Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 11:58 am BST

PDB ID	:	5N7D
Title	:	MAGI-1 complexed with a RSK1 peptide
Authors	:	Gogl, G.; Nyitray, L.
Deposited on	:	2017-02-20
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.227
Clashscore		4
Ramachandran outliers		0.8%
Sidechain outliers		1.6%
RSRZ outliers		13.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
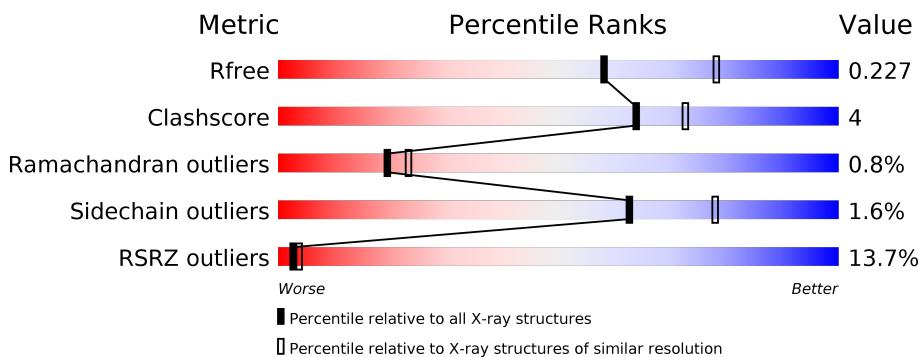
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	427	% 90% 8% ·
1	B	427	25% 85% 13% ··
2	C	49	6% · · 92%
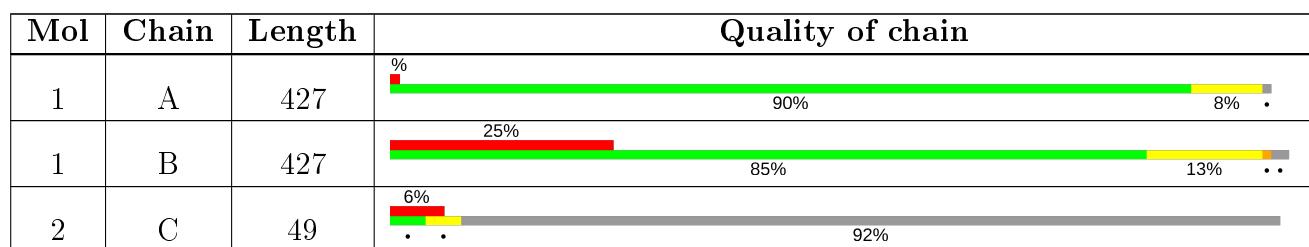
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6750 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 Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1,Annexin A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total 3341	C 2106	N 574	O 647	S 14	0	0	0
1	B	420	Total 3123	C 1959	N 542	O 610	S 12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	GLY	-	expression tag	UNP Q96QZ7
A	453	SER	-	expression tag	UNP Q96QZ7
A	454	MET	-	expression tag	UNP Q96QZ7
A	559	GLY	-	linker	UNP Q96QZ7
A	560	SER	-	linker	UNP Q96QZ7
A	605	GLU	ALA	conflict	UNP P07355
B	452	GLY	-	expression tag	UNP Q96QZ7
B	453	SER	-	expression tag	UNP Q96QZ7
B	454	MET	-	expression tag	UNP Q96QZ7
B	559	GLY	-	linker	UNP Q96QZ7
B	560	SER	-	linker	UNP Q96QZ7
B	605	GLU	ALA	conflict	UNP P07355

- Molecule 2 is a protein called Ribosomal protein S6 kinase alpha-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total 29	C 17	N 4	O 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	687	GLY	-	expression tag	UNP Q15418

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![Worldwide Protein Data Bank logo]

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Chain	Residue	Modelled	Actual	Comment	Reference
C	688	SER	HIS	conflict	UNP Q15418

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
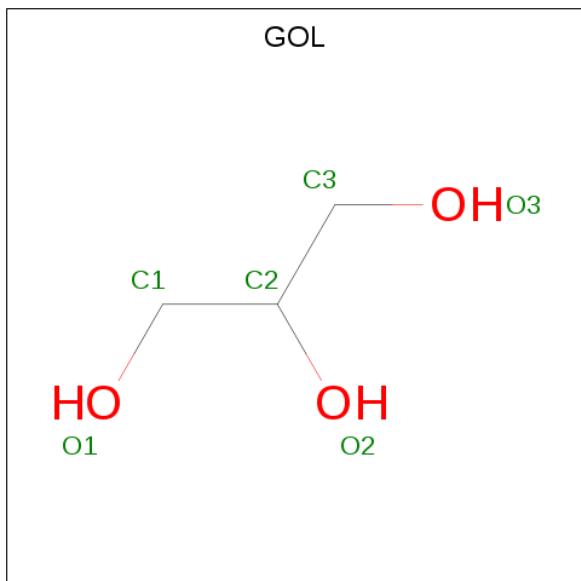
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	Ca 3	0	0
4	A	4	Total 4	Ca 4	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	195	Total O 195 195	0	0
5	B	25	Total O 25 25	0	0

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: Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1,Annexin A2

Chain A:

• Molecule 1: Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1,Annexin A2

Chain B:
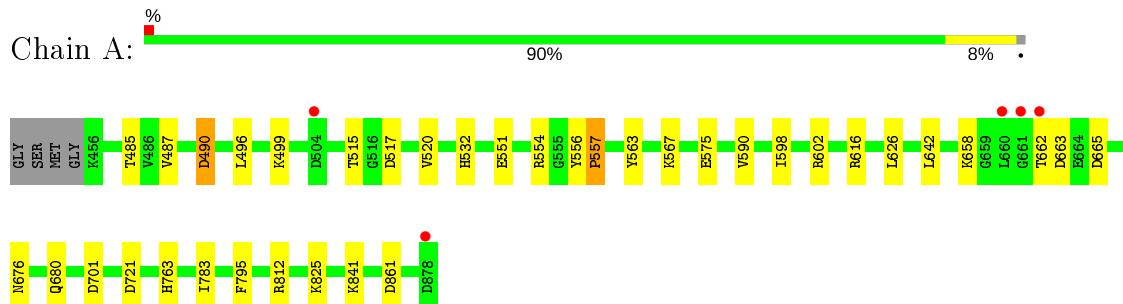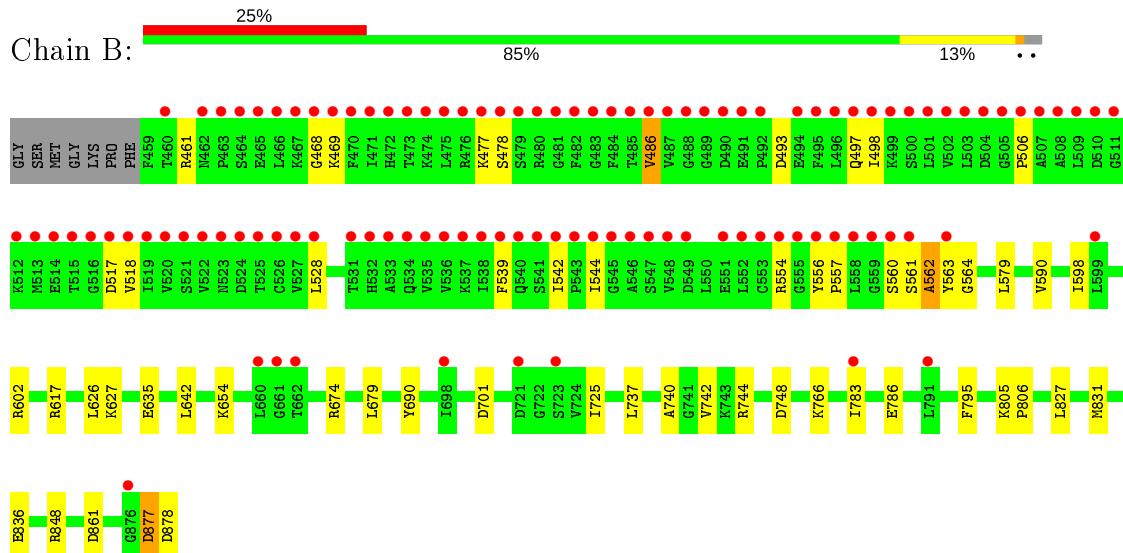
• Molecule 2: Ribosomal protein S6 kinase alpha-1

Chain C:
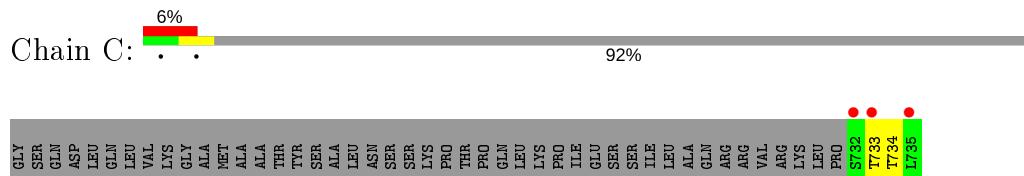
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.81Å 60.68Å 99.71Å 90.00° 98.81° 90.00°	Depositor
Resolution (Å)	49.27 – 2.30 49.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-2.30) 99.9 (49.27-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, R_{free}	0.191 , 0.227 0.191 , 0.227	Depositor DCC
R_{free} test set	2466 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.2	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6750	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CA

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	0.31	1/3392 (0.0%)	0.43	1/4562 (0.0%)
1	B	0.26	0/3167	0.42	1/4281 (0.0%)
2	C	0.18	0/28	0.43	0/36
All	All	0.29	1/6587 (0.0%)	0.42	2/8879 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	PRO	N-CD	5.21	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	556	TYR	C-N-CD	6.06	141.13	128.40
1	A	556	TYR	C-N-CD	5.85	140.68	128.40

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	3341	0	3366	20	0
1	B	3123	0	2959	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	29	0	29	2	0
3	A	18	0	24	3	0
3	B	12	0	16	0	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
5	A	195	0	0	7	1
5	B	25	0	0	2	0
All	All	6750	0	6394	54	1

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 (54) 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:468:GLY:HA3	1:B:554:ARG:O	1.47	1.11
1:A:825:LYS:NZ	5:A:1001:HOH:O	1.89	1.05
1:B:561:SER:CB	1:B:836:GLU:O	2.14	0.94
1:B:737:LEU:O	5:B:1001:HOH:O	1.89	0.90
1:A:812:ARG:NH1	5:A:1002:HOH:O	2.02	0.89
1:B:561:SER:O	1:B:564:GLY:N	2.12	0.75
1:A:515:THR:O	5:A:1003:HOH:O	2.07	0.71
1:A:721:ASP:OD1	5:A:1004:HOH:O	2.07	0.71
1:A:662:THR:OG1	1:A:701:ASP:OD2	2.08	0.70
1:A:532:HIS:NE2	2:C:733:THR:OG1	2.27	0.66
1:B:486:VAL:HG21	1:B:498:ILE:HA	1.78	0.64
1:B:744:ARG:NH1	1:B:748:ASP:HB2	2.15	0.61
1:A:676:ASN:O	1:A:680:GLN:HG2	2.01	0.59
1:B:725:ILE:HD13	1:B:766:LYS:HE2	1.84	0.59
1:B:848:ARG:NH2	5:B:1002:HOH:O	2.35	0.58
1:B:539:PHE:HA	1:B:542:ILE:HD12	1.86	0.58
3:A:902:GOL:O3	5:A:1006:HOH:O	2.17	0.57
1:A:490:ASP:N	1:A:490:ASP:OD1	2.36	0.57
1:B:477:LYS:NZ	1:B:539:PHE:O	2.26	0.57
1:B:783:ILE:HD13	1:B:795:PHE:HB3	1.89	0.54
1:A:485:THR:HG22	2:C:734:THR:HA	1.88	0.53
1:B:561:SER:O	1:B:563:TYR:N	2.42	0.53
1:B:561:SER:O	1:B:562:ALA:C	2.48	0.52
1:B:498:ILE:HD11	1:B:517:ASP:HB2	1.92	0.51
1:A:783:ILE:HD13	1:A:795:PHE:HB3	1.92	0.51
1:B:468:GLY:HA3	1:B:554:ARG:C	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:VAL:HA	1:B:786:GLU:OE2	2.11	0.50
1:A:567:LYS:NZ	5:A:1014:HOH:O	2.41	0.50
1:A:626:LEU:HD12	1:A:642:LEU:HD11	1.94	0.49
1:A:575:GLU:OE2	1:A:616:ARG:NH2	2.44	0.49
1:B:740:ALA:HB1	1:B:748:ASP:HB3	1.95	0.48
1:B:805:LYS:HB3	1:B:806:PRO:HD3	1.96	0.48
1:A:487:VAL:HG13	1:A:499:LYS:HB2	1.96	0.47
1:B:877:ASP:OD1	1:B:877:ASP:N	2.48	0.47
1:B:579:LEU:HD13	1:B:617:ARG:NH1	2.30	0.47
3:A:902:GOL:H32	5:A:1055:HOH:O	2.15	0.46
1:B:461:ARG:HA	1:B:528:LEU:HB3	1.96	0.46
1:B:598:ILE:O	1:B:602:ARG:HG2	2.16	0.46
1:B:478:SER:HB2	1:B:506:PRO:HG3	1.98	0.45
1:B:469:LYS:O	1:B:554:ARG:N	2.50	0.45
1:B:477:LYS:HG2	1:B:544:ILE:HA	1.98	0.45
1:B:626:LEU:HD12	1:B:642:LEU:HD11	1.99	0.44
1:B:654:LYS:NZ	1:B:690:TYR:HB3	2.33	0.44
1:A:825:LYS:HB3	1:A:825:LYS:HE2	1.70	0.44
1:B:674:ARG:HB3	1:B:679:LEU:HG	2.00	0.44
1:A:563:TYR:CD2	1:A:841:LYS:HE3	2.53	0.43
1:B:579:LEU:HB2	1:B:617:ARG:NH2	2.33	0.43
1:B:627:LYS:HG3	1:B:635:GLU:OE2	2.19	0.42
1:A:517:ASP:OD1	1:A:554:ARG:HD3	2.20	0.42
1:B:497:GLN:HA	1:B:518:VAL:HA	2.01	0.42
1:A:520:VAL:HB	1:A:551:GLU:HG2	2.02	0.41
1:A:763:HIS:HB2	3:A:902:GOL:H2	2.02	0.41
1:A:598:ILE:O	1:A:602:ARG:HG2	2.21	0.41
1:B:827:LEU:O	1:B:831:MET:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1058:HOH:O	5:A:1164:HOH:O[4_7512]	2.12	0.08

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	421/427 (99%)	410 (97%)	9 (2%)	2 (0%)	29	35
1	B	418/427 (98%)	394 (94%)	19 (4%)	5 (1%)	13	14
2	C	2/49 (4%)	2 (100%)	0	0	100	100
All	All	841/903 (93%)	806 (96%)	28 (3%)	7 (1%)	19	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	VAL
1	A	663	ASP
1	B	493	ASP
1	B	590	VAL
1	B	562	ALA
1	B	557	PRO
1	B	560	SER

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	365/370 (99%)	359 (98%)	6 (2%)	62	78
1	B	306/370 (83%)	301 (98%)	5 (2%)	62	78
2	C	4/42 (10%)	4 (100%)	0	100	100
All	All	675/782 (86%)	664 (98%)	11 (2%)	62	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	ASP
1	A	496	LEU
1	A	557	PRO
1	A	658	LYS
1	A	665	ASP
1	A	861	ASP
1	B	486	VAL
1	B	701	ASP
1	B	861	ASP
1	B	877	ASP
1	B	878	ASP

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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
3	GOL	B	902	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	A	903	-	5,5,5	0.35	0	5,5,5	0.35	0
3	GOL	A	901	-	5,5,5	0.35	0	5,5,5	0.31	0
3	GOL	B	901	-	5,5,5	0.37	0	5,5,5	0.25	0
3	GOL	A	902	-	5,5,5	0.35	0	5,5,5	0.31	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
3	GOL	B	902	-	-	2/4/4/4	-
3	GOL	A	903	-	-	2/4/4/4	-
3	GOL	A	901	-	-	0/4/4/4	-
3	GOL	B	901	-	-	2/4/4/4	-
3	GOL	A	902	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	GOL	O1-C1-C2-C3
3	B	902	GOL	O1-C1-C2-C3
3	A	903	GOL	O1-C1-C2-O2
3	A	902	GOL	C1-C2-C3-O3
3	B	902	GOL	O1-C1-C2-O2
3	B	901	GOL	O1-C1-C2-O2
3	A	902	GOL	O1-C1-C2-O2
3	B	901	GOL	O1-C1-C2-C3
3	A	902	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GOL	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	423/427 (99%)	0.15	5 (1%)	79	83	29, 53, 86, 149	0
1	B	420/427 (98%)	1.66	108 (25%)	0	0	53, 88, 202, 254	0
2	C	4/49 (8%)	3.09	3 (75%)	0	0	116, 142, 152, 188	0
All	All	847/903 (93%)	0.91	116 (13%)	3	4	29, 71, 188, 254	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	533	ALA	18.4
1	B	554	ARG	13.6
1	B	468	GLY	12.3
1	B	470	PHE	12.2
1	B	531	THR	12.1
1	B	545	GLY	11.9
1	B	555	GLY	11.0
1	B	473	THR	9.5
1	B	556	TYR	9.5
1	B	536	VAL	9.4
1	B	546	ALA	9.2
1	B	553	CYS	9.1
1	B	482	PHE	8.8
1	B	472	HIS	8.7
1	B	535	VAL	8.6
1	B	488	GLY	8.5
1	B	558	LEU	8.3
1	B	532	HIS	8.3
1	B	511	GLY	8.0
1	B	544	ILE	7.9
1	B	502	VAL	7.8
1	B	503	LEU	7.8
1	B	534	GLN	7.8

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Mol	Chain	Res	Type	RSRZ
1	B	525	THR	7.7
1	B	489	GLY	7.7
1	B	513	MET	7.6
1	B	524	ASP	7.5
1	B	508	ALA	7.2
1	B	557	PRO	7.1
1	B	484	PHE	7.1
1	B	520	VAL	7.0
1	B	516	GLY	7.0
1	B	504	ASP	6.7
1	B	485	THR	6.7
1	B	521	SER	6.7
1	B	515	THR	6.7
1	B	490	ASP	6.6
1	B	471	ILE	6.6
1	B	496	LEU	6.6
1	B	507	ALA	6.3
1	B	483	GLY	6.3
1	B	528	LEU	6.2
1	B	497	GLN	6.2
1	B	501	LEU	6.1
1	B	547	SER	6.0
1	B	510	ASP	5.9
1	B	475	LEU	5.9
1	B	522	VAL	5.8
1	B	539	PHE	5.7
1	B	549	ASP	5.7
1	B	469	LYS	5.7
1	B	519	ILE	5.6
1	B	491	GLU	5.6
1	B	466	LEU	5.5
1	B	487	VAL	5.5
1	B	505	GLY	5.3
1	B	492	PRO	5.1
1	B	661	GLY	5.1
1	B	527	VAL	5.0
1	B	498	ILE	5.0
1	B	518	VAL	4.9
1	B	479	SER	4.9
1	B	464	SER	4.9
1	B	465	GLU	4.6
1	B	538	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	662	THR	4.5
1	B	542	ILE	4.4
1	B	552	LEU	4.3
1	B	460	THR	4.3
1	B	560	SER	4.2
1	B	463	PRO	4.1
1	B	517	ASP	4.1
2	C	735	LEU	4.1
2	C	732	SER	4.1
1	B	526	CYS	3.9
1	B	540	GLN	3.9
1	B	561	SER	3.9
1	B	509	LEU	3.9
1	B	660	LEU	3.9
1	A	660	LEU	3.8
1	B	478	SER	3.8
1	B	481	GLY	3.7
1	B	514	GLU	3.7
1	B	486	VAL	3.7
1	B	474	LYS	3.6
1	B	791	LEU	3.6
1	B	512	LYS	3.4
1	B	543	PRO	3.3
1	B	462	ASN	3.3
1	A	662	THR	3.2
1	B	541	SER	3.2
1	B	500	SER	3.1
1	B	523	ASN	3.1
1	B	467	LYS	3.1
1	B	537	LYS	3.0
1	B	476	ARG	2.9
1	B	551	GLU	2.9
1	B	495	PHE	2.7
1	B	548	VAL	2.7
1	B	876	GLY	2.7
1	B	506	PRO	2.7
1	A	878	ASP	2.6
1	A	504	ASP	2.6
2	C	733	THR	2.6
1	B	499	LYS	2.6
1	B	494	GLU	2.5
1	B	477	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	721	ASP	2.3
1	B	783	ILE	2.3
1	B	723	SER	2.3
1	B	599	LEU	2.2
1	B	698	ILE	2.2
1	B	480	ARG	2.1
1	A	661	GLY	2.1
1	B	559	GLY	2.1
1	B	563	TYR	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
4	CA	B	903	1/1	0.58	0.10	121,121,121,121	0
4	CA	A	904	1/1	0.71	0.09	89,89,89,89	0
3	GOL	B	902	6/6	0.86	0.27	75,93,99,102	0
4	CA	A	907	1/1	0.88	0.15	89,89,89,89	0
4	CA	B	904	1/1	0.90	0.08	121,121,121,121	0
3	GOL	A	902	6/6	0.92	0.22	55,68,71,78	0
3	GOL	B	901	6/6	0.93	0.17	71,76,77,83	0
3	GOL	A	903	6/6	0.93	0.14	55,57,62,64	0
4	CA	A	905	1/1	0.95	0.10	54,54,54,54	0
3	GOL	A	901	6/6	0.96	0.18	37,41,47,52	0
4	CA	A	906	1/1	0.99	0.21	36,36,36,36	0
4	CA	B	905	1/1	0.99	0.15	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.