Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 04:23 PM EST

PDB ID	:	4PNR
Title	:	Crystal Structure of human Tankyrase 2 in complex with TIQ-A.
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	:	2014-05-24
Resolution	:	1.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

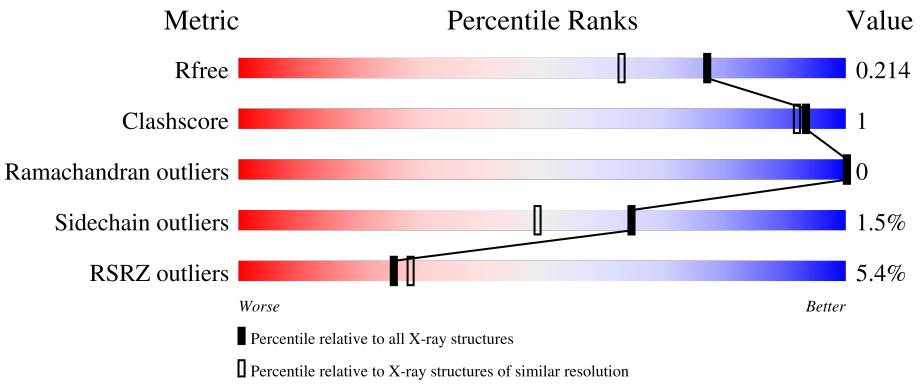
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	227	4% 85% • 12%
1	B	227	4% 87% • 10%
1	C	227	3% 87% 5% 8%
1	D	227	7% 79% • 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7485 atoms, of which 21 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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1619	1020	298	289	12	0	1	0
1	B	204	1654	1045	303	295	11	0	0	0
1	C	208	1690	1068	308	303	11	0	1	0
1	D	189	1526	957	285	273	11	0	0	0

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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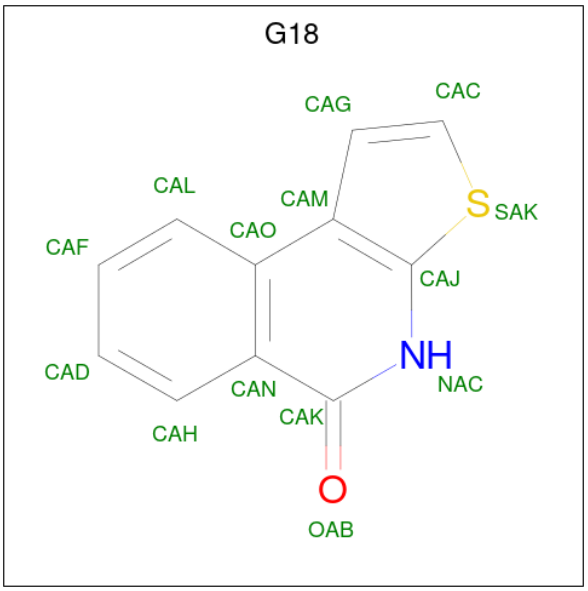
Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	HIS	-	expression tag	UNP Q9H2K2
D	944	HIS	-	expression 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).

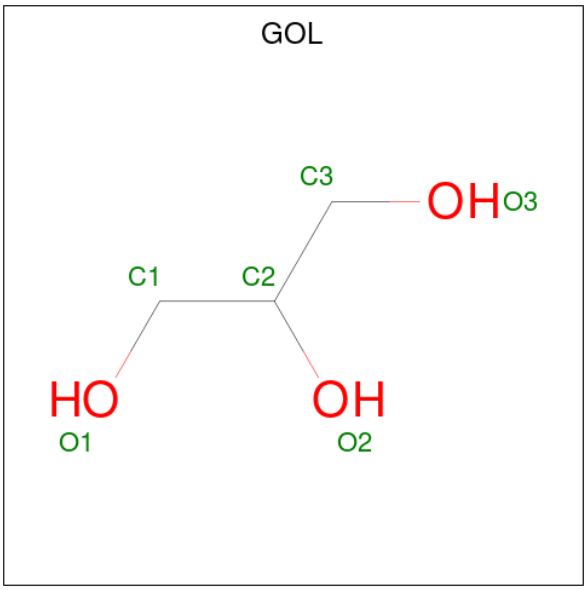
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is 4H-thieno[2,3-c]isoquinolin-5-one (three-letter code: G18) (formula: $C_{11}H_7NOS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
3	A	1	21	11	7	1	1	1	0	0
			Total	C	H	N	O	S		
3	B	1	21	11	7	1	1	1	0	0
			Total	C	H	N	O	S		
3	C	1	21	11	7	1	1	1	0	0

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



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

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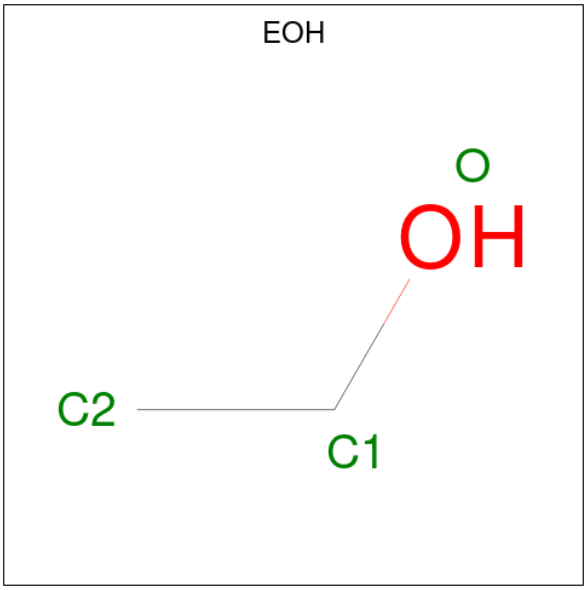
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 3 2 1	0	0

- Molecule 6 is water.

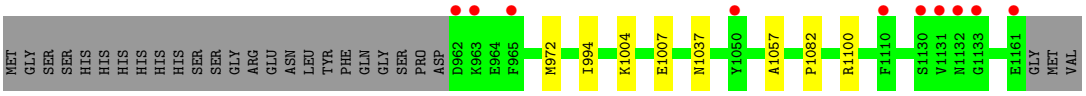
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	231	Total O 231 231	0	0
6	B	245	Total O 245 245	0	0
6	C	237	Total O 237 237	0	0
6	D	189	Total O 189 189	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

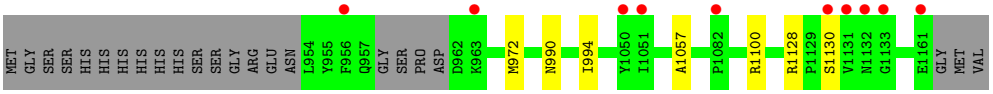
- Molecule 1: Tankyrase-2

Chain A:



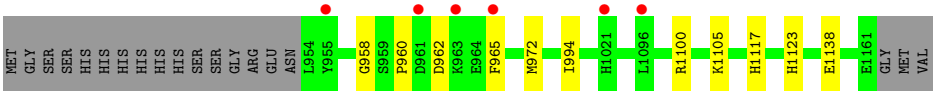
- Molecule 1: Tankyrase-2

Chain B:



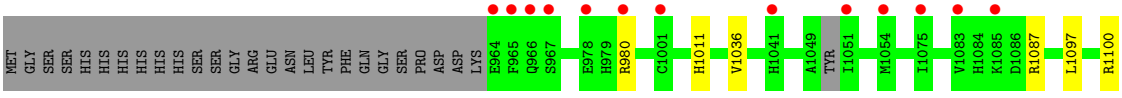
- Molecule 1: Tankyrase-2

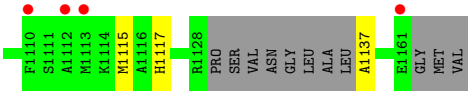
Chain C:



- Molecule 1: Tankyrase-2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.06Å 79.41Å 153.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.04 – 1.71 25.02 – 1.71	Depositor EDS
% Data completeness (in resolution range)	97.4 (25.04-1.71) 97.4 (25.02-1.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 1.71Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.181 , 0.208 0.185 , 0.214	Depositor DCC
R_{free} test set	960 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7485	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EOH, GOL, G18, ZN

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	0.52	0/1665	0.64	0/2237
1	B	0.52	0/1698	0.65	0/2281
1	C	0.52	0/1737	0.65	0/2336
1	D	0.51	0/1564	0.63	0/2097
All	All	0.52	0/6664	0.64	0/8951

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	1619	0	1556	4	1
1	B	1654	0	1583	2	0
1	C	1690	0	1611	9	0
1	D	1526	0	1455	5	1
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
3	A	14	7	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	7	7	0	0
3	C	14	7	7	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	C	3	0	6	1	0
6	A	231	0	0	2	0
6	B	245	0	0	0	0
6	C	237	0	0	1	0
6	D	189	0	0	3	0
All	All	7464	21	6264	18	1

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 1.

All (18) 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:C:1105:LYS:H	1:C:1123:HIS:HD2	1.24	0.82
1:C:972:MET:HG2	1:C:994:ILE:HD11	1.74	0.69
1:A:972:MET:HG2	1:A:994:ILE:HD11	1.77	0.65
1:C:1138:GLU:OE1	5:C:1203:EOH:H22	1.99	0.62
1:B:972:MET:HG2	1:B:994:ILE:HD11	1.80	0.61
1:D:1117:HIS:HD2	6:D:1458:HOH:O	1.86	0.58
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.88	0.56
1:A:1037:ASN:HB2	6:A:1377:HOH:O	2.04	0.56
1:C:962:ASP:OD1	1:C:965[B]:PHE:HD1	1.91	0.54
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.91	0.54
1:D:1011:HIS:HE1	6:D:1463:HOH:O	1.91	0.54
1:C:1105:LYS:H	1:C:1123:HIS:CD2	2.15	0.52
1:C:958:GLY:O	1:C:960:PRO:HD3	2.13	0.48
1:C:1117:HIS:HD2	6:C:1473:HOH:O	1.97	0.46
1:A:1082:PRO:HD2	6:A:1400:HOH:O	2.18	0.44
1:C:972:MET:HG2	1:C:994:ILE:CD1	2.47	0.41
1:D:1137:ALA:N	6:D:1394:HOH:O	2.53	0.41
1:D:1036:VAL:HG13	1:D:1097:LEU:HD21	2.03	0.41

All (1) 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:A:1007:GLU:OE2	1:D:1087:ARG:NH2[4_455]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/227 (88%)	197 (99%)	2 (1%)	0	100	100
1	B	200/227 (88%)	198 (99%)	2 (1%)	0	100	100
1	C	207/227 (91%)	205 (99%)	2 (1%)	0	100	100
1	D	183/227 (81%)	182 (100%)	1 (0%)	0	100	100
All	All	789/908 (87%)	782 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/192 (88%)	168 (99%)	2 (1%)	71	58
1	B	173/192 (90%)	169 (98%)	4 (2%)	50	31
1	C	177/192 (92%)	176 (99%)	1 (1%)	86	80
1	D	159/192 (83%)	156 (98%)	3 (2%)	57	39
All	All	679/768 (88%)	669 (98%)	10 (2%)	65	49

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	LYS
1	A	1100	ARG
1	B	990	ASN
1	B	1100	ARG
1	B	1128	ARG
1	B	1130	SER
1	C	1100	ARG
1	D	980	ARG
1	D	1100	ARG
1	D	1115	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	990	ASN
1	B	1037	ASN
1	B	1070	GLN
1	B	1095	GLN
1	B	1109	GLN
1	C	990	ASN
1	C	1117	HIS
1	C	1123	HIS
1	D	1011	HIS
1	D	1117	HIS

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 (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	G18	B	1202	-	16,16,16	1.73	5 (31%)	13,23,23	1.66	4 (30%)
4	GOL	C	1204	-	5,5,5	0.23	0	5,5,5	0.24	0
5	EOH	C	1203	-	2,2,2	0.97	0	1,1,1	0.34	0
4	GOL	A	1203	-	5,5,5	0.12	0	5,5,5	0.34	0
3	G18	C	1201	-	16,16,16	1.70	5 (31%)	13,23,23	1.61	4 (30%)
4	GOL	D	1202	-	5,5,5	0.24	0	5,5,5	0.39	0
4	GOL	B	1203	-	5,5,5	0.09	0	5,5,5	0.34	0
3	G18	A	1202	-	16,16,16	2.01	5 (31%)	13,23,23	1.59	4 (30%)

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	G18	B	1202	-	-	-	0/3/3/3
4	GOL	C	1204	-	-	0/4/4/4	-
4	GOL	A	1203	-	-	0/4/4/4	-
3	G18	C	1201	-	-	-	0/3/3/3
4	GOL	D	1202	-	-	2/4/4/4	-
4	GOL	B	1203	-	-	0/4/4/4	-
3	G18	A	1202	-	-	-	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	G18	CAF-CAD	4.23	1.49	1.38
3	B	1202	G18	CAJ-SAK	4.05	1.78	1.72
3	A	1202	G18	CAJ-SAK	3.79	1.78	1.72
3	C	1201	G18	CAL-CAO	3.14	1.44	1.40
3	C	1201	G18	CAF-CAD	3.11	1.46	1.38
3	B	1202	G18	CAN-CAO	2.98	1.45	1.40
3	A	1202	G18	CAN-CAO	2.93	1.45	1.40
3	A	1202	G18	CAL-CAO	2.86	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	G18	CAN-CAK	2.37	1.51	1.47
3	C	1201	G18	CAJ-SAK	2.35	1.76	1.72
3	C	1201	G18	CAN-CAK	2.27	1.51	1.47
3	B	1202	G18	CAF-CAD	2.25	1.44	1.38
3	C	1201	G18	CAN-CAO	2.13	1.44	1.40
3	B	1202	G18	CAL-CAO	2.08	1.43	1.40
3	B	1202	G18	CAN-CAK	2.02	1.50	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1202	G18	CAL-CAO-CAM	2.71	127.28	121.57
3	A	1202	G18	CAL-CAO-CAM	2.62	127.09	121.57
3	B	1202	G18	OAB-CAK-NAC	-2.57	117.56	120.95
3	C	1201	G18	CAL-CAO-CAM	2.54	126.93	121.57
3	B	1202	G18	CAN-CAO-CAM	-2.54	116.81	120.14
3	A	1202	G18	CAN-CAO-CAM	-2.50	116.86	120.14
3	C	1201	G18	CAF-CAL-CAO	2.47	124.51	120.33
3	C	1201	G18	CAN-CAO-CAM	-2.39	117.00	120.14
3	B	1202	G18	CAL-CAO-CAN	-2.29	115.44	118.03
3	A	1202	G18	OAB-CAK-NAC	-2.27	117.96	120.95
3	C	1201	G18	OAB-CAK-NAC	-2.21	118.03	120.95
3	A	1202	G18	CAF-CAL-CAO	2.09	123.86	120.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1202	GOL	O2-C2-C3-O3
4	D	1202	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1203	EOH	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 (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	200/227 (88%)	0.09	10 (5%)	28	32	14, 24, 48, 89	0
1	B	204/227 (89%)	0.06	10 (4%)	29	33	13, 22, 47, 84	0
1	C	208/227 (91%)	-0.05	6 (2%)	51	56	13, 21, 45, 73	0
1	D	189/227 (83%)	0.35	17 (8%)	9	10	16, 29, 54, 86	0
All	All	801/908 (88%)	0.11	43 (5%)	25	28	13, 24, 48, 89	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1113	MET	6.1
1	A	1132	ASN	5.8
1	A	1131	VAL	5.6
1	C	965[A]	PHE	5.5
1	D	1051	ILE	5.5
1	B	1131	VAL	5.2
1	C	955	TYR	5.1
1	D	980	ARG	5.0
1	D	966	GLN	4.8
1	B	1132	ASN	4.3
1	D	965	PHE	4.1
1	A	1050	TYR	3.7
1	A	1133	GLY	3.4
1	B	1051	ILE	3.4
1	A	1130	SER	3.4
1	C	961	ASP	3.1
1	A	1110	PHE	3.1
1	C	963	LYS	3.0
1	A	1161	GLU	2.9
1	B	1161	GLU	2.9
1	D	964	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	1041	HIS	2.8
1	D	1001	CYS	2.8
1	B	1050	TYR	2.7
1	B	1133	GLY	2.6
1	D	1083	VAL	2.6
1	D	967	SER	2.6
1	A	962	ASP	2.6
1	D	1075	ILE	2.5
1	D	978	GLU	2.4
1	D	1112	ALA	2.4
1	D	1054	MET	2.3
1	C	1021	HIS	2.3
1	D	1110	PHE	2.3
1	D	1161	GLU	2.3
1	D	1085	LYS	2.3
1	B	963	LYS	2.2
1	B	1082	PRO	2.2
1	B	1130	SER	2.2
1	B	956	PHE	2.1
1	A	963	LYS	2.1
1	A	965	PHE	2.0
1	C	1096	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	EOH	C	1203	3/3	0.60	0.22	19,19,30,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	D	1202	6/6	0.82	0.22	27,41,47,48	0
4	GOL	B	1203	6/6	0.87	0.14	34,39,43,48	0
3	G18	A	1202	14/14	0.88	0.14	16,24,30,30	0
3	G18	B	1202	14/14	0.92	0.13	20,27,30,31	0
4	GOL	A	1203	6/6	0.93	0.09	29,34,38,39	0
4	GOL	C	1204	6/6	0.95	0.10	20,30,33,34	0
3	G18	C	1201	14/14	0.96	0.07	13,19,22,25	0
2	ZN	A	1201	1/1	1.00	0.02	28,28,28,28	0
2	ZN	B	1201	1/1	1.00	0.02	28,28,28,28	0
2	ZN	C	1202	1/1	1.00	0.03	28,28,28,28	0
2	ZN	D	1201	1/1	1.00	0.03	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.