



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:48 am BST

PDB ID : 4BGG
Title : Crystal structure of the ACVR1 kinase in complex with LDN-213844
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Deposited on : 2013-03-26
Resolution : 2.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

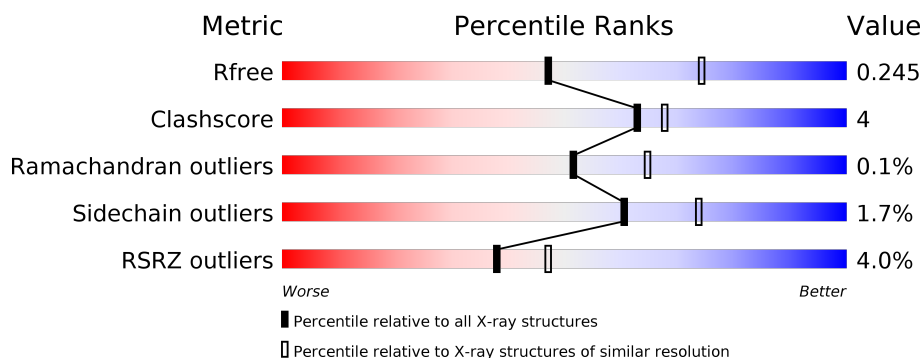
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	301	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> </div>
1	B	301	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div></div> </div> </div>
1	C	301	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>7%</div> </div> </div>
1	D	301	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>5%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	A	1001	-	-	X	-
3	FLC	B	1002	-	-	X	-
3	FLC	C	1001	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9291 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.

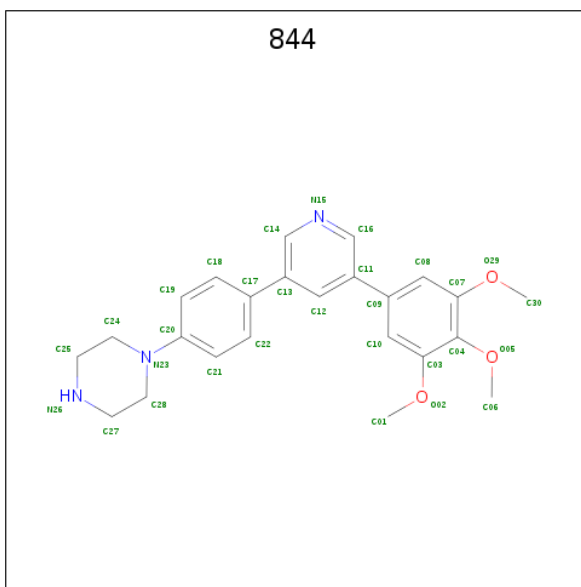
- Molecule 1 is a protein called ACTIVIN RECEPTOR TYPE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2312	1479	392	426	15			
1	B	293	Total	C	N	O	S	0	1	0
			2299	1469	392	423	15			
1	C	279	Total	C	N	O	S	0	2	0
			2112	1353	361	386	12			
1	D	286	Total	C	N	O	S	0	1	0
			2193	1404	374	401	14			

There are 12 discrepancies between the modelled and reference sequences:

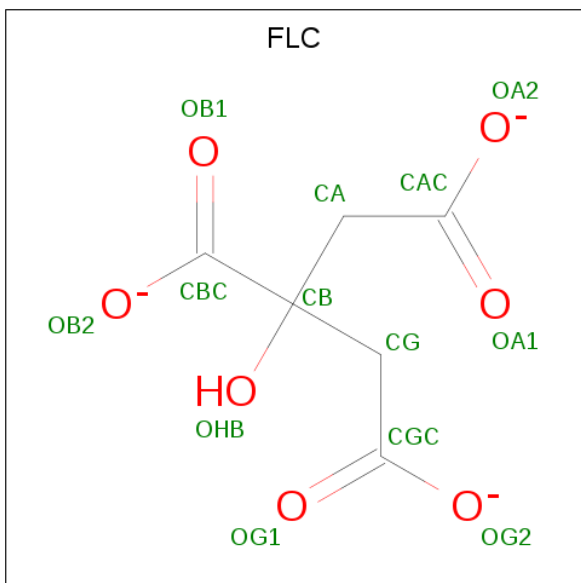
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771
C	199	SER	-	expression tag	UNP Q04771
C	200	MET	-	expression tag	UNP Q04771
C	207	ASP	GLN	engineered mutation	UNP Q04771
D	199	SER	-	expression tag	UNP Q04771
D	200	MET	-	expression tag	UNP Q04771
D	207	ASP	GLN	engineered mutation	UNP Q04771

- Molecule 2 is 1-{4-[5-(3,4,5-trimethoxyphenyl)pyridin-3-yl]phenyl}piperazine (three-letter code: 844) (formula: C₂₄H₂₇N₃O₃).



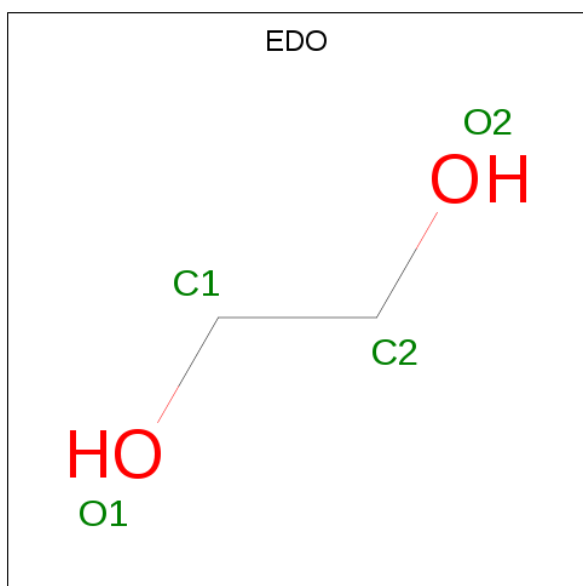
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	24	3	3		
2	B	1	Total	C	N	O	0	0
			30	24	3	3		
2	C	1	Total	C	N	O	0	0
			30	24	3	3		
2	D	1	Total	C	N	O	0	0
			30	24	3	3		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	60	Total	O	0	0
			60	60		

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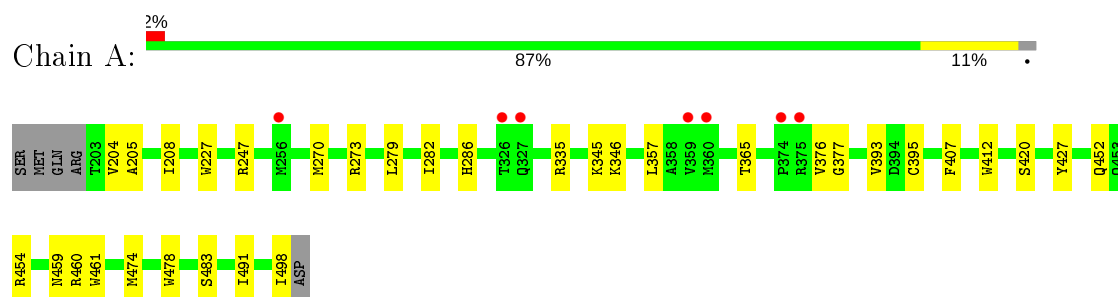
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	21	Total 21	O 21	0	0
5	C	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0
5	D	27	Total 27	O 27	0	0
5	D	1	Total 1	O 1	0	0

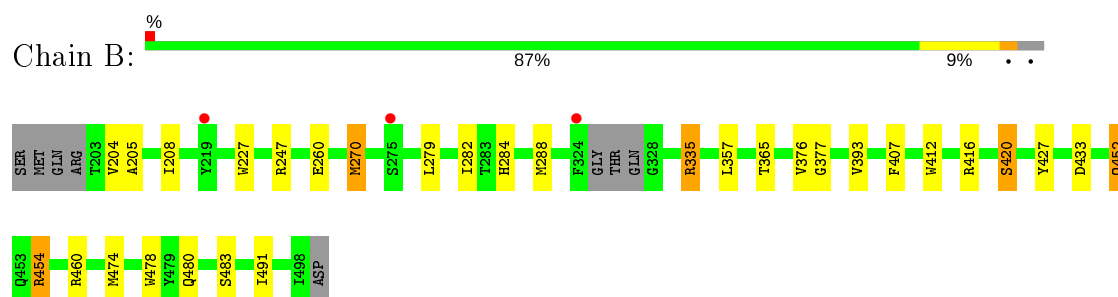
3 Residue-property plots [i](#)

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

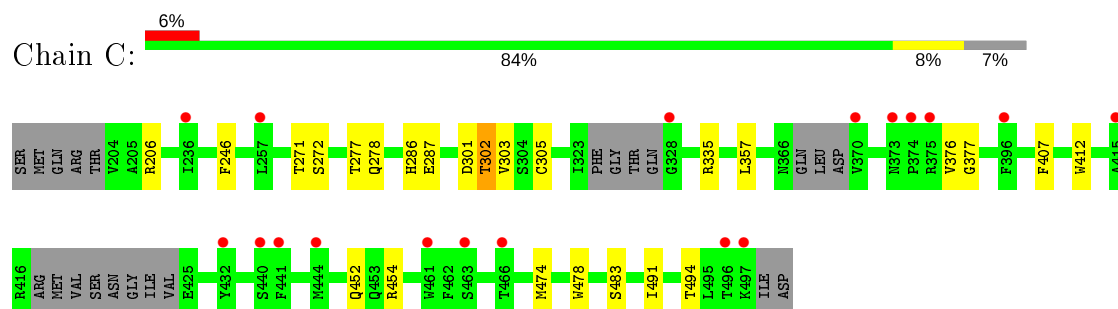
• Molecule 1: ACTIVIN RECEPTOR TYPE-1



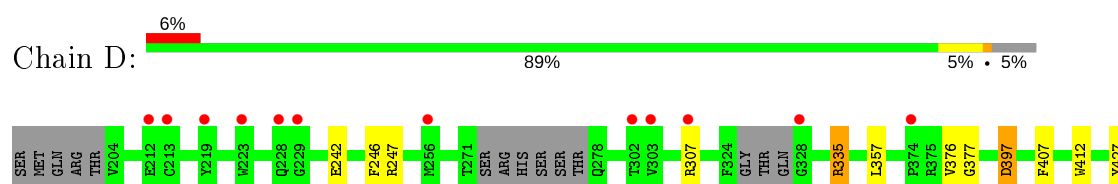
• Molecule 1: ACTIVIN RECEPTOR TYPE-1

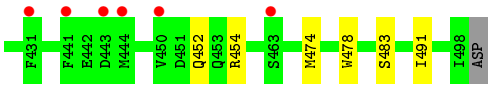


• Molecule 1: ACTIVIN RECEPTOR TYPE-1



• Molecule 1: ACTIVIN RECEPTOR TYPE-1





4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.38Å 99.85Å 187.44Å 90.00° 92.93° 90.00°	Depositor
Resolution (Å)	52.97 – 2.56 52.92 – 2.56	Depositor EDS
% Data completeness (in resolution range)	96.7 (52.97-2.56) 96.7 (52.92-2.56)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.215 , 0.247 0.216 , 0.245	Depositor DCC
R_{free} test set	2487 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9291	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: FLC, 844, EDO

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	0.82	0/2367	0.90	5/3219 (0.2%)
1	B	0.83	2/2353 (0.1%)	0.99	9/3198 (0.3%)
1	C	0.63	0/2163	0.75	2/2951 (0.1%)
1	D	0.59	0/2246	0.79	7/3060 (0.2%)
All	All	0.73	2/9129 (0.0%)	0.87	23/12428 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	420	SER	CB-OG	-5.25	1.35	1.42
1	B	260	GLU	CG-CD	5.18	1.59	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	ARG	NE-CZ-NH2	-20.24	110.18	120.30
1	B	247	ARG	NE-CZ-NH1	19.89	130.24	120.30
1	A	247	ARG	NE-CZ-NH1	-14.75	112.92	120.30
1	A	247	ARG	NE-CZ-NH2	12.47	126.54	120.30
1	D	247	ARG	NE-CZ-NH1	-10.78	114.91	120.30
1	D	247	ARG	NE-CZ-NH2	8.92	124.76	120.30
1	B	270	MET	CG-SD-CE	-6.90	89.16	100.20
1	B	454	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	D	397	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	282	ILE	CG1-CB-CG2	-6.47	97.16	111.40
1	D	454	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	282	ILE	CG1-CB-CG2	-6.27	97.61	111.40
1	B	454	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	498	ILE	CB-CA-C	-5.65	100.29	111.60
1	D	454	ARG	NE-CZ-NH1	5.46	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	454	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	395	CYS	CA-CB-SG	5.30	123.54	114.00
1	B	335	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	D	335	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	B	433	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	454	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	247	ARG	CB-CG-CD	5.02	124.66	111.60
1	D	335	ARG	NE-CZ-NH1	-5.01	117.79	120.30

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	2312	0	2245	22	0
1	B	2299	0	2240	19	0
1	C	2112	0	1953	18	0
1	D	2193	0	2084	9	1
2	A	30	0	27	1	0
2	B	30	0	27	0	0
2	C	30	0	27	0	0
2	D	30	0	27	0	0
3	A	39	0	15	4	0
3	B	39	0	15	8	0
3	C	13	0	5	4	0
4	A	4	0	6	0	0
5	A	49	0	0	1	0
5	B	60	0	0	3	0
5	C	23	0	0	1	0
5	D	28	0	0	1	0
All	All	9291	0	8671	76	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (76) 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)
3:B:1003:FLC:OB1	3:B:1003:FLC:OG2	1.84	0.93
1:A:346:LYS:HG2	3:A:1001:FLC:HA1	1.65	0.79
1:A:420:SER:HB3	1:A:460:ARG:HH21	1.49	0.78
1:B:420:SER:HB3	1:B:460:ARG:HH21	1.52	0.73
1:A:346:LYS:CG	3:A:1001:FLC:HA1	2.23	0.68
1:A:270:MET:HG3	1:A:279:LEU:HD23	1.80	0.64
1:C:286:HIS:ND1	3:C:1001:FLC:HG2	2.14	0.62
3:B:1002:FLC:CG	3:B:1002:FLC:OA2	2.46	0.62
1:B:270:MET:HG3	1:B:279:LEU:HD23	1.80	0.61
1:A:420:SER:HB3	1:A:460:ARG:NH2	2.17	0.60
1:A:412:TRP:HD1	1:A:474:MET:HE1	1.67	0.59
1:A:273:ARG:HD2	5:A:2009:HOH:O	2.03	0.58
1:C:286:HIS:CE1	3:C:1001:FLC:HG2	2.39	0.58
1:B:480:GLN:HG3	5:B:2055:HOH:O	2.05	0.57
1:D:412:TRP:HD1	1:D:474:MET:HE1	1.71	0.56
1:D:242:GLU:O	1:D:246:PHE:HD2	1.90	0.55
1:B:420:SER:HB3	1:B:460:ARG:NH2	2.23	0.54
1:C:303:VAL:O	1:C:303:VAL:CG1	2.56	0.53
1:C:412:TRP:HD1	1:C:474:MET:HE1	1.74	0.53
1:C:272:SER:HA	1:C:277:THR:HA	1.91	0.52
1:A:376:VAL:HG22	1:A:377:GLY:H	1.75	0.52
3:B:1002:FLC:HG2	3:B:1002:FLC:OA2	2.10	0.52
1:C:286:HIS:HA	3:C:1001:FLC:HA1	1.93	0.51
1:A:474:MET:HE3	1:A:478:TRP:CH2	2.46	0.51
1:D:242:GLU:O	1:D:246:PHE:CD2	2.64	0.51
1:C:287:GLU:HG2	3:C:1001:FLC:OA1	2.10	0.50
1:B:270:MET:HG3	1:B:279:LEU:CD2	2.42	0.50
1:C:277:THR:OG1	1:C:278:GLN:N	2.45	0.50
1:C:303:VAL:HG12	1:C:303:VAL:O	2.10	0.49
1:C:301:ASP:O	1:C:303:VAL:N	2.45	0.49
1:A:270:MET:HG3	1:A:279:LEU:CD2	2.43	0.49
1:D:376:VAL:HG22	1:D:377:GLY:H	1.78	0.49
1:B:412:TRP:HD1	1:B:474:MET:HE1	1.78	0.48
1:B:288:MET:HG2	5:B:2012:HOH:O	2.13	0.48
1:D:242:GLU:N	5:D:2005:HOH:O	2.47	0.48
1:C:376:VAL:HG22	1:C:377:GLY:H	1.78	0.47
1:B:376:VAL:HG22	1:B:377:GLY:H	1.79	0.47
1:A:345:LYS:HA	3:A:1001:FLC:CAC	2.45	0.47
1:B:452:GLN:NE2	5:B:2055:HOH:O	2.48	0.47
3:B:1003:FLC:CBC	3:B:1003:FLC:OG2	2.60	0.47
1:C:302:THR:O	1:C:305:CYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ARG:HD3	1:C:357:LEU:O	2.15	0.47
1:D:474:MET:HE3	1:D:478:TRP:CH2	2.51	0.46
1:B:335:ARG:HD3	1:B:357:LEU:O	2.15	0.45
1:C:271:THR:OG1	1:C:278:GLN:HB2	2.16	0.45
1:A:335:ARG:HD3	1:A:357:LEU:O	2.16	0.45
1:B:454:ARG:HD2	1:B:478:TRP:HB3	1.98	0.45
1:D:335:ARG:HD3	1:D:357:LEU:O	2.17	0.45
3:B:1003:FLC:CGC	3:B:1003:FLC:OB1	2.63	0.45
1:A:420:SER:CB	1:A:460:ARG:NH2	2.79	0.44
1:B:420:SER:CB	1:B:460:ARG:HH21	2.26	0.44
1:B:205:ALA:HA	1:B:208:ILE:HD12	2.00	0.44
1:A:420:SER:CB	1:A:460:ARG:HH21	2.27	0.43
1:C:301:ASP:O	1:C:302:THR:C	2.57	0.43
1:B:284:HIS:ND1	3:B:1002:FLC:OA2	2.50	0.43
1:A:460:ARG:HG3	1:A:461:TRP:N	2.33	0.43
1:B:420:SER:CB	1:B:460:ARG:NH2	2.81	0.43
3:B:1001:FLC:CAC	3:B:1002:FLC:OA1	2.67	0.43
1:B:427:TYR:C	1:B:427:TYR:CD2	2.92	0.42
1:B:412:TRP:CZ2	1:B:416:ARG:HD2	2.55	0.42
1:A:205:ALA:HA	1:A:208:ILE:HD12	2.00	0.42
1:C:474:MET:HE3	1:C:478:TRP:CH2	2.54	0.42
1:A:204:VAL:HG13	1:A:227:TRP:CE2	2.55	0.42
1:A:427:TYR:CD2	1:A:427:TYR:C	2.93	0.41
1:D:427:TYR:C	1:D:427:TYR:CD2	2.93	0.41
1:B:204:VAL:HG13	1:B:227:TRP:CE2	2.55	0.41
1:A:286:HIS:ND1	3:A:1001:FLC:OA2	2.29	0.41
1:A:454:ARG:HD2	1:A:478:TRP:HB3	2.03	0.41
1:C:407:PHE:CE2	1:C:491:ILE:HG21	2.55	0.41
1:C:494:THR:O	5:C:2021:HOH:O	2.22	0.41
1:D:407:PHE:CE2	1:D:491:ILE:HG21	2.56	0.41
1:A:474:MET:CE	1:A:478:TRP:CH2	3.04	0.40
1:A:407:PHE:CE2	1:A:491:ILE:HG21	2.57	0.40
1:B:407:PHE:CE2	1:B:491:ILE:HG21	2.55	0.40
2:A:1000:844:H062	2:A:1000:844:O02	2.22	0.40
3:B:1001:FLC:OB1	3:B:1001:FLC:CAC	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ARG:NH2	1:D:307:ARG:NH2[2_755]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/301 (98%)	285 (97%)	10 (3%)	0	100	100
1	B	290/301 (96%)	283 (98%)	7 (2%)	0	100	100
1	C	273/301 (91%)	262 (96%)	10 (4%)	1 (0%)	34	45
1	D	281/301 (93%)	274 (98%)	7 (2%)	0	100	100
All	All	1139/1204 (95%)	1104 (97%)	34 (3%)	1 (0%)	51	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	302	THR

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/270 (90%)	239 (98%)	5 (2%)	55	69
1	B	245/270 (91%)	241 (98%)	4 (2%)	62	76
1	C	207/270 (77%)	203 (98%)	4 (2%)	57	71
1	D	226/270 (84%)	223 (99%)	3 (1%)	69	80
All	All	922/1080 (85%)	906 (98%)	16 (2%)	60	74

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

Mol	Chain	Res	Type
1	A	365	THR
1	A	393	VAL
1	A	452	GLN
1	A	459	ASN
1	A	483	SER
1	B	365	THR
1	B	393	VAL
1	B	452	GLN
1	B	483	SER
1	C	206	ARG
1	C	246	PHE
1	C	452	GLN
1	C	483	SER
1	D	397	ASP
1	D	452	GLN
1	D	483	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	ASN
1	B	452	GLN
1	D	296	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	844	C	1000	-	33,33,33	2.18	11 (33%)	45,45,45	1.60	7 (15%)
3	FLC	A	1003	-	3,12,12	0.77	0	3,17,17	3.47	1 (33%)
2	844	D	1000	-	33,33,33	2.38	10 (30%)	45,45,45	1.33	6 (13%)
3	FLC	B	1003	-	3,12,12	0.69	0	3,17,17	3.01	1 (33%)
3	FLC	A	1002	-	3,12,12	0.92	0	3,17,17	0.70	0
3	FLC	B	1002	-	3,12,12	0.79	0	3,17,17	3.48	3 (100%)
3	FLC	C	1001	-	3,12,12	1.62	1 (33%)	3,17,17	1.48	1 (33%)
3	FLC	B	1001	-	3,12,12	1.68	1 (33%)	3,17,17	2.85	1 (33%)
4	EDO	A	1004	-	3,3,3	0.65	0	2,2,2	0.22	0
3	FLC	A	1001	-	3,12,12	0.85	0	3,17,17	2.85	1 (33%)
2	844	A	1000	-	33,33,33	1.80	10 (30%)	45,45,45	1.49	7 (15%)
2	844	B	1000	-	33,33,33	2.05	10 (30%)	45,45,45	1.44	8 (17%)

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	844	C	1000	-	-	2/18/26/26	0/4/4/4
3	FLC	A	1003	-	-	4/6/16/16	-
2	844	D	1000	-	-	4/18/26/26	0/4/4/4
3	FLC	B	1003	-	-	3/6/16/16	-
3	FLC	A	1002	-	-	4/6/16/16	-
3	FLC	B	1002	-	-	5/6/16/16	-
3	FLC	C	1001	-	-	1/6/16/16	-
3	FLC	B	1001	-	-	6/6/16/16	-
4	EDO	A	1004	-	-	1/1/1/1	-
3	FLC	A	1001	-	-	4/6/16/16	-
2	844	A	1000	-	-	0/18/26/26	0/4/4/4
2	844	B	1000	-	-	0/18/26/26	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1000	844	C22-C21	5.98	1.49	1.38
2	C	1000	844	C22-C21	5.45	1.48	1.38
2	D	1000	844	C19-C18	4.57	1.47	1.38
2	C	1000	844	C08-C07	4.57	1.47	1.38
2	C	1000	844	O29-C07	4.46	1.44	1.37
2	D	1000	844	C10-C09	4.40	1.47	1.39
2	B	1000	844	C08-C07	4.30	1.46	1.38
2	D	1000	844	C08-C07	4.25	1.46	1.38
2	A	1000	844	C22-C21	4.15	1.46	1.38
2	C	1000	844	C19-C18	4.13	1.46	1.38
2	A	1000	844	C19-C18	4.10	1.46	1.38
2	D	1000	844	O02-C03	4.00	1.43	1.37
2	B	1000	844	C10-C09	3.95	1.46	1.39
2	B	1000	844	O29-C07	3.93	1.43	1.37
2	A	1000	844	C08-C07	3.66	1.45	1.38
2	D	1000	844	O29-C07	3.65	1.43	1.37
2	B	1000	844	C24-N23	-3.38	1.41	1.46
2	B	1000	844	C19-C18	3.38	1.44	1.38
2	D	1000	844	O05-C04	3.30	1.44	1.38
2	B	1000	844	C21-C20	-3.29	1.32	1.39
2	B	1000	844	C22-C21	3.26	1.44	1.38
2	C	1000	844	O02-C03	3.23	1.42	1.37
2	A	1000	844	C28-N23	-2.70	1.42	1.46
2	D	1000	844	C19-C20	2.69	1.44	1.39
2	B	1000	844	O02-C01	-2.64	1.34	1.42
2	C	1000	844	C19-C20	2.59	1.44	1.39
2	A	1000	844	C10-C09	2.56	1.44	1.39
2	A	1000	844	O29-C07	2.47	1.41	1.37
3	C	1001	FLC	CG-CB	-2.39	1.51	1.54
2	D	1000	844	C11-C09	2.35	1.54	1.49
2	A	1000	844	C21-C20	-2.34	1.34	1.39
2	C	1000	844	C16-N15	-2.28	1.29	1.34
3	B	1001	FLC	OHB-CB	2.28	1.46	1.43
2	C	1000	844	C24-N23	-2.28	1.43	1.46
2	A	1000	844	C11-C09	2.27	1.54	1.49
2	B	1000	844	C19-C20	2.26	1.43	1.39
2	C	1000	844	C08-C09	2.22	1.43	1.39
2	D	1000	844	C03-C04	2.18	1.45	1.41
2	A	1000	844	O29-C30	-2.18	1.36	1.42
2	C	1000	844	C11-C09	2.18	1.54	1.49
2	B	1000	844	C28-N23	-2.16	1.43	1.46
2	C	1000	844	C21-C20	-2.15	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	844	C19-C20	2.14	1.43	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	FLC	CB-CG-CGC	-5.85	105.62	114.98
3	B	1003	FLC	CB-CA-CAC	-5.18	106.69	114.98
2	C	1000	844	C12-C11-C16	4.77	121.85	117.11
2	A	1000	844	C16-N15-C14	4.71	123.90	117.48
3	B	1001	FLC	CB-CA-CAC	-4.66	107.53	114.98
3	B	1002	FLC	CB-CG-CGC	-4.61	107.61	114.98
3	A	1001	FLC	CB-CG-CGC	-4.49	107.79	114.98
2	C	1000	844	C16-N15-C14	3.79	122.64	117.48
2	B	1000	844	C12-C11-C16	3.68	120.76	117.11
2	D	1000	844	C16-N15-C14	3.45	122.19	117.48
2	A	1000	844	C24-N23-C20	3.44	127.39	118.09
2	C	1000	844	C24-N23-C20	3.44	127.38	118.09
2	B	1000	844	C24-N23-C20	3.42	127.33	118.09
2	D	1000	844	C12-C11-C16	3.37	120.45	117.11
3	B	1002	FLC	CG-CB-CA	3.16	117.79	109.33
2	B	1000	844	C12-C13-C14	3.02	120.10	117.11
2	A	1000	844	C25-C24-N23	2.79	116.52	110.48
2	D	1000	844	C27-C28-N23	2.71	116.35	110.48
2	A	1000	844	C12-C11-C16	2.71	119.79	117.11
2	A	1000	844	C01-O02-C03	-2.65	113.53	117.53
2	C	1000	844	C27-C28-N23	2.64	116.20	110.48
2	C	1000	844	C13-C12-C11	-2.48	117.38	121.31
2	B	1000	844	C16-N15-C14	2.47	120.85	117.48
2	A	1000	844	C12-C13-C14	2.47	119.56	117.11
2	B	1000	844	C12-C11-C09	-2.46	116.80	120.86
2	D	1000	844	C25-C24-N23	2.41	115.69	110.48
2	C	1000	844	C25-C24-N23	2.37	115.61	110.48
2	D	1000	844	C24-N23-C20	2.37	124.49	118.09
3	C	1001	FLC	CB-CA-CAC	-2.32	111.27	114.98
2	B	1000	844	C13-C12-C11	-2.31	117.66	121.31
3	B	1002	FLC	CB-CA-CAC	-2.25	111.38	114.98
2	B	1000	844	C10-C03-C04	2.20	122.71	120.22
2	C	1000	844	O05-C04-C07	-2.20	116.96	120.12
2	B	1000	844	C27-C28-N23	2.16	115.16	110.48
2	A	1000	844	C30-O29-C07	2.13	120.74	117.53
2	D	1000	844	C30-O29-C07	2.10	120.70	117.53

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	FLC	CA-CB-CG-CGC
3	B	1003	FLC	CBC-CB-CG-CGC
3	B	1003	FLC	OHB-CB-CG-CGC
3	A	1002	FLC	CA-CB-CG-CGC
3	A	1002	FLC	CBC-CB-CG-CGC
3	A	1002	FLC	OHB-CB-CG-CGC
3	B	1002	FLC	CBC-CB-CG-CGC
3	B	1001	FLC	CAC-CA-CB-CBC
3	B	1001	FLC	CAC-CA-CB-CG
3	B	1001	FLC	CAC-CA-CB-OHB
3	B	1001	FLC	CBC-CB-CG-CGC
3	B	1001	FLC	OHB-CB-CG-CGC
3	B	1002	FLC	CA-CB-CG-CGC
3	B	1002	FLC	OHB-CB-CG-CGC
3	B	1002	FLC	CAC-CA-CB-OHB
3	A	1001	FLC	CAC-CA-CB-CG
2	D	1000	844	C04-C07-O29-C30
3	A	1003	FLC	CAC-CA-CB-CG
3	B	1001	FLC	CA-CB-CG-CGC
3	C	1001	FLC	CA-CB-CG-CGC
4	A	1004	EDO	O1-C1-C2-O2
3	A	1001	FLC	CAC-CA-CB-OHB
2	D	1000	844	C10-C09-C11-C12
3	A	1003	FLC	CAC-CA-CB-CBC
3	A	1001	FLC	CAC-CA-CB-CBC
2	D	1000	844	C08-C07-O29-C30
3	A	1003	FLC	CAC-CA-CB-OHB
3	A	1002	FLC	CAC-CA-CB-OHB
3	A	1001	FLC	CA-CB-CG-CGC
2	D	1000	844	C08-C09-C11-C12
2	C	1000	844	C08-C09-C11-C16
3	B	1002	FLC	CAC-CA-CB-CG
3	A	1003	FLC	CA-CB-CG-CGC
2	C	1000	844	C08-C09-C11-C12

There are no ring outliers.

6 monomers are involved in 17 short contacts:

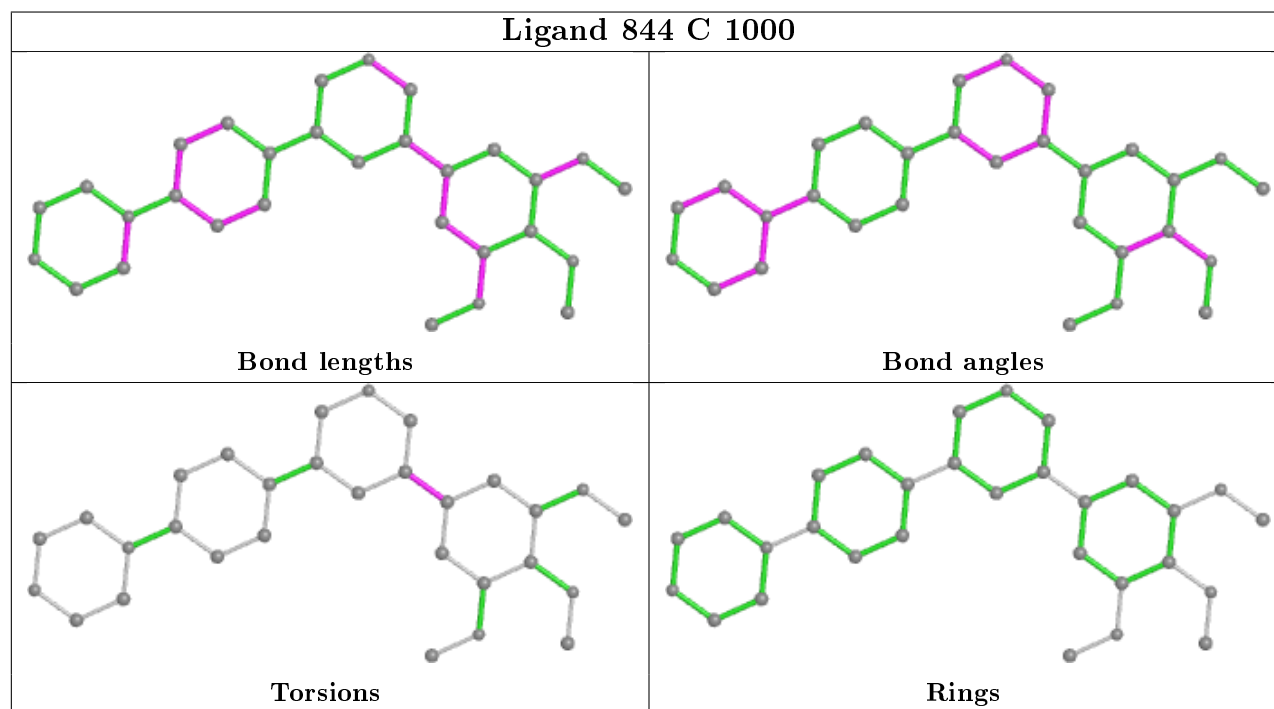
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003	FLC	3	0

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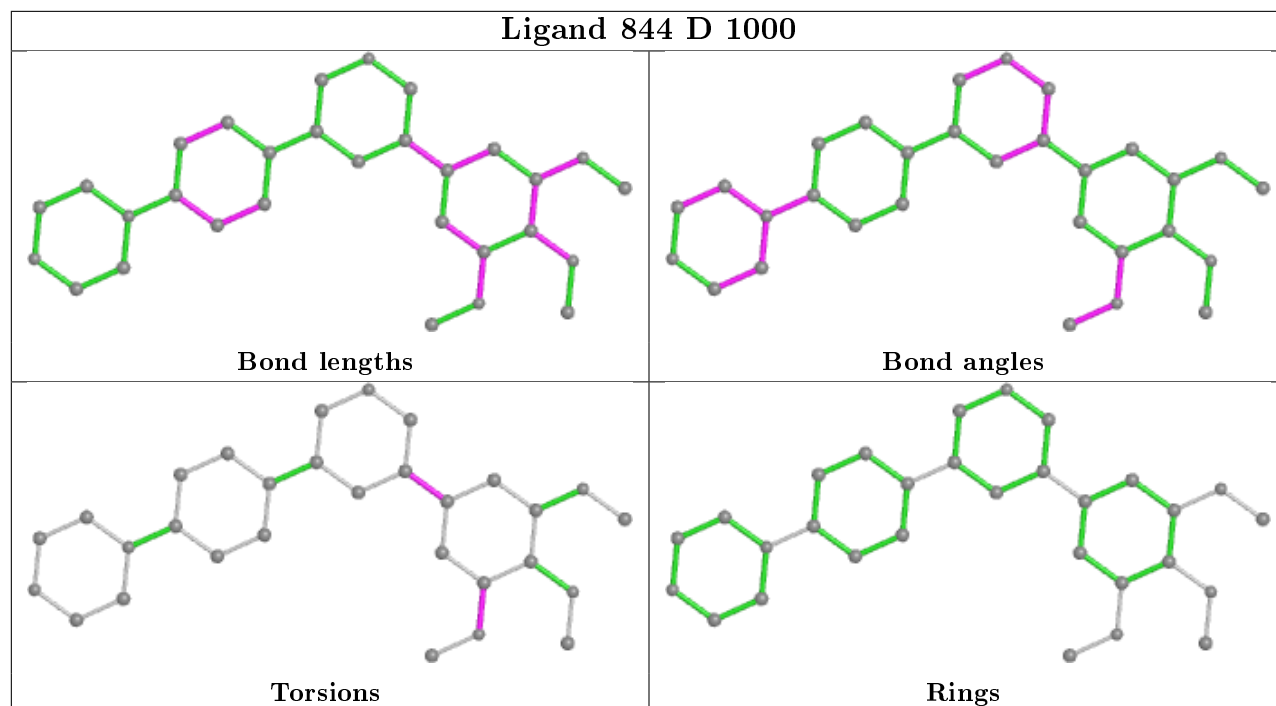
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	FLC	4	0
3	C	1001	FLC	4	0
3	B	1001	FLC	2	0
3	A	1001	FLC	4	0
2	A	1000	844	1	0

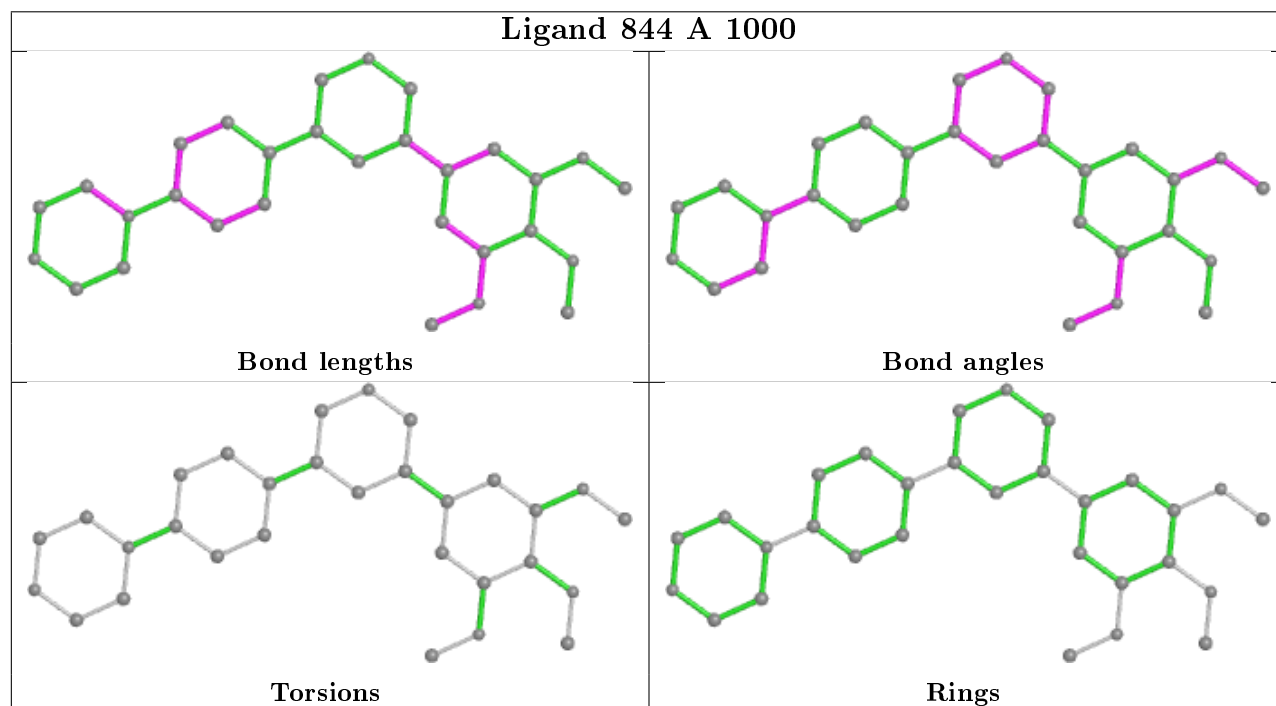
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

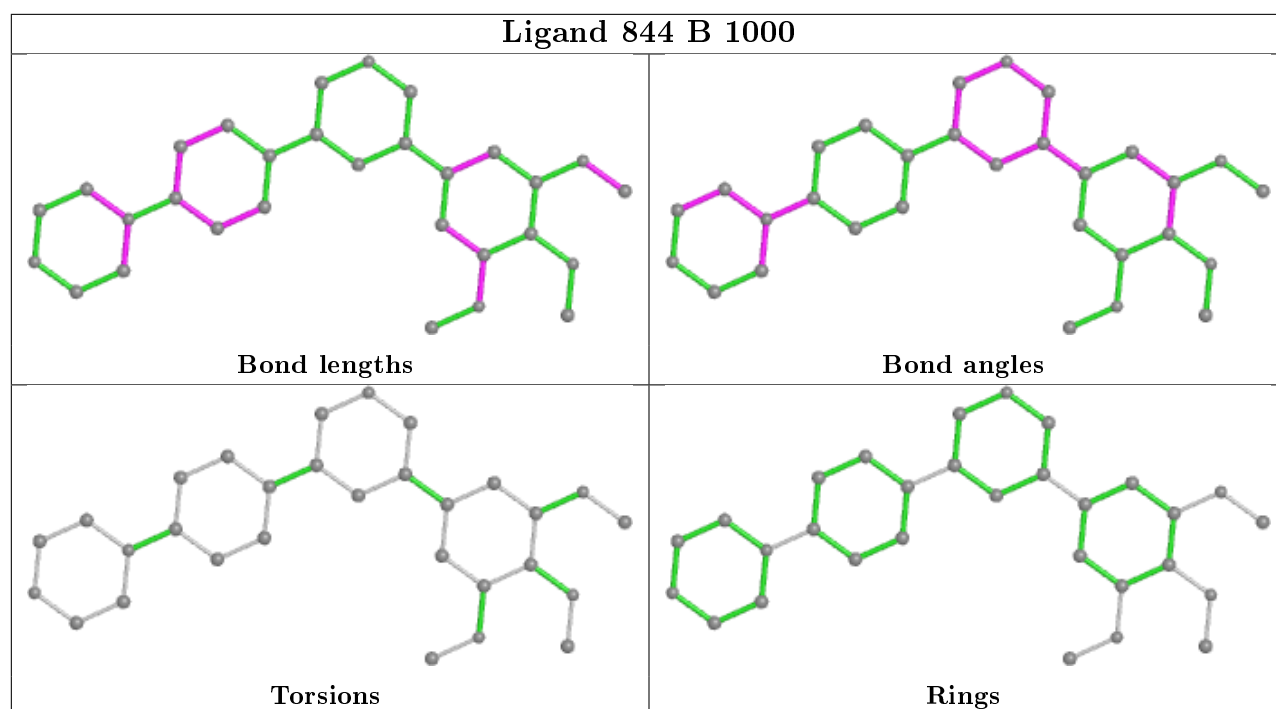


Ligand 844 D 1000



Ligand 844 A 1000





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	296/301 (98%)	-0.03	7 (2%) 59 67	26, 44, 90, 137	0
1	B	293/301 (97%)	-0.11	3 (1%) 82 87	24, 40, 72, 112	0
1	C	279/301 (92%)	0.45	18 (6%) 18 23	46, 79, 147, 171	0
1	D	286/301 (95%)	0.43	18 (6%) 20 25	43, 75, 105, 131	0
All	All	1154/1204 (95%)	0.18	46 (3%) 38 47	24, 59, 117, 171	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	374	PRO	10.9
1	D	303	VAL	6.7
1	C	328	GLY	4.0
1	C	373	ASN	4.0
1	D	223	TRP	3.9
1	C	396	PHE	3.9
1	C	257	LEU	3.8
1	C	441	PHE	3.8
1	C	461	TRP	3.6
1	D	219	TYR	3.5
1	C	466	THR	3.5
1	D	256	MET	3.5
1	B	324	PHE	3.4
1	C	236	ILE	3.3
1	D	228	GLN	3.2
1	C	375	ARG	3.2
1	D	307	ARG	3.2
1	D	443	ASP	3.0
1	C	496	THR	3.0
1	A	375	ARG	2.9
1	D	229	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	497	LYS	2.7
1	B	275	SER	2.7
1	C	463	SER	2.6
1	D	328	GLY	2.6
1	D	302	THR	2.6
1	B	219	TYR	2.5
1	A	359	VAL	2.5
1	A	327	GLN	2.5
1	D	212	GLU	2.5
1	C	440	SER	2.4
1	C	432	TYR	2.4
1	A	326	THR	2.4
1	C	415	ALA	2.3
1	D	441	PHE	2.3
1	D	450	VAL	2.2
1	A	360	MET	2.2
1	C	444	MET	2.2
1	A	374	PRO	2.2
1	C	370	VAL	2.1
1	D	213	CYS	2.1
1	D	463	SER	2.1
1	A	256	MET	2.0
1	D	374	PRO	2.0
1	D	431	PHE	2.0
1	D	444	MET	2.0

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

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

6.3 Carbohydrates ⓘ

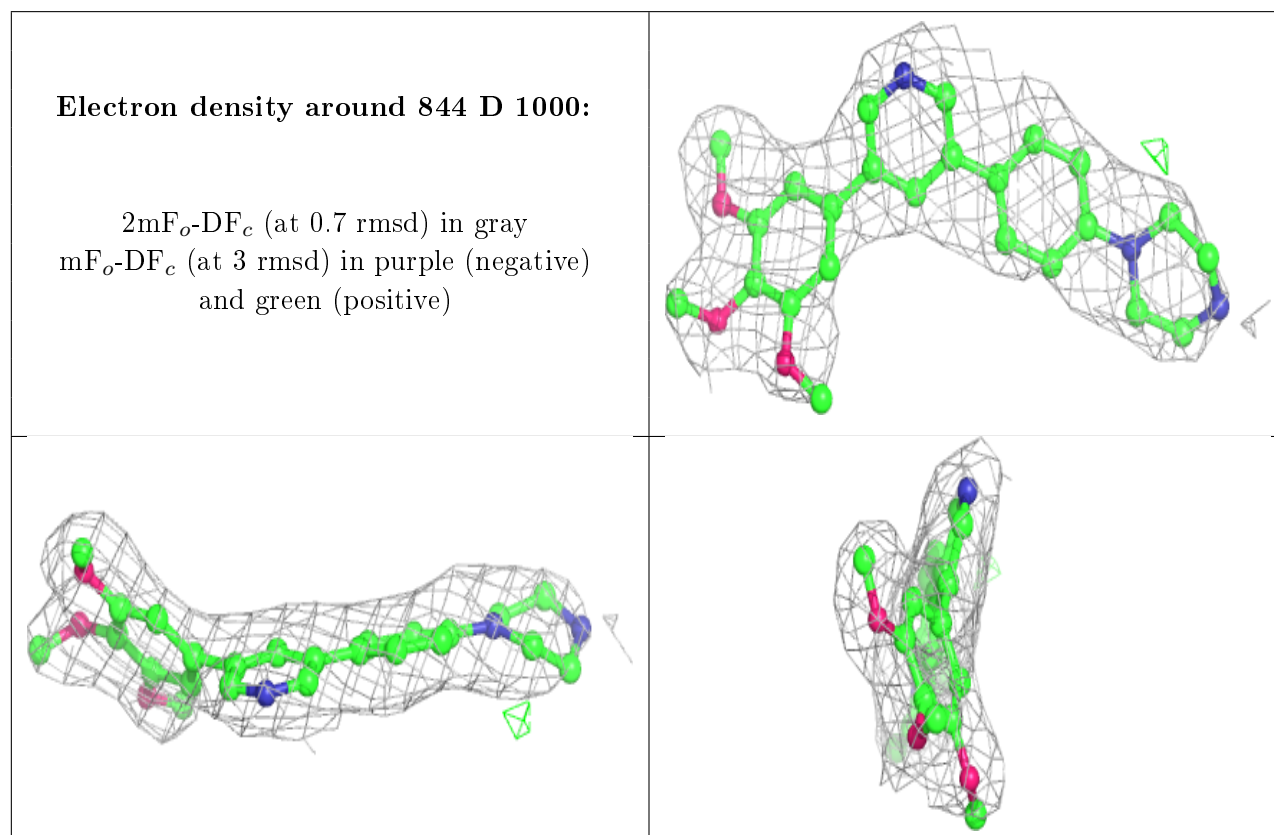
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

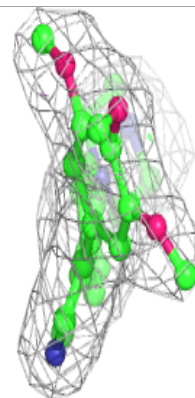
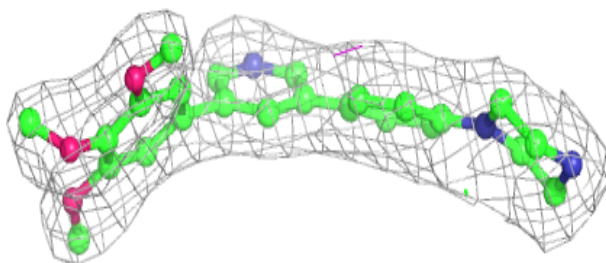
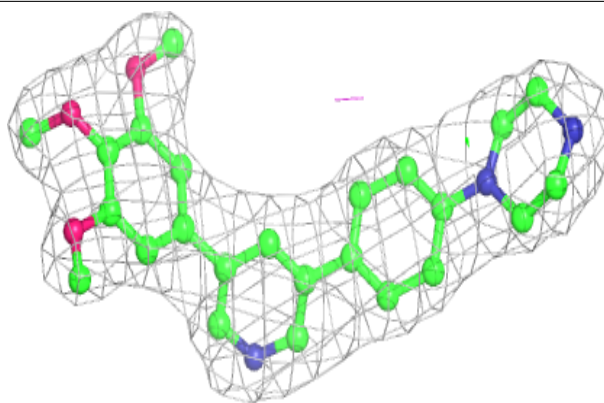
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FLC	B	1003	13/13	0.83	0.23	39,64,78,97	0
3	FLC	A	1003	13/13	0.85	0.18	56,82,97,99	0
3	FLC	B	1002	13/13	0.85	0.21	50,71,80,80	0
3	FLC	A	1001	13/13	0.85	0.18	38,52,72,85	0
3	FLC	A	1002	13/13	0.86	0.34	45,79,97,97	0
3	FLC	C	1001	13/13	0.88	0.14	65,69,89,89	0
3	FLC	B	1001	13/13	0.90	0.20	46,61,71,79	0
4	EDO	A	1004	4/4	0.91	0.22	41,49,53,62	0
2	844	D	1000	30/30	0.92	0.18	46,56,93,99	0
2	844	C	1000	30/30	0.97	0.15	30,40,67,70	0
2	844	B	1000	30/30	0.97	0.16	22,28,45,47	0
2	844	A	1000	30/30	0.98	0.12	25,30,50,51	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.

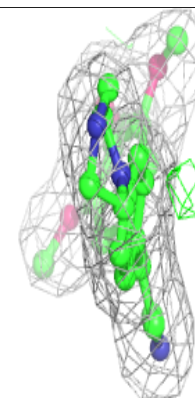
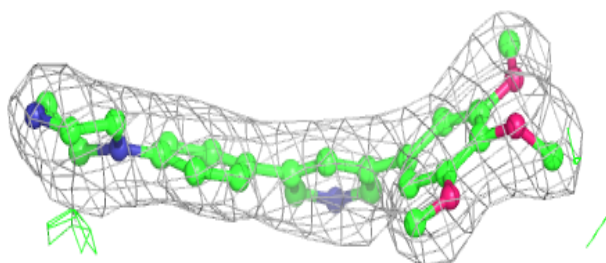
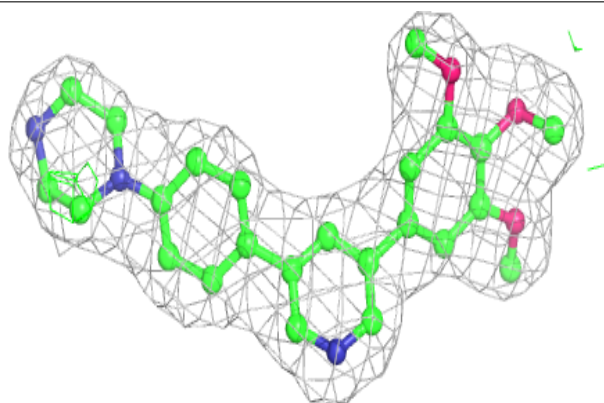


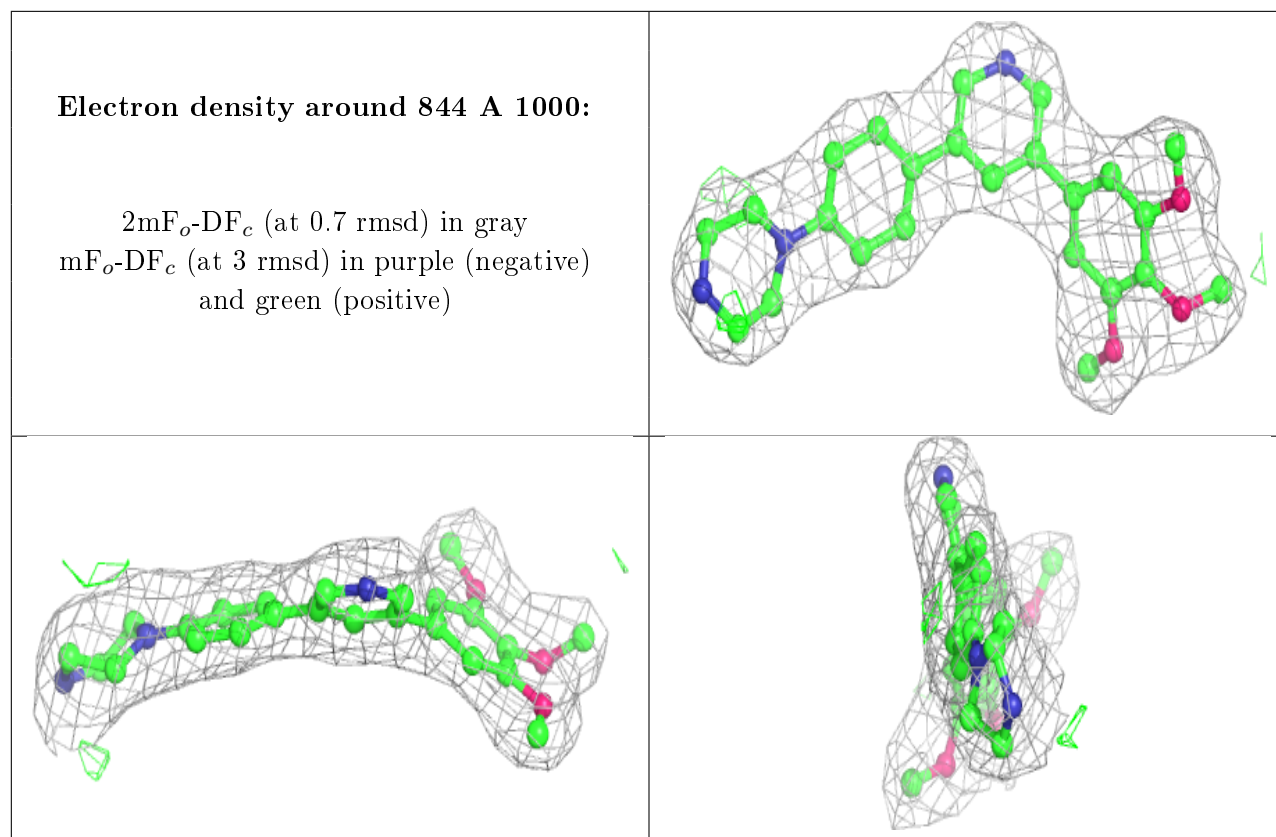
Electron density around 844 C 1000:

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

**Electron density around 844 B 1000:**

$2mF_o-DF_c$ (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.