



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:45 am BST

PDB ID : 5N7F
Title : MAGI-1 complexed with a pRSK1 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 ⓘ 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

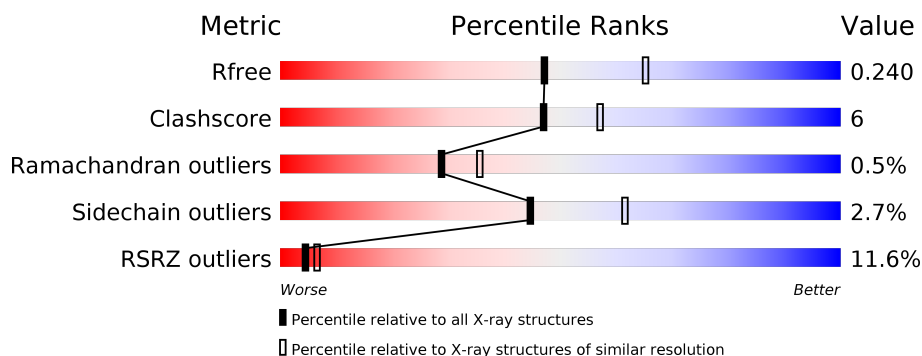
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	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 $\leq 5\%$. 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	427	<div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	B	427	<div> <div>22%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	C	49	<div> <div>8%</div> <div>88%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7311 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	C	N	O	S	0	1	0
			3338	2102	574	648	14			
1	B	416	Total	C	N	O	S	0	0	0
			3249	2041	560	634	14			

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	GLN	conflict	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	GLN	conflict	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	6	Total	C	N	O	P	0	0	0
			45	25	6	13	1			

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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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	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Ca	0	0
			4	4		
4	A	5	Total	Ca	0	0
			5	5		

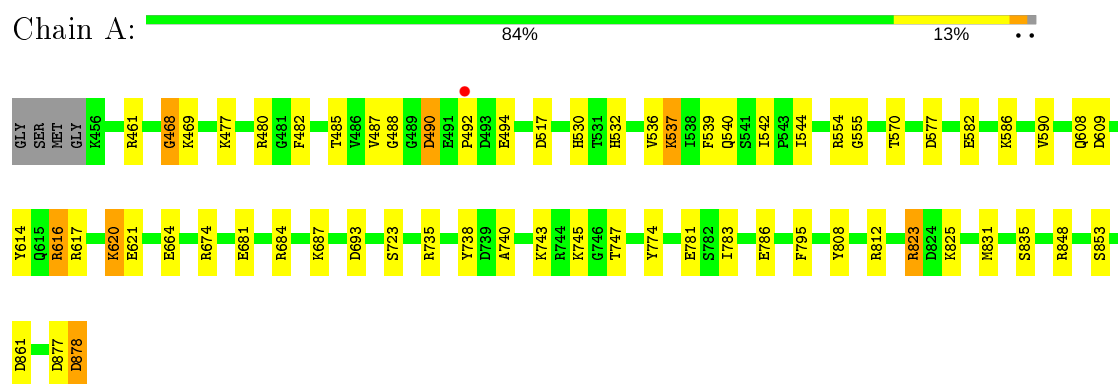
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	369	Total 369	O 369	0	0
5	B	265	Total 265	O 265	0	0

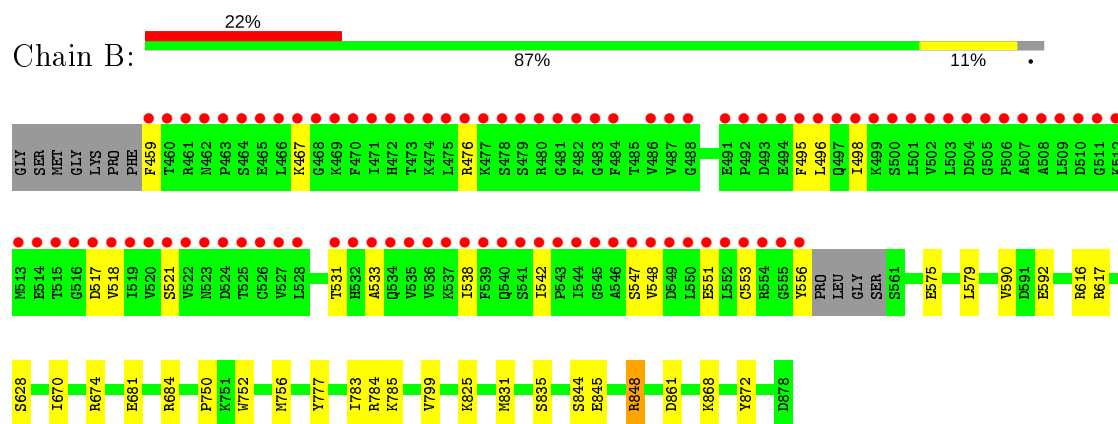
3 Residue-property plots

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.

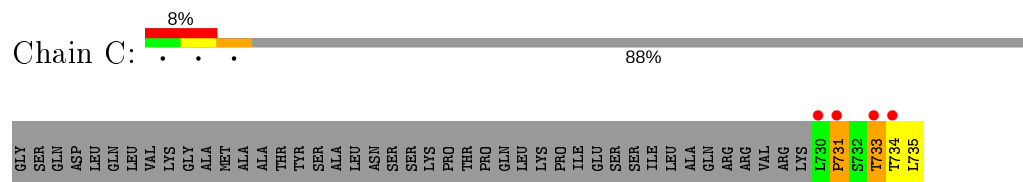
- Molecule 1: Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1, Annexin A2



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



- Molecule 2: Ribosomal protein S6 kinase alpha-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.15Å 98.56Å 200.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 2.30 49.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.73-2.30) 100.0 (49.74-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, R_{free}	0.186 , 0.240 0.186 , 0.240	Depositor DCC
R_{free} test set	2613 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7311	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.32% 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, CA, SEP

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	0.44	0/3389	0.57	0/4560
1	B	0.36	0/3296	0.52	0/4436
2	C	0.38	0/34	0.71	0/44
All	All	0.40	0/6719	0.55	0/9040

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

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	3338	0	3345	55	0
1	B	3249	0	3217	27	0
2	C	45	0	36	8	0
3	A	18	0	24	0	0
3	B	18	0	24	1	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
5	A	369	0	0	21	0
5	B	265	0	0	6	0
All	All	7311	0	6646	83	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 6.

All (83) 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:A:681:GLU:OE2	1:A:684:ARG:NH1	1.95	1.00
1:A:492:PRO:O	5:A:1001:HOH:O	1.80	0.99
1:A:664:GLU:OE2	5:A:1002:HOH:O	1.88	0.92
1:B:476:ARG:HG2	1:B:547:SER:HB3	1.63	0.79
1:A:823:ARG:NH1	1:A:825:LYS:H	1.81	0.79
1:A:608:GLN:OE1	5:A:1003:HOH:O	2.03	0.76
1:A:848:ARG:NH1	5:A:1010:HOH:O	2.16	0.76
1:A:609:ASP:OD2	5:A:1004:HOH:O	2.04	0.74
1:A:480:ARG:NH2	5:A:1013:HOH:O	2.19	0.74
1:A:823:ARG:HH11	1:A:825:LYS:HB2	1.53	0.73
1:A:490:ASP:OD2	2:C:731:PRO:HB3	1.92	0.70
1:A:878:ASP:OD1	5:A:1006:HOH:O	2.11	0.68
1:A:577:ASP:OD1	5:A:1008:HOH:O	2.12	0.67
1:A:781:GLU:OE2	5:A:1007:HOH:O	2.12	0.67
1:A:488:GLY:H	2:C:731:PRO:HG2	1.61	0.65
1:B:575:GLU:OE1	1:B:616:ARG:NH2	2.30	0.64
1:A:485:THR:HG22	2:C:734:THR:HA	1.79	0.63
1:A:823:ARG:HH11	1:A:825:LYS:CB	2.13	0.59
1:A:544:ILE:O	5:A:1011:HOH:O	2.17	0.59
1:A:517:ASP:OD1	1:A:554:ARG:HD3	2.02	0.58
1:A:582:GLU:OE1	1:A:586:LYS:NZ	2.37	0.57
1:A:554:ARG:NH1	5:A:1017:HOH:O	2.27	0.57
1:A:616:ARG:NH1	5:A:1027:HOH:O	2.37	0.57
1:A:745:LYS:NZ	5:A:1025:HOH:O	2.36	0.57
1:B:831:MET:O	1:B:835:SER:HB3	2.05	0.56
1:A:539:PHE:CD2	2:C:735:LEU:HD13	2.40	0.56
1:A:532:HIS:NE2	2:C:733:THR:OG1	2.25	0.56
1:B:531:THR:HG23	1:B:533:ALA:H	1.71	0.55
1:B:518:VAL:HG23	1:B:553:CYS:HB3	1.89	0.54
1:A:738:TYR:CE2	1:A:743:LYS:HD3	2.43	0.54
1:A:848:ARG:HD2	5:A:1326:HOH:O	2.07	0.54
1:A:738:TYR:HE2	1:A:743:LYS:HD3	1.73	0.53
1:A:823:ARG:HB2	5:A:1290:HOH:O	2.08	0.53
1:B:681:GLU:OE1	1:B:684:ARG:NH1	2.42	0.53
1:B:825:LYS:HG2	5:B:1137:HOH:O	2.08	0.53
1:B:825:LYS:NZ	5:B:1003:HOH:O	2.14	0.52
3:B:901:GOL:O1	5:B:1001:HOH:O	1.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ARG:O	5:A:1012:HOH:O	2.18	0.52
1:B:784:ARG:HD3	5:B:1100:HOH:O	2.10	0.52
1:B:496:LEU:O	1:B:518:VAL:HA	2.09	0.51
1:A:812:ARG:NH1	5:A:1031:HOH:O	2.41	0.51
1:B:868:LYS:HE3	1:B:872:TYR:CZ	2.46	0.51
1:A:783:ILE:HD13	1:A:795:PHE:HB3	1.95	0.48
1:B:777:TYR:CZ	1:B:785:LYS:HE3	2.49	0.48
1:B:845:GLU:OE2	1:B:848:ARG:NH1	2.46	0.48
1:B:467:LYS:H	1:B:556:TYR:HE2	1.62	0.48
1:A:747:THR:HB	1:A:786:GLU:OE2	2.13	0.48
1:A:853:SER:OG	1:A:878:ASP:OD1	2.31	0.48
1:B:538:ILE:O	1:B:542:ILE:HD12	2.14	0.48
1:A:490:ASP:OD1	2:C:731:PRO:HG3	2.14	0.47
1:B:459:PHE:HA	1:B:495:PHE:CZ	2.48	0.47
1:A:555:GLY:O	1:A:570:THR:HG22	2.15	0.46
1:A:823:ARG:HE	1:A:825:LYS:HB3	1.81	0.45
1:A:620[A]:LYS:HD3	1:A:621:GLU:N	2.32	0.45
1:A:539:PHE:HD2	2:C:735:LEU:HD13	1.81	0.45
1:A:537:LYS:HD3	1:A:537:LYS:HA	1.82	0.45
1:A:735:ARG:HG2	1:A:774:TYR:CZ	2.52	0.45
1:B:752:TRP:O	1:B:756:MET:HG3	2.17	0.45
1:A:823:ARG:CZ	1:A:825:LYS:H	2.30	0.45
1:B:592:GLU:OE1	5:B:1004:HOH:O	2.21	0.44
1:B:521:SER:OG	1:B:551:GLU:OE2	2.31	0.44
1:A:468:GLY:HA3	1:A:554:ARG:O	2.18	0.43
1:A:808:TYR:CZ	1:A:812:ARG:HD2	2.53	0.43
1:B:579:LEU:HD13	1:B:617:ARG:CZ	2.48	0.43
1:A:745:LYS:HA	1:A:745:LYS:HD3	1.77	0.43
1:B:670:ILE:O	1:B:674:ARG:HG2	2.19	0.43
1:B:750:PRO:HB2	5:B:1008:HOH:O	2.19	0.43
1:A:620[A]:LYS:HA	1:A:620[A]:LYS:HE2	2.01	0.42
1:B:521:SER:OG	1:B:551:GLU:HB3	2.19	0.42
1:B:868:LYS:HA	1:B:868:LYS:HD2	1.62	0.42
1:A:477:LYS:HD3	1:A:542:ILE:O	2.19	0.42
1:A:461:ARG:NH1	5:A:1039:HOH:O	2.52	0.42
1:A:536:VAL:O	1:A:540:GLN:HG3	2.20	0.42
1:A:536:VAL:HG22	2:C:735:LEU:HD21	2.02	0.41
1:B:498:ILE:HG12	1:B:517:ASP:O	2.20	0.41
1:A:614:TYR:OH	5:A:1005:HOH:O	2.05	0.41
1:A:687:LYS:HD2	1:A:693:ASP:OD1	2.19	0.41
1:B:783:ILE:HD11	1:B:799:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LYS:HD2	1:A:482:PHE:CE2	2.56	0.41
1:A:740:ALA:HB2	5:A:1181:HOH:O	2.20	0.41
1:A:831:MET:O	1:A:835:SER:HB3	2.21	0.41
1:B:542:ILE:HD13	1:B:548:VAL:CG1	2.50	0.41
1:A:735:ARG:NH2	5:A:1019:HOH:O	2.29	0.41

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	422/427 (99%)	411 (97%)	9 (2%)	2 (0%)	29	35
1	B	412/427 (96%)	398 (97%)	13 (3%)	1 (0%)	47	58
2	C	3/49 (6%)	2 (67%)	0	1 (33%)	0	0
All	All	837/903 (93%)	811 (97%)	22 (3%)	4 (0%)	29	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	VAL
1	B	590	VAL
2	C	731	PRO
1	A	468	GLY

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	363/370 (98%)	348 (96%)	15 (4%)	30	43
1	B	348/370 (94%)	344 (99%)	4 (1%)	73	86
2	C	4/41 (10%)	3 (75%)	1 (25%)	0	0
All	All	715/781 (92%)	695 (97%)	20 (3%)	44	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	LYS
1	A	487	VAL
1	A	490	ASP
1	A	494	GLU
1	A	530	HIS
1	A	537	LYS
1	A	616	ARG
1	A	617	ARG
1	A	620[A]	LYS
1	A	620[B]	LYS
1	A	723	SER
1	A	823	ARG
1	A	861	ASP
1	A	877	ASP
1	A	878	ASP
1	B	628	SER
1	B	844	SER
1	B	848	ARG
1	B	861	ASP
2	C	733	THR

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 ⓘ

1 non-standard protein/DNA/RNA residue 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	SEP	C	732	2	8,9,10	1.62	1 (12%)	8,12,14	1.55	1 (12%)

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	SEP	C	732	2	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	732	SEP	P-O1P	3.50	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	732	SEP	OG-CB-CA	3.32	111.38	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	732	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	A	903	-	5,5,5	0.32	0	5,5,5	0.49	0
3	GOL	B	901	-	5,5,5	0.37	0	5,5,5	0.62	0
3	GOL	B	902	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	A	902	-	5,5,5	0.35	0	5,5,5	0.29	0
3	GOL	A	901	-	5,5,5	0.34	0	5,5,5	0.54	0
3	GOL	B	903	-	5,5,5	0.43	0	5,5,5	0.18	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	A	903	-	-	2/4/4/4	-
3	GOL	B	901	-	-	0/4/4/4	-
3	GOL	B	902	-	-	3/4/4/4	-
3	GOL	A	902	-	-	2/4/4/4	-
3	GOL	A	901	-	-	0/4/4/4	-
3	GOL	B	903	-	-	2/4/4/4	-

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	C1-C2-C3-O3
3	A	902	GOL	O1-C1-C2-C3

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	GOL	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	423/427 (99%)	-0.40	1 (0%) 95 96	18, 39, 70, 122	0
1	B	416/427 (97%)	0.62	93 (22%) 0 1	22, 40, 164, 184	0
2	C	5/49 (10%)	3.42	4 (80%) 0 0	72, 97, 129, 148	0
All	All	844/903 (93%)	0.13	98 (11%) 4 6	18, 39, 153, 184	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	468	GLY	10.4
2	C	730	LEU	9.2
1	B	503	LEU	8.5
1	B	471	ILE	8.0
1	B	533	ALA	7.8
1	B	482	PHE	7.8
1	B	470	PHE	7.7
1	B	475	LEU	7.0
1	B	509	LEU	6.9
1	B	535	VAL	6.7
1	B	496	LEU	6.5
1	B	472	HIS	6.4
1	B	501	LEU	6.4
1	B	550	LEU	6.3
1	B	511	GLY	6.3
1	B	483	GLY	6.2
1	B	534	GLN	6.2
1	B	541	SER	6.2
1	B	498	ILE	6.0
1	B	549	ASP	6.0
1	B	484	PHE	6.0
1	B	488	GLY	5.9
1	B	505	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	504	ASP	5.6
1	B	553	CYS	5.6
1	B	524	ASP	5.5
1	B	502	VAL	5.4
1	B	552	LEU	5.4
1	B	467	LYS	5.3
1	B	554	ARG	5.1
1	B	481	GLY	5.1
1	B	548	VAL	4.9
1	B	497	GLN	4.9
1	B	538	ILE	4.8
1	B	479	SER	4.8
1	B	478	SER	4.7
1	B	545	GLY	4.6
1	B	528	LEU	4.6
1	B	522	VAL	4.6
1	B	493	ASP	4.5
1	B	516	GLY	4.5
1	B	464	SER	4.4
1	B	459	PHE	4.3
1	B	514	GLU	4.3
1	B	536	VAL	4.3
1	B	460	THR	4.3
1	B	556	TYR	4.1
1	B	508	ALA	4.0
1	B	477	LYS	4.0
1	B	542	ILE	4.0
1	B	539	PHE	4.0
1	B	466	LEU	4.0
1	B	473	THR	3.9
1	B	532	HIS	3.9
1	B	555	GLY	3.9
1	B	531	THR	3.8
1	B	544	ILE	3.7
1	B	506	PRO	3.7
1	B	519	ILE	3.7
1	B	487	VAL	3.5
1	B	495	PHE	3.4
1	B	523	ASN	3.4
1	B	551	GLU	3.4
1	B	513	MET	3.4
1	B	465	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	521	SER	3.2
1	B	492	PRO	3.2
1	B	510	ASP	3.2
1	B	500	SER	3.1
2	C	733	THR	3.1
1	B	512	LYS	3.1
1	B	480	ARG	3.1
1	B	515	THR	3.1
1	B	507	ALA	3.1
1	B	543	PRO	3.0
1	B	525	THR	3.0
1	B	547	SER	2.9
1	B	486	VAL	2.9
1	B	518	VAL	2.9
1	B	469	LYS	2.9
1	B	520	VAL	2.9
1	B	494	GLU	2.8
1	B	476	ARG	2.8
1	B	526	CYS	2.7
1	B	491	GLU	2.5
1	B	546	ALA	2.5
1	B	527	VAL	2.4
1	B	499	LYS	2.4
1	B	540	GLN	2.3
2	C	731	PRO	2.3
1	A	492	PRO	2.3
2	C	734	THR	2.1
1	B	537	LYS	2.1
1	B	517	ASP	2.1
1	B	461	ARG	2.1
1	B	462	ASN	2.1
1	B	463	PRO	2.1
1	B	474	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SEP	C	732	10/11	0.77	0.31	119,140,151,153	0

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(\AA^2)	Q<0.9
4	CA	A	905	1/1	0.87	0.05	71,71,71,71	0
3	GOL	B	902	6/6	0.90	0.14	32,50,60,62	0
4	CA	B	904	1/1	0.90	0.22	118,118,118,118	0
3	GOL	A	902	6/6	0.94	0.14	44,55,64,65	0
4	CA	A	908	1/1	0.94	0.17	97,97,97,97	0
4	CA	B	907	1/1	0.95	0.10	81,81,81,81	0
3	GOL	A	903	6/6	0.96	0.12	37,39,46,46	0
3	GOL	B	903	6/6	0.97	0.18	30,46,54,57	0
3	GOL	B	901	6/6	0.98	0.14	19,28,33,34	0
4	CA	A	904	1/1	0.98	0.10	42,42,42,42	0
3	GOL	A	901	6/6	0.98	0.12	23,35,37,42	0
4	CA	B	905	1/1	0.99	0.10	37,37,37,37	0
4	CA	A	906	1/1	0.99	0.12	32,32,32,32	0
4	CA	B	906	1/1	0.99	0.20	29,29,29,29	0
4	CA	A	907	1/1	0.99	0.10	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.