



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:27 pm BST

PDB ID : 4ELF  
Title : Structure-activity relationship guides enantiomeric preference among potent inhibitors of B. anthracis dihydrofolate reductase  
Authors : Bourne, C.R.; Barrow, W.W.  
Deposited on : 2012-04-10  
Resolution : 2.30 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](mailto: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.

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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

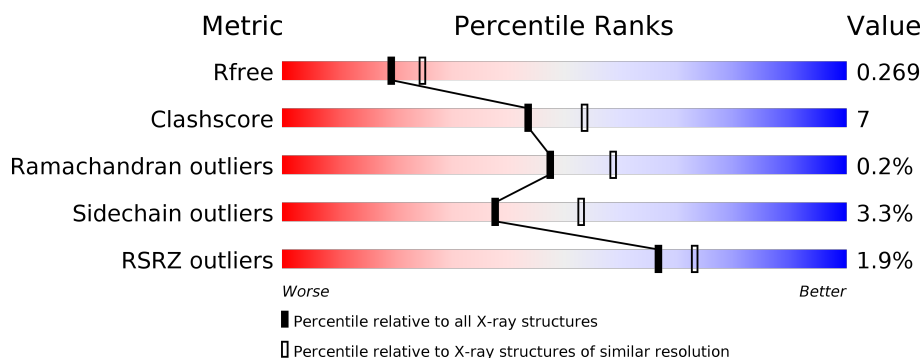
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	166	<div> <div></div> <div>86%13%.</div> </div>
1	B	166	<div> <div></div> <div>89%10%.</div> </div>
1	C	166	<div> <div>2%</div> <div>86%13%.</div> </div>
1	D	166	<div> <div>2%</div> <div>78%17%5%</div> </div>
1	E	166	<div> <div></div> <div>87%12%.</div> </div>
1	F	166	<div> <div>%</div> <div>83%15%.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	166	
1	H	166	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	D	202	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12321 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 Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	B	166	Total	C	N	O	S	0	0	0
			1374	889	225	251	9			
1	C	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	D	166	Total	C	N	O	S	0	1	0
			1386	896	229	252	9			
1	E	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	F	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	G	166	Total	C	N	O	S	0	0	0
			1380	892	228	251	9			
1	H	166	Total	C	N	O	S	0	1	0
			1386	896	229	252	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LEU	-	EXPRESSION TAG	UNP Q81R22
A	164	VAL	-	EXPRESSION TAG	UNP Q81R22
A	165	PRO	-	EXPRESSION TAG	UNP Q81R22
A	166	ARG	-	EXPRESSION TAG	UNP Q81R22
B	163	LEU	-	EXPRESSION TAG	UNP Q81R22
B	164	VAL	-	EXPRESSION TAG	UNP Q81R22
B	165	PRO	-	EXPRESSION TAG	UNP Q81R22
B	166	ARG	-	EXPRESSION TAG	UNP Q81R22
C	163	LEU	-	EXPRESSION TAG	UNP Q81R22
C	164	VAL	-	EXPRESSION TAG	UNP Q81R22
C	165	PRO	-	EXPRESSION TAG	UNP Q81R22
C	166	ARG	-	EXPRESSION TAG	UNP Q81R22
D	163	LEU	-	EXPRESSION TAG	UNP Q81R22

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Chain	Residue	Modelled	Actual	Comment	Reference
D	164	VAL	-	EXPRESSION TAG	UNP Q81R22
D	165	PRO	-	EXPRESSION TAG	UNP Q81R22
D	166	ARG	-	EXPRESSION TAG	UNP Q81R22
E	163	LEU	-	EXPRESSION TAG	UNP Q81R22
E	164	VAL	-	EXPRESSION TAG	UNP Q81R22
E	165	PRO	-	EXPRESSION TAG	UNP Q81R22
E	166	ARG	-	EXPRESSION TAG	UNP Q81R22
F	163	LEU	-	EXPRESSION TAG	UNP Q81R22
F	164	VAL	-	EXPRESSION TAG	UNP Q81R22
F	165	PRO	-	EXPRESSION TAG	UNP Q81R22
F	166	ARG	-	EXPRESSION TAG	UNP Q81R22
G	163	LEU	-	EXPRESSION TAG	UNP Q81R22
G	164	VAL	-	EXPRESSION TAG	UNP Q81R22
G	165	PRO	-	EXPRESSION TAG	UNP Q81R22
G	166	ARG	-	EXPRESSION TAG	UNP Q81R22
H	163	LEU	-	EXPRESSION TAG	UNP Q81R22
H	164	VAL	-	EXPRESSION TAG	UNP Q81R22
H	165	PRO	-	EXPRESSION TAG	UNP Q81R22
H	166	ARG	-	EXPRESSION TAG	UNP Q81R22

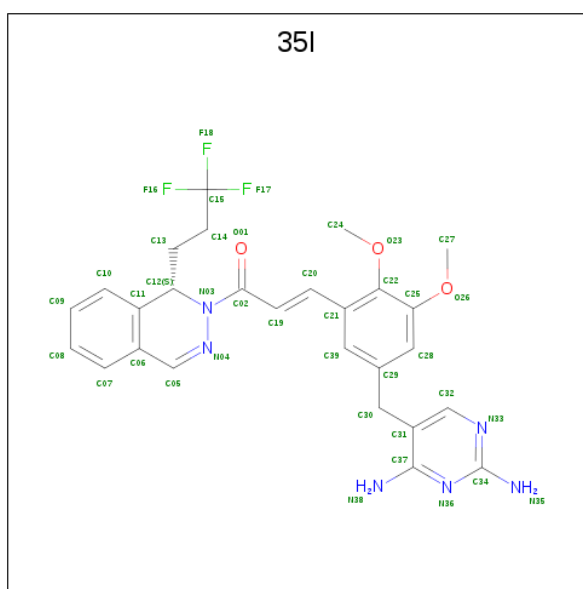
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is (2E)-3-{5-[(2,4-diaminopyrimidin-5-yl)methyl]-2,3-dimethoxyphenyl}-1-[(1S)-1-(3,3,3-trifluoropropyl)phthalazin-2(1H)-yl]prop-2-en-1-one (three-letter code: 35I) (formula: C<sub>27</sub>H<sub>27</sub>F<sub>3</sub>N<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O 39 27 3 6 3	0	0
4	B	1	Total C F N O 39 27 3 6 3	0	0
4	C	1	Total C F N O 39 27 3 6 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	F	N	O	0	0
			39	27	3	6	3		
4	E	1	Total	C	F	N	O	0	0
			39	27	3	6	3		
4	F	1	Total	C	F	N	O	0	0
			39	27	3	6	3		
4	G	1	Total	C	F	N	O	0	0
			39	27	3	6	3		
4	H	1	Total	C	F	N	O	0	0
			39	27	3	6	3		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total	O	0	0
			158	158		
5	B	142	Total	O	0	0
			142	142		
5	C	157	Total	O	0	0
			157	157		
5	D	105	Total	O	0	0
			105	105		
5	E	96	Total	O	0	0
			96	96		
5	F	91	Total	O	0	0
			91	91		
5	G	124	Total	O	0	0
			124	124		
5	H	74	Total	O	0	0
			74	74		

### 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: Dihydrofolate reductase

Chain A: 




- Molecule 1: Dihydrofolate reductase

Chain B: 




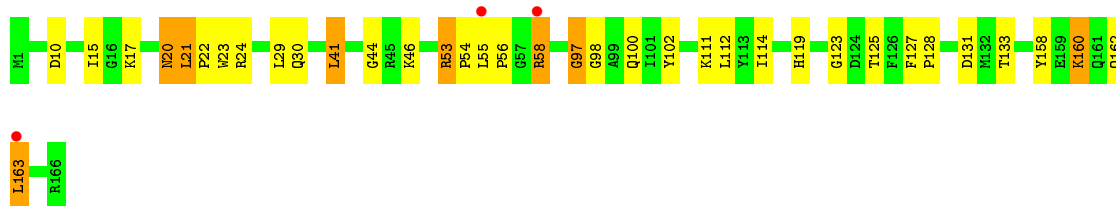
- Molecule 1: Dihydrofolate reductase

Chain C: 



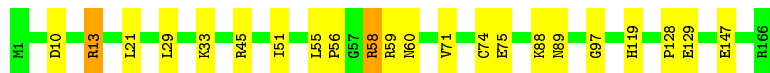
- Molecule 1: Dihydrofolate reductase

Chain D: 



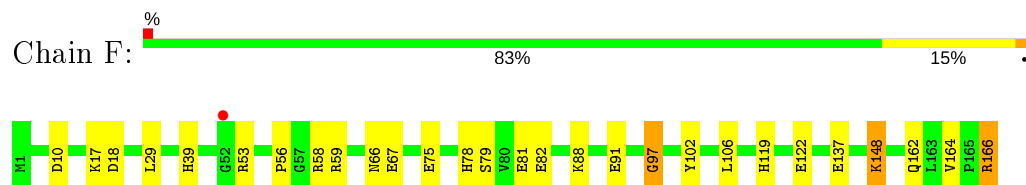
- Molecule 1: Dihydrofolate reductase

Chain E: 

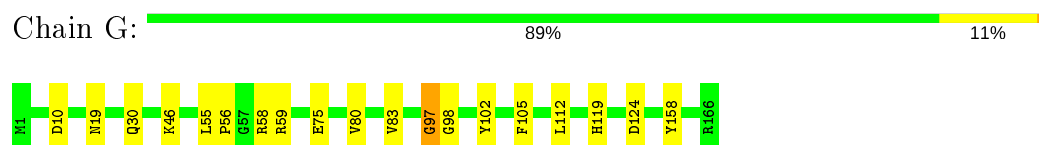




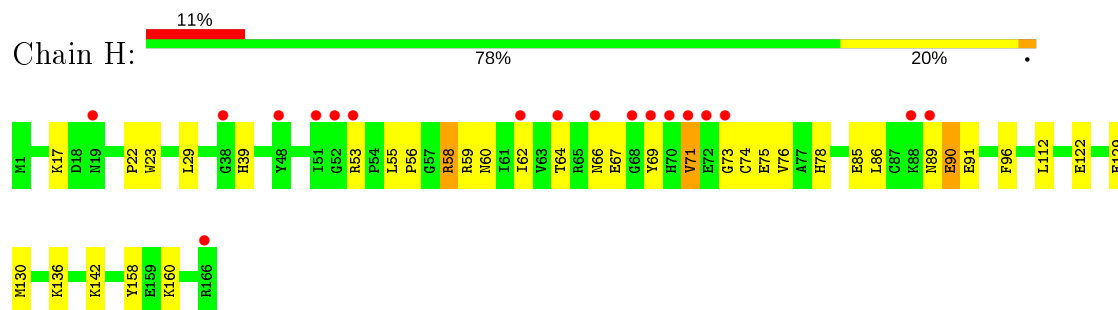
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.27Å 136.12Å 168.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.55 – 2.30 71.63 – 1.78	Depositor EDS
% Data completeness (in resolution range)	95.7 (31.55-2.30) 92.7 (71.63-1.78)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.78Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.228 , 0.290 0.210 , 0.269	Depositor DCC
$R_{free}$ test set	7034 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtrriage
Anisotropy	0.445	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8718e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, 35I, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	0/1418	0.58	1/1918 (0.1%)
1	B	0.47	0/1412	0.58	0/1911
1	C	0.47	0/1418	0.57	1/1918 (0.1%)
1	D	0.45	0/1427	0.55	0/1930
1	E	0.45	0/1418	0.56	0/1918
1	F	0.42	0/1418	0.56	0/1918
1	G	0.46	0/1418	0.57	1/1918 (0.1%)
1	H	0.41	0/1427	0.56	0/1930
All	All	0.45	0/11356	0.57	3/15361 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	GLY	N-CA-C	-5.47	99.42	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	GLY	N-CA-C	-5.08	100.40	113.10
1	G	98	GLY	N-CA-C	-5.08	100.41	113.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	GLY	Peptide
1	B	97	GLY	Peptide
1	C	97	GLY	Peptide
1	D	97	GLY	Peptide
1	E	97	GLY	Peptide
1	F	97	GLY	Peptide
1	G	97	GLY	Peptide

## 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	1380	0	1346	13	0
1	B	1374	0	1335	13	0
1	C	1380	0	1346	14	0
1	D	1386	0	1354	42	0
1	E	1380	0	1346	14	1
1	F	1380	0	1346	22	0
1	G	1380	0	1346	13	0
1	H	1386	0	1354	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	2	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	39	0	27	0	0
4	B	39	0	27	2	0
4	C	39	0	27	1	0
4	D	39	0	27	15	0
4	E	39	0	27	3	0
4	F	39	0	27	4	0
4	G	39	0	27	1	0
4	H	39	0	27	5	0
5	A	158	0	0	5	1
5	B	142	0	0	2	0
5	C	157	0	0	5	0
5	D	105	0	0	5	0
5	E	96	0	0	0	0
5	F	91	0	0	5	0
5	G	124	0	0	3	0
5	H	74	0	0	4	0
All	All	12321	0	10989	149	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 7.

All (149) 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:D:58:ARG:HH12	4:D:203:35I:C07	1.26	1.45
1:D:58:ARG:NH1	4:D:203:35I:H2	1.24	1.45
1:D:24:ARG:HH22	1:E:89:ASN:HD21	1.17	0.90
1:F:17:LYS:HE2	1:F:122:GLU:HG2	1.51	0.90
1:D:58:ARG:HH22	4:D:203:35I:H3	1.38	0.87
1:E:55:LEU:H	1:E:60:ASN:HD21	1.28	0.80
1:D:58:ARG:NH2	4:D:203:35I:H3	1.95	0.80
1:D:58:ARG:HH22	4:D:203:35I:C08	1.96	0.79
1:E:29:LEU:HD22	4:E:203:35I:H12	1.68	0.76
1:D:53:ARG:NE	5:D:382:HOH:O	1.98	0.71
1:E:51:ILE:HA	4:E:203:35I:H15	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:ASP:OD1	5:G:314:HOH:O	2.11	0.69
1:A:1:MET:N	5:A:385:HOH:O	2.26	0.67
1:F:53:ARG:NH2	4:F:203:35I:O01	2.29	0.65
1:A:49:GLU:OE2	5:A:334:HOH:O	2.15	0.65
1:D:55:LEU:N	1:D:55:LEU:HD12	2.12	0.65
1:H:56:PRO:O	1:H:58:ARG:NH1	2.28	0.65
1:D:20:ASN:HA	4:D:203:35I:H16	1.79	0.64
1:D:17:LYS:HB2	1:D:123:GLY:HA2	1.79	0.64
1:E:56:PRO:O	1:E:58:ARG:NH1	2.31	0.63
1:F:119:HIS:ND1	5:F:352:HOH:O	2.30	0.63
1:D:160:LYS:NZ	5:D:309:HOH:O	2.32	0.61
1:B:56:PRO:O	1:B:58:ARG:NH1	2.33	0.61
1:C:32:VAL:HG12	4:C:203:35I:H1	1.83	0.60
1:C:166:ARG:NH2	5:C:379:HOH:O	2.33	0.60
1:G:56:PRO:O	1:G:58:ARG:NH1	2.31	0.60
1:F:56:PRO:O	1:F:58:ARG:NH2	2.34	0.60
1:B:34:LYS:O	5:B:337:HOH:O	2.17	0.59
1:D:30[B]:GLN:NE2	4:D:203:35I:F16	2.25	0.59
1:C:13:ARG:NH1	1:C:128:PRO:O	2.36	0.58
1:H:129:GLU:OE1	1:H:130:MET:N	2.35	0.58
1:H:62:ILE:HD13	1:H:71:VAL:HG11	1.85	0.57
1:D:24:ARG:HH22	1:E:89:ASN:ND2	1.97	0.57
1:E:33:LYS:HG3	1:E:58:ARG:HH21	1.70	0.57
1:D:58:ARG:NH1	4:D:203:35I:C07	2.12	0.57
1:D:55:LEU:HD23	4:D:203:35I:C05	2.35	0.56
1:B:58:ARG:NH1	4:B:203:35I:H3	2.21	0.56
1:E:13:ARG:NH1	1:E:128:PRO:O	2.39	0.55
1:D:127:PHE:CD1	1:D:128:PRO:HD2	2.41	0.55
1:F:148:LYS:NZ	5:F:330:HOH:O	2.29	0.55
1:D:29:LEU:HD22	4:D:203:35I:H12	1.89	0.55
1:H:29:LEU:HB3	4:H:202:35I:H8	1.88	0.55
1:A:39:HIS:HE1	5:A:442:HOH:O	1.89	0.55
1:D:55:LEU:H	1:D:55:LEU:HD12	1.72	0.54
1:F:56:PRO:O	1:F:58:ARG:NH1	2.40	0.54
1:H:59:ARG:HH22	1:H:86:LEU:HB3	1.73	0.54
1:F:58:ARG:HG3	1:F:58:ARG:HH11	1.72	0.53
1:G:10:ASP:HB2	1:G:119:HIS:O	2.08	0.53
1:D:58:ARG:HH12	4:D:203:35I:H2	0.43	0.53
1:E:33:LYS:HG3	1:E:58:ARG:NH2	2.24	0.53
1:H:69:TYR:HB3	1:H:76:VAL:HG21	1.90	0.53
1:C:34:LYS:HE3	5:C:363:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:HG23	1:A:105:PHE:CE1	2.44	0.52
1:E:59:ARG:NE	1:E:75:GLU:OE2	2.39	0.52
1:F:162:GLN:NE2	5:F:380:HOH:O	2.41	0.52
1:F:10:ASP:HB2	1:F:119:HIS:O	2.10	0.51
1:D:44:GLY:HA3	3:D:202:CL:CL	2.47	0.51
1:D:55:LEU:H	1:D:55:LEU:CD1	2.23	0.51
1:D:41:LEU:HD22	1:D:58:ARG:HD2	1.93	0.51
1:H:22:PRO:HG2	1:H:23:TRP:CE3	2.46	0.51
1:D:58:ARG:HH12	4:D:203:35I:C08	2.08	0.51
1:F:137:GLU:O	1:H:142:LYS:HE3	2.11	0.51
1:D:54:PRO:O	1:D:56:PRO:HD3	2.11	0.50
1:C:85:GLU:OE2	1:C:88:LYS:NZ	2.44	0.50
1:H:53:ARG:NH2	4:H:202:35I:H10	2.26	0.50
1:E:10:ASP:HB2	1:E:119:HIS:O	2.11	0.50
1:F:166:ARG:NH2	5:F:328:HOH:O	2.44	0.50
1:H:58:ARG:NH1	4:H:202:35I:H3	2.27	0.50
1:F:67:GLU:HA	1:F:78:HIS:CD2	2.46	0.49
1:F:75:GLU:OE2	5:F:353:HOH:O	2.20	0.49
1:G:83:VAL:HG21	1:G:105:PHE:HZ	1.78	0.49
1:C:13:ARG:NH2	5:C:326:HOH:O	2.42	0.49
1:C:17:LYS:HA	1:C:124:ASP:OD1	2.12	0.49
1:B:60:ASN:HD22	1:B:60:ASN:N	2.09	0.49
1:H:160:LYS:NZ	5:H:355:HOH:O	2.46	0.49
1:G:112:LEU:HB2	1:G:158:TYR:HB2	1.95	0.48
1:B:70:HIS:HB3	5:B:441:HOH:O	2.13	0.48
1:F:58:ARG:NH2	4:F:203:35I:H3	2.28	0.48
1:G:56:PRO:HD2	4:G:203:35I:H4	1.95	0.48
1:C:10:ASP:HB2	1:C:119:HIS:O	2.14	0.48
1:B:10:ASP:HB2	1:B:119:HIS:O	2.14	0.48
1:F:39:HIS:O	1:F:58:ARG:HG2	2.13	0.48
1:H:86:LEU:N	5:H:336:HOH:O	2.38	0.48
1:G:30:GLN:HG2	5:G:412:HOH:O	2.13	0.48
1:D:100:GLN:NE2	5:D:358:HOH:O	2.42	0.47
1:D:112:LEU:HB2	1:D:158:TYR:HB2	1.95	0.47
1:D:58:ARG:NH2	4:D:203:35I:C08	2.66	0.47
1:H:59:ARG:NE	1:H:75:GLU:OE1	2.47	0.47
1:H:60:ASN:O	1:H:74:CYS:HB3	2.15	0.47
1:A:41:LEU:HG	1:A:58:ARG:HG2	1.97	0.47
1:D:58:ARG:NH1	4:D:203:35I:C08	2.75	0.47
1:B:30:GLN:NE2	4:B:203:35I:F18	2.38	0.47
1:D:10:ASP:HB2	1:D:119:HIS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ARG:NH2	5:D:382:HOH:O	2.48	0.47
1:D:55:LEU:N	1:D:55:LEU:CD1	2.76	0.46
1:F:97:GLY:HA2	1:F:102:TYR:CZ	2.51	0.46
1:H:89:ASN:OD1	1:H:90:GLU:N	2.48	0.46
1:E:58:ARG:CZ	4:E:203:35I:H3	2.46	0.46
1:D:53:ARG:CZ	5:D:382:HOH:O	2.55	0.46
1:B:97:GLY:HA2	1:B:102:TYR:CE2	2.51	0.46
1:D:131:ASP:OD1	1:D:133:THR:OG1	2.31	0.46
1:F:29:LEU:HB3	4:F:203:35I:H7	1.98	0.46
1:A:44:GLY:HA3	3:A:202:CL:CL	2.54	0.45
1:D:163:LEU:HD12	1:D:163:LEU:HA	1.82	0.45
1:B:65:ARG:HD3	1:F:164:VAL:O	2.17	0.45
1:D:56:PRO:O	1:D:58:ARG:NH2	2.50	0.45
1:H:55:LEU:HD22	4:H:202:35I:C11	2.47	0.45
1:C:55:LEU:HA	1:C:56:PRO:HD3	1.77	0.44
1:A:97:GLY:HA2	1:A:102:TYR:CZ	2.52	0.44
1:D:15:ILE:HG13	1:D:125:THR:HG23	2.00	0.44
1:G:30:GLN:HG3	5:G:360:HOH:O	2.18	0.44
1:H:136:LYS:NZ	5:H:328:HOH:O	2.49	0.44
1:A:13:ARG:HD3	5:A:389:HOH:O	2.18	0.44
1:C:74:CYS:O	5:C:389:HOH:O	2.21	0.44
1:H:112:LEU:HB2	1:H:158:TYR:HB2	1.99	0.44
1:F:17:LYS:O	1:F:18:ASP:HB2	2.18	0.44
1:B:64:THR:O	1:B:78:HIS:HA	2.18	0.44
1:G:55:LEU:HA	1:G:56:PRO:HD3	1.85	0.43
1:D:97:GLY:HA2	1:D:102:TYR:CE2	2.54	0.43
1:G:59:ARG:NH2	1:G:75:GLU:OE1	2.47	0.43
1:A:134:ASN:HB3	5:A:438:HOH:O	2.18	0.43
1:B:17:LYS:HB2	1:B:123:GLY:HA2	2.01	0.43
1:F:79:SER:OG	1:F:82:GLU:HG3	2.18	0.43
1:C:146:ASP:HB2	1:C:147:GLU:OE1	2.19	0.43
1:H:39:HIS:O	1:H:58:ARG:HB2	2.19	0.43
1:A:10:ASP:HB2	1:A:119:HIS:O	2.18	0.42
1:H:96:PHE:O	4:H:202:35I:N38	2.52	0.42
1:E:71:VAL:HG23	1:E:74:CYS:HB2	2.01	0.42
1:G:19:ASN:HD21	1:G:46:LYS:HD2	1.85	0.42
1:H:85:GLU:N	5:H:336:HOH:O	2.51	0.42
1:D:22:PRO:HD2	1:D:23:TRP:CE3	2.55	0.42
1:A:127:PHE:HA	1:A:128:PRO:HD3	1.94	0.41
1:G:97:GLY:HA2	1:G:102:TYR:CE2	2.55	0.41
1:A:37:MET:HA	1:A:58:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LEU:HG	4:D:203:35I:H17	2.01	0.41
1:F:58:ARG:NH2	4:F:203:35I:C08	2.84	0.41
1:D:41:LEU:HD12	1:D:41:LEU:HA	1.81	0.41
1:H:66:ASN:O	1:H:78:HIS:CD2	2.74	0.41
1:D:98:GLY:HA3	3:D:202:CL:CL	2.57	0.41
1:C:60:ASN:N	1:C:60:ASN:HD22	2.19	0.41
1:F:59:ARG:NH2	1:F:75:GLU:OE2	2.54	0.41
1:B:88:LYS:HE3	1:B:88:LYS:HB2	1.86	0.41
1:E:21:LEU:HD23	1:E:21:LEU:HA	1.95	0.41
1:C:8:ALA:HA	1:C:115:THR:HB	2.02	0.40
1:D:21:LEU:HA	1:D:22:PRO:HD3	1.91	0.40
1:C:70:HIS:HB2	5:C:438:HOH:O	2.20	0.40
1:G:97:GLY:HA2	1:G:102:TYR:CZ	2.57	0.40
1:B:98:GLY:HA3	3:B:202:CL:CL	2.59	0.40
1:A:112:LEU:O	1:A:157:VAL:HA	2.22	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:E:147:GLU:OE2	5:A:418:HOH:O[2_555]	2.10	0.10

## 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	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	B	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	C	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	D	165/166 (99%)	154 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	164/166 (99%)	161 (98%)	3 (2%)	0	100	100
1	F	164/166 (99%)	158 (96%)	5 (3%)	1 (1%)	25	31
1	G	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
1	H	165/166 (99%)	158 (96%)	6 (4%)	1 (1%)	25	31
All	All	1314/1328 (99%)	1275 (97%)	37 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	66	ASN
1	H	73	GLY

### 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	150/150 (100%)	146 (97%)	4 (3%)	44	61
1	B	149/150 (99%)	146 (98%)	3 (2%)	55	72
1	C	150/150 (100%)	148 (99%)	2 (1%)	69	82
1	D	151/150 (101%)	140 (93%)	11 (7%)	14	18
1	E	150/150 (100%)	145 (97%)	5 (3%)	38	53
1	F	150/150 (100%)	144 (96%)	6 (4%)	31	44
1	G	150/150 (100%)	149 (99%)	1 (1%)	84	92
1	H	151/150 (101%)	143 (95%)	8 (5%)	22	31
All	All	1201/1200 (100%)	1161 (97%)	40 (3%)	38	53

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	58	ARG

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Mol	Chain	Res	Type
1	A	59	ARG
1	A	81	GLU
1	B	60	ASN
1	B	162	GLN
1	B	163	LEU
1	C	88	LYS
1	C	106	LEU
1	D	20	ASN
1	D	21	LEU
1	D	41	LEU
1	D	46	LYS
1	D	53	ARG
1	D	58	ARG
1	D	111	LYS
1	D	114	ILE
1	D	160	LYS
1	D	162	GLN
1	D	163	LEU
1	E	13	ARG
1	E	45	ARG
1	E	58	ARG
1	E	88	LYS
1	E	129	GLU
1	F	81	GLU
1	F	88	LYS
1	F	91	GLU
1	F	106	LEU
1	F	148	LYS
1	F	166	ARG
1	G	80	VAL
1	H	17	LYS
1	H	58	ARG
1	H	64	THR
1	H	67	GLU
1	H	71	VAL
1	H	90	GLU
1	H	91	GLU
1	H	122	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	B	70	HIS
1	B	162	GLN
1	E	60	ASN
1	E	89	ASN
1	H	12	ASN
1	H	78	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	35I	H	202	-	42,42,42	2.37	10 (23%)	53,60,60	2.05	16 (30%)
4	35I	F	203	-	42,42,42	2.32	10 (23%)	53,60,60	1.95	13 (24%)
4	35I	D	203	-	42,42,42	2.47	9 (21%)	53,60,60	1.97	12 (22%)
4	35I	G	203	-	42,42,42	2.42	11 (26%)	53,60,60	1.82	14 (26%)
4	35I	B	203	-	42,42,42	2.51	10 (23%)	53,60,60	1.88	13 (24%)
4	35I	E	203	-	42,42,42	2.54	10 (23%)	53,60,60	1.95	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	35I	C	203	-	42,42,42	2.53	9 (21%)	53,60,60	1.94	16 (30%)
4	35I	A	203	-	42,42,42	2.51	10 (23%)	53,60,60	1.84	13 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	35I	H	202	-	-	5/22/36/36	0/3/4/4
4	35I	F	203	-	-	10/22/36/36	0/3/4/4
4	35I	D	203	-	-	6/22/36/36	0/3/4/4
4	35I	G	203	-	-	2/22/36/36	0/3/4/4
4	35I	B	203	-	-	3/22/36/36	0/3/4/4
4	35I	E	203	-	-	9/22/36/36	0/3/4/4
4	35I	C	203	-	-	7/22/36/36	0/3/4/4
4	35I	A	203	-	-	4/22/36/36	0/3/4/4

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	203	35I	C05-N04	10.79	1.42	1.29
4	D	203	35I	C05-N04	10.60	1.42	1.29
4	B	203	35I	C05-N04	10.59	1.42	1.29
4	A	203	35I	C05-N04	10.33	1.41	1.29
4	C	203	35I	C05-N04	10.24	1.41	1.29
4	H	202	35I	C05-N04	10.05	1.41	1.29
4	F	203	35I	C05-N04	9.87	1.41	1.29
4	G	203	35I	C05-N04	9.80	1.41	1.29
4	D	203	35I	C06-C11	-6.10	1.33	1.40
4	G	203	35I	C06-C11	-5.99	1.34	1.40
4	E	203	35I	C06-C11	-5.87	1.34	1.40
4	C	203	35I	C06-C11	-5.78	1.34	1.40
4	B	203	35I	C06-C11	-5.64	1.34	1.40
4	A	203	35I	C06-C11	-5.62	1.34	1.40
4	H	202	35I	C06-C11	-5.47	1.34	1.40
4	F	203	35I	C06-C11	-5.42	1.34	1.40
4	C	203	35I	C21-C20	5.42	1.55	1.47
4	E	203	35I	C21-C20	5.36	1.55	1.47
4	A	203	35I	C21-C20	5.33	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	203	35I	C21-C20	5.28	1.55	1.47
4	D	203	35I	C21-C20	4.93	1.55	1.47
4	G	203	35I	C21-C20	4.71	1.54	1.47
4	H	202	35I	C21-C20	4.62	1.54	1.47
4	C	203	35I	C37-N38	4.54	1.45	1.34
4	B	203	35I	C34-N35	4.47	1.42	1.33
4	F	203	35I	C21-C20	4.40	1.54	1.47
4	A	203	35I	C34-N35	4.31	1.42	1.33
4	G	203	35I	C34-N35	4.19	1.42	1.33
4	D	203	35I	C37-N38	4.12	1.44	1.34
4	E	203	35I	C34-N35	4.11	1.42	1.33
4	H	202	35I	C34-N35	4.11	1.42	1.33
4	D	203	35I	C34-N35	4.07	1.42	1.33
4	C	203	35I	C34-N35	4.06	1.42	1.33
4	B	203	35I	C37-N38	3.90	1.43	1.34
4	A	203	35I	C37-N38	3.86	1.43	1.34
4	G	203	35I	C37-N38	3.74	1.43	1.34
4	F	203	35I	C34-N35	3.66	1.41	1.33
4	E	203	35I	C37-N38	3.62	1.43	1.34
4	F	203	35I	C37-N38	3.61	1.43	1.34
4	E	203	35I	C02-N03	3.51	1.42	1.36
4	A	203	35I	C02-N03	3.47	1.42	1.36
4	C	203	35I	C02-N03	3.39	1.42	1.36
4	H	202	35I	C37-N38	3.29	1.42	1.34
4	D	203	35I	C02-N03	3.20	1.42	1.36
4	F	203	35I	C02-N03	3.06	1.41	1.36
4	B	203	35I	C02-N03	3.04	1.41	1.36
4	A	203	35I	C19-C02	3.00	1.53	1.48
4	E	203	35I	C19-C02	2.90	1.52	1.48
4	H	202	35I	C02-N03	2.84	1.41	1.36
4	C	203	35I	C19-C02	2.67	1.52	1.48
4	E	203	35I	C07-C06	2.67	1.45	1.41
4	G	203	35I	C02-N03	2.65	1.41	1.36
4	C	203	35I	C19-C20	2.51	1.39	1.33
4	H	202	35I	C07-C06	2.49	1.45	1.41
4	B	203	35I	C07-C06	2.47	1.45	1.41
4	E	203	35I	C19-C20	2.46	1.39	1.33
4	A	203	35I	C19-C20	2.44	1.39	1.33
4	B	203	35I	C19-C02	2.42	1.52	1.48
4	G	203	35I	C19-C02	2.39	1.52	1.48
4	C	203	35I	C07-C06	2.38	1.45	1.41
4	H	202	35I	C19-C02	2.35	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	35I	C07-C06	2.34	1.45	1.41
4	G	203	35I	C07-C06	2.33	1.45	1.41
4	G	203	35I	C19-C20	2.33	1.39	1.33
4	B	203	35I	C19-C20	2.31	1.39	1.33
4	H	202	35I	C19-C20	2.28	1.39	1.33
4	H	202	35I	C21-C22	-2.27	1.37	1.41
4	F	203	35I	C19-C02	2.25	1.51	1.48
4	A	203	35I	C21-C22	-2.20	1.37	1.41
4	D	203	35I	C07-C06	2.14	1.44	1.41
4	G	203	35I	C21-C22	-2.13	1.37	1.41
4	B	203	35I	C21-C22	-2.12	1.38	1.41
4	D	203	35I	C19-C02	2.11	1.51	1.48
4	F	203	35I	C10-C11	2.11	1.42	1.39
4	E	203	35I	C10-C11	2.11	1.42	1.39
4	F	203	35I	C19-C20	2.10	1.38	1.33
4	D	203	35I	C19-C20	2.08	1.38	1.33
4	F	203	35I	C07-C06	2.03	1.44	1.41
4	G	203	35I	C10-C11	2.01	1.42	1.39

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	203	35I	C06-C05-N04	-7.33	116.14	125.88
4	H	202	35I	C06-C05-N04	-6.98	116.61	125.88
4	F	203	35I	C06-C05-N04	-6.58	117.14	125.88
4	G	203	35I	C06-C05-N04	-6.37	117.43	125.88
4	A	203	35I	C06-C05-N04	-5.79	118.19	125.88
4	E	203	35I	C06-C05-N04	-5.60	118.45	125.88
4	B	203	35I	C06-C05-N04	-5.42	118.68	125.88
4	C	203	35I	C06-C05-N04	-4.78	119.54	125.88
4	B	203	35I	N33-C34-N36	-4.48	120.24	125.70
4	H	202	35I	C31-C32-N33	-4.47	116.37	123.82
4	E	203	35I	N33-C34-N36	-4.39	120.36	125.70
4	A	203	35I	N33-C34-N36	-4.30	120.47	125.70
4	C	203	35I	C30-C31-C37	-4.22	116.34	122.17
4	G	203	35I	N33-C34-N36	-4.13	120.68	125.70
4	D	203	35I	N33-C34-N36	-3.95	120.89	125.70
4	H	202	35I	C30-C31-C37	-3.79	116.94	122.17
4	H	202	35I	N33-C34-N36	-3.78	121.10	125.70
4	E	203	35I	C19-C02-N03	3.75	122.41	115.91
4	B	203	35I	C34-N36-C37	3.69	121.07	116.99
4	H	202	35I	C32-N33-C34	3.68	123.25	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	203	35I	C34-N36-C37	3.60	120.96	116.99
4	H	202	35I	C21-C20-C19	-3.59	119.79	126.93
4	A	203	35I	C34-N36-C37	3.58	120.94	116.99
4	C	203	35I	C31-C32-N33	-3.51	117.97	123.82
4	D	203	35I	C34-N36-C37	3.50	120.85	116.99
4	F	203	35I	N33-C34-N36	-3.45	121.50	125.70
4	C	203	35I	N38-C37-N36	3.38	121.82	117.03
4	H	202	35I	C06-C11-C12	3.35	120.27	116.94
4	D	203	35I	C19-C02-N03	3.35	121.71	115.91
4	F	203	35I	C19-C02-N03	3.33	121.67	115.91
4	B	203	35I	C11-C12-N03	3.32	112.95	108.00
4	B	203	35I	C06-C11-C12	3.25	120.16	116.94
4	C	203	35I	C11-C12-N03	3.17	112.74	108.00
4	D	203	35I	C30-C31-C37	-3.15	117.82	122.17
4	B	203	35I	O26-C25-C28	-3.14	118.72	124.12
4	F	203	35I	C24-O23-C22	3.12	123.34	114.78
4	E	203	35I	O26-C25-C22	3.12	120.64	115.16
4	F	203	35I	C11-C06-C05	3.10	120.26	117.73
4	F	203	35I	O26-C25-C22	3.09	120.59	115.16
4	B	203	35I	O26-C25-C22	3.08	120.58	115.16
4	B	203	35I	C21-C20-C19	-3.07	120.83	126.93
4	G	203	35I	C34-N36-C37	3.06	120.37	116.99
4	C	203	35I	N33-C34-N36	-3.06	121.97	125.70
4	G	203	35I	C21-C20-C19	-2.99	120.98	126.93
4	D	203	35I	N38-C37-N36	2.99	121.25	117.03
4	A	203	35I	C11-C12-N03	2.99	112.46	108.00
4	E	203	35I	C30-C31-C37	-2.97	118.07	122.17
4	C	203	35I	C32-C31-C37	2.96	119.75	115.72
4	F	203	35I	C21-C20-C19	-2.95	121.08	126.93
4	E	203	35I	C11-C12-N03	2.94	112.39	108.00
4	E	203	35I	O26-C25-C28	-2.90	119.14	124.12
4	B	203	35I	C11-C06-C05	2.87	120.07	117.73
4	G	203	35I	C32-N33-C34	2.85	121.72	116.44
4	D	203	35I	C31-C32-N33	-2.85	119.07	123.82
4	E	203	35I	N38-C37-N36	2.83	121.03	117.03
4	E	203	35I	C31-C32-N33	-2.83	119.11	123.82
4	F	203	35I	C31-C32-N33	-2.82	119.12	123.82
4	G	203	35I	C31-C32-N33	-2.82	119.13	123.82
4	H	202	35I	C31-C30-C29	2.78	120.51	114.22
4	D	203	35I	C21-C20-C19	-2.76	121.45	126.93
4	E	203	35I	C32-N33-C34	2.73	121.50	116.44
4	C	203	35I	C34-N36-C37	2.72	120.00	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	203	35I	C21-C20-C19	-2.71	121.54	126.93
4	A	203	35I	C32-N33-C34	2.69	121.42	116.44
4	A	203	35I	C31-C32-N33	-2.68	119.35	123.82
4	D	203	35I	C32-N33-C34	2.67	121.38	116.44
4	B	203	35I	C32-N33-C34	2.65	121.35	116.44
4	G	203	35I	C06-C11-C12	2.63	119.55	116.94
4	A	203	35I	O26-C25-C22	2.62	119.77	115.16
4	F	203	35I	C32-N33-C34	2.62	121.30	116.44
4	F	203	35I	O26-C25-C28	-2.61	119.62	124.12
4	C	203	35I	C24-O23-C22	2.61	121.92	114.78
4	C	203	35I	C06-C11-C12	2.60	119.52	116.94
4	C	203	35I	C21-C39-C29	-2.59	119.18	122.22
4	E	203	35I	C24-O23-C22	2.58	121.86	114.78
4	H	202	35I	N35-C34-N33	2.57	120.05	117.44
4	H	202	35I	C11-C12-N03	2.57	111.84	108.00
4	B	203	35I	C31-C32-N33	-2.56	119.55	123.82
4	F	203	35I	C34-N36-C37	2.54	119.80	116.99
4	A	203	35I	C13-C14-C15	2.52	119.52	113.94
4	C	203	35I	C11-C06-C05	2.50	119.78	117.73
4	B	203	35I	N35-C34-N33	2.48	119.96	117.44
4	H	202	35I	C32-C31-C37	2.48	119.09	115.72
4	G	203	35I	C07-C06-C11	2.48	120.92	118.64
4	A	203	35I	C06-C11-C12	2.47	119.39	116.94
4	H	202	35I	C24-O23-C22	2.46	121.51	114.78
4	F	203	35I	C30-C31-C37	-2.45	118.79	122.17
4	C	203	35I	C32-N33-C34	2.43	120.94	116.44
4	D	203	35I	O26-C25-C22	2.41	119.40	115.16
4	G	203	35I	N35-C34-N33	2.41	119.88	117.44
4	G	203	35I	C11-C12-N03	2.41	111.59	108.00
4	A	203	35I	C11-C06-C05	2.39	119.68	117.73
4	C	203	35I	C31-C37-N38	-2.37	118.83	122.19
4	G	203	35I	C31-C30-C29	2.36	119.56	114.22
4	E	203	35I	N35-C34-N33	2.33	119.81	117.44
4	G	203	35I	C24-O23-C22	2.32	121.13	114.78
4	H	202	35I	C31-C37-N38	-2.32	118.90	122.19
4	A	203	35I	N35-C34-N33	2.28	119.75	117.44
4	G	203	35I	C11-C06-C05	2.25	119.57	117.73
4	H	202	35I	C07-C06-C11	2.25	120.71	118.64
4	H	202	35I	C21-C39-C29	-2.22	119.61	122.22
4	A	203	35I	O26-C25-C28	-2.18	120.36	124.12
4	F	203	35I	C07-C06-C11	2.16	120.63	118.64
4	H	202	35I	C11-C06-C05	2.14	119.48	117.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	203	35I	C31-C37-N38	-2.12	119.18	122.19
4	E	203	35I	C06-C11-C12	2.11	119.03	116.94
4	D	203	35I	O26-C25-C28	-2.10	120.50	124.12
4	G	203	35I	C13-C14-C15	2.08	118.54	113.94
4	E	203	35I	C13-C14-C15	2.07	118.52	113.94
4	B	203	35I	C24-O23-C22	2.05	120.40	114.78
4	A	203	35I	N38-C37-N36	2.04	119.92	117.03
4	C	203	35I	O26-C25-C22	2.04	118.74	115.16
4	D	203	35I	C32-C31-C37	2.02	118.47	115.72

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	202	35I	N03-C12-C13-C14
4	H	202	35I	C12-C13-C14-C15
4	H	202	35I	C13-C14-C15-F16
4	G	203	35I	C11-C12-C13-C14
4	G	203	35I	C12-C13-C14-C15
4	F	203	35I	O01-C02-C19-C20
4	F	203	35I	N03-C02-C19-C20
4	F	203	35I	C11-C12-C13-C14
4	F	203	35I	C12-C13-C14-C15
4	F	203	35I	C13-C14-C15-F17
4	D	203	35I	O01-C02-C19-C20
4	D	203	35I	N03-C02-C19-C20
4	D	203	35I	C11-C12-C13-C14
4	D	203	35I	C12-C13-C14-C15
4	B	203	35I	N03-C12-C13-C14
4	E	203	35I	O01-C02-C19-C20
4	E	203	35I	N03-C02-C19-C20
4	E	203	35I	N03-C12-C13-C14
4	C	203	35I	N03-C12-C13-C14
4	C	203	35I	C11-C12-C13-C14
4	C	203	35I	C13-C14-C15-F16
4	A	203	35I	N03-C12-C13-C14
4	F	203	35I	C19-C20-C21-C22
4	H	202	35I	C13-C14-C15-F17
4	H	202	35I	C13-C14-C15-F18
4	F	203	35I	C13-C14-C15-F16
4	C	203	35I	C13-C14-C15-F17
4	A	203	35I	C13-C14-C15-F16

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Mol	Chain	Res	Type	Atoms
4	A	203	35I	C13-C14-C15-F17
4	E	203	35I	C22-C25-O26-C27
4	B	203	35I	C22-C25-O26-C27
4	F	203	35I	C19-C20-C21-C39
4	D	203	35I	C19-C20-C21-C39
4	E	203	35I	C28-C25-O26-C27
4	E	203	35I	C19-C20-C21-C22
4	E	203	35I	C19-C20-C21-C39
4	C	203	35I	C22-C25-O26-C27
4	F	203	35I	C13-C14-C15-F18
4	C	203	35I	C13-C14-C15-F18
4	A	203	35I	C13-C14-C15-F18
4	D	203	35I	C19-C20-C21-C22
4	B	203	35I	C28-C25-O26-C27
4	F	203	35I	N03-C12-C13-C14
4	C	203	35I	C28-C25-O26-C27
4	E	203	35I	C13-C14-C15-F16
4	E	203	35I	C13-C14-C15-F18

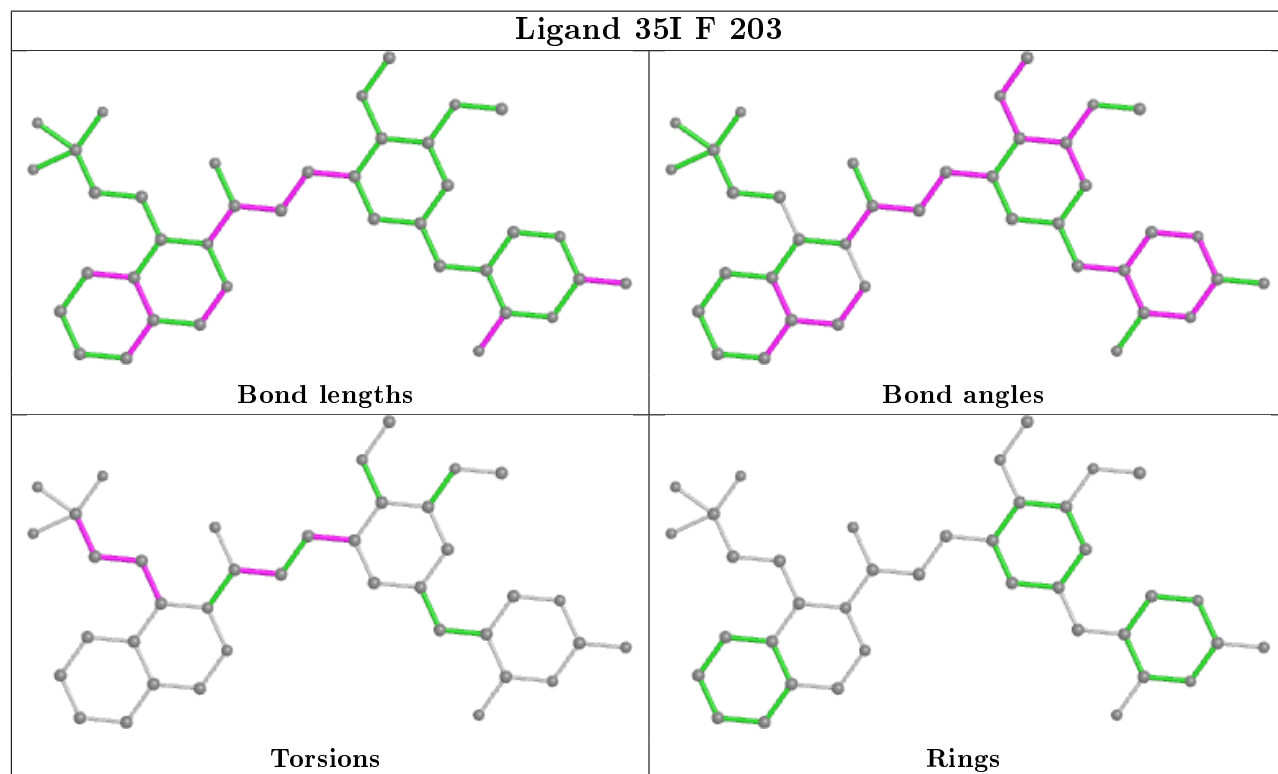
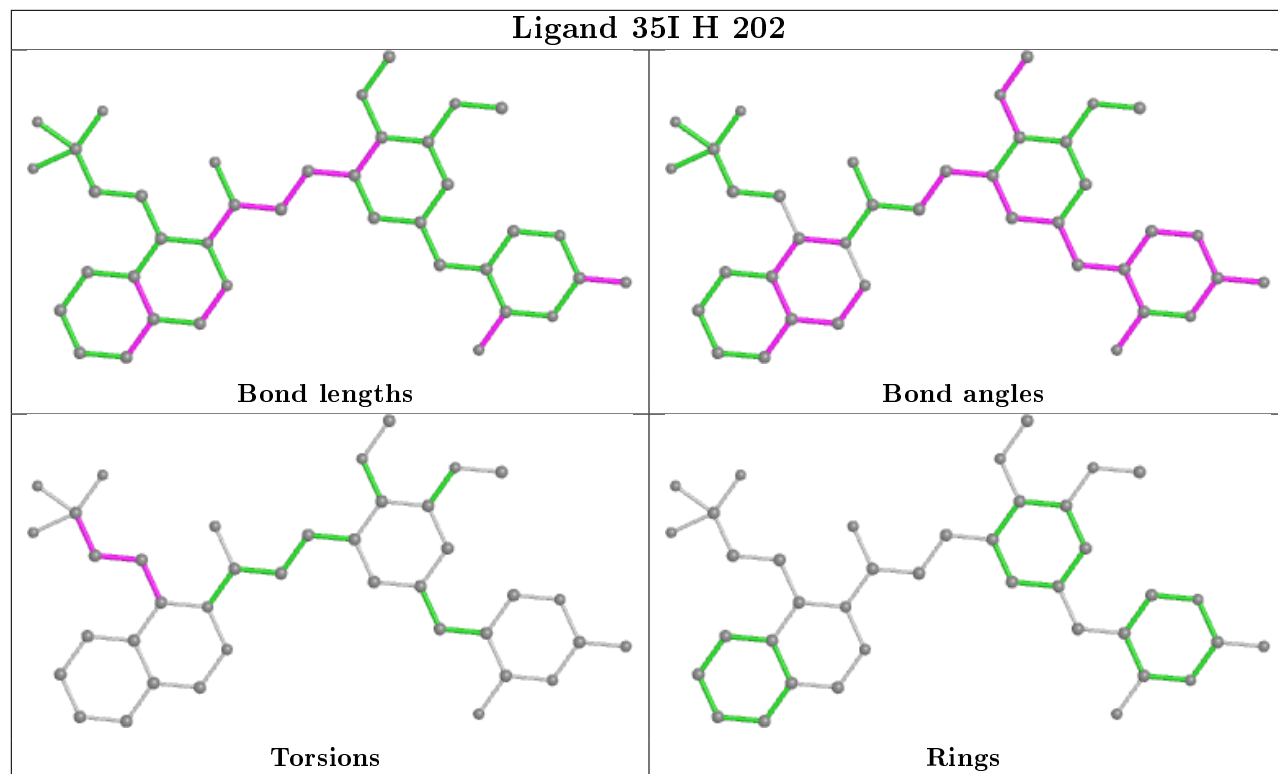
There are no ring outliers.

7 monomers are involved in 31 short contacts:

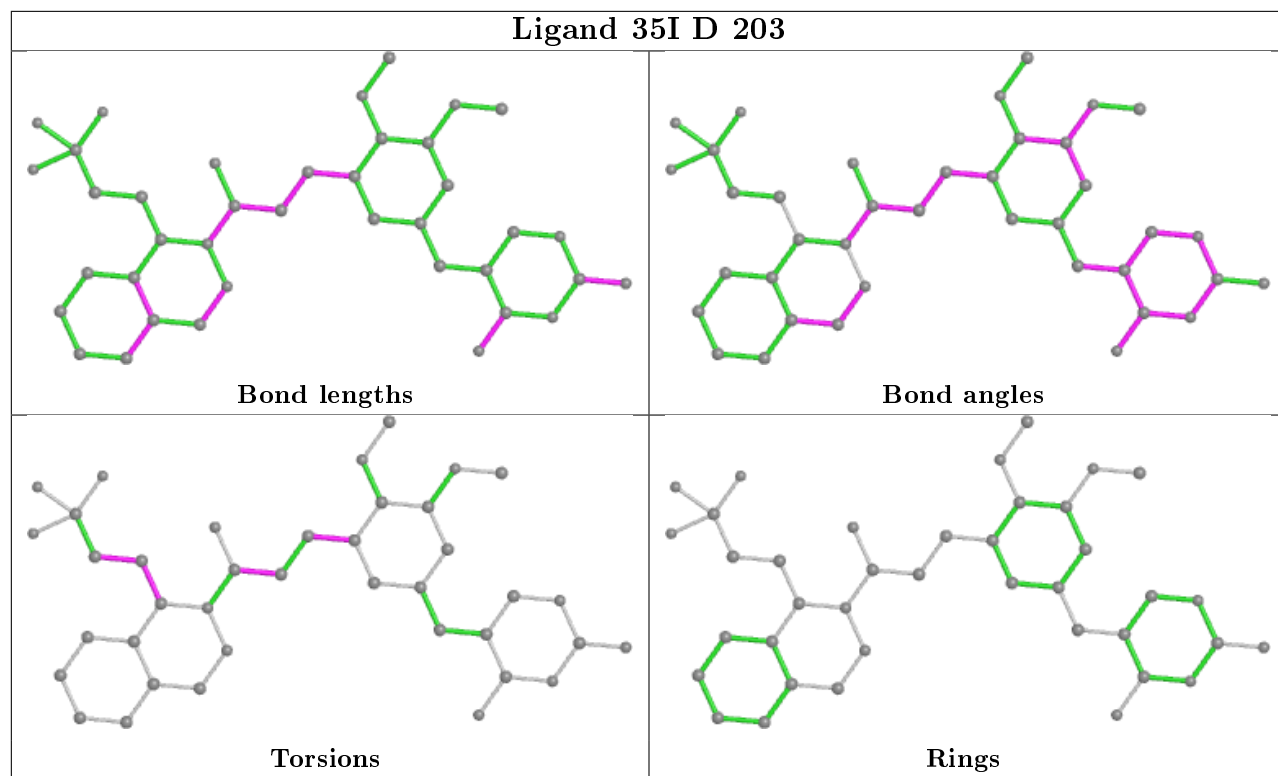
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	202	35I	5	0
4	F	203	35I	4	0
4	D	203	35I	15	0
4	G	203	35I	1	0
4	B	203	35I	2	0
4	E	203	35I	3	0
4	C	203	35I	1	0

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

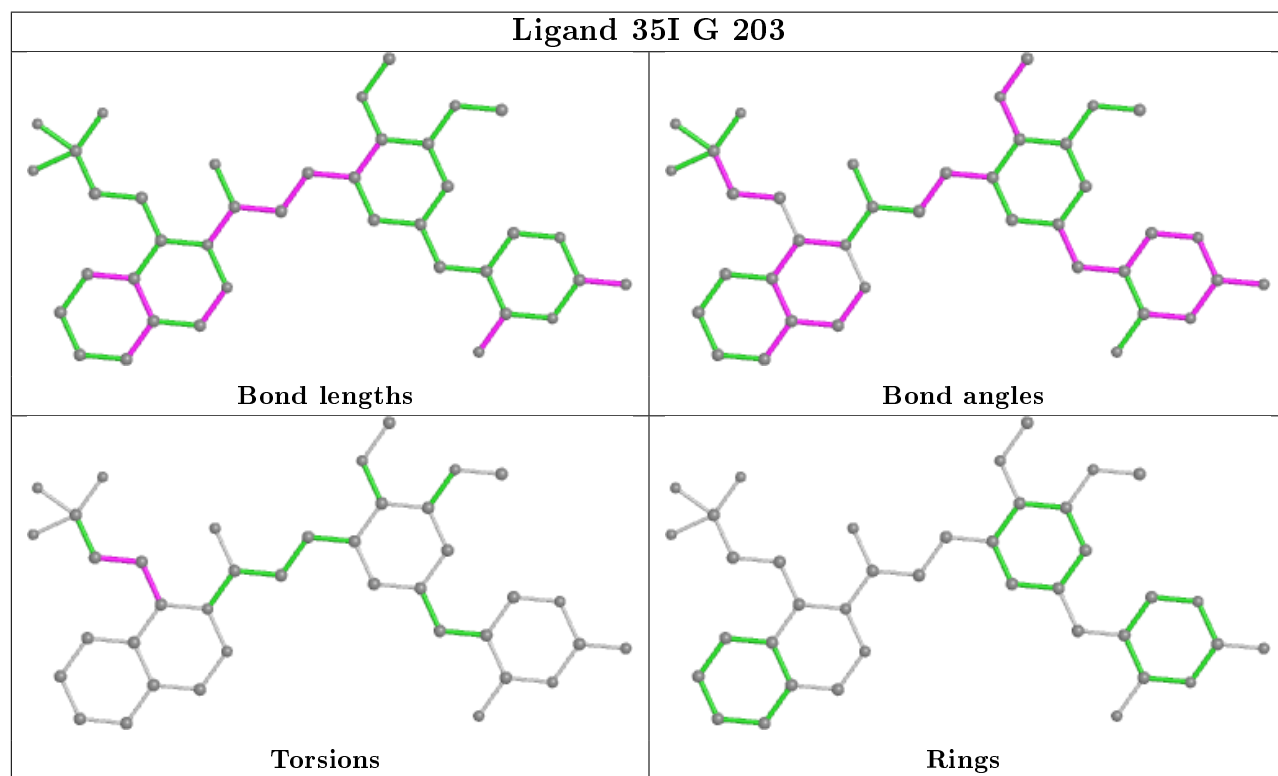
equivalents in the CSD to analyse the geometry.



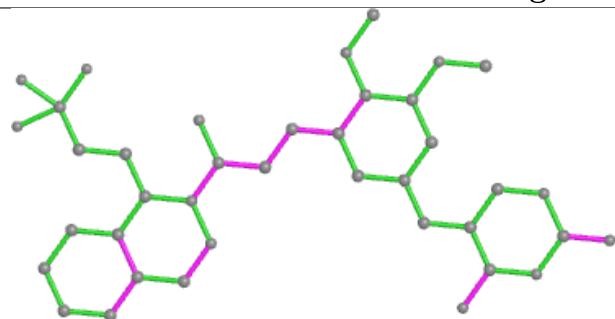
## Ligand 35I D 203



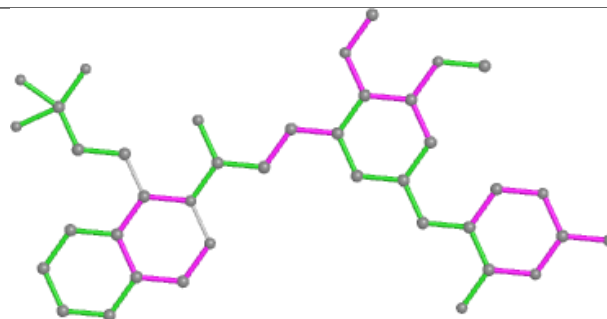
## Ligand 35I G 203



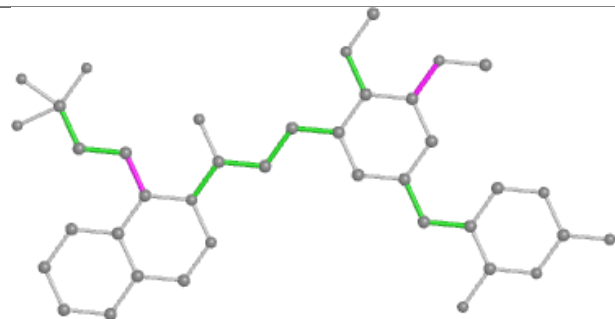
## Ligand 35I B 203



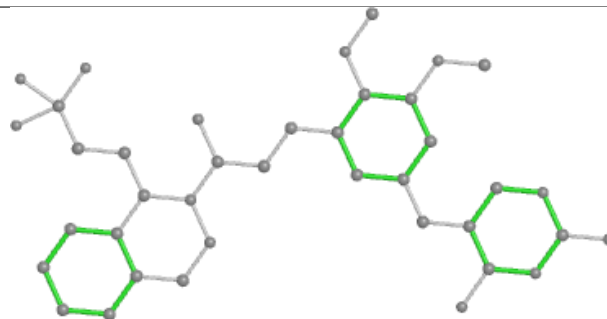
Bond lengths



Bond angles

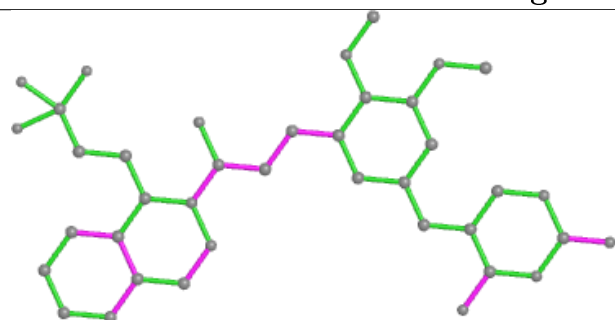


Torsions

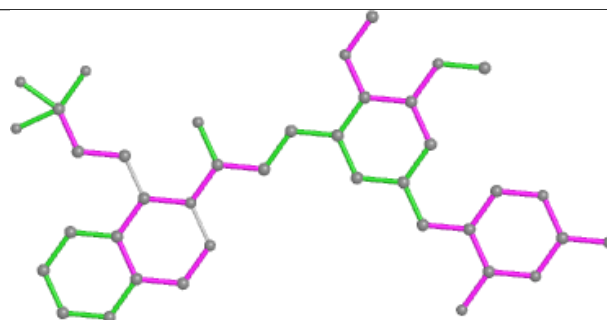


Rings

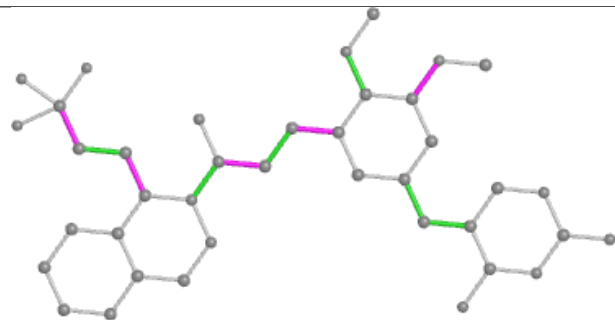
## Ligand 35I E 203



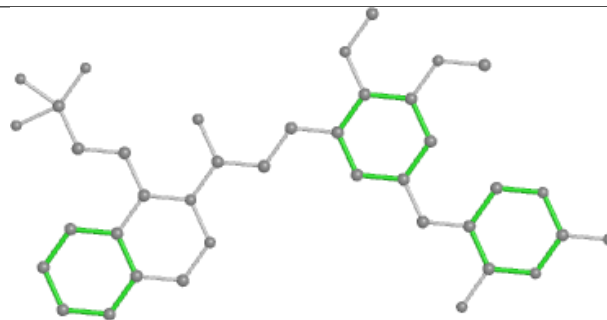
Bond lengths



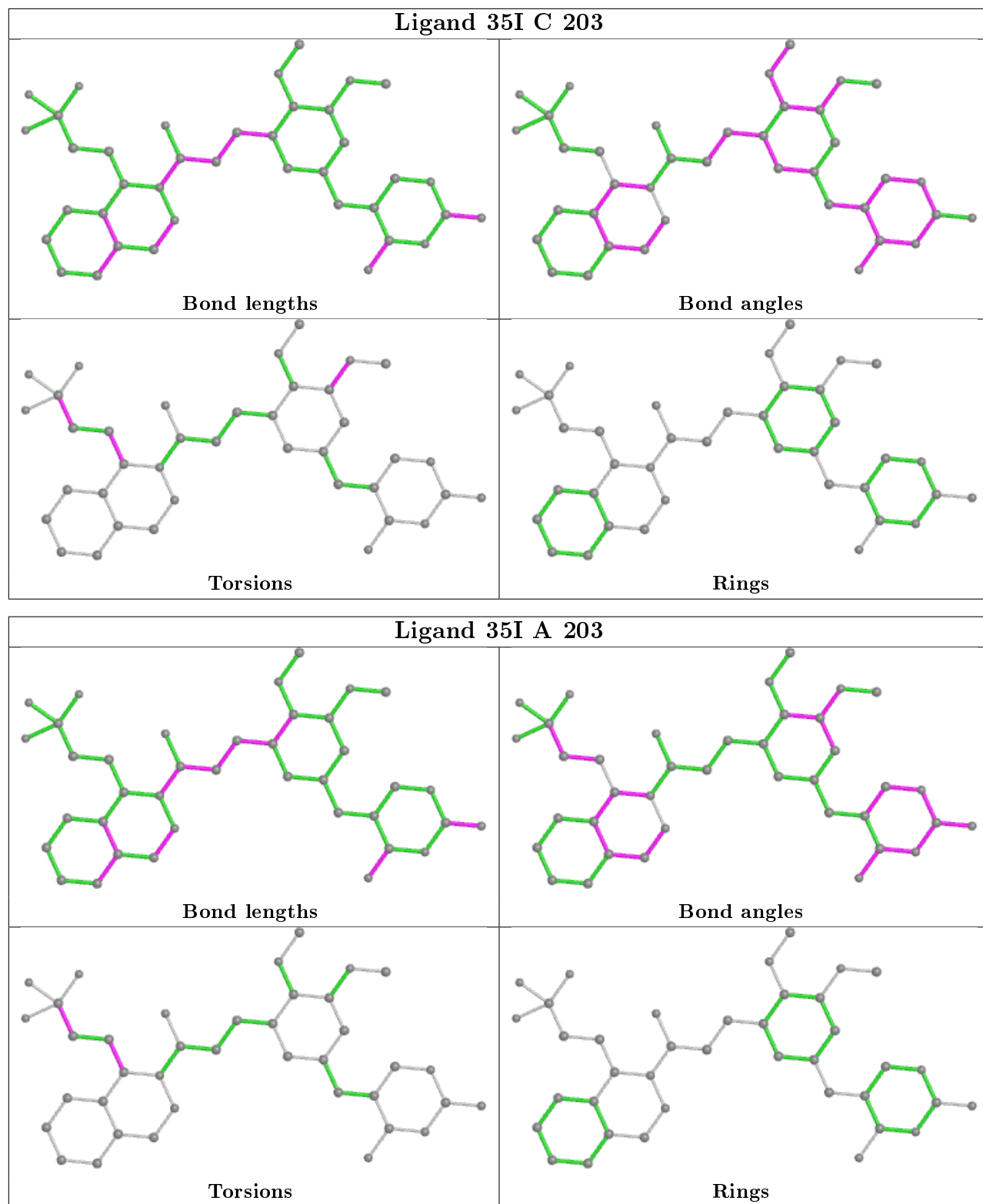
Bond angles



Torsions



Rings



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	166/166 (100%)	-0.22	0 <span>100</span> <span>100</span>	19, 34, 56, 65	0
1	B	166/166 (100%)	-0.34	0 <span>100</span> <span>100</span>	21, 32, 51, 56	0
1	C	166/166 (100%)	-0.25	3 (1%) <span>68</span> <span>74</span>	22, 33, 50, 56	0
1	D	166/166 (100%)	-0.15	3 (1%) <span>68</span> <span>74</span>	21, 37, 69, 98	0
1	E	166/166 (100%)	-0.18	0 <span>100</span> <span>100</span>	21, 39, 60, 72	0
1	F	166/166 (100%)	-0.26	1 (0%) <span>89</span> <span>92</span>	22, 38, 57, 69	0
1	G	166/166 (100%)	-0.26	0 <span>100</span> <span>100</span>	23, 37, 58, 67	0
1	H	166/166 (100%)	0.36	18 (10%) <span>5</span> <span>8</span>	20, 45, 98, 129	0
All	All	1328/1328 (100%)	-0.16	25 (1%) <span>66</span> <span>73</span>	19, 37, 65, 129	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	89	ASN	10.1
1	H	70	HIS	7.8
1	H	69	TYR	5.0
1	H	66	ASN	4.1
1	D	55	LEU	3.8
1	H	51	ILE	3.4
1	H	72	GLU	3.4
1	H	53	ARG	3.1
1	H	19	ASN	3.0
1	H	52	GLY	2.9
1	H	73	GLY	2.8
1	H	88	LYS	2.7
1	H	48	TYR	2.7
1	C	70	HIS	2.5
1	H	68	GLY	2.5
1	H	38	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	166	ARG	2.3
1	H	64	THR	2.2
1	C	19	ASN	2.2
1	H	62	ILE	2.2
1	D	163	LEU	2.2
1	D	58	ARG	2.1
1	C	51	ILE	2.1
1	H	71	VAL	2.0
1	F	52	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CL	H	201	1/1	0.57	0.35	98,98,98,98	0
2	CA	H	203	1/1	0.75	0.10	66,66,66,66	0
4	35I	G	203	39/39	0.79	0.16	28,43,50,50	0
4	35I	F	203	39/39	0.80	0.17	33,58,63,64	0
4	35I	B	203	39/39	0.80	0.17	24,43,66,66	0
4	35I	D	203	39/39	0.81	0.19	27,56,62,62	0
2	CA	A	201	1/1	0.81	0.12	54,54,54,54	0
4	35I	H	202	39/39	0.83	0.15	18,53,60,60	0
4	35I	E	203	39/39	0.84	0.17	25,52,64,64	0
4	35I	A	203	39/39	0.85	0.17	17,40,56,56	0
4	35I	C	203	39/39	0.89	0.14	16,37,56,56	0
3	CL	F	202	1/1	0.91	0.10	54,54,54,54	0
3	CL	B	202	1/1	0.93	0.14	37,37,37,37	0
2	CA	D	201	1/1	0.93	0.15	32,32,32,32	0

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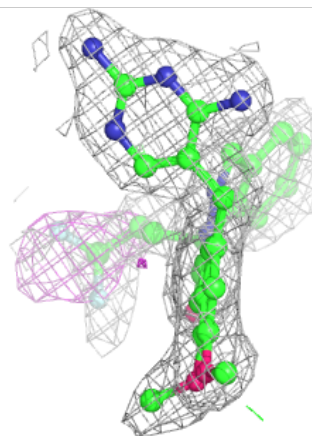
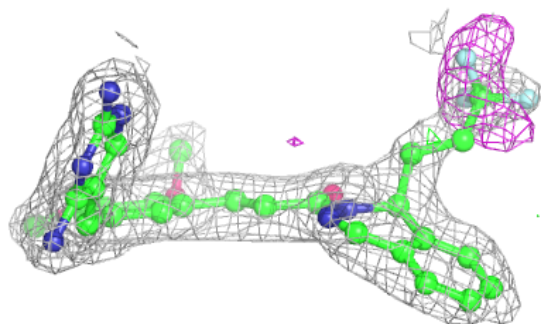
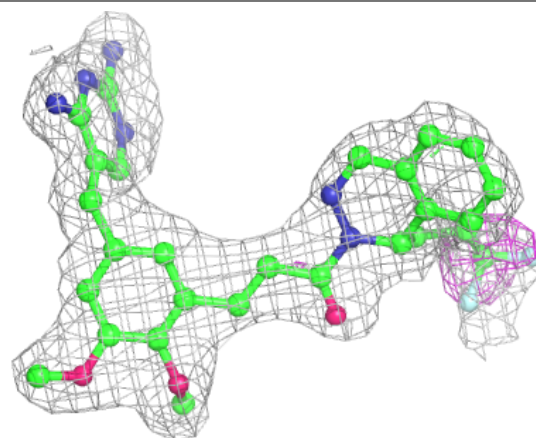
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	F	201	1/1	0.94	0.09	44,44,44,44	0
2	CA	B	201	1/1	0.96	0.12	33,33,33,33	0
2	CA	G	201	1/1	0.97	0.09	39,39,39,39	0
3	CL	G	202	1/1	0.97	0.10	48,48,48,48	0
3	CL	D	202	1/1	0.97	0.13	40,40,40,40	0
2	CA	E	201	1/1	0.98	0.06	39,39,39,39	0
3	CL	A	202	1/1	0.98	0.11	28,28,28,28	0
3	CL	C	202	1/1	0.98	0.18	35,35,35,35	0
3	CL	E	202	1/1	0.98	0.16	49,49,49,49	0
2	CA	C	201	1/1	1.00	0.12	27,27,27,27	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.

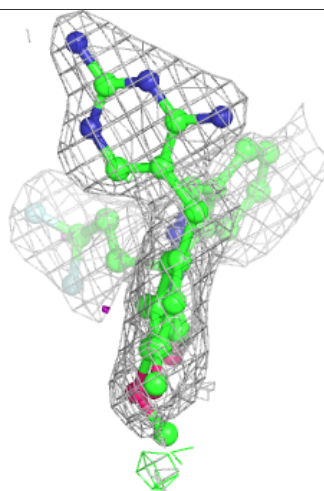
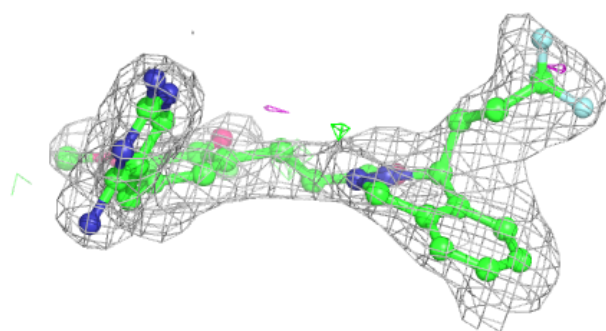
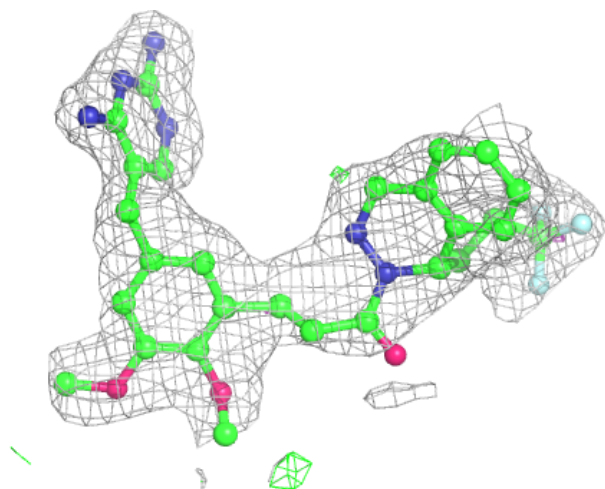
**Electron density around 35I G 203:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



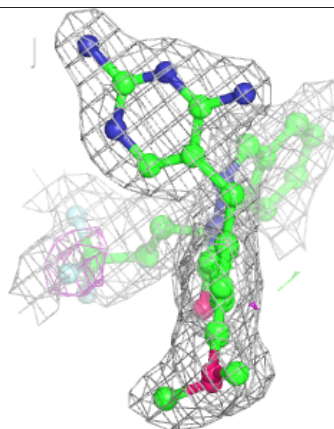
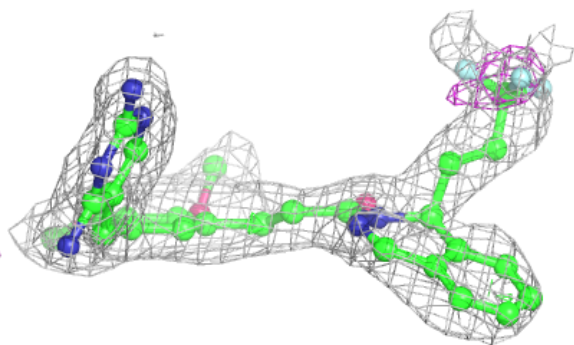
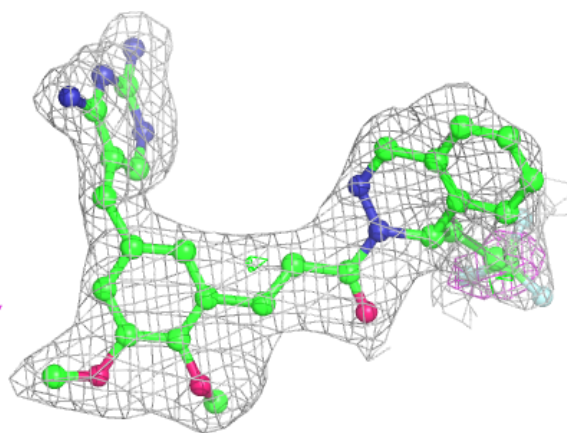
**Electron density around 35I F 203:**

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



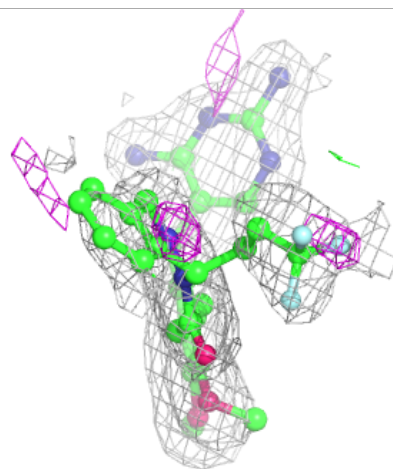
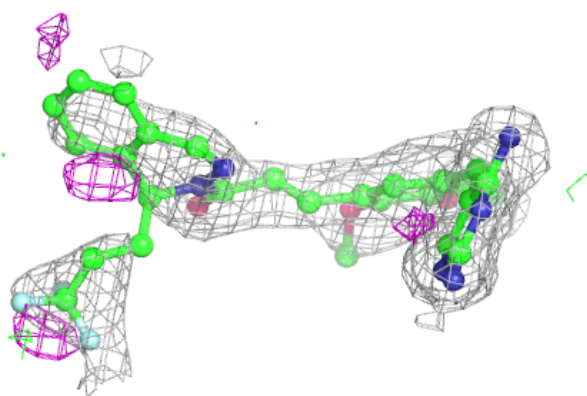
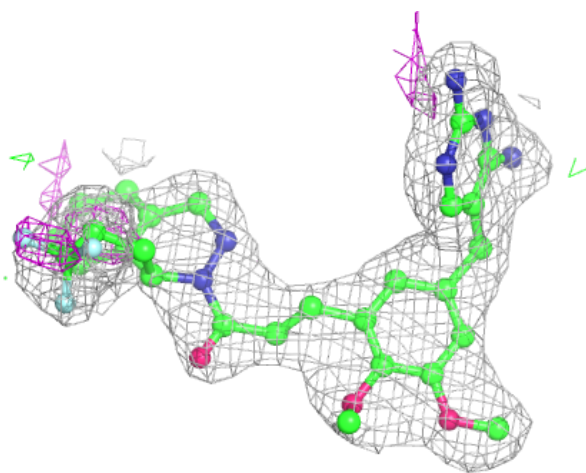
**Electron density around 35I B 203:**

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



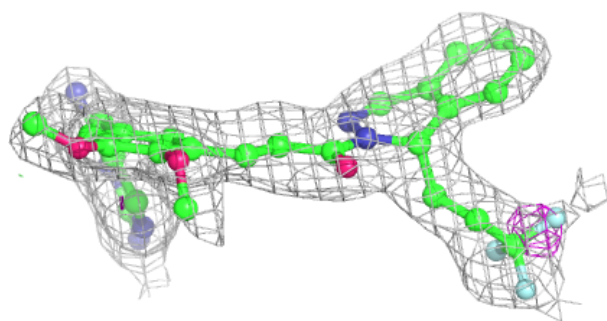
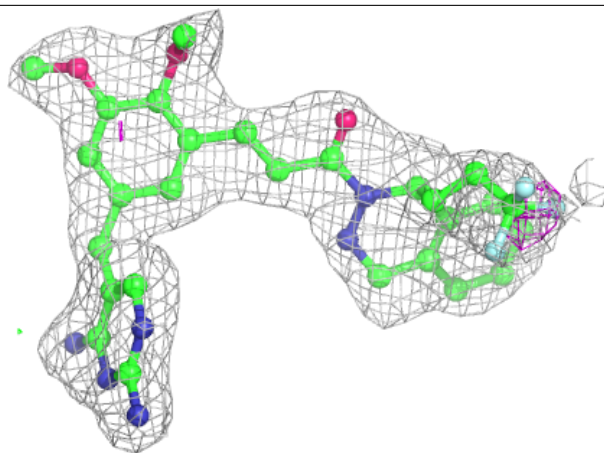
**Electron density around 35I D 203:**

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



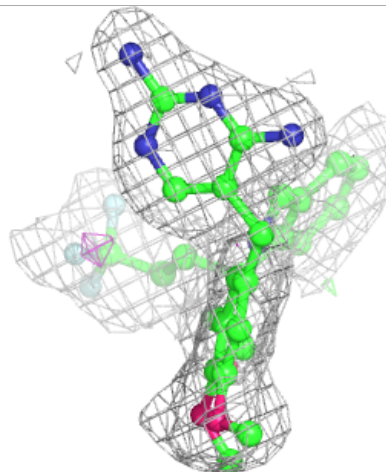
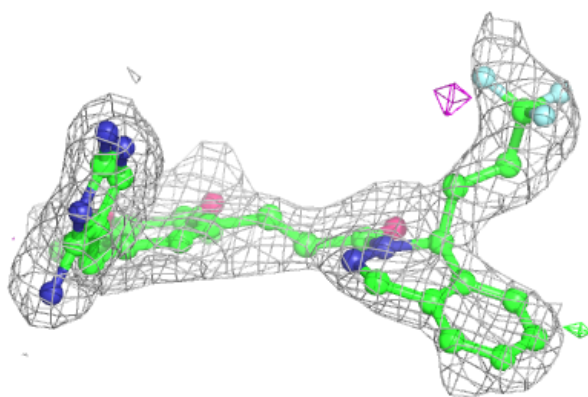
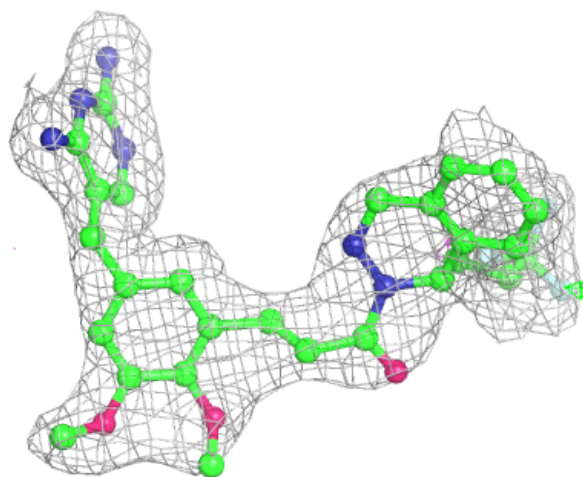
**Electron density around 35I H 202:**

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



**Electron density around 35I E 203:**

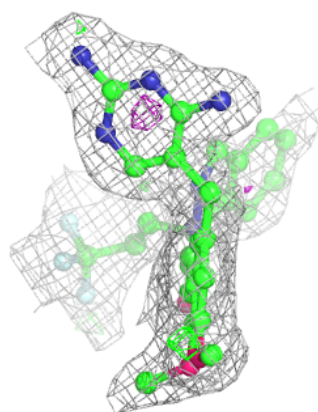
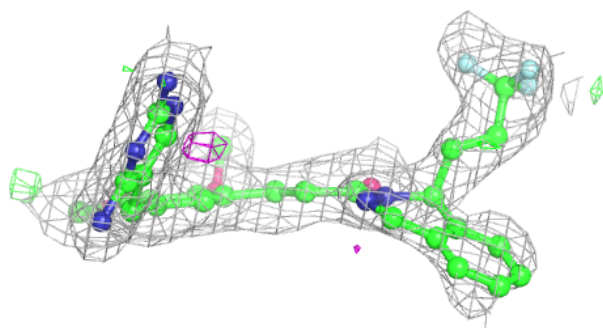
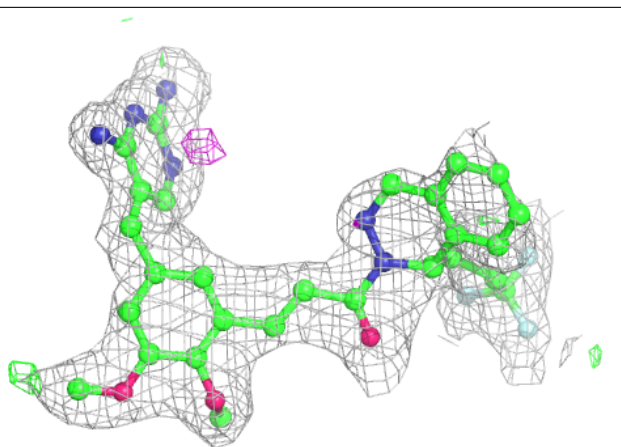
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





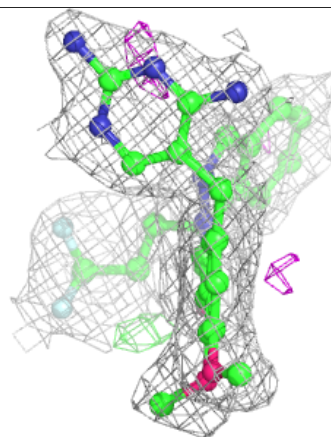
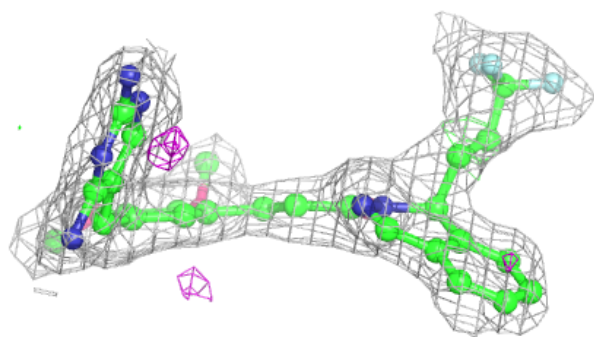
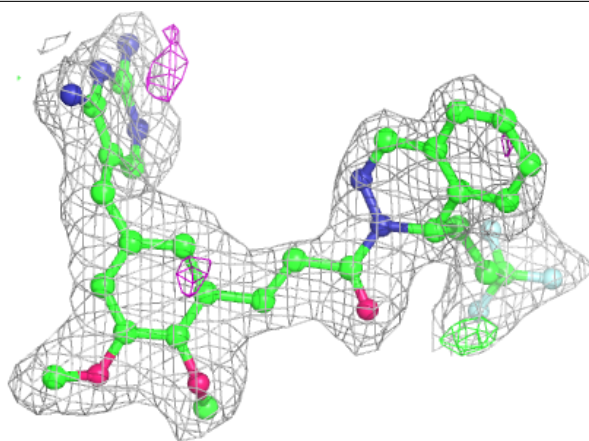
**Electron density around 35I A 203:**

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



**Electron density around 35I C 203:**

$2mF_o - DF_c$  (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.