



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:03 AM UTC

PDB ID : 4TJU / pdb_00004tju
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

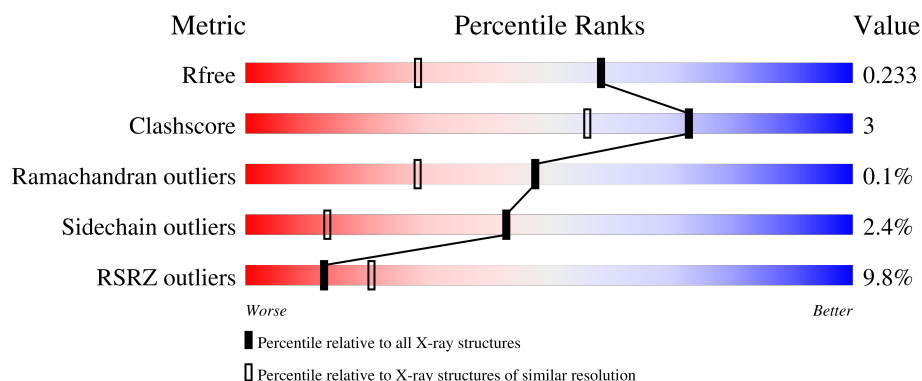
1 Overall quality at a glance

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}	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	7% 77% 9% • 13%
1	B	227	7% 81% 7% • 11%
1	C	227	11% 81% 8% • 9%
1	D	227	9% 76% 6% 17%

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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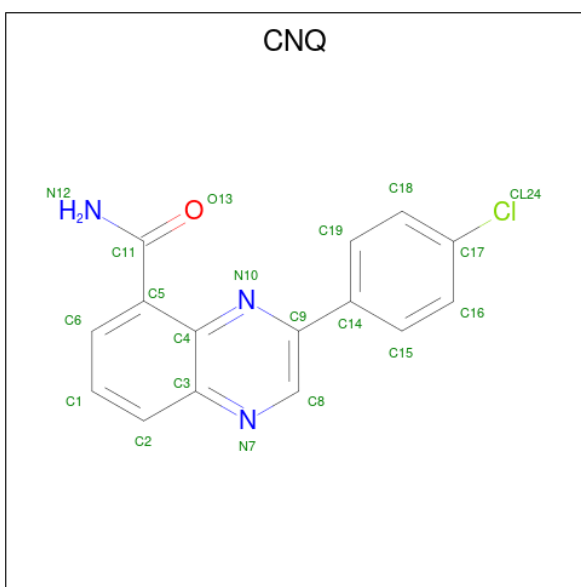
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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is 3-(4-CHLOROPHENYL)QUINOXALINE-5-CARBOXAMIDE (CCD ID: CNQ) (formula: C₁₅H₁₀ClN₃O).



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

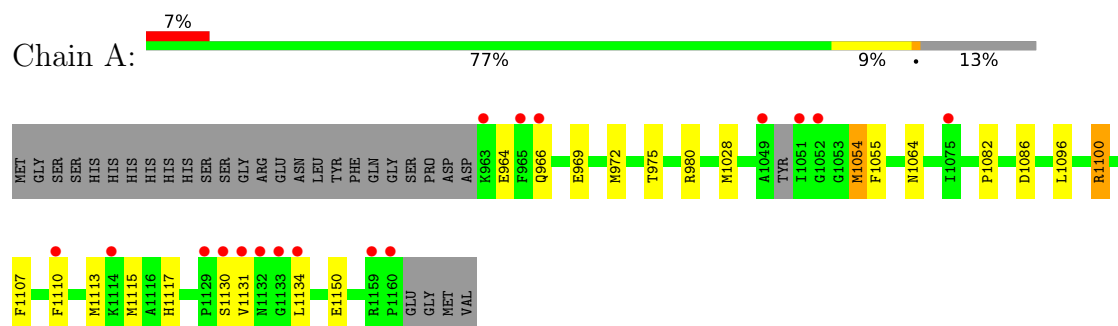
- Molecule 4 is water.

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

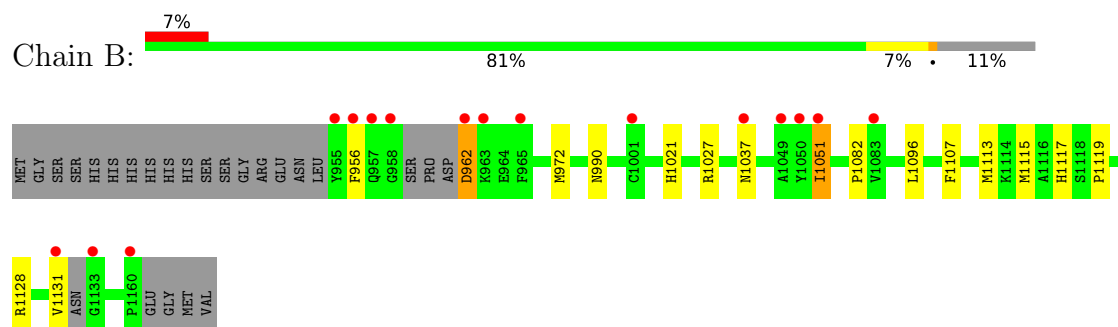
3 Residue-property plots [i](#)

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.

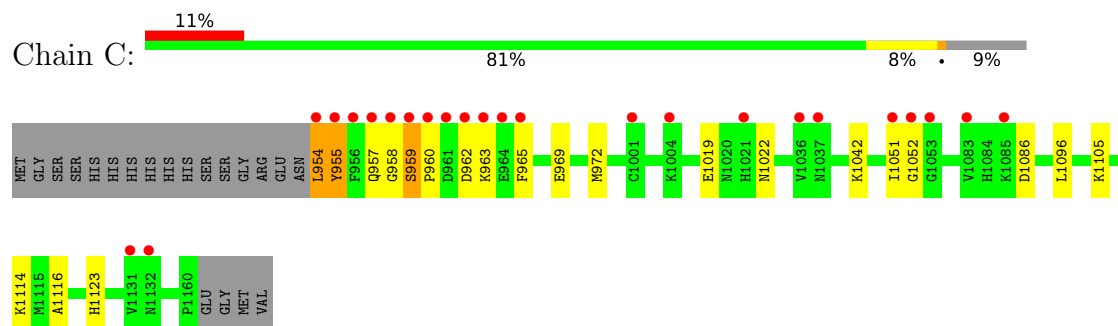
• Molecule 1: Tankyrase-2



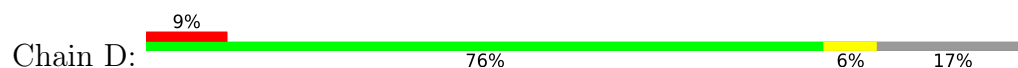
• Molecule 1: Tankyrase-2

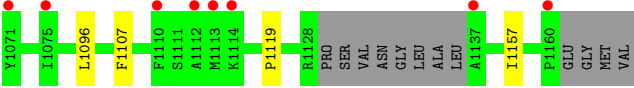
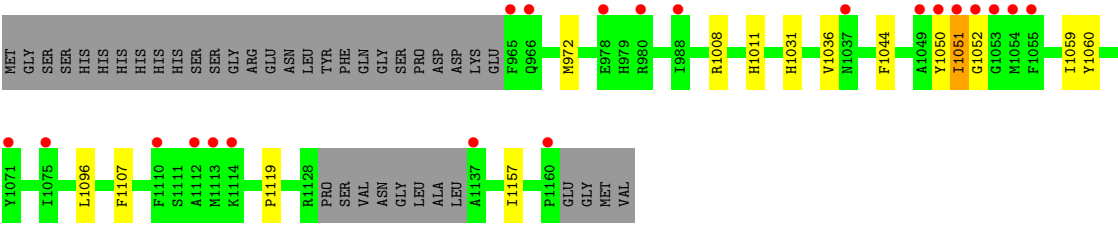


• Molecule 1: Tankyrase-2



• Molecule 1: Tankyrase-2





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 76.68 – 1.57	Depositor EDS
% Data completeness (in resolution range)	92.0 (76.68-1.57) 92.0 (76.68-1.57)	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-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.194 , 0.221 0.197 , 0.233	Depositor DCC
R_{free} test set	1167 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.90	2/1654 (0.1%)	1.13	4/2219 (0.2%)
1	B	0.86	0/1688	1.14	1/2264 (0.0%)
1	C	1.04	1/1729 (0.1%)	1.17	7/2326 (0.3%)
1	D	0.81	0/1601	1.10	1/2148 (0.0%)
All	All	0.91	3/6672 (0.0%)	1.14	13/8957 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	954	LEU	C-N	20.88	1.62	1.33
1	A	1054	MET	SD-CE	-6.49	1.63	1.79
1	A	966	GLN	C-O	-5.43	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	954	LEU	O-C-N	-13.48	101.44	123.00
1	B	956	PHE	N-CA-C	7.86	122.25	109.59
1	C	1116	ALA	N-CA-C	-6.56	105.40	113.41
1	A	1086	ASP	CA-CB-CG	6.56	119.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	969	GLU	CB-CG-CD	6.54	123.71	112.60
1	C	1051	ILE	N-CA-C	6.48	122.81	109.34
1	C	969	GLU	CB-CG-CD	6.32	123.34	112.60
1	C	1022	ASN	N-CA-C	6.06	119.99	112.24
1	C	1052	GLY	N-CA-C	5.94	122.68	115.31
1	A	964	GLU	N-CA-C	-5.63	105.06	111.14
1	A	1150	GLU	N-CA-C	5.38	116.83	111.07
1	C	1086	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	1157	ILE	N-CA-C	-5.18	102.40	109.55

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	12	0
1	B	1637	0	1574	9	0
1	C	1677	0	1605	12	0
1	D	1548	0	1490	9	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7535	0	6264	41	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 (41) 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:B:1113:MET:HE3	1:B:1115[B]:MET:HE1	1.21	1.15
1:A:1054:MET:HE1	1:A:1134:LEU:HD21	1.36	1.06
1:A:1113:MET:HE3	1:A:1115[A]:MET:HE1	1.06	1.02
1:A:1113:MET:HE3	1:A:1115[A]:MET:CE	1.97	0.93
1:A:1113:MET:CE	1:A:1115[A]:MET:HE1	2.00	0.90
1:B:1113:MET:HE3	1:B:1115[B]:MET:CE	2.05	0.87
1:C:1105:LYS:H	1:C:1123:HIS:HD2	1.22	0.85
1:B:1113:MET:CE	1:B:1115[B]:MET:HE1	2.12	0.73
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:C:959:SER:O	1:C:962:ASP:HB2	1.98	0.63
1:A:1054:MET:HE3	1:A:1055:PHE:CE2	2.35	0.61
1:D:1031:HIS:HD2	1:D:1060:TYR:O	1.83	0.61
1:C:955:TYR:CD1	1:C:955:TYR:N	2.69	0.60
1:C:972:MET:HE1	1:C:1096:LEU:HD12	1.88	0.56
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:B:972:MET:HE1	1:B:1096:LEU:HD12	1.89	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:972:MET:HE1	1:A:1096:LEU:HD12	1.91	0.51
1:C:955:TYR:N	1:C:955:TYR:HD1	2.10	0.49
1:D:972:MET:HE1	1:D:1096:LEU:HD12	1.94	0.49
1:C:955:TYR:HD1	1:C:955:TYR:H	1.60	0.49
1:D:1011:HIS:HE1	4:D:1419:HOH:O	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1008:ARG:NH2	4:D:1432:HOH:O	2.51	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:A:1028:MET:SD	1:A:1100:ARG:HG3	2.61	0.41
1:A:1107:PHE:CD2	1:A:1113:MET:HE1	2.56	0.41
1:A:975:THR:HB	1:A:1064:ASN:HA	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 [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	196/227 (86%)	194 (99%)	1 (0%)	1 (0%)	24	9
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%)	48	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1131	VAL

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	169/192 (88%)	167 (99%)	2 (1%)	63	40
1	B	171/192 (89%)	164 (96%)	7 (4%)	27	4
1	C	176/192 (92%)	171 (97%)	5 (3%)	38	9
1	D	163/192 (85%)	161 (99%)	2 (1%)	63	40
All	All	679/768 (88%)	663 (98%)	16 (2%)	43	13

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	980	ARG
1	A	1100	ARG
1	B	962	ASP
1	B	990	ASN
1	B	1027	ARG
1	B	1037	ASN
1	B	1051	ILE
1	B	1128	ARG
1	B	1131	VAL
1	C	955	TYR
1	C	959	SER
1	C	963	LYS
1	C	1042	LYS
1	C	1114	LYS
1	D	1036	VAL
1	D	1051	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1023	HIS
1	A	1037	ASN
1	A	1064	ASN
1	A	1095	GLN
1	B	993	ASN
1	B	1109	GLN
1	C	1011	HIS
1	C	1020	ASN
1	C	1064	ASN

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Mol	Chain	Res	Type
1	C	1123	HIS
1	C	1132	ASN
1	D	984	HIS
1	D	998	GLN
1	D	1011	HIS
1	D	1031	HIS
1	D	1095	GLN
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 oligosaccharides 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	1.85	8 (36%)	31,31,31	1.23	2 (6%)
3	CNQ	C	1202	-	22,22,22	1.88	8 (36%)	31,31,31	1.13	2 (6%)
3	CNQ	D	1202	-	22,22,22	1.76	6 (27%)	31,31,31	1.14	3 (9%)
3	CNQ	B	1202	-	22,22,22	1.73	7 (31%)	31,31,31	1.33	2 (6%)

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	C	1202	-	-	0/8/8/8	0/3/3/3
3	CNQ	D	1202	-	-	0/8/8/8	0/3/3/3
3	CNQ	B	1202	-	-	0/8/8/8	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	CNQ	C1-C6	3.90	1.45	1.38
3	C	1202	CNQ	C1-C6	3.62	1.45	1.38
3	D	1202	CNQ	C8-C9	3.19	1.48	1.39
3	C	1202	CNQ	C3-N7	3.04	1.42	1.37
3	B	1202	CNQ	C1-C6	3.01	1.44	1.38
3	D	1202	CNQ	C4-N10	2.98	1.43	1.37
3	B	1202	CNQ	C5-C4	2.89	1.48	1.43
3	D	1202	CNQ	C11-N12	2.68	1.37	1.33
3	A	1202	CNQ	C4-N10	2.63	1.42	1.37
3	B	1202	CNQ	C3-N7	2.58	1.41	1.37
3	C	1202	CNQ	C16-C15	2.55	1.42	1.38
3	C	1202	CNQ	C8-C9	2.55	1.46	1.39
3	A	1202	CNQ	C19-C14	2.51	1.44	1.39
3	A	1202	CNQ	C1-C2	2.36	1.41	1.36
3	B	1202	CNQ	C19-C18	2.35	1.42	1.38
3	D	1202	CNQ	C5-C4	2.34	1.47	1.43
3	C	1202	CNQ	C11-N12	2.27	1.37	1.33
3	B	1202	CNQ	C19-C14	2.27	1.43	1.39
3	C	1202	CNQ	C19-C14	2.27	1.43	1.39
3	B	1202	CNQ	C4-N10	2.24	1.41	1.37
3	D	1202	CNQ	C1-C6	2.22	1.42	1.38
3	A	1202	CNQ	C5-C4	2.17	1.47	1.43
3	C	1202	CNQ	C4-N10	2.13	1.41	1.37
3	D	1202	CNQ	C4-C3	2.11	1.46	1.42
3	A	1202	CNQ	C8-C9	2.09	1.45	1.39
3	B	1202	CNQ	C9-N10	2.06	1.36	1.33
3	A	1202	CNQ	C2-C3	2.06	1.45	1.41
3	C	1202	CNQ	C4-C3	2.02	1.46	1.42
3	A	1202	CNQ	C11-N12	2.01	1.36	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	CNQ	C5-C4-N10	4.72	123.28	119.56
3	A	1202	CNQ	C4-C5-C11	-4.03	120.99	125.16
3	D	1202	CNQ	C5-C4-N10	3.79	122.54	119.56
3	C	1202	CNQ	C5-C4-N10	3.22	122.10	119.56
3	B	1202	CNQ	C4-C5-C11	-2.94	122.11	125.16
3	A	1202	CNQ	C5-C4-N10	2.54	121.56	119.56
3	C	1202	CNQ	C4-C5-C11	-2.49	122.58	125.16
3	D	1202	CNQ	C4-C5-C11	-2.29	122.79	125.16
3	D	1202	CNQ	C14-C9-N10	2.06	119.78	117.05

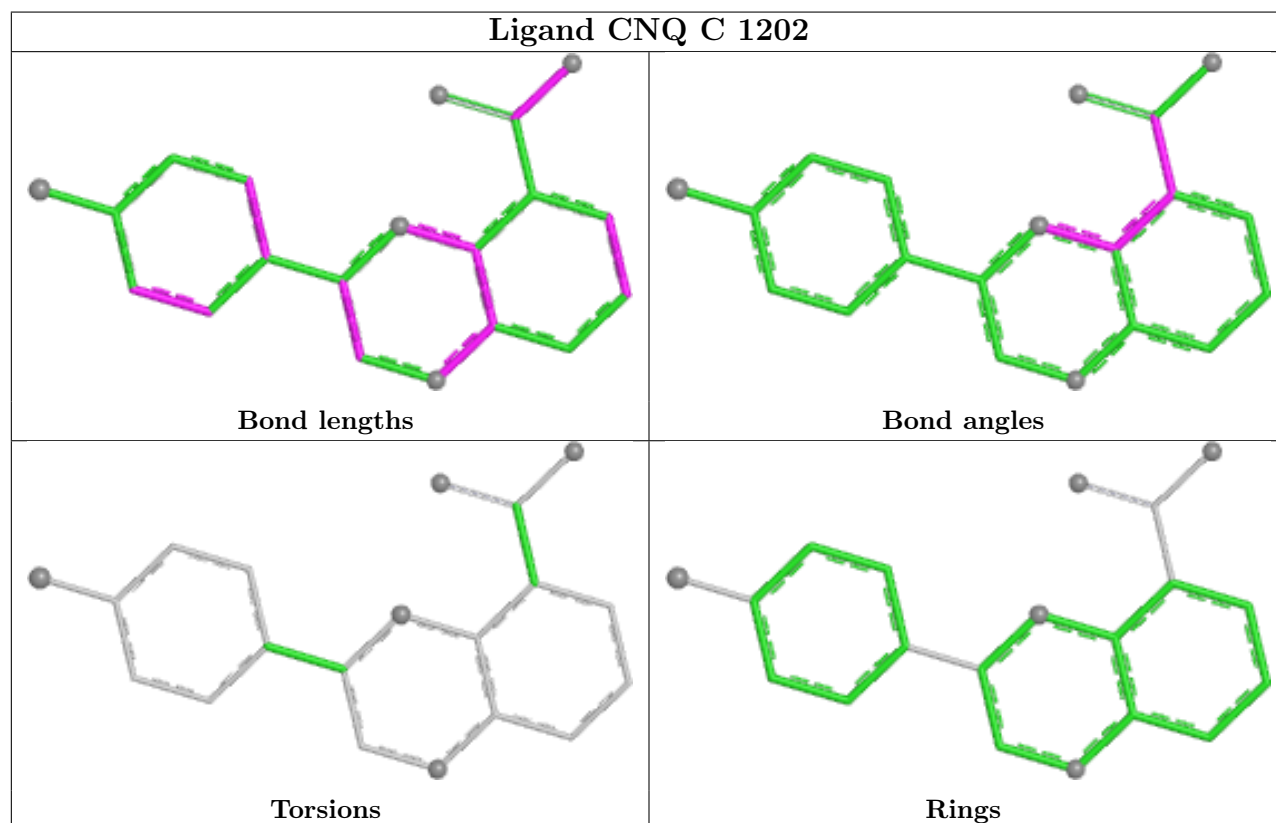
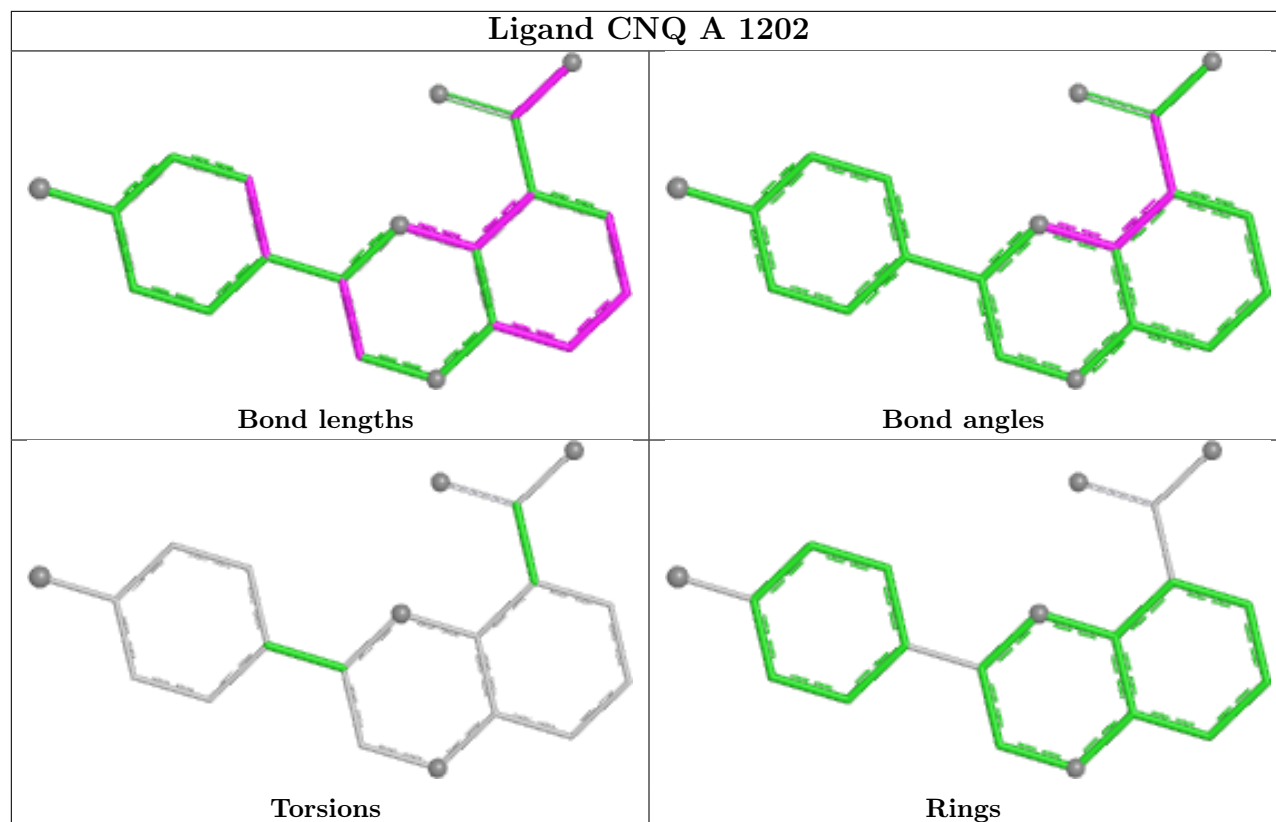
There are no chirality outliers.

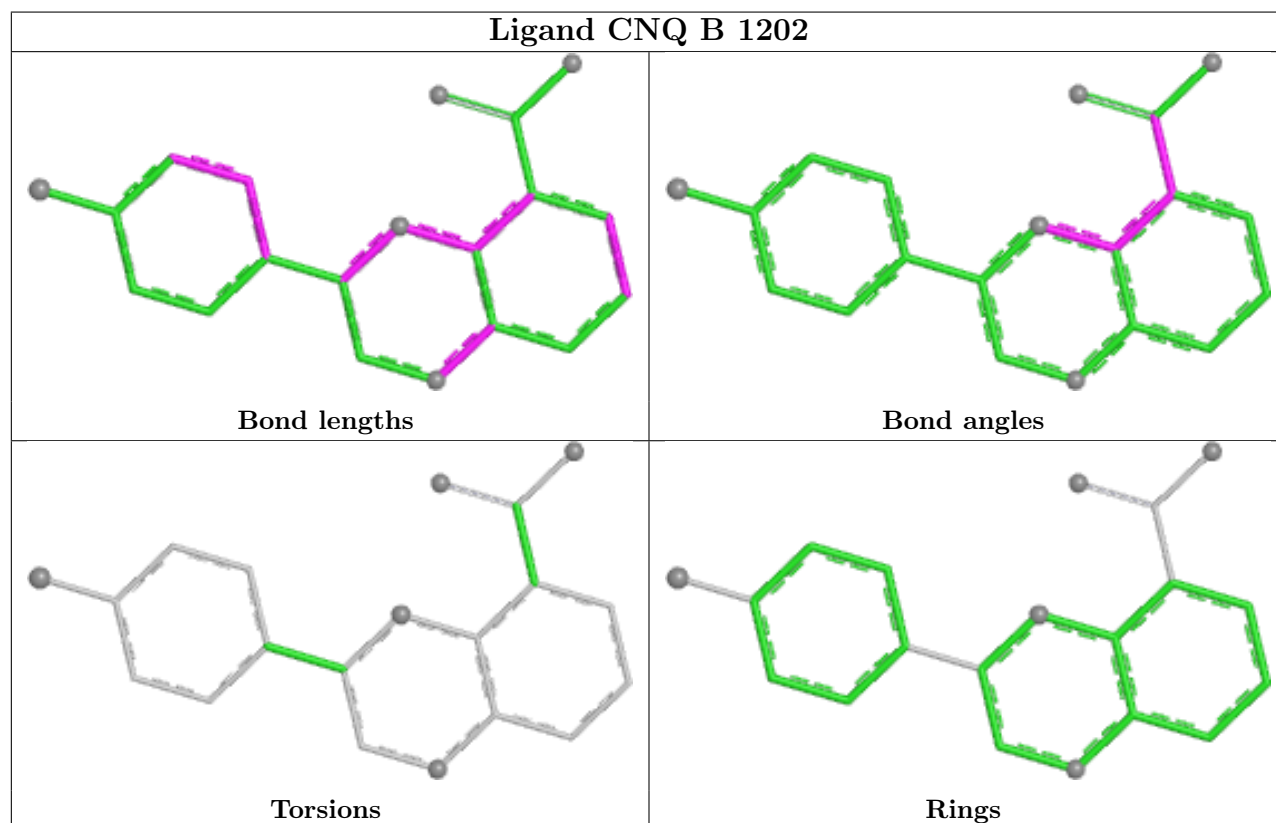
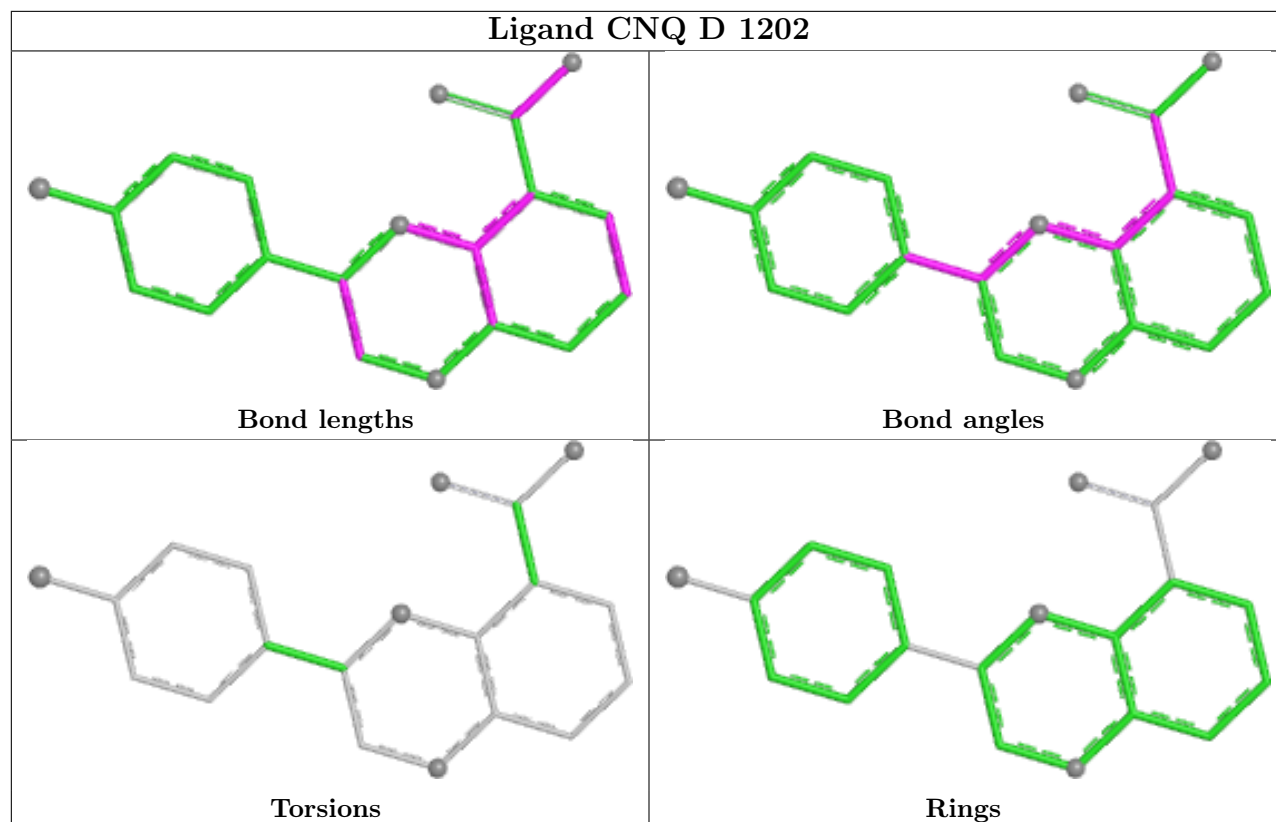
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	0.43	17 (8%)	16 24	12, 21, 44, 66	3 (1%)
1	B	202/227 (88%)	0.43	16 (7%)	18 27	12, 20, 43, 66	3 (1%)
1	C	207/227 (91%)	0.46	24 (11%)	9 15	12, 20, 37, 47	2 (0%)
1	D	188/227 (82%)	0.70	21 (11%)	10 16	13, 24, 52, 70	4 (2%)
All	All	794/908 (87%)	0.51	78 (9%)	13 21	12, 21, 43, 70	12 (1%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	955	TYR	7.8
1	A	1131	VAL	7.3
1	B	955	TYR	6.6
1	B	1131	VAL	6.0
1	C	954	LEU	5.7
1	D	1051	ILE	5.5
1	C	960	PRO	5.4
1	C	961	ASP	5.3
1	D	1110	PHE	5.3
1	B	958	GLY	5.1
1	C	965	PHE	4.9
1	B	956	PHE	4.9
1	C	957	GLN	4.8
1	D	1113	MET	4.6
1	D	1112	ALA	4.6
1	C	1052	GLY	4.4
1	C	958	GLY	4.1
1	D	965	PHE	3.9
1	C	963	LYS	3.7
1	A	1052	GLY	3.7
1	C	1053	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1130	SER	3.6
1	A	1132	ASN	3.6
1	D	1054	MET	3.5
1	C	962	ASP	3.4
1	D	1052	GLY	3.4
1	C	1051	ILE	3.4
1	B	1051	ILE	3.3
1	D	1114	LYS	3.3
1	C	959	SER	3.3
1	B	957	GLN	3.3
1	B	1050	TYR	3.3
1	A	1110	PHE	3.3
1	A	965	PHE	3.2
1	B	1133	GLY	3.2
1	D	1137	ALA	3.2
1	A	1160	PRO	3.1
1	D	1160	PRO	3.1
1	D	1055	PHE	3.0
1	C	1131	VAL	3.0
1	B	963	LYS	3.0
1	C	964	GLU	2.9
1	D	1053	GLY	2.9
1	D	966	GLN	2.9
1	C	1021	HIS	2.9
1	C	956	PHE	2.9
1	D	1071	TYR	2.8
1	A	963	LYS	2.8
1	D	1037[A]	ASN	2.7
1	D	1075	ILE	2.7
1	C	1083	VAL	2.7
1	A	1051	ILE	2.6
1	A	1129	PRO	2.5
1	B	965	PHE	2.5
1	B	1160	PRO	2.5
1	B	1037	ASN	2.5
1	B	962	ASP	2.5
1	D	1049	ALA	2.4
1	A	1133	GLY	2.4
1	C	1132	ASN	2.4
1	D	980	ARG	2.3
1	C	1001	CYS	2.3
1	A	966	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1049	ALA	2.3
1	B	1001	CYS	2.3
1	A	1134	LEU	2.3
1	D	978	GLU	2.3
1	A	1075	ILE	2.1
1	B	1083	VAL	2.1
1	A	1114	LYS	2.1
1	D	988	ILE	2.1
1	D	1050	TYR	2.1
1	A	1049	ALA	2.0
1	A	1159	ARG	2.0
1	C	1004	LYS	2.0
1	C	1085	LYS	2.0
1	C	1036	VAL	2.0
1	C	1037[A]	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

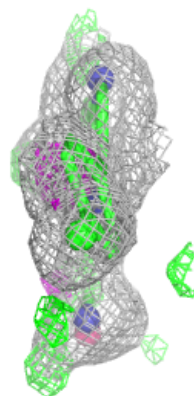
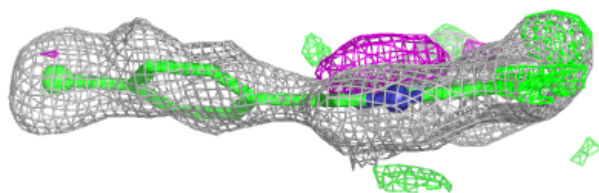
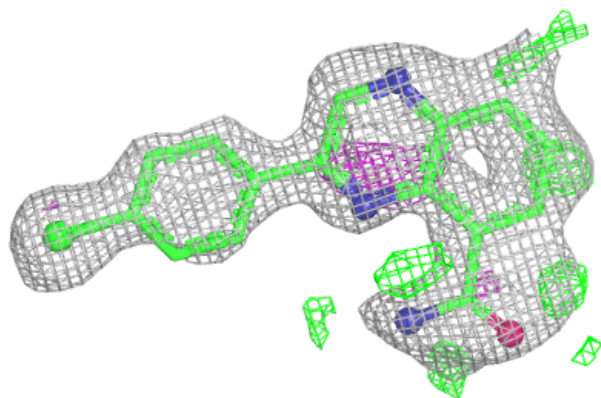
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CNQ	D	1202	20/20	0.79	0.15	34,39,47,50	0
3	CNQ	A	1202	20/20	0.88	0.12	19,23,40,47	0
3	CNQ	B	1202	20/20	0.90	0.11	19,26,39,41	0
3	CNQ	C	1202	20/20	0.95	0.08	12,17,30,33	0
2	ZN	A	1201	1/1	0.97	0.04	26,26,26,26	0
2	ZN	B	1201	1/1	0.97	0.05	24,24,24,24	0
2	ZN	C	1201	1/1	0.97	0.05	26,26,26,26	0
2	ZN	D	1201	1/1	0.97	0.04	27,27,27,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

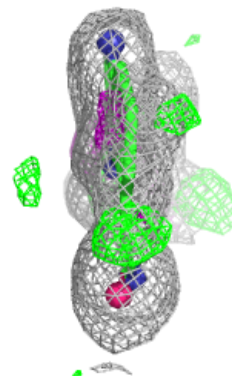
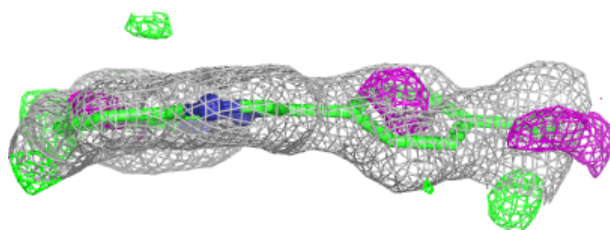
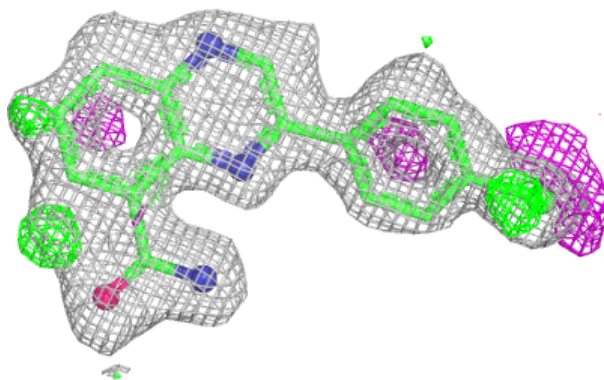
Electron density around CNQ D 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

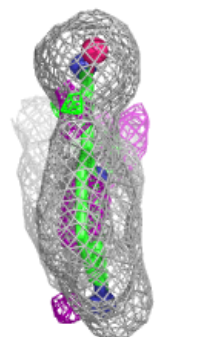
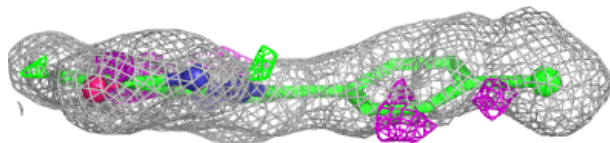
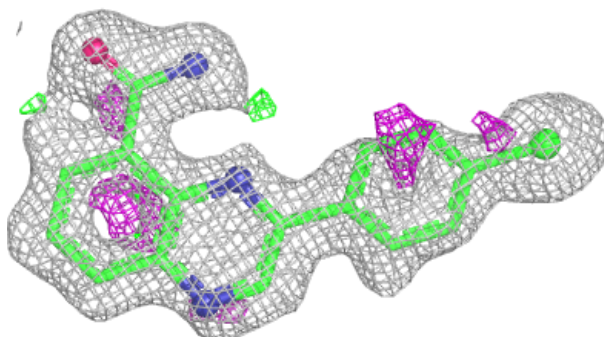


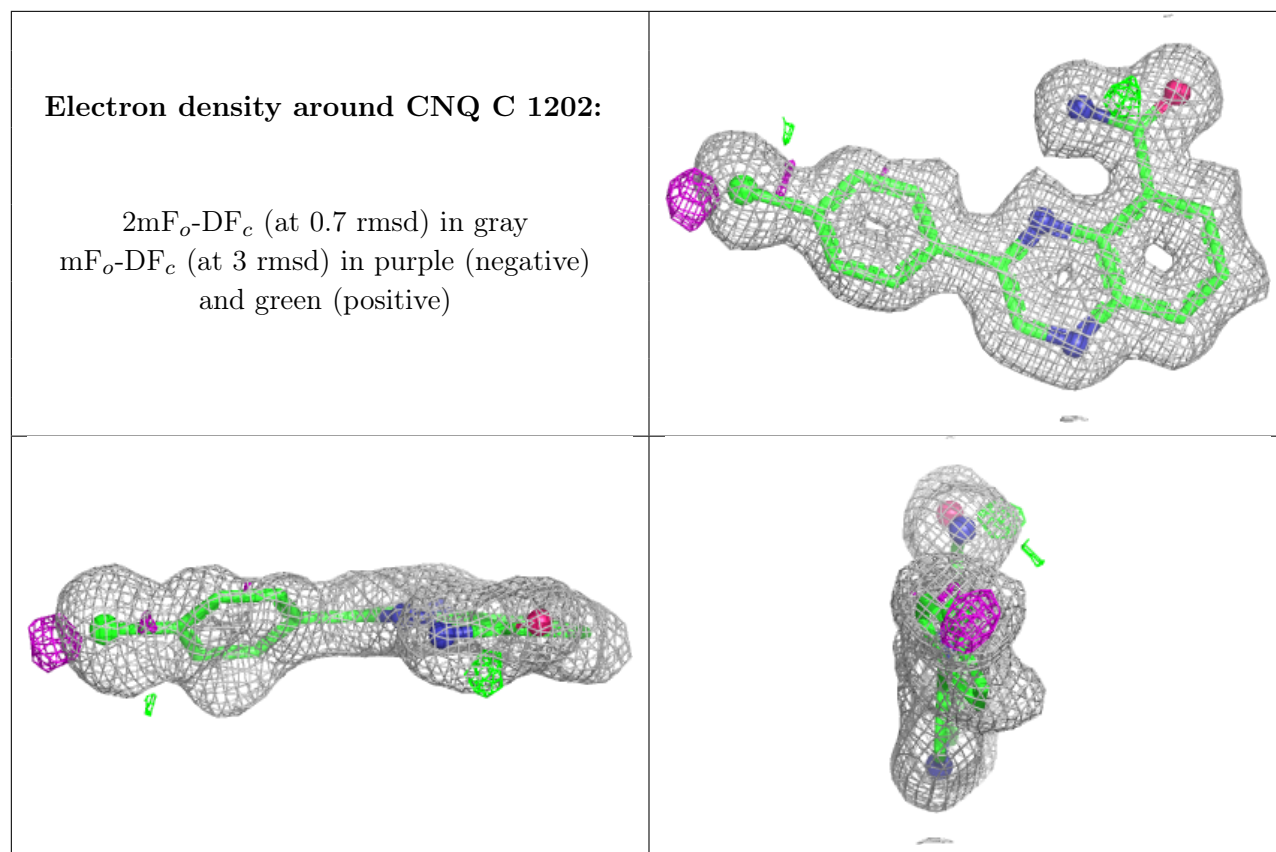
Electron density around CNQ A 1202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CNQ B 1202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.