Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 11:03 AM EST

PDB ID	:	4TJY
Title	:	Crystal Structure of human Tankyrase 2 in complex with ABT-888.
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	:	2014-05-25
Resolution	:	1.90 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:

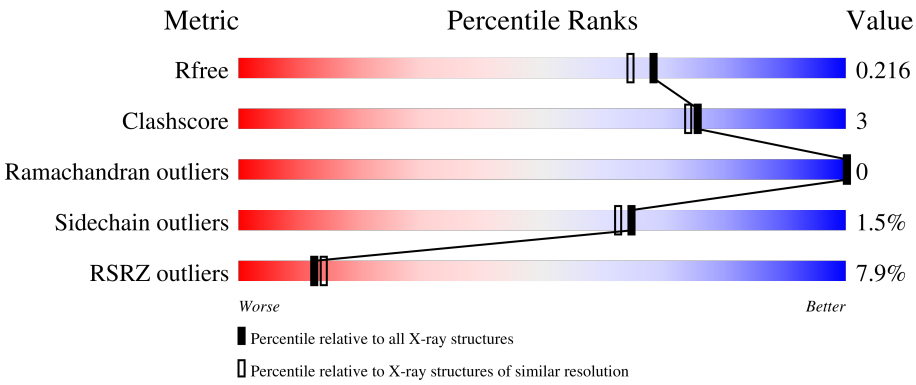
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	6%, 80%, 7% • 12%
1	B	227	6%, 87% • 10%
1	C	227	4%, 84%, 6% • 8%
1	D	227	12%, 78%, 5% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7319 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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1598	1007	296	284	11	0	0	0
1	B	204	1649	1042	303	293	11	0	0	0
1	C	208	1676	1057	308	300	11	0	1	0
1	D	191	1540	971	287	271	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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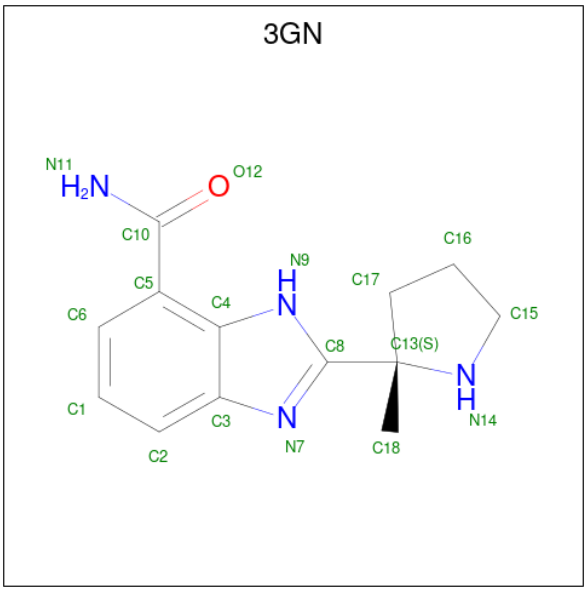
Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	HIS	-	expression tag	UNP Q9H2K2
D	944	HIS	-	expression 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

- Molecule 3 is 2-[(2S)-2-methylpyrrolidin-2-yl]-1H-benzimidazole-7-carboxamide (three-letter code: 3GN) (formula: $C_{13}H_{16}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	18	13	4	1	0	0
			Total	C	N	O		
3	B	1	18	13	4	1	0	0
			Total	C	N	O		
3	C	1	18	13	4	1	0	0

- Molecule 4 is water.

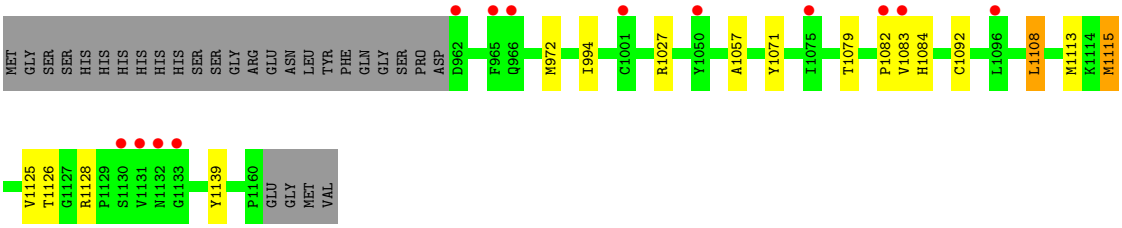
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	204	204	204	0	0
			Total	O		
4	B	194	194	194	0	0
			Total	O		
4	C	230	230	230	0	0
			Total	O		
4	D	171	171	171	0	0

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.

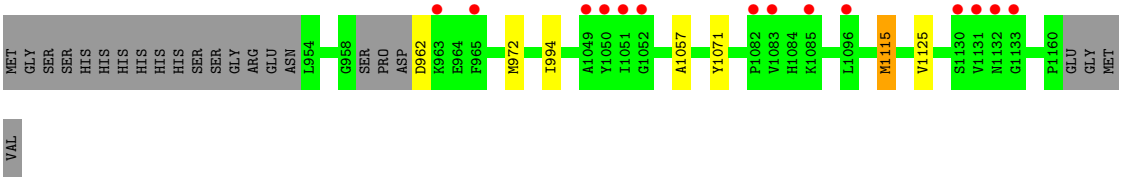
• Molecule 1: Tankyrase-2

Chain A:



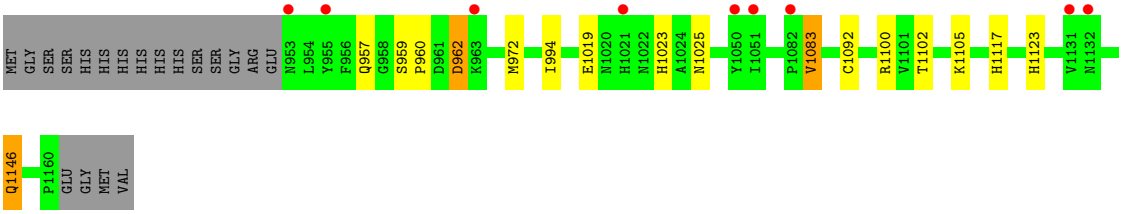
• Molecule 1: Tankyrase-2

Chain B:



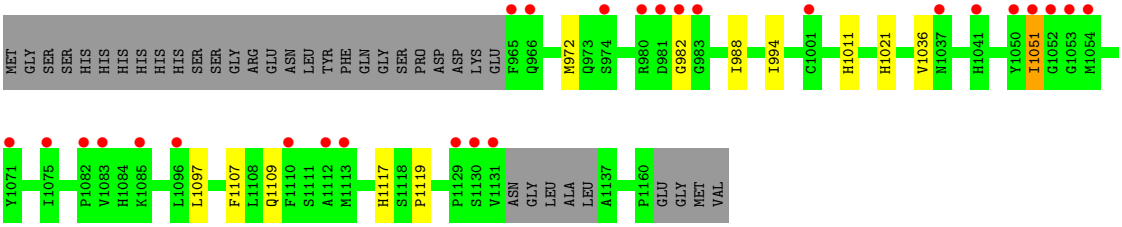
• Molecule 1: Tankyrase-2

Chain C:



• Molecule 1: Tankyrase-2

Chain D:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY SER PRO ASP ASP LYS GLU F965 Q966 N972 Q973 S974 R980 D981 G982 G983 I988 I994 C1001 H1011 H1021 V1036 N1037 H1041 Y1050 I1051 G1052 G1053 M1054
Y1071 I1075 P1082 V1083 H1084 K1085 L1096 L1097 F1107 L1108 Q1109 F1110 S1111 A1112 M1113 H1117 S1118 P1119 P1129 S1130 V1131 ASN GLY LEU ALA LEU A1137 P1160 GLU GLY MET VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.11Å 79.57Å 153.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.94 – 1.90 21.83 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (21.94-1.90) 98.6 (21.83-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.90Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.177 , 0.219 0.176 , 0.216	Depositor DCC
R_{free} test set	1047 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7319	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.14% 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: 3GN, 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	0.53	0/1641	0.67	0/2207
1	B	0.51	0/1693	0.65	1/2274 (0.0%)
1	C	0.52	0/1724	0.65	1/2318 (0.0%)
1	D	0.51	0/1582	0.65	0/2125
All	All	0.52	0/6640	0.66	2/8924 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1115	MET	CB-CG-SD	-5.42	96.14	112.40
1	C	960	PRO	N-CA-CB	5.18	109.52	103.30

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	1598	0	1528	15	0
1	B	1649	0	1580	6	0
1	C	1676	0	1600	10	0
1	D	1540	0	1473	10	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	18	0	16	1	0
3	B	18	0	16	1	0
3	C	18	0	16	0	0
4	A	204	0	0	2	0
4	B	194	0	0	1	0
4	C	230	0	0	1	0
4	D	171	0	0	3	0
All	All	7319	0	6229	39	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 3.

All (39) 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:1023:HIS:HD2	1:C:1025:ASN:H	1.21	0.85
1:C:1105:LYS:H	1:C:1123:HIS:HD2	1.28	0.80
1:B:1115:MET:HE1	1:B:1125:VAL:HG21	1.73	0.69
1:C:1083:VAL:HG13	1:C:1092:CYS:SG	2.41	0.61
1:A:1115:MET:HE1	1:A:1125:VAL:HG21	1.85	0.59
1:A:1079:THR:HG23	4:A:1309:HOH:O	2.04	0.56
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.88	0.56
1:A:972:MET:HG2	1:A:994:ILE:HD11	1.88	0.55
1:C:972:MET:HG2	1:C:994:ILE:HD11	1.89	0.55
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.90	0.54
1:B:972:MET:HG2	1:B:994:ILE:HD11	1.90	0.52
1:A:1083:VAL:HG22	1:A:1092:CYS:SG	2.49	0.52
1:A:1027:ARG:NH1	1:A:1139:TYR:OH	2.43	0.52
1:D:1117:HIS:HD2	4:D:1231:HOH:O	1.93	0.51
1:D:972:MET:HG2	1:D:994:ILE:HD11	1.92	0.51
1:D:1011:HIS:HE1	4:D:1325:HOH:O	1.95	0.50
1:B:1115:MET:HG2	4:B:1478:HOH:O	2.11	0.49
1:A:1082:PRO:HD2	4:A:1425:HOH:O	2.13	0.49
1:A:1071:TYR:CE1	3:A:1202:3GN:H18B	2.47	0.49
1:C:959:SER:HB2	1:C:962:ASP:HB2	1.96	0.48
1:C:1019:GLU:OE1	1:C:1123:HIS:HE1	1.96	0.47
1:C:1117:HIS:HD2	4:C:1339:HOH:O	1.97	0.46
1:B:1115:MET:CE	1:B:1125:VAL:HG21	2.43	0.46
1:C:1023:HIS:CD2	1:C:1025:ASN:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:VAL:HG23	1:A:1084:HIS:CE1	2.52	0.45
1:D:982:GLY:O	1:D:988:ILE:HD11	2.18	0.44
1:D:1107:PHE:CG	1:D:1119:PRO:HG2	2.53	0.44
1:D:1021:HIS:HE1	4:D:1295:HOH:O	2.00	0.44
1:D:1107:PHE:HE2	1:D:1109:GLN:HE21	1.64	0.44
1:A:1083:VAL:CG2	1:A:1092:CYS:SG	3.06	0.44
1:A:1113:MET:CE	1:A:1115:MET:CE	2.96	0.44
1:A:1113:MET:CE	1:A:1115:MET:HE1	2.50	0.42
1:A:1113:MET:HE3	1:A:1115:MET:CE	2.49	0.42
1:C:1102:THR:HB	1:C:1146:GLN:HG2	2.02	0.42
1:A:1108:LEU:HD12	1:A:1126:THR:HB	2.02	0.42
1:B:1071:TYR:CE1	3:B:1202:3GN:H18B	2.55	0.42
1:D:1036:VAL:HG13	1:D:1097:LEU:HD21	2.03	0.41
1:D:1051:ILE:H	1:D:1051:ILE:HG13	1.44	0.41
1:A:1115:MET:CE	1:A:1125:VAL:HG21	2.50	0.41

There are no symmetry-related clashes.

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	197/227 (87%)	195 (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	187/227 (82%)	184 (98%)	3 (2%)	0	100	100
All	All	791/908 (87%)	782 (99%)	9 (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	166/192 (86%)	163 (98%)	3 (2%)	59	55
1	B	172/192 (90%)	171 (99%)	1 (1%)	86	87
1	C	175/192 (91%)	170 (97%)	5 (3%)	42	35
1	D	160/192 (83%)	159 (99%)	1 (1%)	86	87
All	All	673/768 (88%)	663 (98%)	10 (2%)	65	62

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

Mol	Chain	Res	Type
1	A	1108	LEU
1	A	1115	MET
1	A	1128	ARG
1	B	962	ASP
1	C	957	GLN
1	C	962	ASP
1	C	1083	VAL
1	C	1100	ARG
1	C	1146	GLN
1	D	1051	ILE

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

Mol	Chain	Res	Type
1	A	1011	HIS
1	B	1011	HIS
1	B	1048	HIS
1	C	1023	HIS
1	C	1117	HIS
1	C	1123	HIS
1	D	1011	HIS
1	D	1021	HIS
1	D	1109	GLN

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Mol	Chain	Res	Type
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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	3GN	B	1202	-	16,20,20	1.59	4 (25%)	14,30,30	1.47	3 (21%)
3	3GN	C	1202	-	16,20,20	1.39	3 (18%)	14,30,30	1.52	3 (21%)
3	3GN	A	1202	-	16,20,20	1.84	5 (31%)	14,30,30	1.49	3 (21%)

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	3GN	B	1202	-	-	0/4/19/19	0/3/3/3
3	3GN	C	1202	-	-	0/4/19/19	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3GN	A	1202	-	-	2/4/19/19	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	3GN	C17-C13	4.35	1.59	1.54
3	B	1202	3GN	C17-C13	3.42	1.58	1.54
3	A	1202	3GN	C1-C2	3.06	1.43	1.36
3	A	1202	3GN	C10-N11	2.86	1.38	1.33
3	A	1202	3GN	C1-C6	2.75	1.44	1.38
3	B	1202	3GN	C10-N11	2.67	1.38	1.33
3	C	1202	3GN	C10-N11	2.49	1.37	1.33
3	B	1202	3GN	C1-C2	2.44	1.42	1.36
3	C	1202	3GN	C1-C6	2.42	1.44	1.38
3	B	1202	3GN	C1-C6	2.16	1.43	1.38
3	A	1202	3GN	C5-C10	2.15	1.54	1.50
3	C	1202	3GN	C1-C2	2.15	1.41	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1202	3GN	O12-C10-N11	-3.44	117.69	122.58
3	C	1202	3GN	O12-C10-N11	-3.41	117.73	122.58
3	A	1202	3GN	O12-C10-N11	-3.38	117.78	122.58
3	C	1202	3GN	C18-C13-C17	-2.77	107.76	112.78
3	B	1202	3GN	O12-C10-C5	2.71	123.41	120.22
3	A	1202	3GN	O12-C10-C5	2.53	123.21	120.22
3	A	1202	3GN	C16-C17-C13	2.45	106.44	104.18
3	C	1202	3GN	O12-C10-C5	2.36	123.00	120.22
3	B	1202	3GN	C16-C17-C13	2.03	106.05	104.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	3GN	N11-C10-C5-C4
3	A	1202	3GN	O12-C10-C5-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1202	3GN	1	0
3	A	1202	3GN	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	199/227 (87%)	0.32	13 (6%)	18	21	16, 28, 51, 70	0
1	B	204/227 (89%)	0.38	14 (6%)	16	19	16, 28, 50, 73	0
1	C	208/227 (91%)	0.19	9 (4%)	35	38	15, 25, 48, 64	0
1	D	191/227 (84%)	0.72	27 (14%)	2	2	19, 33, 54, 84	0
All	All	802/908 (88%)	0.39	63 (7%)	12	14	15, 28, 51, 84	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1131	VAL	8.0
1	B	1131	VAL	6.6
1	D	1052	GLY	5.6
1	B	1132	ASN	5.4
1	A	1050	TYR	4.9
1	D	1050	TYR	4.7
1	D	1113	MET	4.6
1	C	963	LYS	4.6
1	D	980	ARG	4.4
1	D	1083	VAL	4.4
1	A	1083	VAL	4.3
1	A	1132	ASN	4.1
1	D	1054	MET	4.1
1	D	966	GLN	4.0
1	D	965	PHE	4.0
1	D	1112	ALA	3.9
1	D	1001	CYS	3.8
1	C	1050	TYR	3.7
1	D	1129	PRO	3.6
1	D	1082	PRO	3.6
1	D	1051	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	1041	HIS	3.4
1	A	1133	GLY	3.3
1	B	1130	SER	3.3
1	B	1133	GLY	3.2
1	A	962	ASP	3.1
1	D	1071	TYR	3.1
1	B	1082	PRO	3.1
1	B	1051	ILE	3.1
1	C	955	TYR	3.1
1	B	1083	VAL	3.1
1	A	965	PHE	3.0
1	C	953	ASN	3.0
1	D	1130	SER	3.0
1	D	1096	LEU	2.9
1	A	1130	SER	2.9
1	D	1075	ILE	2.8
1	C	1131	VAL	2.8
1	C	1082	PRO	2.7
1	D	1053	GLY	2.7
1	D	1085	LYS	2.6
1	A	1075	ILE	2.6
1	D	1110	PHE	2.6
1	D	981	ASP	2.6
1	B	1085	LYS	2.5
1	A	1001	CYS	2.5
1	B	1050	TYR	2.4
1	A	1096	LEU	2.4
1	C	1132	ASN	2.4
1	A	1131	VAL	2.4
1	D	1037	ASN	2.3
1	C	1051	ILE	2.3
1	B	1049	ALA	2.3
1	B	1096	LEU	2.3
1	D	982	GLY	2.3
1	D	974	SER	2.3
1	C	1021	HIS	2.2
1	D	983	GLY	2.2
1	B	1052	GLY	2.2
1	A	1082	PRO	2.2
1	B	965	PHE	2.1
1	A	966	GLN	2.1
1	B	963	LYS	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
3	3GN	A	1202	18/18	0.84	0.17	22,32,43,46	0
3	3GN	B	1202	18/18	0.87	0.16	22,33,51,52	0
3	3GN	C	1202	18/18	0.94	0.10	19,23,41,42	0
2	ZN	B	1201	1/1	0.99	0.03	38,38,38,38	0
2	ZN	C	1201	1/1	1.00	0.03	34,34,34,34	0
2	ZN	A	1201	1/1	1.00	0.03	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.