



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 02:53 PM EDT

PDB ID : 5NAF
Title : Co-crystal structure of an MeCP2 peptide with TBLR1 WD40 domain
Authors : Kruusvee, V.; Cook, A.G.
Deposited on : 2017-02-27
Resolution : 2.49 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

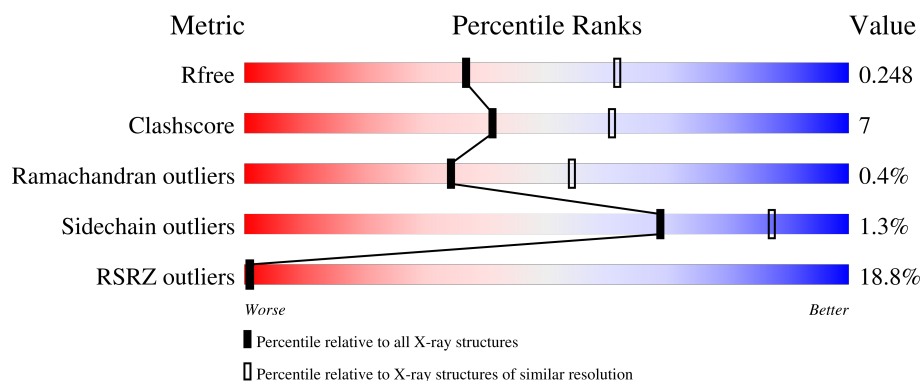
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	402	
1	B	402	
1	C	402	
1	D	402	
2	E	25	

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Mol	Chain	Length	Quality of chain
2	F	25	

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	GOL	D	606	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10400 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 F-box-like/WD repeat-containing protein TBL1XR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2654	1669	457	513	15			
1	B	348	Total	C	N	O	S	0	0	0
			2616	1651	452	498	15			
1	C	339	Total	C	N	O	S	0	0	0
			2235	1395	399	430	11			
1	D	331	Total	C	N	O	S	0	0	0
			2114	1309	384	410	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	MET	-	initiating methionine	UNP Q8BHHJ5
A	114	GLY	-	expression tag	UNP Q8BHHJ5
A	115	SER	-	expression tag	UNP Q8BHHJ5
A	116	SER	-	expression tag	UNP Q8BHHJ5
A	117	HIS	-	expression tag	UNP Q8BHHJ5
A	118	HIS	-	expression tag	UNP Q8BHHJ5
A	119	HIS	-	expression tag	UNP Q8BHHJ5
A	120	HIS	-	expression tag	UNP Q8BHHJ5
A	121	HIS	-	expression tag	UNP Q8BHHJ5
A	122	HIS	-	expression tag	UNP Q8BHHJ5
A	123	SER	-	expression tag	UNP Q8BHHJ5
A	124	SER	-	expression tag	UNP Q8BHHJ5
A	125	GLY	-	expression tag	UNP Q8BHHJ5
A	126	LEU	-	expression tag	UNP Q8BHHJ5
A	127	GLU	-	expression tag	UNP Q8BHHJ5
A	128	VAL	-	expression tag	UNP Q8BHHJ5
A	129	LEU	-	expression tag	UNP Q8BHHJ5
A	130	PHE	-	expression tag	UNP Q8BHHJ5
A	131	GLN	-	expression tag	UNP Q8BHHJ5
A	132	GLY	-	expression tag	UNP Q8BHHJ5
A	133	PRO	-	expression tag	UNP Q8BHHJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	113	MET	-	initiating methionine	UNP Q8BHIJ5
B	114	GLY	-	expression tag	UNP Q8BHIJ5
B	115	SER	-	expression tag	UNP Q8BHIJ5
B	116	SER	-	expression tag	UNP Q8BHIJ5
B	117	HIS	-	expression tag	UNP Q8BHIJ5
B	118	HIS	-	expression tag	UNP Q8BHIJ5
B	119	HIS	-	expression tag	UNP Q8BHIJ5
B	120	HIS	-	expression tag	UNP Q8BHIJ5
B	121	HIS	-	expression tag	UNP Q8BHIJ5
B	122	HIS	-	expression tag	UNP Q8BHIJ5
B	123	SER	-	expression tag	UNP Q8BHIJ5
B	124	SER	-	expression tag	UNP Q8BHIJ5
B	125	GLY	-	expression tag	UNP Q8BHIJ5
B	126	LEU	-	expression tag	UNP Q8BHIJ5
B	127	GLU	-	expression tag	UNP Q8BHIJ5
B	128	VAL	-	expression tag	UNP Q8BHIJ5
B	129	LEU	-	expression tag	UNP Q8BHIJ5
B	130	PHE	-	expression tag	UNP Q8BHIJ5
B	131	GLN	-	expression tag	UNP Q8BHIJ5
B	132	GLY	-	expression tag	UNP Q8BHIJ5
B	133	PRO	-	expression tag	UNP Q8BHIJ5
C	113	MET	-	initiating methionine	UNP Q8BHIJ5
C	114	GLY	-	expression tag	UNP Q8BHIJ5
C	115	SER	-	expression tag	UNP Q8BHIJ5
C	116	SER	-	expression tag	UNP Q8BHIJ5
C	117	HIS	-	expression tag	UNP Q8BHIJ5
C	118	HIS	-	expression tag	UNP Q8BHIJ5
C	119	HIS	-	expression tag	UNP Q8BHIJ5
C	120	HIS	-	expression tag	UNP Q8BHIJ5
C	121	HIS	-	expression tag	UNP Q8BHIJ5
C	122	HIS	-	expression tag	UNP Q8BHIJ5
C	123	SER	-	expression tag	UNP Q8BHIJ5
C	124	SER	-	expression tag	UNP Q8BHIJ5
C	125	GLY	-	expression tag	UNP Q8BHIJ5
C	126	LEU	-	expression tag	UNP Q8BHIJ5
C	127	GLU	-	expression tag	UNP Q8BHIJ5
C	128	VAL	-	expression tag	UNP Q8BHIJ5
C	129	LEU	-	expression tag	UNP Q8BHIJ5
C	130	PHE	-	expression tag	UNP Q8BHIJ5
C	131	GLN	-	expression tag	UNP Q8BHIJ5
C	132	GLY	-	expression tag	UNP Q8BHIJ5
C	133	PRO	-	expression tag	UNP Q8BHIJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	113	MET	-	initiating methionine	UNP Q8BHIJ5
D	114	GLY	-	expression tag	UNP Q8BHIJ5
D	115	SER	-	expression tag	UNP Q8BHIJ5
D	116	SER	-	expression tag	UNP Q8BHIJ5
D	117	HIS	-	expression tag	UNP Q8BHIJ5
D	118	HIS	-	expression tag	UNP Q8BHIJ5
D	119	HIS	-	expression tag	UNP Q8BHIJ5
D	120	HIS	-	expression tag	UNP Q8BHIJ5
D	121	HIS	-	expression tag	UNP Q8BHIJ5
D	122	HIS	-	expression tag	UNP Q8BHIJ5
D	123	SER	-	expression tag	UNP Q8BHIJ5
D	124	SER	-	expression tag	UNP Q8BHIJ5
D	125	GLY	-	expression tag	UNP Q8BHIJ5
D	126	LEU	-	expression tag	UNP Q8BHIJ5
D	127	GLU	-	expression tag	UNP Q8BHIJ5
D	128	VAL	-	expression tag	UNP Q8BHIJ5
D	129	LEU	-	expression tag	UNP Q8BHIJ5
D	130	PHE	-	expression tag	UNP Q8BHIJ5
D	131	GLN	-	expression tag	UNP Q8BHIJ5
D	132	GLY	-	expression tag	UNP Q8BHIJ5
D	133	PRO	-	expression tag	UNP Q8BHIJ5

- Molecule 2 is a protein called Methyl-CpG-binding protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			81	52	18	11			
2	F	10	Total	C	N	O	0	0	0
			72	47	14	11			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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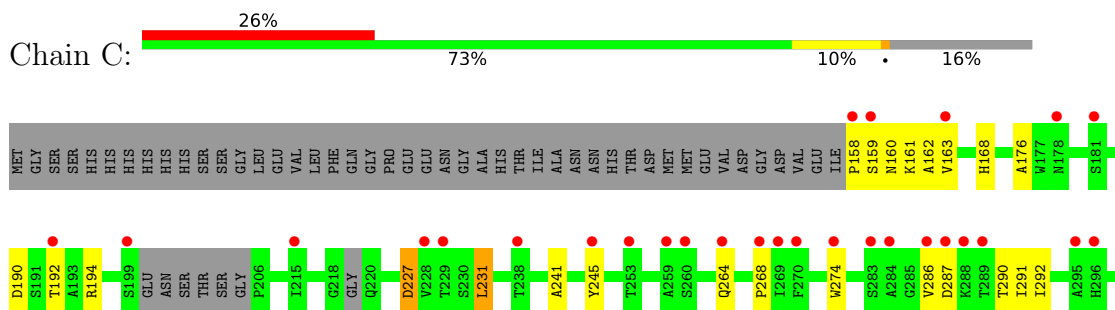
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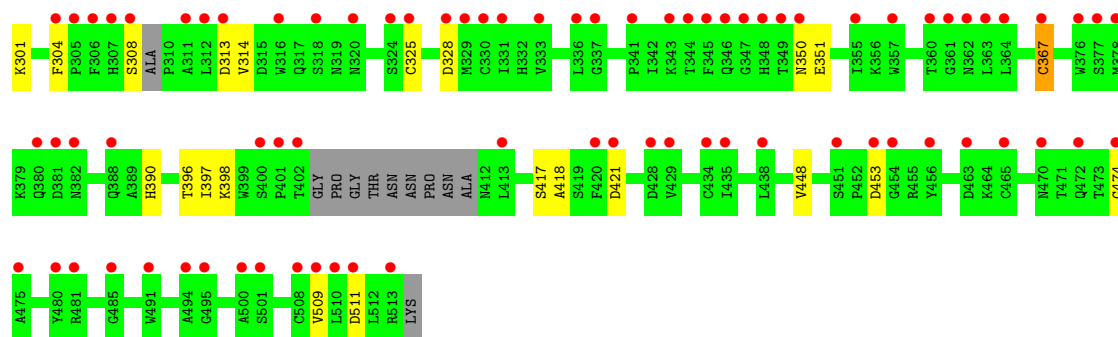
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

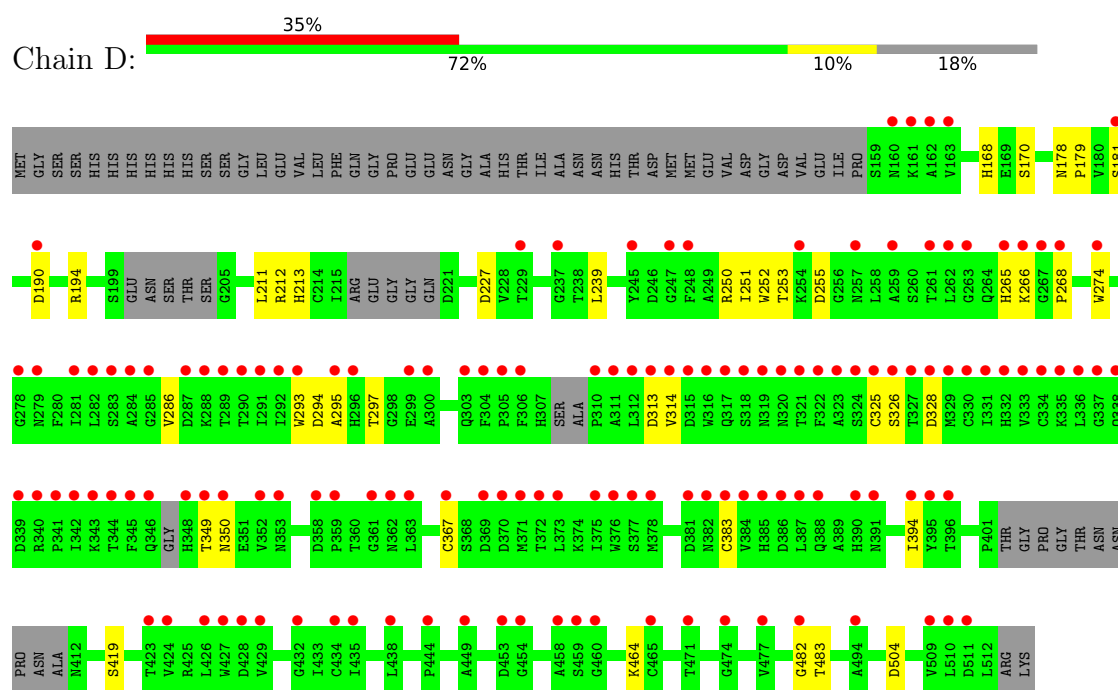
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	202	Total	O	0	0
			202	202		
4	B	187	Total	O	0	0
			187	187		
4	C	74	Total	O	0	0
			74	74		
4	D	40	Total	O	0	0
			40	40		
4	E	5	Total	O	0	0
			5	5		
4	F	6	Total	O	0	0
			6	6		

- Molecule 1: F-box-like/WD repeat-containing protein TBL1XR1

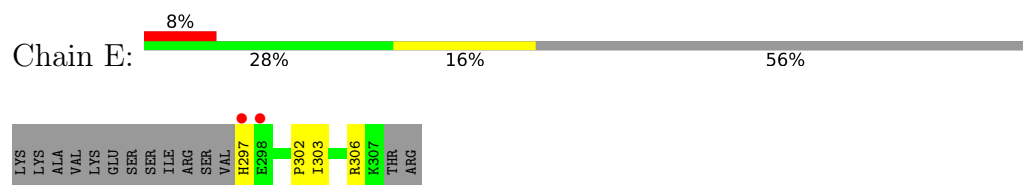




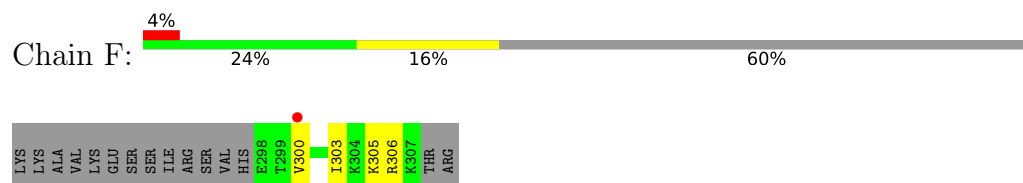
● Molecule 1: F-box-like/WD repeat-containing protein TBL1XR1



● Molecule 2: Methyl-CpG-binding protein 2



● Molecule 2: Methyl-CpG-binding protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.63Å 58.64Å 155.10Å 97.63° 91.17° 90.24°	Depositor
Resolution (Å)	49.64 – 2.49 49.64 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.64-2.49) 97.5 (49.64-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.203 , 0.248 0.203 , 0.248	Depositor DCC
R_{free} test set	2513 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10400	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.55% 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: 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	0.28	0/2720	0.53	0/3710
1	B	0.29	0/2682	0.52	0/3658
1	C	0.30	0/2286	0.57	2/3138 (0.1%)
1	D	0.34	0/2157	0.54	0/2966
2	E	0.26	0/82	0.50	0/109
2	F	0.28	0/72	0.55	0/95
All	All	0.30	0/9999	0.54	2/13676 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	LEU	CB-CG-CD2	-11.20	91.97	111.00
1	C	231	LEU	CB-CG-CD1	5.91	121.05	111.00

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	2654	0	2472	35	0
1	B	2616	0	2456	32	1
1	C	2235	0	1708	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2114	0	1569	27	0
2	E	81	0	77	3	0
2	F	72	0	80	4	0
3	A	42	0	56	0	1
3	B	30	0	40	0	0
3	C	6	0	8	0	0
3	D	36	0	47	0	0
4	A	202	0	0	5	1
4	B	187	0	0	3	1
4	C	74	0	0	7	0
4	D	40	0	0	3	0
4	E	5	0	0	1	0
4	F	6	0	0	0	0
All	All	10400	0	8513	130	2

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 7.

The worst 5 of 130 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:D:265:HIS:HE2	1:D:293:TRP:HZ2	1.11	0.92
1:A:194:ARG:HH11	1:A:208:GLN:NE2	1.68	0.91
1:B:302:GLN:HE22	1:B:337:GLY:H	1.23	0.87
1:A:194:ARG:HH11	1:A:208:GLN:HE21	1.18	0.84
1:D:483:THR:OG1	1:D:504:ASP:OD2	1.95	0.83

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLN:NE2	3:A:605:GOL:O3[1_565]	2.16	0.04
4:A:844:HOH:O	4:B:859:HOH:O[1_545]	2.19	0.01

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	346/402 (86%)	329 (95%)	15 (4%)	2 (1%)	25	43
1	B	342/402 (85%)	328 (96%)	13 (4%)	1 (0%)	41	61
1	C	329/402 (82%)	312 (95%)	16 (5%)	1 (0%)	41	61
1	D	319/402 (79%)	304 (95%)	14 (4%)	1 (0%)	41	61
2	E	9/25 (36%)	9 (100%)	0	0	100	100
2	F	8/25 (32%)	8 (100%)	0	0	100	100
All	All	1353/1658 (82%)	1290 (95%)	58 (4%)	5 (0%)	34	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	266	LYS
1	C	264	GLN
1	A	199	SER
1	A	200	GLU
1	B	213	HIS

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	276/338 (82%)	274 (99%)	2 (1%)	84	94
1	B	273/338 (81%)	270 (99%)	3 (1%)	73	89
1	C	159/338 (47%)	156 (98%)	3 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	141/338 (42%)	138 (98%)	3 (2%)	53	78
2	E	6/24 (25%)	6 (100%)	0	100	100
2	F	7/24 (29%)	7 (100%)	0	100	100
All	All	862/1400 (62%)	851 (99%)	11 (1%)	69	87

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	367	CYS
1	D	213	HIS
1	D	367	CYS
1	D	325	CYS
1	B	462	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	353	ASN
1	B	470	ASN
1	D	160	ASN
1	C	213	HIS
1	B	302	GLN

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

19 ligands 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	$\# Z > 2$
3	GOL	D	601	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	A	607	-	5,5,5	0.36	0	5,5,5	0.19	0
3	GOL	D	603	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	B	605	-	5,5,5	0.36	0	5,5,5	0.25	0
3	GOL	B	602	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	B	601	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	D	606	-	5,5,5	0.77	0	5,5,5	0.60	0
3	GOL	A	601	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	D	604	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	D	605	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	A	604	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	A	605	-	5,5,5	0.36	0	5,5,5	0.38	0
3	GOL	D	602	-	5,5,5	0.37	0	5,5,5	0.28	0
3	GOL	C	601	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	B	604	-	5,5,5	0.40	0	5,5,5	0.24	0
3	GOL	B	603	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	A	606	-	5,5,5	0.37	0	5,5,5	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	601	-	-	2/4/4/4	-
3	GOL	A	607	-	-	2/4/4/4	-
3	GOL	D	603	-	-	2/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	605	-	-	4/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-
3	GOL	B	601	-	-	2/4/4/4	-
3	GOL	D	606	-	-	0/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-
3	GOL	D	604	-	-	2/4/4/4	-
3	GOL	D	605	-	-	2/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	A	605	-	-	0/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-
3	GOL	C	601	-	-	2/4/4/4	-
3	GOL	B	604	-	-	2/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	A	606	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	A	603	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-C3
3	A	607	GOL	O1-C1-C2-C3
3	B	603	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	GOL	0	1

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 [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	352/402 (87%)	0.55	6 (1%) 70 72	17, 28, 50, 127	0
1	B	348/402 (86%)	0.60	7 (2%) 65 68	18, 29, 48, 97	0
1	C	339/402 (84%)	1.63	106 (31%) 0 0	29, 70, 109, 135	0
1	D	331/402 (82%)	2.16	140 (42%) 0 0	32, 75, 125, 155	0
2	E	11/25 (44%)	1.28	2 (18%) 1 1	30, 35, 86, 89	0
2	F	10/25 (40%)	0.85	1 (10%) 7 6	28, 40, 61, 77	0
All	All	1391/1658 (83%)	1.22	262 (18%) 1 1	17, 44, 109, 155	0

The worst 5 of 262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	PHE	10.4
1	D	329	MET	9.4
1	D	330	CYS	8.3
1	D	340	ARG	7.6
1	D	361	GLY	7.4

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 ⓘ

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
3	GOL	D	606	6/6	0.24	0.52	67,70,71,74	0
3	GOL	A	601	6/6	0.43	0.31	64,68,69,69	0
3	GOL	A	606	6/6	0.64	0.33	62,67,69,72	0
3	GOL	A	602	6/6	0.65	0.26	63,65,66,66	0
3	GOL	B	604	6/6	0.69	0.30	40,57,61,62	0
3	GOL	D	605	6/6	0.71	0.21	68,71,73,73	0
3	GOL	D	601	6/6	0.72	0.18	68,74,76,77	0
3	GOL	D	603	6/6	0.72	0.20	58,61,64,65	0
3	GOL	D	602	6/6	0.73	0.21	52,53,54,55	0
3	GOL	B	602	6/6	0.74	0.29	45,49,52,53	0
3	GOL	D	604	6/6	0.76	0.20	68,71,75,78	0
3	GOL	C	601	6/6	0.77	0.21	63,66,67,67	0
3	GOL	B	605	6/6	0.78	0.22	47,50,54,57	0
3	GOL	B	601	6/6	0.79	0.19	60,61,62,64	0
3	GOL	B	603	6/6	0.81	0.35	61,70,75,75	0
3	GOL	A	603	6/6	0.83	0.36	57,60,63,67	0
3	GOL	A	607	6/6	0.83	0.19	53,56,59,59	0
3	GOL	A	604	6/6	0.84	0.35	39,45,46,47	0
3	GOL	A	605	6/6	0.84	0.23	59,60,62,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.