



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:29 PM GMT

PDB ID : 4TJU
Title : Crystal Structure of human Tankyrase 2 in complex with 3,4-CPQ-5-C.
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 : 1.57 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

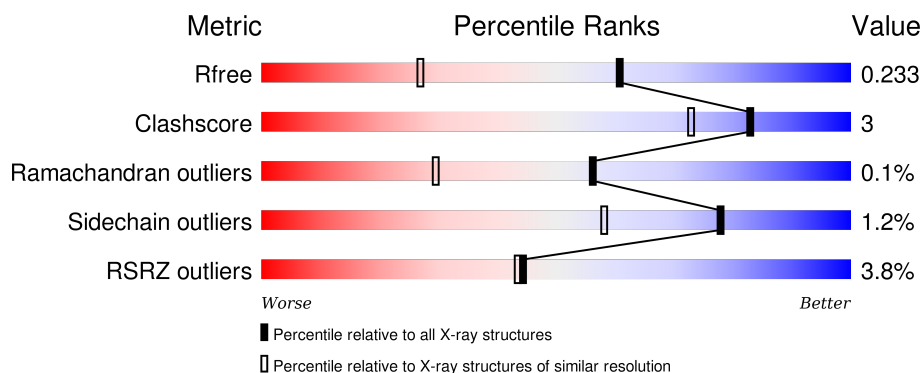
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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}	91344	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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. 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	227	<div> <div>2%</div> <div>81% 6% 13%</div> </div>
1	B	227	<div> <div>2%</div> <div>83% 5% 11%</div> </div>
1	C	227	<div> <div>6%</div> <div>86% • • 9%</div> </div>
1	D	227	<div> <div>4%</div> <div>78% • 17%</div> </div>

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	CNQ	A	1202	-	-	-	X
3	CNQ	B	1202	-	-	-	X
3	CNQ	D	1202	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7535 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
1	A	197	Total	C	N	O	S	0	3	0
			1604	1011	298	283	12			
1	B	202	Total	C	N	O	S	0	3	0
			1637	1036	299	290	12			
1	C	207	Total	C	N	O	S	0	2	0
			1677	1059	307	300	11			
1	D	188	Total	C	N	O	S	0	4	0
			1548	976	288	272	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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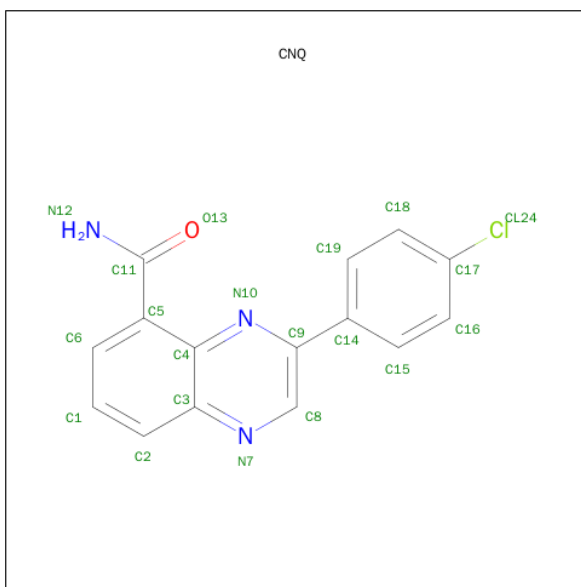
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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	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-(4-CHLOROPHENYL)QUINOXALINE-5-CARBOXAMIDE (three-letter code: CNQ) (formula: C₁₅H₁₀ClN₃O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			20	15	1	3	1		
3	B	1	Total	C	Cl	N	O	0	0
			20	15	1	3	1		
3	C	1	Total	C	Cl	N	O	0	0
			20	15	1	3	1		
3	D	1	Total	C	Cl	N	O	0	0
			20	15	1	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	241	Total	O	0	0
			241	241		
4	B	258	Total	O	0	0
			258	258		
4	C	272	Total	O	0	0
			272	272		
4	D	214	Total	O	0	0
			214	214		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.14Å 79.49Å 153.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.68 – 1.57 70.57 – 1.57	Depositor EDS
% Data completeness (in resolution range)	92.0 (76.68-1.57) 92.0 (70.57-1.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.57Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.194 , 0.221 0.197 , 0.233	Depositor DCC
R_{free} test set	1167 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 116789 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7535	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.59	0/1654	0.66	0/2219
1	B	0.56	0/1688	0.71	0/2264
1	C	0.69	1/1729 (0.1%)	0.77	2/2326 (0.1%)
1	D	0.49	0/1601	0.64	0/2148
All	All	0.59	1/6672 (0.0%)	0.70	2/8957 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	954	LEU	C-N	12.34	1.62	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	954	LEU	O-C-N	-13.29	101.44	122.70
1	C	954	LEU	CA-C-N	6.80	132.16	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	962	ASP	Peptide
1	C	954	LEU	Mainchain

5.2 Too-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 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	1604	0	1555	14	0
1	B	1637	0	1574	8	0
1	C	1677	0	1605	11	0
1	D	1548	0	1490	8	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
3	A	20	0	10	0	0
3	B	20	0	10	0	0
3	C	20	0	10	0	0
3	D	20	0	10	0	0
4	A	241	0	0	1	0
4	B	258	0	0	2	0
4	C	272	0	0	1	0
4	D	214	0	0	2	0
All	All	7535	0	6264	40	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 (40) 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	1.22	0.85
1:C:958:GLY:O	1:C:960:PRO:HD3	1.89	0.72
1:D:1050:TYR:O	1:D:1052:GLY:HA2	1.93	0.69
1:C:1105:LYS:H	1:C:1123:HIS:CD2	2.11	0.66
1:A:1054:MET:HE1	1:A:1134:LEU:HD21	1.79	0.64
1:C:959:SER:O	1:C:962:ASP:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:MET:CE	1:A:1134:LEU:HD21	2.28	0.63
1:D:1031:HIS:HD2	1:D:1060:TYR:O	1.83	0.61
1:C:955:TYR:N	1:C:955:TYR:CD1	2.69	0.60
1:B:1115[B]:MET:HE1	1:B:1125:VAL:HG21	1.83	0.59
1:B:1082:PRO:HD2	4:B:1488:HOH:O	2.06	0.55
1:C:957:GLN:NE2	4:C:1301:HOH:O	1.68	0.55
1:C:958:GLY:HA3	1:C:965:PHE:CZ	2.44	0.53
1:C:958:GLY:HA3	1:C:965:PHE:CE1	2.43	0.53
1:B:1051:ILE:CD1	1:D:1051:ILE:HG21	2.39	0.53
1:A:1113:MET:CE	1:A:1115[A]:MET:HE1	2.41	0.50
1:C:955:TYR:N	1:C:955:TYR:HD1	2.10	0.49
1:C:955:TYR:H	1:C:955:TYR:HD1	1.60	0.49
1:A:1113:MET:CE	1:A:1115[A]:MET:CE	2.90	0.49
1:D:1011:HIS:HE1	4:D:1419:HOH:O	1.98	0.47
1:A:1115[A]:MET:HE1	1:A:1125:VAL:HG21	1.96	0.47
1:B:1021:HIS:HD2	4:B:1303:HOH:O	1.99	0.46
1:B:1115[B]:MET:HG3	1:B:1117:HIS:O	2.17	0.45
1:A:1110:PHE:HD2	1:A:1130:SER:HB3	1.82	0.45
1:D:1107:PHE:CG	1:D:1119:PRO:HG2	2.52	0.45
1:A:1115[A]:MET:HG3	1:A:1117:HIS:O	2.17	0.44
1:C:1019:GLU:OE1	1:C:1123:HIS:HE1	2.01	0.44
1:D:1008:ARG:NH2	4:D:1432:HOH:O	2.51	0.43
1:A:1113:MET:HE3	1:A:1115[A]:MET:HE1	2.00	0.43
1:A:1113:MET:HE2	1:A:1115[A]:MET:CE	2.49	0.43
1:D:1031:HIS:CD2	1:D:1060:TYR:O	2.69	0.42
1:D:1044:PHE:HB3	1:D:1059:ILE:HD13	2.02	0.42
1:B:1113:MET:CE	1:B:1115[B]:MET:CE	2.98	0.41
1:A:1113:MET:HE3	1:A:1115[A]:MET:CE	2.50	0.41
1:B:1113:MET:CE	1:B:1115[B]:MET:HE1	2.50	0.41
1:A:1028:MET:SD	1:A:1100:ARG:HG3	2.61	0.41
1:A:975:THR:HB	1:A:1064:ASN:HA	2.03	0.40
1:A:1113:MET:HE2	1:A:1115[A]:MET:HE1	2.03	0.40
1:A:1082:PRO:HD2	4:A:1461:HOH:O	2.21	0.40
1:B:1107:PHE:CG	1:B:1119:PRO:HG2	2.56	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	196/227 (86%)	194 (99%)	1 (0%)	1 (0%)	34	11
1	B	199/227 (88%)	199 (100%)	0	0	100	100
1	C	207/227 (91%)	206 (100%)	1 (0%)	0	100	100
1	D	188/227 (83%)	183 (97%)	5 (3%)	0	100	100
All	All	790/908 (87%)	782 (99%)	7 (1%)	1 (0%)	56	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1131	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/192 (88%)	168 (99%)	1 (1%)	90	81
1	B	171/192 (89%)	167 (98%)	4 (2%)	58	28
1	C	176/192 (92%)	174 (99%)	2 (1%)	80	61
1	D	163/192 (85%)	162 (99%)	1 (1%)	90	81
All	All	679/768 (88%)	671 (99%)	8 (1%)	78	58

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1100	ARG
1	B	962	ASP
1	B	990	ASN
1	B	1027	ARG
1	B	1037	ASN
1	C	955	TYR
1	C	959	SER
1	D	1051	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1037	ASN
1	B	993	ASN
1	B	1021	HIS
1	C	990	ASN
1	C	1020	ASN
1	C	1123	HIS
1	D	1011	HIS
1	D	1031	HIS
1	D	1109	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	CNQ	A	1202	-	22,22,22	1.77	6 (27%)	29,31,31	0.97	1 (3%)
3	CNQ	B	1202	-	22,22,22	1.65	7 (31%)	29,31,31	0.96	2 (6%)
3	CNQ	C	1202	-	22,22,22	1.80	8 (36%)	29,31,31	0.95	1 (3%)
3	CNQ	D	1202	-	22,22,22	1.76	5 (22%)	29,31,31	0.88	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	CNQ	A	1202	-	-	0/8/8/8	0/3/3/3
3	CNQ	B	1202	-	-	0/8/8/8	0/3/3/3
3	CNQ	C	1202	-	-	0/8/8/8	0/3/3/3
3	CNQ	D	1202	-	-	0/8/8/8	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	CNQ	C4-N10	2.05	1.41	1.37
3	C	1202	CNQ	C11-N12	2.06	1.37	1.33
3	B	1202	CNQ	C19-C18	2.14	1.42	1.38
3	B	1202	CNQ	C4-N10	2.15	1.41	1.37
3	C	1202	CNQ	C19-C14	2.16	1.43	1.39
3	B	1202	CNQ	C19-C14	2.16	1.43	1.39
3	A	1202	CNQ	C1-C2	2.20	1.41	1.36
3	B	1202	CNQ	C8-C9	2.24	1.45	1.40
3	C	1202	CNQ	C4-C3	2.25	1.46	1.42
3	C	1202	CNQ	C16-C15	2.32	1.42	1.38
3	D	1202	CNQ	C4-C3	2.36	1.46	1.42
3	B	1202	CNQ	C3-N7	2.36	1.41	1.37
3	A	1202	CNQ	C5-C4	2.37	1.47	1.43
3	A	1202	CNQ	C19-C14	2.39	1.44	1.39
3	A	1202	CNQ	C8-C9	2.40	1.45	1.40
3	D	1202	CNQ	C11-N12	2.43	1.37	1.33
3	B	1202	CNQ	C1-C6	2.51	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	CNQ	C4-N10	2.53	1.42	1.37
3	D	1202	CNQ	C5-C4	2.53	1.47	1.43
3	C	1202	CNQ	C3-N7	2.78	1.42	1.37
3	D	1202	CNQ	C4-N10	2.86	1.43	1.37
3	C	1202	CNQ	C8-C9	2.98	1.46	1.40
3	C	1202	CNQ	C1-C6	3.02	1.45	1.38
3	B	1202	CNQ	C5-C4	3.07	1.48	1.43
3	A	1202	CNQ	C1-C6	3.24	1.45	1.38
3	D	1202	CNQ	C8-C9	3.79	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	CNQ	C5-C4-C3	-2.03	116.90	119.47
3	A	1202	CNQ	C6-C5-C4	2.10	121.05	118.71
3	B	1202	CNQ	C6-C5-C4	2.15	121.10	118.71
3	C	1202	CNQ	C2-C3-C4	2.27	121.83	119.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	954:LEU	C	955:TYR	N	1.62

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	197/227 (86%)	-0.12	4 (2%) 68 69	12, 21, 44, 66	0
1	B	202/227 (88%)	-0.17	4 (1%) 68 69	13, 21, 43, 66	0
1	C	207/227 (91%)	0.02	13 (6%) 23 22	12, 20, 37, 47	0
1	D	188/227 (82%)	-0.01	9 (4%) 34 32	14, 24, 52, 70	0
All	All	794/908 (87%)	-0.07	30 (3%) 44 43	12, 21, 43, 70	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1131	VAL	9.7
1	C	955	TYR	8.7
1	C	960	PRO	6.6
1	D	1110	PHE	6.0
1	C	961	ASP	5.1
1	C	965	PHE	4.5
1	C	954	LEU	4.4
1	C	957	GLN	4.3
1	D	1113	MET	4.1
1	A	1132	ASN	4.0
1	D	1054	MET	3.9
1	B	1051	ILE	3.9
1	C	959	SER	3.7
1	B	1131	VAL	3.6
1	C	963	LYS	3.2
1	C	958	GLY	3.1
1	D	980	ARG	3.0
1	C	1021	HIS	2.9
1	A	1110	PHE	2.9
1	D	1051	ILE	2.9
1	A	1130	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1052	GLY	2.6
1	D	966	GLN	2.4
1	D	1071	TYR	2.3
1	C	962	ASP	2.3
1	D	1112	ALA	2.2
1	C	964	GLU	2.2
1	B	958	GLY	2.1
1	C	956	PHE	2.0
1	B	955	TYR	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CNQ	B	1202	20/20	0.90	0.17	9.08	19,26,39,41	0
3	CNQ	A	1202	20/20	0.89	0.16	6.16	19,23,40,47	0
3	CNQ	D	1202	20/20	0.77	0.22	3.95	34,39,47,50	0
3	CNQ	C	1202	20/20	0.94	0.09	0.89	12,17,30,33	0
2	ZN	C	1201	1/1	0.97	0.08	-0.02	26,26,26,26	0
2	ZN	D	1201	1/1	0.97	0.06	-0.82	27,27,27,27	0
2	ZN	B	1201	1/1	0.97	0.06	-1.96	24,24,24,24	0
2	ZN	A	1201	1/1	0.95	0.06	-2.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.