Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 07:22 pm GMT

PDB ID	:	6TWY
Title	:	MAGI1_2 complexed with a phosphomimetic RSK1 peptide
Authors	:	Gogl, G.; Cousido-Siah, A.; Trave, G.
Deposited on	:	2020-01-13
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

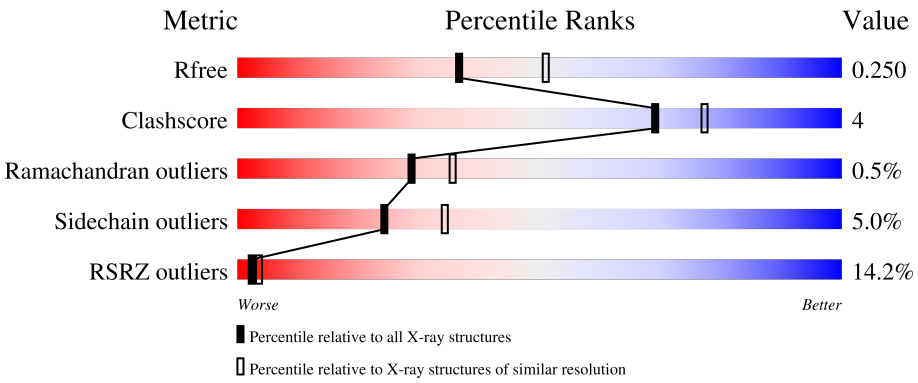
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	21% 86% 12% ••
1	B	427	7% 87% 11% ••
2	C	11	9% 27% 9% 9% 55%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6892 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
			Total	C	N	O	S			
1	A	421	3338	2097	571	656	14	0	4	0
1	B	421	3326	2091	571	650	14	0	1	0

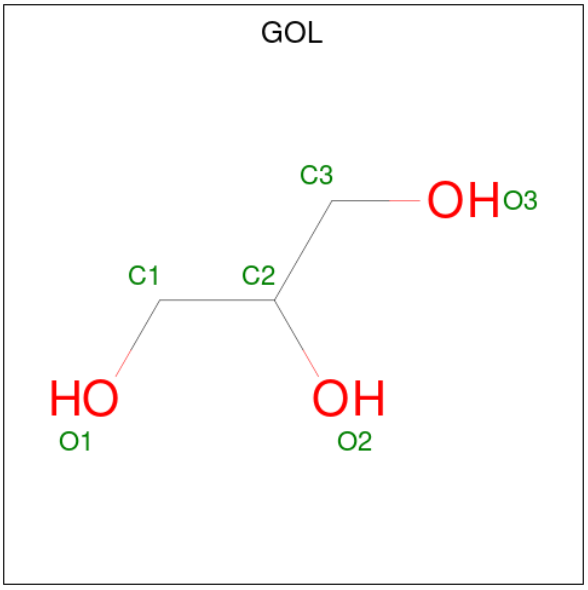
There are 18 discrepancies between the modelled and reference sequences:

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	455	GLY	-	expression tag	UNP Q96QZ7
A	456	LYS	-	expression tag	UNP Q96QZ7
A	457	PRO	-	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	455	GLY	-	expression tag	UNP Q96QZ7
B	456	LYS	-	expression tag	UNP Q96QZ7
B	457	PRO	-	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 Phosphomimetic RSK1 peptide.

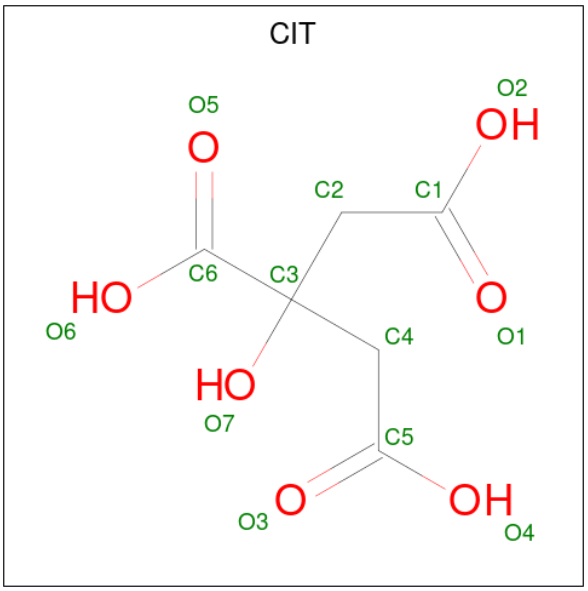
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	39	24	5	10	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Ca 5 5	0	0
5	B	6	Total Ca 6 6	0	0

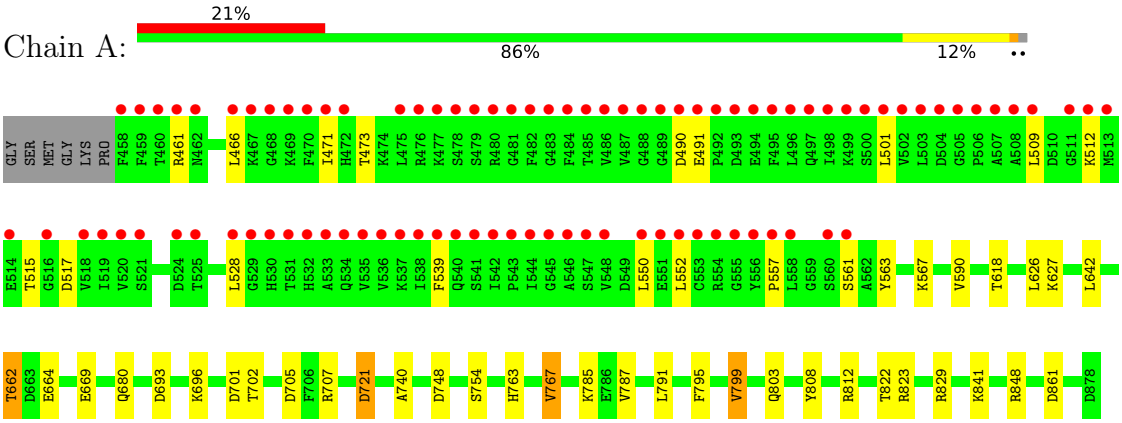
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	58	Total O 58 58	0	0
6	B	63	Total O 63 63	0	0

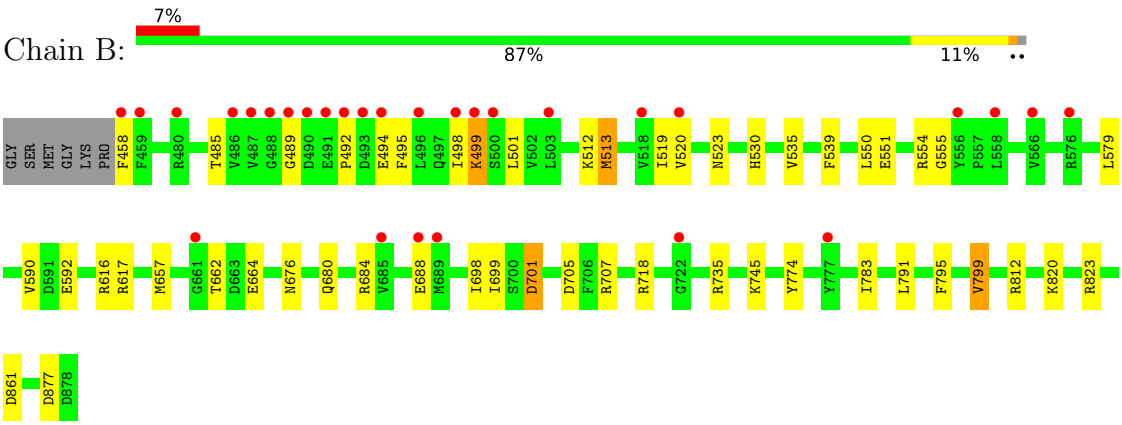
3 Residue-property plots (i)

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

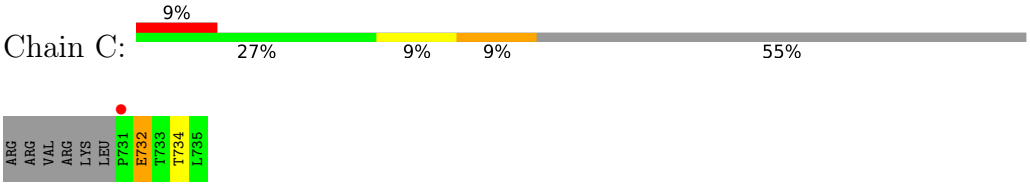
• Molecule 1: Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1,Annexin A2



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



• Molecule 2: Phosphomimetic RSK1 peptide



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.45Å 96.38Å 198.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.19 – 2.30 48.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.19-2.30) 99.0 (48.19-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.205 , 0.250 0.204 , 0.250	Depositor DCC
R_{free} test set	2556 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6892	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, CIT

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	0.30	0/3388	0.45	0/4562
1	B	0.31	0/3376	0.46	0/4542
2	C	0.19	0/39	0.42	0/51
All	All	0.30	0/6803	0.45	0/9155

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	3338	0	3306	23	0
1	B	3326	0	3323	26	0
2	C	39	0	38	2	0
3	A	12	0	16	0	0
3	B	6	0	8	0	0
4	A	13	0	5	1	0
4	B	26	0	10	1	0
5	A	5	0	0	0	0
5	B	6	0	0	0	0
6	A	58	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	63	0	0	3	0
All	All	6892	0	6706	50	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 (50) 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:520:VAL:HB	1:B:551:GLU:HG2	1.60	0.81
1:A:721[A]:ASP:OD1	1:A:721[A]:ASP:N	2.15	0.79
1:A:785:LYS:NZ	6:A:1001:HOH:O	2.20	0.75
1:B:684:ARG:NH1	1:B:688:GLU:OE1	2.23	0.71
1:B:795:PHE:O	1:B:799:VAL:HG12	1.89	0.71
1:B:499:LYS:NZ	2:C:732:GLU:OE2	2.20	0.69
1:B:555:GLY:N	6:B:1005:HOH:O	2.29	0.66
1:A:561:SER:O	1:A:567:LYS:NZ	2.28	0.65
1:B:498:ILE:HD11	1:B:519:ILE:HD11	1.80	0.63
1:A:823:ARG:NH1	6:A:1003:HOH:O	2.31	0.63
1:B:554:ARG:HA	6:B:1005:HOH:O	1.98	0.62
1:B:823:ARG:NH1	6:B:1006:HOH:O	2.34	0.59
1:B:485:THR:HG22	2:C:734:THR:HA	1.84	0.59
1:A:848:ARG:NH2	6:A:1007:HOH:O	2.36	0.58
1:B:783:ILE:HD13	1:B:795:PHE:HB3	1.86	0.57
1:B:662:THR:HG21	1:B:701:ASP:HB3	1.86	0.56
4:B:903:CIT:O2	4:B:903:CIT:O7	2.24	0.55
1:B:512:LYS:O	1:B:554:ARG:NH1	2.40	0.54
1:B:657:MET:HE3	1:B:698:ILE:HG12	1.91	0.52
1:B:735:ARG:HG3	1:B:774:TYR:CE1	2.45	0.52
1:A:461:ARG:HA	1:A:528:LEU:HB3	1.93	0.51
1:A:626:LEU:HD12	1:A:642:LEU:HD11	1.93	0.50
1:B:657:MET:HE1	1:B:698:ILE:HA	1.95	0.49
1:B:699:ILE:HG23	1:B:707:ARG:HH11	1.77	0.49
1:B:820:LYS:O	1:B:823:ARG:NH2	2.41	0.48
1:A:669:GLU:OE1	1:A:829:ARG:HD2	2.14	0.48
1:B:501:LEU:HD21	1:B:513:MET:HG2	1.95	0.47
1:B:684:ARG:NH1	1:B:684:ARG:HG2	2.30	0.45
1:A:795:PHE:O	1:A:799:VAL:HG13	2.16	0.45
1:A:740:ALA:HB1	1:A:748:ASP:HB3	1.99	0.45
1:A:471:ILE:HD12	1:A:512:LYS:HE2	1.98	0.45
1:A:693:ASP:HA	6:A:1023:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:TYR:CZ	1:A:812:ARG:HD2	2.51	0.44
1:A:563:TYR:CD2	1:A:841:LYS:HE3	2.53	0.44
1:A:705:ASP:HB2	1:A:791:LEU:HD22	2.00	0.44
1:A:662:THR:HG21	1:A:701:ASP:HB3	2.00	0.44
1:A:539:PHE:CE1	1:A:550:LEU:HD21	2.53	0.43
1:B:489:GLY:H	1:B:494:GLU:HG3	1.83	0.43
1:A:517:ASP:HB3	1:A:552:LEU:HB3	2.01	0.43
1:B:539:PHE:HE1	1:B:550:LEU:HD21	1.84	0.43
1:A:803:GLN:NE2	6:A:1015:HOH:O	2.52	0.43
1:A:822:THR:O	4:A:902:CIT:O7	2.35	0.43
1:A:763:HIS:O	1:A:767:VAL:HG13	2.18	0.42
1:B:676:ASN:ND2	1:B:718:ARG:O	2.49	0.42
1:B:705:ASP:HB2	1:B:791:LEU:HD22	2.00	0.42
1:A:466:LEU:HD11	1:A:528:LEU:HD11	2.02	0.42
1:A:702:THR:OG1	1:A:707:ARG:HG3	2.18	0.42
1:B:498:ILE:HG13	1:B:513:MET:SD	2.60	0.42
1:B:539:PHE:CE1	1:B:550:LEU:HD21	2.55	0.41
1:B:579:LEU:HG	1:B:617:ARG:CZ	2.51	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	423/427 (99%)	409 (97%)	12 (3%)	2 (0%)	29 35
1	B	420/427 (98%)	409 (97%)	9 (2%)	2 (0%)	29 35
2	C	3/11 (27%)	3 (100%)	0	0	100 100
All	All	846/865 (98%)	821 (97%)	21 (2%)	4 (0%)	29 35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	557	PRO
1	A	590	VAL
1	B	492	PRO
1	B	590	VAL

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	361/370 (98%)	342 (95%)	19 (5%)	22	31
1	B	362/370 (98%)	345 (95%)	17 (5%)	26	37
2	C	5/11 (46%)	4 (80%)	1 (20%)	1	1
All	All	728/751 (97%)	691 (95%)	37 (5%)	24	33

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	473	THR
1	A	490	ASP
1	A	491	GLU
1	A	501	LEU
1	A	509	LEU
1	A	515	THR
1	A	618	THR
1	A	627	LYS
1	A	662	THR
1	A	664	GLU
1	A	680	GLN
1	A	696	LYS
1	A	721[A]	ASP
1	A	721[B]	ASP
1	A	754	SER
1	A	767	VAL
1	A	787	VAL
1	A	799	VAL
1	A	861	ASP

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Mol	Chain	Res	Type
1	B	458	PHE
1	B	495	PHE
1	B	499	LYS
1	B	513	MET
1	B	523	ASN
1	B	530	HIS
1	B	535	VAL
1	B	592	GLU
1	B	616	ARG
1	B	664	GLU
1	B	680	GLN
1	B	701	ASP
1	B	745	LYS
1	B	799	VAL
1	B	812	ARG
1	B	861	ASP
1	B	877	ASP
2	C	732	GLU

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 11 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	0.93	0	5,5,5	0.98	0
3	GOL	B	902	-	5,5,5	0.96	0	5,5,5	1.07	0
4	CIT	A	902	-	12,12,12	1.23	2 (16%)	17,17,17	1.20	1 (5%)
3	GOL	A	901	-	5,5,5	0.74	0	5,5,5	1.22	1 (20%)
4	CIT	B	901	-	12,12,12	0.97	0	17,17,17	1.59	2 (11%)
4	CIT	B	903	-	12,12,12	1.01	0	17,17,17	1.60	2 (11%)

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	-	-	0/4/4/4	-
3	GOL	B	902	-	-	3/4/4/4	-
4	CIT	A	902	-	-	6/16/16/16	-
3	GOL	A	901	-	-	1/4/4/4	-
4	CIT	B	901	-	-	9/16/16/16	-
4	CIT	B	903	-	-	11/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	CIT	O4-C5	-2.23	1.23	1.30
4	A	902	CIT	O2-C1	-2.23	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	CIT	O6-C6-C3	4.18	120.31	113.05
4	B	903	CIT	O6-C6-C3	4.07	120.11	113.05
4	A	902	CIT	O5-C6-C3	-3.07	117.91	122.25
4	B	903	CIT	O2-C1-C2	2.23	121.51	114.35
4	B	901	CIT	O4-C5-C4	2.10	121.09	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	GOL	C3-C2-C1	-2.07	103.65	111.70

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	CIT	C2-C3-C6-O5
4	A	902	CIT	C2-C3-C6-O6
4	A	902	CIT	O7-C3-C6-O5
4	A	902	CIT	O7-C3-C6-O6
4	B	901	CIT	O7-C3-C6-O5
4	B	901	CIT	O7-C3-C6-O6
4	B	901	CIT	C4-C3-C6-O6
4	B	903	CIT	C1-C2-C3-C4
4	B	903	CIT	C1-C2-C3-C6
4	B	903	CIT	C2-C3-C6-O5
4	B	903	CIT	C2-C3-C6-O6
4	B	903	CIT	O7-C3-C6-O5
4	B	903	CIT	O7-C3-C6-O6
4	B	901	CIT	C2-C3-C4-C5
4	B	903	CIT	C1-C2-C3-O7
3	A	901	GOL	C1-C2-C3-O3
3	B	902	GOL	O1-C1-C2-C3
4	B	901	CIT	C2-C3-C6-O5
4	B	901	CIT	C4-C3-C6-O5
3	B	902	GOL	O1-C1-C2-O2
4	B	901	CIT	C2-C3-C6-O6
4	B	903	CIT	O1-C1-C2-C3
3	B	902	GOL	O2-C2-C3-O3
4	B	901	CIT	C6-C3-C4-C5
4	B	903	CIT	O2-C1-C2-C3
4	B	901	CIT	O7-C3-C4-C5
4	A	902	CIT	C3-C4-C5-O3
4	A	902	CIT	C3-C4-C5-O4
4	B	903	CIT	C6-C3-C4-C5
4	B	903	CIT	O7-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	CIT	1	0
4	B	903	CIT	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 (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(Å^2)	Q<0.9
1	A	421/427 (98%)	1.25	90 (21%) 0 1	44, 72, 172, 210	0
1	B	421/427 (98%)	0.49	29 (6%) 16 22	44, 79, 125, 177	0
2	C	5/11 (45%)	1.56	1 (20%) 1 1	100, 106, 122, 139	0
All	All	847/865 (97%)	0.87	120 (14%) 2 3	44, 75, 162, 210	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	LEU	12.2
1	A	533	ALA	9.0
1	A	492	PRO	8.1
1	A	557	PRO	8.1
1	A	553	CYS	7.9
1	A	499	LYS	7.8
1	B	490	ASP	7.7
1	A	487	VAL	7.7
1	A	539	PHE	7.6
1	A	528	LEU	7.3
1	A	542	ILE	7.3
1	A	459	PHE	6.9
1	A	482	PHE	6.8
1	A	496	LEU	6.7
1	A	479	SER	6.6
1	B	491	GLU	6.5
1	A	458	PHE	6.5
1	A	483	GLY	6.3
1	A	484	PHE	6.3
1	A	503	LEU	6.3
1	A	518	VAL	6.2
1	A	552	LEU	6.0
1	A	529	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	532	HIS	5.9
1	A	507	ALA	5.9
1	A	556	TYR	5.9
1	A	491	GLU	5.7
1	A	502	VAL	5.7
1	A	460	THR	5.7
1	A	550	LEU	5.7
1	A	468	GLY	5.5
1	B	500	SER	5.5
1	A	536	VAL	5.5
1	A	493	ASP	5.5
1	A	466	LEU	5.4
1	A	535	VAL	5.4
1	A	509	LEU	5.3
1	A	504	ASP	5.3
1	A	519	ILE	5.3
1	A	506	PRO	5.3
1	A	486	VAL	5.2
1	A	498	ILE	5.1
1	B	492	PRO	5.1
1	A	554	ARG	5.0
1	A	475	LEU	5.0
1	A	513	MET	4.9
1	A	537	LYS	4.8
1	A	495	PHE	4.7
1	A	470	PHE	4.7
1	A	485	THR	4.7
1	A	472	HIS	4.6
1	B	489	GLY	4.6
1	A	469	LYS	4.6
1	A	508	ALA	4.5
1	A	555	GLY	4.4
1	A	531	THR	4.2
1	B	486	VAL	4.2
1	A	530	HIS	4.2
1	A	538	ILE	4.2
1	A	514	GLU	4.1
1	A	477	LYS	4.1
2	C	731	PRO	4.1
1	A	544	ILE	4.0
1	A	480	ARG	4.0
1	A	540	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	461	ARG	3.8
1	A	478	SER	3.7
1	A	546	ALA	3.6
1	A	524	ASP	3.6
1	A	500	SER	3.6
1	A	476	ARG	3.6
1	A	541	SER	3.6
1	A	481	GLY	3.5
1	A	490	ASP	3.5
1	B	576	ARG	3.5
1	A	558	LEU	3.4
1	A	560	SER	3.4
1	A	488	GLY	3.3
1	A	551	GLU	3.3
1	B	458	PHE	3.2
1	B	487	VAL	3.2
1	A	505	GLY	3.1
1	A	525	THR	3.1
1	A	512	LYS	3.0
1	A	543	PRO	3.0
1	A	520	VAL	3.0
1	B	496	LEU	2.9
1	A	494	GLU	2.9
1	B	503	LEU	2.9
1	B	722	GLY	2.8
1	A	497	GLN	2.8
1	A	471	ILE	2.8
1	B	777	TYR	2.8
1	A	489	GLY	2.7
1	B	518	VAL	2.7
1	A	521	SER	2.6
1	B	689	MET	2.6
1	B	459	PHE	2.5
1	A	547	SER	2.5
1	A	545	GLY	2.4
1	B	494	GLU	2.4
1	B	499	LYS	2.4
1	B	558	LEU	2.3
1	B	493	ASP	2.3
1	A	511	GLY	2.3
1	A	467	LYS	2.3
1	A	534	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	548	VAL	2.3
1	B	498	ILE	2.2
1	A	516	GLY	2.2
1	B	480	ARG	2.2
1	B	566	VAL	2.2
1	B	688	GLU	2.1
1	B	556	TYR	2.1
1	B	685	VAL	2.1
1	A	462	ASN	2.1
1	B	520	VAL	2.1
1	B	661	GLY	2.0
1	B	488	GLY	2.0
1	A	561	SER	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 monosaccharides 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	CIT	B	903	13/13	0.65	0.23	107,123,127,131	0
5	CA	B	907	1/1	0.66	0.33	163,163,163,163	0
5	CA	B	908	1/1	0.71	0.11	118,118,118,118	0
4	CIT	A	902	13/13	0.75	0.17	93,111,127,135	0
5	CA	B	905	1/1	0.80	0.17	129,129,129,129	0
4	CIT	B	901	13/13	0.81	0.33	99,141,148,150	0
5	CA	A	907	1/1	0.82	0.10	101,101,101,101	0
5	CA	A	904	1/1	0.82	0.10	123,123,123,123	0
5	CA	A	906	1/1	0.84	0.07	139,139,139,139	0
5	CA	B	906	1/1	0.84	0.17	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	903	6/6	0.89	0.21	64,92,100,102	0
5	CA	B	904	1/1	0.92	0.20	107,107,107,107	0
5	CA	B	909	1/1	0.93	0.06	80,80,80,80	0
3	GOL	B	902	6/6	0.95	0.18	53,63,69,70	0
5	CA	A	905	1/1	0.96	0.09	129,129,129,129	0
5	CA	A	908	1/1	0.96	0.16	87,87,87,87	0
3	GOL	A	901	6/6	0.97	0.23	52,62,64,74	0

6.5 Other polymers (i)

There are no such residues in this entry.