



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:36 pm BST

PDB ID : 5JQH
Title : Structure of beta2 adrenoceptor bound to carazolol and inactive-state stabilizing nanobody, Nb60
Authors : Staus, D.P.; Strachan, R.T.; Manglik, A.; Pani, B.; Kahsai, A.W.; Kim, T.H.; Wingler, L.M.; Ahn, S.; Chatterjee, A.; Masoudi, A.; Kruse, A.C.; Pardon, E.; Steyaert, J.; Weis, W.I.; Prosser, R.S.; Kobilka, B.K.; Costa, T.; Lefkowitz, R.J.
Deposited on : 2016-05-05
Resolution : 3.20 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

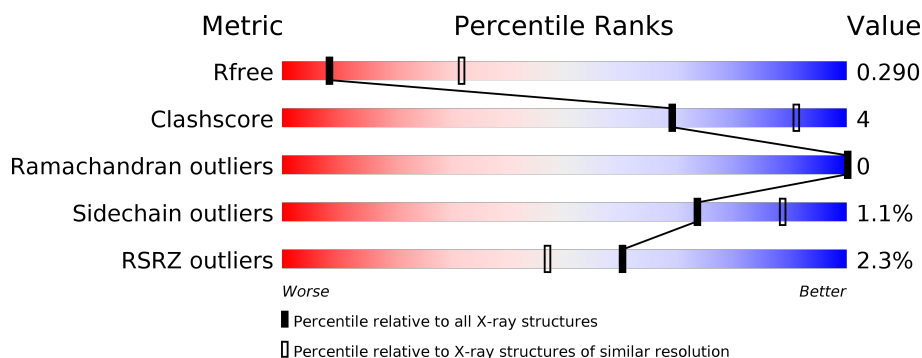
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	471	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 77% 6% 17% </div> </div>
1	B	471	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 78% 7% 15% </div> </div>
2	C	125	<div> <div style="width: 82%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 82% 14% • </div> </div>
2	D	125	<div> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 81% 11% • 6% </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CLR	A	1402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7701 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 Endolysin,Beta-2 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			2915	1912	478	505	20			
1	B	402	Total	C	N	O	S	0	0	0
			2989	1953	494	521	21			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	852	ASP	-	expression tag	UNP P00720
A	853	TYR	-	expression tag	UNP P00720
A	854	LYS	-	expression tag	UNP P00720
A	855	ASP	-	expression tag	UNP P00720
A	856	ASP	-	expression tag	UNP P00720
A	857	ASP	-	expression tag	UNP P00720
A	858	ASP	-	expression tag	UNP P00720
A	859	ALA	-	expression tag	UNP P00720
A	860	GLU	-	expression tag	UNP P00720
A	861	ASN	-	expression tag	UNP P00720
A	862	LEU	-	expression tag	UNP P00720
A	863	TYR	-	expression tag	UNP P00720
A	864	PHE	-	expression tag	UNP P00720
A	865	GLN	-	expression tag	UNP P00720
A	866	GLY	-	expression tag	UNP P00720
A	877	GLY	ARG	conflict	UNP P00720
A	919	THR	CYS	engineered mutation	UNP P00720
A	962	ALA	CYS	engineered mutation	UNP P00720
A	1002	ARG	ILE	conflict	UNP P00720
A	1027	ALA	-	linker	UNP P00720
A	1028	ALA	-	linker	UNP P00720
A	1029	ASP	-	linker	UNP P00720
A	1096	THR	MET	engineered mutation	UNP P07550
A	1098	THR	MET	engineered mutation	UNP P07550
A	1187	GLU	ASN	engineered mutation	UNP P07550

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P07550
A	?	-	SER	deletion	UNP P07550
A	?	-	GLU	deletion	UNP P07550
A	?	-	GLY	deletion	UNP P07550
A	?	-	ARG	deletion	UNP P07550
A	?	-	PHE	deletion	UNP P07550
A	?	-	HIS	deletion	UNP P07550
A	?	-	VAL	deletion	UNP P07550
A	?	-	GLN	deletion	UNP P07550
A	?	-	ASN	deletion	UNP P07550
A	?	-	LEU	deletion	UNP P07550
A	?	-	SER	deletion	UNP P07550
A	?	-	GLN	deletion	UNP P07550
A	?	-	VAL	deletion	UNP P07550
A	?	-	GLU	deletion	UNP P07550
A	?	-	GLN	deletion	UNP P07550
A	?	-	ASP	deletion	UNP P07550
A	?	-	GLY	deletion	UNP P07550
A	?	-	ARG	deletion	UNP P07550
A	?	-	THR	deletion	UNP P07550
A	?	-	GLY	deletion	UNP P07550
A	?	-	HIS	deletion	UNP P07550
A	?	-	GLY	deletion	UNP P07550
A	?	-	LEU	deletion	UNP P07550
A	?	-	ARG	deletion	UNP P07550
A	?	-	ARG	deletion	UNP P07550
A	1261	ILE	SER	conflict	UNP P07550
A	1262	ASP	SER	conflict	UNP P07550
A	1265	ALA	CYS	engineered mutation	UNP P07550
B	852	ASP	-	expression tag	UNP P00720
B	853	TYR	-	expression tag	UNP P00720
B	854	LYS	-	expression tag	UNP P00720
B	855	ASP	-	expression tag	UNP P00720
B	856	ASP	-	expression tag	UNP P00720
B	857	ASP	-	expression tag	UNP P00720
B	858	ASP	-	expression tag	UNP P00720
B	859	ALA	-	expression tag	UNP P00720
B	860	GLU	-	expression tag	UNP P00720
B	861	ASN	-	expression tag	UNP P00720
B	862	LEU	-	expression tag	UNP P00720
B	863	TYR	-	expression tag	UNP P00720
B	864	PHE	-	expression tag	UNP P00720

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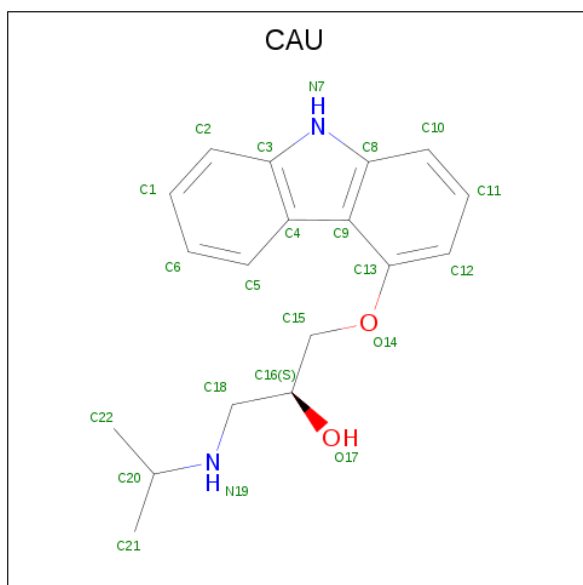
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Chain	Residue	Modelled	Actual	Comment	Reference
B	865	GLN	-	expression tag	UNP P00720
B	866	GLY	-	expression tag	UNP P00720
B	877	GLY	ARG	conflict	UNP P00720
B	919	THR	CYS	engineered mutation	UNP P00720
B	962	ALA	CYS	engineered mutation	UNP P00720
B	1002	ARG	ILE	conflict	UNP P00720
B	1027	ALA	-	linker	UNP P00720
B	1028	ALA	-	linker	UNP P00720
B	1029	ASP	-	linker	UNP P00720
B	1096	THR	MET	engineered mutation	UNP P07550
B	1098	THR	MET	engineered mutation	UNP P07550
B	1187	GLU	ASN	engineered mutation	UNP P07550
B	?	-	LYS	deletion	UNP P07550
B	?	-	SER	deletion	UNP P07550
B	?	-	GLU	deletion	UNP P07550
B	?	-	GLY	deletion	UNP P07550
B	?	-	ARG	deletion	UNP P07550
B	?	-	PHE	deletion	UNP P07550
B	?	-	HIS	deletion	UNP P07550
B	?	-	VAL	deletion	UNP P07550
B	?	-	GLN	deletion	UNP P07550
B	?	-	ASN	deletion	UNP P07550
B	?	-	LEU	deletion	UNP P07550
B	?	-	SER	deletion	UNP P07550
B	?	-	GLN	deletion	UNP P07550
B	?	-	VAL	deletion	UNP P07550
B	?	-	GLU	deletion	UNP P07550
B	?	-	GLN	deletion	UNP P07550
B	?	-	ASP	deletion	UNP P07550
B	?	-	GLY	deletion	UNP P07550
B	?	-	ARG	deletion	UNP P07550
B	?	-	THR	deletion	UNP P07550
B	?	-	GLY	deletion	UNP P07550
B	?	-	HIS	deletion	UNP P07550
B	?	-	GLY	deletion	UNP P07550
B	?	-	LEU	deletion	UNP P07550
B	?	-	ARG	deletion	UNP P07550
B	?	-	ARG	deletion	UNP P07550
B	1261	ILE	SER	conflict	UNP P07550
B	1262	ASP	SER	conflict	UNP P07550
B	1265	ALA	CYS	engineered mutation	UNP P07550

- Molecule 2 is a protein called Nanobody60, Nb60.

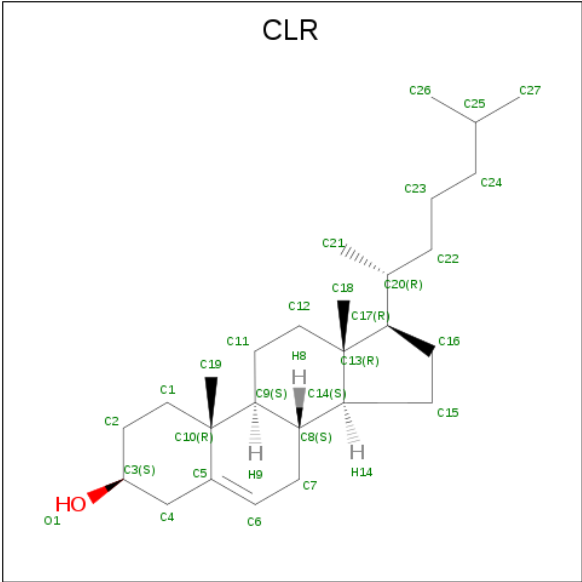
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	117	Total	C	N	O	S	0	0	0
			838	522	145	167	4			
2	C	120	Total	C	N	O	S	0	1	0
			859	537	149	169	4			

- Molecule 3 is (2S)-1-(9H-Carbazol-4-yloxy)-3-(isopropylamino)propan-2-ol (three-letter code: CAU) (formula: C₁₈H₂₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	18	2	2		
3	B	1	Total	C	N	O	0	0
			22	18	2	2		

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).

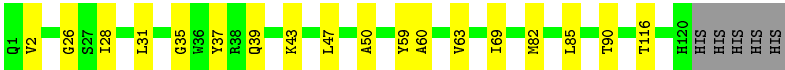


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	B	1	Total	C	O	0	0
			28	27	1		

Chain C:

82%

14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.92Å 164.49Å 218.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.87 – 3.20 32.87 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.4 (32.87-3.20) 84.6 (32.87-3.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.246 , 0.290 0.246 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (7.33%)	wwPDB-VP
Wilson B-factor (Å ²)	92.9	Xtriage
Anisotropy	0.821	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7701	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5285e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/2985	0.36	0/4092
1	B	0.23	0/3057	0.36	0/4189
2	C	0.25	0/874	0.43	0/1189
2	D	0.25	0/852	0.43	0/1158
All	All	0.24	0/7768	0.38	0/10628

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2915	0	2751	16	0
1	B	2989	0	2811	19	0
2	C	859	0	795	10	0
2	D	838	0	769	9	0
3	A	22	0	22	0	0
3	B	22	0	22	0	0
4	A	28	0	46	1	0
4	B	28	0	46	1	0
All	All	7701	0	7262	55	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 4.

All (55) 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)
2:C:82:MET:HB3	2:C:85:LEU:HD21	1.71	0.71
1:B:1340:LEU:HD12	1:B:1341:CYS:H	1.59	0.67
2:C:90:THR:HG23	2:C:116:THR:HA	1.76	0.66
1:B:1205:ILE:HA	1:B:1209:TYR:HB2	1.79	0.64
1:B:991:TRP:HB3	1:B:1019:ARG:HA	1.81	0.61
1:A:991:TRP:HB3	1:A:1019:ARG:HA	1.83	0.60
1:A:1205:ILE:HA	1:A:1209:TYR:HB2	1.83	0.59
1:B:929:GLU:O	1:B:933:ASN:ND2	2.36	0.59
2:C:39:GLN:NE2	2:C:43:LYS:O	2.36	0.58
2:D:2:VAL:HA	2:D:26:GLY:HA3	1.86	0.57
1:B:957:ASP:OD2	1:B:960:ARG:NH1	2.38	0.55
1:A:952:VAL:HG21	1:A:983:LEU:HB3	1.89	0.55
1:B:1172:HIS:CG	1:B:1175:ARG:HE	2.25	0.55
2:D:44:LEU:HD23	2:D:44:LEU:H	1.72	0.54
2:D:35:GLY:HA2	2:D:50:ALA:HA	1.90	0.54
1:A:979:PHE:HB3	1:A:982:SER:HB2	1.89	0.53
1:A:1058:ILE:HD13	1:A:1069:ASN:HB3	1.92	0.52
1:A:1115:LEU:HD22	1:A:1166:PHE:HE1	1.75	0.52
2:D:90:THR:HG23	2:D:116:THR:HA	1.92	0.51
1:B:1115:LEU:HD22	1:B:1166:PHE:HE1	1.76	0.51
1:A:1142:GLN:HE22	2:C:28:ILE:H	1.57	0.51
1:B:981:ASN:HA	1:B:984:ARG:HH12	1.75	0.50
2:D:38:ARG:NH1	2:D:89:ASP:HA	2.26	0.50
2:D:60:ALA:HB3	2:D:63:VAL:HG22	1.93	0.50
1:B:981:ASN:HA	1:B:984:ARG:NH1	2.27	0.50
2:C:35:GLY:HA2	2:C:50:ALA:HA	1.94	0.49
1:A:1063:ARG:HH12	1:A:1331:ASP:HA	1.77	0.49
1:A:875:ASP:OD1	1:A:1013:ARG:NH2	2.46	0.49
2:D:29:PHE:HA	2:D:32:ASN:HD21	1.76	0.49
1:B:953:TYR:O	1:B:961:ARG:NE	2.45	0.49
1:A:1178:HIS:HD2	1:A:1180:GLU:HB3	1.78	0.48
2:C:60:ALA:HB3	2:C:63:VAL:HG22	1.96	0.48
2:D:98:LYS:HG2	2:D:107:ASP:OD1	2.14	0.48
1:B:1292:VAL:HG13	1:B:1303:ILE:HD12	1.97	0.47
1:A:1098:THR:HB	1:A:1189:THR:HG22	1.95	0.47
1:B:1175:ARG:NH1	1:B:1185:TYR:CG	2.84	0.46
1:A:1133:PHE:HB3	1:A:1144:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:TYR:CZ	2:C:47:LEU:HD13	2.51	0.45
1:B:1058:ILE:HD13	1:B:1069:ASN:HB3	1.99	0.44
1:A:1130:ASP:OD1	1:A:1143:SER:OG	2.23	0.44
1:A:1277:ILE:HG22	1:A:1325:ILE:HD13	1.99	0.44
1:B:1219:TYR:OH	1:B:1272:LEU:O	2.28	0.44
1:B:1277:ILE:HG22	1:B:1325:ILE:HD13	2.00	0.43
1:B:953:TYR:HD1	1:B:964:LEU:HD23	1.82	0.43
2:C:59:TYR:CZ	2:C:69:ILE:HG22	2.53	0.43
2:C:28:ILE:HG22	2:C:31:LEU:H	1.83	0.43
4:B:1402:CLR:H232	4:B:1402:CLR:H211	1.79	0.43
1:A:1178:HIS:CD2	1:A:1180:GLU:HB3	2.54	0.42
2:D:47:LEU:HD11	2:D:50:ALA:HB2	2.02	0.42
4:A:1402:CLR:H211	4:A:1402:CLR:H232	1.83	0.42
1:B:1122:GLU:OE1	1:B:1161:SER:OG	2.34	0.41
2:C:2:VAL:HA	2:C:26:GLY:HA3	2.02	0.41
1:A:1051:ASN:O	1:A:1055:ILE:HG12	2.21	0.40
1:B:1281:THR:HG22	1:B:1318:ASN:ND2	2.36	0.40
1:B:1296:HIS:CE1	1:B:1303:ILE:HB	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	385/471 (82%)	372 (97%)	13 (3%)	0	100	100
1	B	394/471 (84%)	383 (97%)	11 (3%)	0	100	100
2	C	118/125 (94%)	114 (97%)	4 (3%)	0	100	100
2	D	115/125 (92%)	112 (97%)	3 (3%)	0	100	100
All	All	1012/1192 (85%)	981 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	280/407 (69%)	278 (99%)	2 (1%)	84	94
1	B	287/407 (70%)	283 (99%)	4 (1%)	67	86
2	C	82/99 (83%)	82 (100%)	0	100	100
2	D	79/99 (80%)	77 (98%)	2 (2%)	47	77
All	All	728/1012 (72%)	720 (99%)	8 (1%)	73	88

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

Mol	Chain	Res	Type
1	A	1189	THR
1	A	1312	ASN
1	B	1223	PHE
1	B	1312	ASN
1	B	1340	LEU
1	B	1342	LEU
2	D	32	ASN
2	D	44	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1142	GLN
1	A	1170	GLN
1	A	1178	HIS
1	A	1197	GLN
1	B	933	ASN
1	B	1179	GLN
1	B	1183	ASN
1	B	1197	GLN
1	B	1229	GLN
1	B	1296	HIS
1	B	1299	GLN

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Mol	Chain	Res	Type
2	D	3	GLN
2	D	13	GLN
2	C	32	ASN
2	C	114	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](#)

4 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	$\# Z > 2$
4	CLR	A	1402	-	31,31,31	1.90	6 (19%)	48,48,48	1.73	12 (25%)
4	CLR	B	1402	-	31,31,31	1.90	6 (19%)	48,48,48	1.72	12 (25%)
3	CAU	A	1401	-	22,24,24	2.05	5 (22%)	31,33,33	0.94	0
3	CAU	B	1401	-	22,24,24	2.05	5 (22%)	31,33,33	0.95	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
4	CLR	A	1402	-	-	8/10/68/68	0/4/4/4
4	CLR	B	1402	-	-	8/10/68/68	0/4/4/4
3	CAU	A	1401	-	-	0/10/10/10	0/3/3/3
3	CAU	B	1401	-	-	0/10/10/10	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1402	CLR	C10-C5	-5.87	1.41	1.52
4	B	1402	CLR	C10-C5	-5.86	1.41	1.52
4	B	1402	CLR	C4-C5	-5.08	1.40	1.51
4	A	1402	CLR	C4-C5	-5.05	1.40	1.51
3	B	1401	CAU	C10-C8	-4.77	1.33	1.41
4	B	1402	CLR	C7-C6	-4.77	1.39	1.50
3	A	1401	CAU	C10-C8	-4.76	1.33	1.41
4	A	1402	CLR	C7-C6	-4.75	1.40	1.50
3	B	1401	CAU	C2-C3	-4.72	1.33	1.41
3	A	1401	CAU	C2-C3	-4.68	1.33	1.41
3	B	1401	CAU	C13-C9	-3.64	1.34	1.41
3	A	1401	CAU	C13-C9	-3.64	1.34	1.41
3	A	1401	CAU	C5-C4	-3.47	1.34	1.41
3	B	1401	CAU	C5-C4	-3.47	1.34	1.41
4	A	1402	CLR	C6-C5	3.27	1.40	1.33
3	A	1401	CAU	C4-C3	-3.24	1.33	1.42
4	B	1402	CLR	C6-C5	3.24	1.40	1.33
3	B	1401	CAU	C4-C3	-3.22	1.34	1.42
4	B	1402	CLR	C10-C9	-2.33	1.52	1.56
4	A	1402	CLR	C13-C14	-2.31	1.50	1.55
4	A	1402	CLR	C10-C9	-2.26	1.52	1.56
4	B	1402	CLR	C13-C14	-2.26	1.50	1.55

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1402	CLR	C4-C5-C10	3.90	121.61	116.42
4	A	1402	CLR	C4-C5-C10	3.78	121.45	116.42
4	A	1402	CLR	C13-C17-C20	-3.76	113.60	119.49
4	B	1402	CLR	C15-C14-C8	-3.63	113.11	119.08
4	A	1402	CLR	C15-C14-C8	-3.55	113.24	119.08
4	A	1402	CLR	C16-C17-C13	-3.46	99.67	103.84
4	B	1402	CLR	C13-C17-C20	-3.45	114.09	119.49
4	A	1402	CLR	C1-C2-C3	-3.39	106.11	110.47
4	B	1402	CLR	C16-C17-C13	-3.38	99.77	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1402	CLR	C1-C2-C3	-3.33	106.20	110.47
4	A	1402	CLR	C11-C9-C10	-3.10	109.00	113.08
4	B	1402	CLR	C10-C9-C8	-3.06	108.14	112.73
4	B	1402	CLR	C11-C9-C10	-3.00	109.12	113.08
4	A	1402	CLR	C10-C9-C8	-2.92	108.36	112.73
4	B	1402	CLR	C17-C13-C14	-2.77	96.80	100.07
4	A	1402	CLR	C17-C13-C14	-2.64	96.95	100.07
4	B	1402	CLR	C4-C5-C6	-2.53	116.96	120.61
4	A	1402	CLR	C13-C14-C8	-2.51	110.66	114.38
4	A	1402	CLR	C11-C12-C13	-2.49	108.51	112.78
4	B	1402	CLR	C11-C12-C13	-2.46	108.56	112.78
4	A	1402	CLR	C4-C5-C6	-2.46	117.07	120.61
4	B	1402	CLR	C13-C14-C8	-2.44	110.77	114.38
4	B	1402	CLR	C19-C10-C9	-2.36	108.86	111.68
4	A	1402	CLR	C19-C10-C9	-2.36	108.87	111.68

There are no chirality outliers.

All (16) torsion outliers are listed below:

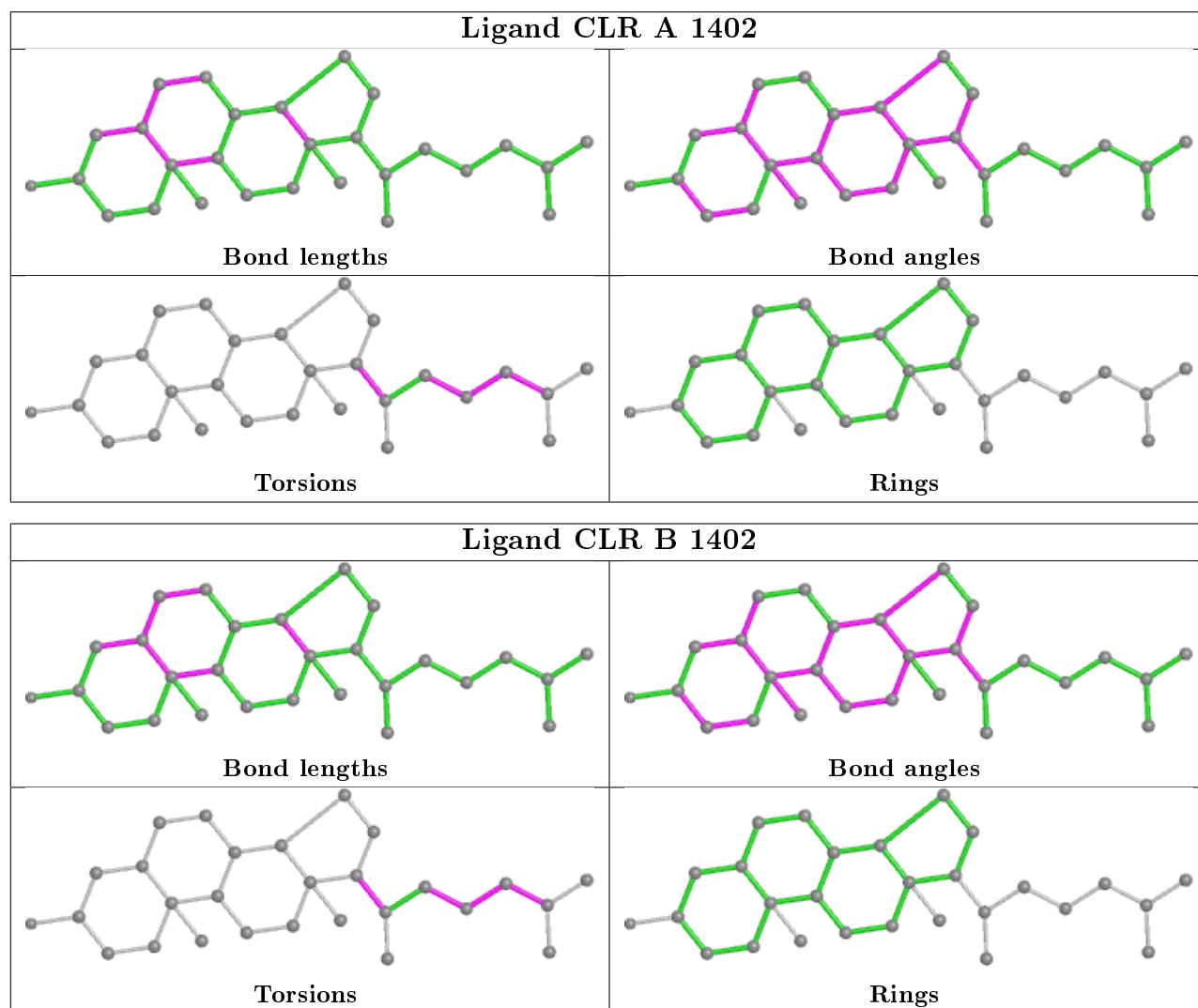
Mol	Chain	Res	Type	Atoms
4	A	1402	CLR	C13-C17-C20-C21
4	B	1402	CLR	C13-C17-C20-C21
4	A	1402	CLR	C13-C17-C20-C22
4	A	1402	CLR	C20-C22-C23-C24
4	B	1402	CLR	C20-C22-C23-C24
4	B	1402	CLR	C13-C17-C20-C22
4	B	1402	CLR	C23-C24-C25-C26
4	B	1402	CLR	C23-C24-C25-C27
4	A	1402	CLR	C23-C24-C25-C26
4	A	1402	CLR	C23-C24-C25-C27
4	A	1402	CLR	C16-C17-C20-C21
4	B	1402	CLR	C16-C17-C20-C21
4	A	1402	CLR	C16-C17-C20-C22
4	B	1402	CLR	C22-C23-C24-C25
4	B	1402	CLR	C16-C17-C20-C22
4	A	1402	CLR	C22-C23-C24-C25

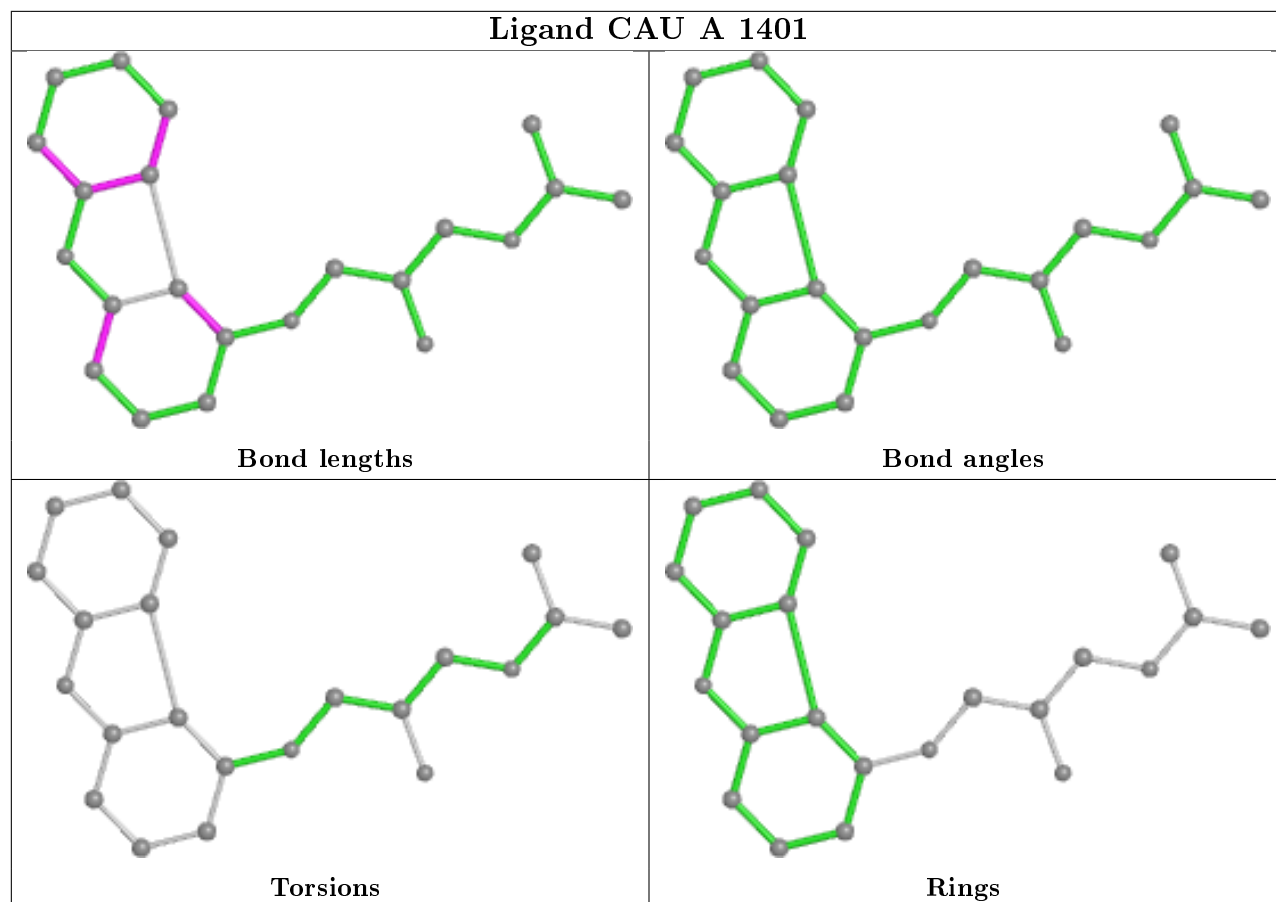
There are no ring outliers.

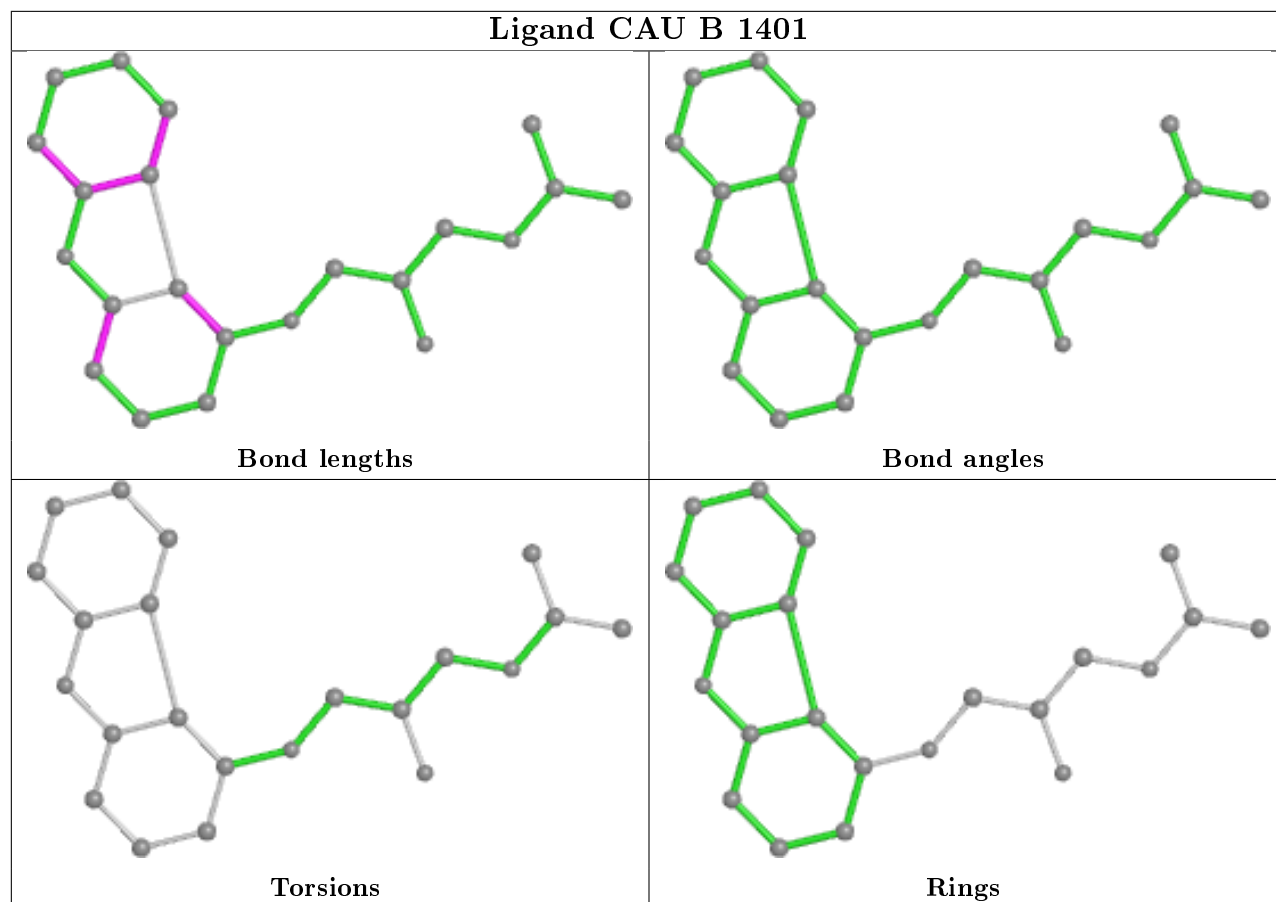
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1402	CLR	1	0
4	B	1402	CLR	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.







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	391/471 (83%)	0.03	6 (1%) 73 61	73, 125, 204, 255	0
1	B	402/471 (85%)	0.06	18 (4%) 33 21	84, 130, 206, 262	0
2	C	120/125 (96%)	-0.25	0 100 100	82, 113, 147, 188	0
2	D	117/125 (93%)	0.04	0 100 100	90, 120, 183, 198	0
All	All	1030/1192 (86%)	0.01	24 (2%) 60 47	73, 123, 201, 262	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	926	ASP	4.2
1	A	1003	TRP	3.8
1	B	968	VAL	3.7
1	B	1095	LEU	3.4
1	A	982	SER	3.4
1	A	998	LEU	3.3
1	A	1095	LEU	3.0
1	B	969	PHE	2.9
1	B	928	ALA	2.9
1	B	925	LYS	2.8
1	B	935	ASP	2.6
1	B	953	TYR	2.5
1	B	971	MET	2.5
1	B	924	THR	2.5
1	B	949	LEU	2.5
1	B	1006	GLN	2.3
1	B	966	ASN	2.3
1	B	964	LEU	2.2
1	B	923	ILE	2.2
1	B	965	ILE	2.2
1	B	1319	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	929	GLU	2.1
1	A	1298	ILE	2.1
1	A	983	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

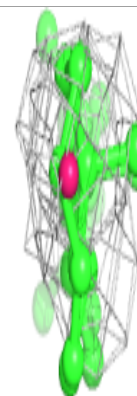
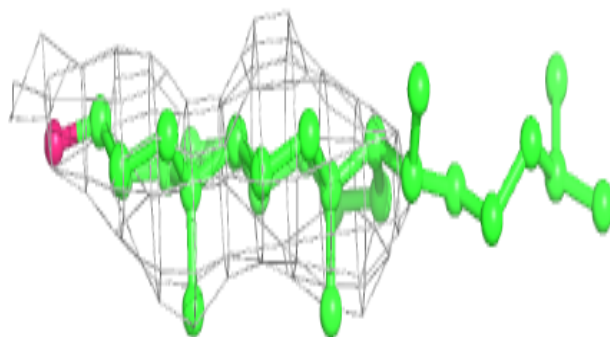
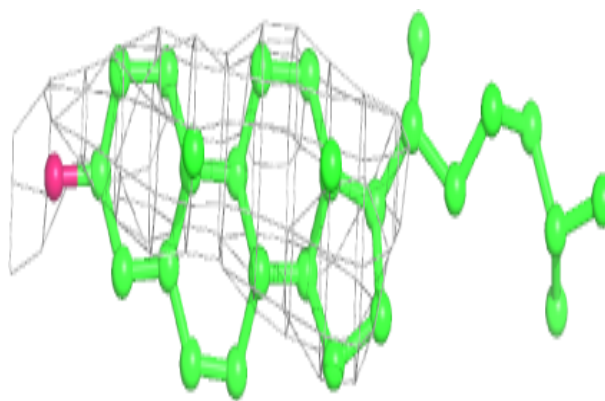
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CLR	A	1402	28/28	0.76	0.68	161,168,175,177	0
4	CLR	B	1402	28/28	0.83	0.75	142,159,166,168	0
3	CAU	B	1401	22/22	0.90	0.26	86,115,129,134	0
3	CAU	A	1401	22/22	0.94	0.27	97,123,139,142	0

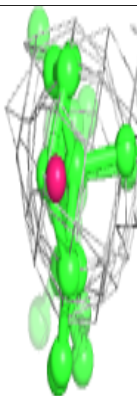
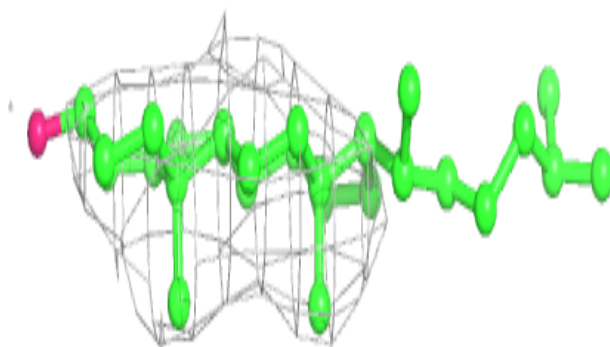
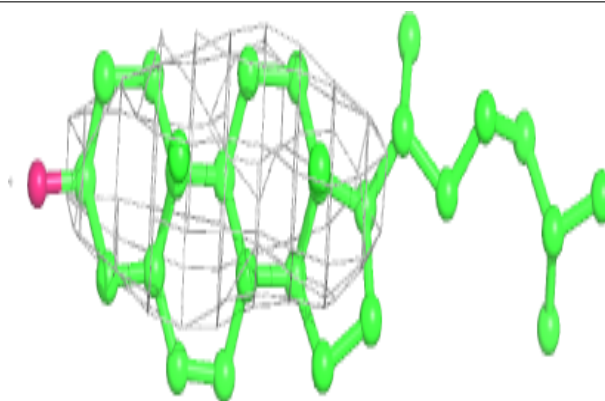
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLR A 1402:

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

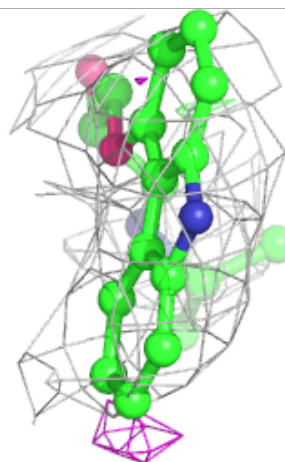
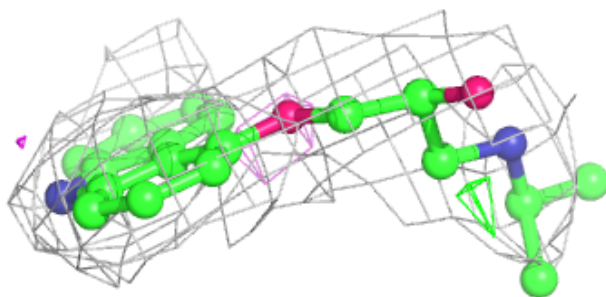
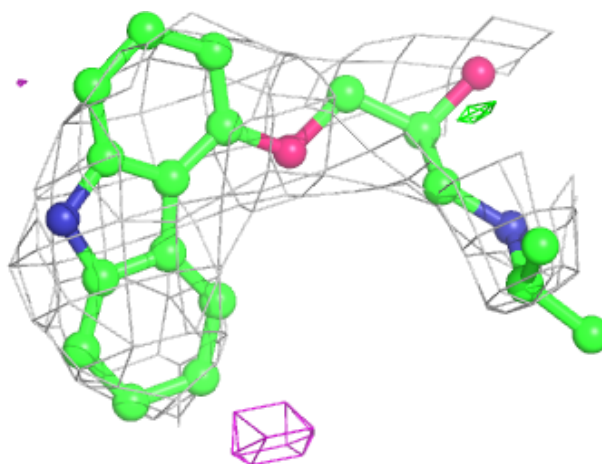
**Electron density around CLR B 1402:**

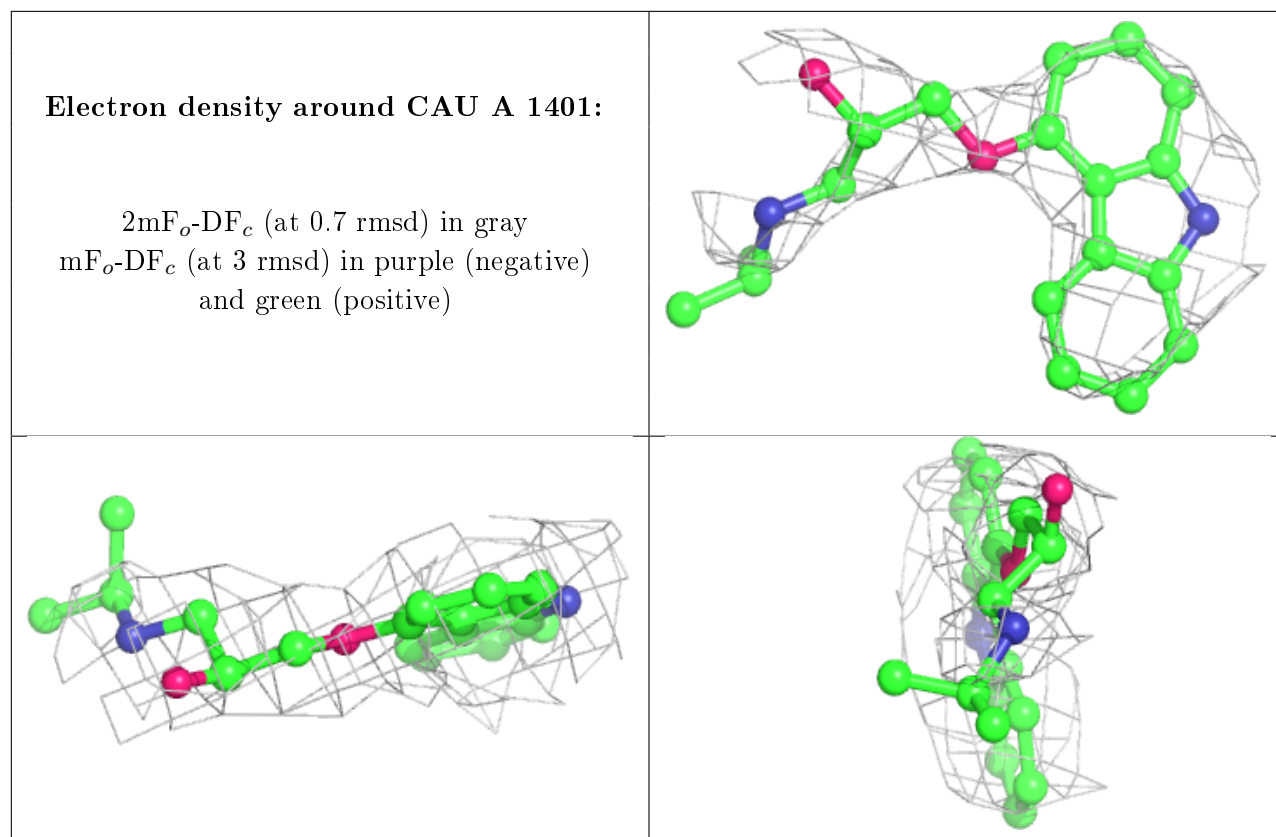
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CAU B 1401:

$2mF_o-DF_c$ (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.