



Full wwPDB X-ray Structure Validation Report

Oct 8, 2014 – 12:24 AM EDT

PDB ID : 4PML
Title : Crystal Structure of human Tankyrase 2 in complex with 3-amino-benzamide.
Authors : Qiu, W.; Lam, R.; Romanov, V.; Gordon, R.; Gebremeskel, S.; Vodsedalek, J.; Thompson, C.; Beletskaya, I.; Battaile, K.P.; Pai, E.F.; Chirgadze, N.Y.
Deposited on : 2014-05-22
Resolution : 1.87 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

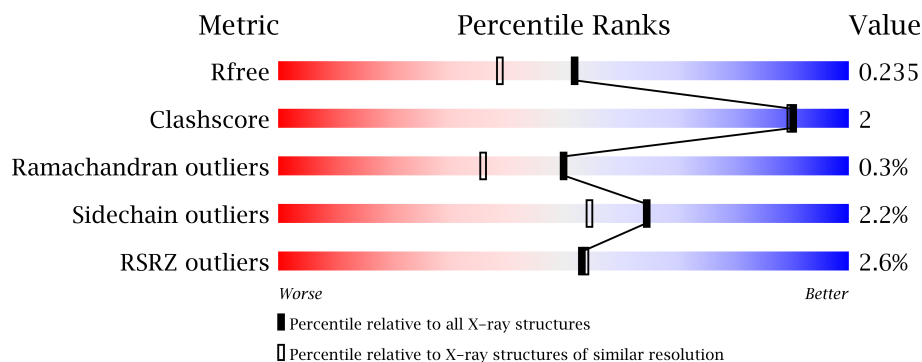
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 1.87 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}	66092	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	227	
1	B	227	
1	C	227	
1	D	227	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	1203	-	X
4	GOL	B	1203	-	X
4	GOL	D	1203	-	X
5	EDO	B	1206	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	B	1207	-	X
6	DMS	A	1205	-	X
6	DMS	C	1204	-	X
7	IPA	B	1204	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7313 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1598	1008	295	284	11			
1	B	205	Total	C	N	O	S	0	0	0
			1662	1049	304	298	11			
1	C	208	Total	C	N	O	S	0	0	0
			1678	1058	308	301	11			
1	D	198	Total	C	N	O	S	0	1	0
			1590	1002	293	283	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	938	MET	-	initiating methionine	UNP Q9H2K2
A	939	GLY	-	expression tag	UNP Q9H2K2
A	940	SER	-	expression tag	UNP Q9H2K2
A	941	SER	-	expression tag	UNP Q9H2K2
A	942	HIS	-	expression tag	UNP Q9H2K2
A	943	HIS	-	expression tag	UNP Q9H2K2
A	944	HIS	-	expression tag	UNP Q9H2K2
A	945	HIS	-	expression tag	UNP Q9H2K2
A	946	HIS	-	expression tag	UNP Q9H2K2
A	947	HIS	-	expression tag	UNP Q9H2K2
A	948	SER	-	expression tag	UNP Q9H2K2
A	949	SER	-	expression tag	UNP Q9H2K2
A	950	GLY	-	expression tag	UNP Q9H2K2
A	951	ARG	-	expression tag	UNP Q9H2K2
A	952	GLU	-	expression tag	UNP Q9H2K2
A	953	ASN	-	expression tag	UNP Q9H2K2
A	954	LEU	-	expression tag	UNP Q9H2K2
A	955	TYR	-	expression tag	UNP Q9H2K2
A	956	PHE	-	expression tag	UNP Q9H2K2
A	957	GLN	-	expression tag	UNP Q9H2K2
A	958	GLY	-	expression tag	UNP Q9H2K2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	938	MET	-	initiating methionine	UNP Q9H2K2
B	939	GLY	-	expression tag	UNP Q9H2K2
B	940	SER	-	expression tag	UNP Q9H2K2
B	941	SER	-	expression tag	UNP Q9H2K2
B	942	HIS	-	expression tag	UNP Q9H2K2
B	943	HIS	-	expression tag	UNP Q9H2K2
B	944	HIS	-	expression tag	UNP Q9H2K2
B	945	HIS	-	expression tag	UNP Q9H2K2
B	946	HIS	-	expression tag	UNP Q9H2K2
B	947	HIS	-	expression tag	UNP Q9H2K2
B	948	SER	-	expression tag	UNP Q9H2K2
B	949	SER	-	expression tag	UNP Q9H2K2
B	950	GLY	-	expression tag	UNP Q9H2K2
B	951	ARG	-	expression tag	UNP Q9H2K2
B	952	GLU	-	expression tag	UNP Q9H2K2
B	953	ASN	-	expression tag	UNP Q9H2K2
B	954	LEU	-	expression tag	UNP Q9H2K2
B	955	TYR	-	expression tag	UNP Q9H2K2
B	956	PHE	-	expression tag	UNP Q9H2K2
B	957	GLN	-	expression tag	UNP Q9H2K2
B	958	GLY	-	expression tag	UNP Q9H2K2
C	938	MET	-	initiating methionine	UNP Q9H2K2
C	939	GLY	-	expression tag	UNP Q9H2K2
C	940	SER	-	expression tag	UNP Q9H2K2
C	941	SER	-	expression tag	UNP Q9H2K2
C	942	HIS	-	expression tag	UNP Q9H2K2
C	943	HIS	-	expression tag	UNP Q9H2K2
C	944	HIS	-	expression tag	UNP Q9H2K2
C	945	HIS	-	expression tag	UNP Q9H2K2
C	946	HIS	-	expression tag	UNP Q9H2K2
C	947	HIS	-	expression tag	UNP Q9H2K2
C	948	SER	-	expression tag	UNP Q9H2K2
C	949	SER	-	expression tag	UNP Q9H2K2
C	950	GLY	-	expression tag	UNP Q9H2K2
C	951	ARG	-	expression tag	UNP Q9H2K2
C	952	GLU	-	expression tag	UNP Q9H2K2
C	953	ASN	-	expression tag	UNP Q9H2K2
C	954	LEU	-	expression tag	UNP Q9H2K2
C	955	TYR	-	expression tag	UNP Q9H2K2
C	956	PHE	-	expression tag	UNP Q9H2K2
C	957	GLN	-	expression tag	UNP Q9H2K2
C	958	GLY	-	expression tag	UNP Q9H2K2

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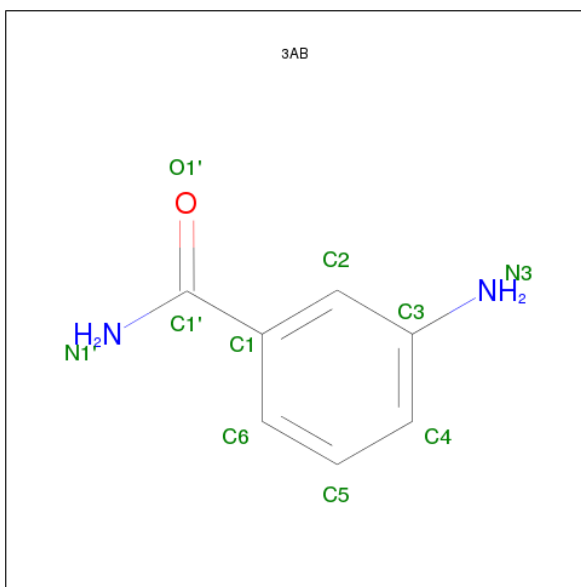
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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	HIS	-	expression tag	UNP Q9H2K2
D	944	HIS	-	expression tag	UNP Q9H2K2
D	945	HIS	-	expression tag	UNP Q9H2K2
D	946	HIS	-	expression tag	UNP Q9H2K2
D	947	HIS	-	expression tag	UNP Q9H2K2
D	948	SER	-	expression tag	UNP Q9H2K2
D	949	SER	-	expression tag	UNP Q9H2K2
D	950	GLY	-	expression tag	UNP Q9H2K2
D	951	ARG	-	expression tag	UNP Q9H2K2
D	952	GLU	-	expression tag	UNP Q9H2K2
D	953	ASN	-	expression tag	UNP Q9H2K2
D	954	LEU	-	expression tag	UNP Q9H2K2
D	955	TYR	-	expression tag	UNP Q9H2K2
D	956	PHE	-	expression tag	UNP Q9H2K2
D	957	GLN	-	expression tag	UNP Q9H2K2
D	958	GLY	-	expression tag	UNP Q9H2K2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

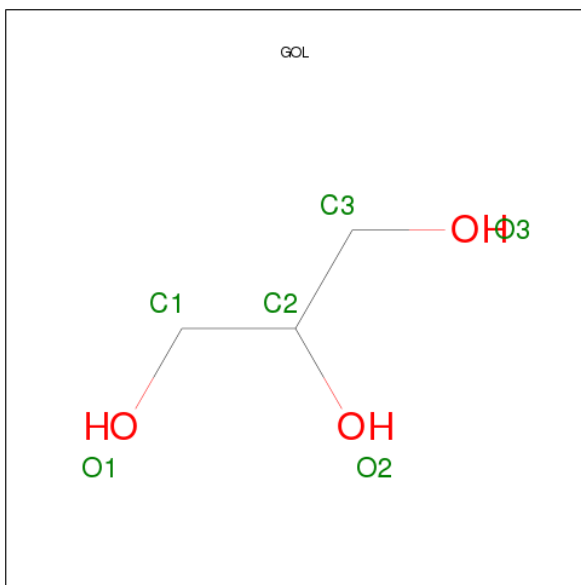
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 3-aminobenzamide (three-letter code: 3AB) (formula: C₇H₈N₂O).



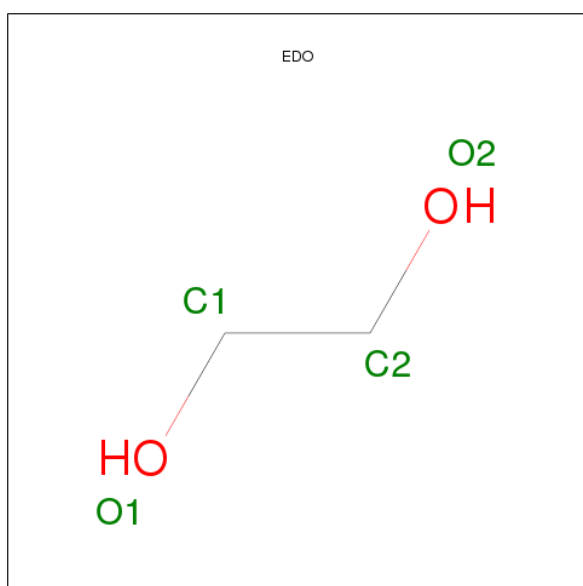
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	2	1		
3	B	1	Total	C	N	O	0	0
			10	7	2	1		
3	C	1	Total	C	N	O	0	0
			10	7	2	1		
3	D	1	Total	C	N	O	0	0
			10	7	2	1		

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



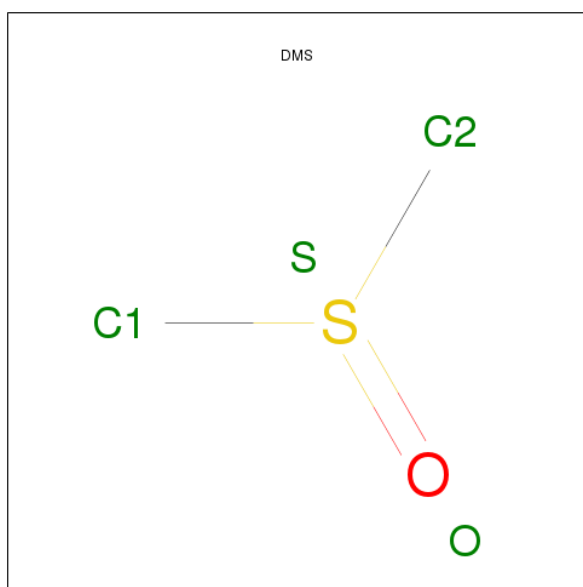
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



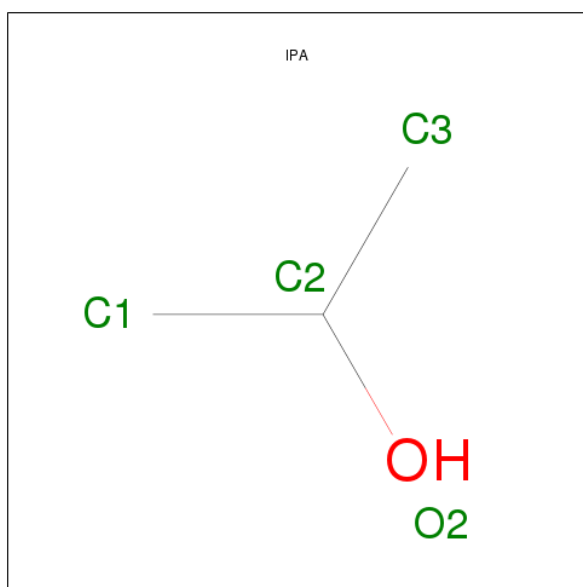
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



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

- Molecule 8 is water.

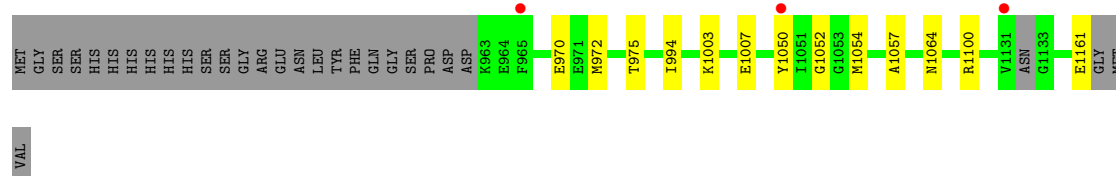
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	191	Total 191	O 191	0	0
8	B	167	Total 167	O 167	0	0
8	C	192	Total 192	O 192	0	0
8	D	135	Total 135	O 135	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

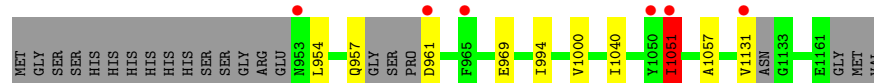
• Molecule 1: Tankyrase-2

Chain A: 



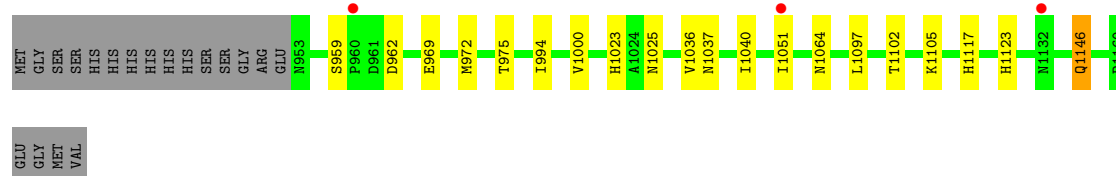
• Molecule 1: Tankyrase-2

Chain B: 



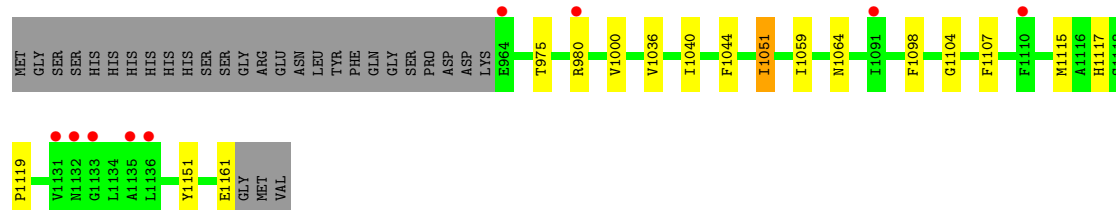
• Molecule 1: Tankyrase-2

Chain C: 



• Molecule 1: Tankyrase-2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.02Å 79.80Å 153.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.34 – 1.87 39.90 – 1.87	Depositor EDS
% Data completeness (in resolution range)	95.8 (44.34-1.87) 95.8 (39.90-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.87Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.201 , 0.223 0.213 , 0.235	Depositor DCC
R_{free} test set	1074 reflections (1.50%)	DCC
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72800 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7313	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, IPA, 3AB, EDO, DMS

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	0.36	0/1640	0.56	0/2202
1	B	0.36	0/1705	0.58	0/2289
1	C	0.36	0/1724	0.58	0/2319
1	D	0.37	0/1636	0.56	0/2202
All	All	0.36	0/6705	0.57	0/9012

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1598	0	1536	6	0
1	B	1662	0	1586	4	0
1	C	1678	0	1603	10	0
1	D	1590	0	1513	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	8	0	0
3	B	10	0	8	0	0
3	C	10	0	8	0	0
3	D	10	0	8	0	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	1	0
5	A	4	0	6	0	0
5	B	8	0	12	0	0
5	D	4	0	6	1	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
7	B	4	0	8	0	0
8	A	191	0	0	0	0
8	B	167	0	0	0	0
8	C	192	0	0	0	0
8	D	135	0	0	0	0
All	All	7313	0	6352	27	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1105:LYS:H	1:C:1123:HIS:HD2	1.36	0.73
1:B:1000:VAL:HG21	1:B:1040:ILE:HD12	1.73	0.70
1:C:1000:VAL:HG21	1:C:1040:ILE:HD12	1.82	0.62
1:C:1040:ILE:HD11	1:C:1097:LEU:HD21	1.85	0.59
1:C:959:SER:HB2	1:C:962:ASP:HB2	1.84	0.58
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.87	0.57
1:C:972:MET:HG2	1:C:994:ILE:HD11	1.85	0.57
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.91	0.53
1:C:1023:HIS:HD2	1:C:1025:ASN:H	1.59	0.51
1:D:1115[A]:MET:HE1	1:D:1119:PRO:HG3	1.96	0.48
1:A:1054:MET:HB2	4:A:1203:GOL:H32	1.95	0.48
1:D:1044:PHE:HB3	1:D:1059:ILE:HD13	1.95	0.48
1:D:1107:PHE:CG	1:D:1119:PRO:HG2	2.50	0.46
1:A:975:THR:HB	1:A:1064:ASN:HA	1.98	0.46
1:B:969:GLU:HG3	1:B:994:ILE:HG13	1.97	0.46
1:D:1104:GLY:O	5:D:1204:EDO:H12	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:969:GLU:HG3	1:C:994:ILE:HG13	1.97	0.45
1:C:1102:THR:HB	1:C:1146:GLN:HG2	2.00	0.44
1:A:972:MET:HG2	1:A:994:ILE:HD11	1.99	0.43
1:B:1051:ILE:HD13	1:D:1051:ILE:HD13	2.00	0.43
1:D:1098:PHE:HB3	1:D:1151:TYR:HB2	1.99	0.43
1:A:1003:LYS:O	1:A:1007:GLU:HG2	2.19	0.43
1:D:975:THR:HB	1:D:1064:ASN:HA	2.01	0.42
1:A:1050:TYR:CZ	1:A:1052:GLY:HA3	2.55	0.42
1:D:1059:ILE:HG12	4:D:1203:GOL:H31	2.01	0.41
1:C:975:THR:HB	1:C:1064:ASN:HA	2.02	0.41
1:D:1000:VAL:HG21	1:D:1040:ILE:HG12	2.01	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	194/227 (86%)	189 (97%)	5 (3%)	0	100	100
1	B	199/227 (88%)	196 (98%)	2 (1%)	1 (0%)	38	22
1	C	206/227 (91%)	204 (99%)	2 (1%)	0	100	100
1	D	197/227 (87%)	191 (97%)	5 (2%)	1 (0%)	38	22
All	All	796/908 (88%)	780 (98%)	14 (2%)	2 (0%)	50	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1051	ILE
1	B	1051	ILE

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	167/192 (87%)	164 (98%)	3 (2%)	71	63
1	B	174/192 (91%)	169 (97%)	5 (3%)	55	41
1	C	176/192 (92%)	172 (98%)	4 (2%)	63	52
1	D	165/192 (86%)	162 (98%)	3 (2%)	71	63
All	All	682/768 (89%)	667 (98%)	15 (2%)	64	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	970	GLU
1	A	1100	ARG
1	A	1161	GLU
1	B	954	LEU
1	B	957	GLN
1	B	961	ASP
1	B	1051	ILE
1	B	1131	VAL
1	C	1036	VAL
1	C	1037	ASN
1	C	1051	ILE
1	C	1146	GLN
1	D	980	ARG
1	D	1036	VAL
1	D	1161	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	HIS
1	A	1048	HIS
1	B	957	GLN
1	B	1011	HIS
1	B	1021	HIS
1	B	1048	HIS

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Mol	Chain	Res	Type
1	C	1023	HIS
1	C	1117	HIS
1	C	1123	HIS
1	D	1011	HIS
1	D	1109	GLN
1	D	1117	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	3AB	A	1202	-	10,10,10	1.06	1 (10%)	13,13,13	0.73	0
4	GOL	A	1203	-	5,5,5	0.15	0	5,5,5	0.23	0
5	EDO	A	1204	-	3,3,3	0.62	0	2,2,2	0.41	0
6	DMS	A	1205	-	3,3,3	0.32	0	3,3,3	0.32	0
3	3AB	B	1202	-	10,10,10	0.99	1 (10%)	13,13,13	0.68	0
4	GOL	B	1203	-	5,5,5	0.14	0	5,5,5	0.20	0
7	IPA	B	1204	-	3,3,3	0.65	0	3,3,3	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	B	1205	-	3,3,3	0.27	0	3,3,3	0.59	0
5	EDO	B	1206	-	3,3,3	0.61	0	2,2,2	0.39	0
5	EDO	B	1207	-	3,3,3	0.51	0	2,2,2	0.60	0
3	3AB	C	1201	-	10,10,10	1.17	1 (10%)	13,13,13	0.70	0
4	GOL	C	1203	-	5,5,5	0.15	0	5,5,5	0.18	0
6	DMS	C	1204	-	3,3,3	0.30	0	3,3,3	0.28	0
3	3AB	D	1202	-	10,10,10	1.04	1 (10%)	13,13,13	0.67	0
4	GOL	D	1203	-	5,5,5	0.14	0	5,5,5	0.24	0
5	EDO	D	1204	-	3,3,3	0.60	0	2,2,2	0.24	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	3AB	A	1202	-	-	0/4/4/4	0/1/1/1
4	GOL	A	1203	-	-	0/4/4/4	0/0/0/0
5	EDO	A	1204	-	-	0/1/1/1	0/0/0/0
6	DMS	A	1205	-	-	0/0/0/0	0/0/0/0
3	3AB	B	1202	-	-	0/4/4/4	0/1/1/1
4	GOL	B	1203	-	-	0/4/4/4	0/0/0/0
7	IPA	B	1204	-	-	0/0/0/0	0/0/0/0
6	DMS	B	1205	-	-	0/0/0/0	0/0/0/0
5	EDO	B	1206	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1207	-	-	0/1/1/1	0/0/0/0
3	3AB	C	1201	-	-	0/4/4/4	0/1/1/1
4	GOL	C	1203	-	-	0/4/4/4	0/0/0/0
6	DMS	C	1204	-	-	0/0/0/0	0/0/0/0
3	3AB	D	1202	-	-	0/4/4/4	0/1/1/1
4	GOL	D	1203	-	-	0/4/4/4	0/0/0/0
5	EDO	D	1204	-	-	0/1/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1201	3AB	C1-C1'	2.91	1.55	1.50
3	A	1202	3AB	C1-C1'	2.55	1.54	1.50
3	D	1202	3AB	C1-C1'	2.42	1.54	1.50
3	B	1202	3AB	C1-C1'	2.30	1.54	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	198/227 (87%)	0.02	3 (1%) 70 71	15, 26, 45, 74	0
1	B	205/227 (90%)	0.10	6 (2%) 49 49	15, 27, 53, 81	0
1	C	208/227 (91%)	0.10	3 (1%) 72 73	13, 25, 46, 61	0
1	D	198/227 (87%)	0.47	9 (4%) 32 32	17, 33, 54, 81	0
All	All	809/908 (89%)	0.17	21 (2%) 53 54	13, 27, 51, 81	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1131	VAL	9.4
1	B	1131	VAL	3.3
1	A	1050	TYR	3.3
1	D	1110	PHE	3.1
1	D	1132	ASN	3.0
1	C	1132	ASN	2.9
1	B	1051	ILE	2.9
1	D	964	GLU	2.7
1	B	953	ASN	2.4
1	B	961	ASP	2.4
1	D	1136	LEU	2.3
1	C	960	PRO	2.3
1	D	1135	ALA	2.3
1	D	980	ARG	2.2
1	C	1051	ILE	2.2
1	B	1050	TYR	2.2
1	A	965	PHE	2.2
1	D	1091	ILE	2.1
1	D	1133	GLY	2.1
1	A	1131	VAL	2.1
1	B	965	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	B	1203	6/6	0.25	11.46	53,53,54,55	0
4	GOL	D	1203	6/6	0.28	9.15	36,38,39,40	0
6	DMS	A	1205	4/4	0.36	7.88	97,97,97,97	0
6	DMS	C	1204	4/4	0.51	7.32	97,98,98,98	0
5	EDO	B	1207	4/4	0.29	5.94	42,43,43,44	0
4	GOL	A	1203	6/6	0.17	5.64	39,42,42,44	0
5	EDO	B	1206	4/4	0.17	5.09	34,36,36,37	0
7	IPA	B	1204	4/4	0.16	2.94	50,50,50,51	0
6	DMS	B	1205	4/4	0.20	0.90	86,86,86,86	0
5	EDO	D	1204	4/4	0.12	0.71	29,30,30,33	0
3	3AB	C	1201	10/10	0.10	0.50	14,16,19,20	0
3	3AB	D	1202	10/10	0.10	-0.16	28,28,28,29	0
4	GOL	C	1203	6/6	0.11	-0.18	30,31,35,37	0
3	3AB	A	1202	10/10	0.08	-0.50	13,14,17,20	0
2	ZN	C	1202	1/1	0.08	-0.91	34,34,34,34	0
5	EDO	A	1204	4/4	0.10	-1.60	50,50,50,51	0
2	ZN	B	1201	1/1	0.07	-1.72	38,38,38,38	0
2	ZN	A	1201	1/1	0.07	-1.80	32,32,32,32	0
3	3AB	B	1202	10/10	0.06	-1.94	17,18,19,20	0
2	ZN	D	1201	1/1	0.05	-2.83	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.