



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 02:57 am BST

PDB ID : 3LW0
Title : IGF-1RK in complex with ligand MSC1609119A-1
Authors : Graedler, U.; Heinrich, T.; Boettcher, H.; Blaukat, A.; Shutes, A.; Askew, B.
Deposited on : 2010-02-23
Resolution : 1.79 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

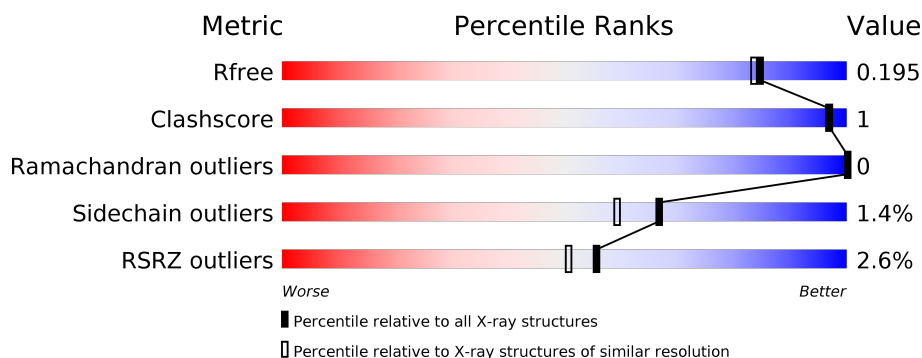
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	304	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>
1	B	304	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	C	304	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	D	304	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10929 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.

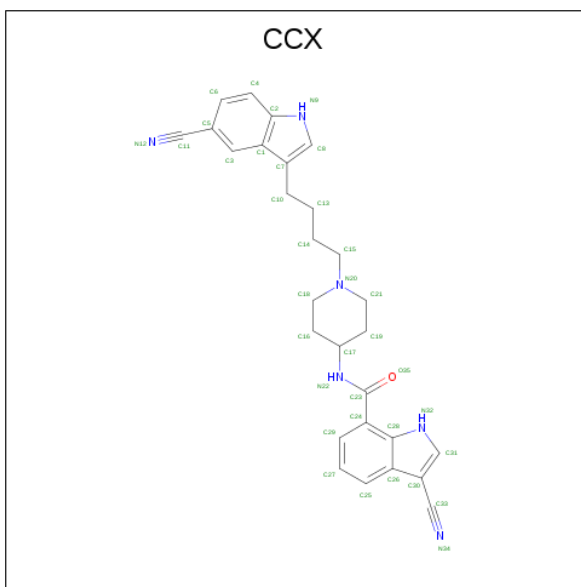
- Molecule 1 is a protein called Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	23	6	0
			2392	1518	398	451	25			
1	B	292	Total	C	N	O	S	10	8	0
			2407	1526	401	455	25			
1	C	292	Total	C	N	O	S	12	6	0
			2392	1518	398	451	25			
1	D	292	Total	C	N	O	S	21	6	0
			2393	1519	398	451	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1097	ALA	GLU	engineered mutation	UNP P08069
A	1099	ALA	GLU	engineered mutation	UNP P08069
B	1097	ALA	GLU	engineered mutation	UNP P08069
B	1099	ALA	GLU	engineered mutation	UNP P08069
C	1097	ALA	GLU	engineered mutation	UNP P08069
C	1099	ALA	GLU	engineered mutation	UNP P08069
D	1097	ALA	GLU	engineered mutation	UNP P08069
D	1099	ALA	GLU	engineered mutation	UNP P08069

- Molecule 2 is 3-cyano-N-{1-[4-(5-cyano-1H-indol-3-yl)butyl]piperidin-4-yl}-1H-indole-7-carboxamide (three-letter code: CCX) (formula: C₂₈H₂₈N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	13	0
			35	28	6	1		
2	A	1	Total	C	N	O	0	0
			35	28	6	1		
2	B	1	Total	C	N	O	13	0
			35	28	6	1		
2	B	1	Total	C	N	O	0	0
			35	28	6	1		
2	C	1	Total	C	N	O	14	0
			35	28	6	1		
2	C	1	Total	C	N	O	0	0
			35	28	6	1		
2	D	1	Total	C	N	O	13	0
			35	28	6	1		
2	D	1	Total	C	N	O	0	0
			35	28	6	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

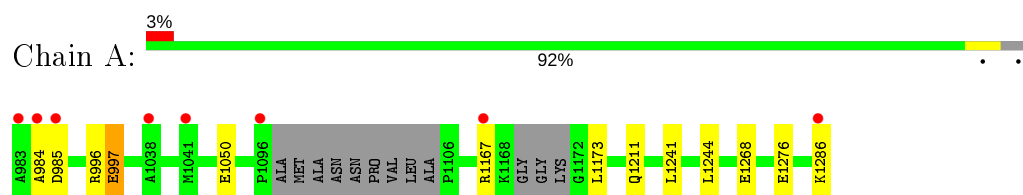
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total	O	0	1
			280	280		
4	B	254	Total	O	0	1
			255	255		
4	C	263	Total	O	0	1
			264	264		
4	D	253	Total	O	0	1
			254	254		

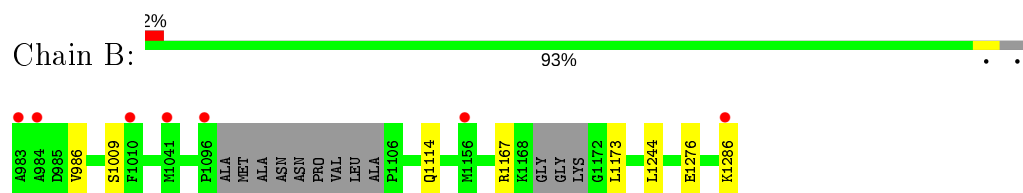
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

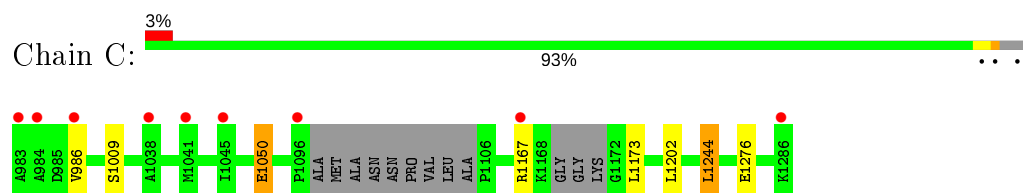
- Molecule 1: Insulin-like growth factor 1 receptor



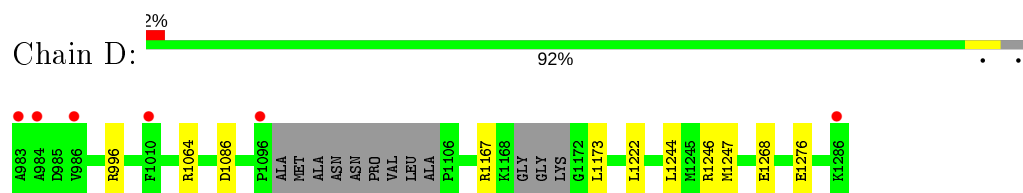
- Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	189.35Å 189.35Å 115.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.79 94.66 – 1.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.79) 99.7 (94.66-1.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.157 , 0.185 0.169 , 0.195	Depositor DCC
R_{free} test set	4956 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.025 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.025 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.467 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.470 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.467 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10929	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, CCX

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	0.55	1/2441 (0.0%)	0.64	0/3287
1	B	0.53	0/2456	0.61	0/3308
1	C	0.55	1/2441 (0.0%)	0.63	0/3287
1	D	0.53	0/2442	0.62	0/3289
All	All	0.54	2/9780 (0.0%)	0.63	0/13171

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1050	GLU	CG-CD	6.98	1.62	1.51
1	A	1050	GLU	CG-CD	6.29	1.61	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1050	GLU	Sidechain

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	2392	0	2346	6	0
1	B	2407	0	2358	5	0
1	C	2392	0	2346	4	0
1	D	2393	0	2349	5	0
2	A	70	0	56	0	0
2	B	70	0	56	0	0
2	C	70	0	56	0	0
2	D	70	0	56	0	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
4	A	280	0	0	1	0
4	B	255	0	0	1	0
4	C	264	0	0	1	0
4	D	254	0	0	3	0
All	All	10929	0	9639	18	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 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:A:1276[A]:GLU:OE2	1:D:1276[A]:GLU:OE2	2.05	0.74
1:D:1247[B]:MET:SD	4:D:773:HOH:O	2.56	0.62
1:B:1276[A]:GLU:OE2	1:C:1276[A]:GLU:OE2	2.24	0.56
1:A:997:GLU:CD	1:A:997:GLU:H	2.08	0.55
1:B:1114:GLN:HG3	3:B:1:GOL:H12	1.89	0.55
1:D:1167:ARG:HB2	1:D:1173:LEU:HD23	1.91	0.52
1:D:1246:ARG:NH1	4:D:685:HOH:O	2.42	0.51
1:B:1286:LYS:OXT	1:B:1286:LYS:HG3	2.12	0.50
1:C:1009:SER:HB3	4:C:1301:HOH:O	2.12	0.49
1:A:1286:LYS:HG3	1:A:1286:LYS:OXT	2.13	0.49
1:B:1009:SER:HB3	4:B:781:HOH:O	2.13	0.49
1:D:1064:ARG:HD2	4:D:897:HOH:O	2.13	0.48
1:C:1167:ARG:HB2	1:C:1173:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1167:ARG:HB2	1:B:1173:LEU:HD23	1.98	0.45
1:A:1211:GLN:HG3	4:A:388:HOH:O	2.15	0.45
1:A:984:ALA:O	1:A:985:ASP:HB2	2.17	0.45
1:A:1167:ARG:HB2	1:A:1173:LEU:HD23	2.00	0.43
1:C:1202:LEU:HD11	1:C:1244:LEU:HD13	2.00	0.43

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	292/304 (96%)	286 (98%)	6 (2%)	0	100	100
1	B	294/304 (97%)	288 (98%)	6 (2%)	0	100	100
1	C	292/304 (96%)	285 (98%)	7 (2%)	0	100	100
1	D	292/304 (96%)	286 (98%)	6 (2%)	0	100	100
All	All	1170/1216 (96%)	1145 (98%)	25 (2%)	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	262/263 (100%)	257 (98%)	5 (2%)	57	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	264/263 (100%)	262 (99%)	2 (1%)	81	78
1	C	262/263 (100%)	260 (99%)	2 (1%)	81	78
1	D	262/263 (100%)	257 (98%)	5 (2%)	57	46
All	All	1050/1052 (100%)	1036 (99%)	14 (1%)	67	62

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	996	ARG
1	A	997	GLU
1	A	1241	LEU
1	A	1244	LEU
1	A	1268	GLU
1	B	986	VAL
1	B	1244	LEU
1	C	986	VAL
1	C	1244	LEU
1	D	996	ARG
1	D	1086	ASP
1	D	1222	LEU
1	D	1244	LEU
1	D	1268	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1214	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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$
2	CCX	D	4	-	36,39,39	1.16	2 (5%)	39,54,54	1.76	5 (12%)
3	GOL	C	2	-	5,5,5	0.40	0	5,5,5	0.40	0
2	CCX	A	1287	-	36,39,39	1.18	4 (11%)	39,54,54	1.13	3 (7%)
2	CCX	C	3	-	36,39,39	1.42	4 (11%)	39,54,54	1.37	6 (15%)
2	CCX	B	2	-	36,39,39	1.35	3 (8%)	39,54,54	1.13	5 (12%)
2	CCX	B	1287	-	36,39,39	1.21	4 (11%)	39,54,54	1.21	5 (12%)
2	CCX	C	1287	-	36,39,39	1.16	4 (11%)	39,54,54	1.18	3 (7%)
2	CCX	A	1	-	36,39,39	1.40	3 (8%)	39,54,54	1.26	7 (17%)
3	GOL	B	1	-	5,5,5	0.39	0	5,5,5	0.51	0
2	CCX	D	1287	-	36,39,39	1.27	4 (11%)	39,54,54	1.20	6 (15%)

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
2	CCX	D	4	-	-	3/17/29/29	0/5/5/5
3	GOL	C	2	-	-	2/4/4/4	-
2	CCX	A	1287	-	-	8/17/29/29	0/5/5/5
2	CCX	C	3	-	-	1/17/29/29	0/5/5/5
2	CCX	B	2	-	-	1/17/29/29	0/5/5/5
2	CCX	B	1287	-	-	8/17/29/29	0/5/5/5
2	CCX	C	1287	-	-	8/17/29/29	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CCX	A	1	-	-	1/17/29/29	0/5/5/5
3	GOL	B	1	-	-	0/4/4/4	-
2	CCX	D	1287	-	-	8/17/29/29	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	CCX	C33-N34	4.65	1.25	1.14
2	A	1	CCX	C23-N22	4.48	1.43	1.34
2	B	2	CCX	C23-N22	4.08	1.43	1.34
2	A	1	CCX	C30-C26	-3.39	1.37	1.42
2	D	4	CCX	C30-C26	-3.17	1.37	1.42
2	B	2	CCX	C30-C26	-3.00	1.38	1.42
2	C	3	CCX	C30-C26	-2.97	1.38	1.42
2	C	3	CCX	C24-C28	-2.89	1.39	1.43
2	D	1287	CCX	C24-C28	-2.85	1.39	1.43
2	B	2	CCX	C24-C28	-2.84	1.39	1.43
2	A	1	CCX	C24-C28	-2.83	1.39	1.43
2	D	4	CCX	C24-C28	-2.79	1.39	1.43
2	D	1287	CCX	C30-C26	-2.58	1.38	1.42
2	B	1287	CCX	C30-C26	-2.41	1.38	1.42
2	B	1287	CCX	C24-C28	-2.38	1.40	1.43
2	A	1287	CCX	C23-N22	2.32	1.39	1.34
2	D	1287	CCX	C23-N22	2.24	1.39	1.34
2	B	1287	CCX	C23-N22	2.23	1.39	1.34
2	A	1287	CCX	C24-C28	-2.22	1.40	1.43
2	C	3	CCX	C23-N22	2.17	1.38	1.34
2	A	1287	CCX	C25-C26	-2.15	1.37	1.42
2	C	1287	CCX	C30-C26	-2.15	1.39	1.42
2	C	1287	CCX	C23-N22	2.12	1.38	1.34
2	C	1287	CCX	C3-C1	-2.10	1.38	1.42
2	B	1287	CCX	C24-C23	-2.06	1.47	1.50
2	C	1287	CCX	C4-C2	-2.06	1.38	1.41
2	A	1287	CCX	C30-C26	-2.05	1.39	1.42
2	D	1287	CCX	C3-C1	-2.03	1.38	1.42

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	CCX	C17-N22-C23	8.05	133.70	122.55
2	C	3	CCX	C30-C33-N34	-4.61	164.11	176.74
2	A	1	CCX	C5-C3-C1	-3.55	117.48	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1287	CCX	C19-C17-N22	-3.41	103.50	110.56
2	B	1287	CCX	C19-C17-N22	-3.27	103.80	110.56
2	D	1287	CCX	C19-C17-N22	-3.18	103.98	110.56
2	B	2	CCX	C5-C3-C1	-3.16	117.88	121.05
2	D	4	CCX	C5-C3-C1	-3.15	117.89	121.05
2	C	1287	CCX	C19-C17-N22	-3.07	104.21	110.56
2	C	3	CCX	C5-C3-C1	-3.01	118.03	121.05
2	C	1287	CCX	C5-C3-C1	-2.84	118.21	121.05
2	D	4	CCX	C3-C1-C2	2.75	122.02	118.26
2	B	2	CCX	C3-C1-C2	2.69	121.93	118.26
2	D	4	CCX	C24-C23-N22	2.60	121.59	116.79
2	D	1287	CCX	O35-C23-C24	-2.56	118.18	121.72
2	A	1	CCX	C3-C1-C2	2.51	121.70	118.26
2	B	1287	CCX	C5-C3-C1	-2.50	118.54	121.05
2	B	1287	CCX	C21-C19-C17	2.43	114.77	110.50
2	C	3	CCX	C3-C1-C2	2.39	121.52	118.26
2	A	1287	CCX	C5-C3-C1	-2.36	118.68	121.05
2	B	2	CCX	O35-C23-C24	-2.36	118.45	121.72
2	A	1	CCX	C19-C17-C16	-2.22	106.96	110.82
2	C	3	CCX	C24-C23-N22	2.22	120.88	116.79
2	D	1287	CCX	C3-C5-C11	2.20	121.56	119.65
2	C	3	CCX	C17-N22-C23	2.19	125.58	122.55
2	A	1	CCX	O35-C23-C24	-2.14	118.77	121.72
2	C	1287	CCX	C3-C1-C2	2.12	121.16	118.26
2	B	1287	CCX	C3-C1-C2	2.12	121.15	118.26
2	A	1	CCX	C6-C4-C2	-2.11	118.18	120.84
2	B	1287	CCX	C24-C23-N22	2.11	120.67	116.79
2	B	2	CCX	C24-C23-N22	2.08	120.62	116.79
2	D	1287	CCX	C24-C23-N22	2.06	120.59	116.79
2	A	1	CCX	C27-C25-C26	-2.06	118.04	120.89
2	D	4	CCX	C27-C25-C26	-2.05	118.05	120.89
2	A	1287	CCX	C24-C23-N22	2.05	120.58	116.79
2	A	1	CCX	C18-C16-C17	-2.03	106.94	110.50
2	D	1287	CCX	C3-C1-C2	2.03	121.03	118.26
2	C	3	CCX	C27-C25-C26	-2.03	118.08	120.89
2	B	2	CCX	C27-C25-C26	-2.01	118.11	120.89
2	D	1287	CCX	C17-N22-C23	2.00	125.32	122.55

There are no chirality outliers.

All (40) torsion outliers are listed below:

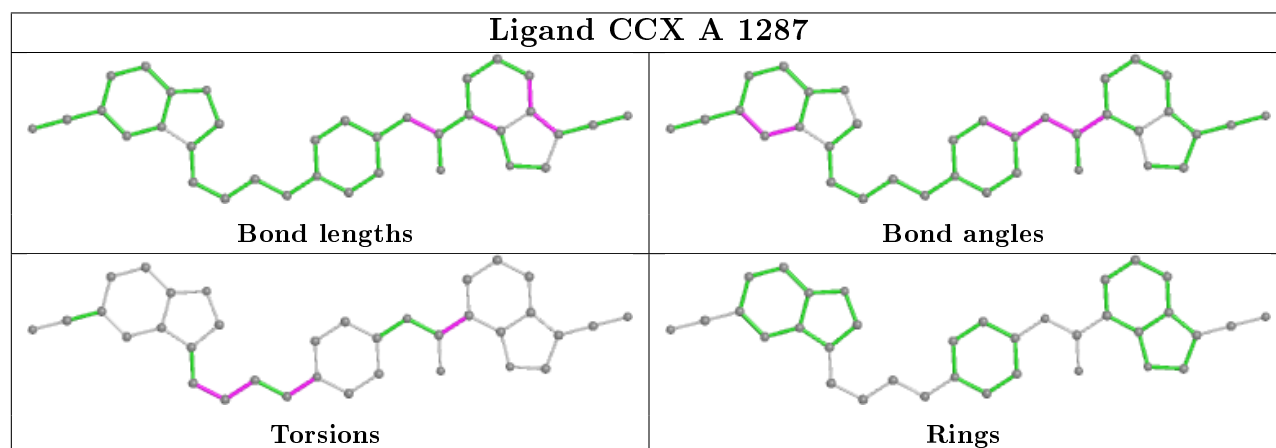
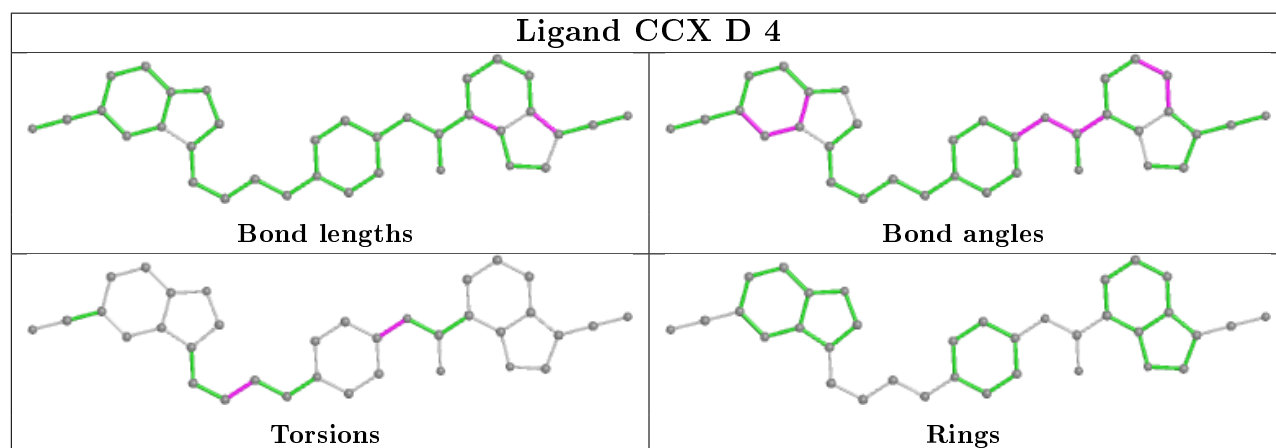
Mol	Chain	Res	Type	Atoms
3	C	2	GOL	C1-C2-C3-O3
2	A	1287	CCX	N22-C23-C24-C28
2	A	1287	CCX	N22-C23-C24-C29
2	A	1287	CCX	O35-C23-C24-C28
2	A	1287	CCX	O35-C23-C24-C29
2	B	1287	CCX	N22-C23-C24-C28
2	B	1287	CCX	N22-C23-C24-C29
2	B	1287	CCX	O35-C23-C24-C28
2	B	1287	CCX	O35-C23-C24-C29
2	C	1287	CCX	N22-C23-C24-C28
2	C	1287	CCX	N22-C23-C24-C29
2	C	1287	CCX	O35-C23-C24-C28
2	C	1287	CCX	O35-C23-C24-C29
2	D	1287	CCX	N22-C23-C24-C28
2	D	1287	CCX	N22-C23-C24-C29
2	D	1287	CCX	O35-C23-C24-C28
2	D	1287	CCX	O35-C23-C24-C29
2	D	1287	CCX	C7-C10-C13-C14
2	C	1287	CCX	C7-C10-C13-C14
2	A	1287	CCX	C7-C10-C13-C14
2	B	1287	CCX	C7-C10-C13-C14
3	C	2	GOL	O2-C2-C3-O3
2	A	1287	CCX	C14-C15-N20-C18
2	A	1287	CCX	C14-C15-N20-C21
2	C	1287	CCX	C14-C15-N20-C21
2	B	1287	CCX	C14-C15-N20-C21
2	B	1287	CCX	C14-C15-N20-C18
2	B	1287	CCX	C10-C13-C14-C15
2	A	1287	CCX	C10-C13-C14-C15
2	C	1287	CCX	C14-C15-N20-C18
2	C	1287	CCX	C10-C13-C14-C15
2	D	1287	CCX	C10-C13-C14-C15
2	D	1287	CCX	C14-C15-N20-C21
2	D	4	CCX	C19-C17-N22-C23
2	D	1287	CCX	C14-C15-N20-C18
2	B	2	CCX	C10-C13-C14-C15
2	D	4	CCX	C10-C13-C14-C15
2	C	3	CCX	C10-C13-C14-C15
2	A	1	CCX	C10-C13-C14-C15
2	D	4	CCX	C16-C17-N22-C23

There are no ring outliers.

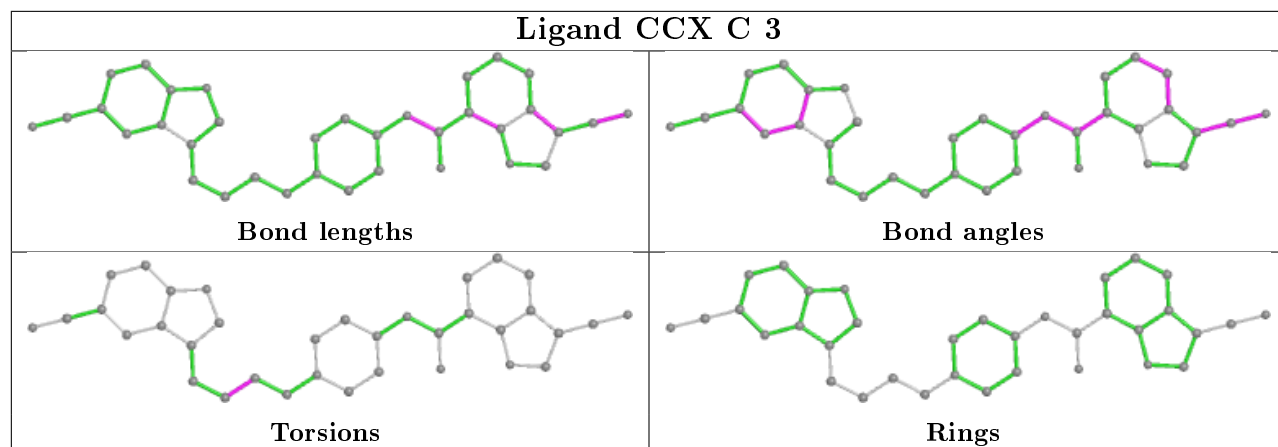
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	GOL	1	0

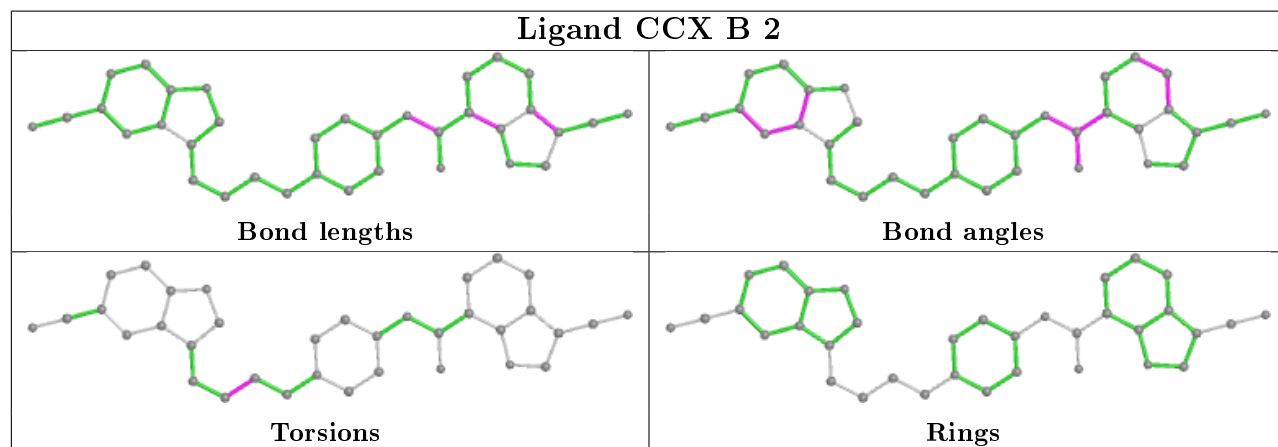
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



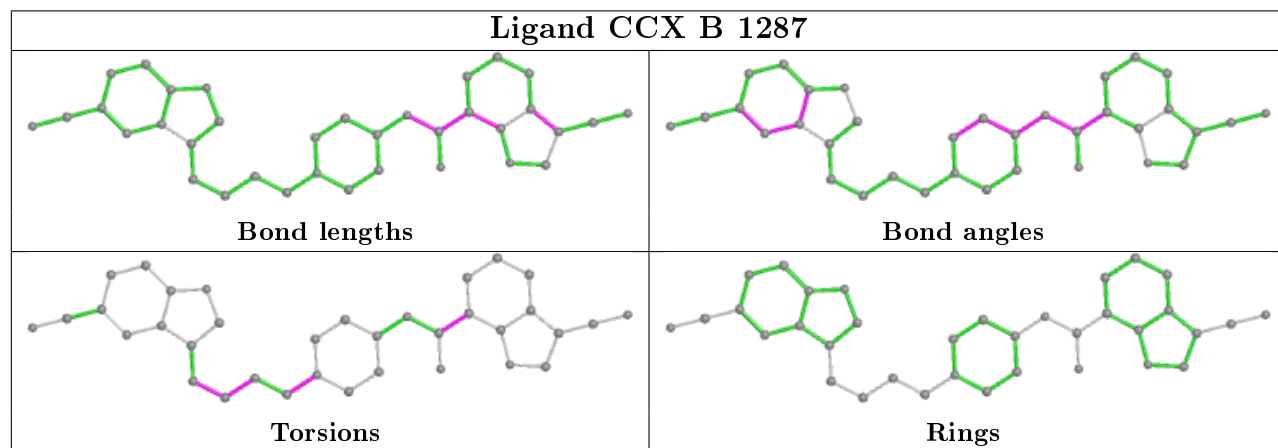
Ligand CCX C 3

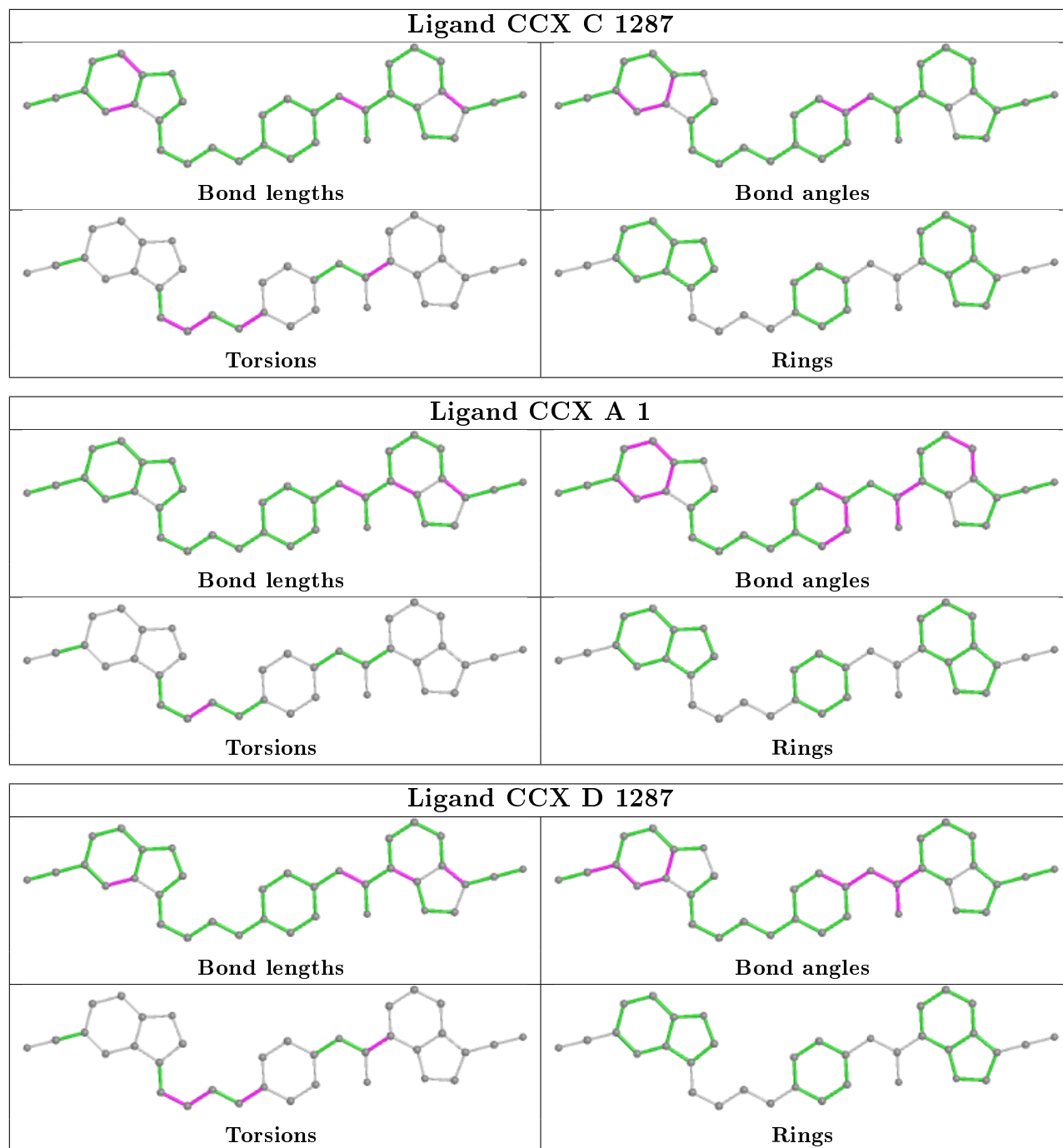


Ligand CCX B 2



Ligand CCX B 1287





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 ⓘ

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	292/304 (96%)	-0.03	8 (2%) 54 49	4, 12, 23, 35	15 (5%)
1	B	292/304 (96%)	-0.01	7 (2%) 59 54	3, 12, 23, 35	9 (3%)
1	C	292/304 (96%)	-0.04	9 (3%) 49 43	4, 12, 23, 34	7 (2%)
1	D	292/304 (96%)	-0.02	6 (2%) 63 59	4, 12, 24, 34	15 (5%)
All	All	1168/1216 (96%)	-0.03	30 (2%) 56 51	3, 12, 24, 35	46 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	983	ALA	4.8
1	A	1096	PRO	4.5
1	D	984	ALA	4.3
1	D	1286	LYS	4.3
1	D	983	ALA	4.2
1	C	983	ALA	4.2
1	C	1096	PRO	3.9
1	B	983	ALA	3.7
1	C	984	ALA	3.6
1	B	1041	MET	3.5
1	B	984	ALA	3.5
1	D	1096	PRO	3.4
1	A	984	ALA	3.1
1	B	1096	PRO	2.9
1	A	1041	MET	2.7
1	C	1038	ALA	2.7
1	C	1286	LYS	2.6
1	D	986	VAL	2.5
1	C	986	VAL	2.4
1	C	1045	ILE	2.3
1	B	1286	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1010	PHE	2.2
1	B	1156	MET	2.2
1	A	1038	ALA	2.2
1	C	1167	ARG	2.1
1	B	1010	PHE	2.1
1	A	985	ASP	2.1
1	A	1167	ARG	2.1
1	C	1041	MET	2.0
1	A	1286	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 carbohydrates in this entry.

6.4 Ligands [i](#)

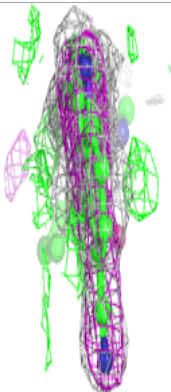
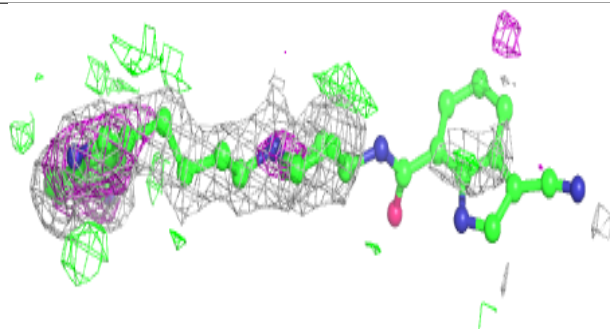
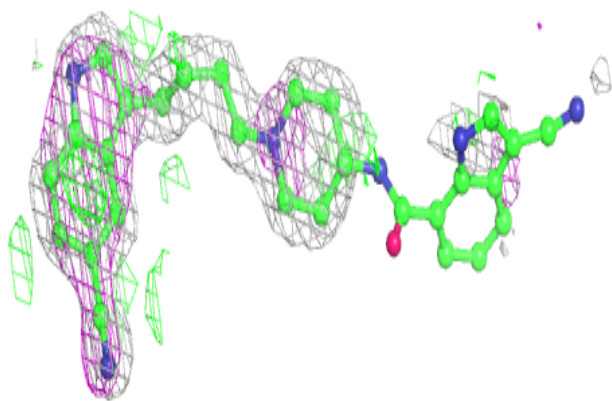
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	1	6/6	0.80	0.17	48,49,49,49	0
2	CCX	C	3	35/35	0.90	0.24	14,22,24,24	14
3	GOL	C	2	6/6	0.91	0.10	42,44,45,48	0
2	CCX	A	1	35/35	0.91	0.22	12,23,31,34	13
2	CCX	B	2	35/35	0.92	0.21	13,23,30,32	13
2	CCX	D	4	35/35	0.93	0.21	13,22,32,35	13
2	CCX	B	1287	35/35	0.96	0.08	4,10,15,18	0
2	CCX	C	1287	35/35	0.96	0.08	5,10,15,17	0
2	CCX	A	1287	35/35	0.96	0.08	4,10,15,18	0
2	CCX	D	1287	35/35	0.96	0.08	3,9,14,18	0

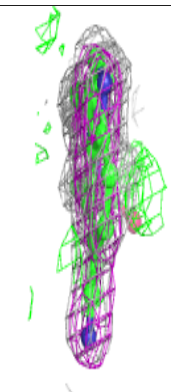
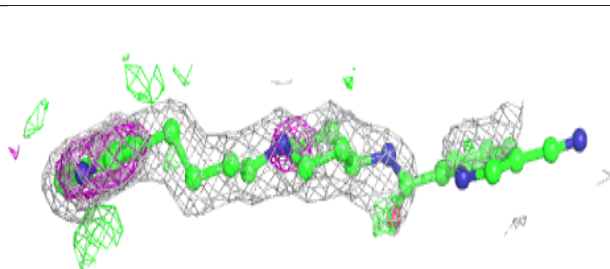
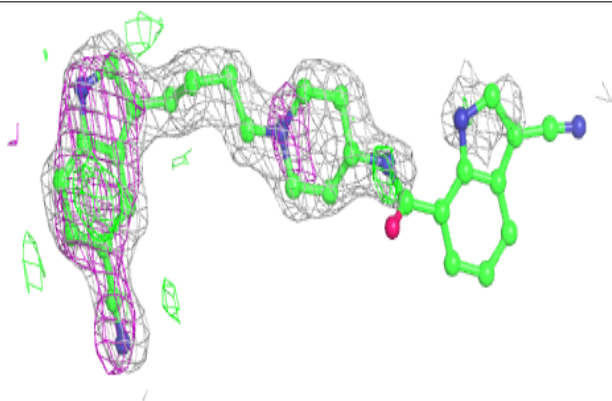
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CCX C 3:

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

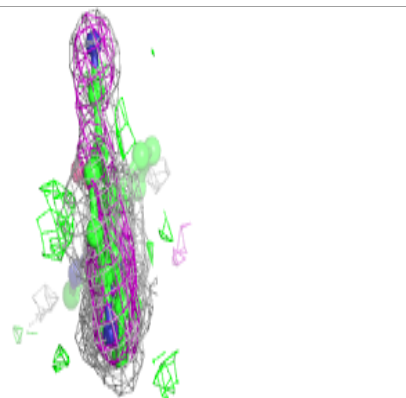
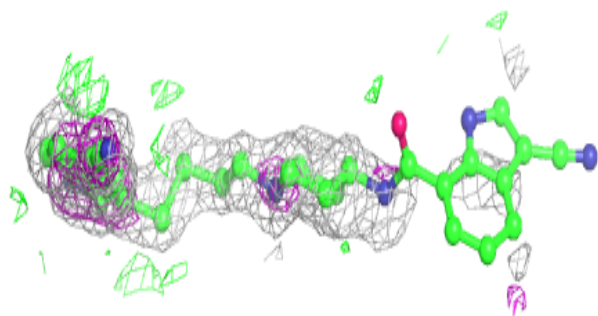
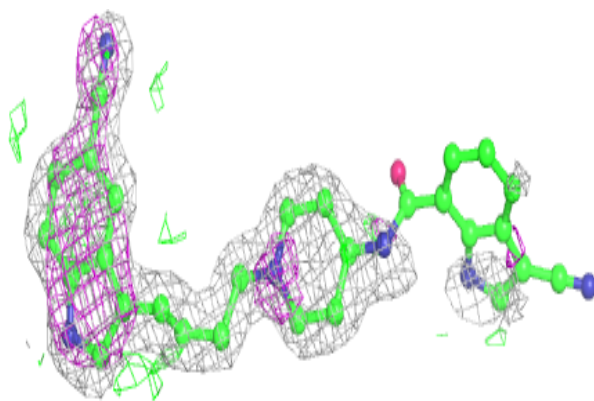
**Electron density around CCX A 1:**

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

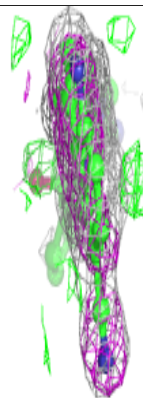
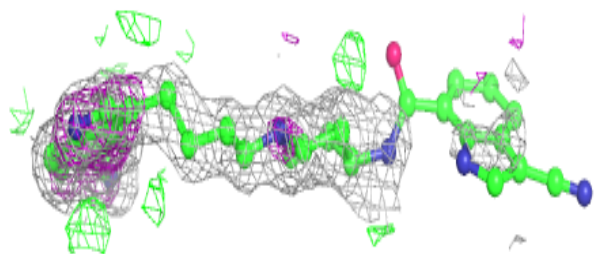
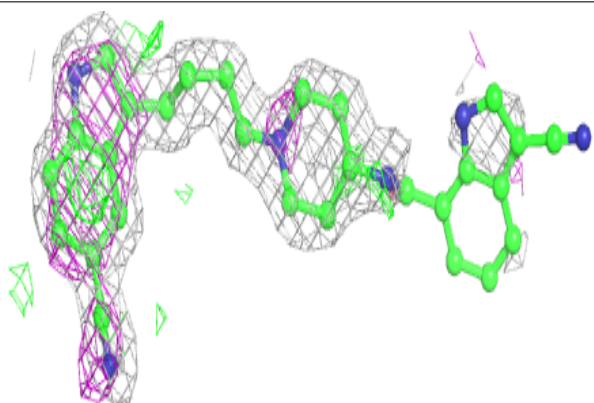


Electron density around CCX B 2:

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

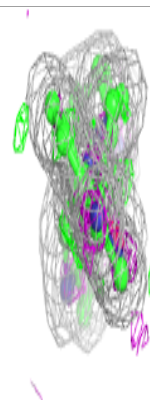
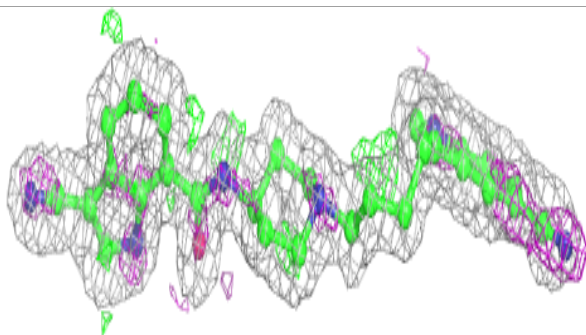
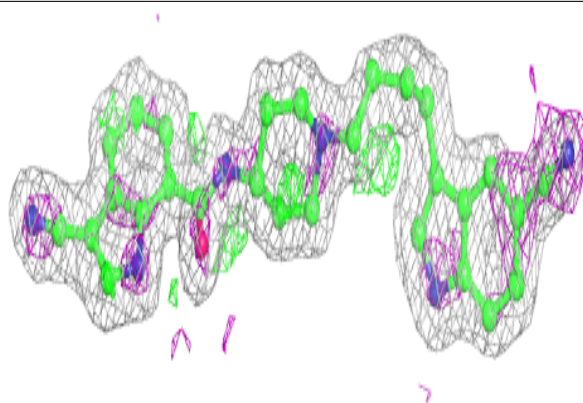
**Electron density around CCX D 4:**

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

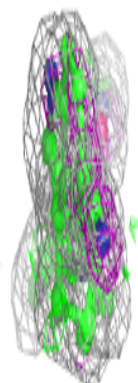
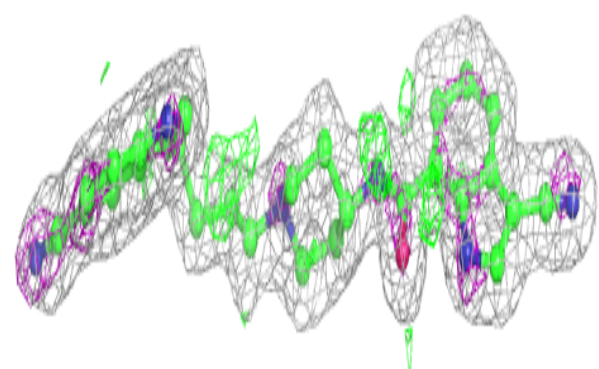
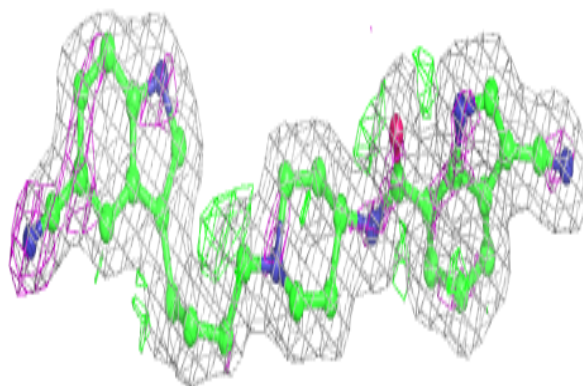


Electron density around CCX B 1287:

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

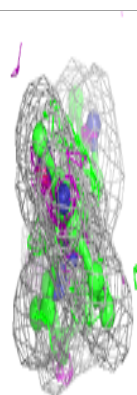
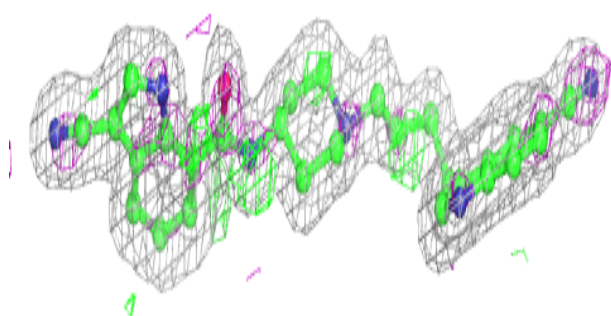
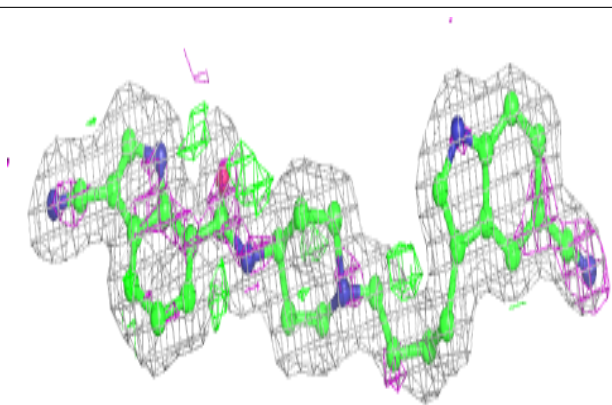
**Electron density around CCX C 1287:**

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

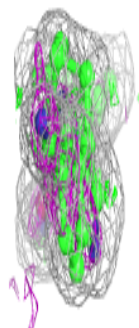
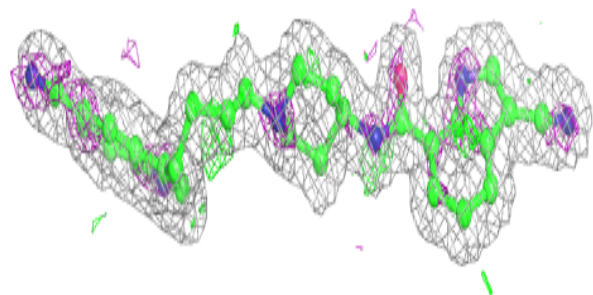
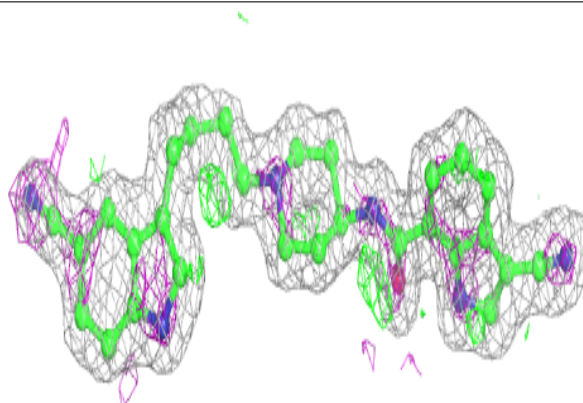


Electron density around CCX A 1287:

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

**Electron density around CCX D 1287:**

$2mF_o-DF_c$ (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.