Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 05:01 pm GMT

PDB ID	:	6TWQ
Title	:	MAGI1_2 complexed with a 16E6 peptide
Authors	:	Gogl, G.; Cousido-Siah, A.; Trave, G.
Deposited on	:	2020-01-13
Resolution	:	2.65 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
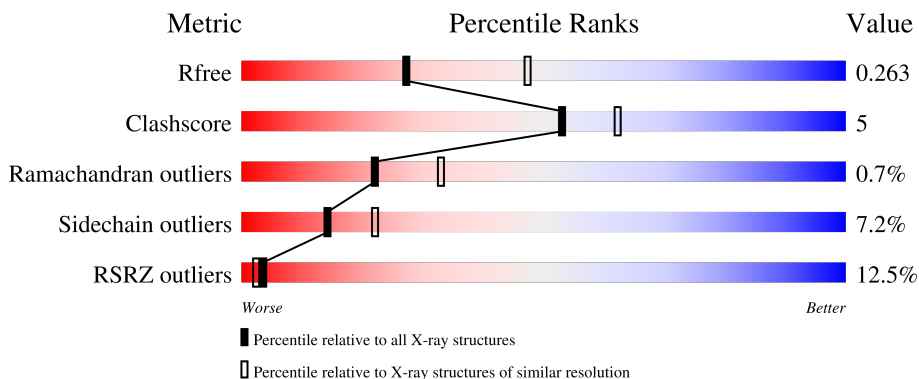http://www.wwpdb.org/validation/2017/FAQs#types.

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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 2.65 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		0.263
Clashscore		5
Ramachandran outliers		0.7%
Sidechain outliers		7.2%
RSRZ outliers		12.5%

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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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% / 82% / 15% / ••
1	B	427	2% / 81% / 16% / ••
2	C	10	20% / 40% / 30% / 30%
2	D	10	70% / 40% / 30% / 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	A	902	-	-	X	-
3	CIT	B	901	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6883 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	B	422	Total 3328	C 2095	N 571	O 648	S 14	0	0	0
1	A	421	Total 3312	C 2085	N 570	O 643	S 14	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	452	GLY	-	expression tag	UNP H7C535
B	453	SER	-	expression tag	UNP H7C535
B	454	MET	-	expression tag	UNP H7C535
B	559	GLY	-	linker	UNP H7C535
B	560	SER	-	linker	UNP H7C535
B	605	GLU	ALA	conflict	UNP P07355
A	452	GLY	-	expression tag	UNP H7C535
A	453	SER	-	expression tag	UNP H7C535
A	454	MET	-	expression tag	UNP H7C535
A	559	GLY	-	linker	UNP H7C535
A	560	SER	-	linker	UNP H7C535
A	605	GLU	ALA	conflict	UNP P07355

- Molecule 2 is a protein called THR-ARG-ARG-GLU-THR-GLN-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total 61	C 35	N 14	O 12	0	0	0
2	D	7	Total 61	C 35	N 14	O 12	0	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	28	Total 28	O 28	0	0
6	A	31	Total 31	O 31	0	0

3 Residue-property plots ⓘ

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
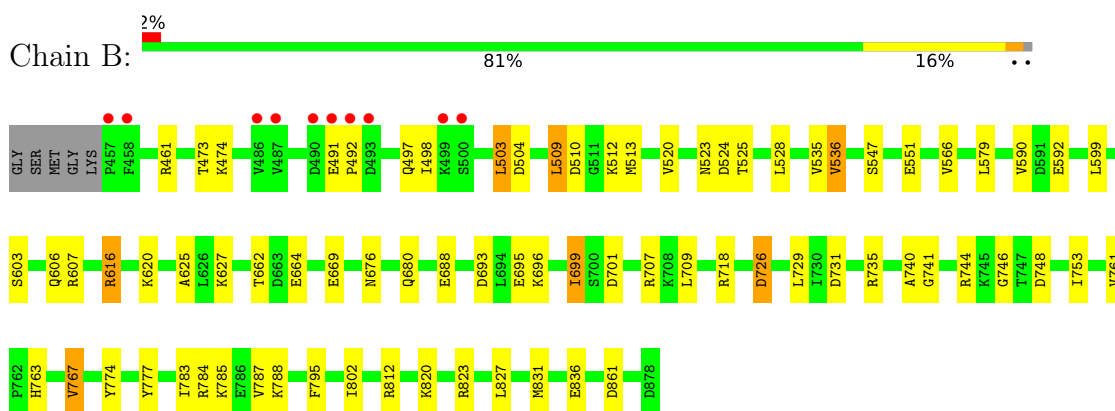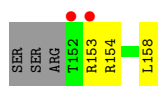

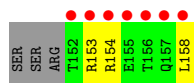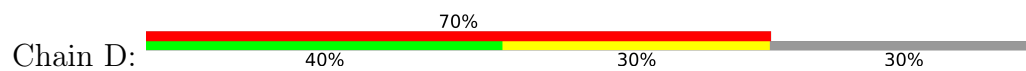• Molecule 1: Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1,Annexin A2
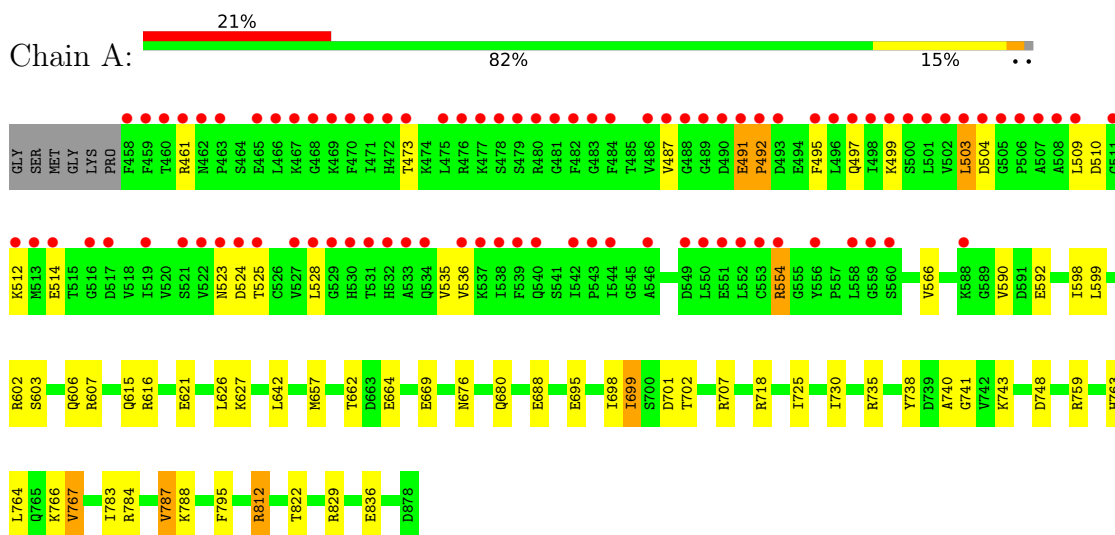
• Molecule 2: THR-ARG-ARG-GLU-THR-GLN-LEU

• Molecule 2: THR-ARG-ARG-GLU-THR-GLN-LEU

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.81Å 97.13Å 201.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.65 48.56 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.56-2.65) 99.2 (48.56-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.239 , 0.262 0.239 , 0.263	Depositor DCC
R_{free} test set	1739 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	70.2	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6883	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 18.24% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, CA, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.25	0/3362	0.42	0/4524
1	B	0.24	0/3379	0.40	0/4546
2	C	0.20	0/60	0.43	0/77
2	D	0.20	0/60	0.45	0/77
All	All	0.25	0/6861	0.41	0/9224

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	3312	0	3310	36	0
1	B	3328	0	3337	33	0
2	C	61	0	59	1	0
2	D	61	0	59	1	0
3	A	13	0	5	6	0
3	B	26	0	10	2	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	0	0	0
6	A	31	0	0	0	0
6	B	28	0	0	0	0
All	All	6883	0	6796	73	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 (73) 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:514:GLU:CB	1:A:554:ARG:HH11	1.94	0.80
1:A:514:GLU:CB	1:A:554:ARG:NH1	2.45	0.80
1:B:669:GLU:OE2	1:B:812:ARG:NH1	2.21	0.73
1:B:599:LEU:O	1:B:607:ARG:NH1	2.27	0.67
1:B:784:ARG:O	1:B:788:LYS:NZ	2.28	0.67
1:A:784:ARG:O	1:A:788:LYS:NZ	2.29	0.66
1:A:566:VAL:HG23	1:A:836:GLU:HG3	1.79	0.65
1:B:662:THR:HG21	1:B:701:ASP:HB3	1.78	0.65
1:A:599:LEU:O	1:A:607:ARG:NH1	2.32	0.62
1:A:822:THR:H	3:A:902:CIT:H41	1.65	0.62
1:A:822:THR:H	3:A:902:CIT:C4	2.13	0.61
1:A:695:GLU:O	1:A:699:ILE:HG12	2.01	0.61
1:B:695:GLU:O	1:B:699:ILE:HG12	2.00	0.61
3:A:902:CIT:O2	3:A:902:CIT:O7	2.15	0.59
1:A:740:ALA:HB1	1:A:748:ASP:HB3	1.86	0.58
1:B:566:VAL:HG23	1:B:836:GLU:HG3	1.84	0.58
1:A:662:THR:HG21	1:A:701:ASP:HB3	1.86	0.58
1:B:620:LYS:HE3	1:B:625:ALA:HB2	1.85	0.57
1:B:783:ILE:HD13	1:B:795:PHE:HB3	1.87	0.57
1:B:520:VAL:HB	1:B:551:GLU:HG2	1.87	0.56
1:B:744:ARG:HH21	1:B:746:GLY:HA3	1.70	0.56
1:B:726:ASP:HB3	1:B:729:LEU:HB3	1.88	0.55
1:A:783:ILE:HD13	1:A:795:PHE:HB3	1.89	0.55
1:A:676:ASN:ND2	1:A:718:ARG:O	2.43	0.52
1:B:740:ALA:HB1	1:B:748:ASP:HB3	1.93	0.51
1:A:503:LEU:H	1:A:503:LEU:HD23	1.76	0.50
1:B:536:VAL:HG22	2:C:158:LEU:HD21	1.94	0.50
1:B:699:ILE:HG22	1:B:707:ARG:HH11	1.77	0.49
3:B:903:CIT:O2	3:B:903:CIT:O7	2.30	0.49
1:B:676:ASN:ND2	1:B:718:ARG:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:LEU:HD21	1:A:536:VAL:HG22	1.93	0.49
1:B:761:VAL:HG13	1:B:802:ILE:HG23	1.94	0.48
1:A:699:ILE:HG23	1:A:707:ARG:HD3	1.94	0.48
1:B:699:ILE:HG23	1:B:707:ARG:HD3	1.94	0.48
1:A:725:ILE:HD13	1:A:766:LYS:HE2	1.96	0.48
1:B:731:ASP:OD1	1:B:774:TYR:OH	2.22	0.47
1:B:503:LEU:H	1:B:503:LEU:HD23	1.80	0.46
1:A:615:GLN:HG3	1:A:621:GLU:OE2	2.15	0.46
1:A:822:THR:O	3:A:902:CIT:C4	2.64	0.45
1:B:827:LEU:O	1:B:831:MET:HG2	2.17	0.45
1:B:820:LYS:O	1:B:823:ARG:NH2	2.48	0.45
1:A:491:GLU:HG3	1:A:492:PRO:HD2	1.99	0.45
1:A:699:ILE:HG12	1:A:699:ILE:H	1.47	0.44
1:B:709:LEU:HD13	1:B:753:ILE:HG12	1.99	0.44
1:B:509:LEU:HD13	1:B:509:LEU:HA	1.81	0.44
1:A:787:VAL:O	1:A:788:LYS:NZ	2.46	0.44
1:B:498:ILE:HG21	1:B:513:MET:HE3	1.99	0.44
1:A:626:LEU:HD12	1:A:642:LEU:HD11	1.98	0.44
1:A:759:ARG:HB2	1:A:764:LEU:HG	2.00	0.44
1:B:603:SER:OG	1:B:606:GLN:HG3	2.18	0.43
1:A:763:HIS:O	1:A:767:VAL:HG13	2.18	0.43
1:A:822:THR:O	3:A:902:CIT:O7	2.34	0.43
1:B:510:ASP:OD1	1:B:512:LYS:HB2	2.18	0.43
1:A:603:SER:OG	1:A:606:GLN:HG3	2.18	0.43
1:A:698:ILE:O	1:A:702:THR:OG1	2.25	0.43
1:A:699:ILE:HG22	1:A:707:ARG:HH11	1.84	0.42
1:A:730:ILE:HG13	1:A:763:HIS:CE1	2.54	0.42
1:A:812:ARG:HH21	1:A:812:ARG:CG	2.33	0.42
1:A:461:ARG:HA	1:A:528:LEU:HB3	2.01	0.42
1:A:738:TYR:CE2	1:A:743:LYS:HB2	2.55	0.42
1:B:461:ARG:HA	1:B:528:LEU:HB3	2.02	0.42
1:B:777:TYR:CE2	1:B:785:LYS:HD2	2.55	0.41
1:B:616:ARG:HE	1:B:616:ARG:HB3	1.55	0.41
1:B:695:GLU:HG2	1:B:699:ILE:HD11	2.02	0.41
1:B:763:HIS:O	1:B:767:VAL:HG13	2.20	0.41
1:B:474:LYS:HE2	1:B:547:SER:OG	2.21	0.41
1:A:510:ASP:OD1	1:A:512:LYS:HB2	2.20	0.41
1:B:693:ASP:HB2	1:B:696:LYS:HG3	2.03	0.41
1:A:669:GLU:OE2	1:A:829:ARG:NH1	2.54	0.41
1:A:657:MET:HE1	1:A:698:ILE:HG12	2.03	0.40
3:B:903:CIT:O3	3:B:903:CIT:C6	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ILE:O	1:A:602:ARG:HG2	2.21	0.40
3:A:902:CIT:O6	3:A:902:CIT:C5	2.70	0.40

There are no symmetry-related clashes.

5.3   Torsion angles   ⓘ

5.3.1   Protein backbone   ⓘ

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	419/427 (98%)	406 (97%)	10 (2%)	3 (1%)	22	33
1	B	420/427 (98%)	407 (97%)	10 (2%)	3 (1%)	22	33
2	C	5/10 (50%)	5 (100%)	0	0	100	100
2	D	5/10 (50%)	5 (100%)	0	0	100	100
All	All	849/874 (97%)	823 (97%)	20 (2%)	6 (1%)	22	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	492	PRO
1	A	492	PRO
1	B	590	VAL
1	B	741	GLY
1	A	590	VAL
1	A	741	GLY

5.3.2   Protein sidechains   ⓘ

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	358/370 (97%)	333 (93%)	25 (7%)	15	23
1	B	363/370 (98%)	339 (93%)	24 (7%)	16	25
2	C	6/10 (60%)	4 (67%)	2 (33%)	0	0
2	D	6/10 (60%)	4 (67%)	2 (33%)	0	0
All	All	733/760 (96%)	680 (93%)	53 (7%)	14	22

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	473	THR
1	B	491	GLU
1	B	497	GLN
1	B	503	LEU
1	B	504	ASP
1	B	509	LEU
1	B	523	ASN
1	B	524	ASP
1	B	525	THR
1	B	535	VAL
1	B	536	VAL
1	B	579	LEU
1	B	592	GLU
1	B	616	ARG
1	B	627	LYS
1	B	664	GLU
1	B	680	GLN
1	B	688	GLU
1	B	699	ILE
1	B	726	ASP
1	B	735	ARG
1	B	767	VAL
1	B	787	VAL
1	B	861	ASP
2	C	153	ARG
2	C	154	ARG
2	D	153	ARG
2	D	154	ARG
1	A	473	THR
1	A	487	VAL

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Mol	Chain	Res	Type
1	A	491	GLU
1	A	495	PHE
1	A	497	GLN
1	A	499	LYS
1	A	503	LEU
1	A	504	ASP
1	A	509	LEU
1	A	523	ASN
1	A	524	ASP
1	A	525	THR
1	A	535	VAL
1	A	554	ARG
1	A	592	GLU
1	A	616	ARG
1	A	627	LYS
1	A	664	GLU
1	A	680	GLN
1	A	688	GLU
1	A	699	ILE
1	A	735	ARG
1	A	767	VAL
1	A	787	VAL
1	A	812	ARG

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 (i)

Of 16 ligands modelled in this entry, 11 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	#$|Z| > 2$
4	GOL	B	902	-	5,5,5	0.93	0	5,5,5	1.03	0
3	CIT	B	901	-	12,12,12	1.01	0	17,17,17	1.55	2 (11%)
3	CIT	A	902	-	12,12,12	1.15	1 (8%)	17,17,17	1.58	2 (11%)
4	GOL	A	901	-	5,5,5	0.94	0	5,5,5	1.01	0
3	CIT	B	903	-	12,12,12	1.14	0	17,17,17	1.17	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
4	GOL	B	902	-	-	0/4/4/4	-
3	CIT	B	901	-	-	11/16/16/16	-
3	CIT	A	902	-	-	11/16/16/16	-
4	GOL	A	901	-	-	2/4/4/4	-
3	CIT	B	903	-	-	12/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	CIT	O4-C5	-2.07	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	CIT	O5-C6-C3	-4.22	116.28	122.25
3	B	901	CIT	O6-C6-C3	3.98	119.96	113.05
3	A	902	CIT	O6-C6-C3	3.22	118.64	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	903	CIT	O5-C6-C3	-3.01	117.99	122.25
3	B	903	CIT	O6-C6-C3	2.03	116.58	113.05
3	B	901	CIT	O4-C5-C4	2.02	120.85	114.35

There are no chirality outliers.

All (36) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	A	902	CIT	C1-C2-C3-O7
3	A	902	CIT	C1-C2-C3-C6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	CIT	6	0
3	B	903	CIT	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	421/427 (98%)	1.23	88 (20%)	1	1	46, 75, 162, 171	0
1	B	422/427 (98%)	0.24	10 (2%)	59	54	47, 84, 114, 128	0
2	C	7/10 (70%)	2.31	2 (28%)	0	0	88, 99, 118, 119	0
2	D	7/10 (70%)	7.61	7 (100%)	0	0	155, 165, 170, 171	0
All	All	857/874 (98%)	0.80	107 (12%)	3	2	46, 83, 158, 171	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	553	CYS	12.8
1	A	468	GLY	10.1
2	D	158	LEU	9.6
2	D	156	THR	9.6
1	A	516	GLY	9.5
1	A	514	GLU	9.4
1	A	501	LEU	9.2
1	A	513	MET	8.8
2	D	152	THR	8.7
2	D	153	ARG	8.4
1	A	470	PHE	8.3
1	A	469	LYS	7.7
1	A	487	VAL	7.5
1	A	533	ALA	7.4
1	A	499	LYS	7.4
1	A	509	LEU	7.3
1	A	461	ARG	7.0
1	A	502	VAL	6.9
2	C	152	THR	6.5
1	A	556	TYR	6.5
2	D	157	GLN	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	504	ASP	6.3
1	A	486	VAL	6.3
1	A	519	ILE	6.2
1	A	507	ALA	6.0
2	D	154	ARG	6.0
1	A	536	VAL	5.9
1	A	550	LEU	5.8
1	A	532	HIS	5.8
1	A	492	PRO	5.7
1	A	460	THR	5.7
1	A	471	ILE	5.5
1	A	493	ASP	5.5
1	A	552	LEU	5.3
1	A	528	LEU	5.3
1	A	490	ASP	5.3
1	A	484	PHE	5.2
1	A	496	LEU	4.9
1	A	517	ASP	4.8
1	A	537	LYS	4.7
1	A	481	GLY	4.7
1	A	527	VAL	4.7
1	A	551	GLU	4.7
1	A	482	PHE	4.6
2	D	155	GLU	4.5
1	A	543	PRO	4.5
1	A	472	HIS	4.4
2	C	153	ARG	4.4
1	A	476	ARG	4.3
1	A	459	PHE	4.2
1	A	558	LEU	4.2
1	A	458	PHE	4.2
1	A	488	GLY	4.2
1	A	491	GLU	4.2
1	A	503	LEU	4.2
1	A	531	THR	4.1
1	A	489	GLY	4.0
1	A	534	GLN	4.0
1	A	512	LYS	3.9
1	A	540	GLN	3.8
1	A	498	ILE	3.8
1	A	521	SER	3.8
1	A	505	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	478	SER	3.7
1	A	539	PHE	3.7
1	A	479	SER	3.6
1	A	483	GLY	3.6
1	A	467	LYS	3.5
1	A	525	THR	3.5
1	A	463	PRO	3.4
1	A	544	ILE	3.4
1	A	560	SER	3.4
1	A	475	LEU	3.4
1	A	497	GLN	3.3
1	B	492	PRO	3.3
1	A	511	GLY	3.3
1	A	466	LEU	3.3
1	A	522	VAL	3.2
1	A	529	GLY	3.2
1	A	554	ARG	3.1
1	A	477	LYS	3.1
1	A	549	ASP	3.1
1	A	524	ASP	3.0
1	A	473	THR	3.0
1	B	486	VAL	2.9
1	A	462	ASN	2.9
1	A	508	ALA	2.8
1	A	500	SER	2.7
1	A	465	GLU	2.6
1	B	500	SER	2.6
1	B	458	PHE	2.6
1	B	490	ASP	2.5
1	A	523	ASN	2.4
1	B	487	VAL	2.4
1	A	542	ILE	2.4
1	A	588	LYS	2.4
1	A	506	PRO	2.4
1	B	499	LYS	2.3
1	A	530	HIS	2.3
1	B	457	PRO	2.2
1	A	480	ARG	2.2
1	A	495	PHE	2.2
1	A	538	ILE	2.2
1	A	559	GLY	2.2
1	B	491	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	546	ALA	2.1
1	B	493	ASP	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	CA	B	906	1/1	0.19	0.15	141,141,141,141	0
5	CA	B	908	1/1	0.23	0.11	126,126,126,126	0
5	CA	B	905	1/1	0.32	0.18	128,128,128,128	0
5	CA	A	905	1/1	0.36	0.29	154,154,154,154	0
5	CA	A	907	1/1	0.54	0.13	95,95,95,95	0
3	CIT	B	901	13/13	0.55	0.53	120,141,149,149	0
5	CA	A	903	1/1	0.72	0.18	135,135,135,135	0
3	CIT	B	903	13/13	0.79	0.22	65,93,103,104	0
5	CA	B	904	1/1	0.79	0.29	98,98,98,98	0
5	CA	A	906	1/1	0.80	0.23	143,143,143,143	0
4	GOL	A	901	6/6	0.81	0.51	86,99,173,227	0
5	CA	B	909	1/1	0.82	0.10	105,105,105,105	0
3	CIT	A	902	13/13	0.86	0.15	87,102,110,110	0
5	CA	B	907	1/1	0.92	0.29	173,173,173,173	0
4	GOL	B	902	6/6	0.94	0.18	62,63,72,78	0
5	CA	A	904	1/1	0.95	0.07	114,114,114,114	0

6.5 Other polymers ⓘ

There are no such residues in this entry.