Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 12:06 PM EDT

PDB ID	:	7S3P
Title	:	BD2 domain of human BRD3 bound to Physachenolide C
Authors	:	Horton, N.C.; Chapman, E.; Sivinski, J.; Zerio, C.; Ghadirian, N.
Deposited on	:	2021-09-07
Resolution	:	2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

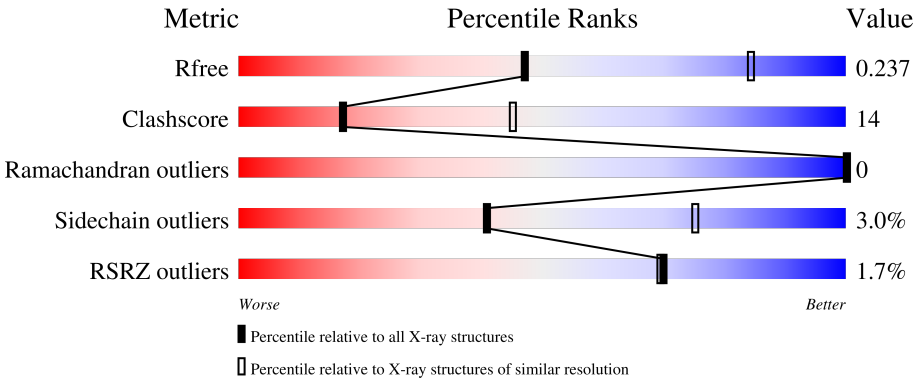
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	112	73% 22%
1	B	112	2% 79% 17%
1	C	112	4% 82% 13%
1	D	112	65% 31%
1	E	112	2% 77% 18%

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Mol	Chain	Length	Quality of chain
1	F	112	4% 74% 21%
1	G	112	79% 16%
1	H	112	2% 66% 29%
1	I	112	% 72% 23%
1	J	112	2% 71% 25%
1	K	112	3% 72% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	502	-	-	-	X
3	CL	C	502	-	-	-	X
3	CL	F	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9984 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 Bromodomain-containing protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	108	Total	C	N	O	S	0	0	0
			855	550	142	154	9			
1	A	108	Total	C	N	O	S	0	0	0
			873	559	151	154	9			
1	B	108	Total	C	N	O	S	0	0	0
			869	557	147	156	9			
1	C	108	Total	C	N	O	S	0	0	0
			857	549	143	156	9			
1	D	108	Total	C	N	O	S	0	0	0
			869	556	150	154	9			
1	E	109	Total	C	N	O	S	0	0	0
			881	565	152	155	9			
1	F	108	Total	C	N	O	S	0	0	0
			869	556	150	154	9			
1	G	108	Total	C	N	O	S	0	0	0
			850	546	143	152	9			
1	H	108	Total	C	N	O	S	0	0	0
			863	553	147	154	9			
1	I	108	Total	C	N	O	S	0	0	0
			841	541	137	154	9			
1	J	108	Total	C	N	O	S	0	0	0
			851	548	142	152	9			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	305	GLY	-	expression tag	UNP Q15059
A	305	GLY	-	expression tag	UNP Q15059
B	305	GLY	-	expression tag	UNP Q15059
C	305	GLY	-	expression tag	UNP Q15059
D	305	GLY	-	expression tag	UNP Q15059
E	305	GLY	-	expression tag	UNP Q15059
F	305	GLY	-	expression tag	UNP Q15059

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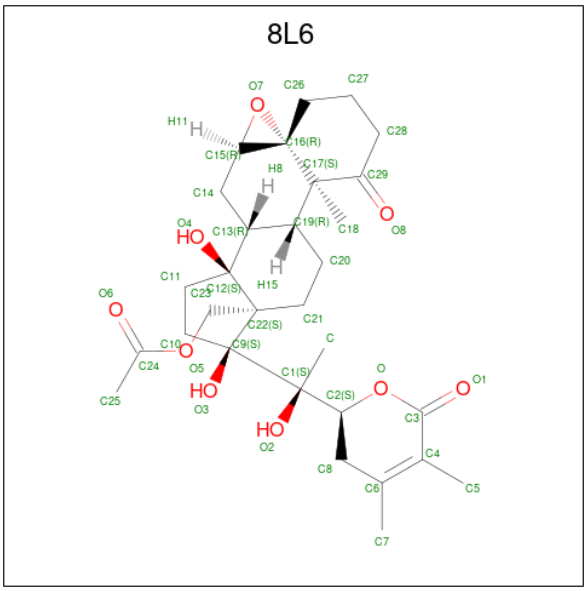
Chain	Residue	Modelled	Actual	Comment	Reference
G	305	GLY	-	expression tag	UNP Q15059
H	305	GLY	-	expression tag	UNP Q15059
I	305	GLY	-	expression tag	UNP Q15059
J	305	GLY	-	expression tag	UNP Q15059

- Molecule 2 is Physachenolide C (three-letter code: 8L6) (formula: $C_{30}H_{42}O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total C O 39 30 9	0	0
2	A	1	Total C O 39 30 9	0	0
2	B	1	Total C O 39 30 9	0	0
2	C	1	Total C O 39 30 9	0	0
2	D	1	Total C O 39 30 9	0	0
2	E	1	Total C O 39 30 9	0	0
2	F	1	Total C O 39 30 9	0	0
2	G	1	Total C O 39 30 9	0	0
2	H	1	Total C O 39 30 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total C O 39 30 9	0	0
2	J	1	Total C O 39 30 9	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	6	Total O 6 6	0	0
4	A	9	Total O 9 9	0	0
4	B	4	Total O 4 4	0	0
4	C	5	Total O 5 5	0	0
4	D	8	Total O 8 8	0	0
4	E	8	Total O 8 8	0	0
4	F	6	Total O 6 6	0	0
4	G	7	Total O 7 7	0	0
4	H	9	Total O 9 9	0	0

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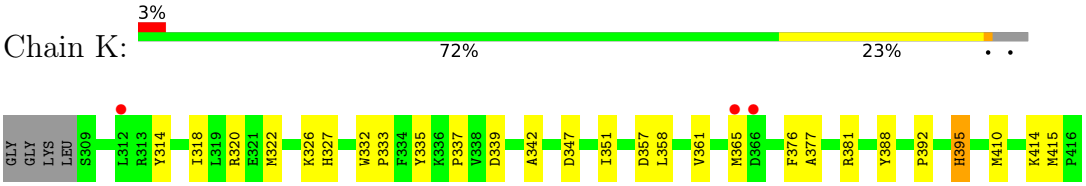
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	6	Total O 6 6	0	0
4	J	3	Total O 3 3	0	0

3 Residue-property plots

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.

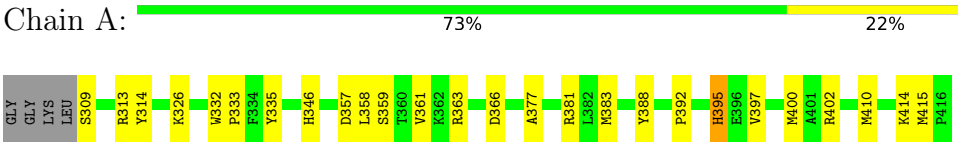
• Molecule 1: Bromodomain-containing protein 3

Chain K:



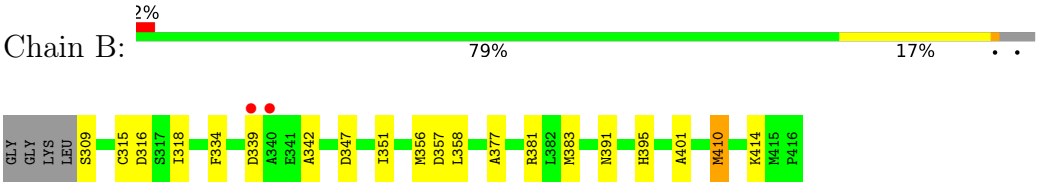
• Molecule 1: Bromodomain-containing protein 3

Chain A:



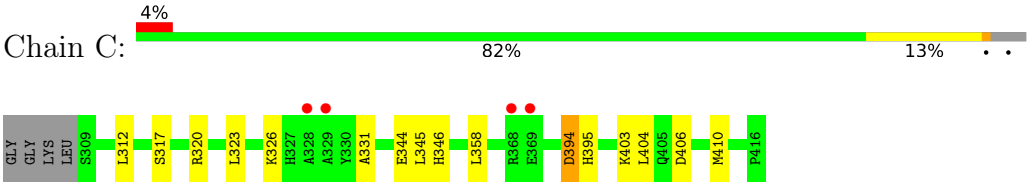
• Molecule 1: Bromodomain-containing protein 3

Chain B:



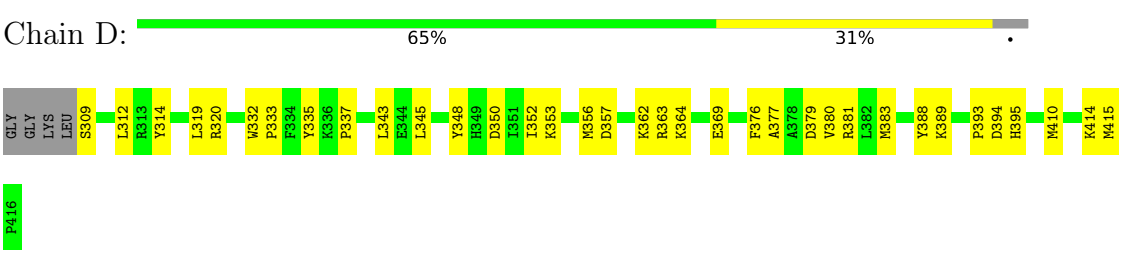
• Molecule 1: Bromodomain-containing protein 3

Chain C:



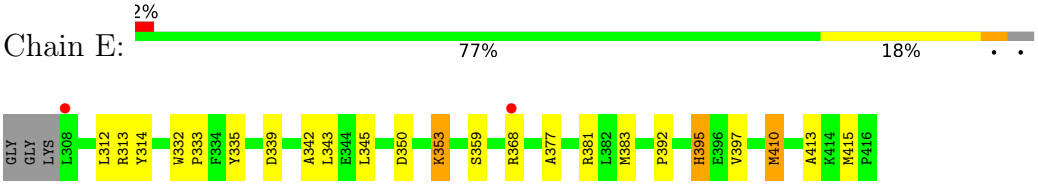
• Molecule 1: Bromodomain-containing protein 3

Chain D:



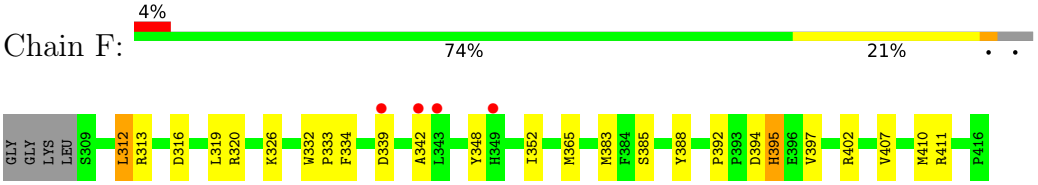
• Molecule 1: Bromodomain-containing protein 3

Chain E:



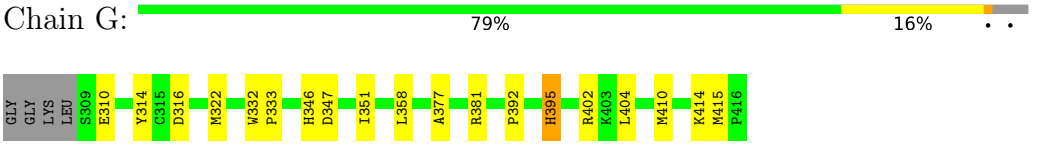
• Molecule 1: Bromodomain-containing protein 3

Chain F:



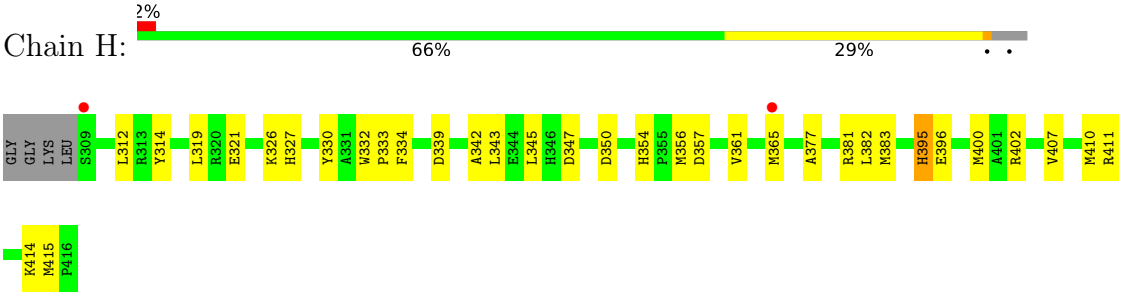
• Molecule 1: Bromodomain-containing protein 3

Chain G:



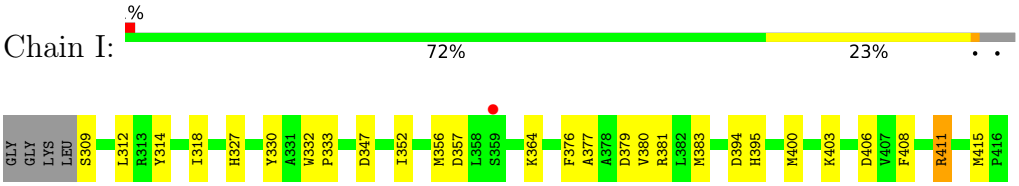
• Molecule 1: Bromodomain-containing protein 3

Chain H:



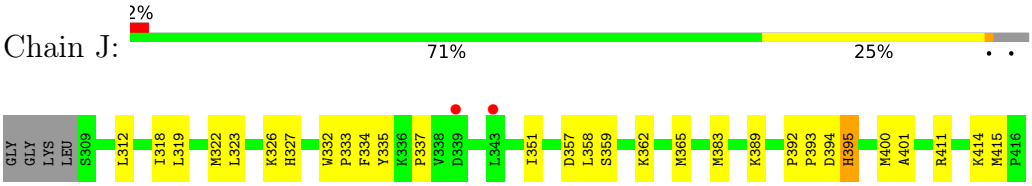
• Molecule 1: Bromodomain-containing protein 3

Chain I:



• Molecule 1: Bromodomain-containing protein 3

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.45Å 158.53Å 293.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.49 – 2.89 39.49 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.49-2.89) 99.9 (39.49-2.89)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19_4158	Depositor
R, R_{free}	0.207 , 0.240 0.203 , 0.237	Depositor DCC
R_{free} test set	1996 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9984	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8L6, CL

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	0.46	0/899	0.60	0/1215
1	B	0.53	0/895	0.64	0/1211
1	C	0.51	0/883	0.66	0/1198
1	D	0.46	0/895	0.66	0/1211
1	E	0.45	0/907	0.63	0/1226
1	F	0.50	0/895	0.65	0/1211
1	G	0.46	0/876	0.64	0/1189
1	H	0.42	0/889	0.59	0/1204
1	I	0.54	0/867	0.63	0/1179
1	J	0.49	0/877	0.63	0/1189
1	K	0.44	0/881	0.64	0/1194
All	All	0.48	0/9764	0.63	0/13227

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

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	873	0	821	26	0
1	B	869	0	807	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	857	0	781	13	0
1	D	869	0	810	27	0
1	E	881	0	832	20	0
1	F	869	0	810	25	0
1	G	850	0	775	19	0
1	H	863	0	799	38	0
1	I	841	0	755	17	0
1	J	851	0	784	37	0
1	K	855	0	788	39	0
2	A	39	0	0	2	0
2	B	39	0	0	1	0
2	C	39	0	0	1	0
2	D	39	0	0	1	0
2	E	39	0	0	1	0
2	F	39	0	0	1	0
2	G	39	0	0	1	0
2	H	39	0	0	1	0
2	I	39	0	0	4	0
2	J	39	0	0	5	0
2	K	39	0	0	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	2	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	A	9	0	0	0	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	8	0	0	1	0
4	E	8	0	0	0	0
4	F	6	0	0	1	0
4	G	7	0	0	0	0
4	H	9	0	0	0	0
4	I	6	0	0	0	0
4	J	3	0	0	0	0
4	K	6	0	0	1	0
All	All	9984	0	8762	259	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 14.

All (259) 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:I:364:LYS:HE3	1:I:379:ASP:OD2	1.67	0.94
1:A:402:ARG:HH21	1:H:410:MET:HE3	1.38	0.89
1:H:330:TYR:HA	1:H:400:MET:HE3	1.55	0.88
1:K:410:MET:HE2	1:J:393:PRO:HB3	1.59	0.85
1:H:314:TYR:HD2	1:H:415:MET:HE2	1.42	0.82
1:B:410:MET:HE1	1:B:414:LYS:HE2	1.63	0.80
1:K:410:MET:HE3	1:K:414:LYS:HE3	1.64	0.79
1:A:397:VAL:HA	1:A:400:MET:HE3	1.66	0.77
1:K:318:ILE:HG22	1:K:322:MET:CE	2.14	0.77
1:A:397:VAL:HA	1:A:400:MET:CE	2.15	0.76
1:D:350:ASP:O	1:D:353:LYS:HE2	1.85	0.76
1:G:314:TYR:HD2	1:G:415:MET:CE	2.01	0.74
1:G:410:MET:HE1	1:G:414:LYS:HE2	1.70	0.73
1:K:410:MET:HE3	1:K:414:LYS:CE	2.19	0.72
1:J:392:PRO:HG2	1:J:395:HIS:CE1	2.25	0.72
1:K:388:TYR:O	1:J:414:LYS:HE2	1.91	0.71
1:K:410:MET:CE	1:K:414:LYS:HE3	2.21	0.70
1:D:389:LYS:HG3	1:E:413:ALA:O	1.90	0.70
1:H:343:LEU:O	1:H:345:LEU:CD1	2.40	0.69
1:H:356:MET:HB2	1:H:382:LEU:HD23	1.73	0.69
1:K:318:ILE:HG22	1:K:322:MET:HE2	1.74	0.69
1:J:312:LEU:HD22	1:J:365:MET:HE3	1.75	0.69
1:H:314:TYR:CE2	1:H:415:MET:HA	2.29	0.68
1:K:365:MET:HE1	1:K:376:PHE:CD1	2.30	0.67
1:G:314:TYR:HD2	1:G:415:MET:HE2	1.60	0.66
1:E:350:ASP:O	1:E:353:LYS:HE2	1.96	0.66
1:J:392:PRO:HG2	1:J:395:HIS:ND1	2.10	0.66
1:F:395:HIS:HB3	1:F:397:VAL:HG12	1.78	0.66
1:A:402:ARG:NH2	1:H:410:MET:HE3	2.11	0.66
1:C:346:HIS:CD2	1:F:316:ASP:OD2	2.49	0.66
1:K:318:ILE:CG2	1:K:322:MET:HE2	2.26	0.65
1:K:410:MET:CE	1:K:414:LYS:CE	2.73	0.65
1:C:317:SER:OG	1:C:320:ARG:NH2	2.30	0.65
1:J:400:MET:CE	2:J:501:8L6:C28	2.75	0.64
1:G:402:ARG:HG3	1:G:402:ARG:HH11	1.62	0.64
1:H:332:TRP:CG	1:H:333:PRO:HD3	2.33	0.64
1:K:365:MET:CE	1:K:376:PHE:CD1	2.81	0.63
1:H:314:TYR:CD2	1:H:415:MET:HE2	2.29	0.63
1:I:400:MET:CE	2:I:501:8L6:O8	2.46	0.63
1:C:394:ASP:OD1	1:F:326:LYS:NZ	2.32	0.63
1:G:322:MET:HG2	1:G:404:LEU:HD11	1.79	0.63
2:K:501:8L6:O4	2:K:501:8L6:O2	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:400:MET:HE1	2:I:501:8L6:O8	1.98	0.63
2:J:501:8L6:O2	2:J:501:8L6:O4	2.16	0.63
1:E:339:ASP:OD2	1:E:342:ALA:HB2	1.99	0.62
1:D:364:LYS:HG2	1:D:369:GLU:OE1	1.98	0.62
1:J:337:PRO:HG3	1:J:357:ASP:OD2	1.99	0.62
1:E:339:ASP:OD2	1:E:342:ALA:CB	2.48	0.62
1:C:326:LYS:HD2	1:C:326:LYS:O	2.00	0.61
1:A:388:TYR:O	1:H:414:LYS:NZ	2.25	0.61
1:I:403:LYS:O	1:I:406:ASP:HB2	2.00	0.61
1:C:346:HIS:HD2	1:F:316:ASP:OD2	1.83	0.60
1:J:312:LEU:HD22	1:J:365:MET:CE	2.30	0.60
1:K:365:MET:CE	1:K:376:PHE:CE1	2.84	0.60
2:F:502:8L6:O2	2:F:502:8L6:O4	2.19	0.60
1:H:377:ALA:O	1:H:381:ARG:HG3	2.01	0.60
1:F:319:LEU:O	1:F:319:LEU:HD12	2.00	0.60
1:H:343:LEU:O	1:H:345:LEU:HD13	2.00	0.60
1:B:347:ASP:O	1:B:351:ILE:HD12	2.02	0.59
1:G:402:ARG:HG3	1:G:402:ARG:NH1	2.18	0.59
1:K:318:ILE:HG22	1:K:322:MET:HE3	1.82	0.59
1:J:319:LEU:HD21	1:J:362:LYS:HA	1.84	0.59
1:H:339:ASP:O	1:H:343:LEU:HD23	2.03	0.59
1:K:410:MET:CE	1:J:393:PRO:HB3	2.30	0.59
1:F:394:ASP:OD1	1:F:394:ASP:N	2.34	0.58
1:F:407:VAL:O	1:F:411:ARG:HG2	2.03	0.58
1:K:339:ASP:OD2	1:K:342:ALA:CB	2.52	0.58
1:F:339:ASP:OD2	1:F:342:ALA:HB2	2.02	0.58
1:H:357:ASP:HA	1:H:383:MET:HG3	1.84	0.58
1:A:314:TYR:CE2	1:A:415:MET:HA	2.39	0.58
1:G:377:ALA:O	1:G:381:ARG:HG3	2.03	0.58
1:B:347:ASP:OD1	1:B:347:ASP:N	2.33	0.57
1:K:410:MET:HE2	1:J:393:PRO:CB	2.33	0.57
1:D:343:LEU:HB2	1:D:345:LEU:HG	1.86	0.57
1:F:365:MET:HE3	3:F:501:CL:CL	2.41	0.57
1:D:376:PHE:O	1:D:380:VAL:HG23	2.05	0.57
1:D:337:PRO:HG3	1:D:357:ASP:OD2	2.05	0.57
1:D:364:LYS:HA	1:D:369:GLU:OE1	2.04	0.57
1:A:377:ALA:O	1:A:381:ARG:HG3	2.05	0.57
1:F:334:PHE:HB3	1:F:383:MET:CE	2.35	0.57
1:H:343:LEU:C	1:H:345:LEU:HD13	2.24	0.57
1:J:337:PRO:N	1:J:357:ASP:OD2	2.38	0.57
1:H:319:LEU:HD22	1:H:361:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:318:ILE:O	1:J:322:MET:HG3	2.06	0.56
1:J:319:LEU:CD2	1:J:362:LYS:HA	2.36	0.56
1:J:326:LYS:HD3	1:J:327:HIS:CE1	2.41	0.56
1:J:337:PRO:CG	1:J:357:ASP:OD2	2.53	0.56
1:K:332:TRP:CG	1:K:333:PRO:HD3	2.41	0.55
2:E:501:8L6:O2	2:E:501:8L6:O4	2.24	0.55
1:K:332:TRP:HA	1:K:335:TYR:CD2	2.42	0.55
1:E:335:TYR:O	1:E:359:SER:OG	2.21	0.55
1:I:314:TYR:CD2	1:I:415:MET:HG3	2.42	0.55
1:C:403:LYS:O	1:C:406:ASP:HB2	2.07	0.55
1:K:337:PRO:CD	1:K:357:ASP:OD2	2.55	0.54
1:G:314:TYR:CE2	1:G:415:MET:HA	2.42	0.54
1:I:376:PHE:O	1:I:380:VAL:HG23	2.06	0.54
1:I:377:ALA:O	1:I:381:ARG:HG3	2.07	0.54
1:H:343:LEU:CB	1:H:345:LEU:HD13	2.37	0.54
1:K:410:MET:CE	1:K:414:LYS:HE2	2.37	0.54
1:A:309:SER:O	1:A:313:ARG:HG3	2.07	0.54
2:D:501:8L6:O4	2:D:501:8L6:O2	2.25	0.54
1:G:314:TYR:HD2	1:G:415:MET:HE3	1.73	0.54
1:J:335:TYR:O	1:J:359:SER:OG	2.23	0.54
1:H:347:ASP:O	1:H:350:ASP:HB2	2.09	0.53
1:K:337:PRO:N	1:K:357:ASP:OD2	2.41	0.53
1:H:339:ASP:O	1:H:343:LEU:CD2	2.56	0.53
1:A:326:LYS:NZ	1:J:394:ASP:OD2	2.36	0.53
1:A:410:MET:HG3	1:H:402:ARG:NH2	2.23	0.53
1:A:400:MET:HE1	2:A:501:8L6:O8	2.09	0.53
1:F:334:PHE:HB3	1:F:383:MET:HE3	1.90	0.53
1:A:397:VAL:HA	1:A:400:MET:HE2	1.91	0.52
1:I:347:ASP:OD1	1:I:347:ASP:N	2.41	0.52
1:J:358:LEU:HD21	1:J:383:MET:HE1	1.92	0.51
1:D:393:PRO:HA	1:E:410:MET:CE	2.40	0.51
1:K:339:ASP:OD2	1:K:342:ALA:N	2.37	0.51
1:B:334:PHE:CZ	1:B:401:ALA:HB2	2.46	0.51
1:C:345:LEU:HA	1:F:320:ARG:HH12	1.76	0.51
1:A:400:MET:CE	2:A:501:8L6:O8	2.58	0.51
1:H:339:ASP:OD2	1:H:342:ALA:CB	2.59	0.51
1:J:337:PRO:CD	1:J:357:ASP:OD2	2.58	0.51
1:K:347:ASP:O	1:K:351:ILE:HG13	2.10	0.51
1:H:339:ASP:OD2	1:H:342:ALA:HB2	2.11	0.51
1:K:326:LYS:HZ2	1:H:395:HIS:CE1	2.27	0.50
1:D:410:MET:HE3	1:D:414:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:332:TRP:CG	1:J:333:PRO:HD3	2.46	0.50
1:I:327:HIS:HD1	1:I:330:TYR:HH	1.59	0.50
1:A:332:TRP:CG	1:A:333:PRO:HD3	2.46	0.50
1:K:326:LYS:HD3	1:K:327:HIS:NE2	2.27	0.50
1:K:357:ASP:OD1	1:K:357:ASP:C	2.50	0.50
1:E:332:TRP:CG	1:E:333:PRO:HD3	2.47	0.50
1:J:351:ILE:HG22	1:J:389:LYS:HD3	1.93	0.50
1:B:391:ASN:OD1	2:B:501:8L6:C	2.60	0.49
1:D:319:LEU:HD21	1:D:362:LYS:HA	1.94	0.49
1:F:339:ASP:OD2	1:F:342:ALA:CB	2.61	0.49
1:B:316:ASP:OD2	1:D:363:ARG:HD3	2.13	0.49
1:E:377:ALA:O	1:E:381:ARG:HG3	2.12	0.49
1:F:392:PRO:HG2	1:F:395:HIS:CE1	2.48	0.49
1:B:377:ALA:O	1:B:381:ARG:HG3	2.13	0.49
1:K:326:LYS:HD3	1:K:327:HIS:CE1	2.47	0.48
1:H:321:GLU:OE2	1:H:411:ARG:NH1	2.46	0.48
1:J:400:MET:HE3	2:J:501:8L6:C28	2.43	0.48
1:A:346:HIS:O	1:E:313:ARG:HD2	2.14	0.48
1:H:334:PHE:HB3	1:H:383:MET:SD	2.53	0.48
1:J:319:LEU:HD21	1:J:362:LYS:CA	2.43	0.48
1:K:314:TYR:CD2	1:K:415:MET:HG3	2.49	0.48
1:K:332:TRP:HA	1:K:335:TYR:CE2	2.49	0.48
1:A:392:PRO:HG2	1:A:395:HIS:ND1	2.29	0.48
1:F:334:PHE:CB	1:F:383:MET:HE3	2.44	0.48
1:H:354:HIS:O	1:H:382:LEU:HD21	2.13	0.48
1:I:332:TRP:CG	1:I:333:PRO:HD3	2.49	0.48
1:B:357:ASP:N	1:B:357:ASP:OD1	2.47	0.47
1:K:392:PRO:HG2	1:K:395:HIS:CE1	2.49	0.47
1:B:334:PHE:HZ	1:B:401:ALA:HB2	1.78	0.47
1:D:332:TRP:HA	1:D:335:TYR:CD2	2.49	0.47
1:F:410:MET:HE3	1:F:410:MET:O	2.14	0.47
1:G:347:ASP:O	1:G:351:ILE:HG13	2.15	0.47
1:D:388:TYR:HB3	1:E:410:MET:SD	2.55	0.47
1:D:356:MET:HE3	1:D:379:ASP:OD1	2.15	0.47
1:E:314:TYR:CE2	1:E:415:MET:HA	2.50	0.47
1:H:326:LYS:HD3	1:H:327:HIS:CE1	2.50	0.47
1:G:332:TRP:CG	1:G:333:PRO:HD3	2.50	0.46
1:I:400:MET:HE2	2:I:501:8L6:O8	2.14	0.46
1:A:363:ARG:NH1	3:F:501:CL:CL	2.86	0.46
1:D:314:TYR:CD2	1:D:415:MET:HG3	2.51	0.46
1:K:365:MET:HE2	1:K:376:PHE:CD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:PRO:HB3	1:E:410:MET:CE	2.46	0.46
1:K:377:ALA:O	1:K:381:ARG:HG3	2.16	0.46
1:B:315:CYS:HA	1:B:318:ILE:HD12	1.98	0.46
1:H:314:TYR:CE2	1:H:415:MET:CA	2.98	0.46
1:C:331:ALA:HB2	1:C:404:LEU:HD13	1.98	0.46
1:F:388:TYR:OH	1:F:402:ARG:HD2	2.15	0.46
1:I:356:MET:O	1:I:383:MET:HG3	2.16	0.46
1:H:327:HIS:CE1	1:H:407:VAL:HG21	2.51	0.46
1:K:357:ASP:O	1:K:361:VAL:HG23	2.16	0.46
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.67	0.45
2:G:501:8L6:O4	2:G:501:8L6:O2	2.34	0.45
1:H:314:TYR:HD2	1:H:415:MET:CE	2.22	0.45
1:G:415:MET:HE3	1:G:415:MET:HB2	1.47	0.45
1:H:415:MET:HE3	1:H:415:MET:HB2	1.73	0.45
1:G:392:PRO:HG2	1:G:395:HIS:ND1	2.31	0.45
1:J:400:MET:HE1	2:J:501:8L6:C28	2.47	0.45
1:A:358:LEU:HD23	1:A:383:MET:CE	2.46	0.45
1:E:395:HIS:HB3	1:E:397:VAL:HG12	1.99	0.45
1:J:392:PRO:CG	1:J:395:HIS:CE1	2.97	0.45
1:D:364:LYS:HA	1:D:369:GLU:CD	2.37	0.45
1:H:396:GLU:O	1:H:400:MET:HG3	2.17	0.45
2:H:501:8L6:O5	2:H:501:8L6:O3	2.34	0.45
1:E:343:LEU:HB2	1:E:345:LEU:HG	1.99	0.45
1:I:318:ILE:HG12	1:I:411:ARG:HB3	1.98	0.45
2:C:501:8L6:O2	2:C:501:8L6:O4	2.35	0.44
1:C:410:MET:HE2	1:C:410:MET:HB3	1.83	0.44
1:B:339:ASP:OD2	1:B:342:ALA:HB2	2.17	0.44
1:F:312:LEU:HD12	1:F:312:LEU:HA	1.88	0.44
1:A:410:MET:HG3	1:H:402:ARG:HH21	1.81	0.44
1:D:377:ALA:O	1:D:381:ARG:HG3	2.18	0.44
1:J:400:MET:CE	2:J:501:8L6:O8	2.66	0.44
1:J:337:PRO:CA	1:J:357:ASP:OD2	2.66	0.44
1:A:357:ASP:O	1:A:361:VAL:HG23	2.18	0.43
1:F:348:TYR:CZ	1:F:352:ILE:HG13	2.53	0.43
1:C:344:GLU:O	1:F:320:ARG:NH1	2.52	0.43
1:H:343:LEU:HB2	1:H:345:LEU:HD13	1.99	0.43
1:A:332:TRP:HA	1:A:335:TYR:CD2	2.53	0.43
1:K:410:MET:HE1	1:K:414:LYS:CE	2.48	0.43
1:D:314:TYR:CE2	1:D:415:MET:HA	2.54	0.43
1:F:402:ARG:NH2	4:F:601:HOH:O	2.51	0.43
1:J:358:LEU:HD23	1:J:358:LEU:HA	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:ASP:OD1	1:D:394:ASP:N	2.52	0.43
1:E:339:ASP:OD2	1:E:342:ALA:HB3	2.17	0.43
1:G:402:ARG:HH11	1:G:402:ARG:CG	2.31	0.43
1:K:339:ASP:OD2	1:K:342:ALA:HB2	2.19	0.43
1:D:320:ARG:NH1	4:D:602:HOH:O	2.41	0.43
1:D:348:TYR:CE1	1:D:352:ILE:HG13	2.53	0.43
1:H:332:TRP:CD1	1:H:333:PRO:HD3	2.54	0.43
1:I:380:VAL:HG11	1:I:408:PHE:CD1	2.54	0.43
2:I:501:8L6:O4	2:I:501:8L6:O2	2.36	0.43
1:J:334:PHE:HZ	1:J:401:ALA:HB2	1.84	0.42
1:G:314:TYR:CD2	1:G:415:MET:HB2	2.54	0.42
1:F:402:ARG:HD2	1:F:402:ARG:HA	1.81	0.42
1:G:358:LEU:HD23	1:G:358:LEU:HA	1.88	0.42
1:K:365:MET:HE2	1:K:376:PHE:CE1	2.55	0.42
1:A:410:MET:HE1	1:A:414:LYS:HE2	2.02	0.42
1:H:319:LEU:CD2	1:H:361:VAL:HG12	2.50	0.42
1:K:337:PRO:HG3	1:K:357:ASP:OD2	2.20	0.42
1:A:410:MET:CE	1:A:414:LYS:HE2	2.50	0.42
1:B:356:MET:HE3	1:B:356:MET:HB2	1.93	0.41
1:D:312:LEU:HA	1:D:312:LEU:HD23	1.64	0.41
1:D:363:ARG:HD2	1:G:346:HIS:CD2	2.55	0.41
1:H:332:TRP:CD2	1:H:333:PRO:HD3	2.55	0.41
1:J:312:LEU:CD2	1:J:365:MET:CE	2.97	0.41
1:A:314:TYR:CD2	1:A:415:MET:HA	2.55	0.41
1:E:332:TRP:N	1:E:333:PRO:CD	2.84	0.41
1:K:320:ARG:NH1	4:K:601:HOH:O	2.49	0.41
1:C:323:LEU:HD23	1:C:323:LEU:HA	1.91	0.41
1:J:312:LEU:CD2	1:J:365:MET:HE1	2.51	0.41
1:F:332:TRP:N	1:F:333:PRO:CD	2.84	0.41
1:J:319:LEU:HD12	1:J:319:LEU:HA	1.87	0.41
1:H:312:LEU:O	1:H:365:MET:HE1	2.21	0.41
1:A:332:TRP:HA	1:A:335:TYR:CE2	2.56	0.41
1:B:358:LEU:HD23	1:B:358:LEU:HA	1.83	0.41
1:C:312:LEU:HA	1:C:312:LEU:HD23	1.81	0.41
1:D:332:TRP:N	1:D:333:PRO:CD	2.83	0.41
1:D:356:MET:O	1:D:383:MET:HG3	2.21	0.41
1:D:393:PRO:HA	1:E:410:MET:HE2	2.03	0.41
1:E:392:PRO:HG2	1:E:395:HIS:CE1	2.56	0.41
1:G:410:MET:HE2	1:G:410:MET:HB3	1.76	0.41
1:I:312:LEU:HD23	1:I:312:LEU:HA	1.91	0.41
1:K:358:LEU:HD23	1:K:358:LEU:HA	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:TRP:N	1:G:333:PRO:CD	2.84	0.40
1:I:332:TRP:N	1:I:333:PRO:CD	2.84	0.40
1:E:312:LEU:HD23	1:E:312:LEU:HA	1.94	0.40
1:J:318:ILE:HG12	1:J:411:ARG:HB3	2.03	0.40
1:J:334:PHE:HB3	1:J:383:MET:SD	2.61	0.40
1:J:415:MET:HE2	1:J:415:MET:HB2	1.91	0.40
1:A:366:ASP:HB3	1:F:313:ARG:NH1	2.36	0.40
1:F:319:LEU:HD12	1:F:319:LEU:C	2.40	0.40
1:B:334:PHE:HB3	1:B:383:MET:SD	2.61	0.40
1:I:352:ILE:HD13	1:I:352:ILE:N	2.35	0.40
1:J:323:LEU:HD23	1:J:323:LEU:HA	1.77	0.40
1:E:392:PRO:HG2	1:E:395:HIS:ND1	2.36	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	106/112 (95%)	106 (100%)	0	0	100	100
1	B	106/112 (95%)	105 (99%)	1 (1%)	0	100	100
1	C	106/112 (95%)	106 (100%)	0	0	100	100
1	D	106/112 (95%)	105 (99%)	1 (1%)	0	100	100
1	E	107/112 (96%)	106 (99%)	1 (1%)	0	100	100
1	F	106/112 (95%)	105 (99%)	1 (1%)	0	100	100
1	G	106/112 (95%)	106 (100%)	0	0	100	100
1	H	106/112 (95%)	106 (100%)	0	0	100	100
1	I	106/112 (95%)	106 (100%)	0	0	100	100
1	J	106/112 (95%)	105 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	106/112 (95%)	105 (99%)	1 (1%)	0	100	100
All	All	1167/1232 (95%)	1161 (100%)	6 (0%)	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	88/97 (91%)	86 (98%)	2 (2%)	50	80
1	B	87/97 (90%)	84 (97%)	3 (3%)	37	71
1	C	85/97 (88%)	83 (98%)	2 (2%)	49	79
1	D	87/97 (90%)	85 (98%)	2 (2%)	50	80
1	E	89/97 (92%)	84 (94%)	5 (6%)	21	52
1	F	87/97 (90%)	84 (97%)	3 (3%)	37	71
1	G	83/97 (86%)	80 (96%)	3 (4%)	35	69
1	H	86/97 (89%)	85 (99%)	1 (1%)	71	91
1	I	82/97 (84%)	77 (94%)	5 (6%)	18	48
1	J	84/97 (87%)	83 (99%)	1 (1%)	71	91
1	K	85/97 (88%)	84 (99%)	1 (1%)	71	91
All	All	943/1067 (88%)	915 (97%)	28 (3%)	41	75

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	395	HIS
1	A	359	SER
1	A	395	HIS
1	B	309	SER
1	B	395	HIS
1	B	410	MET

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Mol	Chain	Res	Type
1	C	394	ASP
1	C	395	HIS
1	D	309	SER
1	D	395	HIS
1	E	353	LYS
1	E	368	ARG
1	E	383	MET
1	E	395	HIS
1	E	410	MET
1	F	312	LEU
1	F	385	SER
1	F	395	HIS
1	G	310	GLU
1	G	316	ASP
1	G	395	HIS
1	H	395	HIS
1	I	309	SER
1	I	357	ASP
1	I	394	ASP
1	I	395	HIS
1	I	411	ARG
1	J	395	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
2	8L6	A	501	-	40,44,44	2.12	10 (25%)	53,76,76	2.47	19 (35%)
2	8L6	F	502	-	40,44,44	2.08	11 (27%)	53,76,76	2.33	18 (33%)
2	8L6	B	501	-	40,44,44	2.08	10 (25%)	53,76,76	2.35	18 (33%)
2	8L6	H	501	-	40,44,44	2.12	11 (27%)	53,76,76	2.46	18 (33%)
2	8L6	K	501	-	40,44,44	2.06	9 (22%)	53,76,76	2.35	19 (35%)
2	8L6	J	501	-	40,44,44	2.06	9 (22%)	53,76,76	2.38	20 (37%)
2	8L6	D	501	-	40,44,44	2.10	10 (25%)	53,76,76	2.44	18 (33%)
2	8L6	C	501	-	40,44,44	2.13	11 (27%)	53,76,76	2.37	18 (33%)
2	8L6	G	501	-	40,44,44	2.11	10 (25%)	53,76,76	2.48	19 (35%)
2	8L6	I	501	-	40,44,44	2.11	11 (27%)	53,76,76	2.40	19 (35%)
2	8L6	E	501	-	40,44,44	2.08	10 (25%)	53,76,76	2.40	18 (33%)

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	8L6	A	501	-	-	12/16/118/118	0/6/6/6
2	8L6	F	502	-	-	11/16/118/118	0/6/6/6
2	8L6	B	501	-	-	9/16/118/118	0/6/6/6
2	8L6	H	501	-	-	9/16/118/118	0/6/6/6
2	8L6	K	501	-	-	8/16/118/118	0/6/6/6
2	8L6	J	501	-	-	11/16/118/118	0/6/6/6
2	8L6	D	501	-	-	11/16/118/118	0/6/6/6
2	8L6	C	501	-	-	10/16/118/118	0/6/6/6
2	8L6	G	501	-	-	9/16/118/118	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8L6	I	501	-	-	8/16/118/118	0/6/6/6
2	8L6	E	501	-	-	10/16/118/118	0/6/6/6

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	8L6	C16-C15	6.94	1.56	1.47
2	A	501	8L6	C16-C15	6.87	1.56	1.47
2	D	501	8L6	C16-C15	6.83	1.56	1.47
2	G	501	8L6	C16-C15	6.78	1.56	1.47
2	E	501	8L6	C16-C15	6.70	1.56	1.47
2	F	502	8L6	C16-C15	6.69	1.56	1.47
2	J	501	8L6	C16-C15	6.67	1.56	1.47
2	K	501	8L6	C16-C15	6.65	1.56	1.47
2	B	501	8L6	C16-C15	6.64	1.56	1.47
2	C	501	8L6	C16-C15	6.63	1.56	1.47
2	I	501	8L6	C16-C15	6.62	1.56	1.47
2	J	501	8L6	C27-C28	-5.07	1.35	1.52
2	K	501	8L6	C27-C28	-5.06	1.35	1.52
2	B	501	8L6	C27-C28	-5.06	1.35	1.52
2	F	502	8L6	C27-C28	-5.06	1.35	1.52
2	D	501	8L6	C27-C28	-5.03	1.35	1.52
2	E	501	8L6	C27-C28	-5.02	1.35	1.52
2	G	501	8L6	C27-C28	-5.01	1.35	1.52
2	H	501	8L6	C27-C28	-4.99	1.35	1.52
2	I	501	8L6	C27-C28	-4.99	1.35	1.52
2	A	501	8L6	C27-C28	-4.98	1.35	1.52
2	C	501	8L6	C27-C28	-4.97	1.35	1.52
2	K	501	8L6	O-C2	-4.61	1.40	1.46
2	G	501	8L6	O-C2	-4.56	1.41	1.46
2	C	501	8L6	O-C2	-4.52	1.41	1.46
2	B	501	8L6	O-C2	-4.48	1.41	1.46
2	J	501	8L6	O-C2	-4.39	1.41	1.46
2	E	501	8L6	O-C2	-4.35	1.41	1.46
2	A	501	8L6	O-C2	-4.32	1.41	1.46
2	H	501	8L6	O-C2	-4.25	1.41	1.46
2	F	502	8L6	O-C2	-4.22	1.41	1.46
2	I	501	8L6	O-C2	-4.17	1.41	1.46
2	D	501	8L6	O-C2	-4.11	1.41	1.46
2	C	501	8L6	C21-C22	-4.02	1.47	1.54
2	E	501	8L6	C21-C22	-3.98	1.47	1.54
2	H	501	8L6	C21-C22	-3.98	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	8L6	C21-C22	-3.98	1.47	1.54
2	G	501	8L6	C21-C22	-3.96	1.47	1.54
2	B	501	8L6	C21-C22	-3.95	1.47	1.54
2	F	502	8L6	C21-C22	-3.85	1.47	1.54
2	J	501	8L6	C21-C22	-3.80	1.47	1.54
2	A	501	8L6	C21-C22	-3.76	1.47	1.54
2	D	501	8L6	O2-C1	3.75	1.49	1.43
2	K	501	8L6	C21-C22	-3.73	1.47	1.54
2	D	501	8L6	C21-C22	-3.67	1.47	1.54
2	E	501	8L6	O2-C1	3.64	1.49	1.43
2	J	501	8L6	O2-C1	3.53	1.49	1.43
2	F	502	8L6	O2-C1	3.50	1.49	1.43
2	I	501	8L6	O2-C1	3.36	1.49	1.43
2	G	501	8L6	O2-C1	3.35	1.49	1.43
2	A	501	8L6	O2-C1	3.33	1.49	1.43
2	C	501	8L6	O2-C1	3.28	1.49	1.43
2	C	501	8L6	C17-C19	3.26	1.62	1.56
2	K	501	8L6	O2-C1	3.24	1.49	1.43
2	A	501	8L6	C17-C19	3.15	1.61	1.56
2	B	501	8L6	O2-C1	3.14	1.48	1.43
2	H	501	8L6	O2-C1	3.08	1.48	1.43
2	D	501	8L6	C17-C19	3.02	1.61	1.56
2	A	501	8L6	C10-C9	2.92	1.58	1.54
2	I	501	8L6	C10-C9	2.92	1.58	1.54
2	H	501	8L6	C21-C20	-2.90	1.47	1.53
2	C	501	8L6	C10-C9	2.89	1.58	1.54
2	H	501	8L6	C10-C9	2.88	1.58	1.54
2	G	501	8L6	C21-C20	-2.87	1.47	1.53
2	B	501	8L6	C10-C9	2.85	1.58	1.54
2	F	502	8L6	C10-C9	2.83	1.58	1.54
2	G	501	8L6	C10-C9	2.82	1.58	1.54
2	I	501	8L6	C17-C19	2.80	1.61	1.56
2	K	501	8L6	C21-C20	-2.78	1.47	1.53
2	E	501	8L6	C21-C20	-2.78	1.47	1.53
2	I	501	8L6	C21-C20	-2.78	1.47	1.53
2	J	501	8L6	C21-C20	-2.77	1.47	1.53
2	D	501	8L6	C21-C20	-2.75	1.47	1.53
2	F	502	8L6	C21-C20	-2.73	1.47	1.53
2	J	501	8L6	C10-C9	2.70	1.58	1.54
2	B	501	8L6	C21-C20	-2.69	1.47	1.53
2	K	501	8L6	C10-C9	2.68	1.58	1.54
2	D	501	8L6	C10-C9	2.67	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	8L6	C10-C9	2.66	1.58	1.54
2	C	501	8L6	C21-C20	-2.65	1.47	1.53
2	H	501	8L6	C12-C13	2.64	1.58	1.54
2	H	501	8L6	C17-C19	2.60	1.61	1.56
2	I	501	8L6	C8-C2	2.54	1.57	1.52
2	A	501	8L6	C21-C20	-2.52	1.48	1.53
2	G	501	8L6	C17-C19	2.42	1.60	1.56
2	A	501	8L6	C8-C2	2.37	1.56	1.52
2	G	501	8L6	O4-C12	-2.32	1.40	1.44
2	B	501	8L6	C12-C22	-2.31	1.53	1.57
2	G	501	8L6	C12-C22	-2.26	1.53	1.57
2	B	501	8L6	O4-C12	-2.23	1.40	1.44
2	E	501	8L6	C17-C19	2.22	1.60	1.56
2	F	502	8L6	C8-C2	2.22	1.56	1.52
2	A	501	8L6	O4-C12	-2.21	1.40	1.44
2	H	501	8L6	O4-C12	-2.19	1.40	1.44
2	J	501	8L6	C8-C2	2.18	1.56	1.52
2	E	501	8L6	C8-C2	2.17	1.56	1.52
2	F	502	8L6	C12-C13	2.16	1.57	1.54
2	K	501	8L6	C8-C2	2.16	1.56	1.52
2	B	501	8L6	C17-C19	2.14	1.60	1.56
2	C	501	8L6	O4-C12	-2.13	1.40	1.44
2	F	502	8L6	C17-C19	2.12	1.60	1.56
2	I	501	8L6	C14-C15	-2.12	1.47	1.52
2	D	501	8L6	O4-C12	-2.12	1.40	1.44
2	C	501	8L6	C12-C13	2.11	1.57	1.54
2	I	501	8L6	O4-C12	-2.10	1.40	1.44
2	K	501	8L6	O4-C12	-2.10	1.40	1.44
2	D	501	8L6	C8-C2	2.06	1.56	1.52
2	C	501	8L6	C8-C2	2.05	1.56	1.52
2	J	501	8L6	O4-C12	-2.03	1.40	1.44
2	E	501	8L6	O4-C12	-2.03	1.40	1.44
2	F	502	8L6	O4-C12	-2.02	1.40	1.44
2	H	501	8L6	C8-C2	2.02	1.56	1.52

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	8L6	O7-C16-C26	-9.24	96.21	114.70
2	G	501	8L6	O7-C16-C26	-9.22	96.26	114.70
2	A	501	8L6	O7-C16-C26	-9.20	96.29	114.70
2	H	501	8L6	O7-C16-C26	-8.93	96.82	114.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	8L6	O7-C16-C26	-8.82	97.05	114.70
2	I	501	8L6	O7-C16-C26	-8.57	97.56	114.70
2	C	501	8L6	O7-C16-C26	-8.44	97.80	114.70
2	F	502	8L6	O7-C16-C26	-8.33	98.04	114.70
2	K	501	8L6	O7-C16-C26	-8.28	98.13	114.70
2	B	501	8L6	O7-C16-C26	-8.19	98.31	114.70
2	J	501	8L6	O7-C16-C26	-7.71	99.27	114.70
2	J	501	8L6	C22-C12-C13	-5.72	106.58	113.85
2	H	501	8L6	C22-C12-C13	-5.14	107.32	113.85
2	A	501	8L6	C27-C28-C29	5.05	123.34	112.09
2	G	501	8L6	C27-C28-C29	5.01	123.25	112.09
2	D	501	8L6	C27-C28-C29	4.99	123.20	112.09
2	H	501	8L6	C16-O7-C15	4.91	63.95	60.88
2	I	501	8L6	C27-C28-C29	4.90	123.00	112.09
2	H	501	8L6	C27-C28-C29	4.88	122.95	112.09
2	E	501	8L6	C27-C28-C29	4.87	122.93	112.09
2	D	501	8L6	C16-O7-C15	4.85	63.92	60.88
2	G	501	8L6	C16-O7-C15	4.80	63.89	60.88
2	A	501	8L6	C16-O7-C15	4.80	63.88	60.88
2	C	501	8L6	C27-C28-C29	4.77	122.71	112.09
2	E	501	8L6	C22-C12-C13	-4.76	107.80	113.85
2	B	501	8L6	C22-C12-C13	-4.72	107.85	113.85
2	C	501	8L6	C16-C17-C29	-4.67	99.93	107.97
2	K	501	8L6	C16-O7-C15	4.66	63.80	60.88
2	B	501	8L6	C16-O7-C15	4.60	63.76	60.88
2	E	501	8L6	C16-O7-C15	4.59	63.75	60.88
2	I	501	8L6	C16-O7-C15	4.58	63.75	60.88
2	A	501	8L6	C16-C17-C29	-4.56	100.12	107.97
2	J	501	8L6	C16-O7-C15	4.52	63.71	60.88
2	I	501	8L6	C16-C17-C29	-4.51	100.22	107.97
2	C	501	8L6	C16-O7-C15	4.50	63.70	60.88
2	K	501	8L6	C27-C28-C29	4.49	122.08	112.09
2	F	502	8L6	C27-C28-C29	4.49	122.08	112.09
2	F	502	8L6	C16-O7-C15	4.47	63.68	60.88
2	D	501	8L6	C16-C17-C29	-4.46	100.29	107.97
2	B	501	8L6	C27-C28-C29	4.42	121.92	112.09
2	I	501	8L6	C22-C12-C13	-4.41	108.24	113.85
2	G	501	8L6	C22-C12-C13	-4.30	108.38	113.85
2	B	501	8L6	C16-C17-C29	-4.27	100.62	107.97
2	F	502	8L6	C22-C12-C13	-4.24	108.46	113.85
2	A	501	8L6	C22-C12-C13	-4.23	108.47	113.85
2	K	501	8L6	C22-C12-C13	-4.18	108.53	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	501	8L6	C26-C27-C28	4.17	120.70	111.38
2	D	501	8L6	C22-C12-C13	-4.12	108.61	113.85
2	F	502	8L6	C16-C17-C29	-4.03	101.03	107.97
2	J	501	8L6	C16-C17-C29	-4.03	101.04	107.97
2	K	501	8L6	C16-C17-C29	-4.02	101.05	107.97
2	J	501	8L6	C27-C28-C29	4.02	121.03	112.09
2	I	501	8L6	O-C3-O1	-4.01	111.03	117.64
2	G	501	8L6	C16-C17-C29	-3.99	101.10	107.97
2	C	501	8L6	C22-C12-C13	-3.99	108.78	113.85
2	D	501	8L6	C26-C27-C28	3.97	120.24	111.38
2	G	501	8L6	O-C3-O1	-3.96	111.11	117.64
2	H	501	8L6	C16-C17-C29	-3.95	101.17	107.97
2	E	501	8L6	C16-C17-C29	-3.92	101.22	107.97
2	J	501	8L6	O-C3-O1	-3.90	111.20	117.64
2	H	501	8L6	O-C3-O1	-3.89	111.22	117.64
2	D	501	8L6	O-C3-O1	-3.88	111.23	117.64
2	A	501	8L6	C26-C27-C28	3.87	120.02	111.38
2	B	501	8L6	O-C3-O1	-3.84	111.30	117.64
2	H	501	8L6	C26-C27-C28	3.84	119.96	111.38
2	E	501	8L6	O-C3-O1	-3.83	111.32	117.64
2	E	501	8L6	C26-C27-C28	3.79	119.86	111.38
2	C	501	8L6	O-C3-O1	-3.77	111.41	117.64
2	J	501	8L6	O5-C23-C22	3.75	114.16	108.83
2	I	501	8L6	C26-C27-C28	3.74	119.73	111.38
2	K	501	8L6	O-C3-O1	-3.73	111.49	117.64
2	J	501	8L6	C27-C26-C16	-3.69	104.34	112.03
2	B	501	8L6	C27-C26-C16	-3.69	104.35	112.03
2	J	501	8L6	C18-C17-C19	-3.66	107.08	112.02
2	F	502	8L6	C18-C17-C19	-3.64	107.10	112.02
2	A	501	8L6	O-C3-O1	-3.64	111.63	117.64
2	K	501	8L6	C18-C17-C19	-3.63	107.13	112.02
2	F	502	8L6	O-C3-O1	-3.60	111.71	117.64
2	H	501	8L6	C18-C17-C19	-3.59	107.17	112.02
2	B	501	8L6	C18-C17-C19	-3.57	107.20	112.02
2	K	501	8L6	C27-C26-C16	-3.54	104.65	112.03
2	C	501	8L6	C18-C17-C19	-3.53	107.26	112.02
2	G	501	8L6	O5-C23-C22	3.51	113.82	108.83
2	F	502	8L6	C27-C26-C16	-3.50	104.74	112.03
2	C	501	8L6	C26-C27-C28	3.49	119.19	111.38
2	E	501	8L6	C18-C17-C19	-3.45	107.36	112.02
2	A	501	8L6	C18-C17-C19	-3.44	107.37	112.02
2	C	501	8L6	C27-C26-C16	-3.41	104.92	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	8L6	O5-C23-C22	3.40	113.67	108.83
2	F	502	8L6	O5-C23-C22	3.39	113.65	108.83
2	D	501	8L6	O5-C23-C22	3.34	113.57	108.83
2	G	501	8L6	C7-C6-C8	3.32	120.51	114.36
2	F	502	8L6	C26-C27-C28	3.31	118.78	111.38
2	G	501	8L6	C18-C17-C19	-3.31	107.56	112.02
2	K	501	8L6	C26-C27-C28	3.26	118.66	111.38
2	B	501	8L6	C26-C27-C28	3.23	118.59	111.38
2	B	501	8L6	C7-C6-C8	3.22	120.33	114.36
2	D	501	8L6	C18-C17-C19	-3.22	107.67	112.02
2	C	501	8L6	C7-C6-C8	3.17	120.23	114.36
2	K	501	8L6	C7-C6-C8	3.17	120.22	114.36
2	A	501	8L6	C7-C6-C8	3.16	120.20	114.36
2	H	501	8L6	C7-C6-C8	3.15	120.19	114.36
2	H	501	8L6	O5-C23-C22	3.10	113.23	108.83
2	I	501	8L6	C7-C6-C8	3.09	120.08	114.36
2	I	501	8L6	O5-C23-C22	3.08	113.21	108.83
2	I	501	8L6	C27-C26-C16	-3.07	105.63	112.03
2	I	501	8L6	C18-C17-C19	-3.05	107.91	112.02
2	J	501	8L6	C7-C6-C8	3.02	119.95	114.36
2	E	501	8L6	C7-C6-C8	3.01	119.93	114.36
2	J	501	8L6	C26-C27-C28	3.00	118.08	111.38
2	E	501	8L6	O5-C23-C22	2.93	113.00	108.83
2	E	501	8L6	C27-C26-C16	-2.93	105.93	112.03
2	A	501	8L6	O8-C29-C28	-2.88	116.45	121.56
2	K	501	8L6	O5-C23-C22	2.87	112.92	108.83
2	H	501	8L6	C27-C26-C16	-2.86	106.07	112.03
2	F	502	8L6	C7-C6-C8	2.85	119.64	114.36
2	A	501	8L6	C27-C26-C16	-2.85	106.09	112.03
2	D	501	8L6	C7-C6-C8	2.84	119.61	114.36
2	B	501	8L6	O5-C23-C22	2.82	112.83	108.83
2	C	501	8L6	O8-C29-C28	-2.81	116.57	121.56
2	C	501	8L6	O5-C23-C22	2.80	112.81	108.83
2	J	501	8L6	O7-C15-C16	-2.75	57.92	59.77
2	H	501	8L6	O7-C15-C16	-2.73	57.94	59.77
2	K	501	8L6	C10-C9-C1	2.71	116.24	111.48
2	D	501	8L6	O8-C29-C28	-2.71	116.75	121.56
2	I	501	8L6	O8-C29-C28	-2.69	116.78	121.56
2	B	501	8L6	C10-C9-C1	2.68	116.19	111.48
2	G	501	8L6	O8-C29-C28	-2.68	116.80	121.56
2	D	501	8L6	O7-C15-C16	-2.68	57.97	59.77
2	B	501	8L6	O-C3-C4	2.67	123.76	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	501	8L6	O8-C29-C28	-2.67	116.82	121.56
2	H	501	8L6	O-C3-C4	2.66	123.73	118.98
2	D	501	8L6	C27-C26-C16	-2.65	106.50	112.03
2	F	502	8L6	C10-C9-C1	2.64	116.12	111.48
2	F	502	8L6	O7-C15-C16	-2.62	58.01	59.77
2	I	501	8L6	O7-C15-C16	-2.62	58.01	59.77
2	A	501	8L6	O7-C15-C16	-2.62	58.01	59.77
2	A	501	8L6	C7-C6-C4	-2.60	119.41	123.84
2	G	501	8L6	C10-C9-C1	2.60	116.05	111.48
2	G	501	8L6	O7-C15-C16	-2.59	58.03	59.77
2	D	501	8L6	C10-C9-C1	2.59	116.02	111.48
2	E	501	8L6	O7-C15-C16	-2.58	58.04	59.77
2	J	501	8L6	C10-C9-C1	2.57	116.00	111.48
2	H	501	8L6	C10-C9-C1	2.57	115.99	111.48
2	K	501	8L6	O7-C15-C16	-2.56	58.05	59.77
2	B	501	8L6	O7-C15-C16	-2.56	58.05	59.77
2	E	501	8L6	C5-C4-C3	2.56	120.48	115.38
2	I	501	8L6	C7-C6-C4	-2.56	119.50	123.84
2	G	501	8L6	C5-C4-C3	2.55	120.46	115.38
2	I	501	8L6	O-C3-C4	2.54	123.52	118.98
2	I	501	8L6	C5-C4-C3	2.53	120.43	115.38
2	K	501	8L6	O-C3-C4	2.53	123.50	118.98
2	K	501	8L6	C7-C6-C4	-2.53	119.55	123.84
2	F	502	8L6	C5-C4-C3	2.53	120.42	115.38
2	E	501	8L6	O8-C29-C28	-2.53	117.08	121.56
2	C	501	8L6	C10-C9-C1	2.52	115.90	111.48
2	H	501	8L6	C5-C4-C3	2.52	120.40	115.38
2	A	501	8L6	C5-C4-C3	2.51	120.39	115.38
2	A	501	8L6	C10-C9-C1	2.51	115.89	111.48
2	E	501	8L6	C10-C9-C1	2.50	115.87	111.48
2	C	501	8L6	O7-C15-C16	-2.50	58.09	59.77
2	H	501	8L6	C7-C6-C4	-2.49	119.61	123.84
2	J	501	8L6	O-C3-C4	2.46	123.38	118.98
2	B	501	8L6	O8-C29-C28	-2.46	117.19	121.56
2	I	501	8L6	C10-C9-C1	2.45	115.78	111.48
2	C	501	8L6	O-C3-C4	2.45	123.36	118.98
2	C	501	8L6	C7-C6-C4	-2.44	119.70	123.84
2	D	501	8L6	C5-C4-C3	2.43	120.22	115.38
2	G	501	8L6	O-C3-C4	2.43	123.32	118.98
2	E	501	8L6	C7-C6-C4	-2.41	119.75	123.84
2	J	501	8L6	C5-C4-C3	2.41	120.18	115.38
2	F	502	8L6	O8-C29-C28	-2.40	117.29	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	8L6	C5-C4-C3	2.40	120.17	115.38
2	K	501	8L6	C5-C4-C3	2.39	120.16	115.38
2	D	501	8L6	O-C3-C4	2.38	123.24	118.98
2	D	501	8L6	O5-C24-C25	2.37	122.72	112.38
2	F	502	8L6	C7-C6-C4	-2.37	119.82	123.84
2	K	501	8L6	O2-C1-C	-2.36	103.04	107.84
2	G	501	8L6	O5-C24-C25	2.35	122.63	112.38
2	G	501	8L6	C27-C26-C16	-2.35	107.14	112.03
2	E	501	8L6	O5-C24-C25	2.34	122.59	112.38
2	B	501	8L6	C7-C6-C4	-2.34	119.86	123.84
2	G	501	8L6	O-C2-C8	-2.34	107.22	110.05
2	A	501	8L6	O-C3-C4	2.33	123.16	118.98
2	E	501	8L6	O-C3-C4	2.33	123.15	118.98
2	K	501	8L6	O8-C29-C28	-2.33	117.43	121.56
2	B	501	8L6	O5-C24-C25	2.32	122.49	112.38
2	H	501	8L6	O5-C24-C25	2.32	122.48	112.38
2	J	501	8L6	C7-C6-C4	-2.31	119.92	123.84
2	G	501	8L6	C7-C6-C4	-2.30	119.93	123.84
2	K	501	8L6	O5-C24-C25	2.28	122.32	112.38
2	I	501	8L6	O5-C24-C25	2.28	122.31	112.38
2	F	502	8L6	O5-C24-C25	2.28	122.31	112.38
2	C	501	8L6	O5-C24-C25	2.27	122.30	112.38
2	A	501	8L6	O5-C24-C25	2.27	122.27	112.38
2	D	501	8L6	C7-C6-C4	-2.27	119.99	123.84
2	B	501	8L6	C5-C4-C3	2.24	119.85	115.38
2	J	501	8L6	O5-C24-C25	2.21	122.01	112.38
2	J	501	8L6	O8-C29-C28	-2.21	117.64	121.56
2	I	501	8L6	O2-C1-C	-2.20	103.37	107.84
2	J	501	8L6	O2-C1-C	-2.18	103.41	107.84
2	J	501	8L6	C20-C21-C22	2.15	120.21	113.82
2	F	502	8L6	O-C3-C4	2.06	122.67	118.98
2	A	501	8L6	O2-C1-C	-2.03	103.72	107.84

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	501	8L6	C9-C1-C2-C8
2	K	501	8L6	O2-C1-C2-O
2	K	501	8L6	C-C1-C9-C10
2	K	501	8L6	C-C1-C9-C22
2	K	501	8L6	C-C1-C9-O3

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Mol	Chain	Res	Type	Atoms
2	K	501	8L6	O2-C1-C9-C10
2	A	501	8L6	C-C1-C2-C8
2	A	501	8L6	C9-C1-C2-O
2	A	501	8L6	C9-C1-C2-C8
2	A	501	8L6	O2-C1-C2-O
2	A	501	8L6	O2-C1-C2-C8
2	A	501	8L6	C-C1-C9-C10
2	A	501	8L6	C-C1-C9-C22
2	A	501	8L6	C-C1-C9-O3
2	A	501	8L6	O2-C1-C9-C10
2	B	501	8L6	C9-C1-C2-C8
2	B	501	8L6	C-C1-C9-C10
2	B	501	8L6	C-C1-C9-C22
2	B	501	8L6	C-C1-C9-O3
2	B	501	8L6	O2-C1-C9-C10
2	C	501	8L6	C-C1-C2-C8
2	C	501	8L6	C9-C1-C2-O
2	C	501	8L6	C9-C1-C2-C8
2	C	501	8L6	O2-C1-C2-O
2	C	501	8L6	O2-C1-C2-C8
2	C	501	8L6	C-C1-C9-C10
2	C	501	8L6	C-C1-C9-C22
2	C	501	8L6	C-C1-C9-O3
2	C	501	8L6	O2-C1-C9-C10
2	D	501	8L6	C9-C1-C2-O
2	D	501	8L6	C9-C1-C2-C8
2	D	501	8L6	O2-C1-C2-O
2	D	501	8L6	C-C1-C9-C10
2	D	501	8L6	C-C1-C9-C22
2	D	501	8L6	C-C1-C9-O3
2	D	501	8L6	O2-C1-C9-C10
2	E	501	8L6	C-C1-C2-C8
2	E	501	8L6	C9-C1-C2-O
2	E	501	8L6	C9-C1-C2-C8
2	E	501	8L6	O2-C1-C2-O
2	E	501	8L6	O2-C1-C2-C8
2	E	501	8L6	C-C1-C9-C10
2	E	501	8L6	C-C1-C9-C22
2	E	501	8L6	C-C1-C9-O3
2	E	501	8L6	O2-C1-C9-C10
2	F	502	8L6	C-C1-C2-C8
2	F	502	8L6	C9-C1-C2-O

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Mol	Chain	Res	Type	Atoms
2	F	502	8L6	C9-C1-C2-C8
2	F	502	8L6	O2-C1-C2-O
2	F	502	8L6	O2-C1-C2-C8
2	F	502	8L6	C-C1-C9-C10
2	F	502	8L6	C-C1-C9-C22
2	F	502	8L6	C-C1-C9-O3
2	F	502	8L6	O2-C1-C9-C10
2	G	501	8L6	C-C1-C9-C10
2	G	501	8L6	C-C1-C9-C22
2	G	501	8L6	C-C1-C9-O3
2	G	501	8L6	O2-C1-C9-C10
2	H	501	8L6	C9-C1-C2-C8
2	H	501	8L6	C-C1-C9-C10
2	H	501	8L6	C-C1-C9-C22
2	H	501	8L6	C-C1-C9-O3
2	H	501	8L6	O2-C1-C9-C10
2	I	501	8L6	C9-C1-C2-C8
2	I	501	8L6	O2-C1-C2-O
2	I	501	8L6	C-C1-C9-C10
2	I	501	8L6	C-C1-C9-C22
2	I	501	8L6	C-C1-C9-O3
2	I	501	8L6	O2-C1-C9-C10
2	J	501	8L6	C9-C1-C2-O
2	J	501	8L6	C9-C1-C2-C8
2	J	501	8L6	O2-C1-C2-O
2	J	501	8L6	C-C1-C9-C10
2	J	501	8L6	C-C1-C9-C22
2	J	501	8L6	C-C1-C9-O3
2	J	501	8L6	O2-C1-C9-C10
2	E	501	8L6	C-C1-C2-O
2	J	501	8L6	C25-C24-O5-C23
2	B	501	8L6	O2-C1-C2-O
2	G	501	8L6	O2-C1-C2-O
2	H	501	8L6	O2-C1-C2-O
2	K	501	8L6	O2-C1-C2-C8
2	B	501	8L6	O2-C1-C2-C8
2	D	501	8L6	O2-C1-C2-C8
2	H	501	8L6	O2-C1-C2-C8
2	I	501	8L6	O2-C1-C2-C8
2	J	501	8L6	O2-C1-C2-C8
2	A	501	8L6	C-C1-C2-O
2	A	501	8L6	C25-C24-O5-C23

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Mol	Chain	Res	Type	Atoms
2	J	501	8L6	O6-C24-O5-C23
2	D	501	8L6	C25-C24-O5-C23
2	C	501	8L6	C-C1-C2-O
2	G	501	8L6	C25-C24-O5-C23
2	K	501	8L6	C9-C1-C2-O
2	B	501	8L6	C9-C1-C2-O
2	H	501	8L6	C9-C1-C2-O
2	I	501	8L6	C9-C1-C2-O
2	F	502	8L6	C-C1-C2-O
2	D	501	8L6	C-C1-C2-C8
2	J	501	8L6	C-C1-C2-C8
2	A	501	8L6	O6-C24-O5-C23
2	H	501	8L6	C25-C24-O5-C23
2	F	502	8L6	C25-C24-O5-C23
2	B	501	8L6	C25-C24-O5-C23
2	D	501	8L6	O6-C24-O5-C23
2	G	501	8L6	O2-C1-C2-C8
2	G	501	8L6	O6-C24-O5-C23
2	G	501	8L6	C9-C1-C2-C8

There are no ring outliers.

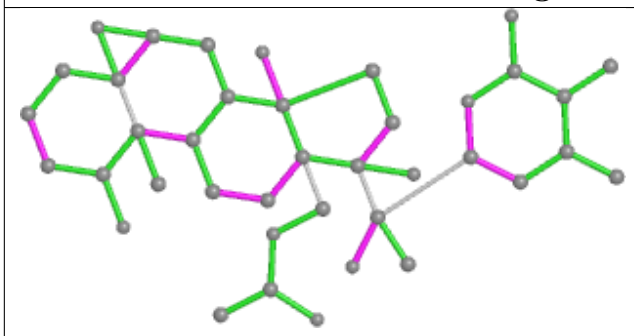
11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	8L6	2	0
2	F	502	8L6	1	0
2	B	501	8L6	1	0
2	H	501	8L6	1	0
2	K	501	8L6	1	0
2	J	501	8L6	5	0
2	D	501	8L6	1	0
2	C	501	8L6	1	0
2	G	501	8L6	1	0
2	I	501	8L6	4	0
2	E	501	8L6	1	0

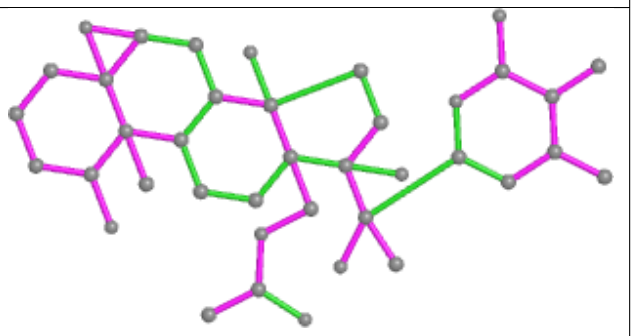
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

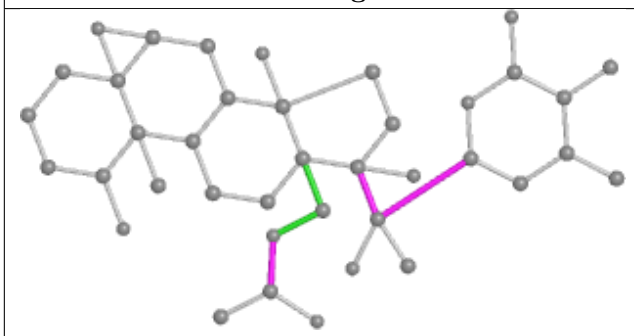
Ligand 8L6 A 501



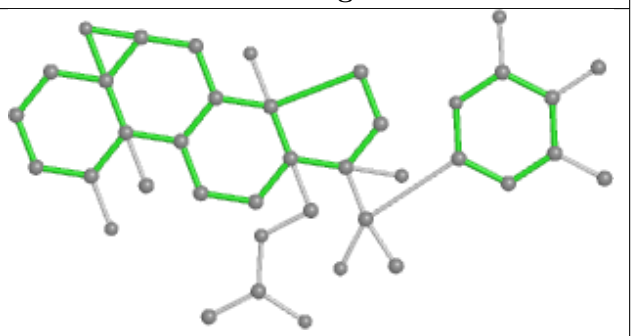
Bond lengths



Bond angles

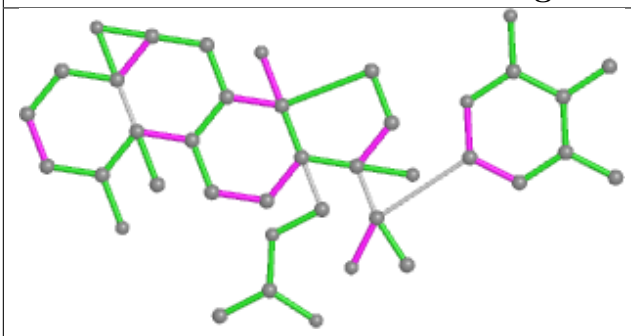


Torsions

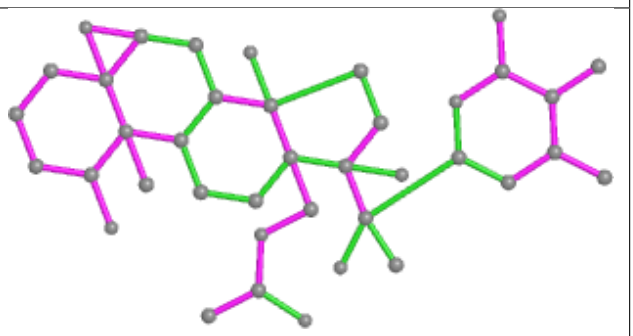


Rings

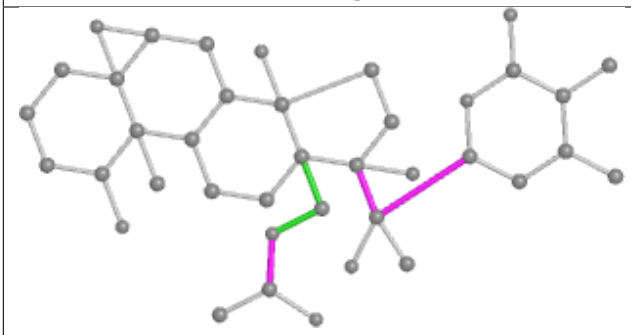
Ligand 8L6 F 502



Bond lengths



Bond angles



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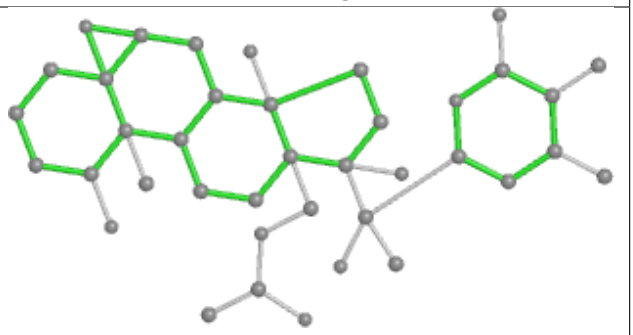
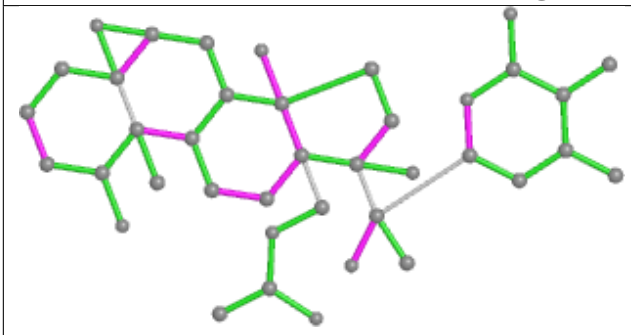
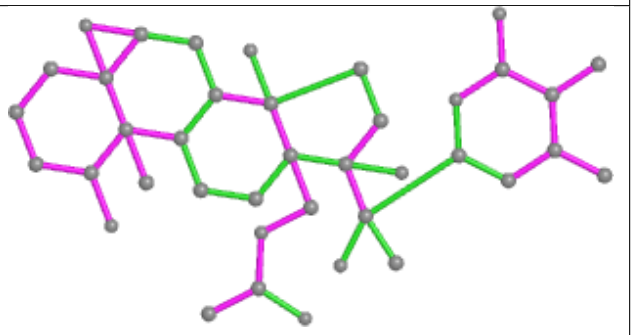


Rings

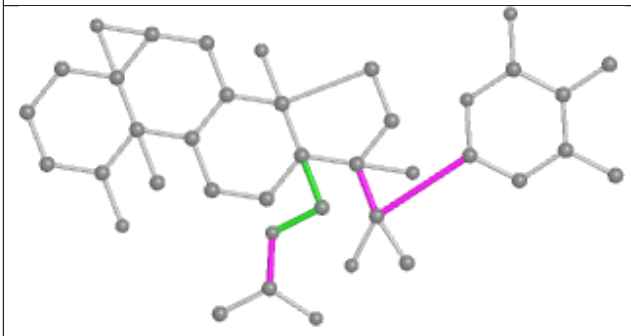
Ligand 8L6 B 501



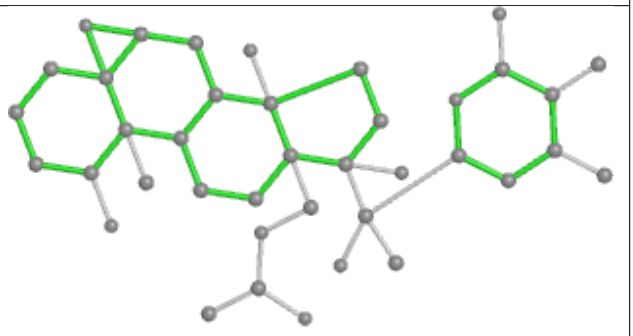
Bond lengths



Bond angles

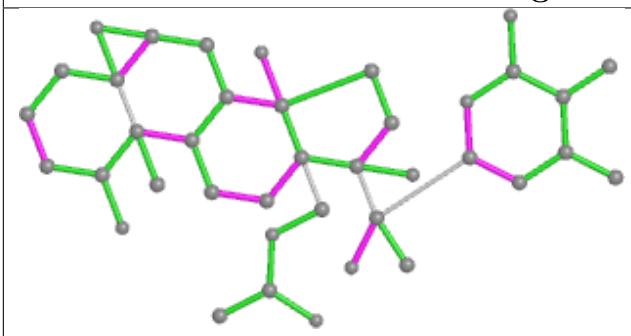


Torsions

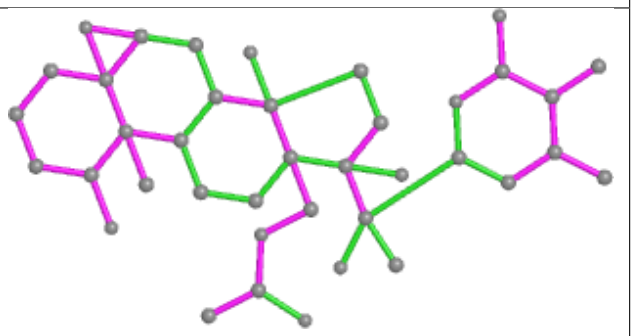


Rings

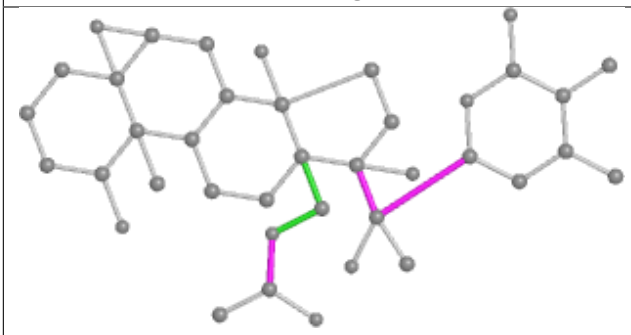
Ligand 8L6 H 501



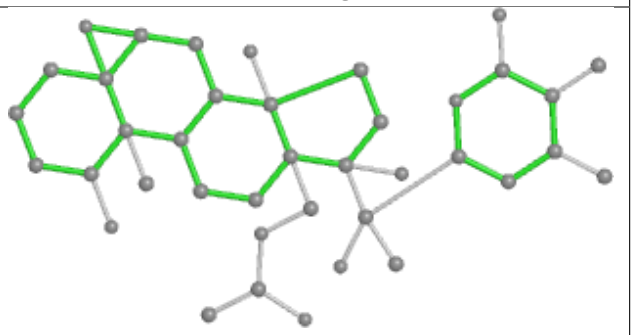
Bond lengths



Bond angles

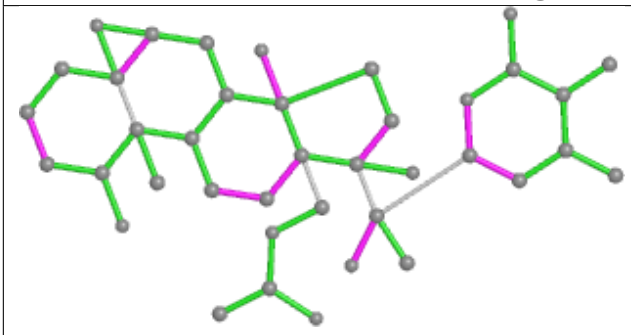


Torsions

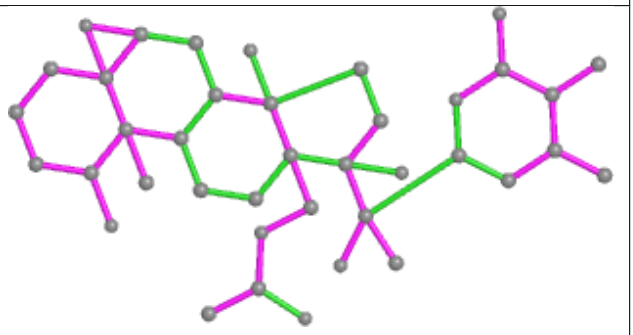


Rings

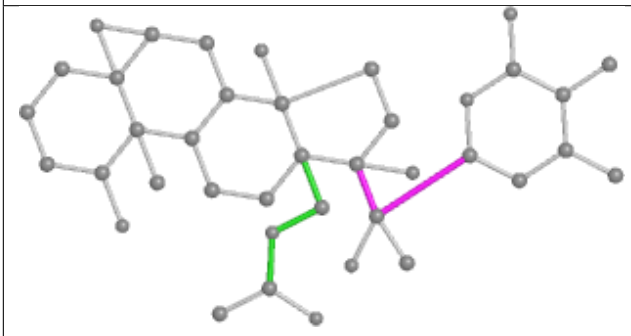
Ligand 8L6 K 501



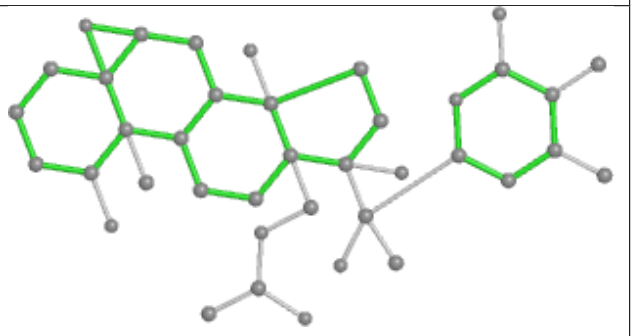
Bond lengths



Bond angles

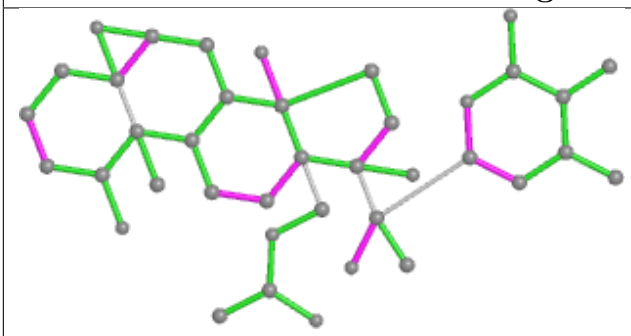


Torsions

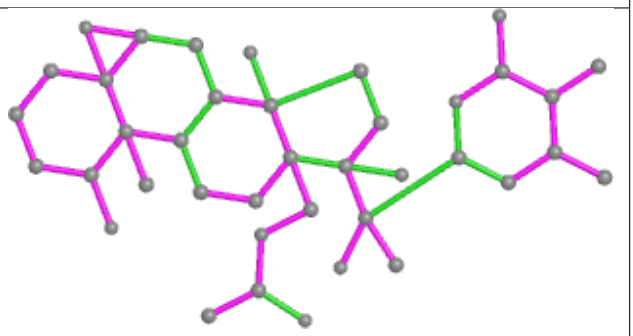


Rings

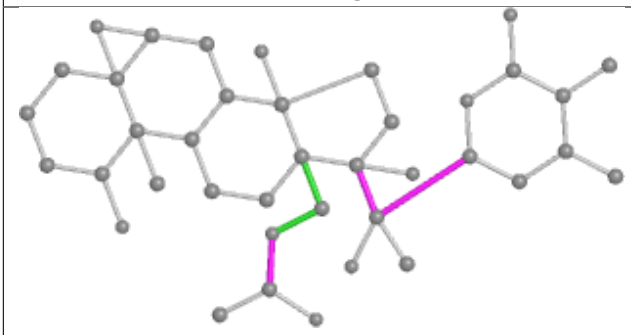
Ligand 8L6 J 501



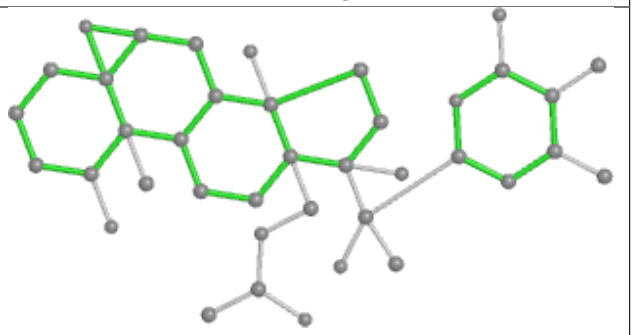
Bond lengths



Bond angles

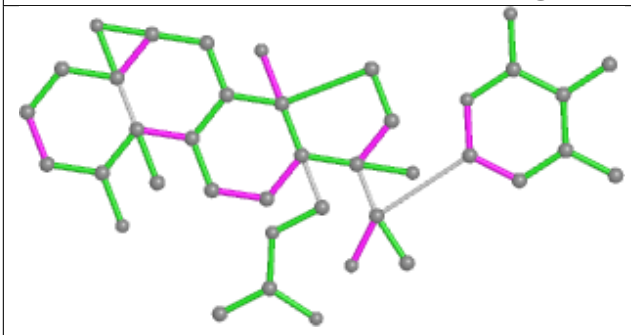


Torsions

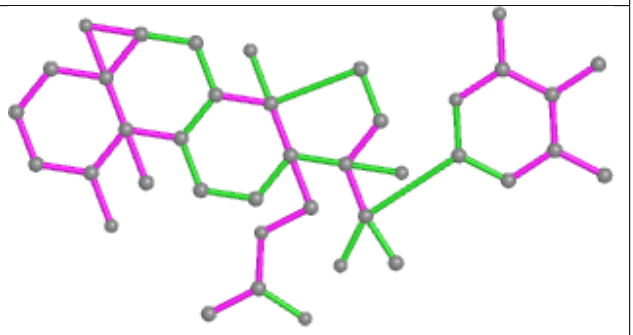


Rings

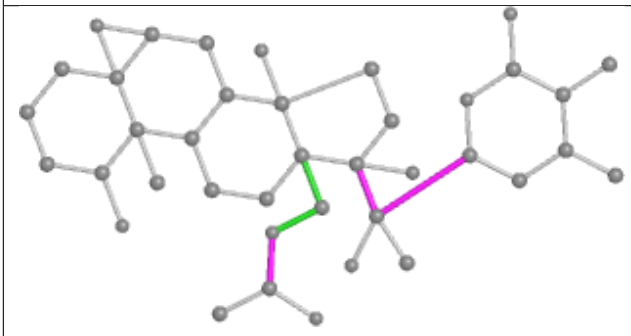
Ligand 8L6 D 501



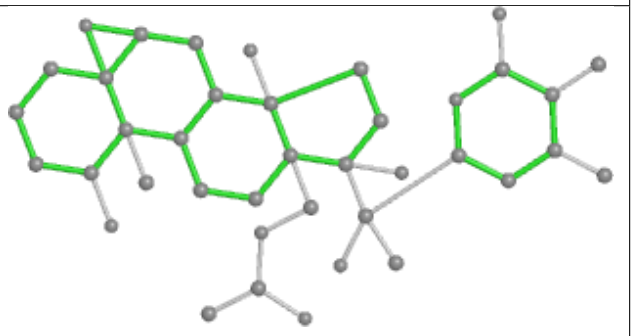
Bond lengths



Bond angles

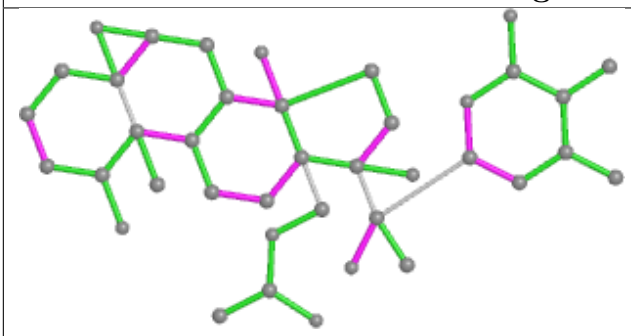


Torsions

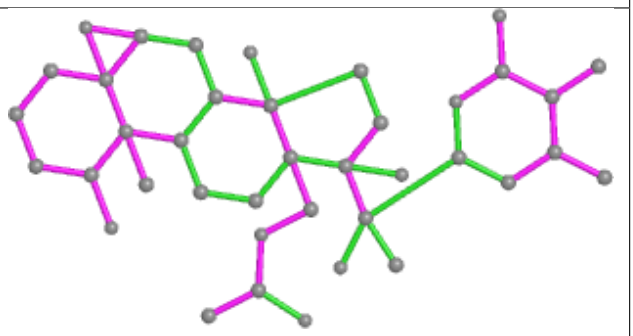


Rings

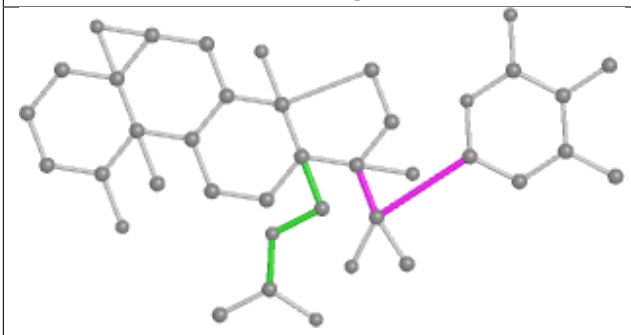
Ligand 8L6 C 501



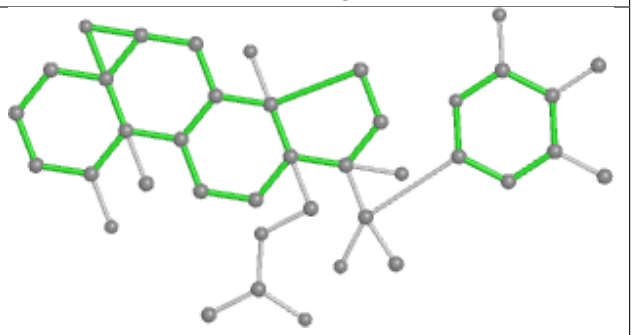
Bond lengths



Bond angles

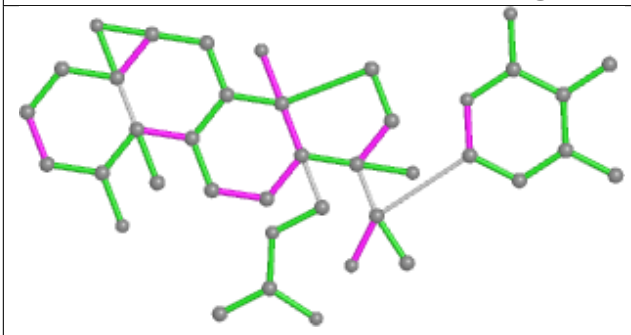


Torsions

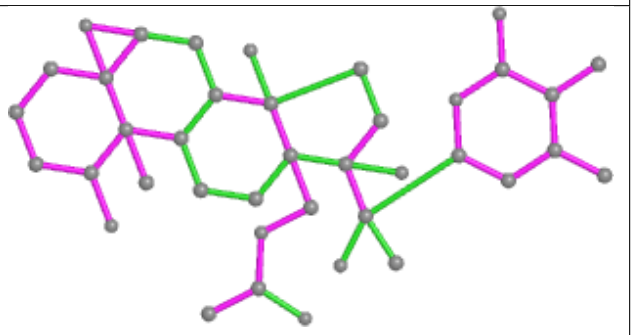


Rings

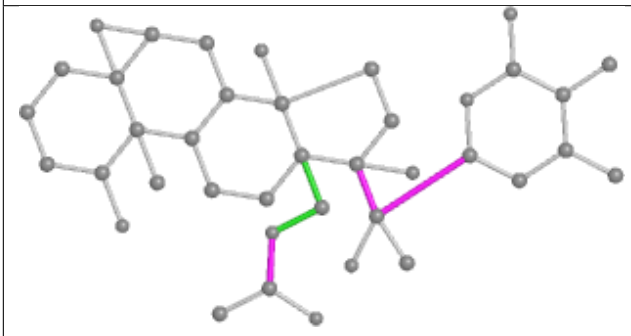
Ligand 8L6 G 501



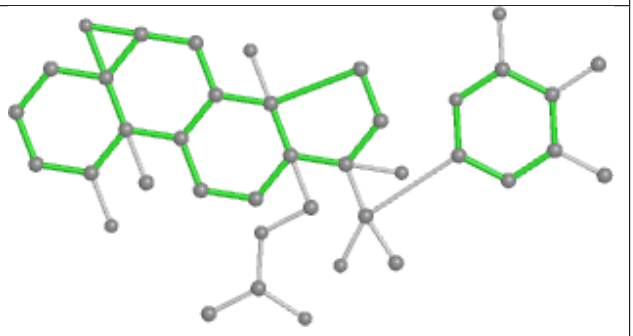
Bond lengths



Bond angles

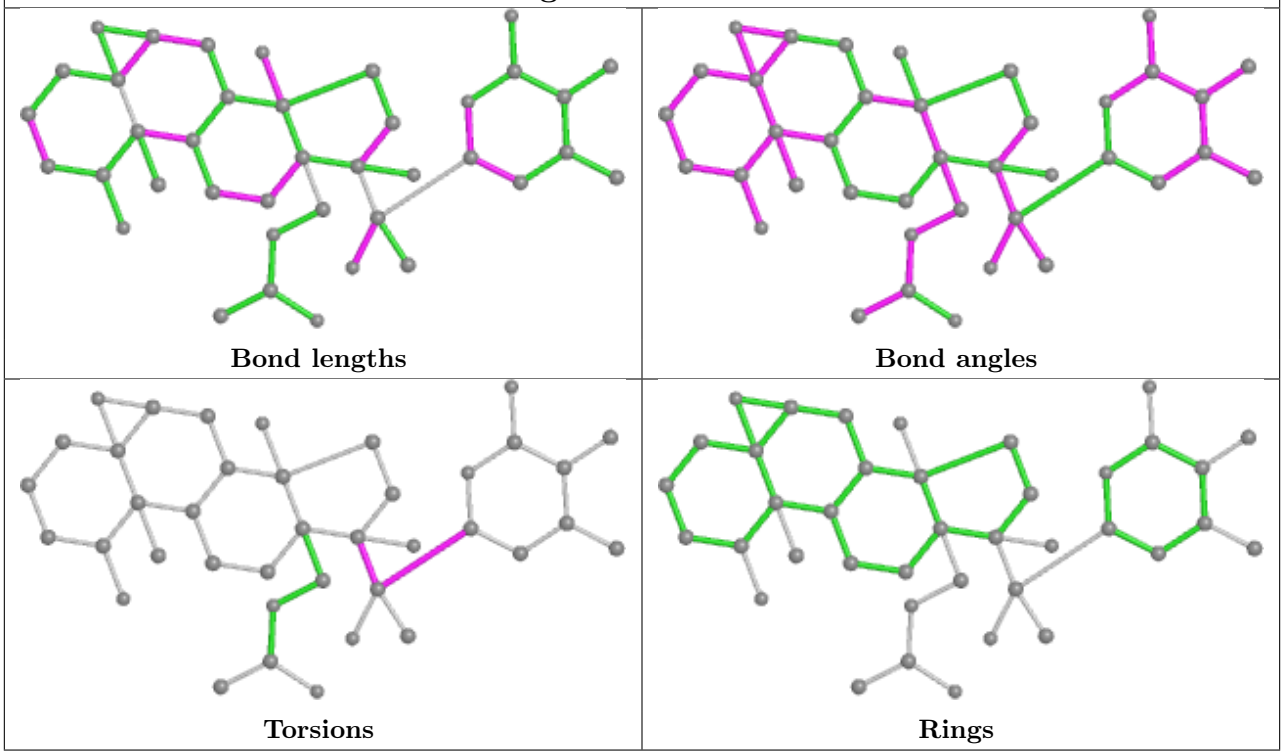


Torsions

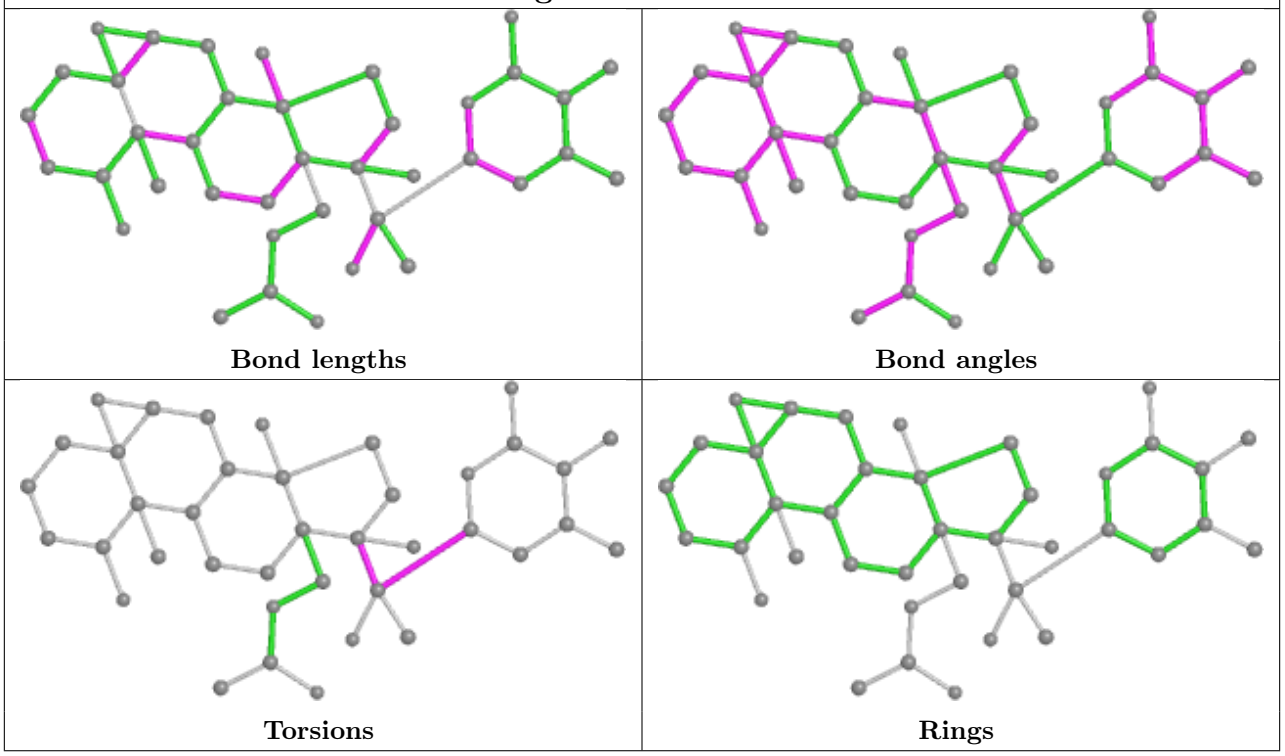


Rings

Ligand 8L6 I 501



Ligand 8L6 E 501



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, 95^{th} 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	108/112 (96%)	-0.05	0 100 100	35, 46, 59, 69	0
1	B	108/112 (96%)	0.05	2 (1%) 66 65	32, 44, 57, 64	0
1	C	108/112 (96%)	0.09	4 (3%) 41 37	32, 47, 64, 73	0
1	D	108/112 (96%)	0.01	0 100 100	32, 43, 56, 60	0
1	E	109/112 (97%)	0.09	2 (1%) 68 67	33, 45, 63, 69	0
1	F	108/112 (96%)	0.17	4 (3%) 41 37	35, 49, 64, 71	0
1	G	108/112 (96%)	0.03	0 100 100	32, 43, 59, 68	0
1	H	108/112 (96%)	0.21	2 (1%) 66 65	36, 52, 65, 72	0
1	I	108/112 (96%)	0.10	1 (0%) 84 84	34, 47, 60, 69	0
1	J	108/112 (96%)	0.04	2 (1%) 66 65	39, 51, 67, 74	0
1	K	108/112 (96%)	0.16	3 (2%) 53 49	34, 48, 65, 76	0
All	All	1189/1232 (96%)	0.08	20 (1%) 70 69	32, 47, 63, 76	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	366	ASP	4.0
1	B	339	ASP	3.1
1	E	308	LEU	3.0
1	J	339	ASP	3.0
1	C	369	GLU	3.0
1	C	329	ALA	2.9
1	K	365	MET	2.8
1	J	343	LEU	2.7
1	K	312	LEU	2.6
1	H	365	MET	2.5
1	F	343	LEU	2.4
1	C	368	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	349	HIS	2.3
1	C	328	ALA	2.3
1	H	309	SER	2.3
1	F	342	ALA	2.2
1	E	368	ARG	2.2
1	I	359	SER	2.1
1	F	339	ASP	2.1
1	B	340	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	F	501	1/1	-0.14	0.40	85,85,85,85	0
3	CL	A	502	1/1	0.40	0.43	70,70,70,70	0
3	CL	C	502	1/1	0.74	0.41	73,73,73,73	0
3	CL	G	502	1/1	0.85	0.41	69,69,69,69	0
3	CL	K	502	1/1	0.86	0.31	67,67,67,67	0
2	8L6	F	502	39/39	0.92	0.28	46,59,69,71	0
3	CL	I	502	1/1	0.92	0.39	67,67,67,67	0
2	8L6	K	501	39/39	0.93	0.20	34,50,61,62	0
2	8L6	J	501	39/39	0.93	0.25	44,55,67,69	0
2	8L6	A	501	39/39	0.93	0.22	37,47,64,68	0
2	8L6	E	501	39/39	0.93	0.21	34,51,63,64	0
2	8L6	C	501	39/39	0.94	0.23	37,51,72,78	0
2	8L6	H	501	39/39	0.94	0.24	43,56,67,69	0
2	8L6	B	501	39/39	0.94	0.26	36,47,59,62	0
2	8L6	D	501	39/39	0.95	0.21	35,49,59,64	0

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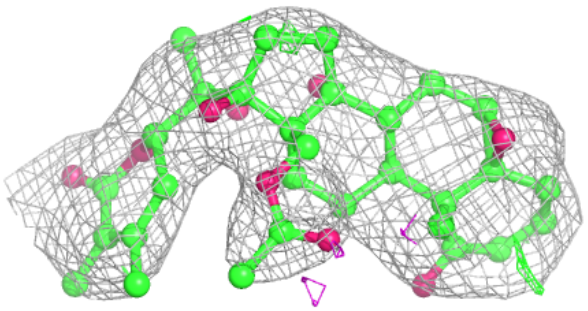
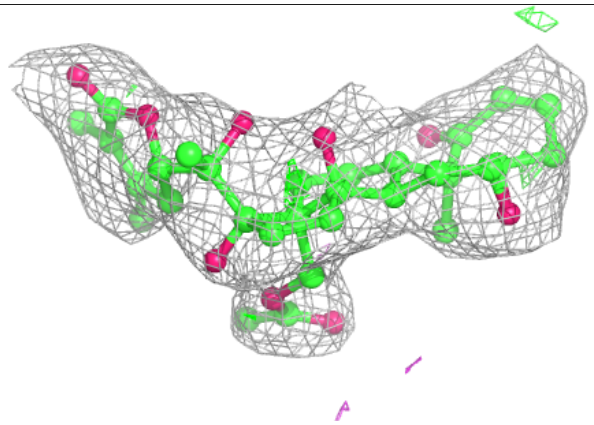
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	8L6	I	501	39/39	0.95	0.22	26,53,65,75	0
2	8L6	G	501	39/39	0.95	0.18	32,47,61,65	0

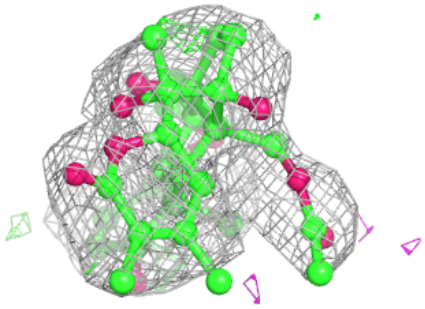
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8L6 F 502:

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

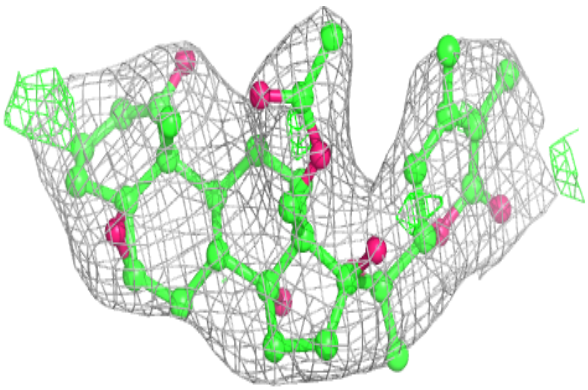


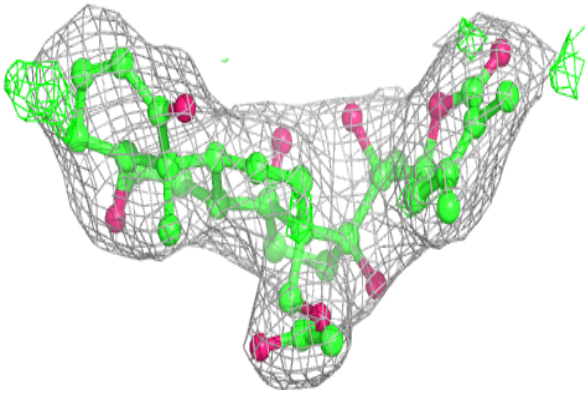


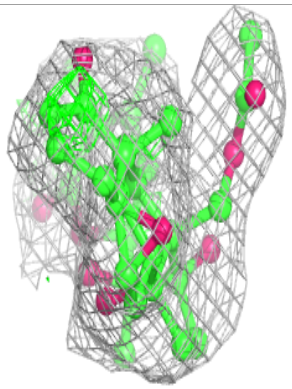


Electron density around 8L6 K 501:

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

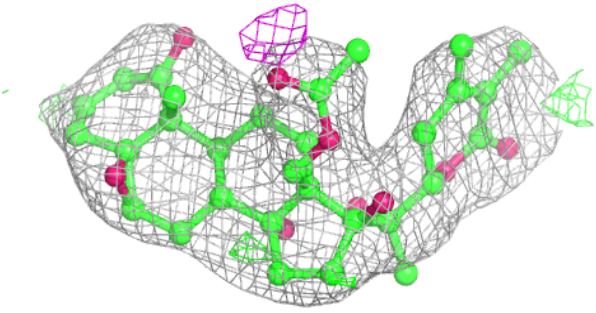


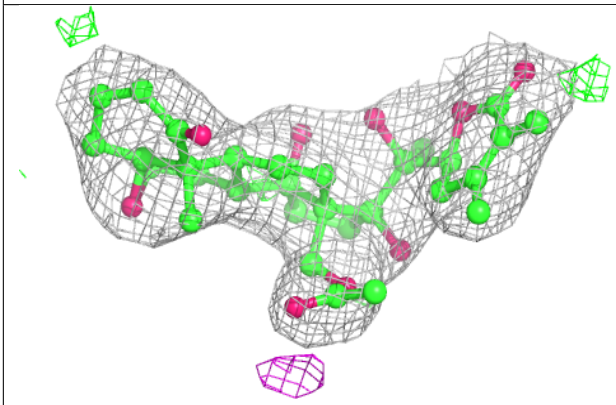


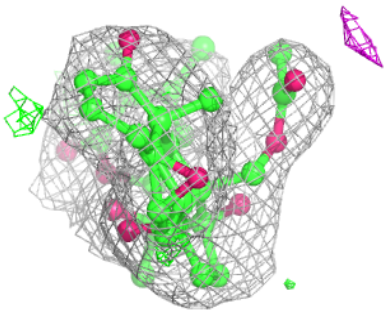


Electron density around 8L6 J 501:

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

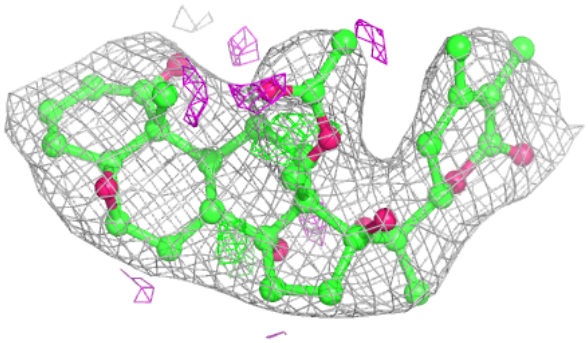


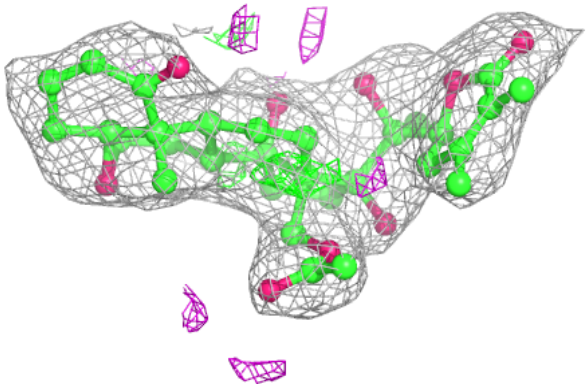


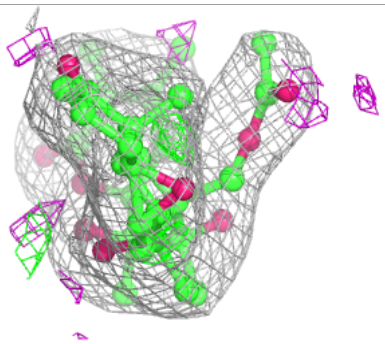


Electron density around 8L6 A 501:

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

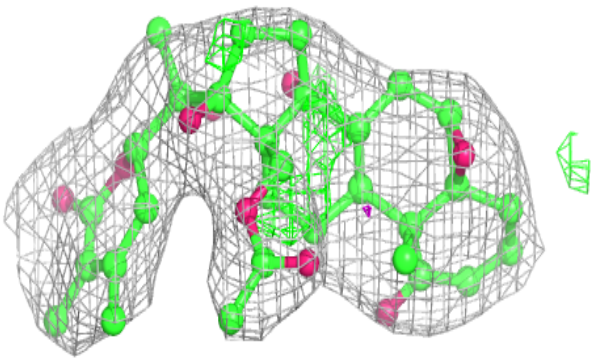


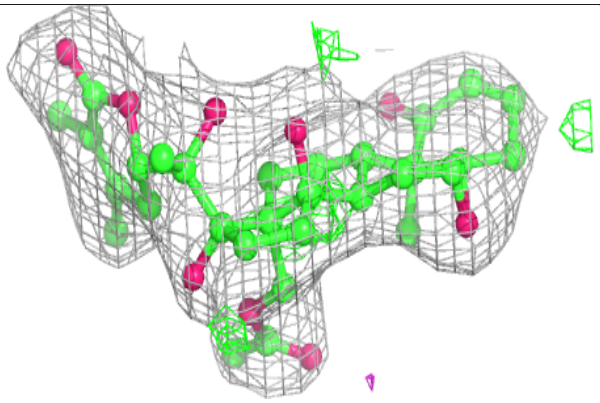


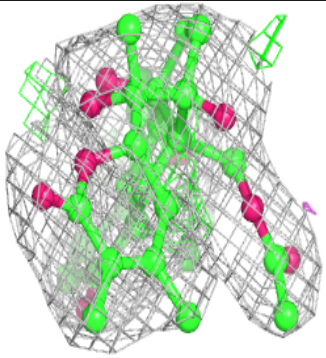


Electron density around 8L6 E 501:

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

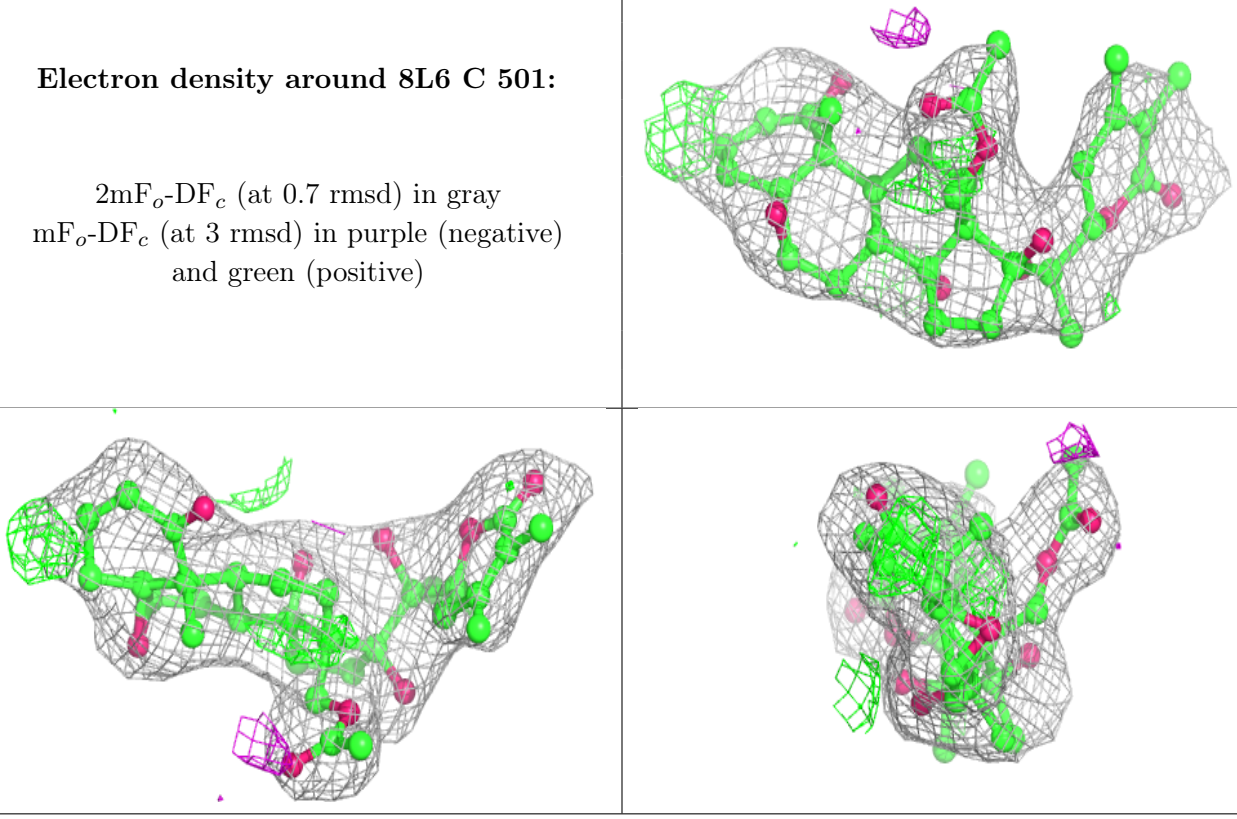






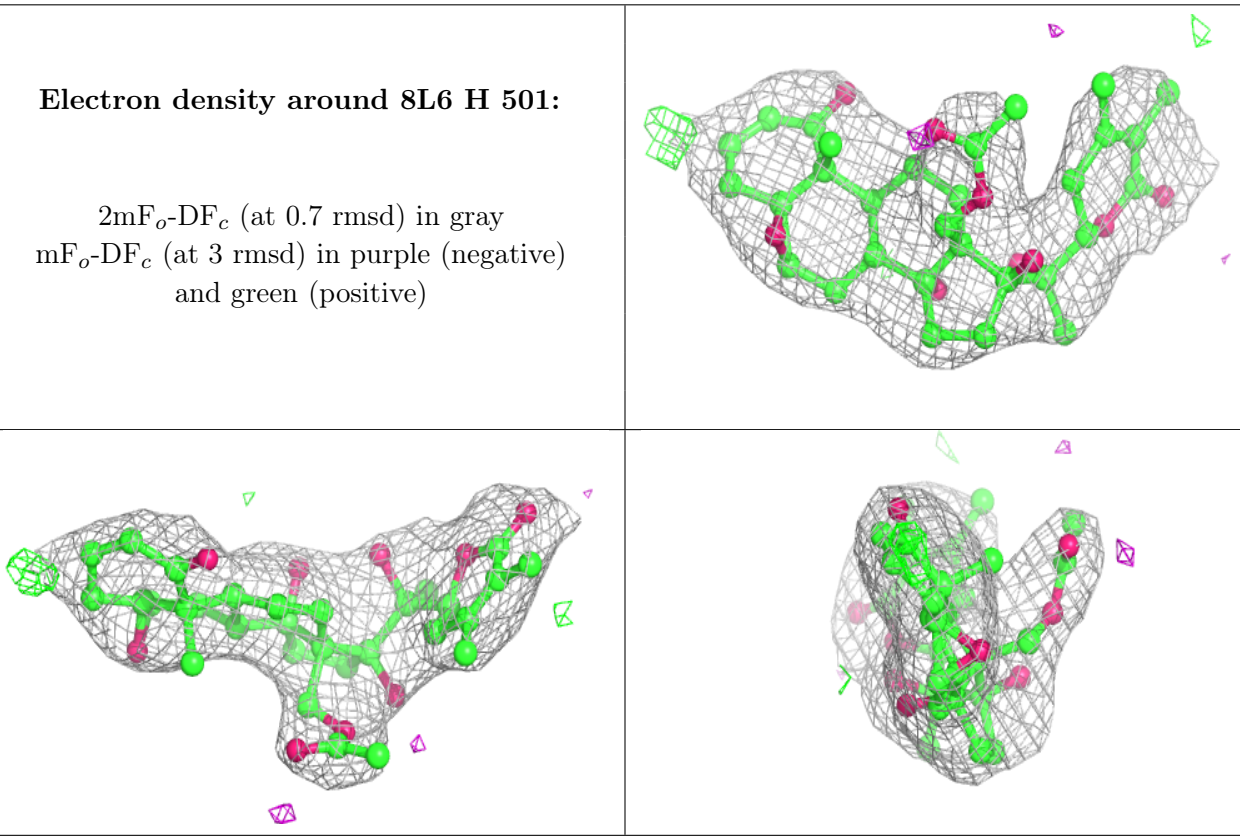
Electron density around 8L6 C 501:

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



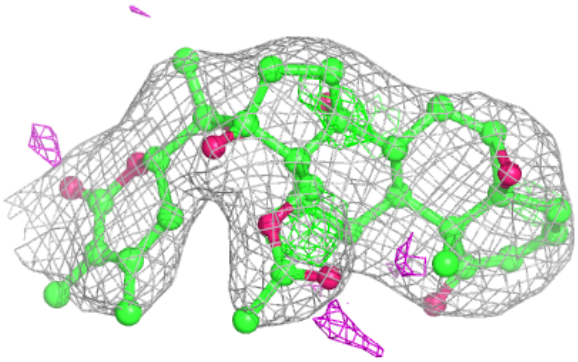
Electron density around 8L6 H 501:

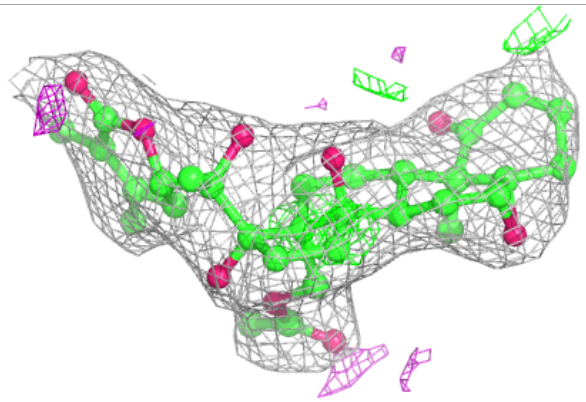
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

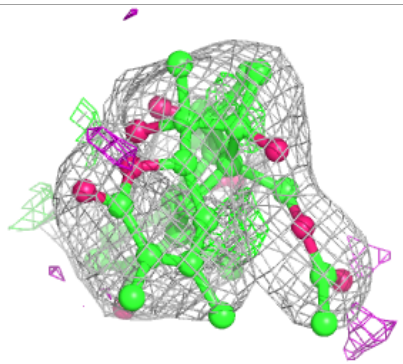


Electron density around 8L6 B 501:

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

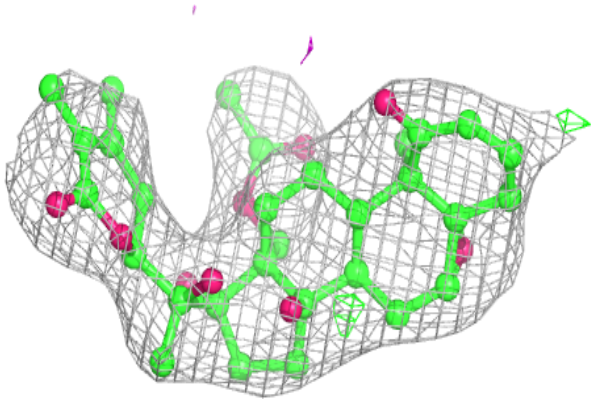


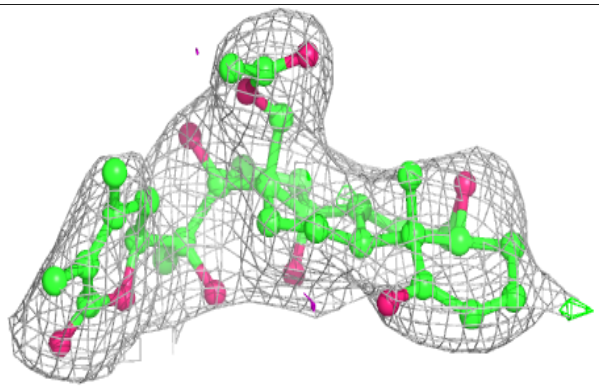


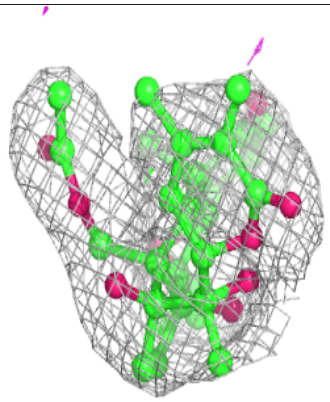


Electron density around 8L6 D 501:

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

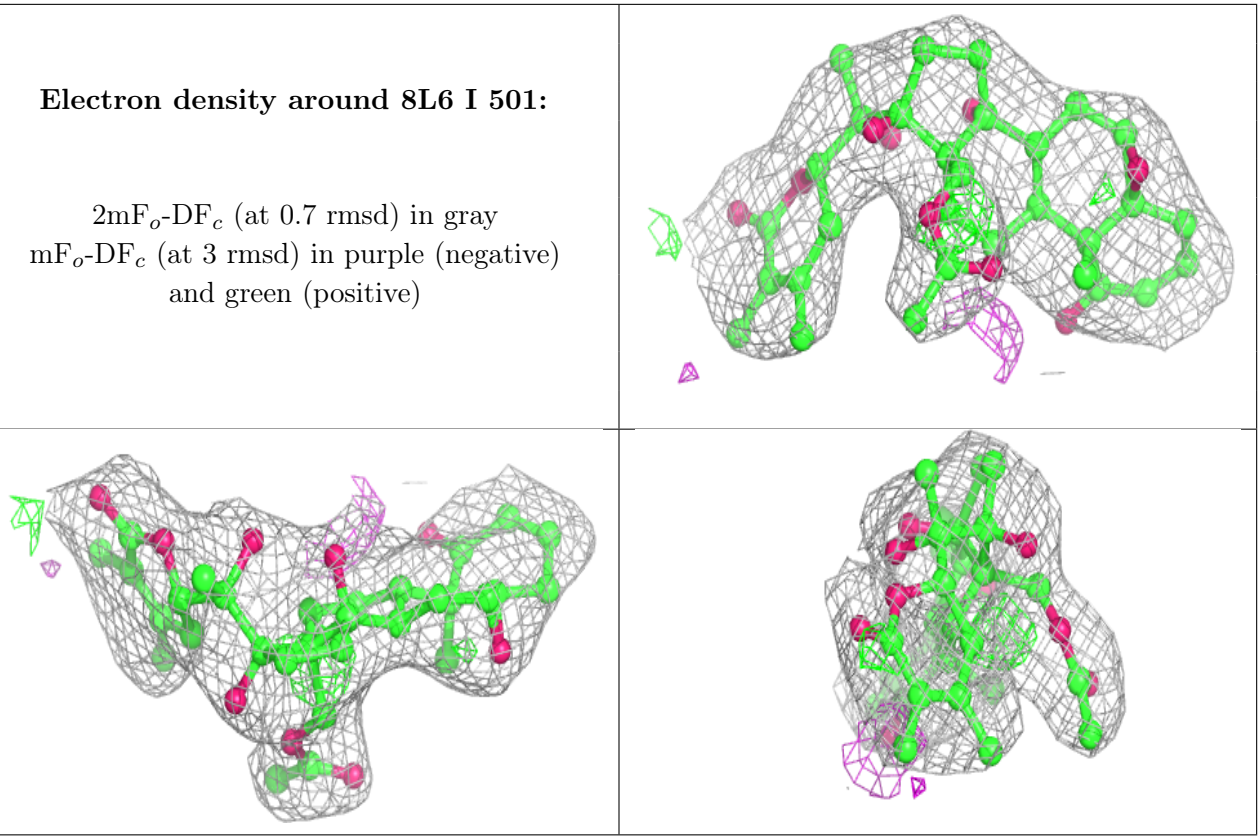






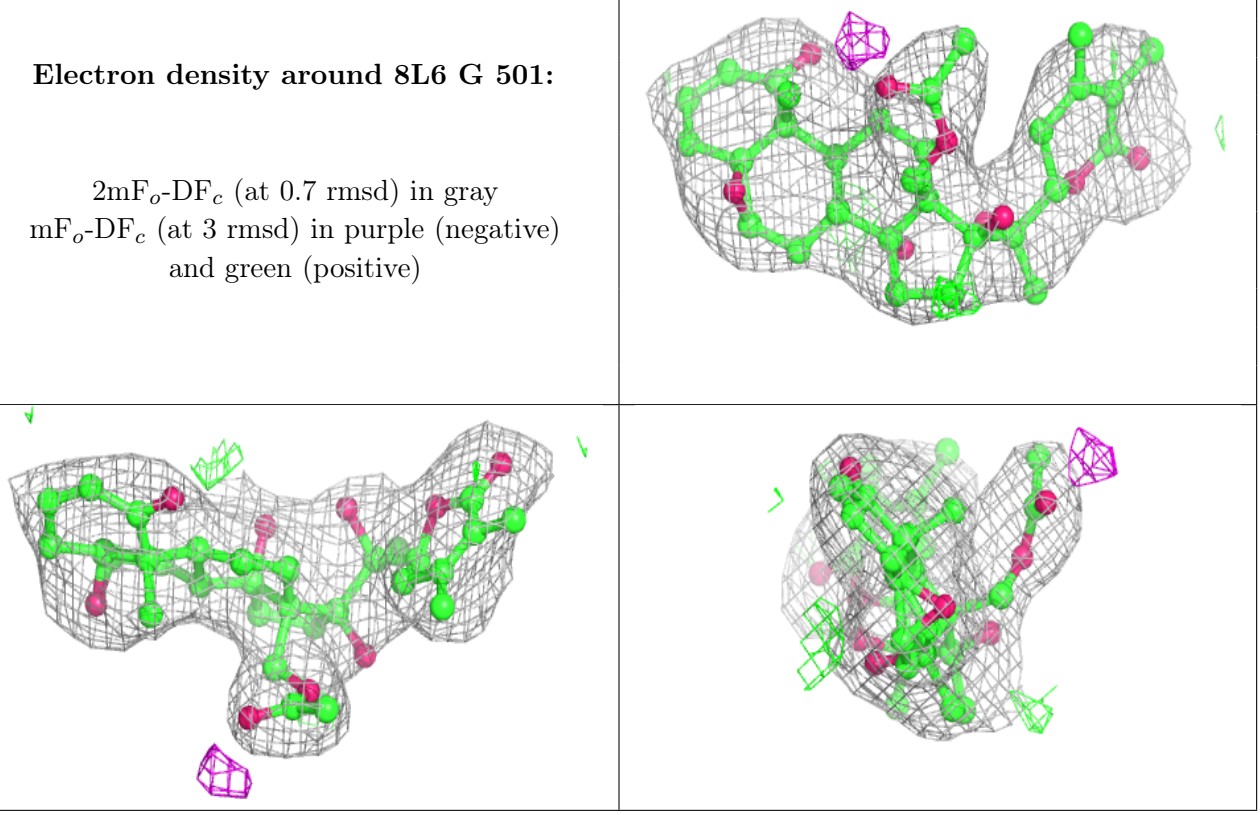
Electron density around 8L6 I 501:

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



Electron density around 8L6 G 501:

$2mF_o$-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.