



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 6TWX / pdb_00006twx
Title : MAGI1_2 complexed with a phosphorylated 16E6 peptide
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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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

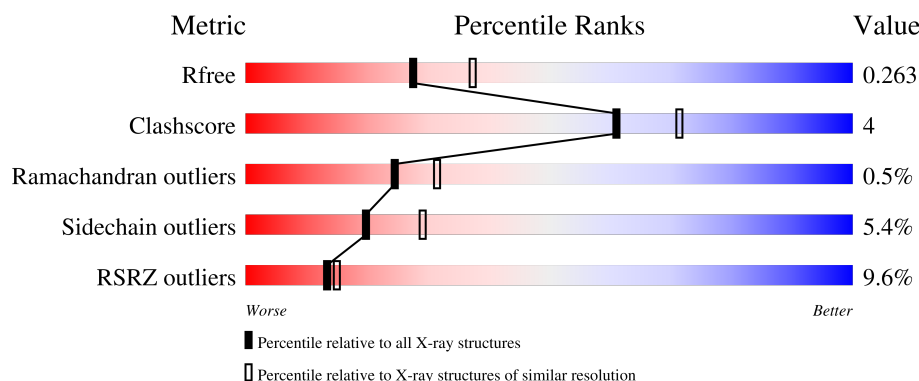
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	12% 85% 12% ..
1	B	427	7% 83% 15% ..
2	C	10	30% 10% 60%
2	D	10	20% 20% 10% 70%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6920 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	1	0
			3319	2088	568	649	14			
1	B	421	Total	C	N	O	S	0	1	0
			3326	2091	571	650	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	-	expression tag	UNP Q96QZ7
A	559	GLY	-	linker	UNP Q96QZ7
A	560	SER	-	linker	UNP Q96QZ7
A	605	GLU	ALA	conflict	UNP P07355
B	452	GLY	-	expression tag	UNP Q96QZ7
B	453	SER	-	expression tag	UNP Q96QZ7
B	454	MET	-	expression tag	UNP Q96QZ7
B	559	GLY	-	linker	UNP Q96QZ7
B	560	SER	-	linker	UNP Q96QZ7
B	605	GLU	ALA	conflict	UNP P07355

- Molecule 2 is a protein called 16E6 peptide.

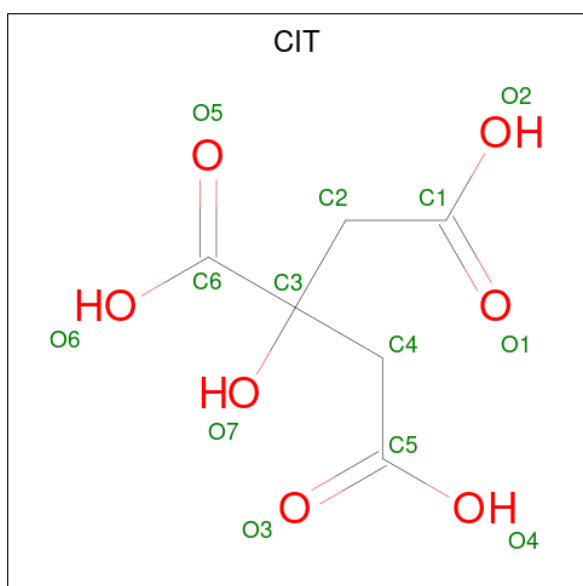
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	P	0	0	0
			38	20	5	12	1			
2	D	3	Total	C	N	O	P	0	0	0
			29	15	4	9	1			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

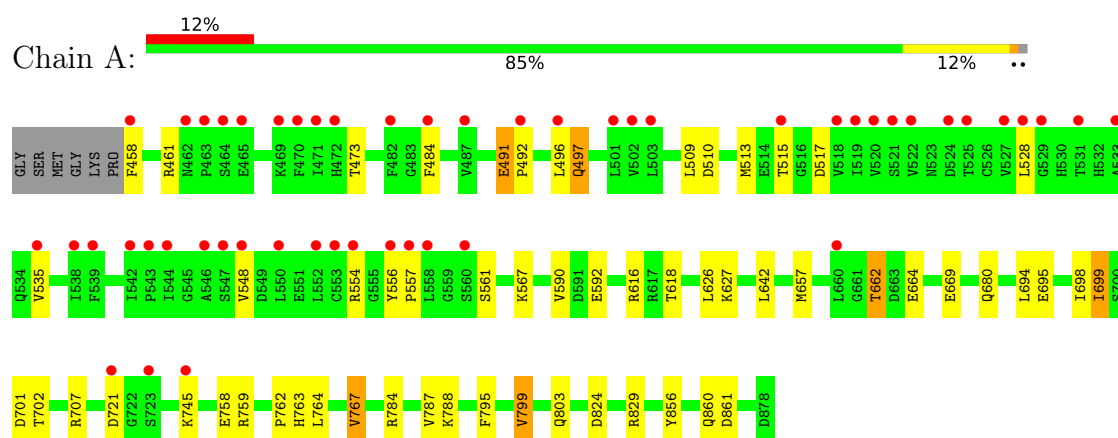
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	68	Total	O	0	0
			68	68		
6	B	78	Total	O	0	0
			78	78		

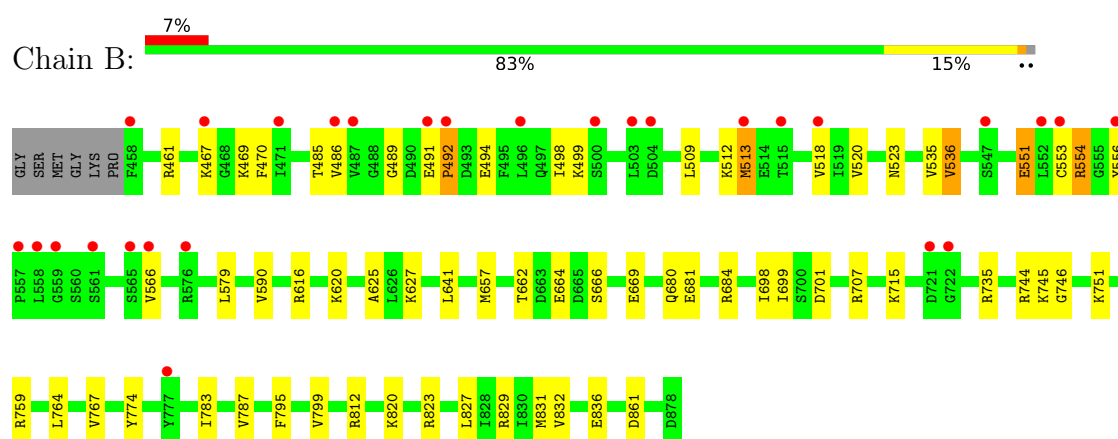
3 Residue-property plots [i](#)

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.

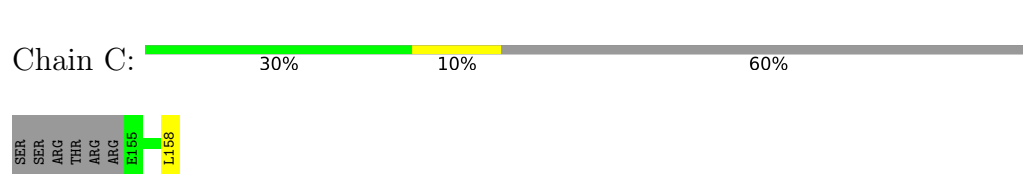
- Molecule 1: Membrane-associated guanylate kinase, WW and PDZ domain-containing protein 1, Annexin A2



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



- Molecule 2: 16E6 peptide



- Molecule 2: 16E6 peptide

Chain D:



SER	T156	Q157
SER		L158
ARG		
THR		
ARG		
ARG		
GLU		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.47Å 96.55Å 198.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 2.30 46.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.91-2.30) 98.8 (46.91-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.209 , 0.259 0.214 , 0.263	Depositor DCC
R_{free} test set	2561 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6920	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.63% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/3369	0.37	0/4534
1	B	0.22	0/3376	0.40	0/4542
2	C	0.10	0/25	0.27	0/29
2	D	0.08	0/17	0.25	0/20
All	All	0.22	0/6787	0.38	0/9125

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	3319	0	3309	26	0
1	B	3326	0	3323	31	0
2	C	38	0	30	1	0
2	D	29	0	26	0	0
3	A	6	0	8	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	0	0	0
6	A	68	0	0	1	0
6	B	78	0	0	3	0
All	All	6920	0	6719	57	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 (57) 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:657:MET:HE1	1:A:698:ILE:HG12	1.59	0.85
1:B:657:MET:HE1	1:B:698:ILE:HA	1.65	0.78
1:B:520:VAL:HB	1:B:551:GLU:HG2	1.68	0.76
1:B:795:PHE:O	1:B:799:VAL:HG12	1.93	0.68
1:B:518:VAL:HB	1:B:553:CYS:HB3	1.74	0.68
1:A:561:SER:O	1:A:567:LYS:NZ	2.24	0.67
1:B:662:THR:HG21	1:B:701:ASP:HB3	1.76	0.67
1:B:512:LYS:O	1:B:554:ARG:NH1	2.28	0.64
1:B:812:ARG:NH2	6:B:1005:HOH:O	2.29	0.64
1:B:566:VAL:HG23	1:B:836:GLU:HG3	1.80	0.63
1:B:681:GLU:OE2	1:B:684:ARG:NH2	2.27	0.63
1:B:669:GLU:OE2	1:B:812:ARG:NH1	2.32	0.63
1:B:783:ILE:HD13	1:B:795:PHE:HB3	1.82	0.62
1:A:824:ASP:OD2	4:A:902:CIT:O7	2.22	0.58
1:B:536:VAL:HG22	2:C:158:LEU:HD21	1.88	0.56
1:B:735:ARG:HG3	1:B:774:TYR:CE1	2.43	0.54
1:A:626:LEU:HD12	1:A:642:LEU:HD11	1.90	0.54
1:A:662:THR:HG21	1:A:701:ASP:HB3	1.90	0.53
1:A:491:GLU:HG3	1:A:492:PRO:HD2	1.90	0.53
1:B:620:LYS:HE3	1:B:625:ALA:HB2	1.89	0.52
1:A:473:THR:OG1	1:A:510:ASP:OD2	2.23	0.52
1:A:461:ARG:HA	1:A:528:LEU:HB3	1.91	0.52
1:B:489:GLY:H	1:B:494:GLU:HG3	1.75	0.52
1:A:787:VAL:O	1:A:788:LYS:NZ	2.43	0.50
1:A:803:GLN:NE2	6:A:1005:HOH:O	2.43	0.50
1:A:795:PHE:O	1:A:799:VAL:HG13	2.11	0.49
1:A:758:GLU:OE1	1:B:751:LYS:NZ	2.44	0.49
1:A:721:ASP:CG	1:A:762:PRO:HG2	2.38	0.49
1:B:827:LEU:O	1:B:831:MET:HG2	2.14	0.48
1:A:694:LEU:O	1:A:698:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:903:CIT:O2	4:B:903:CIT:O7	2.23	0.46
1:A:695:GLU:O	1:A:699:ILE:HG12	2.15	0.46
1:A:484:PHE:CG	1:A:513:MET:HE1	2.49	0.46
1:B:823:ARG:NH1	6:B:1018:HOH:O	2.49	0.46
1:A:497:GLN:HA	1:A:517:ASP:O	2.17	0.45
1:B:469:LYS:O	1:B:553:CYS:HA	2.17	0.45
1:B:498:ILE:HG13	1:B:513:MET:SD	2.56	0.45
1:A:763:HIS:O	1:A:767:VAL:HG13	2.18	0.43
1:B:744:ARG:HH21	1:B:746:GLY:HA3	1.82	0.43
1:A:759:ARG:HB2	1:A:764:LEU:HG	2.01	0.43
1:B:666:SER:OG	1:B:829:ARG:NH2	2.51	0.43
1:B:820:LYS:O	1:B:823:ARG:NH2	2.42	0.42
1:B:715:LYS:NZ	6:B:1019:HOH:O	2.51	0.42
1:B:469:LYS:N	1:B:554:ARG:O	2.30	0.42
1:B:759:ARG:HB2	1:B:764:LEU:HG	2.01	0.42
1:B:491:GLU:O	1:B:492:PRO:C	2.62	0.42
1:B:470:PHE:HE1	1:B:520:VAL:HG21	1.85	0.42
1:A:702:THR:OG1	1:A:707:ARG:HG3	2.20	0.42
1:B:641:LEU:HD23	1:B:832:VAL:HG13	2.00	0.42
1:A:458:PHE:HD2	1:A:556:TYR:HE1	1.66	0.42
1:A:496:LEU:HD13	1:A:535:VAL:HG21	2.02	0.41
1:A:784:ARG:O	1:A:788:LYS:NZ	2.50	0.41
1:A:517:ASP:OD1	1:A:554:ARG:HB3	2.21	0.41
1:A:669:GLU:OE1	1:A:829:ARG:HD2	2.20	0.40
1:B:657:MET:HE2	1:B:701:ASP:HB2	2.03	0.40
1:B:699:ILE:O	1:B:707:ARG:NH1	2.54	0.40
1:A:856:TYR:O	1:A:860:GLN:HG2	2.21	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	420/427 (98%)	409 (97%)	9 (2%)	2 (0%)	24	31
1	B	420/427 (98%)	409 (97%)	9 (2%)	2 (0%)	24	31
2	C	1/10 (10%)	1 (100%)	0	0	100	100
2	D	1/10 (10%)	1 (100%)	0	0	100	100
All	All	842/874 (96%)	820 (97%)	18 (2%)	4 (0%)	24	31

All (4) Ramachandran outliers are listed below:

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

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	360/370 (97%)	343 (95%)	17 (5%)	23	35
1	B	362/370 (98%)	340 (94%)	22 (6%)	17	24
2	C	3/9 (33%)	3 (100%)	0	100	100
2	D	2/9 (22%)	2 (100%)	0	100	100
All	All	727/758 (96%)	688 (95%)	39 (5%)	20	29

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	GLU
1	A	497	GLN
1	A	509	LEU
1	A	515	THR
1	A	548	VAL
1	A	592	GLU
1	A	616	ARG

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Mol	Chain	Res	Type
1	A	618	THR
1	A	627	LYS
1	A	662	THR
1	A	664	GLU
1	A	680	GLN
1	A	699	ILE
1	A	745	LYS
1	A	767	VAL
1	A	799	VAL
1	A	861	ASP
1	B	461	ARG
1	B	467	LYS
1	B	485	THR
1	B	486	VAL
1	B	499	LYS
1	B	509	LEU
1	B	513	MET
1	B	523	ASN
1	B	535	VAL
1	B	536	VAL
1	B	551	GLU
1	B	554	ARG
1	B	556	TYR
1	B	579	LEU
1	B	616	ARG
1	B	627	LYS
1	B	664	GLU
1	B	680	GLN
1	B	745	LYS
1	B	767	VAL
1	B	787	VAL
1	B	861	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	680	GLN
1	A	800	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	TPO	C	156	2	8,10,11	1.27	0	10,14,16	1.27	0
2	TPO	D	156	2	8,10,11	1.28	0	10,14,16	1.36	1 (10%)

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	TPO	C	156	2	-	3/9/11/13	-
2	TPO	D	156	2	-	6/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	156	TPO	P-OG1-CB	-2.72	115.93	123.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	156	TPO	CG2-CB-OG1-P
2	D	156	TPO	N-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
2	D	156	TPO	N-CA-CB-OG1
2	D	156	TPO	C-CA-CB-CG2
2	D	156	TPO	CG2-CB-OG1-P
2	D	156	TPO	CB-OG1-P-O2P
2	C	156	TPO	CB-OG1-P-O2P
2	C	156	TPO	C-CA-CB-CG2
2	D	156	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	GOL	A	901	-	5,5,5	0.84	0	5,5,5	1.23	1 (20%)
4	CIT	B	903	-	12,12,12	1.05	0	17,17,17	1.50	3 (17%)
3	GOL	B	902	-	5,5,5	1.00	0	5,5,5	1.23	0
4	CIT	B	901	-	12,12,12	1.05	0	17,17,17	1.48	2 (11%)
4	CIT	A	902	-	12,12,12	1.20	2 (16%)	17,17,17	1.09	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	-	-	3/4/4/4	-
4	CIT	B	901	-	-	9/16/16/16	-
4	CIT	A	902	-	-	6/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	CIT	O2-C1	-2.19	1.23	1.30
4	A	902	CIT	O4-C5	-2.17	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	CIT	O6-C6-C3	3.69	120.22	113.14
4	B	901	CIT	O6-C6-C3	3.66	120.15	113.14
4	A	902	CIT	O5-C6-C3	-2.58	117.10	122.09
4	B	903	CIT	O2-C1-C2	2.29	121.60	114.35
4	B	903	CIT	O4-C5-C4	2.25	121.47	114.35
4	A	902	CIT	O6-C6-C3	2.19	117.34	113.14
4	B	901	CIT	O4-C5-C4	2.16	121.20	114.35
3	A	901	GOL	C3-C2-C1	-2.16	103.87	111.80

There are no chirality outliers.

All (29) 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	C2-C3-C4-C5
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-O7
4	B	903	CIT	C1-C2-C3-C4
4	B	903	CIT	C1-C2-C3-C6
4	B	903	CIT	C2-C3-C6-O5

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	CIT	1	0
4	A	902	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 ⓘ

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%)	0.55	51 (12%) 8 9	25, 69, 153, 209	1 (0%)
1	B	421/427 (98%)	0.51	28 (6%) 24 26	41, 74, 121, 167	1 (0%)
2	C	3/10 (30%)	1.36	0 100 100	115, 115, 123, 130	0
2	D	2/10 (20%)	2.50	2 (100%) 0 0	142, 142, 142, 162	0
All	All	847/874 (96%)	0.54	81 (9%) 13 15	25, 72, 144, 209	2 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	VAL	4.6
1	A	520	VAL	4.4
1	A	560	SER	4.1
1	B	487	VAL	4.0
1	B	566	VAL	4.0
1	A	519	ILE	4.0
1	B	503	LEU	3.8
1	A	471	ILE	3.8
1	A	544	ILE	3.6
1	A	463	PRO	3.5
1	A	542	ILE	3.5
1	A	458	PHE	3.5
1	A	470	PHE	3.5
1	A	524	ASP	3.5
1	A	503	LEU	3.5
1	B	458	PHE	3.4
1	B	471	ILE	3.4
1	A	528	LEU	3.3
1	A	531	THR	3.3
1	A	502	VAL	3.3
1	A	527	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	518	VAL	3.3
1	B	486	VAL	3.2
1	A	547	SER	3.2
1	B	722	GLY	3.2
1	B	557	PRO	3.1
1	A	538	ILE	3.1
1	A	557	PRO	3.1
1	B	500	SER	3.1
1	B	565	SER	3.1
1	A	553	CYS	3.0
1	A	496	LEU	3.0
1	B	552	LEU	3.0
2	D	158	LEU	3.0
1	A	472	HIS	3.0
1	A	721	ASP	2.9
1	A	745	LYS	2.8
1	B	576	ARG	2.8
1	A	515	THR	2.8
1	B	556	TYR	2.8
1	A	558	LEU	2.8
1	A	521	SER	2.8
1	B	559	GLY	2.8
1	A	723	SER	2.7
1	B	561	SER	2.7
1	A	533	ALA	2.7
1	A	660	LEU	2.7
1	A	548	VAL	2.7
1	A	464	SER	2.7
1	A	522	VAL	2.6
1	A	501	LEU	2.6
1	A	462	ASN	2.6
1	B	553	CYS	2.6
1	B	513	MET	2.6
1	A	525	THR	2.5
1	A	469	LYS	2.5
1	A	492	PRO	2.5
1	A	484	PHE	2.5
1	A	518	VAL	2.5
1	A	546	ALA	2.5
1	B	558	LEU	2.4
1	A	539	PHE	2.4
1	B	496	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	554	ARG	2.4
1	A	550	LEU	2.4
1	A	465	GLU	2.3
1	A	556	TYR	2.3
1	B	504	ASP	2.2
1	B	547	SER	2.2
1	B	515	THR	2.2
1	A	482	PHE	2.2
1	B	492	PRO	2.2
1	B	491	GLU	2.2
1	A	529	GLY	2.2
1	B	777	TYR	2.1
1	A	543	PRO	2.1
1	B	467	LYS	2.1
1	B	721[A]	ASP	2.1
2	D	157	GLN	2.0
1	A	552	LEU	2.0
1	A	487	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TPO	D	156	11/12	0.58	0.12	102,134,154,158	0
2	TPO	C	156	11/12	0.81	0.15	126,142,147,147	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	CA	B	907	1/1	0.43	0.11	160,160,160,160	0
4	CIT	A	902	13/13	0.51	0.15	102,129,135,136	0
4	CIT	B	903	13/13	0.56	0.18	116,122,133,135	0
5	CA	A	903	1/1	0.57	0.13	135,135,135,135	0
5	CA	A	905	1/1	0.59	0.15	133,133,133,133	0
5	CA	A	906	1/1	0.62	0.25	108,108,108,108	0
5	CA	B	905	1/1	0.71	0.10	122,122,122,122	0
5	CA	B	906	1/1	0.77	0.13	140,140,140,140	0
4	CIT	B	901	13/13	0.77	0.15	75,116,131,132	0
5	CA	B	908	1/1	0.85	0.13	112,112,112,112	0
5	CA	B	904	1/1	0.92	0.12	85,85,85,85	0
3	GOL	B	902	6/6	0.95	0.10	45,59,61,63	0
5	CA	A	904	1/1	0.95	0.08	128,128,128,128	0
3	GOL	A	901	6/6	0.95	0.15	52,55,96,120	0
5	CA	B	909	1/1	0.95	0.07	87,87,87,87	0
5	CA	A	907	1/1	0.99	0.10	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.