



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:06 PM UTC

PDB ID : 4BGG / pdb_00004bgg
Title : Crystal structure of the ACVR1 kinase in complex with LDN-213844
Authors : Sanvitale, C.; Canning, P.; Cooper, C.; Wang, Y.; Mohedas, A.H.; Choi, S.; Yu, P.B.; Cuny, G.D.; Nowak, R.; Coutandin, D.; Vollmar, M.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Bullock, A.; Structural Genomics Consortium (SGC)
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 types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) 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

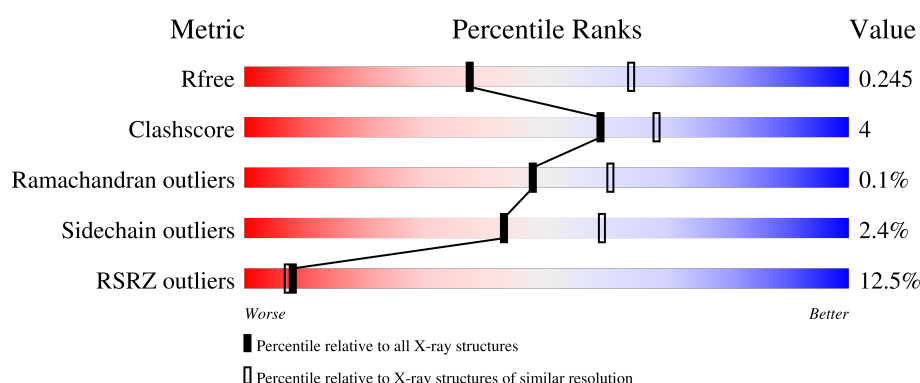
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (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 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	301	7% 87% 11% ..
1	B	301	4% 87% 10% ..
1	C	301	23% 84% 8% 7%
1	D	301	13% 89% 6% 5%

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	FLC	A	1001	-	X	X	-
3	FLC	B	1002	-	X	X	-
3	FLC	B	1003	-	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.

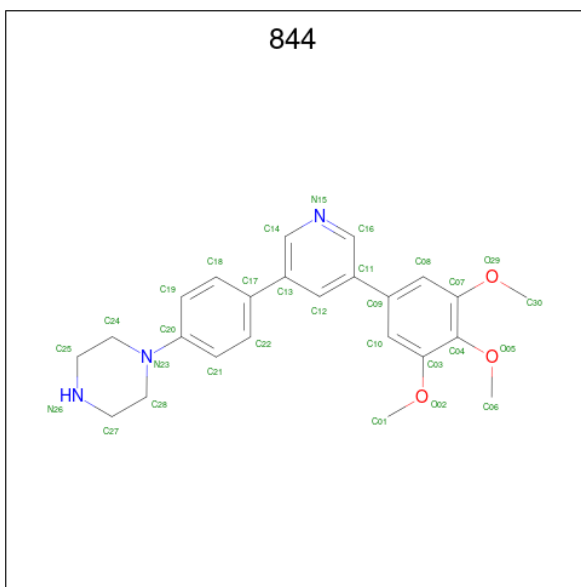
- Molecule 1 is a protein called ACTIVIN RECEPTOR TYPE-1.

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:

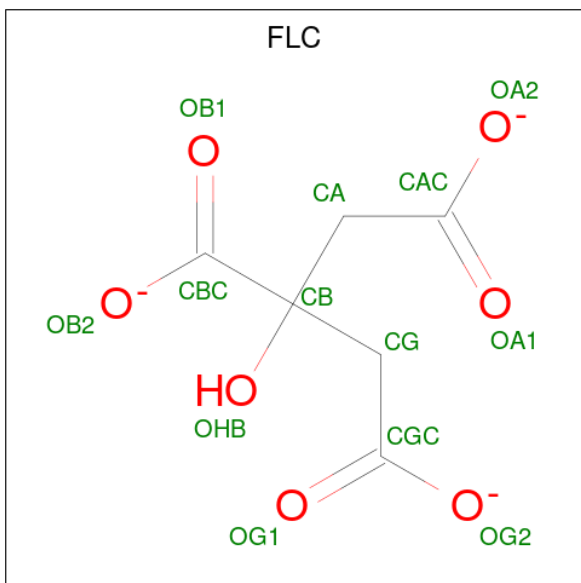
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q04771
A	200	MET	-	expression tag	UNP Q04771
A	207	ASP	GLN	engineered mutation	UNP Q04771
B	199	SER	-	expression tag	UNP Q04771
B	200	MET	-	expression tag	UNP Q04771
B	207	ASP	GLN	engineered mutation	UNP Q04771
C	199	SER	-	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 (CCD ID: 844) (formula: C₂₄H₂₇N₃O₃).



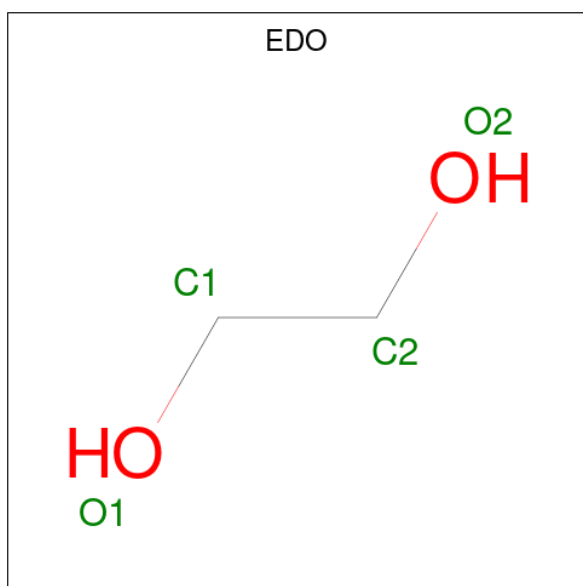
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	24	3	3		
2	B	1	Total	C	N	O	0	0
			30	24	3	3		
2	C	1	Total	C	N	O	0	0
			30	24	3	3		
2	D	1	Total	C	N	O	0	0
			30	24	3	3		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

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

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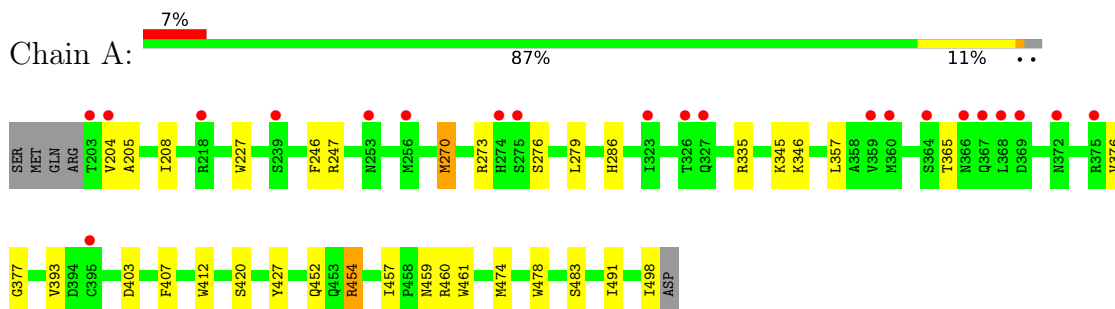
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	21	Total 21	O 21	0	0
5	C	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0
5	D	27	Total 27	O 27	0	0
5	D	1	Total 1	O 1	0	0

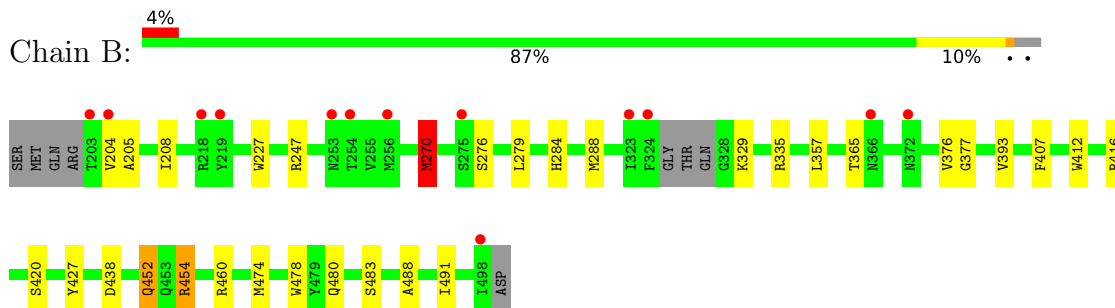
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

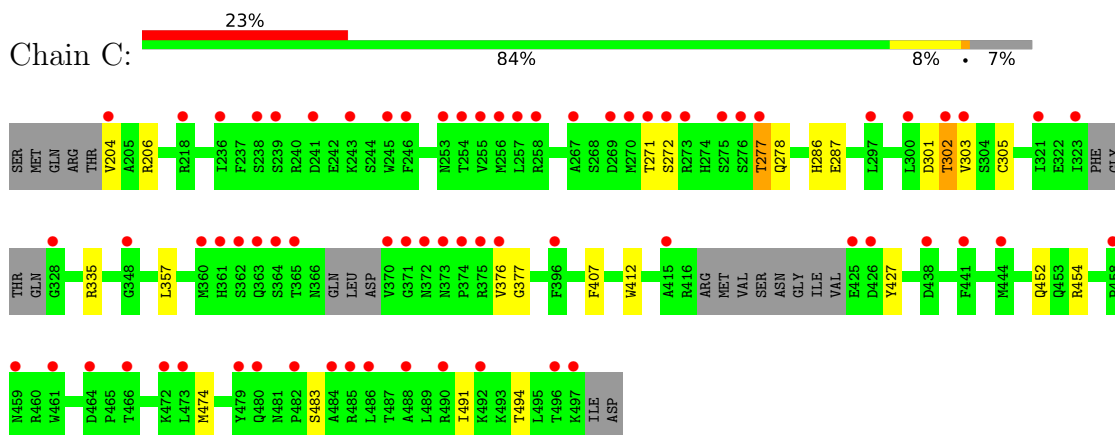
• Molecule 1: ACTIVIN RECEPTOR TYPE-1



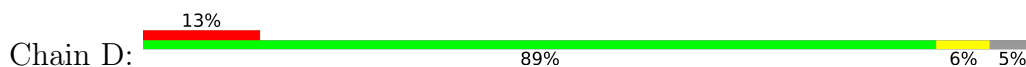
• Molecule 1: ACTIVIN RECEPTOR TYPE-1

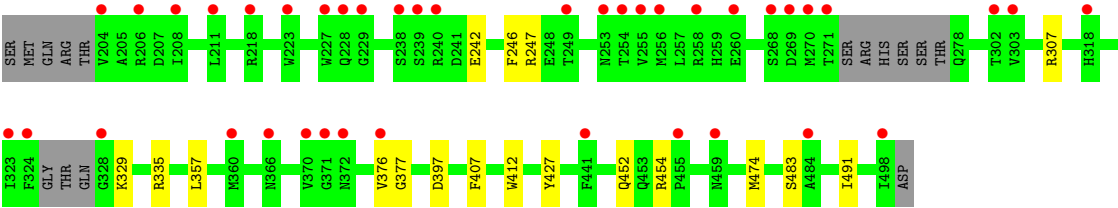


• Molecule 1: ACTIVIN RECEPTOR TYPE-1



• 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 52.97 – 2.56	Depositor EDS
% Data completeness (in resolution range)	96.7 (52.97-2.56) 96.7 (52.97-2.56)	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	2488 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)	0.31 , 43.5	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: EDO, 844, FLC

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	1.10	3/2367 (0.1%)	1.03	4/3219 (0.1%)
1	B	1.12	2/2353 (0.1%)	1.04	7/3198 (0.2%)
1	C	0.86	0/2163	0.93	1/2951 (0.0%)
1	D	0.83	0/2246	0.94	4/3060 (0.1%)
All	All	0.99	5/9129 (0.1%)	0.99	16/12428 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	438	ASP	C-O	-7.40	1.20	1.23
1	A	457	ILE	N-CA	-5.74	1.42	1.46
1	A	403	ASP	N-CA	5.51	1.53	1.46
1	B	488	ALA	N-CA	-5.37	1.39	1.46
1	A	246	PHE	C-O	-5.00	1.18	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	ARG	NE-CZ-NH2	-10.02	110.18	119.20
1	B	247	ARG	NE-CZ-NH1	8.74	130.24	121.50
1	A	247	ARG	NE-CZ-NH1	-8.57	112.92	121.50
1	A	247	ARG	NE-CZ-NH2	8.15	126.54	119.20
1	C	277	THR	N-CA-C	8.12	121.25	110.53
1	B	276	SER	N-CA-C	6.61	118.59	108.42
1	D	247	ARG	NE-CZ-NH1	-6.59	114.91	121.50
1	A	276	SER	N-CA-C	6.46	118.36	108.42
1	D	247	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	D	329	LYS	CA-C-N	-6.07	114.38	120.21
1	D	329	LYS	C-N-CA	-6.07	114.38	120.21
1	B	329	LYS	CA-C-N	-5.87	114.58	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	LYS	C-N-CA	-5.87	114.58	120.21
1	B	247	ARG	CB-CG-CD	5.81	124.66	111.30
1	A	498	ILE	CB-CA-C	-5.65	100.29	111.60
1	B	270	MET	CG-SD-CE	-5.34	89.16	100.90

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	23	0
1	B	2299	0	2240	19	0
1	C	2112	0	1953	19	0
1	D	2193	0	2084	8	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	9	0
3	C	13	0	5	5	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	78	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 (78) 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:OA2	3:B:1002:FLC:CG	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: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: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:CG1	1:C:303:VAL:O	2.56	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:OA2	3:B:1002:FLC:HG2	2.10	0.52
1:C:286:HIS:HA	3:C:1001:FLC:HA1	1.93	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:303:VAL:O	1:C:303:VAL:HG12	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:C:277:THR:OG1	1:C:278:GLN:N	2.45	0.48
1:B:288:MET:HG2	5:B:2012:HOH:O	2.13	0.48
1:A:412:TRP:HD1	1:A:474:MET:HE1	1.79	0.48
1:C:301:ASP:O	1:C:302:THR:C	2.57	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:B:427:TYR:C	1:B:427:TYR:CD2	2.92	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:OG2	3:B:1003:FLC:CBC	2.60	0.47
1:C:302:THR:O	1:C:305:CYS:HB3	2.14	0.47
1:C:335:ARG:HD3	1:C:357:LEU:O	2.15	0.47
1:A:427:TYR:CD2	1:A:427:TYR:C	2.93	0.46
1:B:412:TRP:HD1	1:B:474:MET:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:TYR:CD2	1:D:427:TYR:C	2.93	0.46
1:B:335:ARG:HD3	1:B:357:LEU:O	2.15	0.45
1:D:412:TRP:HD1	1:D:474:MET:HE1	1.81	0.45
1:C:271:THR:OG1	1:C:278:GLN:HB2	2.16	0.45
1:C:412:TRP:HD1	1:C:474:MET:HE1	1.81	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
1:C:427:TYR:CD2	1:C:427:TYR:C	2.95	0.45
3:B:1003:FLC:OB1	3:B:1003:FLC:CGC	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
3:B:1002:FLC:OG1	3:B:1002:FLC:OHB	2.34	0.43
1:A:420:SER:CB	1:A:460:ARG:HH21	2.27	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: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:A:204:VAL:HG13	1:A:227:TRP:CE2	2.55	0.42
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:C:286:HIS:HD1	3:C:1001:FLC:HG2	1.82	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:A:474:MET:HE3	1:A:478:TRP:CH2	2.56	0.40
1:A:412:TRP:HB2	1:A:474:MET:HE3	2.03	0.40
1:B:407:PHE:CE2	1:B:491:ILE:HG21	2.55	0.40
2:A:1000:844:O02	2:A:1000:844:H062	2.22	0.40
3:B:1001:FLC:CAC	3:B:1001:FLC:OB1	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 [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	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%)	30	39
1	D	281/301 (93%)	274 (98%)	7 (2%)	0	100	100
All	All	1139/1204 (95%)	1104 (97%)	34 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	302	THR

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	244/270 (90%)	237 (97%)	7 (3%)	37	53
1	B	245/270 (91%)	239 (98%)	6 (2%)	43	59
1	C	207/270 (77%)	202 (98%)	5 (2%)	43	59
1	D	226/270 (84%)	222 (98%)	4 (2%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	922/1080 (85%)	900 (98%)	22 (2%)	43 59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	MET
1	A	365	THR
1	A	393	VAL
1	A	452	GLN
1	A	454	ARG
1	A	459	ASN
1	A	483	SER
1	B	270	MET
1	B	365	THR
1	B	393	VAL
1	B	452	GLN
1	B	454	ARG
1	B	483	SER
1	C	204	VAL
1	C	206	ARG
1	C	452	GLN
1	C	454	ARG
1	C	483	SER
1	D	397	ASP
1	D	452	GLN
1	D	454	ARG
1	D	483	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	261	ASN
1	A	296	GLN
1	A	452	GLN
1	B	228	GLN
1	B	261	ASN
1	B	296	GLN
1	B	318	HIS
1	B	421	ASN
1	B	452	GLN

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Mol	Chain	Res	Type
1	C	228	GLN
1	C	253	ASN
1	C	261	ASN
1	C	296	GLN
1	C	452	GLN
1	D	261	ASN
1	D	286	HIS
1	D	296	GLN
1	D	421	ASN
1	D	452	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 oligosaccharides 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$
3	FLC	B	1002	-	12,12,12	1.37	1 (8%)	17,17,17	1.91	8 (47%)
2	844	B	1000	-	33,33,33	2.11	9 (27%)	45,45,45	1.43	8 (17%)
3	FLC	A	1003	-	12,12,12	1.13	1 (8%)	17,17,17	1.59	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	844	D	1000	-	33,33,33	2.48	11 (33%)	45,45,45	1.34	6 (13%)
4	EDO	A	1004	-	3,3,3	0.61	0	2,2,2	0.21	0
2	844	C	1000	-	33,33,33	2.28	11 (33%)	45,45,45	1.59	7 (15%)
3	FLC	A	1002	-	12,12,12	1.04	0	17,17,17	1.74	2 (11%)
3	FLC	C	1001	-	12,12,12	1.83	1 (8%)	17,17,17	1.19	2 (11%)
3	FLC	B	1001	-	12,12,12	1.51	3 (25%)	17,17,17	2.71	3 (17%)
3	FLC	B	1003	-	12,12,12	1.78	1 (8%)	17,17,17	2.79	6 (35%)
3	FLC	A	1001	-	12,12,12	2.16	1 (8%)	17,17,17	3.52	10 (58%)
2	844	A	1000	-	33,33,33	1.90	11 (33%)	45,45,45	1.50	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	B	1002	-	-	12/16/16/16	-
2	844	B	1000	-	-	0/18/26/26	0/4/4/4
3	FLC	A	1003	-	-	4/16/16/16	-
2	844	D	1000	-	-	4/18/26/26	0/4/4/4
4	EDO	A	1004	-	-	1/1/1/1	-
2	844	C	1000	-	-	1/18/26/26	0/4/4/4
3	FLC	A	1002	-	-	10/16/16/16	-
3	FLC	C	1001	-	-	6/16/16/16	-
3	FLC	B	1001	-	-	6/16/16/16	-
3	FLC	B	1003	-	-	11/16/16/16	-
3	FLC	A	1001	-	-	8/16/16/16	-
2	844	A	1000	-	-	0/18/26/26	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1000	844	C22-C21	6.69	1.49	1.38
3	A	1001	FLC	OA1-CAC	6.32	1.42	1.22
2	C	1000	844	C22-C21	6.10	1.48	1.38
2	D	1000	844	C19-C18	5.11	1.47	1.38
3	C	1001	FLC	CB-CBC	-4.93	1.48	1.53
2	C	1000	844	C08-C07	4.86	1.47	1.38
2	A	1000	844	C22-C21	4.64	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	844	C19-C18	4.62	1.46	1.38
2	A	1000	844	C19-C18	4.58	1.46	1.38
2	B	1000	844	C08-C07	4.58	1.46	1.38
2	D	1000	844	C08-C07	4.52	1.46	1.38
3	B	1003	FLC	CB-CBC	4.52	1.58	1.53
2	D	1000	844	C10-C09	4.39	1.47	1.39
2	C	1000	844	O29-C07	4.37	1.44	1.37
2	B	1000	844	C10-C09	3.94	1.46	1.39
2	D	1000	844	O02-C03	3.92	1.43	1.37
2	A	1000	844	C08-C07	3.89	1.45	1.38
2	B	1000	844	O29-C07	3.86	1.43	1.37
2	B	1000	844	C19-C18	3.77	1.44	1.38
2	B	1000	844	C22-C21	3.63	1.44	1.38
2	D	1000	844	O29-C07	3.58	1.43	1.37
2	B	1000	844	C21-C20	-3.45	1.32	1.39
2	D	1000	844	O05-C04	3.30	1.44	1.38
2	C	1000	844	O02-C03	3.17	1.42	1.37
2	B	1000	844	C24-N23	-3.11	1.41	1.46
2	B	1000	844	O02-C01	-2.87	1.34	1.42
2	D	1000	844	C19-C20	2.81	1.44	1.39
2	C	1000	844	C19-C20	2.71	1.44	1.39
2	A	1000	844	C10-C09	2.55	1.44	1.39
3	B	1001	FLC	OA1-CAC	2.50	1.30	1.22
2	A	1000	844	C28-N23	-2.48	1.42	1.46
2	A	1000	844	C21-C20	-2.46	1.34	1.39
2	D	1000	844	C11-C09	2.45	1.54	1.49
2	A	1000	844	O29-C07	2.42	1.41	1.37
2	A	1000	844	O29-C30	-2.38	1.36	1.42
2	A	1000	844	C11-C09	2.37	1.54	1.49
2	B	1000	844	C19-C20	2.36	1.43	1.39
2	C	1000	844	C16-N15	-2.33	1.29	1.34
2	C	1000	844	C11-C09	2.27	1.54	1.49
3	B	1001	FLC	CB-CBC	-2.27	1.51	1.53
2	C	1000	844	C21-C20	-2.26	1.35	1.39
3	A	1003	FLC	OA1-CAC	2.25	1.29	1.22
2	A	1000	844	C19-C20	2.23	1.43	1.39
2	C	1000	844	C08-C09	2.21	1.43	1.39
2	D	1000	844	C03-C04	2.20	1.45	1.41
3	B	1002	FLC	OA1-CAC	2.14	1.29	1.22
3	B	1001	FLC	OB2-CBC	-2.13	1.22	1.30
2	C	1000	844	C24-N23	-2.10	1.43	1.46
2	D	1000	844	O29-C30	-2.02	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	844	O02-C01	-2.01	1.37	1.42

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	FLC	OHB-CB-CBC	-9.32	95.74	108.96
3	B	1003	FLC	OB2-CBC-CB	7.73	127.97	113.14
3	A	1001	FLC	OA2-CAC-CA	-6.92	92.41	114.35
3	B	1003	FLC	OB1-CBC-CB	-5.65	111.15	122.09
3	A	1001	FLC	OB2-CBC-CB	5.64	123.96	113.14
3	A	1001	FLC	OHB-CB-CG	-5.58	96.64	109.38
2	A	1000	844	C16-N15-C14	4.70	123.90	117.51
3	A	1002	FLC	OB2-CBC-CB	4.68	122.11	113.14
2	C	1000	844	C12-C11-C16	4.42	121.85	117.10
3	A	1001	FLC	CG-CB-CBC	4.29	119.52	110.03
3	A	1001	FLC	CA-CB-CBC	-4.12	100.91	110.03
3	B	1001	FLC	OHB-CB-CG	4.11	118.75	109.38
3	A	1001	FLC	OA2-CAC-OA1	3.96	133.53	123.33
3	A	1001	FLC	OA1-CAC-CA	3.92	134.06	122.95
3	A	1003	FLC	OB2-CBC-CB	3.82	120.47	113.14
2	C	1000	844	C16-N15-C14	3.78	122.64	117.51
3	A	1002	FLC	OB1-CBC-CB	-3.51	115.30	122.09
2	D	1000	844	C16-N15-C14	3.44	122.19	117.51
2	B	1000	844	C12-C11-C16	3.41	120.76	117.10
2	A	1000	844	C24-N23-C20	3.40	127.39	118.11
2	C	1000	844	C24-N23-C20	3.40	127.38	118.11
2	B	1000	844	C24-N23-C20	3.38	127.33	118.11
3	B	1002	FLC	CG-CB-CA	3.30	117.79	109.31
2	D	1000	844	C12-C11-C16	3.12	120.45	117.10
3	A	1003	FLC	CB-CG-CGC	-3.04	105.62	113.92
3	A	1001	FLC	OHB-CB-CA	3.02	116.27	109.38
3	B	1002	FLC	OHB-CB-CBC	2.90	113.07	108.96
2	A	1000	844	C25-C24-N23	2.82	116.52	110.38
2	B	1000	844	C12-C13-C14	2.80	120.10	117.10
2	D	1000	844	C27-C28-N23	2.75	116.35	110.38
2	A	1000	844	C01-O02-C03	-2.72	113.53	117.51
3	B	1003	FLC	CG-CB-CBC	2.71	116.02	110.03
3	B	1003	FLC	OHB-CB-CG	-2.70	103.22	109.38
2	C	1000	844	C27-C28-N23	2.68	116.20	110.38
3	B	1002	FLC	OHB-CB-CA	-2.65	103.33	109.38
3	B	1003	FLC	CB-CA-CAC	-2.65	106.69	113.92
2	C	1000	844	C13-C12-C11	-2.60	117.38	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	FLC	CG-CB-CBC	-2.56	104.37	110.03
2	A	1000	844	C12-C11-C16	2.51	119.79	117.10
2	B	1000	844	C16-N15-C14	2.46	120.85	117.51
2	D	1000	844	C25-C24-N23	2.44	115.69	110.38
2	B	1000	844	C13-C12-C11	-2.42	117.66	121.30
2	B	1000	844	C12-C11-C09	-2.41	116.80	120.84
2	C	1000	844	C25-C24-N23	2.40	115.61	110.38
3	C	1001	FLC	OG1-CGC-CG	-2.37	116.23	122.95
3	C	1001	FLC	OB1-CBC-CB	-2.35	117.54	122.09
2	D	1000	844	C24-N23-C20	2.34	124.49	118.11
3	B	1001	FLC	CB-CA-CAC	-2.34	107.53	113.92
3	A	1001	FLC	OB1-CBC-CB	-2.34	117.57	122.09
3	B	1002	FLC	CB-CG-CGC	-2.31	107.61	113.92
3	B	1002	FLC	OHB-CB-CG	-2.30	104.13	109.38
2	A	1000	844	C12-C13-C14	2.30	119.56	117.10
3	A	1001	FLC	CB-CG-CGC	-2.24	107.79	113.92
2	B	1000	844	C10-C03-C04	2.24	122.71	120.22
2	C	1000	844	O05-C04-C07	-2.20	116.96	120.12
2	A	1000	844	C30-O29-C07	2.20	120.74	117.51
2	B	1000	844	C27-C28-N23	2.20	115.16	110.38
2	D	1000	844	C30-O29-C07	2.17	120.70	117.51
3	B	1002	FLC	OB2-CBC-CB	2.17	117.30	113.14
3	B	1002	FLC	OG1-CGC-CG	-2.09	117.04	122.95
3	B	1003	FLC	OHB-CB-CA	-2.02	104.76	109.38

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	FLC	CG-CB-CBC-OB1
3	A	1001	FLC	CG-CB-CBC-OB2
3	A	1001	FLC	OHB-CB-CBC-OB1
3	A	1001	FLC	OHB-CB-CBC-OB2
3	A	1002	FLC	OHB-CB-CG-CGC
3	B	1001	FLC	CAC-CA-CB-CG
3	B	1001	FLC	OHB-CB-CG-CGC
3	B	1002	FLC	OHB-CB-CBC-OB2
3	B	1003	FLC	CA-CB-CBC-OB1
3	B	1003	FLC	CA-CB-CBC-OB2
3	B	1003	FLC	OHB-CB-CBC-OB1
3	B	1003	FLC	OHB-CB-CBC-OB2
3	B	1003	FLC	OHB-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
3	A	1002	FLC	CA-CB-CG-CGC
3	A	1002	FLC	CBC-CB-CG-CGC
3	B	1001	FLC	CAC-CA-CB-CBC
3	B	1001	FLC	CAC-CA-CB-OHB
3	B	1003	FLC	CA-CB-CG-CGC
3	B	1003	FLC	CBC-CB-CG-CGC
3	B	1002	FLC	CA-CB-CG-CGC
3	B	1002	FLC	OHB-CB-CG-CGC
3	A	1002	FLC	CA-CB-CBC-OB2
3	B	1001	FLC	CBC-CB-CG-CGC
3	B	1002	FLC	CBC-CB-CG-CGC
3	A	1001	FLC	CAC-CA-CB-CG
2	D	1000	844	C04-C07-O29-C30
3	A	1002	FLC	OHB-CB-CBC-OB2
3	B	1002	FLC	OHB-CB-CBC-OB1
3	A	1002	FLC	CG-CB-CBC-OB2
3	B	1002	FLC	CA-CB-CBC-OB2
3	A	1003	FLC	CAC-CA-CB-CG
3	B	1001	FLC	CA-CB-CG-CGC
3	C	1001	FLC	CA-CB-CG-CGC
3	C	1001	FLC	CBC-CB-CG-CGC
3	A	1002	FLC	CA-CB-CBC-OB1
3	B	1002	FLC	CA-CB-CBC-OB1
3	B	1003	FLC	CG-CB-CBC-OB1
3	B	1003	FLC	CG-CB-CBC-OB2
3	C	1001	FLC	CA-CB-CBC-OB2
3	C	1001	FLC	CG-CB-CBC-OB2
3	A	1001	FLC	CAC-CA-CB-CBC
3	A	1001	FLC	CAC-CA-CB-OHB
3	B	1002	FLC	CAC-CA-CB-OHB
4	A	1004	EDO	O1-C1-C2-O2
2	D	1000	844	C08-C07-O29-C30
3	A	1003	FLC	CAC-CA-CB-CBC
3	A	1002	FLC	CG-CB-CBC-OB1
2	D	1000	844	C10-C09-C11-C12
3	A	1001	FLC	CA-CB-CG-CGC
3	A	1003	FLC	CAC-CA-CB-OHB
3	B	1002	FLC	CB-CA-CAC-OA2
2	D	1000	844	C08-C09-C11-C12
3	C	1001	FLC	CG-CB-CBC-OB1
3	A	1002	FLC	CAC-CA-CB-OHB
2	C	1000	844	C08-C09-C11-C16

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Mol	Chain	Res	Type	Atoms
3	B	1002	FLC	CB-CA-CAC-OA1
3	A	1002	FLC	OHB-CB-CBC-OB1
3	C	1001	FLC	OHB-CB-CBC-OB2
3	B	1002	FLC	CG-CB-CBC-OB1
3	A	1003	FLC	CBC-CB-CG-CGC
3	B	1003	FLC	CB-CG-CGC-OG2
3	B	1003	FLC	CB-CG-CGC-OG1
3	B	1002	FLC	CAC-CA-CB-CG

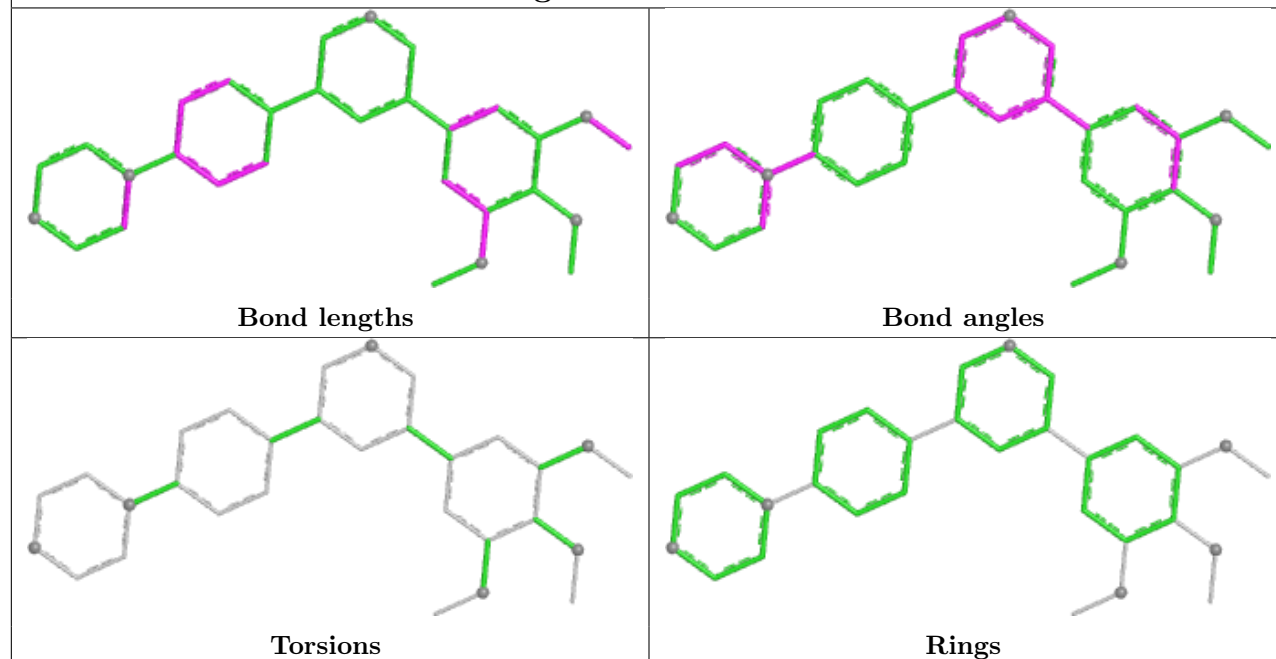
There are no ring outliers.

6 monomers are involved in 19 short contacts:

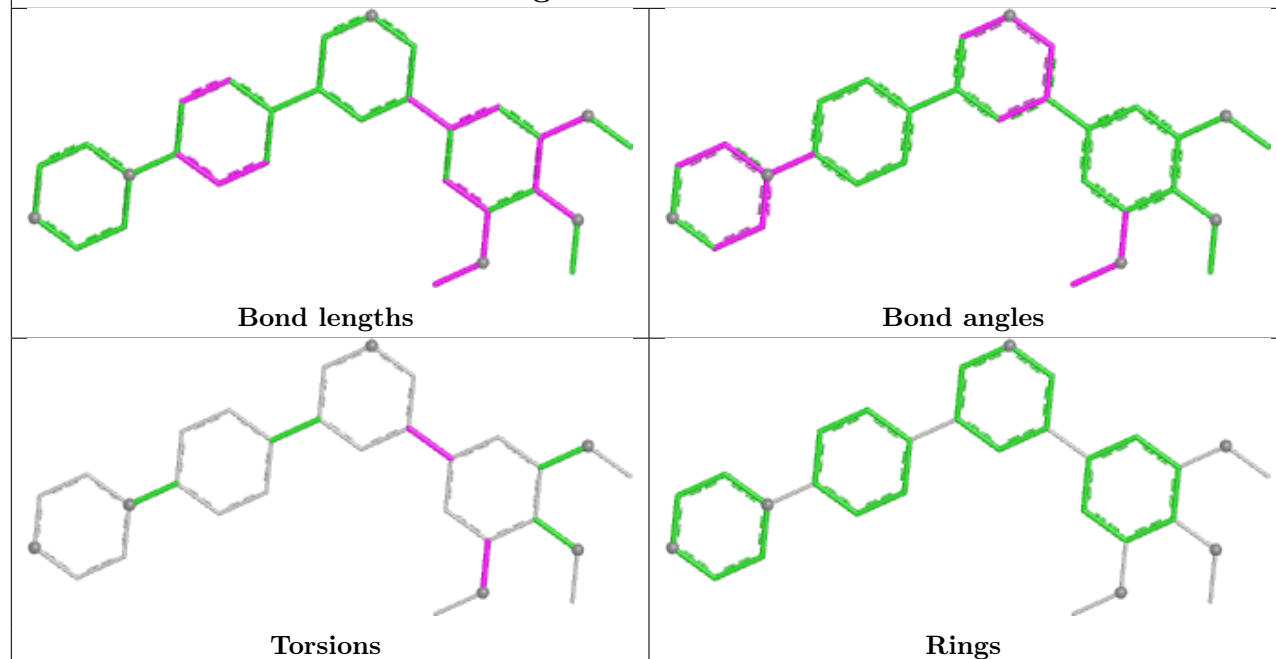
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	FLC	5	0
3	C	1001	FLC	5	0
3	B	1001	FLC	2	0
3	B	1003	FLC	3	0
3	A	1001	FLC	4	0
2	A	1000	844	1	0

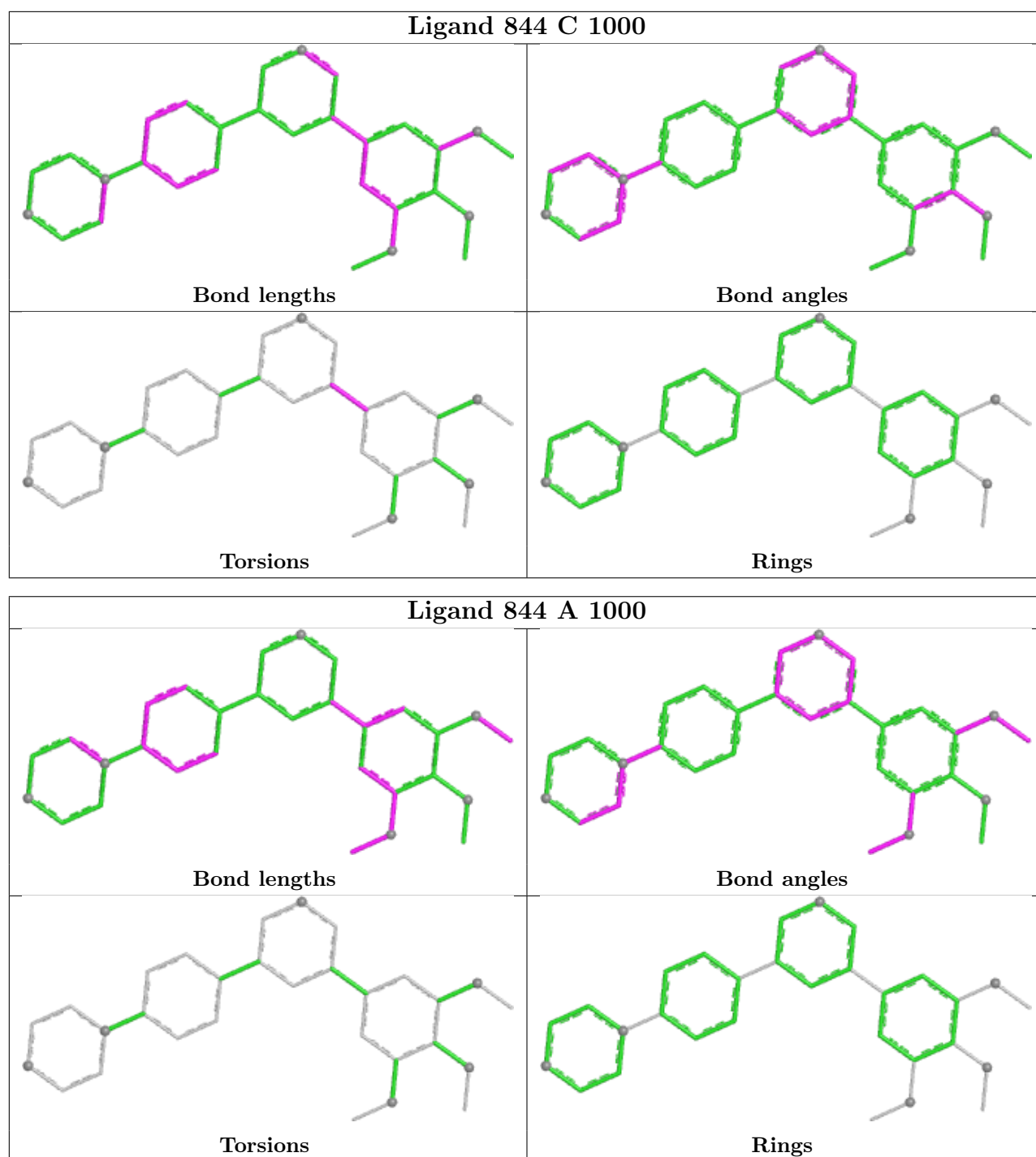
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 B 1000



Ligand 844 D 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%)	0.09	21 (7%) 22 21	24, 44, 90, 137	1 (0%)
1	B	293/301 (97%)	-0.04	13 (4%) 39 40	22, 40, 72, 112	1 (0%)
1	C	279/301 (92%)	1.21	70 (25%) 1 1	40, 78, 146, 171	2 (0%)
1	D	286/301 (95%)	0.97	40 (13%) 6 6	41, 75, 105, 131	1 (0%)
All	All	1154/1204 (95%)	0.54	144 (12%) 8 7	22, 59, 117, 171	5 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	374	PRO	7.7
1	C	370	VAL	6.2
1	D	372	ASN	5.9
1	D	204	VAL	5.6
1	C	204	VAL	5.2
1	C	275	SER	5.0
1	C	372	ASN	5.0
1	C	257	LEU	4.8
1	C	302	THR	4.7
1	D	228	GLN	4.6
1	B	324	PHE	4.5
1	C	364	SER	4.5
1	C	328	GLY	4.4
1	D	229	GLY	4.3
1	D	256	MET	4.2
1	C	497	LYS	4.2
1	C	396	PHE	4.1
1	C	459	ASN	4.1
1	D	238	SER	4.1
1	C	496	THR	4.0
1	C	239	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	326	THR	3.9
1	A	359	VAL	3.7
1	A	360	MET	3.7
1	C	488	ALA	3.6
1	D	254	THR	3.6
1	D	208	ILE	3.5
1	A	327	GLN	3.5
1	D	328	GLY	3.4
1	B	275	SER	3.4
1	C	415	ALA	3.4
1	A	256	MET	3.4
1	D	324	PHE	3.4
1	C	466	THR	3.3
1	D	302	THR	3.3
1	C	323	ILE	3.3
1	C	371	GLY	3.2
1	D	239	SER	3.2
1	D	260	GLU	3.1
1	D	303	VAL	3.1
1	D	271	THR	3.1
1	C	363	GLN	3.1
1	C	254	THR	3.1
1	D	227	TRP	3.1
1	C	482	PRO	3.0
1	A	275	SER	3.0
1	B	253	ASN	3.0
1	C	486	LEU	3.0
1	C	441	PHE	2.9
1	D	498	ILE	2.9
1	D	318	HIS	2.9
1	A	375	ARG	2.9
1	D	323	ILE	2.9
1	D	269	ASP	2.9
1	C	256	MET	2.9
1	C	461	TRP	2.8
1	B	372	ASN	2.8
1	C	276	SER	2.8
1	C	321	ILE	2.8
1	C	373	ASN	2.8
1	D	240	ARG	2.8
1	C	272	SER	2.8
1	A	366	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	366	ASN	2.7
1	B	203	THR	2.7
1	A	369	ASP	2.7
1	D	376	VAL	2.7
1	D	360	MET	2.7
1	D	253	ASN	2.7
1	C	376	VAL	2.7
1	C	365	THR	2.7
1	C	426	ASP	2.6
1	C	246	PHE	2.6
1	C	375	ARG	2.6
1	D	371	GLY	2.6
1	C	238	SER	2.6
1	D	459	ASN	2.6
1	C	362	SER	2.6
1	C	360	MET	2.6
1	C	473	LEU	2.6
1	B	254	THR	2.6
1	B	323	ILE	2.5
1	A	203	THR	2.5
1	A	253	ASN	2.5
1	C	255	VAL	2.5
1	D	366	ASN	2.5
1	B	256	MET	2.5
1	D	370	VAL	2.5
1	C	438	ASP	2.5
1	C	258	ARG	2.4
1	D	249	THR	2.4
1	C	245	TRP	2.4
1	A	239	SER	2.4
1	D	258	ARG	2.4
1	C	479	TYR	2.4
1	A	204	VAL	2.3
1	C	472	LYS	2.3
1	C	458	PRO	2.3
1	D	455	PRO	2.3
1	C	297	LEU	2.3
1	C	269	ASP	2.3
1	D	268	SER	2.3
1	A	274	HIS	2.3
1	D	255	VAL	2.3
1	C	273	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	218	ARG	2.3
1	A	323	ILE	2.3
1	C	425	GLU	2.3
1	D	206	ARG	2.3
1	C	300	LEU	2.2
1	D	211	LEU	2.2
1	D	270	MET	2.2
1	D	441	PHE	2.2
1	C	271	THR	2.2
1	A	368	LEU	2.2
1	B	218	ARG	2.2
1	B	204	VAL	2.2
1	C	253	ASN	2.2
1	C	236	ILE	2.2
1	C	490	ARG	2.2
1	C	267	ALA	2.2
1	A	395	CYS	2.2
1	C	243	LYS	2.2
1	C	303	VAL	2.1
1	A	367	GLN	2.1
1	A	372	ASN	2.1
1	C	218	ARG	2.1
1	C	361	HIS	2.1
1	B	219	TYR	2.1
1	B	498	ILE	2.1
1	D	484	ALA	2.1
1	C	485	ARG	2.1
1	C	277	THR	2.1
1	C	241	ASP	2.1
1	C	464	ASP	2.1
1	A	364	SER	2.1
1	C	270	MET	2.1
1	C	484	ALA	2.0
1	C	348	GLY	2.0
1	C	444	MET	2.0
1	C	480	GLN	2.0
1	A	218	ARG	2.0
1	C	492	LYS	2.0
1	D	223	TRP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

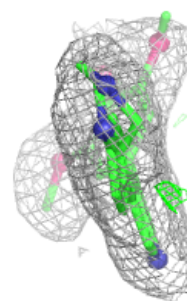
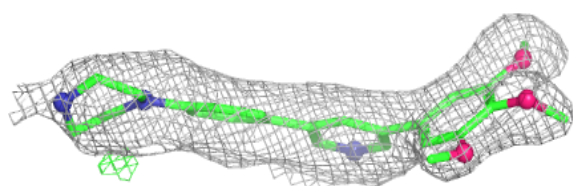
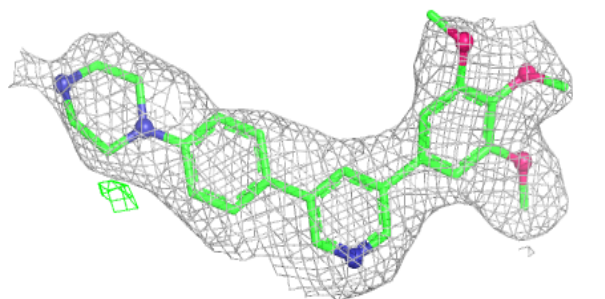
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FLC	B	1003	13/13	0.74	0.16	39,64,78,97	0
3	FLC	C	1001	13/13	0.74	0.13	65,69,89,89	0
3	FLC	A	1001	13/13	0.75	0.14	38,52,72,85	0
3	FLC	A	1002	13/13	0.75	0.13	45,79,97,97	0
3	FLC	B	1002	13/13	0.77	0.15	50,71,80,80	0
3	FLC	A	1003	13/13	0.82	0.15	56,82,97,99	0
3	FLC	B	1001	13/13	0.86	0.11	46,61,71,79	0
2	844	D	1000	30/30	0.86	0.14	46,56,93,99	0
4	EDO	A	1004	4/4	0.92	0.11	41,49,53,62	0
2	844	C	1000	30/30	0.94	0.09	30,40,67,70	0
2	844	A	1000	30/30	0.97	0.06	25,30,50,51	0
2	844	B	1000	30/30	0.97	0.07	22,28,45,47	0

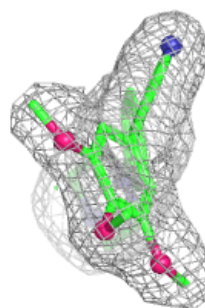
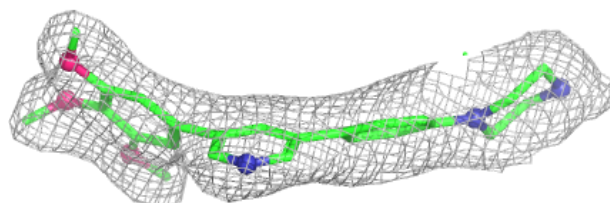
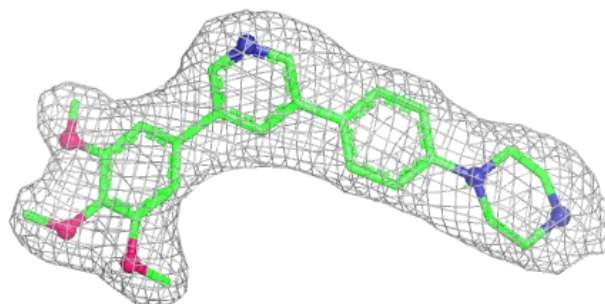
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 844 D 1000:

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

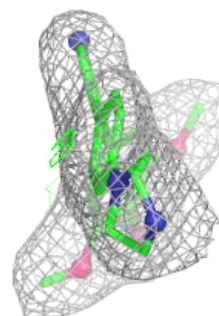
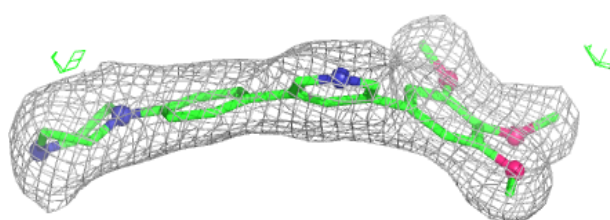
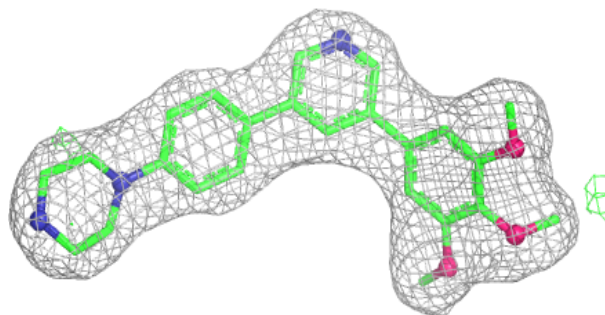
**Electron density around 844 C 1000:**

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

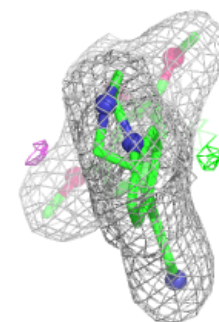
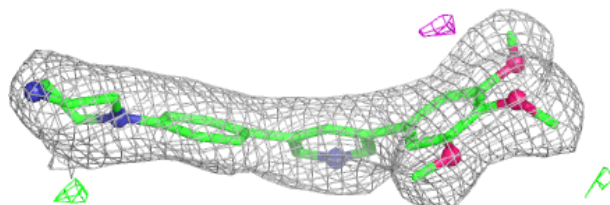
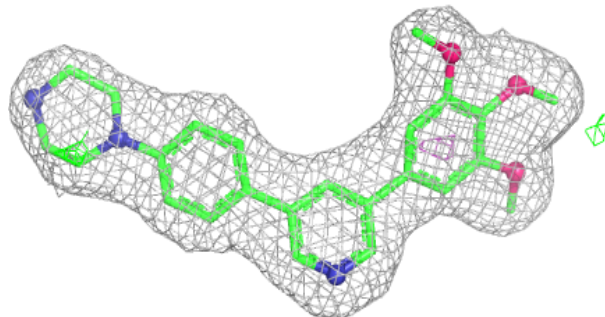


Electron density around 844 A 1000:

$2mF_o-DF_c$ (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.