



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 5UIS / pdb_00005uis
Title : Crystal structure of IRAK4 in complex with compound 12
Authors : Han, S.; Chang, J.S.
Deposited on : 2017-01-14
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

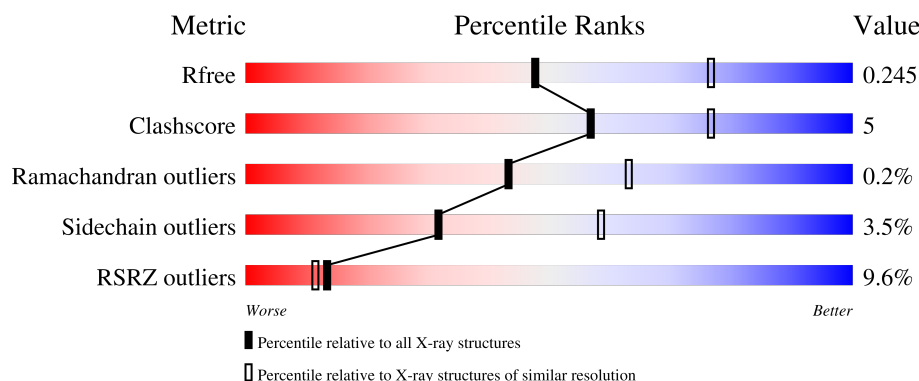
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	323	7% 70% 12% • 16%
1	B	323	8% 67% 17% • 15%
1	C	323	8% 70% 13% • 16%
1	D	323	8% 66% 12% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8743 atoms, of which 92 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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	P	S	0	0	0
			2124	1337	359	413	1	14			
1	B	275	Total	C	N	O	P	S	0	0	0
			2159	1360	365	419	1	14			
1	C	271	Total	C	N	O	P	S	0	1	0
			2146	1353	364	413	1	15			
1	D	251	Total	C	N	O	P	S	0	0	0
			1989	1259	335	380	1	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	initiating methionine	UNP Q9NWZ3
A	139	HIS	-	expression tag	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	HIS	-	expression tag	UNP Q9NWZ3
A	145	GLY	-	expression tag	UNP Q9NWZ3
A	146	GLY	-	expression tag	UNP Q9NWZ3
A	147	GLU	-	expression tag	UNP Q9NWZ3
A	148	ASN	-	expression tag	UNP Q9NWZ3
A	149	LEU	-	expression tag	UNP Q9NWZ3
A	150	TYR	-	expression tag	UNP Q9NWZ3
A	151	PHE	-	expression tag	UNP Q9NWZ3
A	152	GLN	-	expression tag	UNP Q9NWZ3
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	138	MET	-	initiating methionine	UNP Q9NWZ3
B	139	HIS	-	expression tag	UNP Q9NWZ3
B	140	HIS	-	expression tag	UNP Q9NWZ3
B	141	HIS	-	expression tag	UNP Q9NWZ3
B	142	HIS	-	expression tag	UNP Q9NWZ3

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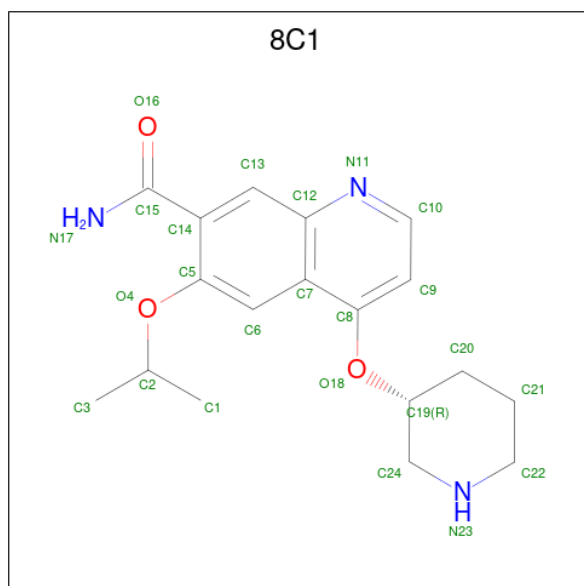
Chain	Residue	Modelled	Actual	Comment	Reference
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	HIS	-	expression tag	UNP Q9NWZ3
B	145	GLY	-	expression tag	UNP Q9NWZ3
B	146	GLY	-	expression tag	UNP Q9NWZ3
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3
B	149	LEU	-	expression tag	UNP Q9NWZ3
B	150	TYR	-	expression tag	UNP Q9NWZ3
B	151	PHE	-	expression tag	UNP Q9NWZ3
B	152	GLN	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3
C	138	MET	-	initiating methionine	UNP Q9NWZ3
C	139	HIS	-	expression tag	UNP Q9NWZ3
C	140	HIS	-	expression tag	UNP Q9NWZ3
C	141	HIS	-	expression tag	UNP Q9NWZ3
C	142	HIS	-	expression tag	UNP Q9NWZ3
C	143	HIS	-	expression tag	UNP Q9NWZ3
C	144	HIS	-	expression tag	UNP Q9NWZ3
C	145	GLY	-	expression tag	UNP Q9NWZ3
C	146	GLY	-	expression tag	UNP Q9NWZ3
C	147	GLU	-	expression tag	UNP Q9NWZ3
C	148	ASN	-	expression tag	UNP Q9NWZ3
C	149	LEU	-	expression tag	UNP Q9NWZ3
C	150	TYR	-	expression tag	UNP Q9NWZ3
C	151	PHE	-	expression tag	UNP Q9NWZ3
C	152	GLN	-	expression tag	UNP Q9NWZ3
C	153	GLY	-	expression tag	UNP Q9NWZ3
D	138	MET	-	initiating methionine	UNP Q9NWZ3
D	139	HIS	-	expression tag	UNP Q9NWZ3
D	140	HIS	-	expression tag	UNP Q9NWZ3
D	141	HIS	-	expression tag	UNP Q9NWZ3
D	142	HIS	-	expression tag	UNP Q9NWZ3
D	143	HIS	-	expression tag	UNP Q9NWZ3
D	144	HIS	-	expression tag	UNP Q9NWZ3
D	145	GLY	-	expression tag	UNP Q9NWZ3
D	146	GLY	-	expression tag	UNP Q9NWZ3
D	147	GLU	-	expression tag	UNP Q9NWZ3
D	148	ASN	-	expression tag	UNP Q9NWZ3
D	149	LEU	-	expression tag	UNP Q9NWZ3
D	150	TYR	-	expression tag	UNP Q9NWZ3
D	151	PHE	-	expression tag	UNP Q9NWZ3
D	152	GLN	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 4-[[[(3R)-piperidin-3-yl]oxy}-6-[(propan-2-yl)oxy]quinoline-7-carboxamide (CCD ID: 8C1) (formula: C₁₈H₂₃N₃O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			47	18	23	3	3		
2	B	1	Total	C	H	N	O	0	0
			47	18	23	3	3		
2	C	1	Total	C	H	N	O	0	0
			47	18	23	3	3		
2	D	1	Total	C	H	N	O	0	0
			47	18	23	3	3		

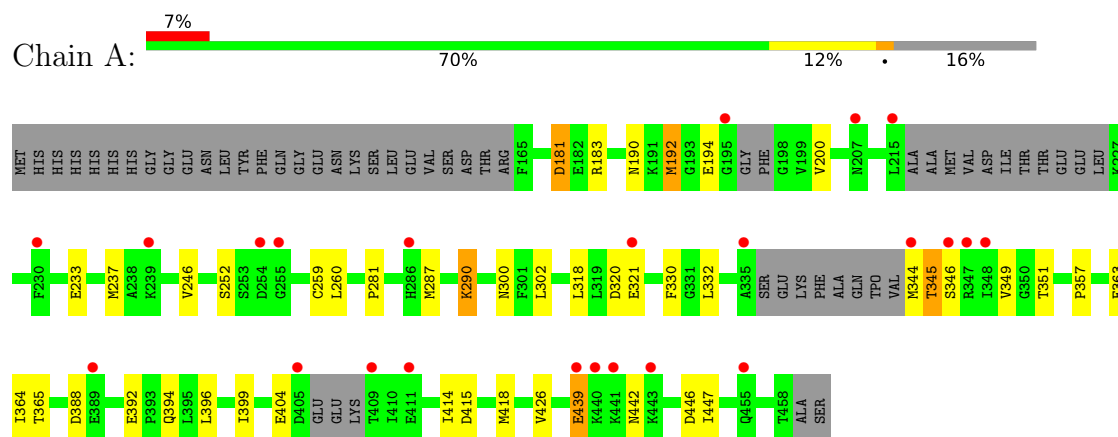
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	36	Total	O	0	0
			36	36		
3	C	38	Total	O	0	0
			38	38		
3	D	29	Total	O	0	0
			29	29		

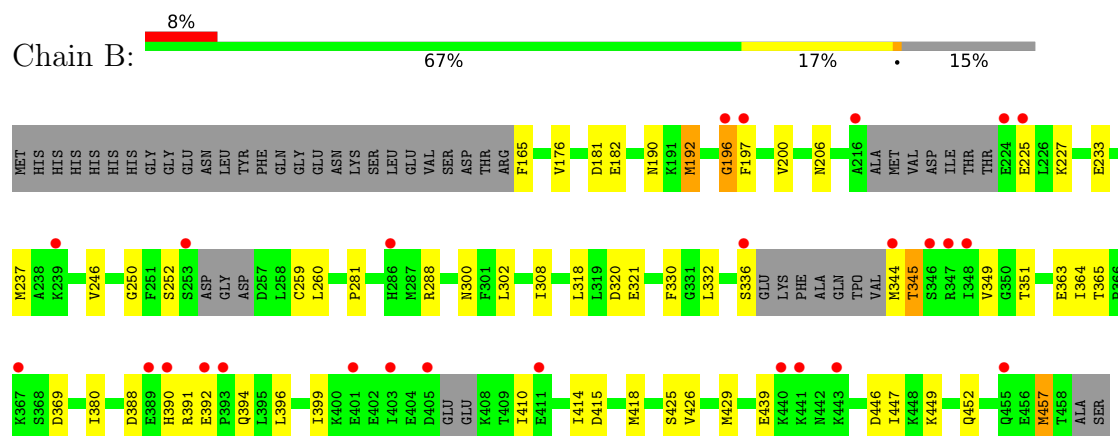
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

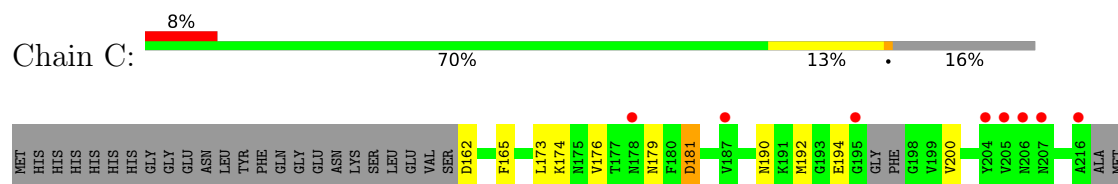
- Molecule 1: Interleukin-1 receptor-associated kinase 4

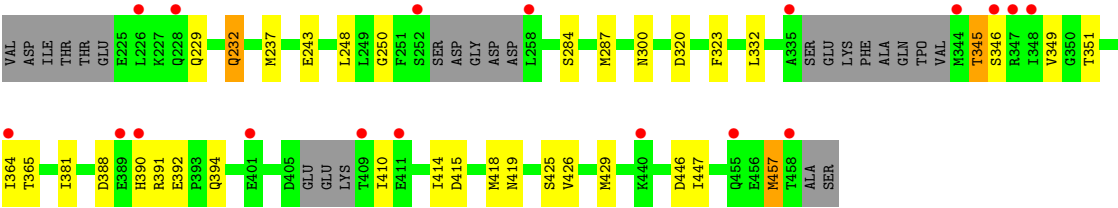


- Molecule 1: Interleukin-1 receptor-associated kinase 4

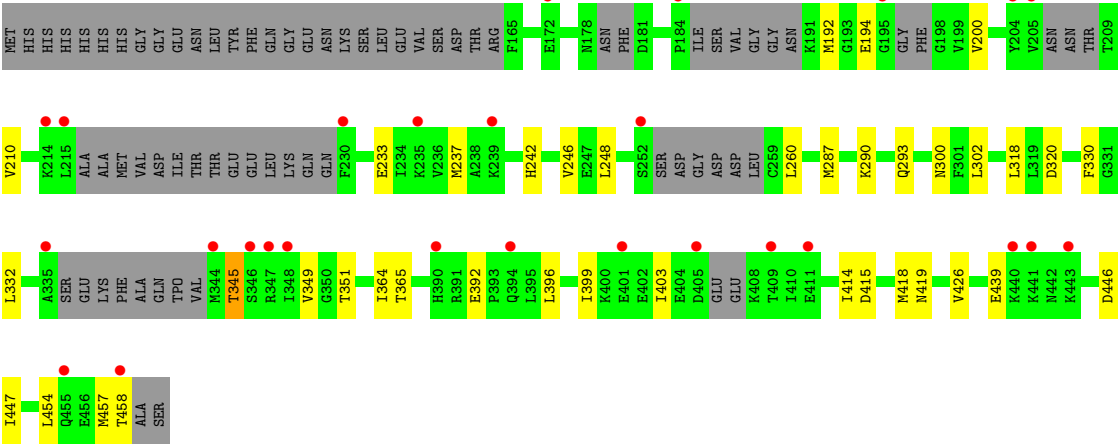


- Molecule 1: Interleukin-1 receptor-associated kinase 4





● Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.14Å 141.13Å 87.44Å 90.00° 124.72° 90.00°	Depositor
Resolution (Å)	25.36 – 2.50 25.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.36-2.50) 99.4 (25.36-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.234 , 0.250 0.227 , 0.245	Depositor DCC
R_{free} test set	2517 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.098 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8743	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8C1, TPO

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	0.81	1/2146 (0.0%)	1.36	6/2888 (0.2%)
1	B	0.81	2/2181 (0.1%)	1.33	6/2934 (0.2%)
1	C	0.81	1/2167 (0.0%)	1.33	11/2914 (0.4%)
1	D	0.79	0/2006	1.34	9/2691 (0.3%)
All	All	0.81	4/8500 (0.0%)	1.34	32/11427 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	MET	SD-CE	-7.68	1.60	1.79
1	C	457	MET	SD-CE	-7.40	1.61	1.79
1	A	192	MET	SD-CE	-6.49	1.63	1.79
1	B	457	MET	SD-CE	-5.00	1.67	1.79

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	HIS	CA-C-N	7.29	131.03	120.38
1	D	242	HIS	C-N-CA	7.29	131.03	120.38
1	B	369	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	181	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	446	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	351	THR	CA-C-N	5.69	129.36	120.82
1	A	351	THR	C-N-CA	5.69	129.36	120.82
1	B	351	THR	CA-C-N	5.65	129.30	120.82
1	B	351	THR	C-N-CA	5.65	129.30	120.82
1	B	388	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	351	THR	CA-C-N	5.51	129.09	120.82
1	D	351	THR	C-N-CA	5.51	129.09	120.82
1	C	351	THR	CA-C-N	5.48	129.04	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	351	THR	C-N-CA	5.48	129.04	120.82
1	A	388	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	446	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	446	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	446	ASP	CA-CB-CG	5.34	117.94	112.60
1	C	388	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	320	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	419	ASN	CA-CB-CG	5.24	117.84	112.60
1	C	419	ASN	CA-CB-CG	5.18	117.78	112.60
1	D	320	ASP	CA-CB-CG	5.16	117.75	112.60
1	C	229	GLN	CA-C-N	5.14	127.44	120.44
1	C	229	GLN	C-N-CA	5.14	127.44	120.44
1	C	320	ASP	CA-C-N	5.13	127.87	120.38
1	C	320	ASP	C-N-CA	5.13	127.87	120.38
1	C	232	GLN	CA-CB-CG	-5.13	103.85	114.10
1	C	181	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	320	ASP	CA-C-N	5.10	127.82	120.38
1	D	320	ASP	C-N-CA	5.10	127.82	120.38
1	A	320	ASP	CA-CB-CG	5.05	117.65	112.60

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	2124	0	2095	19	0
1	B	2159	0	2135	27	0
1	C	2146	0	2128	20	0
1	D	1989	0	1979	15	0
2	A	24	23	0	0	0
2	B	24	23	0	0	0
2	C	24	23	0	0	0
2	D	24	23	0	0	0
3	A	34	0	0	0	0
3	B	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	38	0	0	0	0
3	D	29	0	0	0	0
All	All	8651	92	8337	77	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 5.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:HG3	1:B:281:PRO:HD3	1.64	0.79
1:C:284:SER:H	1:C:287[B]:MET:HE3	1.45	0.77
1:B:192:MET:HE3	1:B:200:VAL:HG12	1.72	0.70
1:B:196:GLY:H	1:B:197:PHE:HA	1.55	0.70
1:D:192:MET:HE3	1:D:200:VAL:HG12	1.74	0.70
1:C:192:MET:HE3	1:C:200:VAL:HG12	1.75	0.68
1:A:192:MET:HE3	1:A:200:VAL:HG12	1.74	0.68
1:D:246:VAL:HG11	1:D:318:LEU:HD12	1.78	0.65
1:B:196:GLY:N	1:B:197:PHE:HA	2.13	0.64
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.80	0.64
1:C:237:MET:HG2	1:C:248:LEU:HB2	1.81	0.62
1:B:429:MET:HE3	1:B:457:MET:HE1	1.80	0.62
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.84	0.60
1:D:399:ILE:O	1:D:403:ILE:HG12	2.01	0.60
1:B:390:HIS:O	1:C:391:ARG:HA	2.02	0.59
1:B:391:ARG:HA	1:C:390:HIS:O	2.03	0.59
1:C:237:MET:HG2	1:C:248:LEU:CB	2.35	0.56
1:D:293:GLN:HE22	1:D:458:THR:HB	1.71	0.56
1:A:237:MET:HA	1:A:237:MET:HE2	1.89	0.54
1:C:429:MET:HE3	1:C:457:MET:HE1	1.89	0.54
1:A:357:PRO:HG3	1:A:439:GLU:HG3	1.90	0.53
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.90	0.53
1:D:237:MET:HG2	1:D:248:LEU:HB2	1.92	0.52
1:C:381:ILE:HG21	1:C:410:ILE:HD11	1.92	0.51
1:C:181:ASP:HB3	1:C:190:ASN:HD22	1.75	0.51
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.92	0.51
1:B:415:ASP:HB3	1:B:418:MET:HE2	1.93	0.51
1:D:414:ILE:HG12	1:D:426:VAL:HG11	1.93	0.50
1:A:233:GLU:HG2	1:A:260:LEU:HD13	1.93	0.49
1:B:165:PHE:HB3	1:B:250:GLY:HA2	1.94	0.49
1:C:287[A]:MET:HE2	1:C:323:PHE:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.95	0.49
1:A:181:ASP:HB3	1:A:190:ASN:HD22	1.77	0.49
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.94	0.49
1:A:344:MET:HE2	1:A:363:GLU:HG2	1.95	0.49
1:B:344:MET:HE2	1:B:363:GLU:HG2	1.94	0.48
1:D:415:ASP:HB3	1:D:418:MET:HE2	1.95	0.48
1:B:332:LEU:HD22	1:B:349:VAL:HG21	1.97	0.47
1:C:165:PHE:HB3	1:C:250:GLY:HA2	1.96	0.47
1:A:281:PRO:HD3	1:B:321:GLU:HG3	1.97	0.47
1:C:173:LEU:HA	1:C:176:VAL:HG22	1.95	0.47
1:D:237:MET:HG2	1:D:248:LEU:CB	2.45	0.46
1:B:302:LEU:HD11	1:B:330:PHE:HE1	1.80	0.46
1:D:332:LEU:HD22	1:D:349:VAL:HG21	1.98	0.46
1:A:332:LEU:HD22	1:A:349:VAL:HG21	1.97	0.45
1:A:302:LEU:HD11	1:A:330:PHE:HE1	1.81	0.45
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.98	0.45
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.99	0.44
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.99	0.44
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.99	0.44
1:C:174:LYS:HG2	1:C:179:ASN:HA	2.00	0.44
1:B:396:LEU:O	1:B:399:ILE:HG12	2.18	0.44
1:A:414:ILE:HG12	1:A:426:VAL:HG11	2.00	0.44
1:C:425:SER:O	1:C:457:MET:HE3	2.17	0.44
1:B:181:ASP:HB3	1:B:190:ASN:HD22	1.82	0.43
1:C:414:ILE:HG12	1:C:426:VAL:HG11	1.99	0.43
1:C:300:ASN:HA	1:C:447:ILE:HG21	2.01	0.43
1:D:233:GLU:HG2	1:D:260:LEU:HD13	2.01	0.43
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.00	0.43
1:D:396:LEU:O	1:D:399:ILE:HG12	2.19	0.43
1:A:396:LEU:O	1:A:399:ILE:HG12	2.19	0.43
1:A:287:MET:CE	1:A:290:LYS:HD2	2.48	0.43
1:C:287[A]:MET:HE2	1:C:323:PHE:CB	2.49	0.42
1:B:425:SER:O	1:B:457:MET:HE3	2.19	0.42
1:B:345:TPO:HB	1:B:364:ILE:HD11	2.01	0.42
1:B:410:ILE:O	1:B:414:ILE:HG13	2.20	0.42
1:C:345:TPO:HB	1:C:364:ILE:HD11	2.02	0.42
1:D:345:TPO:HB	1:D:364:ILE:HD11	2.02	0.42
1:A:181:ASP:OD1	1:A:183:ARG:HD3	2.19	0.42
1:D:454:LEU:O	1:D:457:MET:HG2	2.20	0.42
1:B:288:ARG:HB3	1:B:380:ILE:HG23	2.01	0.42
1:D:302:LEU:HD11	1:D:330:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:LEU:HD22	1:C:349:VAL:HG21	2.02	0.41
1:B:237:MET:HA	1:B:237:MET:HE2	2.02	0.41
1:B:449:LYS:HA	1:B:452:GLN:HG2	2.03	0.41
1:A:345:TPO:HB	1:A:364:ILE:HD11	2.02	0.41
1:B:308:ILE:HD11	1:B:336:SER:HB3	2.02	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	259/323 (80%)	249 (96%)	9 (4%)	1 (0%)	30	49
1	B	264/323 (82%)	256 (97%)	7 (3%)	1 (0%)	30	49
1	C	259/323 (80%)	252 (97%)	7 (3%)	0	100	100
1	D	232/323 (72%)	227 (98%)	5 (2%)	0	100	100
All	All	1014/1292 (78%)	984 (97%)	28 (3%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	GLU
1	B	196	GLY

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	234/279 (84%)	226 (97%)	8 (3%)	32	60
1	B	237/279 (85%)	228 (96%)	9 (4%)	29	56
1	C	236/279 (85%)	228 (97%)	8 (3%)	32	60
1	D	219/279 (78%)	212 (97%)	7 (3%)	34	62
All	All	926/1116 (83%)	894 (96%)	32 (4%)	32	58

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	290	LYS
1	A	346	SER
1	A	365	THR
1	A	392	GLU
1	A	394	GLN
1	A	439	GLU
1	A	442	ASN
1	B	176	VAL
1	B	182	GLU
1	B	206	ASN
1	B	225	GLU
1	B	227	LYS
1	B	365	THR
1	B	392	GLU
1	B	394	GLN
1	B	439	GLU
1	C	162	ASP
1	C	194	GLU
1	C	232	GLN
1	C	243	GLU
1	C	346	SER
1	C	365	THR
1	C	392	GLU
1	C	394	GLN
1	D	194	GLU
1	D	210	VAL
1	D	287	MET
1	D	290	LYS
1	D	365	THR
1	D	392	GLU

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Mol	Chain	Res	Type
1	D	439	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	206	ASN
1	A	207	ASN
1	A	419	ASN
1	B	190	ASN
1	B	207	ASN
1	B	390	HIS
1	B	394	GLN
1	B	442	ASN
1	C	190	ASN
1	D	175	ASN
1	D	232	GLN
1	D	293	GLN
1	D	297	ASN
1	D	390	HIS
1	D	419	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	345	1	8,10,11	1.11	0	10,14,16	1.25	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	B	345	1	8,10,11	1.40	1 (12%)	10,14,16	1.41	3 (30%)
1	TPO	C	345	1	8,10,11	1.25	0	10,14,16	1.17	1 (10%)
1	TPO	D	345	1	8,10,11	1.17	0	10,14,16	1.35	1 (10%)

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
1	TPO	A	345	1	-	2/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	C	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	P-OG1	-2.90	1.54	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	TPO	O2P-P-OG1	2.93	117.26	105.85
1	A	345	TPO	O2P-P-OG1	2.85	116.94	105.85
1	B	345	TPO	P-OG1-CB	-2.36	116.91	123.33
1	B	345	TPO	O2P-P-OG1	2.36	115.05	105.85
1	C	345	TPO	OG1-P-O1P	2.26	117.38	109.33
1	B	345	TPO	CG2-CB-CA	2.03	117.22	113.26

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O1P

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	345	TPO	1	0
1	B	345	TPO	1	0
1	C	345	TPO	1	0
1	D	345	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
2	8C1	B	801	-	25,26,26	0.35	0	32,36,36	0.85	2 (6%)
2	8C1	A	800	-	25,26,26	0.26	0	32,36,36	0.88	1 (3%)
2	8C1	D	501	-	25,26,26	0.30	0	32,36,36	0.82	1 (3%)
2	8C1	C	501	-	25,26,26	0.33	0	32,36,36	1.00	1 (3%)

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	8C1	B	801	-	-	0/12/32/32	0/3/3/3
2	8C1	A	800	-	-	0/12/32/32	0/3/3/3
2	8C1	D	501	-	-	0/12/32/32	0/3/3/3
2	8C1	C	501	-	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	8C1	C8-O18-C19	4.08	125.53	119.11
2	A	800	8C1	C8-O18-C19	2.78	123.49	119.11
2	D	501	8C1	C8-O18-C19	2.56	123.14	119.11
2	B	801	8C1	C8-O18-C19	2.51	123.06	119.11
2	B	801	8C1	C5-O4-C2	2.06	123.33	119.53

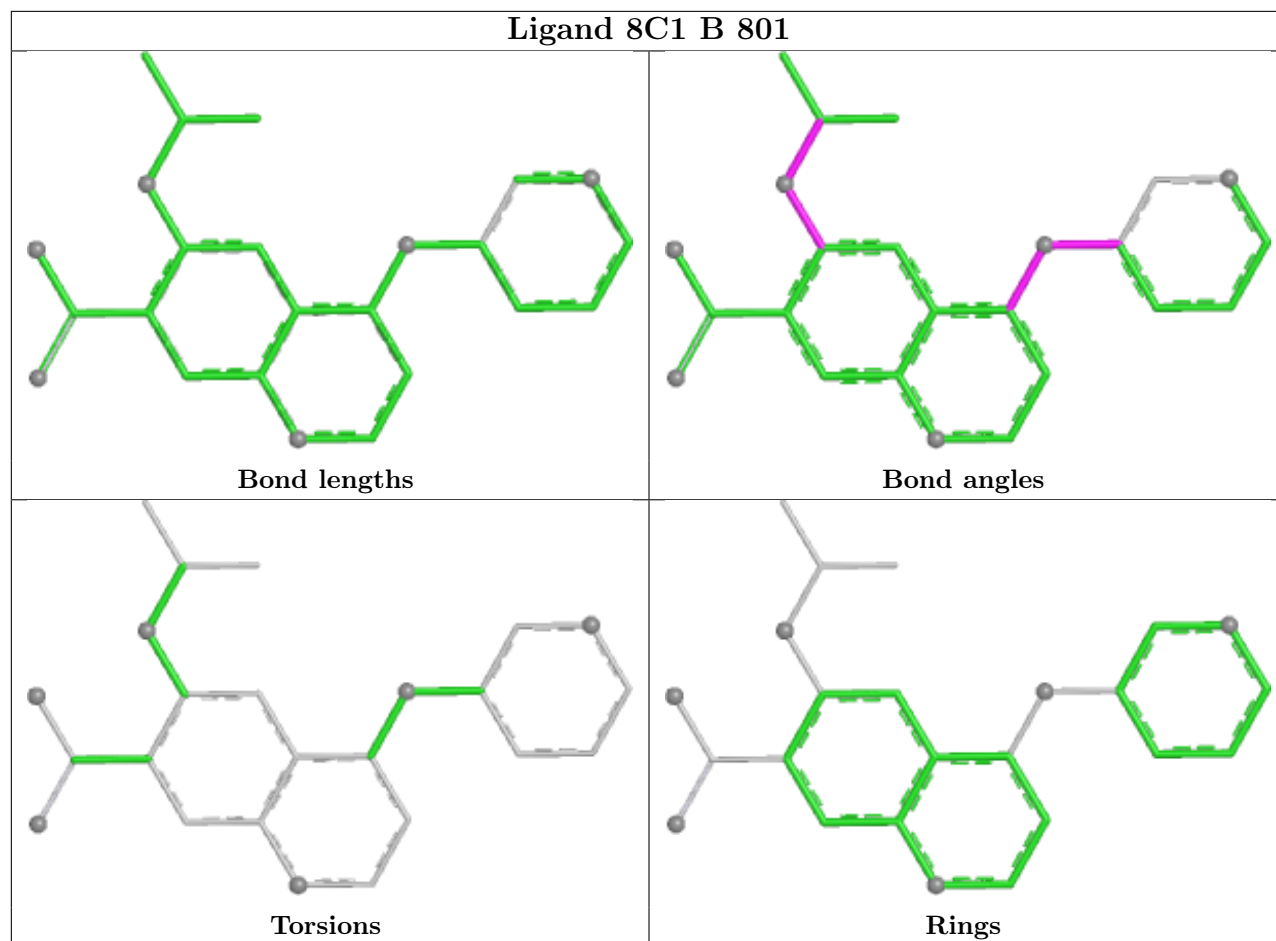
There are no chirality outliers.

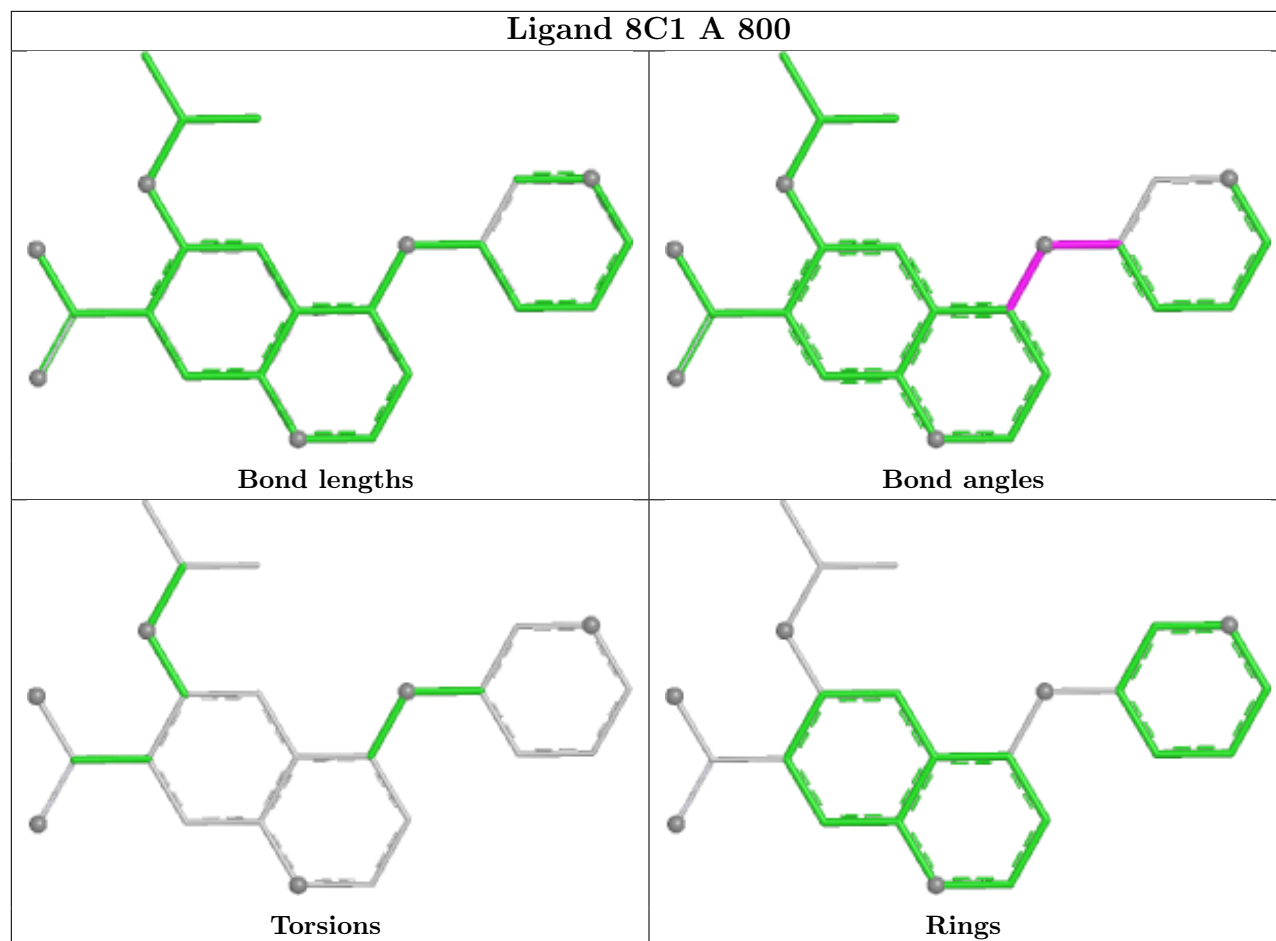
There are no torsion outliers.

There are no ring outliers.

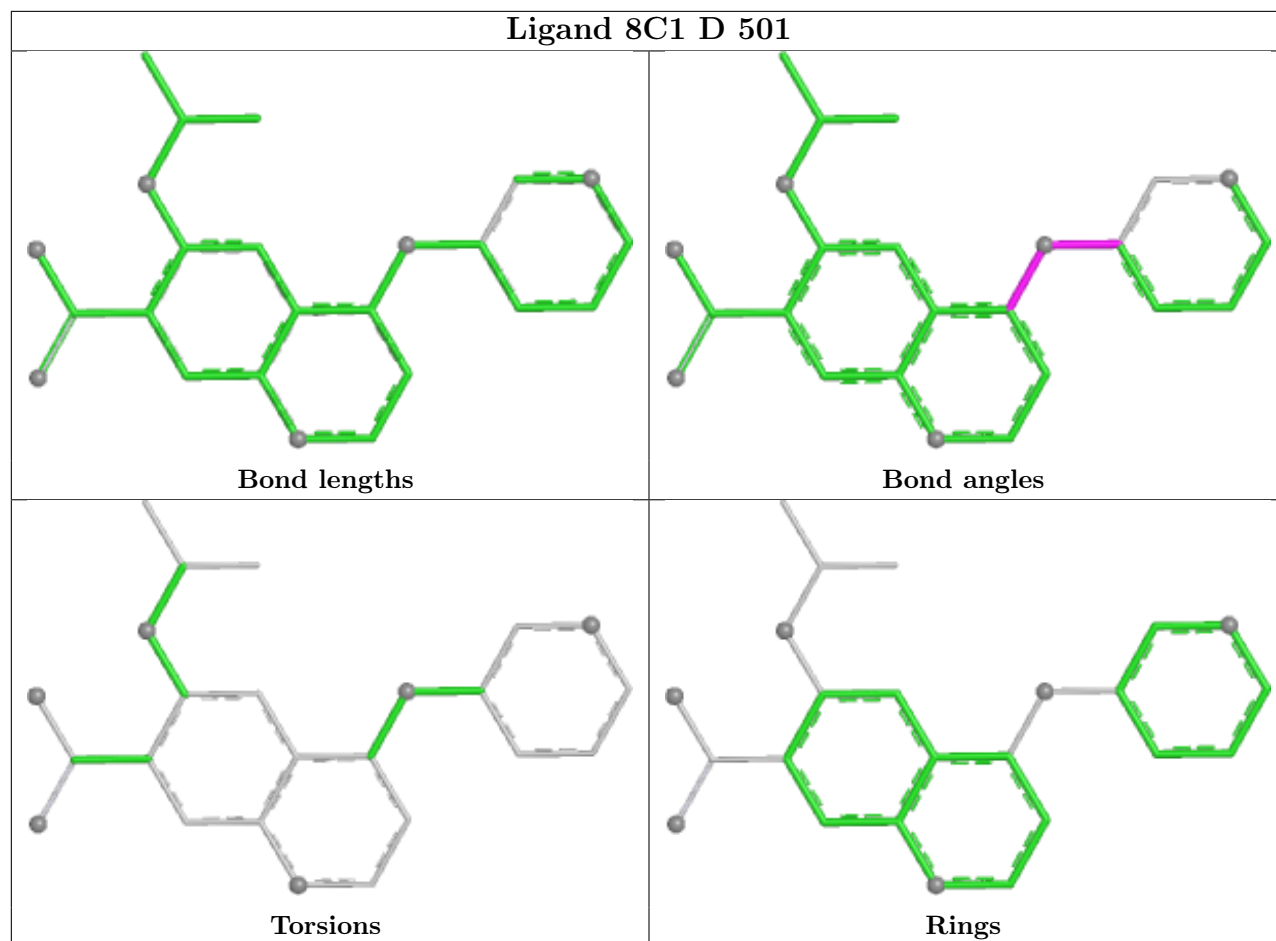
No monomer is involved in short contacts.

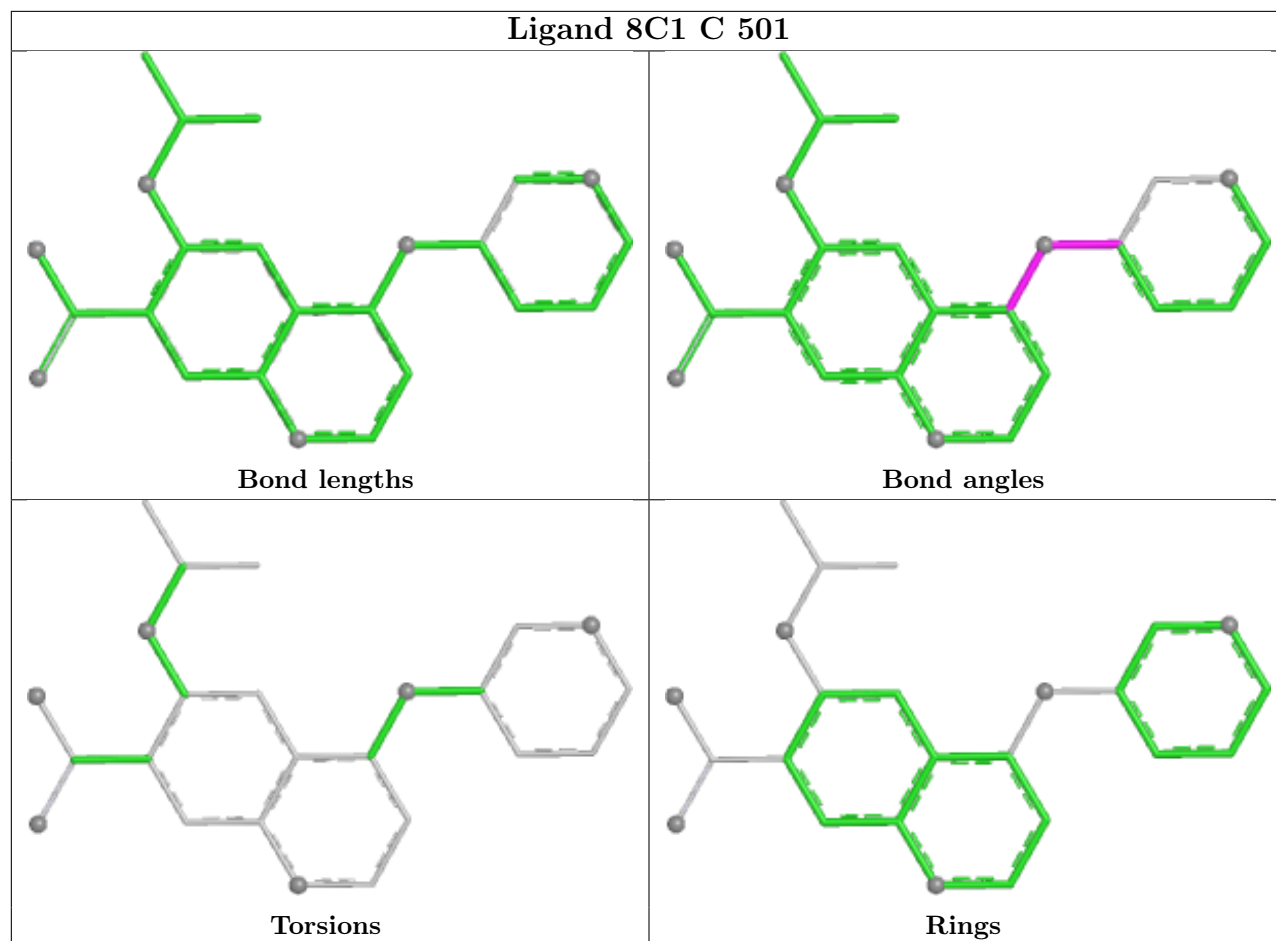
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand 8C1 D 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, 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	269/323 (83%)	0.35	23 (8%)	16 14	29, 47, 71, 90	18 (6%)
1	B	274/323 (84%)	0.44	26 (9%)	14 12	30, 49, 72, 97	18 (6%)
1	C	270/323 (83%)	0.47	26 (9%)	13 11	18, 49, 82, 111	18 (6%)
1	D	250/323 (77%)	0.55	27 (10%)	11 9	30, 49, 82, 98	18 (7%)
All	All	1063/1292 (82%)	0.45	102 (9%)	13 11	18, 48, 78, 111	72 (6%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	GLY	5.2
1	C	344	MET	4.7
1	A	344	MET	4.6
1	A	195	GLY	4.5
1	A	335	ALA	4.5
1	D	252	SER	4.3
1	D	347	ARG	4.3
1	C	195	GLY	4.3
1	B	344	MET	4.2
1	D	205	VAL	4.2
1	D	204	TYR	4.0
1	B	443	LYS	3.9
1	D	344	MET	3.8
1	B	390	HIS	3.6
1	A	348	ILE	3.6
1	A	455	GLN	3.6
1	A	347	ARG	3.6
1	C	347	ARG	3.5
1	B	455	GLN	3.5
1	A	346	SER	3.5
1	B	348	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	346	SER	3.4
1	B	401	GLU	3.3
1	C	348	ILE	3.3
1	A	207	ASN	3.3
1	D	239	LYS	3.3
1	C	411	GLU	3.3
1	B	253	SER	3.2
1	D	348	ILE	3.2
1	A	439	GLU	3.2
1	D	335	ALA	3.1
1	D	195	GLY	3.1
1	A	286	HIS	3.1
1	D	409	THR	3.1
1	B	346	SER	3.0
1	A	411	GLU	3.0
1	D	411	GLU	3.0
1	D	455	GLN	3.0
1	B	347	ARG	3.0
1	A	405	ASP	3.0
1	D	214	LYS	3.0
1	C	390	HIS	2.9
1	D	458	THR	2.8
1	C	335	ALA	2.8
1	C	389	GLU	2.8
1	C	206	ASN	2.8
1	C	440	LYS	2.7
1	D	440	LYS	2.7
1	A	409	THR	2.7
1	B	440	LYS	2.7
1	D	230	PHE	2.6
1	A	255	GLY	2.6
1	C	216	ALA	2.6
1	C	458	THR	2.6
1	C	205	VAL	2.5
1	B	216	ALA	2.5
1	D	184	PRO	2.5
1	C	401	GLU	2.5
1	D	401	GLU	2.5
1	C	258	LEU	2.5
1	A	443	LYS	2.5
1	D	441	LYS	2.5
1	D	346	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	215	LEU	2.4
1	C	207	ASN	2.4
1	B	225	GLU	2.4
1	D	443	LYS	2.4
1	B	403	ILE	2.4
1	B	393	PRO	2.4
1	A	230	PHE	2.4
1	B	441	LYS	2.4
1	B	367	LYS	2.3
1	C	252	SER	2.3
1	D	215	LEU	2.3
1	B	197	PHE	2.3
1	A	440	LYS	2.3
1	B	411	GLU	2.3
1	C	409	THR	2.2
1	C	226	LEU	2.2
1	C	178	ASN	2.2
1	B	336	SER	2.2
1	A	254	ASP	2.2
1	B	392	GLU	2.2
1	C	455	GLN	2.2
1	A	441	LYS	2.2
1	C	187	VAL	2.1
1	B	405	ASP	2.1
1	D	390	HIS	2.1
1	D	172	GLU	2.1
1	B	239	LYS	2.1
1	D	235	LYS	2.1
1	D	394	GLN	2.1
1	C	364	ILE	2.1
1	C	228	GLN	2.0
1	A	321	GLU	2.0
1	A	389	GLU	2.0
1	B	389	GLU	2.0
1	A	239	LYS	2.0
1	C	204	TYR	2.0
1	D	405	ASP	2.0
1	B	286	HIS	2.0
1	B	224	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	TPO	C	345	11/12	0.87	0.10	71,76,80,80	0
1	TPO	D	345	11/12	0.87	0.11	82,88,92,94	0
1	TPO	A	345	11/12	0.88	0.13	74,77,80,81	0
1	TPO	B	345	11/12	0.94	0.12	71,75,79,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

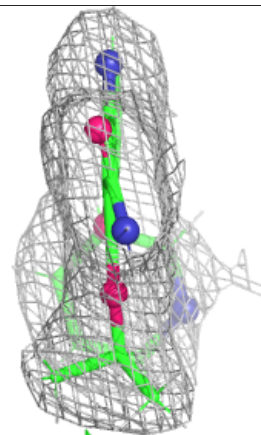
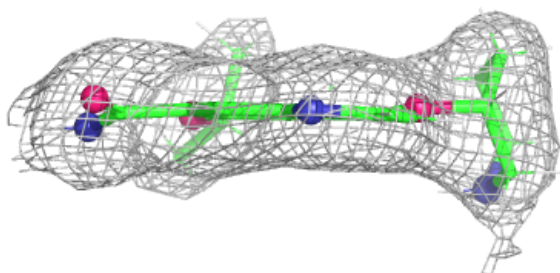
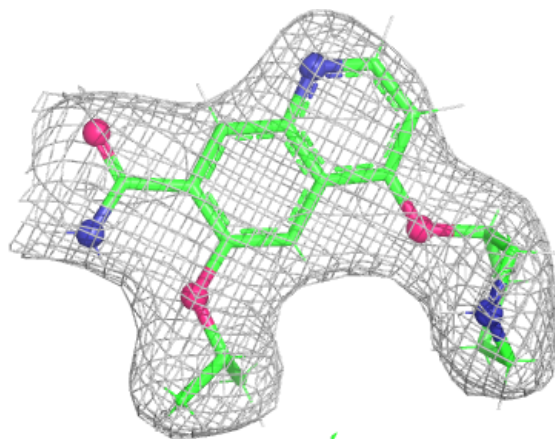
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8C1	D	501	24/24	0.93	0.07	42,45,52,53	0
2	8C1	C	501	24/24	0.94	0.07	36,40,47,47	0
2	8C1	A	800	24/24	0.95	0.07	31,36,41,43	0
2	8C1	B	801	24/24	0.95	0.07	39,43,47,48	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.

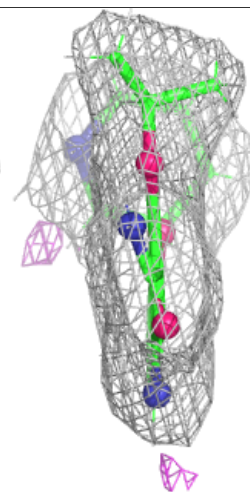
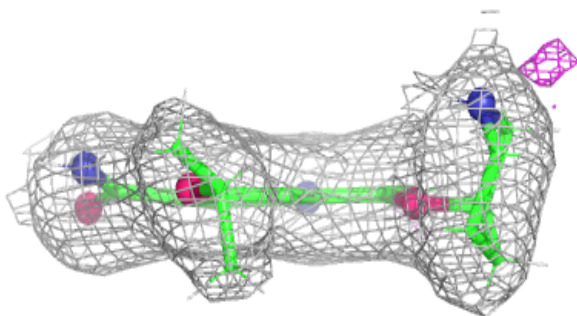
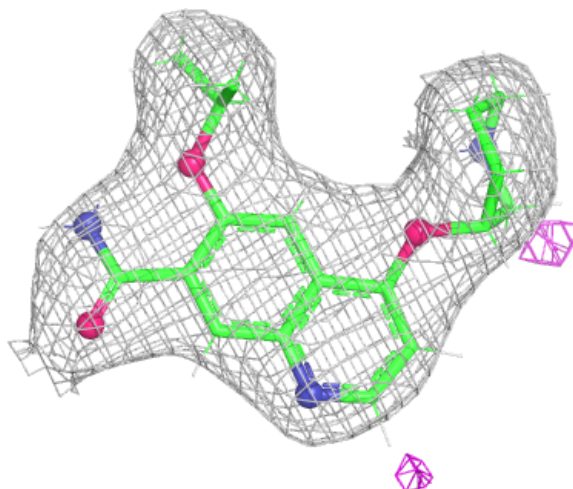
Electron density around 8C1 D 501:

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



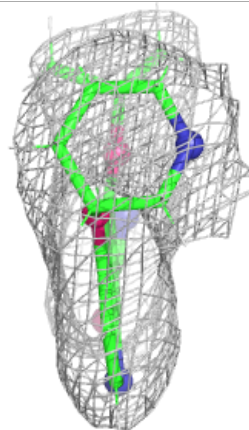
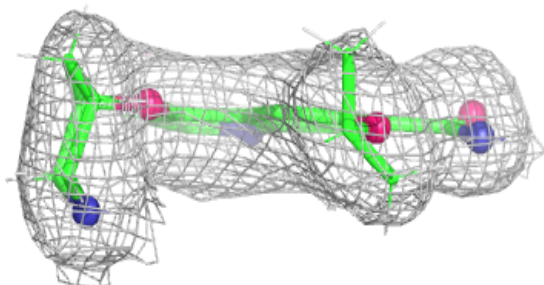
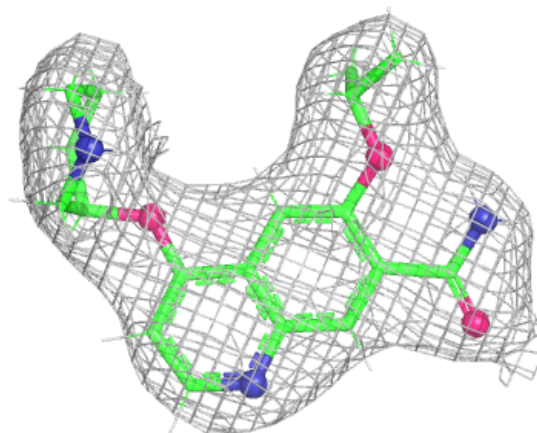
Electron density around 8C1 C 501:

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



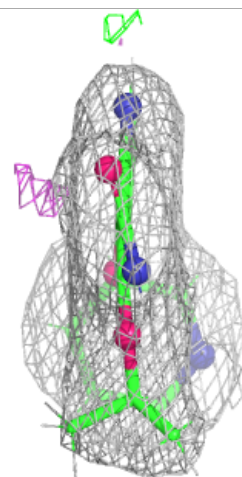
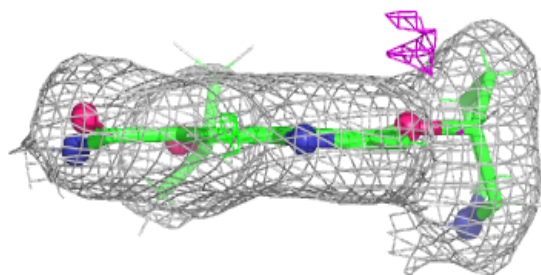
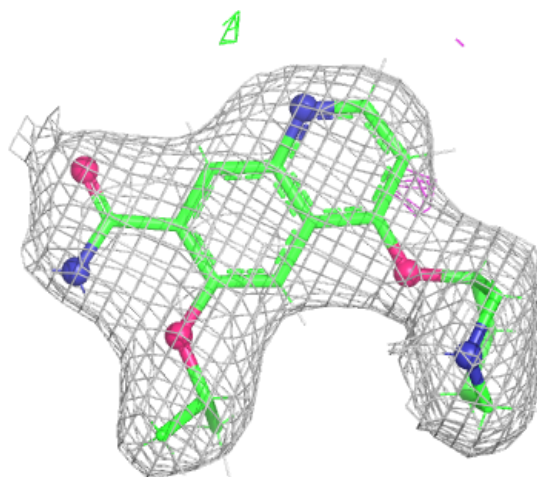
Electron density around 8C1 A 800:

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



Electron density around 8C1 B 801:

$2mF_o-DF_c$ (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.