Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 10:42 pm GMT

PDB ID	:	6TWU
Title	:	MAGI1_2 complexed with a phosphomimetic 16E6 peptide
Authors	:	Gogl, G.; Cousido-Siah, A.; Trave, G.
Deposited on	:	2020-01-13
Resolution	:	2.40 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:

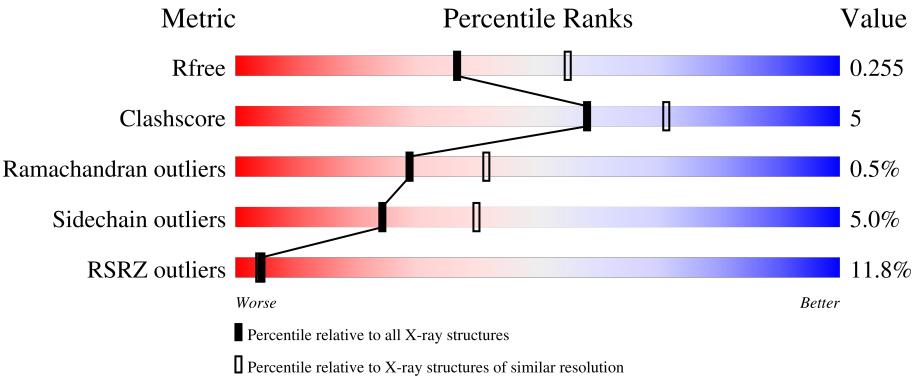
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	18% 83% 15%
1	B	427	6% 86% 11%
2	C	10	30% 70%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6821 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	421	Total	C	N	O	S	0	4	0
			3338	2097	571	656	14			
1	B	421	Total	C	N	O	S	0	1	0
			3326	2091	571	650	14			

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

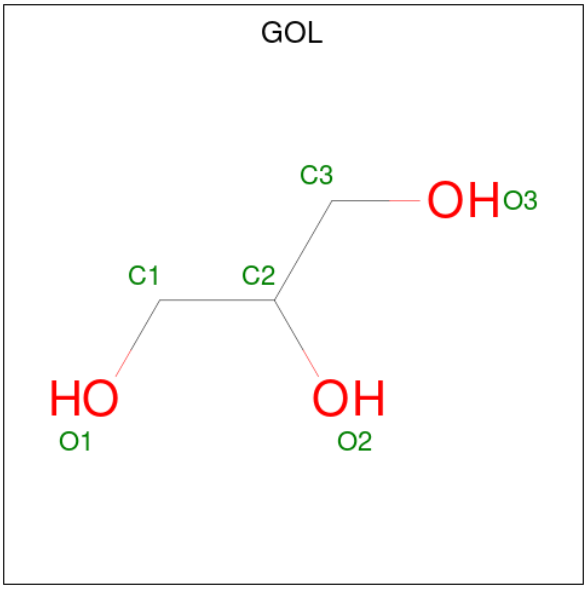
- Molecule 2 is a protein called Protein E6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	3	Total C N O 27 16 4 7	0	0	0

There is a discrepancy between the modelled and reference sequences:

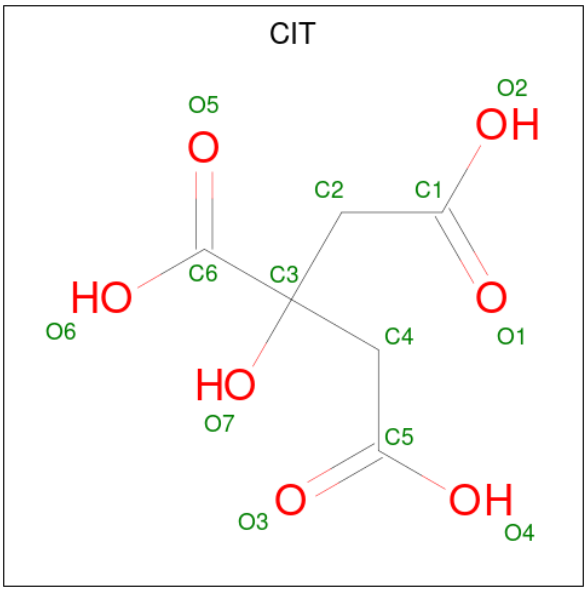
Chain	Residue	Modelled	Actual	Comment	Reference
C	156	GLU	THR	conflict	UNP P03126

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

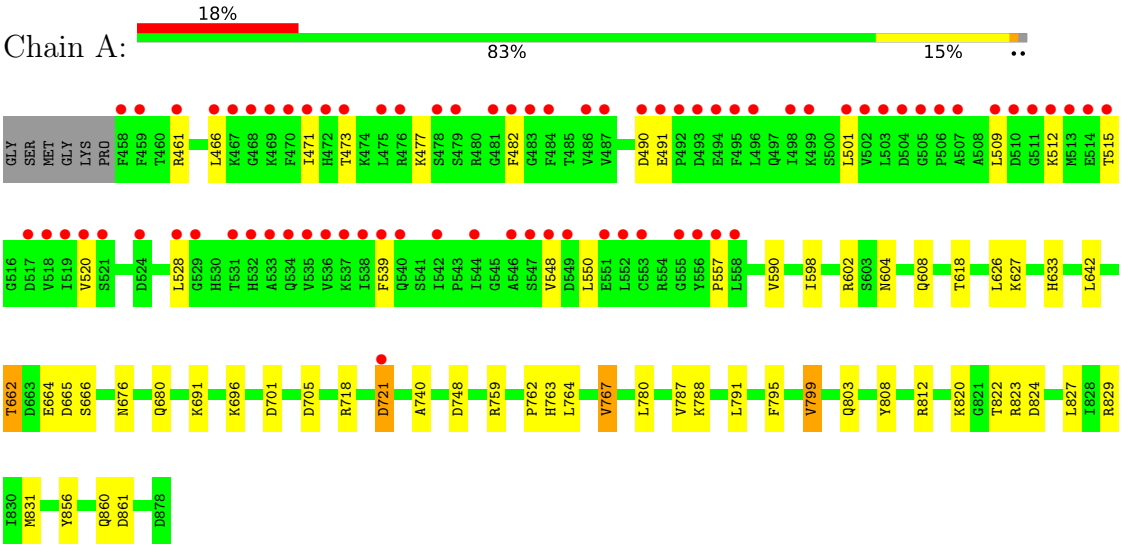
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	30	Total O 30 30	0	0
6	B	32	Total O 32 32	0	0

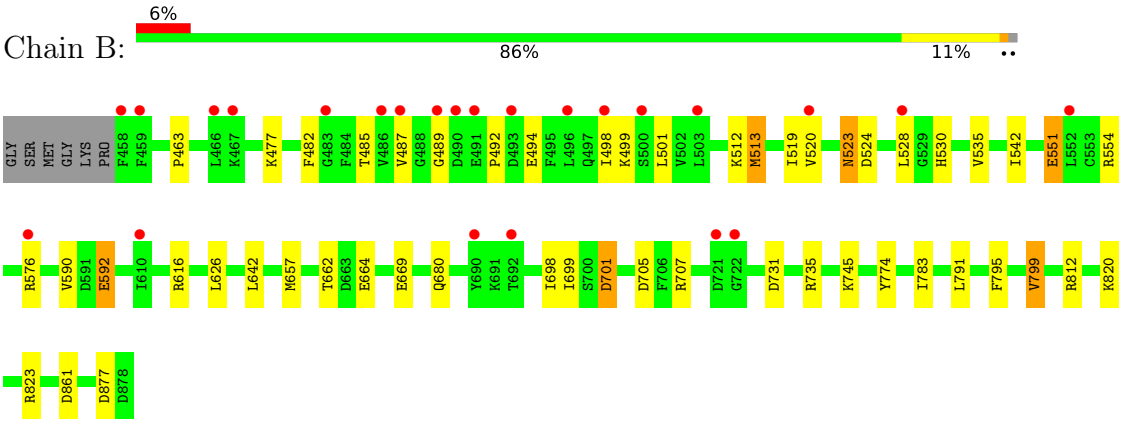
3 Residue-property plots (i)

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: Protein E6


SER
SER
ARG
THR
ARG
ARG
GLU
E156
Q157
L158

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.16Å 96.44Å 197.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.40 48.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.22-2.40) 99.9 (48.22-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.216 , 0.255 0.216 , 0.255	Depositor DCC
R_{free} test set	2306 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6821	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, 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	0.29	0/3388	0.43	0/4562
1	B	0.28	0/3376	0.43	0/4542
2	C	0.58	0/26	0.61	0/32
All	All	0.28	0/6790	0.43	0/9136

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	3306	30	0
1	B	3326	0	3323	31	0
2	C	27	0	24	5	0
3	A	12	0	16	0	0
3	B	6	0	8	1	0
4	A	13	0	5	2	0
4	B	26	0	10	2	0
5	A	5	0	0	0	0
5	B	6	0	0	0	0
6	A	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	32	0	0	4	0
All	All	6821	0	6692	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (65) 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	1.58	0.85
1:B:485:THR:HG22	2:C:156:GLU:O	1.76	0.82
1:A:721[A]:ASP:OD1	1:A:721[A]:ASP:N	2.16	0.79
1:A:665[B]:ASP:OD1	1:A:812:ARG:NH2	2.24	0.70
1:A:633:HIS:NE2	1:A:824:ASP:OD2	2.25	0.69
1:A:803:GLN:NE2	6:A:1002:HOH:O	2.26	0.69
1:B:520:VAL:HG13	1:B:528:LEU:HD11	1.76	0.66
1:A:822:THR:H	4:A:902:CIT:H42	1.60	0.64
1:B:795:PHE:O	1:B:799:VAL:HG12	1.98	0.63
1:B:657:MET:HE1	1:B:698:ILE:HA	1.80	0.62
1:B:820:LYS:O	1:B:823:ARG:NH2	2.32	0.62
1:B:485:THR:HA	2:C:156:GLU:O	2.00	0.62
1:B:482:PHE:N	2:C:158:LEU:O	2.33	0.61
1:B:783:ILE:HD13	1:B:795:PHE:HB3	1.83	0.61
1:A:471:ILE:HD12	1:A:512:LYS:HE2	1.85	0.59
1:A:626:LEU:HD12	1:A:642:LEU:HD11	1.86	0.57
1:B:498:ILE:HD11	1:B:519:ILE:HD11	1.86	0.56
4:B:903:CIT:O2	4:B:903:CIT:O7	2.23	0.55
4:A:902:CIT:O1	4:A:902:CIT:O7	2.21	0.55
1:B:485:THR:CG2	2:C:156:GLU:O	2.50	0.54
1:B:520:VAL:HG13	1:B:528:LEU:CD1	2.37	0.54
1:A:666:SER:OG	1:A:829:ARG:NH2	2.39	0.53
1:B:669:GLU:OE2	1:B:812:ARG:NH1	2.42	0.53
1:B:501:LEU:HD21	1:B:513:MET:HG2	1.90	0.53
1:B:699:ILE:HG23	1:B:707:ARG:HH11	1.75	0.51
1:B:489:GLY:H	1:B:494:GLU:HG3	1.76	0.51
1:B:812:ARG:NH2	6:B:1012:HOH:O	2.37	0.51
1:B:662:THR:HG21	1:B:701:ASP:HB3	1.92	0.51
1:B:523:ASN:O	1:B:524:ASP:HB2	2.11	0.50
1:A:740:ALA:HB1	1:A:748:ASP:HB3	1.93	0.50
1:B:487:VAL:HB	1:B:499:LYS:HD2	1.94	0.49
1:A:808:TYR:CZ	1:A:812:ARG:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ARG:HA	1:A:528:LEU:HB3	1.95	0.48
1:B:463:PRO:HG3	1:B:528:LEU:HD12	1.95	0.48
1:B:592:GLU:H	1:B:592:GLU:HG2	1.37	0.48
4:B:903:CIT:H42	6:B:1016:HOH:O	2.15	0.47
1:B:498:ILE:HG13	1:B:513:MET:SD	2.55	0.47
1:B:485:THR:CB	2:C:156:GLU:O	2.62	0.47
1:A:721[A]:ASP:HB3	1:A:762:PRO:HG2	1.97	0.46
1:A:520:VAL:HG13	1:A:528:LEU:HD11	1.97	0.45
1:A:662:THR:HG21	1:A:701:ASP:HB3	1.98	0.45
1:A:763:HIS:O	1:A:767:VAL:HG13	2.15	0.45
1:B:735:ARG:HG3	1:B:774:TYR:CE1	2.52	0.45
1:A:795:PHE:O	1:A:799:VAL:HG13	2.17	0.44
1:A:820:LYS:O	1:A:823:ARG:NH2	2.41	0.44
1:A:759:ARG:HB2	1:A:764:LEU:HG	2.00	0.44
1:A:466:LEU:HD11	1:A:528:LEU:HD11	2.00	0.44
1:A:604:ASN:O	1:A:608:GLN:HG2	2.17	0.44
1:B:512:LYS:O	1:B:554:ARG:NH1	2.51	0.44
1:A:705:ASP:HB2	1:A:791:LEU:HD22	2.00	0.44
1:A:827:LEU:O	1:A:831:MET:HG2	2.18	0.43
1:B:705:ASP:HB2	1:B:791:LEU:HD22	2.00	0.43
1:B:477:LYS:HD2	1:B:542:ILE:HB	2.00	0.43
1:B:731:ASP:HB3	6:B:1008:HOH:O	2.18	0.43
1:A:676:ASN:ND2	1:A:718:ARG:O	2.48	0.42
1:A:477:LYS:HB2	1:A:482:PHE:CZ	2.54	0.42
1:B:626:LEU:HD12	1:B:642:LEU:HD11	2.02	0.42
1:A:598:ILE:O	1:A:602:ARG:HG2	2.20	0.42
1:A:780:LEU:HD23	1:A:780:LEU:HA	1.89	0.42
1:A:856:TYR:O	1:A:860:GLN:HG2	2.20	0.41
1:A:539:PHE:CE1	1:A:550:LEU:HD21	2.56	0.41
1:A:665[B]:ASP:CG	1:A:812:ARG:HH22	2.23	0.41
1:A:721[B]:ASP:CG	1:A:762:PRO:HG2	2.41	0.41
3:B:902:GOL:O3	6:B:1001:HOH:O	2.22	0.40
1:B:699:ILE:O	1:B:707:ARG:NH1	2.55	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	423/427 (99%)	409 (97%)	12 (3%)	2 (0%)	29 41
1	B	420/427 (98%)	406 (97%)	12 (3%)	2 (0%)	29 41
2	C	1/10 (10%)	1 (100%)	0	0	100 100
All	All	844/864 (98%)	816 (97%)	24 (3%)	4 (0%)	29 41

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%)	340 (94%)	21 (6%)	20 32
1	B	362/370 (98%)	347 (96%)	15 (4%)	30 48
2	C	3/10 (30%)	2 (67%)	1 (33%)	0 0
All	All	726/750 (97%)	689 (95%)	37 (5%)	24 39

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	548	VAL
1	A	618	THR
1	A	627	LYS
1	A	662	THR
1	A	664	GLU
1	A	680	GLN
1	A	691	LYS
1	A	696	LYS
1	A	721[A]	ASP
1	A	721[B]	ASP
1	A	767	VAL
1	A	787	VAL
1	A	788	LYS
1	A	799	VAL
1	A	861	ASP
1	B	513	MET
1	B	523	ASN
1	B	530	HIS
1	B	535	VAL
1	B	551	GLU
1	B	576	ARG
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	861	ASP
1	B	877	ASP
2	C	157	GLN

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	901	-	5,5,5	0.83	0	5,5,5	1.02	0
4	CIT	B	903	-	12,12,12	1.03	0	17,17,17	1.59	2 (11%)
3	GOL	B	902	-	5,5,5	0.85	0	5,5,5	0.98	0
3	GOL	A	903	-	5,5,5	0.89	0	5,5,5	1.01	0
4	CIT	B	901	-	12,12,12	0.97	0	17,17,17	1.52	2 (11%)
4	CIT	A	902	-	12,12,12	1.20	3 (25%)	17,17,17	1.56	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	901	-	-	2/4/4/4	-
4	CIT	B	903	-	-	9/16/16/16	-
3	GOL	B	902	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	903	-	-	0/4/4/4	-
4	CIT	B	901	-	-	9/16/16/16	-
4	CIT	A	902	-	-	10/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	CIT	O2-C1	-2.12	1.23	1.30
4	A	902	CIT	C3-C6	2.10	1.55	1.53
4	A	902	CIT	O4-C5	-2.03	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	903	CIT	O6-C6-C3	4.07	120.12	113.05
4	A	902	CIT	O5-C6-C3	-3.97	116.64	122.25
4	B	901	CIT	O6-C6-C3	3.92	119.85	113.05
4	A	902	CIT	O6-C6-C3	3.37	118.91	113.05
4	B	903	CIT	O2-C1-C2	2.16	121.28	114.35
4	B	901	CIT	O4-C5-C4	2.13	121.19	114.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	CIT	C2-C3-C4-C5
4	A	902	CIT	O7-C3-C4-C5
4	A	902	CIT	C6-C3-C4-C5
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-O5
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

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

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	CIT	2	0
3	B	902	GOL	1	0
4	A	902	CIT	2	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, 95^{th} 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%)	1.02	76 (18%) 1 1	46, 77, 154, 164	0
1	B	421/427 (98%)	0.52	24 (5%) 23 22	48, 83, 117, 135	0
2	C	3/10 (30%)	0.88	0 100 100	118, 118, 128, 135	0
All	All	845/864 (97%)	0.77	100 (11%) 4 4	46, 81, 152, 164	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	LEU	13.5
1	A	553	CYS	8.9
1	A	533	ALA	8.6
1	A	557	PRO	8.2
1	B	500	SER	7.7
1	A	528	LEU	7.7
1	A	513	MET	7.6
1	A	518	VAL	6.9
1	A	492	PRO	6.9
1	A	503	LEU	6.4
1	A	493	ASP	6.3
1	A	512	LYS	6.3
1	A	484	PHE	6.1
1	A	482	PHE	6.0
1	A	511	GLY	5.9
1	A	466	LEU	5.9
1	A	472	HIS	5.7
1	A	502	VAL	5.6
1	A	504	ASP	5.5
1	A	486	VAL	5.3
1	A	520	VAL	5.2
1	A	483	GLY	5.2
1	A	532	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	509	LEU	5.1
1	B	722	GLY	5.0
1	A	535	VAL	4.8
1	A	496	LEU	4.8
1	B	489	GLY	4.7
1	A	458	PHE	4.7
1	B	503	LEU	4.7
1	A	556	TYR	4.6
1	A	471	ILE	4.4
1	A	539	PHE	4.3
1	A	537	LYS	4.3
1	A	459	PHE	4.2
1	B	496	LEU	4.1
1	B	490	ASP	4.1
1	A	547	SER	4.1
1	A	519	ILE	4.1
1	A	499	LYS	4.1
1	A	514	GLU	3.9
1	B	486	VAL	3.8
1	A	510	ASP	3.8
1	A	491	GLU	3.8
1	A	498	ILE	3.7
1	A	551	GLU	3.7
1	A	468	GLY	3.7
1	A	470	PHE	3.7
1	A	461	ARG	3.7
1	A	542	ILE	3.6
1	A	479	SER	3.6
1	A	506	PRO	3.5
1	A	524	ASP	3.5
1	B	458	PHE	3.5
1	A	475	LEU	3.4
1	A	552	LEU	3.2
1	A	487	VAL	3.2
1	A	476	ARG	3.1
1	A	521	SER	3.0
1	A	517	ASP	3.0
1	A	473	THR	3.0
1	A	490	ASP	3.0
1	A	534	GLN	2.9
1	B	528	LEU	2.9
1	B	487	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	507	ALA	2.8
1	B	467	LYS	2.8
1	B	491	GLU	2.8
1	B	493	ASP	2.8
1	A	515	THR	2.8
1	A	478	SER	2.7
1	A	540	GLN	2.7
1	A	536	VAL	2.7
1	A	469	LYS	2.7
1	B	692	THR	2.6
1	A	531	THR	2.6
1	B	721[A]	ASP	2.6
1	A	549	ASP	2.5
1	B	498	ILE	2.5
1	A	555	GLY	2.4
1	A	538	ILE	2.4
1	B	459	PHE	2.4
1	A	481	GLY	2.4
1	A	529	GLY	2.4
1	A	548	VAL	2.4
1	A	495	PHE	2.4
1	A	558	LEU	2.3
1	B	552	LEU	2.3
1	B	576	ARG	2.3
1	A	544	ILE	2.2
1	A	505	GLY	2.2
1	B	466	LEU	2.2
1	B	483	GLY	2.1
1	B	610	ILE	2.1
1	A	546	ALA	2.1
1	B	690	TYR	2.1
1	A	721[A]	ASP	2.1
1	A	467	LYS	2.1
1	B	520	VAL	2.1
1	A	494	GLU	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, 95^{th} 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
5	CA	B	907	1/1	0.04	0.40	186,186,186,186	0
5	CA	B	905	1/1	0.67	0.27	131,131,131,131	0
4	CIT	B	903	13/13	0.69	0.20	116,128,133,134	0
5	CA	B	908	1/1	0.72	0.12	115,115,115,115	0
4	CIT	A	902	13/13	0.79	0.19	96,101,112,117	0
5	CA	A	907	1/1	0.81	0.14	101,101,101,101	0
4	CIT	B	901	13/13	0.81	0.32	105,139,150,150	0
5	CA	A	906	1/1	0.84	0.06	139,139,139,139	0
5	CA	A	904	1/1	0.86	0.13	142,142,142,142	0
3	GOL	A	903	6/6	0.87	0.21	80,95,103,104	0
5	CA	A	905	1/1	0.88	0.15	163,163,163,163	0
5	CA	B	906	1/1	0.88	0.07	140,140,140,140	0
5	CA	B	904	1/1	0.89	0.27	99,99,99,99	0
3	GOL	A	901	6/6	0.92	0.26	56,63,72,81	0
5	CA	B	909	1/1	0.93	0.08	94,94,94,94	0
3	GOL	B	902	6/6	0.94	0.18	52,64,70,77	0
5	CA	A	908	1/1	0.97	0.08	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.