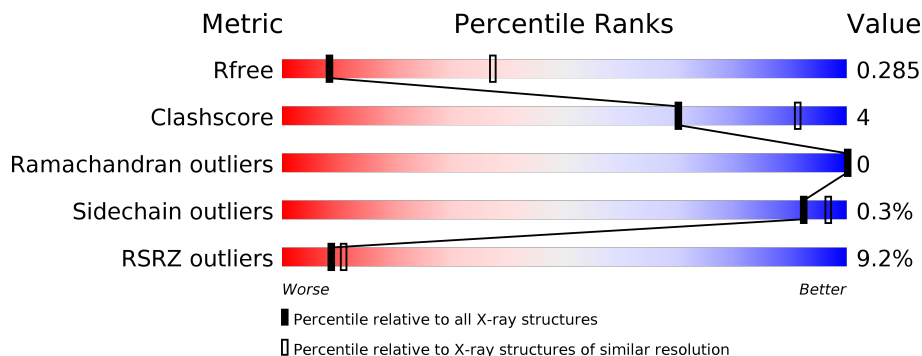
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	414	 7% 66% 6% 28%
1	B	414	 6% 66% 6% 28%
1	C	414	 6% 67% 5% 28%
1	D	414	 8% 67% 5% 28%
1	E	414	 6% 66% 5% 28%
1	F	414	 8% 69% 5% 28%

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Mol	Chain	Length	Quality of chain
1	G	414	
1	H	414	

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
2	GOL	A	1901	-	-	-	X
2	GOL	A	1902	-	-	-	X
2	GOL	B	1901	-	-	-	X
2	GOL	B	1902	-	-	-	X
2	GOL	C	1901	-	-	-	X
2	GOL	D	1901	-	-	-	X
2	GOL	E	1901	-	-	-	X
2	GOL	G	1901	-	-	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18304 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 Nucleoporin NUP188.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	298	2282	1474	394	404	8	2	0	0	0
1	B	298	2282	1474	394	404	8	2	0	0	0
1	C	298	2282	1474	394	404	8	2	0	0	0
1	D	298	2282	1474	394	404	8	2	0	0	0
1	E	298	2282	1474	394	404	8	2	0	0	0
1	F	298	2282	1474	394	404	8	2	0	0	0
1	G	298	2282	1474	394	404	8	2	0	0	0
1	H	298	2282	1474	394	404	8	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

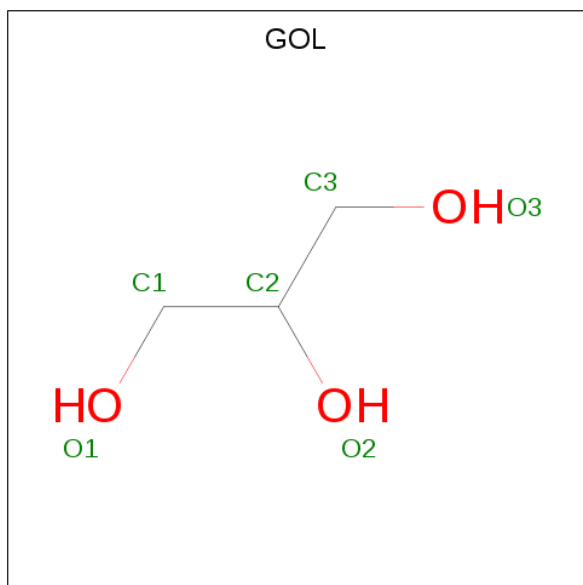
Chain	Residue	Modelled	Actual	Comment	Reference
A	1445	SER	-	expression tag	UNP G0SFH5
A	1446	MSE	-	expression tag	UNP G0SFH5
B	1445	SER	-	expression tag	UNP G0SFH5
B	1446	MSE	-	expression tag	UNP G0SFH5
C	1445	SER	-	expression tag	UNP G0SFH5
C	1446	MSE	-	expression tag	UNP G0SFH5
D	1445	SER	-	expression tag	UNP G0SFH5
D	1446	MSE	-	expression tag	UNP G0SFH5
E	1445	SER	-	expression tag	UNP G0SFH5
E	1446	MSE	-	expression tag	UNP G0SFH5
F	1445	SER	-	expression tag	UNP G0SFH5
F	1446	MSE	-	expression tag	UNP G0SFH5
G	1445	SER	-	expression tag	UNP G0SFH5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1446	MSE	-	expression tag	UNP G0SFH5
H	1445	SER	-	expression tag	UNP G0SFH5
H	1446	MSE	-	expression tag	UNP G0SFH5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

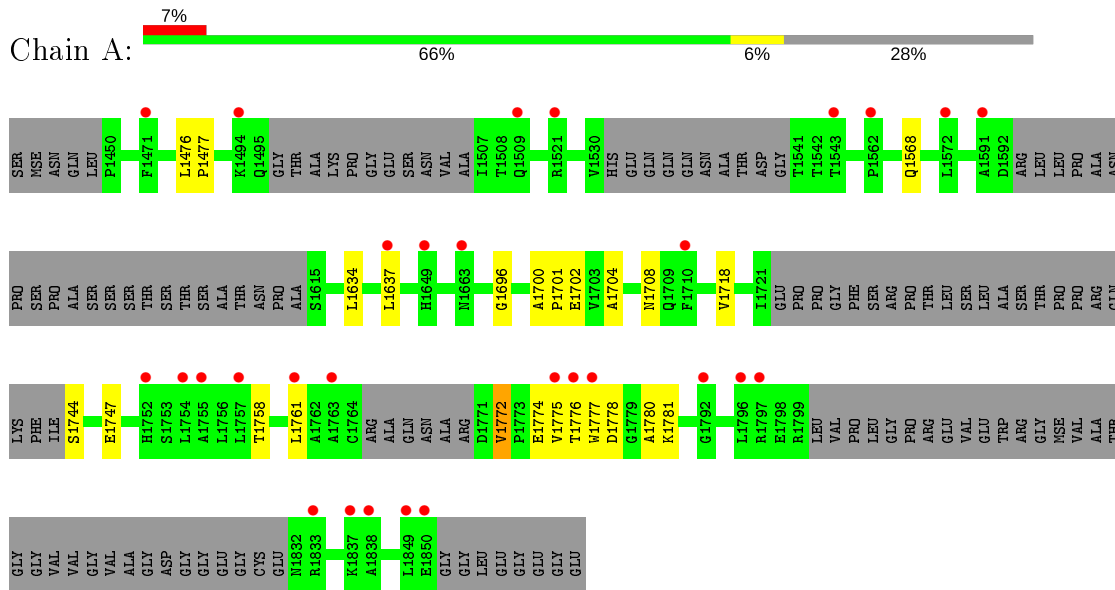


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

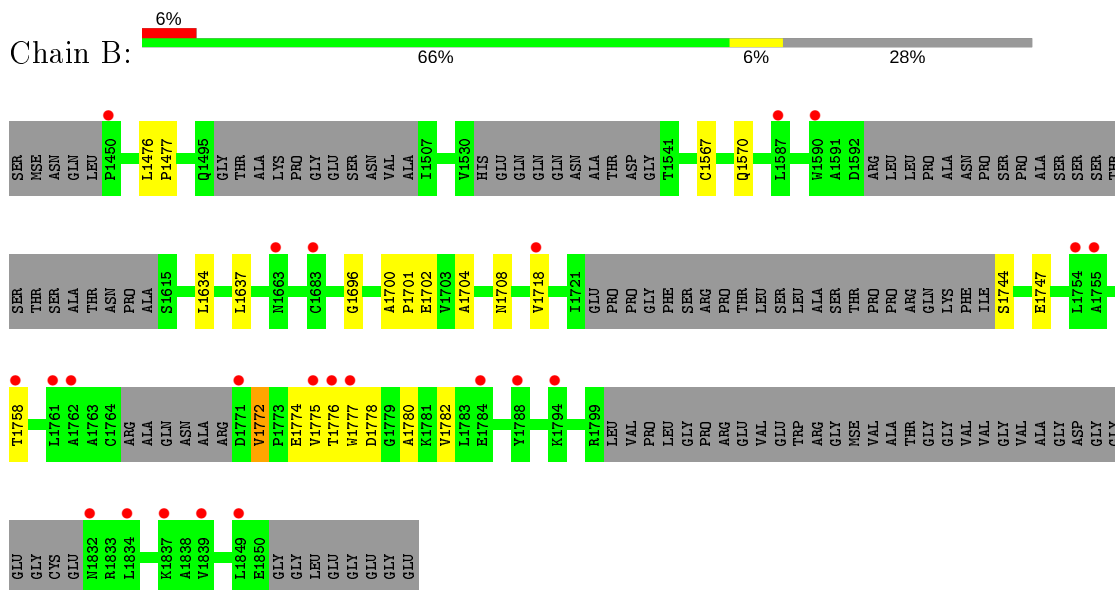
3 Residue-property plots i

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.

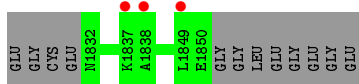
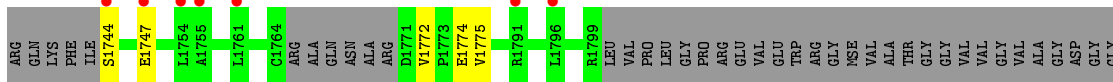
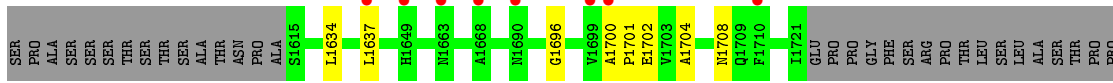
- Molecule 1: Nucleoporin NUP188



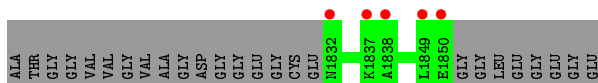
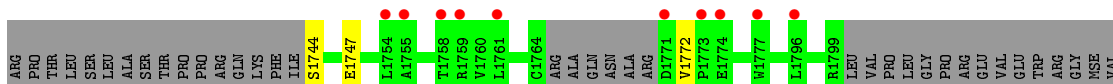
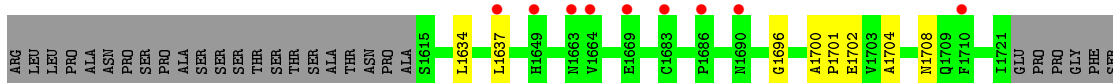
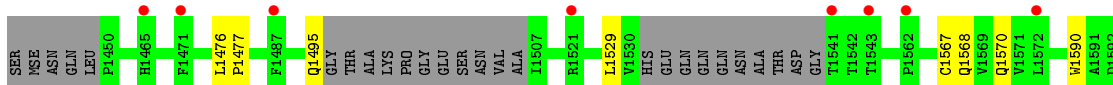
- Molecule 1: Nucleoporin NUP188



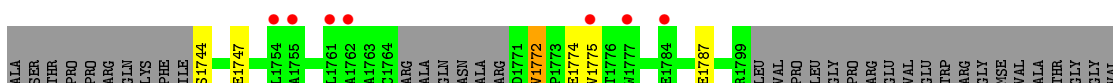
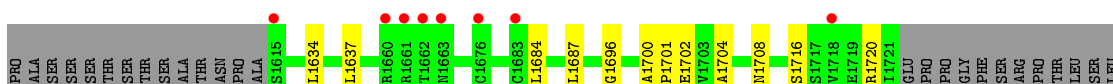
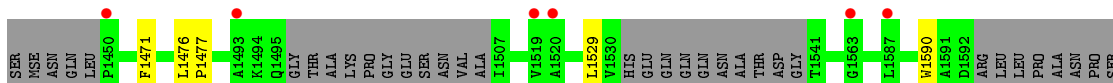
- Molecule 1: Nucleoporin NUP188

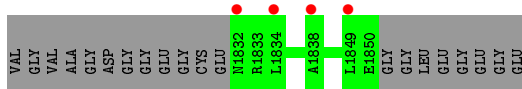


- Molecule 1: Nucleoporin NUP188

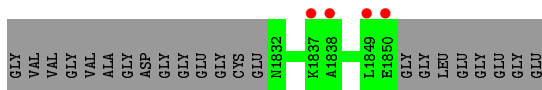
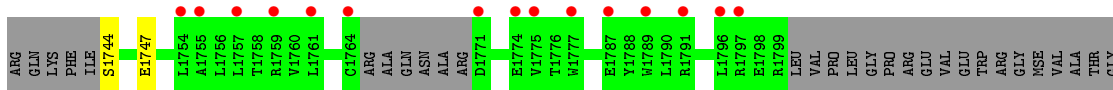
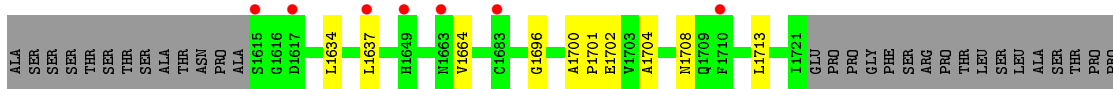
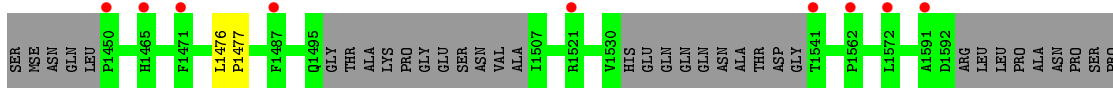


- Molecule 1: Nucleoporin NUP188

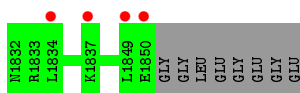
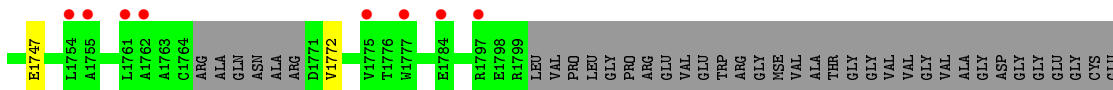
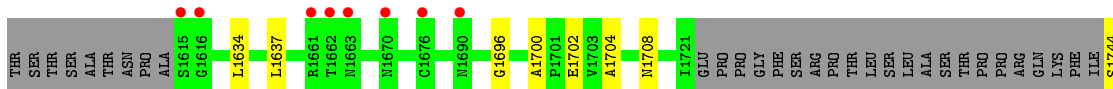
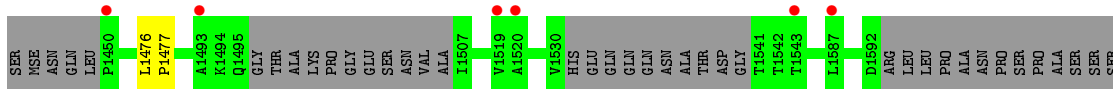




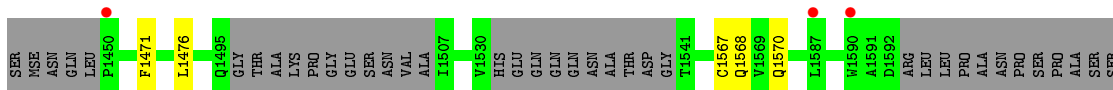
- Molecule 1: Nucleoporin NUP188

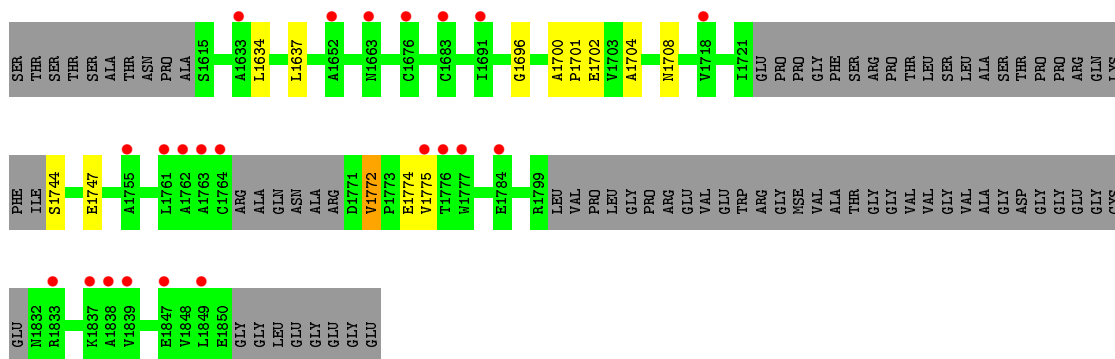


- Molecule 1: Nucleoporin NUP188



- Molecule 1: Nucleoporin NUP188





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.28Å 65.28Å 155.55Å 90.00° 89.95° 90.01°	Depositor
Resolution (Å)	19.85 – 3.35 19.85 – 3.31	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.85-3.35) 89.9 (19.85-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 3.29Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.246 , 0.279 0.252 , 0.285	Depositor DCC
R_{free} test set	1858 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	118.5	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.418 for k,-h,l 0.418 for -k,h,l 0.417 for h,-k,-l 0.417 for -h,k,-l 0.429 for -h,-k,l 0.418 for k,h,-l 0.418 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18304	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: 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	0.27	0/2315	0.43	0/3148
1	B	0.27	0/2315	0.42	0/3148
1	C	0.26	0/2315	0.42	0/3148
1	D	0.25	0/2315	0.43	0/3148
1	E	0.25	0/2315	0.41	0/3148
1	F	0.24	0/2315	0.42	0/3148
1	G	0.25	0/2315	0.42	0/3148
1	H	0.24	0/2315	0.42	0/3148
All	All	0.25	0/18520	0.42	0/25184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2282	0	2371	39	0
1	B	2282	0	2371	38	0
1	C	2282	0	2371	11	0
1	D	2282	0	2371	11	0
1	E	2282	0	2371	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2282	0	2371	8	0
1	G	2282	0	2371	6	0
1	H	2282	0	2371	11	0
2	A	12	0	16	0	0
2	B	12	0	16	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	G	6	0	8	0	0
All	All	18304	0	19032	136	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 4.

All (136) 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:1701:PRO:CG	1:B:1772:VAL:HG21	1.60	1.30
1:B:1701:PRO:CB	1:B:1772:VAL:HG21	1.60	1.29
1:A:1701:PRO:CB	1:A:1772:VAL:HG21	1.64	1.27
1:A:1708:ASN:OD1	1:A:1776:THR:HG23	1.27	1.26
1:A:1758:THR:CG2	1:A:1775:VAL:HG11	1.70	1.20
1:B:1701:PRO:HG3	1:B:1772:VAL:CG2	1.76	1.15
1:A:1701:PRO:HB3	1:A:1772:VAL:CG2	1.81	1.10
1:B:1701:PRO:HG3	1:B:1772:VAL:HG21	1.22	1.09
1:A:1701:PRO:HA	1:A:1772:VAL:HG11	1.09	1.09
1:B:1701:PRO:HB3	1:B:1772:VAL:HG21	1.28	1.09
1:B:1758:THR:HG22	1:B:1775:VAL:HG21	1.31	1.08
1:A:1758:THR:HG21	1:A:1775:VAL:HG11	1.17	1.06
1:B:1701:PRO:CA	1:B:1772:VAL:HG11	1.87	1.04
1:B:1718:VAL:CG2	1:B:1777:TRP:HE1	1.69	1.04
1:A:1718:VAL:HG23	1:A:1777:TRP:HE1	1.22	1.03
1:B:1718:VAL:HG23	1:B:1777:TRP:HE1	1.21	1.00
1:B:1701:PRO:HA	1:B:1772:VAL:CG1	1.92	0.99
1:B:1718:VAL:CG2	1:B:1777:TRP:NE1	2.24	0.99
1:B:1701:PRO:HA	1:B:1772:VAL:HG11	0.98	0.97
1:A:1701:PRO:HB3	1:A:1772:VAL:HG21	0.96	0.95
1:A:1701:PRO:CA	1:A:1772:VAL:HG11	2.00	0.92
1:A:1718:VAL:CG2	1:A:1777:TRP:NE1	2.35	0.90
1:A:1708:ASN:OD1	1:A:1776:THR:CG2	2.18	0.90
1:A:1718:VAL:CG2	1:A:1777:TRP:HE1	1.83	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1701:PRO:HB3	1:B:1772:VAL:CG2	2.01	0.89
1:A:1701:PRO:CG	1:A:1772:VAL:HG21	2.06	0.85
1:A:1758:THR:CG2	1:A:1775:VAL:CG1	2.56	0.83
1:A:1701:PRO:HA	1:A:1772:VAL:CG1	2.04	0.81
1:A:1758:THR:HG21	1:A:1775:VAL:CG1	2.09	0.79
1:B:1701:PRO:CG	1:B:1772:VAL:CG2	2.45	0.79
1:A:1758:THR:HG22	1:A:1775:VAL:HG11	1.68	0.74
1:A:1718:VAL:HG23	1:A:1777:TRP:NE1	1.98	0.73
1:B:1718:VAL:HG23	1:B:1777:TRP:NE1	1.96	0.71
1:D:1744:SER:N	1:D:1747:GLU:OE1	2.24	0.70
1:B:1744:SER:N	1:B:1747:GLU:OE1	2.26	0.69
1:C:1744:SER:N	1:C:1747:GLU:OE1	2.27	0.68
1:B:1718:VAL:HG22	1:B:1777:TRP:NE1	2.10	0.67
1:A:1761:LEU:HD12	1:A:1775:VAL:CG2	2.25	0.67
1:E:1744:SER:N	1:E:1747:GLU:OE1	2.27	0.67
1:H:1744:SER:N	1:H:1747:GLU:OE1	2.29	0.66
1:A:1758:THR:HG22	1:A:1775:VAL:HG21	1.77	0.66
1:F:1744:SER:N	1:F:1747:GLU:OE1	2.29	0.66
1:A:1744:SER:N	1:A:1747:GLU:OE1	2.29	0.66
1:A:1758:THR:HG22	1:A:1775:VAL:CG1	2.25	0.65
1:G:1744:SER:N	1:G:1747:GLU:OE1	2.31	0.64
1:B:1701:PRO:CB	1:B:1772:VAL:CG2	2.54	0.64
1:A:1701:PRO:HG3	1:A:1772:VAL:HG21	1.81	0.63
1:B:1758:THR:HG22	1:B:1775:VAL:CG2	2.18	0.63
1:B:1758:THR:CG2	1:B:1775:VAL:HG21	2.18	0.63
1:C:1567:CYS:SG	1:C:1570:GLN:NE2	2.72	0.62
1:C:1696:GLY:O	1:C:1700:ALA:N	2.33	0.61
1:A:1718:VAL:HG22	1:A:1777:TRP:CZ2	2.35	0.61
1:H:1696:GLY:O	1:H:1700:ALA:N	2.34	0.61
1:D:1696:GLY:O	1:D:1700:ALA:N	2.35	0.59
1:B:1758:THR:CG2	1:B:1775:VAL:HG11	2.32	0.59
1:A:1758:THR:HG22	1:A:1775:VAL:CG2	2.32	0.59
1:A:1696:GLY:O	1:A:1700:ALA:N	2.35	0.59
1:H:1567:CYS:SG	1:H:1570:GLN:NE2	2.74	0.58
1:E:1704:ALA:O	1:E:1708:ASN:ND2	2.36	0.57
1:B:1696:GLY:O	1:B:1700:ALA:N	2.36	0.57
1:E:1774:GLU:HG2	1:E:1775:VAL:H	1.69	0.57
1:G:1696:GLY:O	1:G:1700:ALA:N	2.38	0.57
1:B:1708:ASN:OD1	1:B:1776:THR:HG23	2.04	0.57
1:F:1696:GLY:O	1:F:1700:ALA:N	2.38	0.57
1:F:1704:ALA:O	1:F:1708:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1704:ALA:O	1:B:1708:ASN:ND2	2.38	0.55
1:A:1704:ALA:O	1:A:1708:ASN:ND2	2.39	0.55
1:G:1704:ALA:O	1:G:1708:ASN:ND2	2.40	0.54
1:D:1704:ALA:O	1:D:1708:ASN:ND2	2.40	0.54
1:H:1704:ALA:O	1:H:1708:ASN:ND2	2.39	0.54
1:B:1758:THR:HG21	1:B:1775:VAL:HG11	1.90	0.54
1:B:1718:VAL:HG22	1:B:1777:TRP:CE2	2.44	0.53
1:C:1704:ALA:O	1:C:1708:ASN:ND2	2.40	0.53
1:H:1701:PRO:HB3	1:H:1772:VAL:HG21	1.90	0.52
1:E:1696:GLY:O	1:E:1700:ALA:N	2.42	0.52
1:A:1718:VAL:HG22	1:A:1777:TRP:CE2	2.45	0.52
1:A:1718:VAL:CG2	1:A:1777:TRP:CE2	2.93	0.51
1:B:1777:TRP:CH2	1:B:1782:VAL:HG21	2.46	0.50
1:A:1701:PRO:HG3	1:A:1772:VAL:CG2	2.41	0.50
1:H:1701:PRO:HA	1:H:1772:VAL:HG11	1.95	0.49
1:B:1701:PRO:HG3	1:B:1772:VAL:HG23	1.82	0.48
1:H:1774:GLU:HG2	1:H:1775:VAL:H	1.79	0.48
1:B:1778:ASP:C	1:B:1780:ALA:H	2.17	0.48
1:A:1778:ASP:C	1:A:1780:ALA:H	2.17	0.48
1:B:1774:GLU:HG2	1:B:1775:VAL:H	1.79	0.48
1:A:1634:LEU:HD11	1:A:1637:LEU:HD13	1.96	0.47
1:D:1567:CYS:SG	1:D:1570:GLN:NE2	2.87	0.47
1:D:1529:LEU:HD12	1:D:1590:TRP:CZ2	2.49	0.47
1:H:1634:LEU:HD11	1:H:1637:LEU:HD13	1.97	0.47
1:C:1701:PRO:HB3	1:C:1772:VAL:HG21	1.97	0.47
1:G:1634:LEU:HD11	1:G:1637:LEU:HD13	1.96	0.47
1:A:1778:ASP:OD2	1:A:1781:LYS:HG3	2.14	0.47
1:F:1634:LEU:HD11	1:F:1637:LEU:HD13	1.97	0.46
1:D:1634:LEU:HD11	1:D:1637:LEU:HD13	1.98	0.46
1:B:1567:CYS:SG	1:B:1570:GLN:NE2	2.89	0.46
1:B:1718:VAL:HG22	1:B:1777:TRP:HE1	1.69	0.46
1:A:1774:GLU:HG2	1:A:1775:VAL:H	1.80	0.46
1:E:1701:PRO:HB3	1:E:1772:VAL:HG21	1.98	0.45
1:G:1702:GLU:OE2	1:G:1702:GLU:N	2.49	0.45
1:B:1634:LEU:HD11	1:B:1637:LEU:HD13	1.99	0.45
1:D:1702:GLU:N	1:D:1702:GLU:OE2	2.50	0.45
1:B:1476:LEU:N	1:B:1477:PRO:HD2	2.31	0.45
1:C:1634:LEU:HD11	1:C:1637:LEU:HD13	1.98	0.45
1:F:1476:LEU:N	1:F:1477:PRO:HD2	2.32	0.45
1:G:1476:LEU:N	1:G:1477:PRO:HD2	2.32	0.45
1:A:1758:THR:CG2	1:A:1775:VAL:HG21	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1701:PRO:HG3	1:B:1772:VAL:CB	2.45	0.44
1:C:1702:GLU:N	1:C:1702:GLU:OE2	2.48	0.44
1:E:1634:LEU:HD11	1:E:1637:LEU:HD13	1.99	0.44
1:E:1702:GLU:N	1:E:1702:GLU:OE2	2.51	0.44
1:D:1495:GLN:NE2	1:E:1787:GLU:OE1	2.51	0.44
1:D:1701:PRO:HB3	1:D:1772:VAL:HG21	2.00	0.43
1:E:1529:LEU:HD12	1:E:1590:TRP:CZ2	2.53	0.43
1:A:1702:GLU:N	1:A:1702:GLU:OE2	2.50	0.43
1:B:1702:GLU:N	1:B:1702:GLU:OE2	2.48	0.43
1:A:1476:LEU:N	1:A:1477:PRO:HD2	2.33	0.43
1:E:1476:LEU:N	1:E:1477:PRO:HD2	2.33	0.43
1:H:1702:GLU:OE2	1:H:1702:GLU:N	2.49	0.43
1:A:1758:THR:CB	1:A:1775:VAL:HG21	2.49	0.43
1:H:1568:GLN:HB2	1:H:1634:LEU:HD13	2.01	0.43
1:F:1702:GLU:N	1:F:1702:GLU:OE2	2.48	0.43
1:D:1476:LEU:N	1:D:1477:PRO:HD2	2.34	0.43
1:E:1716:SER:O	1:E:1720:ARG:N	2.53	0.42
1:C:1774:GLU:HG2	1:C:1775:VAL:H	1.84	0.42
1:D:1568:GLN:HB2	1:D:1634:LEU:HD13	2.02	0.42
1:C:1568:GLN:HB2	1:C:1634:LEU:HD13	2.02	0.42
1:C:1476:LEU:N	1:C:1477:PRO:HD2	2.34	0.42
1:B:1700:ALA:HB3	1:B:1701:PRO:HD3	2.02	0.41
1:B:1758:THR:HG22	1:B:1775:VAL:HG11	2.01	0.41
1:C:1471:PHE:HA	1:C:1476:LEU:HD13	2.02	0.41
1:A:1568:GLN:HB2	1:A:1634:LEU:HD13	2.02	0.41
1:F:1700:ALA:HB3	1:F:1701:PRO:HD3	2.02	0.41
1:E:1471:PHE:HA	1:E:1476:LEU:HD13	2.04	0.40
1:F:1664:VAL:HG11	1:F:1713:LEU:HD21	2.04	0.40
1:H:1471:PHE:HA	1:H:1476:LEU:HD13	2.03	0.40
1:E:1684:LEU:O	1:E:1687:LEU:N	2.54	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	284/414 (69%)	252 (89%)	32 (11%)	0	100	100
1	B	284/414 (69%)	251 (88%)	33 (12%)	0	100	100
1	C	284/414 (69%)	253 (89%)	31 (11%)	0	100	100
1	D	284/414 (69%)	255 (90%)	29 (10%)	0	100	100
1	E	284/414 (69%)	255 (90%)	29 (10%)	0	100	100
1	F	284/414 (69%)	255 (90%)	29 (10%)	0	100	100
1	G	284/414 (69%)	253 (89%)	31 (11%)	0	100	100
1	H	284/414 (69%)	254 (89%)	30 (11%)	0	100	100
All	All	2272/3312 (69%)	2028 (89%)	244 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	241/324 (74%)	240 (100%)	1 (0%)	91	95
1	B	241/324 (74%)	240 (100%)	1 (0%)	91	95
1	C	241/324 (74%)	241 (100%)	0	100	100
1	D	241/324 (74%)	241 (100%)	0	100	100
1	E	241/324 (74%)	240 (100%)	1 (0%)	91	95
1	F	241/324 (74%)	241 (100%)	0	100	100
1	G	241/324 (74%)	240 (100%)	1 (0%)	91	95
1	H	241/324 (74%)	240 (100%)	1 (0%)	91	95
All	All	1928/2592 (74%)	1923 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1772	VAL
1	B	1772	VAL
1	E	1772	VAL
1	G	1772	VAL
1	H	1772	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1570	GLN
1	A	1640	HIS
1	C	1640	HIS
1	D	1570	GLN
1	D	1640	HIS
1	E	1640	HIS
1	F	1640	HIS
1	G	1640	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are 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	A	1902	-	5,5,5	0.37	0	5,5,5	0.31	0
2	GOL	G	1901	-	5,5,5	0.38	0	5,5,5	0.29	0
2	GOL	E	1901	-	5,5,5	0.39	0	5,5,5	0.22	0
2	GOL	C	1901	-	5,5,5	0.35	0	5,5,5	0.24	0
2	GOL	D	1901	-	5,5,5	0.39	0	5,5,5	0.09	0
2	GOL	A	1901	-	5,5,5	0.36	0	5,5,5	0.34	0
2	GOL	B	1901	-	5,5,5	0.37	0	5,5,5	0.36	0
2	GOL	B	1902	-	5,5,5	0.37	0	5,5,5	0.27	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	A	1902	-	-	4/4/4/4	-
2	GOL	G	1901	-	-	2/4/4/4	-
2	GOL	E	1901	-	-	1/4/4/4	-
2	GOL	C	1901	-	-	3/4/4/4	-
2	GOL	D	1901	-	-	2/4/4/4	-
2	GOL	A	1901	-	-	0/4/4/4	-
2	GOL	B	1901	-	-	2/4/4/4	-
2	GOL	B	1902	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1902	GOL	O1-C1-C2-C3
2	G	1901	GOL	O1-C1-C2-C3
2	D	1901	GOL	O1-C1-C2-O2
2	D	1901	GOL	O1-C1-C2-C3
2	B	1902	GOL	O1-C1-C2-C3
2	C	1901	GOL	O1-C1-C2-O2
2	C	1901	GOL	O1-C1-C2-C3
2	A	1902	GOL	O1-C1-C2-O2
2	G	1901	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	1902	GOL	O1-C1-C2-O2
2	A	1902	GOL	O2-C2-C3-O3
2	B	1901	GOL	O1-C1-C2-O2
2	B	1901	GOL	O1-C1-C2-C3
2	E	1901	GOL	O1-C1-C2-C3
2	C	1901	GOL	C1-C2-C3-O3
2	A	1902	GOL	C1-C2-C3-O3

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	296/414 (71%)	0.38	29 (9%) 7 9	31, 95, 181, 244	0
1	B	296/414 (71%)	0.41	23 (7%) 13 15	33, 91, 195, 244	0
1	C	296/414 (71%)	0.39	23 (7%) 13 15	36, 94, 177, 244	0
1	D	296/414 (71%)	0.46	32 (10%) 5 6	26, 95, 185, 244	0
1	E	296/414 (71%)	0.36	25 (8%) 11 13	37, 91, 183, 245	0
1	F	296/414 (71%)	0.45	35 (11%) 4 5	29, 91, 180, 244	0
1	G	296/414 (71%)	0.39	26 (8%) 10 11	36, 93, 188, 244	0
1	H	296/414 (71%)	0.40	25 (8%) 11 13	36, 93, 187, 244	0
All	All	2368/3312 (71%)	0.40	218 (9%) 9 11	26, 93, 186, 245	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1850	GLU	8.5
1	G	1663	ASN	7.4
1	B	1775	VAL	7.1
1	D	1849	LEU	6.8
1	E	1663	ASN	6.6
1	H	1755	ALA	6.1
1	A	1649	HIS	5.9
1	H	1784	GLU	5.9
1	G	1762	ALA	5.6
1	B	1784	GLU	5.3
1	B	1663	ASN	5.2
1	H	1450	PRO	5.2
1	E	1755	ALA	5.1
1	C	1754	LEU	4.9
1	F	1761	LEU	4.8
1	G	1587	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	1615	SER	4.8
1	E	1761	LEU	4.7
1	B	1837	LYS	4.7
1	D	1649	HIS	4.7
1	F	1838	ALA	4.6
1	B	1762	ALA	4.6
1	D	1754	LEU	4.6
1	C	1710	PHE	4.5
1	A	1775	VAL	4.5
1	B	1587	LEU	4.5
1	D	1690	ASN	4.5
1	D	1543	THR	4.4
1	F	1755	ALA	4.4
1	E	1520	ALA	4.4
1	E	1777	TRP	4.4
1	F	1562	PRO	4.3
1	H	1849	LEU	4.3
1	C	1649	HIS	4.3
1	H	1761	LEU	4.3
1	F	1775	VAL	4.2
1	E	1762	ALA	4.2
1	B	1683	CYS	4.2
1	F	1850	GLU	4.2
1	E	1784	GLU	4.2
1	B	1755	ALA	4.2
1	E	1838	ALA	4.1
1	D	1837	LYS	4.1
1	B	1777	TRP	4.0
1	H	1762	ALA	4.0
1	C	1849	LEU	3.9
1	E	1849	LEU	3.9
1	H	1763	ALA	3.8
1	G	1761	LEU	3.8
1	C	1755	ALA	3.8
1	H	1775	VAL	3.8
1	E	1450	PRO	3.7
1	E	1587	LEU	3.7
1	G	1784	GLU	3.7
1	D	1541	THR	3.6
1	G	1520	ALA	3.6
1	B	1839	VAL	3.6
1	F	1849	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	1683	CYS	3.5
1	A	1663	ASN	3.5
1	C	1663	ASN	3.5
1	F	1572	LEU	3.5
1	H	1838	ALA	3.5
1	C	1838	ALA	3.5
1	A	1710	PHE	3.5
1	H	1847	GLU	3.5
1	D	1664	VAL	3.4
1	D	1761	LEU	3.4
1	B	1754	LEU	3.4
1	H	1837	LYS	3.4
1	G	1834	LEU	3.4
1	B	1761	LEU	3.4
1	D	1838	ALA	3.4
1	G	1777	TRP	3.4
1	H	1587	LEU	3.3
1	C	1637	LEU	3.3
1	F	1837	LYS	3.3
1	A	1850	GLU	3.3
1	D	1832	ASN	3.3
1	A	1796	LEU	3.3
1	G	1519	VAL	3.3
1	E	1519	VAL	3.2
1	G	1754	LEU	3.2
1	C	1837	LYS	3.2
1	F	1591	ALA	3.2
1	H	1590	TRP	3.2
1	F	1774	GLU	3.2
1	A	1837	LYS	3.2
1	A	1757	LEU	3.1
1	D	1637	LEU	3.1
1	A	1562	PRO	3.1
1	F	1796	LEU	3.1
1	H	1764	CYS	3.1
1	G	1837	LYS	3.0
1	A	1797	ARG	3.0
1	B	1849	LEU	3.0
1	F	1771	ASP	3.0
1	A	1754	LEU	3.0
1	F	1450	PRO	3.0
1	A	1637	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	1615	SER	2.9
1	F	1649	HIS	2.9
1	G	1775	VAL	2.9
1	E	1683	CYS	2.9
1	D	1562	PRO	2.9
1	F	1764	CYS	2.9
1	G	1616	GLY	2.9
1	F	1757	LEU	2.9
1	G	1797	ARG	2.9
1	F	1471	PHE	2.9
1	B	1590	TRP	2.8
1	D	1521	ARG	2.8
1	D	1758	THR	2.8
1	G	1849	LEU	2.8
1	A	1494	LYS	2.8
1	D	1773	PRO	2.8
1	A	1838	ALA	2.8
1	F	1754	LEU	2.8
1	E	1832	ASN	2.8
1	B	1771	ASP	2.8
1	A	1849	LEU	2.8
1	F	1615	SER	2.8
1	C	1761	LEU	2.8
1	C	1699	VAL	2.7
1	G	1670	ASN	2.7
1	H	1839	VAL	2.7
1	G	1662	THR	2.7
1	E	1834	LEU	2.7
1	A	1777	TRP	2.7
1	B	1776	THR	2.7
1	A	1521	ARG	2.7
1	F	1487	PHE	2.7
1	B	1450	PRO	2.7
1	H	1777	TRP	2.6
1	D	1710	PHE	2.6
1	D	1774	GLU	2.6
1	F	1521	ARG	2.6
1	A	1776	THR	2.6
1	F	1710	PHE	2.6
1	E	1563	GLY	2.6
1	E	1662	THR	2.6
1	D	1777	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	1797	ARG	2.5
1	D	1471	PHE	2.5
1	A	1471	PHE	2.5
1	A	1755	ALA	2.5
1	D	1465	HIS	2.5
1	G	1755	ALA	2.5
1	C	1487	PHE	2.5
1	H	1683	CYS	2.5
1	H	1663	ASN	2.5
1	B	1788	TYR	2.5
1	B	1834	LEU	2.5
1	E	1493	ALA	2.5
1	A	1509	GLN	2.4
1	F	1663	ASN	2.4
1	G	1690	ASN	2.4
1	G	1676	CYS	2.4
1	C	1791	ARG	2.4
1	B	1758	THR	2.4
1	C	1562	PRO	2.4
1	A	1543	THR	2.4
1	F	1683	CYS	2.4
1	G	1493	ALA	2.4
1	H	1633	ALA	2.4
1	F	1789	TRP	2.4
1	C	1744	SER	2.4
1	G	1450	PRO	2.4
1	A	1792	GLY	2.3
1	A	1572	LEU	2.3
1	A	1752	HIS	2.3
1	F	1617	ASP	2.3
1	B	1832	ASN	2.3
1	D	1755	ALA	2.3
1	D	1663	ASN	2.3
1	G	1661	ARG	2.3
1	F	1465	HIS	2.3
1	C	1521	ARG	2.3
1	C	1747	GLU	2.3
1	C	1796	LEU	2.3
1	D	1572	LEU	2.3
1	E	1676	CYS	2.3
1	E	1754	LEU	2.2
1	C	1471	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	1775	VAL	2.2
1	E	1718	VAL	2.2
1	H	1691	ILE	2.2
1	H	1652	ALA	2.2
1	B	1794	LYS	2.2
1	C	1700	ALA	2.2
1	E	1660	ARG	2.2
1	F	1787	GLU	2.1
1	B	1718	VAL	2.1
1	H	1676	CYS	2.1
1	G	1850	GLU	2.1
1	A	1833	ARG	2.1
1	D	1771	ASP	2.1
1	F	1791	ARG	2.1
1	D	1686	PRO	2.1
1	C	1516	ASP	2.1
1	E	1661	ARG	2.1
1	A	1761	LEU	2.1
1	A	1591	ALA	2.1
1	A	1763	ALA	2.1
1	C	1668	ALA	2.1
1	F	1541	THR	2.1
1	D	1669	GLU	2.0
1	H	1718	VAL	2.0
1	D	1796	LEU	2.0
1	D	1487	PHE	2.0
1	F	1777	TRP	2.0
1	F	1637	LEU	2.0
1	C	1690	ASN	2.0
1	D	1759	ARG	2.0
1	H	1833	ARG	2.0
1	H	1776	THR	2.0
1	G	1543	THR	2.0
1	F	1759	ARG	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. 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
2	GOL	C	1901	6/6	0.50	0.56	52,60,67,67	0
2	GOL	B	1902	6/6	0.56	1.60	83,99,114,117	0
2	GOL	A	1901	6/6	0.59	0.46	54,61,63,64	0
2	GOL	A	1902	6/6	0.60	1.62	76,85,101,127	0
2	GOL	D	1901	6/6	0.61	0.79	77,86,98,114	0
2	GOL	B	1901	6/6	0.64	0.50	53,69,79,80	0
2	GOL	E	1901	6/6	0.65	0.49	73,86,103,109	0
2	GOL	G	1901	6/6	0.72	1.19	60,64,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.