



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:57 AM EDT

PDB ID : 6EG7
Title : BbvCI B2 dimer with I3C clusters
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2018-08-19
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

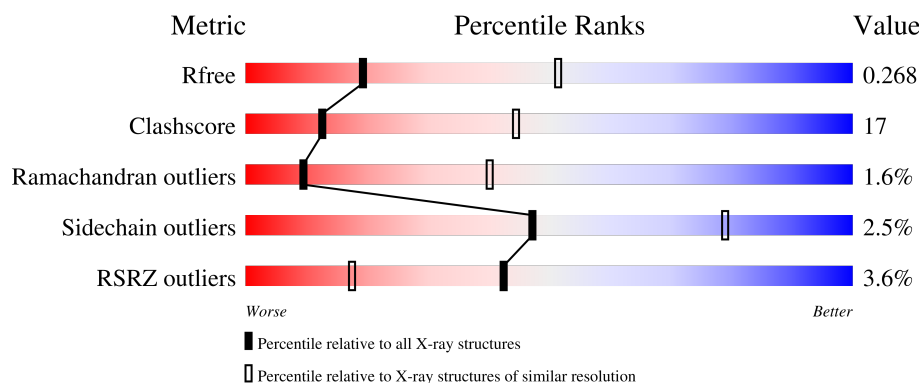
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	285	<div> <div>4%</div> <div>70%</div> <div>24%</div> <div>• •</div> </div>
1	B	285	<div> <div>3%</div> <div>66%</div> <div>27%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	301	-	X	-	-
4	I3C	A	306	-	-	X	-

2 Entry composition [i](#)

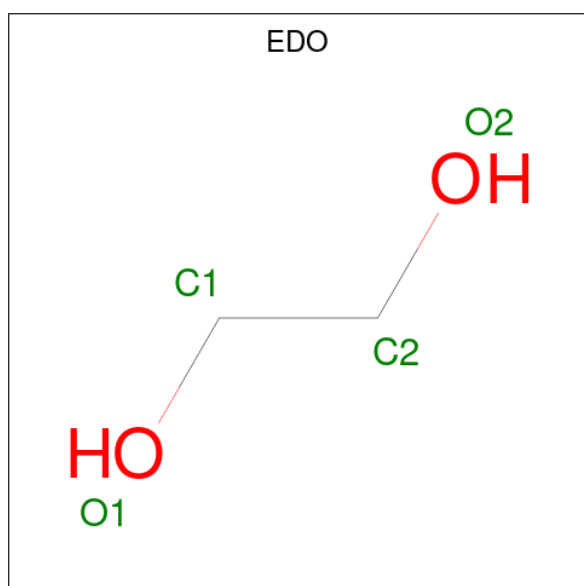
There are 5 unique types of molecules in this entry. The entry contains 4626 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BbvCI endonuclease subunit 2.

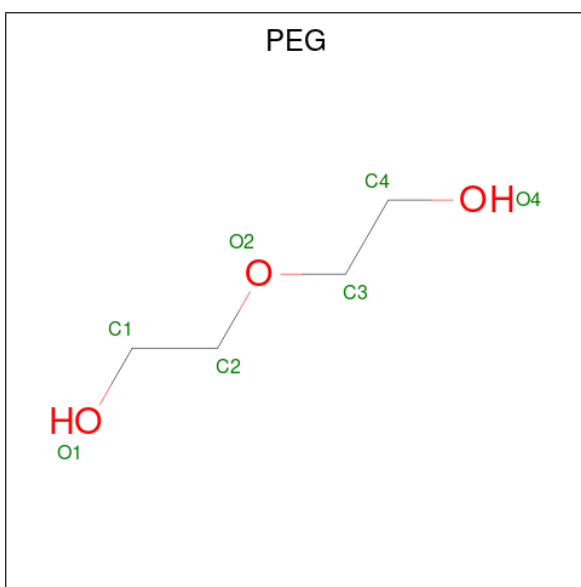
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2244	1431	385	420	8			
1	B	276	Total	C	N	O	S	0	0	0
			2219	1417	378	416	8			

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



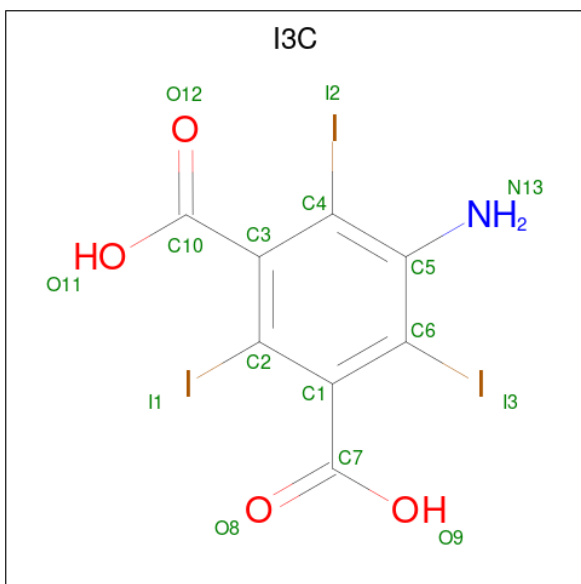
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 5-amino-2,4,6-triodobenzene-1,3-dicarboxylic acid (three-letter code: I3C) (formula: $C_8H_4I_3NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	I	N	O	0	0
			16	8	3	1	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	I	N	O	0	0
			16	8	3	1	4		
4	A	1	Total	C	I	N	O	0	0
			16	8	3	1	4		
4	A	1	Total	C	I	N	O	0	0
			16	8	3	1	4		
4	B	1	Total	C	I	N	O	0	0
			16	8	3	1	4		
4	B	1	Total	C	I	N	O	0	0
			16	8	3	1	4		
4	B	1	Total	C	I	N	O	0	0
			16	8	3	1	4		
4	B	1	Total	C	I	N	O	0	0
			16	8	3	1	4		

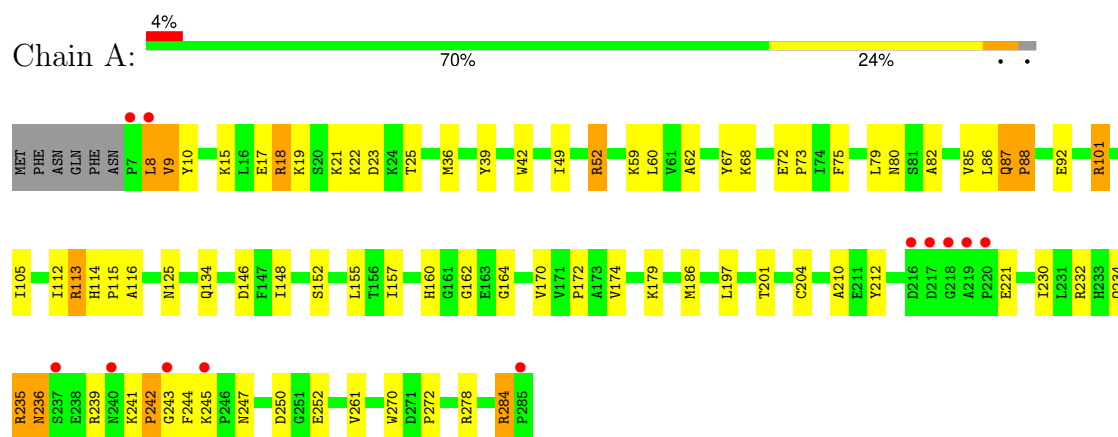
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	2	Total	O	0	0
			2	2		

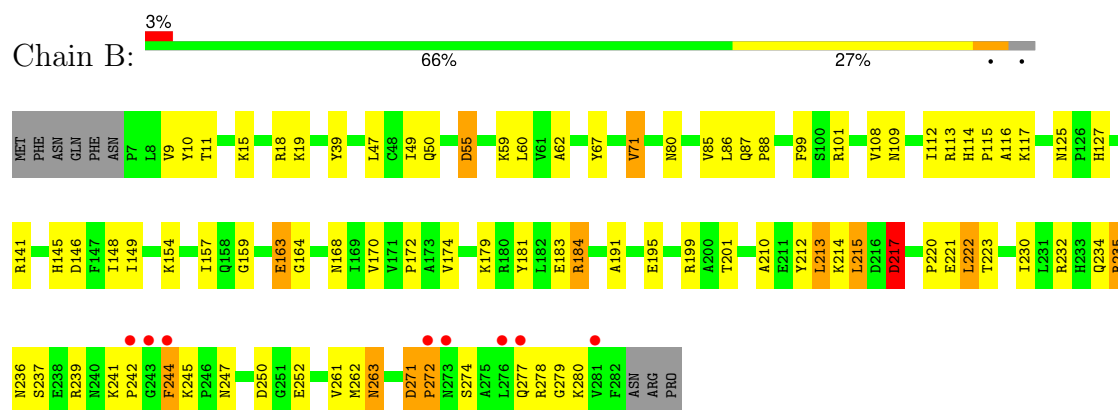
3 Residue-property plots

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

• Molecule 1: BbvCI endonuclease subunit 2



• Molecule 1: BbvCI endonuclease subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	93.89Å 168.25Å 106.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.38 – 3.00 30.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (30.38-3.00) 94.0 (30.36-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.60 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.213 , 0.262 0.218 , 0.268	Depositor DCC
R_{free} test set	821 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4626	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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, I3C, PEG

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	0.52	1/2296 (0.0%)	0.88	3/3107 (0.1%)
1	B	0.52	1/2270 (0.0%)	0.91	5/3072 (0.2%)
All	All	0.52	2/4566 (0.0%)	0.89	8/6179 (0.1%)

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	6
1	B	0	6
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	PRO	N-CD	-8.12	1.36	1.47
1	A	88	PRO	N-CD	-7.06	1.38	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	PRO	CA-N-CD	6.05	120.17	111.70
1	A	88	PRO	CA-N-CD	5.99	120.09	111.70
1	B	71	VAL	N-CA-C	5.44	125.70	111.00
1	A	236	ASN	N-CA-CB	5.37	120.27	110.60
1	B	263	ASN	CB-CA-C	-5.26	99.88	110.40
1	B	271	ASP	CB-CA-C	5.26	120.92	110.40
1	B	163	GLU	C-N-CA	-5.16	111.47	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	PRO	N-CA-CB	-5.07	97.02	102.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	113	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	235	ARG	Sidechain
1	A	278	ARG	Sidechain
1	A	52	ARG	Sidechain
1	B	101	ARG	Sidechain
1	B	113	ARG	Sidechain
1	B	141	ARG	Sidechain
1	B	18	ARG	Sidechain
1	B	184	ARG	Sidechain
1	B	199	ARG	Sidechain

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	2244	0	2222	82	0
1	B	2219	0	2200	71	1
2	A	12	0	17	2	0
3	A	7	0	10	2	1
3	B	7	0	10	2	0
4	A	64	0	8	14	0
4	B	64	0	8	7	0
5	A	7	0	0	0	0
5	B	2	0	0	1	0
All	All	4626	0	4475	152	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 17.

All (152) 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:B:235:ARG:NH2	1:B:237:SER:HB3	1.30	1.40
1:B:195:GLU:OE2	1:B:223:THR:CG2	1.79	1.30
1:B:195:GLU:OE2	1:B:223:THR:HG21	1.37	1.13
1:B:235:ARG:NH2	1:B:237:SER:CB	2.12	1.11
1:B:195:GLU:OE2	1:B:223:THR:HG22	1.57	1.03
1:B:235:ARG:HH21	1:B:237:SER:CB	1.72	1.02
1:A:241:LYS:HB3	1:A:242:PRO:HD2	1.43	1.00
1:A:15:LYS:HD3	1:A:85:VAL:HG22	1.46	0.96
1:B:235:ARG:HH22	1:B:237:SER:HB3	1.06	0.87
1:A:236:ASN:O	1:A:236:ASN:OD1	1.93	0.86
1:B:215:LEU:H	1:B:235:ARG:HE	1.23	0.86
1:A:221:GLU:N	1:A:221:GLU:OE1	2.10	0.84
1:A:19:LYS:HA	1:A:22:LYS:HE3	1.60	0.83
1:A:235:ARG:HG3	1:A:236:ASN:H	1.47	0.80
1:A:79:LEU:HD12	1:A:82:ALA:HB2	1.65	0.79
1:B:263:ASN:ND2	5:B:401:HOH:O	2.16	0.78
1:B:174:VAL:HG21	1:B:261:VAL:HG13	1.66	0.77
1:B:11:THR:HG23	4:B:305:I3C:O9	1.85	0.77
1:B:244:PHE:CD1	1:B:245:LYS:N	2.52	0.72
1:B:213:LEU:HB3	1:B:230:ILE:HG12	1.73	0.69
1:A:235:ARG:HG3	1:A:236:ASN:N	2.06	0.67
1:B:127:HIS:ND1	4:B:304:I3C:N13	2.43	0.67
1:A:79:LEU:CD1	1:A:82:ALA:HB2	2.24	0.67
1:A:212:TYR:CE2	1:A:239:ARG:HD3	2.29	0.67
1:B:67:TYR:O	1:B:71:VAL:HG22	1.95	0.67
1:A:52:ARG:NH1	1:A:60:LEU:HD11	2.11	0.66
1:B:234:GLN:HG3	1:B:247:ASN:HD22	1.61	0.66
1:B:234:GLN:HG3	1:B:247:ASN:ND2	2.10	0.65
1:A:85:VAL:HG11	4:A:306:I3C:C1	2.26	0.65
1:B:195:GLU:CD	1:B:223:THR:HG21	2.16	0.65
1:A:212:TYR:CZ	1:A:239:ARG:HD3	2.32	0.64
1:A:116:ALA:HB3	1:A:148:ILE:HD12	1.79	0.63
1:B:15:LYS:HE2	4:B:303:I3C:O12	1.99	0.63
1:B:116:ALA:HB3	1:B:148:ILE:HD12	1.79	0.63
1:A:79:LEU:HD12	1:A:82:ALA:CB	2.28	0.63
1:A:170:VAL:HG23	2:A:302:EDO:H11	1.80	0.62
1:A:72:GLU:OE2	1:A:87:GLN:NE2	2.30	0.62
1:A:146:ASP:OD1	4:A:305:I3C:I3	2.88	0.62
1:A:241:LYS:HB3	1:A:242:PRO:CD	2.26	0.62
1:B:241:LYS:HB3	1:B:242:PRO:HD2	1.81	0.62
1:B:244:PHE:HD1	1:B:245:LYS:H	1.38	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LYS:HB2	4:A:306:I3C:I1	2.70	0.61
1:A:22:LYS:NZ	4:A:306:I3C:O12	2.31	0.61
1:A:87:GLN:N	1:A:88:PRO:CD	2.64	0.60
1:A:174:VAL:HG21	1:A:261:VAL:HG13	1.82	0.60
1:B:39:TYR:HA	1:B:67:TYR:CE1	2.36	0.60
1:A:234:GLN:HG3	1:A:247:ASN:ND2	2.17	0.60
1:B:232:ARG:NH1	1:B:247:ASN:O	2.36	0.59
1:A:39:TYR:HA	1:A:67:TYR:CE1	2.38	0.59
1:B:55:ASP:N	1:B:55:ASP:OD1	2.35	0.59
1:B:154:LYS:HD3	1:B:168:ASN:OD1	2.03	0.58
1:B:213:LEU:CB	1:B:230:ILE:HG12	2.33	0.58
1:A:172:PRO:HD2	1:A:201:THR:HG21	1.86	0.57
1:A:75:PHE:O	1:A:79:LEU:HB2	2.04	0.57
1:A:241:LYS:CB	1:A:242:PRO:HD2	2.27	0.57
1:A:114:HIS:HB2	1:A:115:PRO:HD2	1.86	0.56
1:A:85:VAL:HG22	1:A:85:VAL:O	2.05	0.56
1:B:220:PRO:HG2	1:B:222:LEU:HD21	1.87	0.55
1:B:181:TYR:HA	1:B:212:TYR:O	2.06	0.55
1:B:67:TYR:CZ	1:B:71:VAL:HG21	2.42	0.55
1:A:15:LYS:CD	1:A:85:VAL:HG22	2.29	0.54
1:B:172:PRO:HD2	1:B:201:THR:HG21	1.87	0.54
1:B:271:ASP:OD2	1:B:274:SER:HB3	2.08	0.54
1:B:47:LEU:O	1:B:50:GLN:NE2	2.41	0.54
1:A:232:ARG:NH1	1:A:247:ASN:O	2.39	0.54
1:A:49:ILE:HD12	1:A:60:LEU:HD23	1.90	0.54
1:B:212:TYR:CE2	1:B:239:ARG:HD2	2.43	0.53
1:B:271:ASP:OD1	1:B:272:PRO:HD2	2.09	0.53
1:A:179:LYS:O	1:A:210:ALA:HA	2.09	0.53
1:B:49:ILE:HD12	1:B:60:LEU:HD23	1.90	0.53
1:B:114:HIS:HB2	1:B:115:PRO:HD2	1.90	0.53
1:B:179:LYS:O	1:B:210:ALA:HA	2.08	0.52
1:A:9:VAL:HG11	1:A:114:HIS:HB3	1.91	0.52
1:A:85:VAL:HG11	4:A:306:I3C:C6	2.40	0.52
1:A:152:SER:O	3:A:303:PEG:H12	2.10	0.52
1:A:134:GLN:OE1	1:A:160:HIS:HB3	2.10	0.51
1:A:52:ARG:NH1	1:A:60:LEU:CD1	2.73	0.51
1:B:146:ASP:OD1	4:B:302:I3C:I2	2.98	0.51
1:B:59:LYS:O	1:B:62:ALA:HB3	2.10	0.51
1:B:87:GLN:HB3	1:B:88:PRO:HD3	1.92	0.50
1:B:244:PHE:CG	1:B:245:LYS:N	2.80	0.50
1:A:179:LYS:HE2	1:A:186:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD1	1:A:252:GLU:HB2	2.13	0.49
1:A:59:LYS:O	1:A:62:ALA:HB3	2.13	0.49
1:B:15:LYS:HZ3	1:B:85:VAL:HG21	1.78	0.49
1:B:212:TYR:CZ	1:B:232:ARG:HD2	2.48	0.48
1:A:92:GLU:OE2	2:A:301:EDO:O2	2.32	0.48
1:A:36:MET:HB3	4:A:307:I3C:I3	2.84	0.48
1:A:272:PRO:HB2	1:B:215:LEU:HD12	1.95	0.48
1:B:234:GLN:CG	1:B:247:ASN:ND2	2.77	0.48
1:B:99:PHE:CD1	1:B:262:MET:HE3	2.48	0.48
1:A:157:ILE:O	1:A:164:GLY:HA2	2.14	0.47
1:B:191:ALA:HB2	1:B:221:GLU:O	2.14	0.47
1:B:214:LYS:HE2	1:B:236:ASN:ND2	2.28	0.47
1:A:101:ARG:O	1:A:105:ILE:HD12	2.14	0.47
1:A:234:GLN:HG3	1:A:247:ASN:HD22	1.78	0.47
1:B:9:VAL:O	1:B:10:TYR:CD1	2.67	0.47
1:B:168:ASN:HB3	3:B:301:PEG:H12	1.97	0.47
1:A:42:TRP:HB2	1:A:67:TYR:HB2	1.97	0.47
1:A:52:ARG:HH12	1:A:60:LEU:HD11	1.79	0.47
1:A:18:ARG:HD3	4:A:306:I3C:O8	2.15	0.47
1:A:114:HIS:HB2	1:A:115:PRO:CD	2.45	0.47
4:B:302:I3C:O9	4:B:305:I3C:N13	2.48	0.47
1:A:79:LEU:CD1	1:A:86:LEU:HD23	2.45	0.46
1:B:157:ILE:O	1:B:164:GLY:HA2	2.15	0.46
1:A:22:LYS:HZ1	4:A:306:I3C:C10	2.26	0.46
1:B:277:GLN:HG3	1:B:278:ARG:N	2.30	0.45
1:A:22:LYS:CE	4:A:306:I3C:I1	3.34	0.45
1:B:170:VAL:HG23	3:B:301:PEG:H31	1.97	0.45
1:B:271:ASP:HA	1:B:272:PRO:HD2	1.56	0.45
1:A:152:SER:C	3:A:303:PEG:H12	2.37	0.45
1:A:9:VAL:HG11	1:A:114:HIS:CB	2.47	0.45
1:B:250:ASP:OD1	1:B:252:GLU:HB2	2.17	0.45
1:A:22:LYS:HE2	4:A:306:I3C:I1	2.87	0.45
1:A:17:GLU:O	1:A:21:LYS:HB2	2.17	0.45
1:B:114:HIS:HB2	1:B:115:PRO:CD	2.46	0.45
1:B:145:HIS:HD2	1:B:148:ILE:HD11	1.81	0.45
1:A:52:ARG:HH12	1:A:60:LEU:CD1	2.30	0.44
1:A:85:VAL:HG11	4:A:306:I3C:C2	2.48	0.44
1:A:284:ARG:O	1:A:284:ARG:HG3	2.17	0.44
1:B:184:ARG:HD2	1:B:217:ASP:O	2.18	0.44
1:A:36:MET:CB	4:A:307:I3C:I3	3.36	0.44
1:A:85:VAL:CG1	4:A:306:I3C:C2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HB3	1:A:80:ASN:H	1.69	0.43
1:A:114:HIS:HD2	1:A:115:PRO:O	2.01	0.43
1:A:197:LEU:HD21	1:A:204:CYS:HB3	2.00	0.43
1:B:86:LEU:HD12	1:B:86:LEU:HA	1.89	0.42
1:A:23:ASP:OD1	1:A:25:THR:HB	2.19	0.42
1:B:232:ARG:O	1:B:234:GLN:HG3	2.19	0.42
1:B:215:LEU:HB2	1:B:235:ARG:HG3	2.01	0.42
1:A:15:LYS:HE3	1:A:85:VAL:CG2	2.50	0.42
1:B:241:LYS:HB3	1:B:242:PRO:CD	2.49	0.42
1:A:270:TRP:O	1:A:270:TRP:CE3	2.73	0.42
1:A:10:TYR:CD1	1:A:10:TYR:N	2.86	0.42
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.88	0.42
1:A:221:GLU:H	1:A:221:GLU:CD	2.18	0.42
1:A:72:GLU:N	1:A:73:PRO:CD	2.83	0.41
1:A:243:GLY:O	1:A:245:LYS:HG2	2.21	0.41
1:B:11:THR:CG2	4:B:305:I3C:O9	2.63	0.41
1:A:113:ARG:HA	1:A:148:ILE:O	2.21	0.41
1:B:112:ILE:O	1:B:149:ILE:HA	2.21	0.41
1:B:15:LYS:NZ	1:B:85:VAL:HG21	2.34	0.41
1:B:19:LYS:HD2	4:B:303:I3C:O9	2.20	0.41
1:A:155:LEU:C	1:A:155:LEU:HD23	2.40	0.41
1:A:230:ILE:O	1:B:280:LYS:HD2	2.21	0.41
1:A:68:LYS:HB3	1:A:72:GLU:OE1	2.21	0.41
1:A:112:ILE:HD11	1:A:152:SER:OG	2.21	0.41
1:A:22:LYS:HZ3	4:A:306:I3C:C3	2.34	0.40
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.79	0.40
1:B:108:VAL:HG22	1:B:109:ASN:N	2.36	0.40
1:B:183:GLU:HA	1:B:214:LYS:HG3	2.03	0.40
1:B:99:PHE:HD1	1:B:262:MET:HE3	1.86	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:B:159:GLY:O	3:A:303:PEG:O1[3_655]	2.16	0.04

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	277/285 (97%)	244 (88%)	29 (10%)	4 (1%)	11	43
1	B	274/285 (96%)	248 (90%)	21 (8%)	5 (2%)	8	37
All	All	551/570 (97%)	492 (89%)	50 (9%)	9 (2%)	9	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	PHE
1	B	244	PHE
1	A	8	LEU
1	A	162	GLY
1	A	242	PRO
1	B	80	ASN
1	B	215	LEU
1	B	217	ASP
1	B	279	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/250 (98%)	240 (98%)	4 (2%)	62	86
1	B	241/250 (96%)	233 (97%)	8 (3%)	38	73
All	All	485/500 (97%)	473 (98%)	12 (2%)	47	79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	87	GLN
1	A	125	ASN
1	A	284	ARG
1	B	55	ASP
1	B	117	LYS
1	B	125	ASN
1	B	163	GLU
1	B	213	LEU
1	B	217	ASP
1	B	222	LEU
1	B	235	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	B	236	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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
4	I3C	A	307	-	16,16,16	3.78	6 (37%)	24,24,24	1.58	5 (20%)
2	EDO	A	304	-	3,3,3	0.27	0	2,2,2	0.48	0
4	I3C	B	305	-	16,16,16	3.77	6 (37%)	24,24,24	1.57	5 (20%)
4	I3C	B	304	-	16,16,16	3.78	6 (37%)	24,24,24	1.57	5 (20%)
4	I3C	B	303	-	16,16,16	3.78	6 (37%)	24,24,24	1.59	5 (20%)
4	I3C	A	308	-	16,16,16	3.78	6 (37%)	24,24,24	1.57	5 (20%)
2	EDO	A	301	-	3,3,3	3.19	1 (33%)	2,2,2	2.45	1 (50%)
3	PEG	B	301	-	6,6,6	0.21	0	5,5,5	0.52	0
3	PEG	A	303	-	6,6,6	0.40	0	5,5,5	0.79	0
4	I3C	A	305	-	16,16,16	3.78	6 (37%)	24,24,24	1.58	5 (20%)
2	EDO	A	302	-	3,3,3	0.19	0	2,2,2	0.30	0
4	I3C	B	302	-	16,16,16	3.77	6 (37%)	24,24,24	1.58	5 (20%)
4	I3C	A	306	-	16,16,16	3.78	6 (37%)	24,24,24	1.55	5 (20%)

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	I3C	A	307	-	-	4/8/8/8	0/1/1/1
2	EDO	A	304	-	-	1/1/1/1	-
4	I3C	B	305	-	-	0/8/8/8	0/1/1/1
4	I3C	B	304	-	-	0/8/8/8	0/1/1/1
4	I3C	B	303	-	-	0/8/8/8	0/1/1/1
4	I3C	A	308	-	-	0/8/8/8	0/1/1/1
2	EDO	A	301	-	-	1/1/1/1	-
3	PEG	B	301	-	-	3/4/4/4	-
3	PEG	A	303	-	-	1/4/4/4	-
4	I3C	A	305	-	-	0/8/8/8	0/1/1/1
2	EDO	A	302	-	-	1/1/1/1	-
4	I3C	B	302	-	-	0/8/8/8	0/1/1/1
4	I3C	A	306	-	-	0/8/8/8	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	305	I3C	C3-C2	6.16	1.49	1.39
4	A	307	I3C	C3-C4	6.15	1.49	1.39
4	B	304	I3C	C1-C6	6.14	1.49	1.39
4	A	305	I3C	C1-C6	6.14	1.49	1.39
4	B	305	I3C	C3-C4	6.13	1.49	1.39
4	A	306	I3C	C3-C2	6.12	1.49	1.39
4	B	304	I3C	C3-C4	6.12	1.49	1.39
4	A	307	I3C	C1-C6	6.12	1.49	1.39
4	A	308	I3C	C1-C6	6.11	1.49	1.39
4	A	308	I3C	C3-C4	6.11	1.49	1.39
4	A	307	I3C	C3-C2	6.11	1.49	1.39
4	A	308	I3C	C3-C2	6.11	1.49	1.39
4	B	303	I3C	C3-C2	6.11	1.49	1.39
4	B	302	I3C	C1-C2	6.11	1.49	1.39
4	A	308	I3C	C1-C2	6.11	1.49	1.39
4	B	303	I3C	C1-C6	6.10	1.49	1.39
4	B	303	I3C	C3-C4	6.10	1.49	1.39
4	B	302	I3C	C1-C6	6.10	1.49	1.39
4	B	305	I3C	C1-C2	6.10	1.49	1.39
4	B	303	I3C	C1-C2	6.10	1.49	1.39
4	A	306	I3C	C1-C2	6.10	1.49	1.39
4	A	307	I3C	C1-C2	6.09	1.49	1.39
4	B	304	I3C	C3-C2	6.09	1.49	1.39
4	B	305	I3C	C3-C2	6.08	1.49	1.39
4	A	306	I3C	C1-C6	6.08	1.49	1.39
4	A	306	I3C	C3-C4	6.08	1.49	1.39
4	B	302	I3C	C3-C2	6.08	1.49	1.39
4	A	305	I3C	C3-C4	6.08	1.49	1.39
4	A	305	I3C	C1-C2	6.08	1.49	1.39
4	B	302	I3C	C3-C4	6.07	1.49	1.39
4	B	304	I3C	C1-C2	6.07	1.49	1.39
4	B	305	I3C	C1-C6	6.04	1.49	1.39
4	A	306	I3C	C5-C6	6.04	1.49	1.41
4	B	304	I3C	C5-C4	6.02	1.49	1.41
4	B	305	I3C	C5-C6	6.02	1.49	1.41
4	A	306	I3C	C5-C4	6.01	1.49	1.41
4	B	302	I3C	C5-C6	6.01	1.49	1.41
4	A	307	I3C	C5-C6	6.00	1.49	1.41
4	A	308	I3C	C5-C6	6.00	1.49	1.41
4	A	305	I3C	C5-C6	5.99	1.49	1.41
4	B	303	I3C	C5-C6	5.99	1.49	1.41
4	A	308	I3C	C5-C4	5.99	1.49	1.41
4	B	305	I3C	C5-C4	5.98	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	I3C	C5-C4	5.98	1.49	1.41
4	B	302	I3C	C5-C4	5.97	1.49	1.41
4	A	307	I3C	C5-C4	5.96	1.49	1.41
4	A	305	I3C	C5-C4	5.96	1.49	1.41
4	B	304	I3C	C5-C6	5.93	1.49	1.41
2	A	301	EDO	O2-C2	-5.48	1.14	1.42

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	I3C	C4-C5-C6	4.14	120.05	116.39
4	B	302	I3C	C4-C5-C6	4.11	120.03	116.39
4	A	307	I3C	C4-C5-C6	4.10	120.02	116.39
4	A	305	I3C	C4-C5-C6	4.10	120.01	116.39
4	B	304	I3C	C4-C5-C6	4.08	120.00	116.39
4	A	308	I3C	C4-C5-C6	4.08	120.00	116.39
4	B	305	I3C	C4-C5-C6	4.06	119.98	116.39
4	A	306	I3C	C4-C5-C6	4.02	119.94	116.39
2	A	301	EDO	O2-C2-C1	3.44	138.60	112.39
4	B	303	I3C	C3-C4-C5	-3.05	119.95	122.27
4	B	302	I3C	C3-C4-C5	-3.03	119.97	122.27
4	B	304	I3C	C1-C6-C5	-3.01	119.98	122.27
4	A	305	I3C	C1-C6-C5	-3.01	119.99	122.27
4	A	307	I3C	C3-C4-C5	-3.01	119.99	122.27
4	A	307	I3C	C1-C6-C5	-3.00	119.99	122.27
4	B	302	I3C	C1-C6-C5	-3.00	119.99	122.27
4	B	305	I3C	C3-C4-C5	-3.00	120.00	122.27
4	B	303	I3C	C1-C6-C5	-2.99	120.00	122.27
4	A	308	I3C	C3-C4-C5	-2.99	120.00	122.27
4	A	308	I3C	C1-C6-C5	-2.98	120.00	122.27
4	B	304	I3C	C3-C4-C5	-2.97	120.01	122.27
4	A	305	I3C	C3-C4-C5	-2.97	120.02	122.27
4	A	306	I3C	C1-C6-C5	-2.96	120.02	122.27
4	B	305	I3C	C1-C6-C5	-2.96	120.02	122.27
4	A	306	I3C	C3-C4-C5	-2.94	120.04	122.27
4	B	302	I3C	C6-C5-N13	-2.20	119.95	121.76
4	A	305	I3C	C6-C5-N13	-2.19	119.96	121.76
4	A	308	I3C	C6-C5-N13	-2.18	119.97	121.76
4	B	303	I3C	C4-C5-N13	-2.18	119.97	121.76
4	A	307	I3C	C4-C5-N13	-2.17	119.98	121.76
4	B	303	I3C	C6-C5-N13	-2.17	119.98	121.76
4	B	304	I3C	C4-C5-N13	-2.15	120.00	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	305	I3C	C4-C5-N13	-2.15	120.00	121.76
4	A	307	I3C	C6-C5-N13	-2.14	120.00	121.76
4	B	304	I3C	C6-C5-N13	-2.14	120.00	121.76
4	A	306	I3C	C6-C5-N13	-2.13	120.01	121.76
4	B	305	I3C	C6-C5-N13	-2.12	120.02	121.76
4	B	302	I3C	C4-C5-N13	-2.11	120.02	121.76
4	A	305	I3C	C4-C5-N13	-2.11	120.03	121.76
4	A	308	I3C	C4-C5-N13	-2.10	120.04	121.76
4	A	306	I3C	C4-C5-N13	-2.09	120.05	121.76

There are no chirality outliers.

All (11) torsion outliers are listed below:

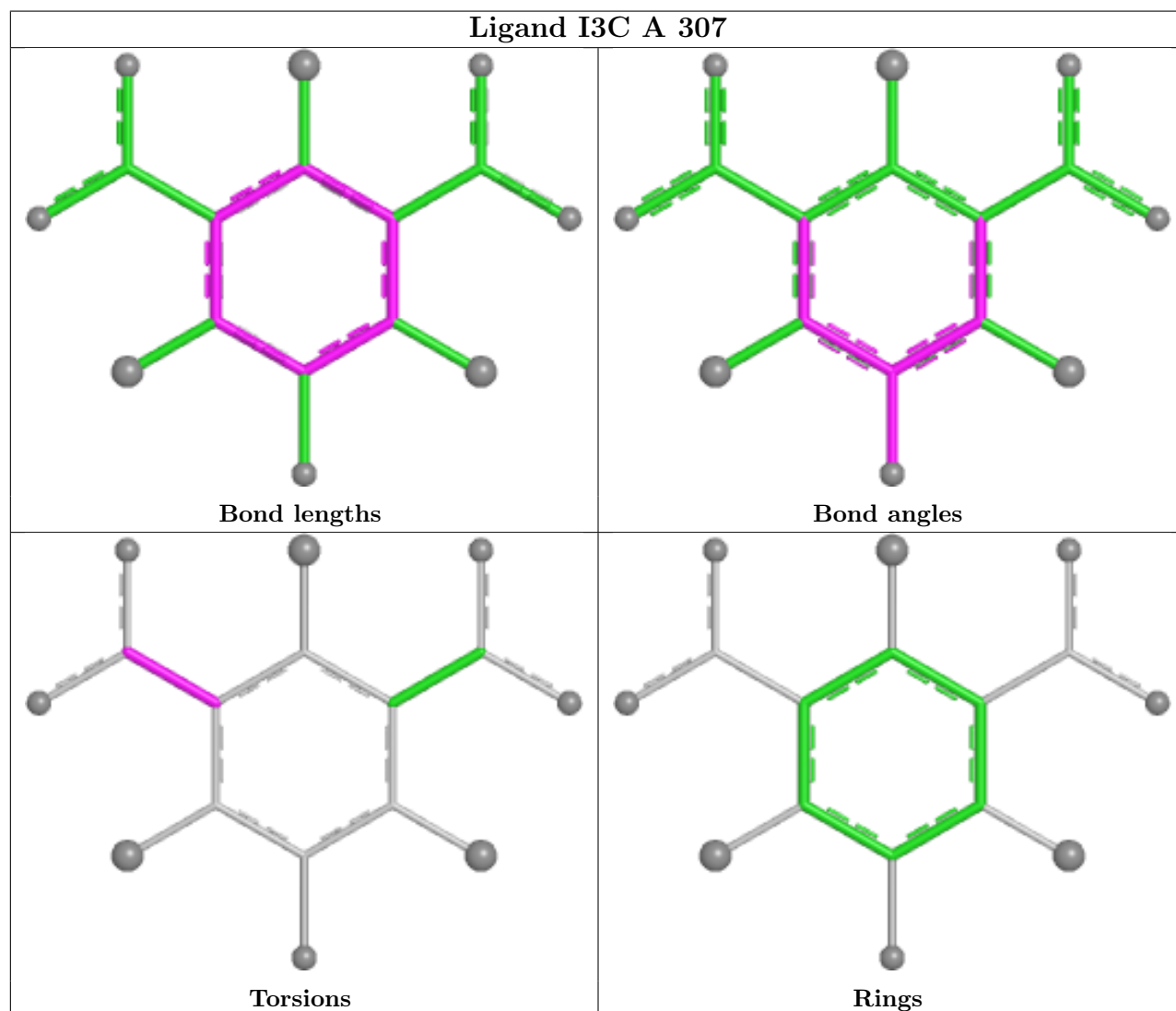
Mol	Chain	Res	Type	Atoms
4	A	307	I3C	O11-C10-C3-C4
4	A	307	I3C	O11-C10-C3-C2
4	A	307	I3C	O12-C10-C3-C4
4	A	307	I3C	O12-C10-C3-C2
3	B	301	PEG	C1-C2-O2-C3
3	B	301	PEG	O1-C1-C2-O2
2	A	304	EDO	O1-C1-C2-O2
3	A	303	PEG	C1-C2-O2-C3
3	B	301	PEG	O2-C3-C4-O4
2	A	302	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

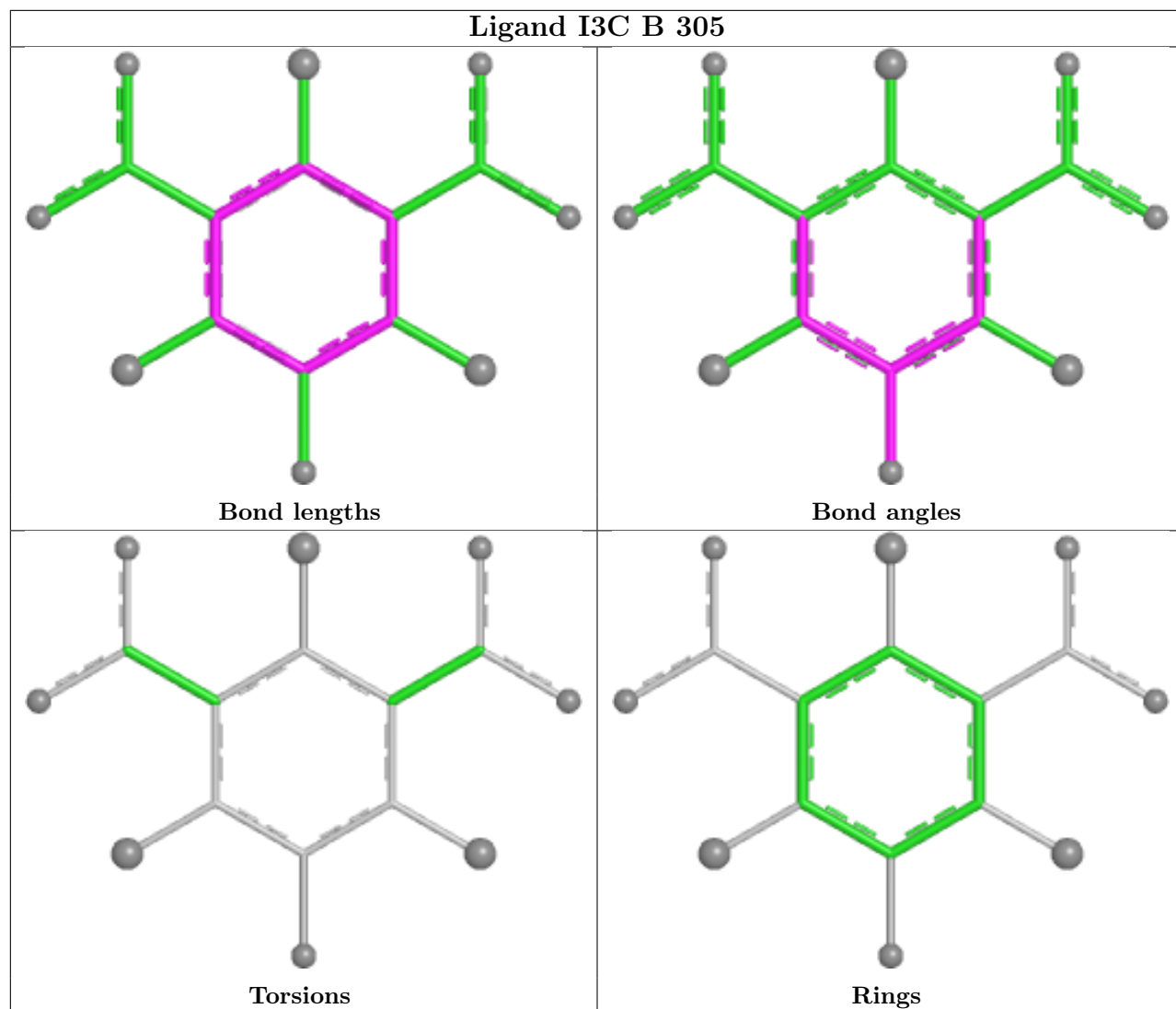
11 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	307	I3C	2	0
4	B	305	I3C	3	0
4	B	304	I3C	1	0
4	B	303	I3C	2	0
2	A	301	EDO	1	0
3	B	301	PEG	2	0
3	A	303	PEG	2	1
4	A	305	I3C	1	0
2	A	302	EDO	1	0
4	B	302	I3C	2	0
4	A	306	I3C	11	0

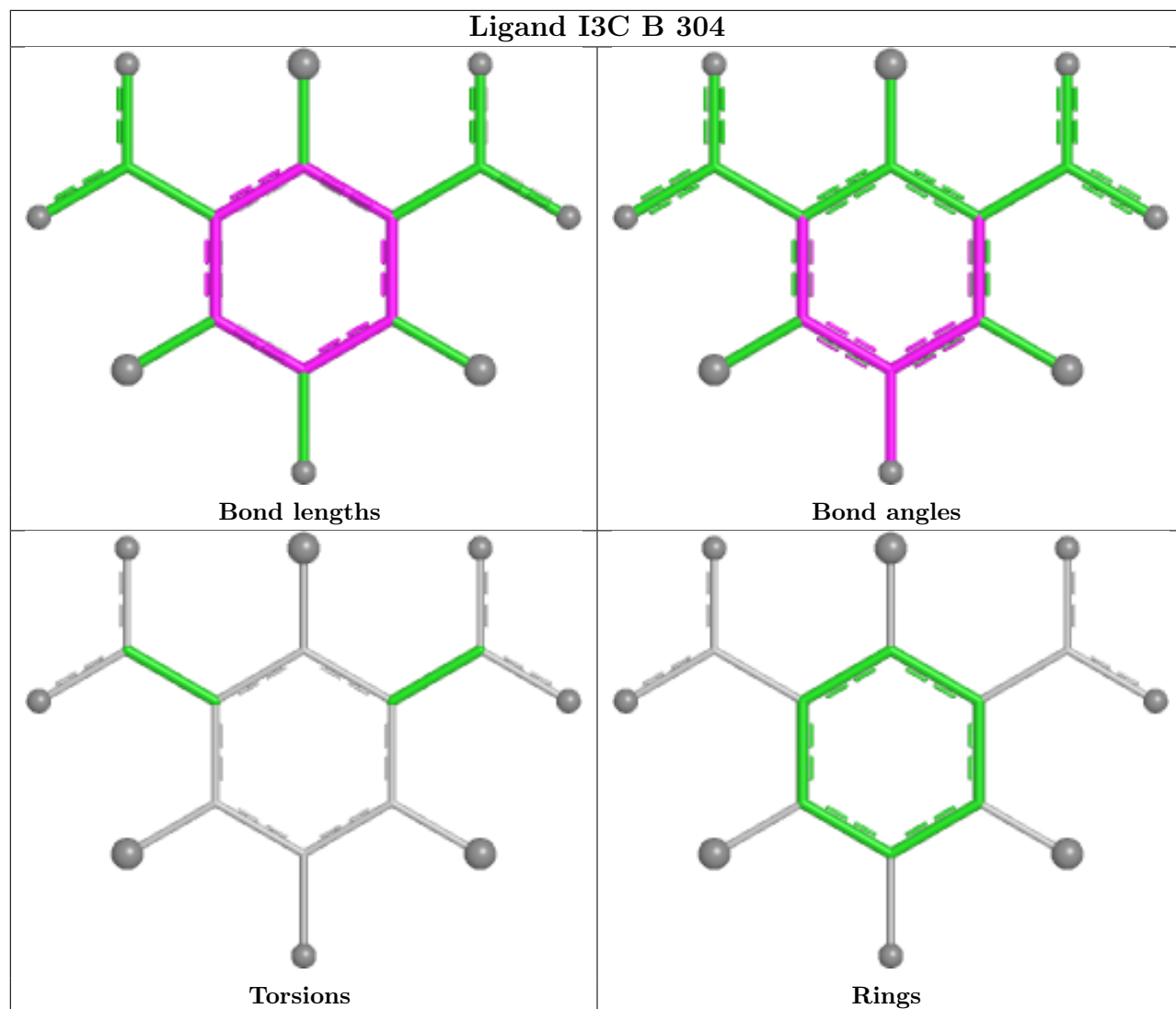
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



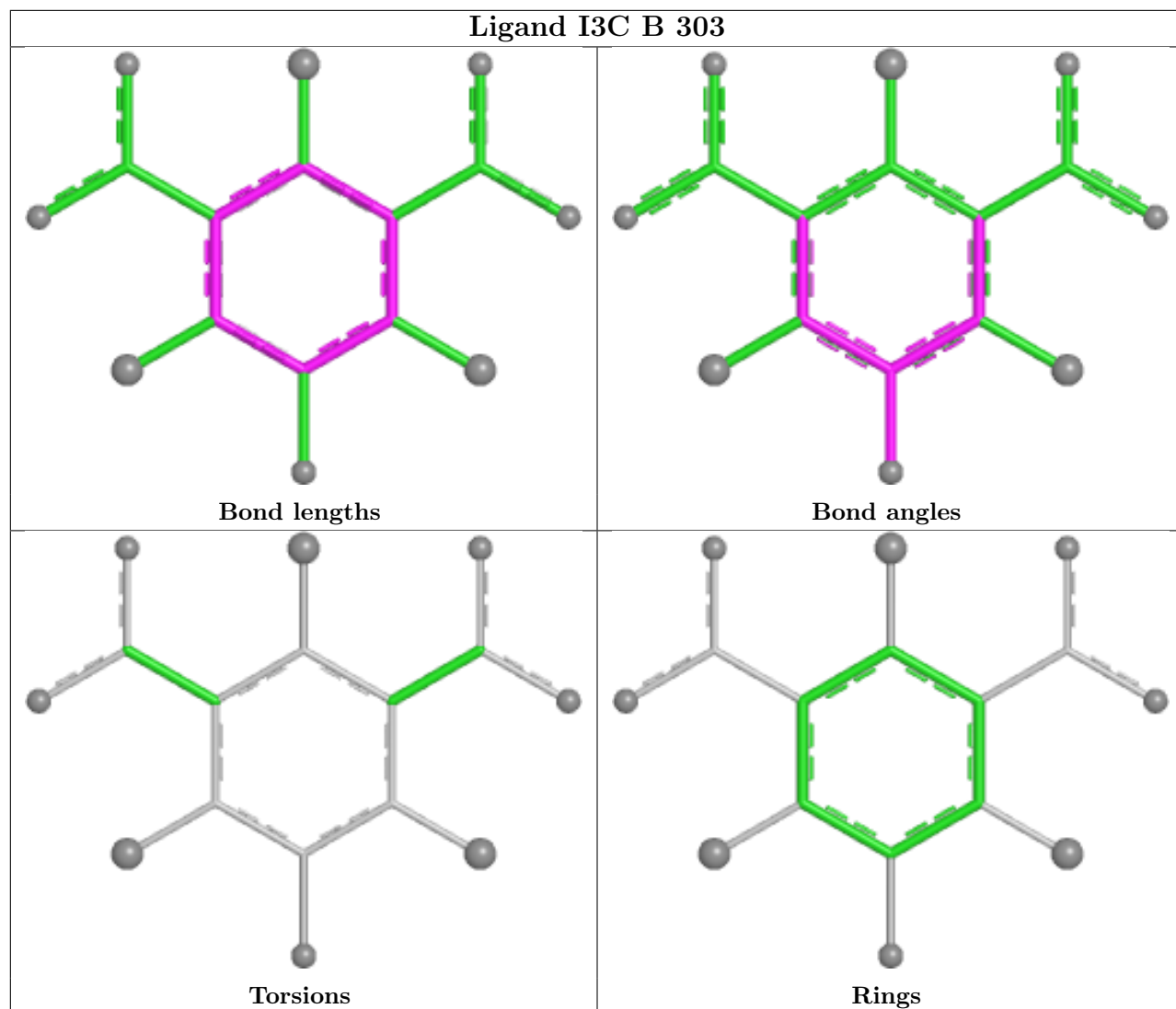
Ligand I3C B 305



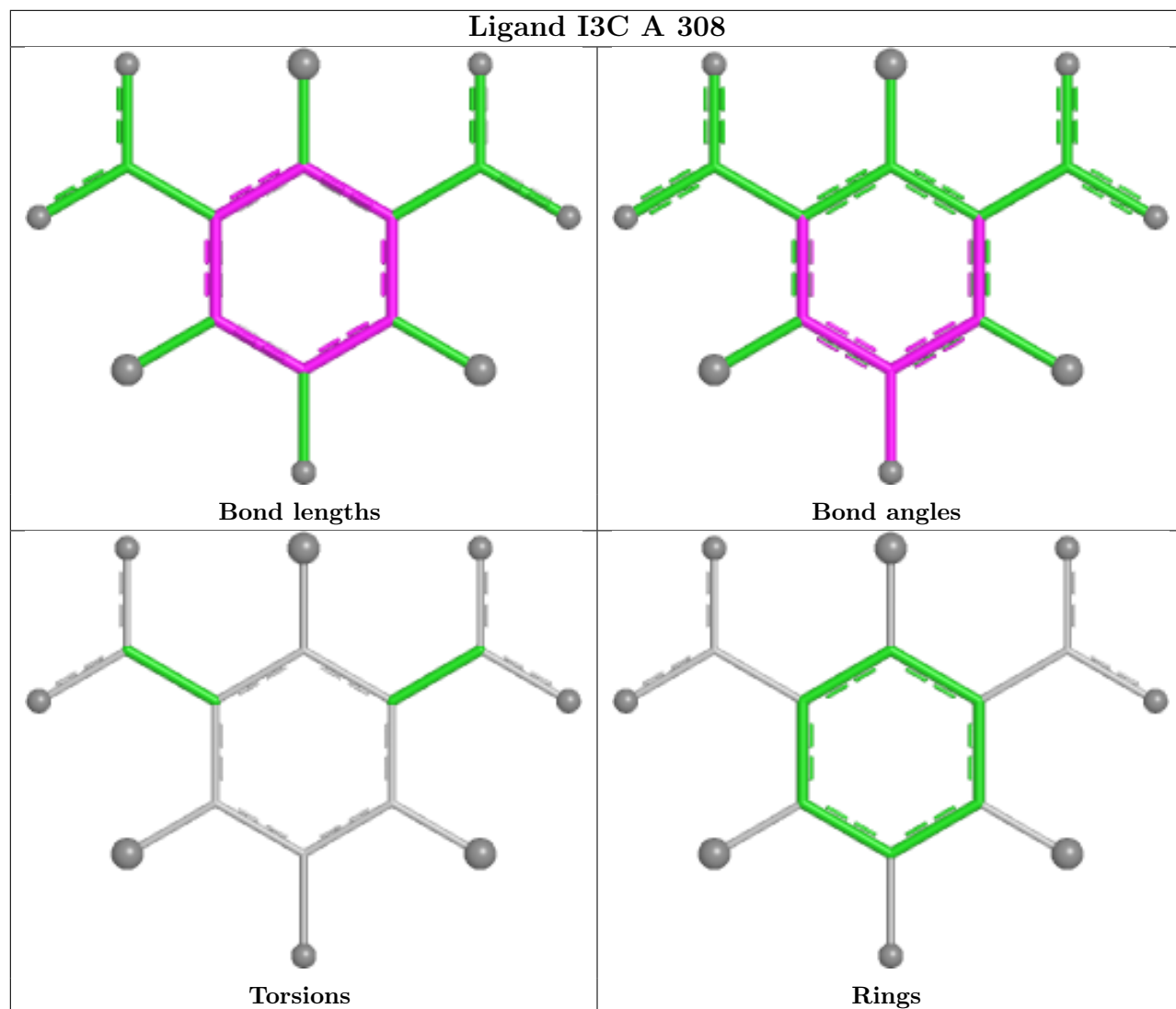
Ligand I3C B 304



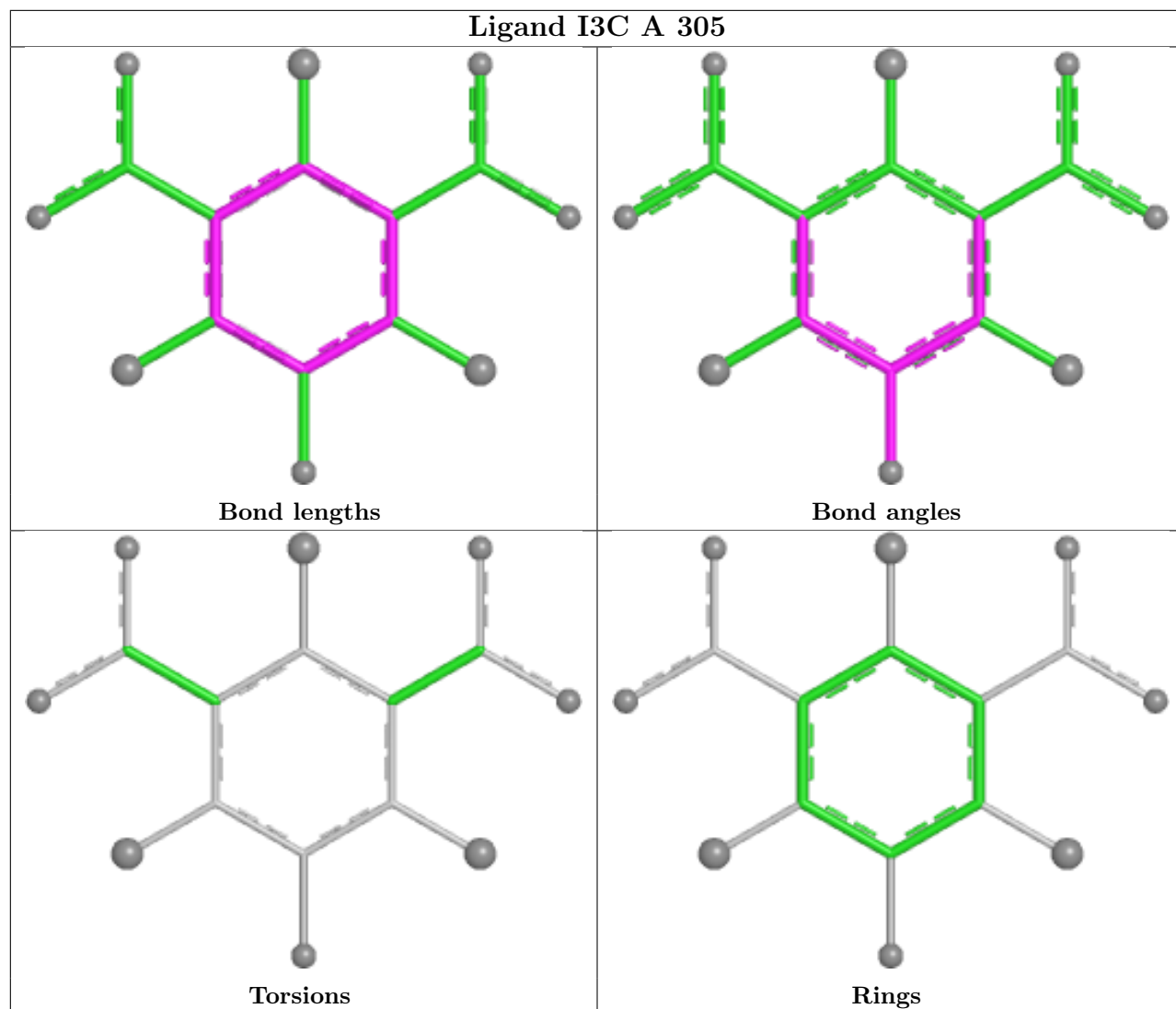
Ligand I3C B 303



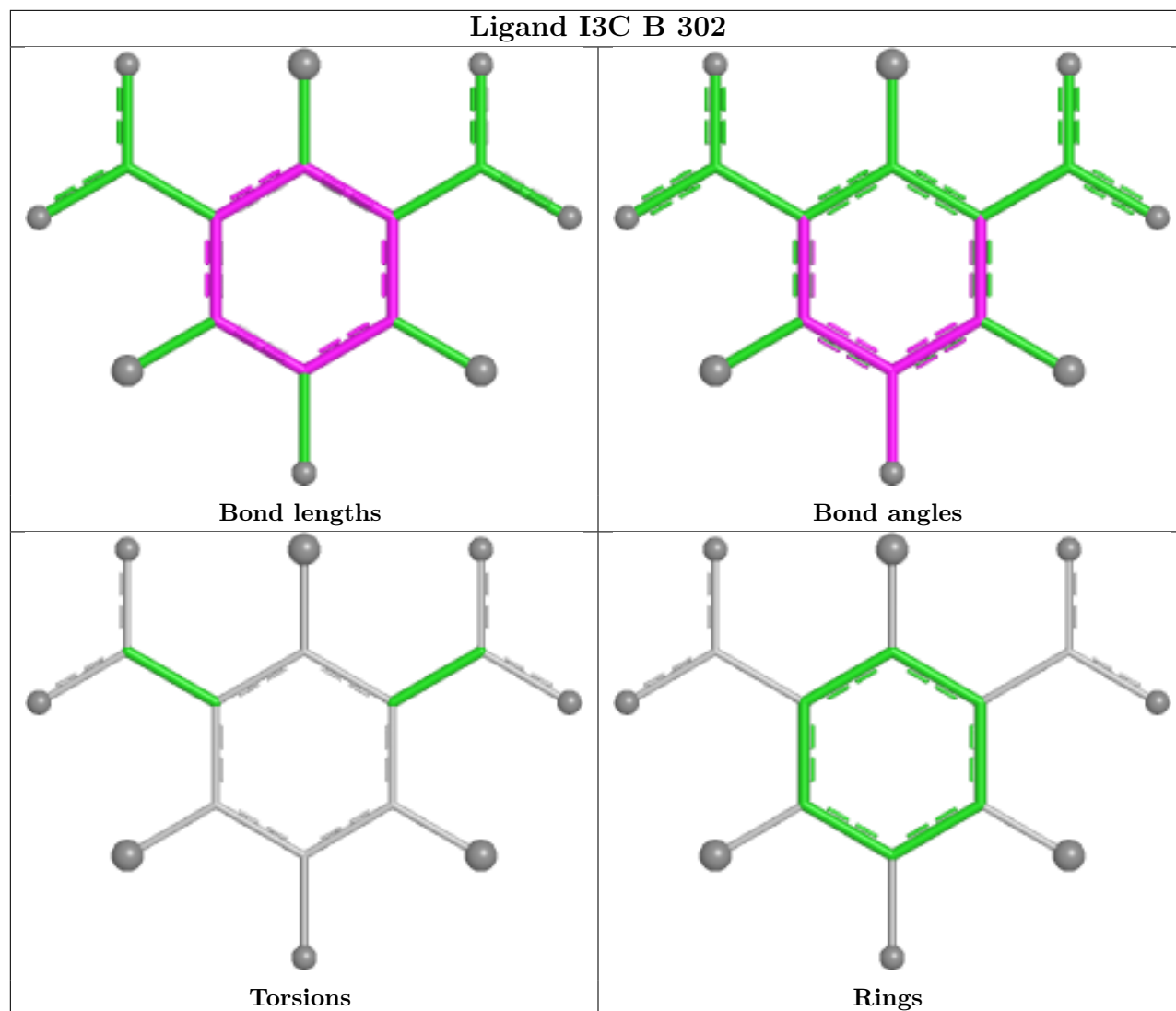
Ligand I3C A 308

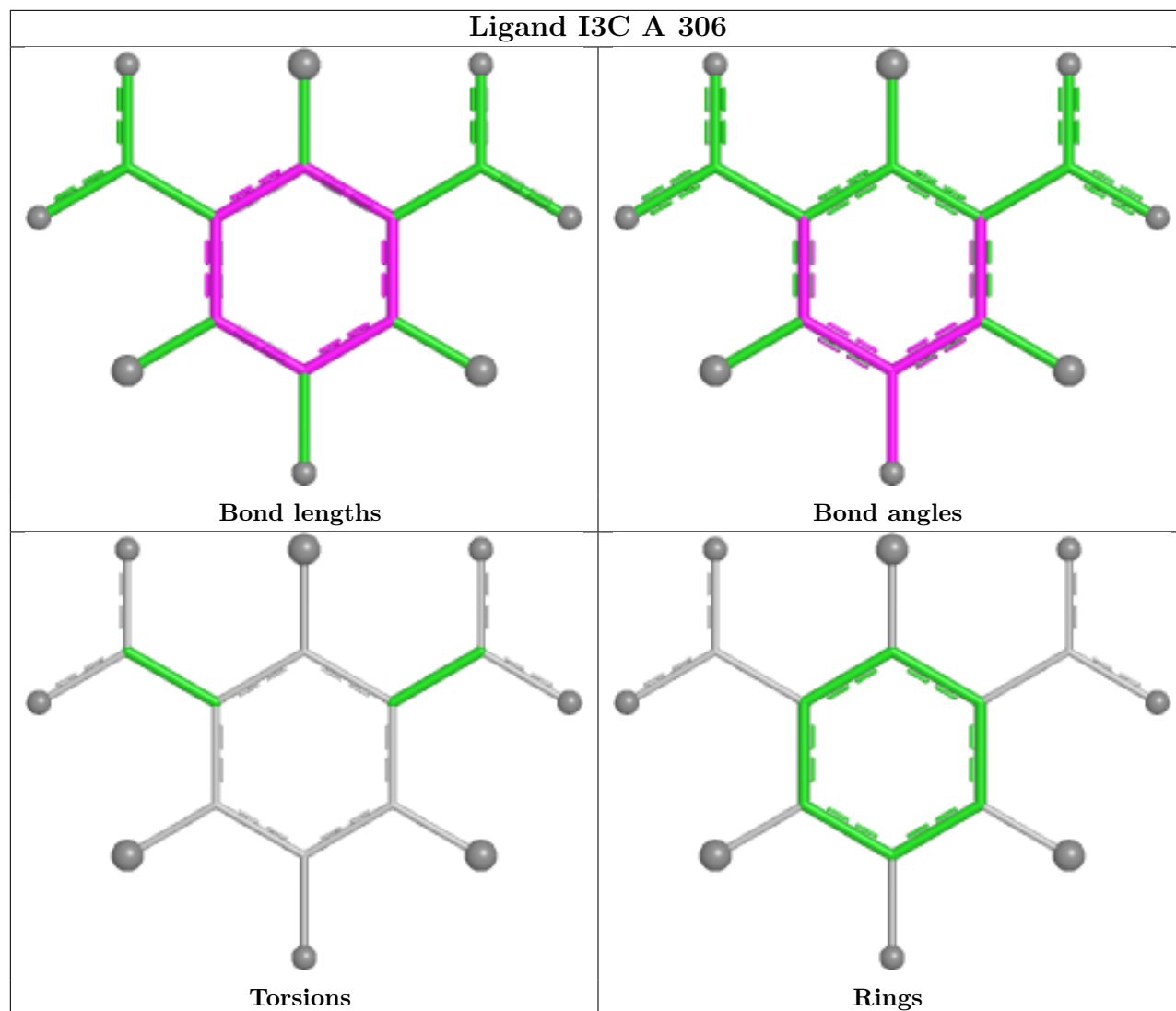


Ligand I3C A 305



Ligand I3C B 302





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	279/285 (97%)	-0.26	12 (4%) 35 13	12, 31, 91, 125	0
1	B	276/285 (96%)	-0.30	8 (2%) 51 23	10, 28, 99, 141	0
All	All	555/570 (97%)	-0.28	20 (3%) 42 17	10, 30, 97, 141	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	GLY	5.3
1	A	217	ASP	5.0
1	A	7	PRO	4.5
1	B	273	ASN	4.3
1	A	216	ASP	4.2
1	A	285	PRO	4.1
1	A	243	GLY	4.1
1	B	272	PRO	3.8
1	A	218	GLY	3.7
1	A	237	SER	3.3
1	A	220	PRO	3.2
1	B	281	VAL	2.9
1	A	8	LEU	2.7
1	B	277	GLN	2.7
1	A	219	ALA	2.6
1	B	276	LEU	2.5
1	B	242	PRO	2.3
1	A	240	ASN	2.3
1	A	245	LYS	2.2
1	B	244	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

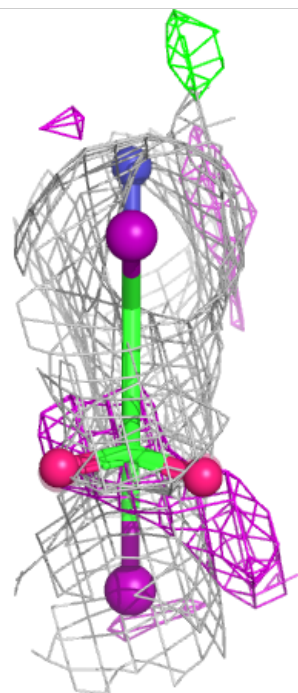
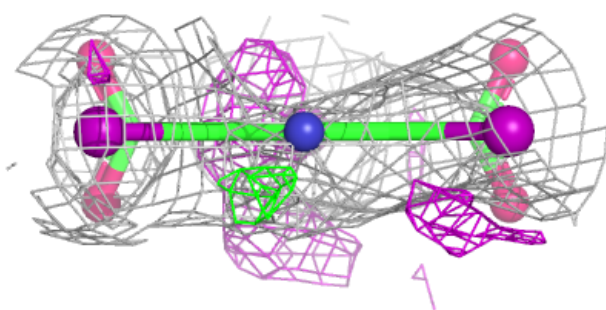
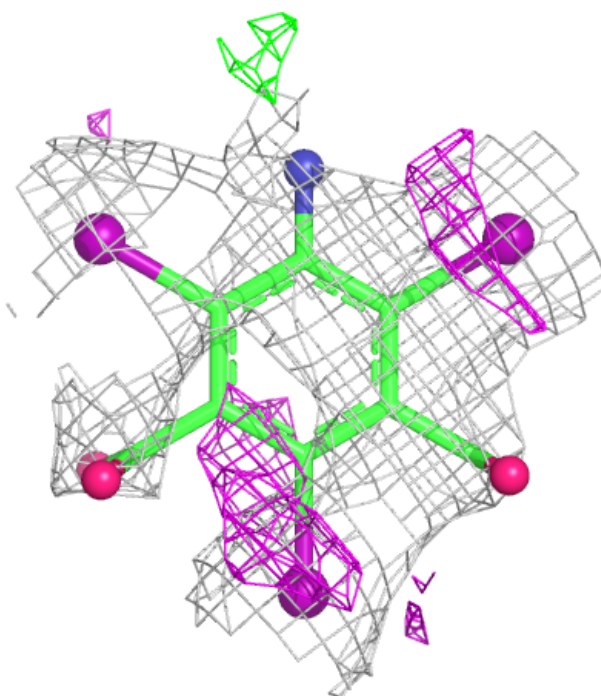
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	301	4/4	0.69	0.39	20,20,20,20	0
3	PEG	A	303	7/7	0.81	0.23	20,20,20,20	0
4	I3C	B	304	16/16	0.84	0.38	83,109,153,167	0
4	I3C	B	305	16/16	0.90	0.41	121,159,173,174	0
4	I3C	A	308	16/16	0.94	0.27	83,124,170,186	0
2	EDO	A	302	4/4	0.94	0.13	20,20,20,20	0
3	PEG	B	301	7/7	0.94	0.28	20,20,20,20	0
2	EDO	A	304	4/4	0.95	0.28	20,20,20,20	0
4	I3C	A	305	16/16	0.96	0.20	64,83,111,152	0
4	I3C	B	302	16/16	0.97	0.20	54,71,82,92	0
4	I3C	A	307	16/16	0.97	0.11	39,49,62,73	0
4	I3C	A	306	16/16	0.97	0.19	51,66,94,110	0
4	I3C	B	303	16/16	0.98	0.16	40,57,83,84	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.

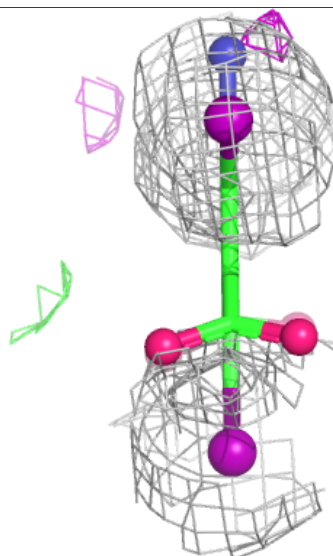
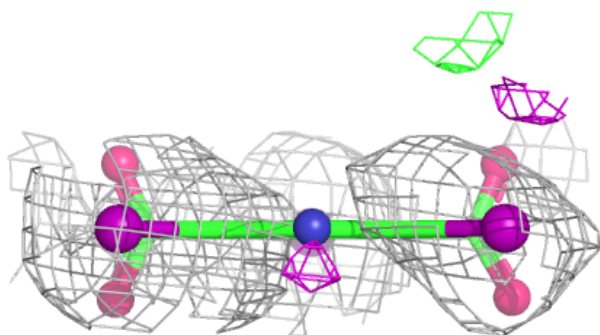
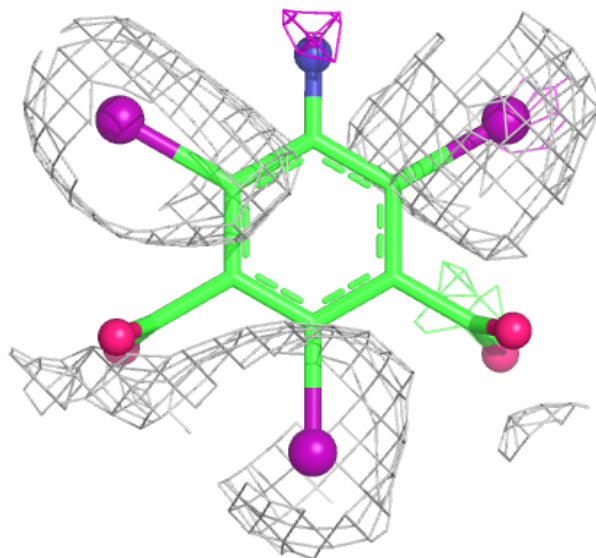
Electron density around I3C B 304:

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



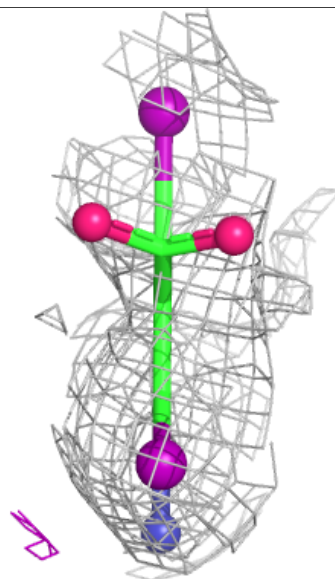
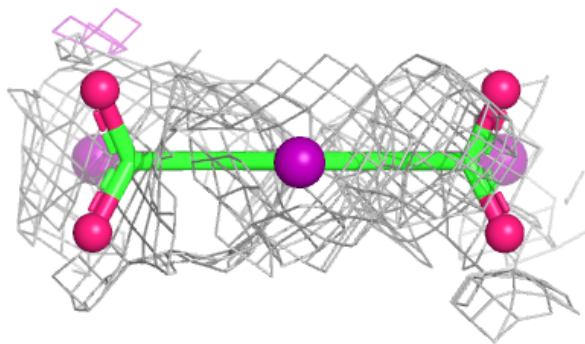
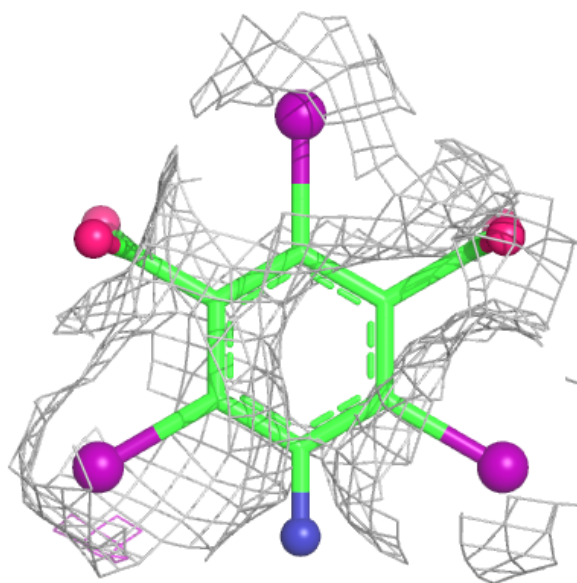
Electron density around I3C B 305:

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



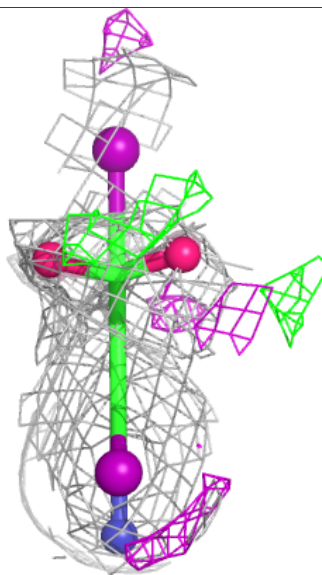
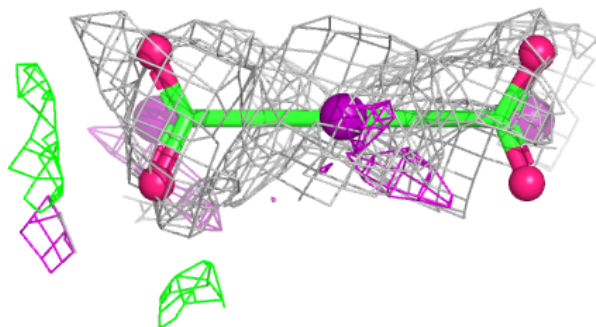
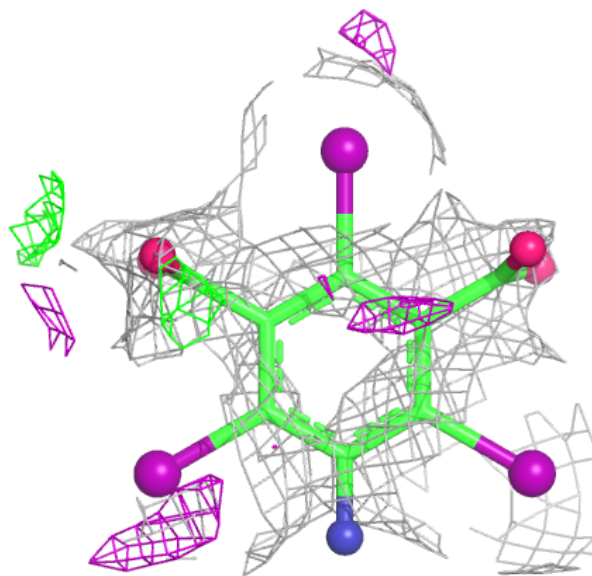
Electron density around I3C A 308:

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



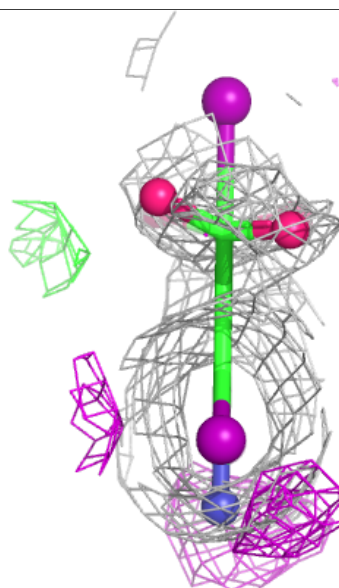
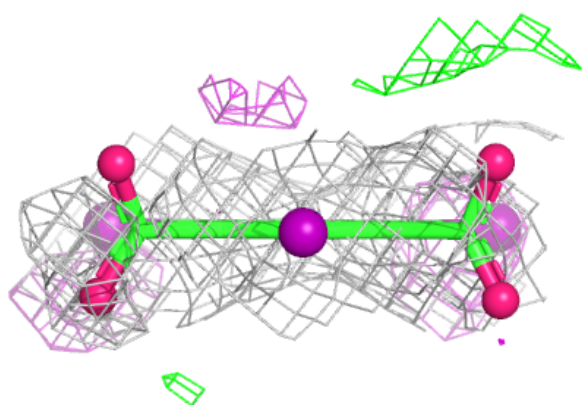
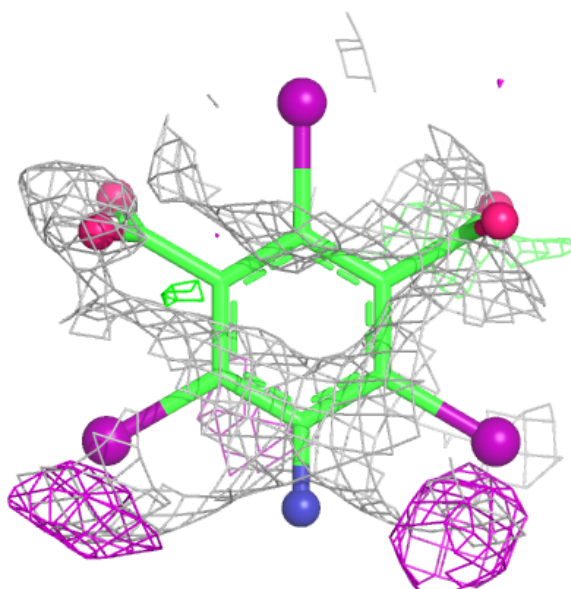
Electron density around I3C A 305:

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



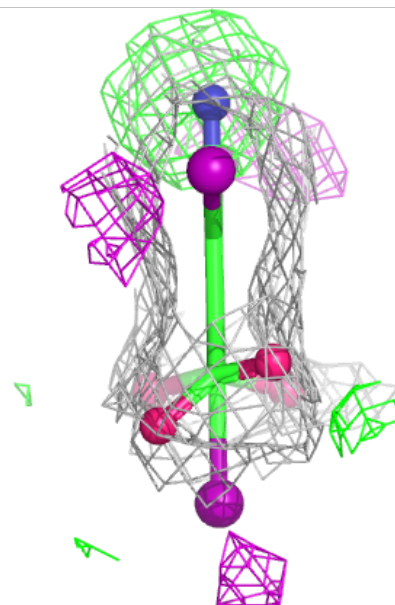
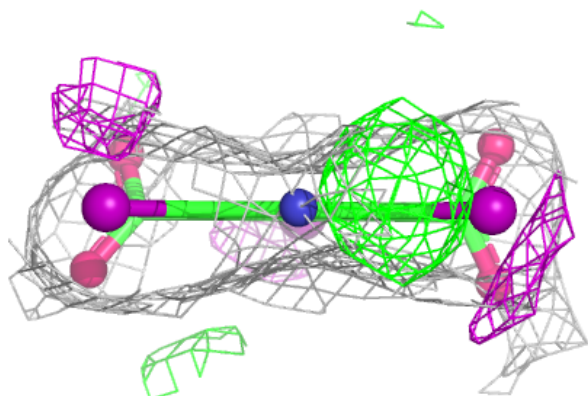
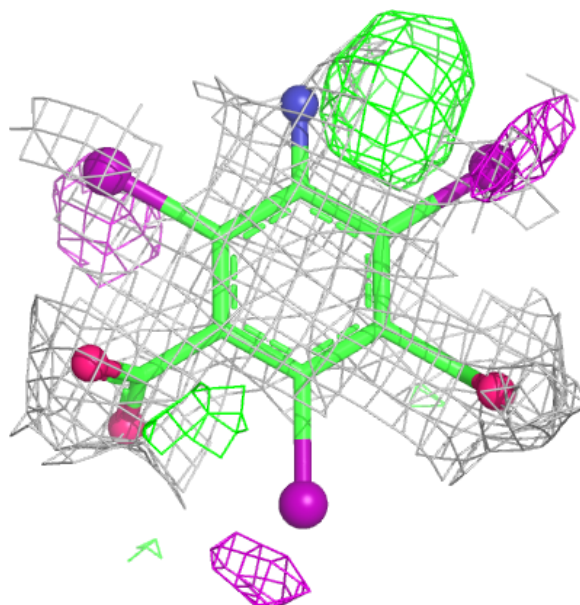
Electron density around I3C B 302:

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



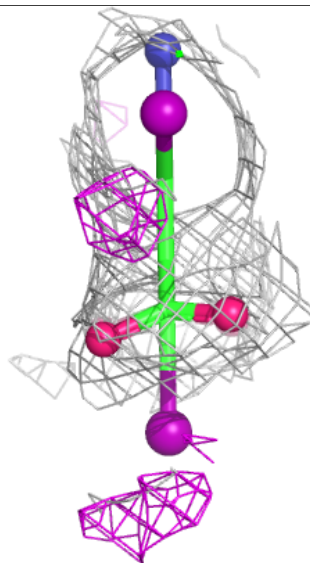
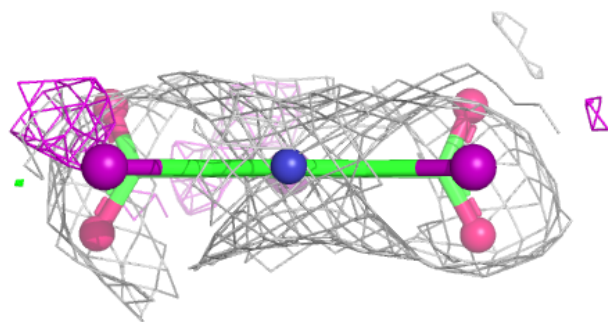
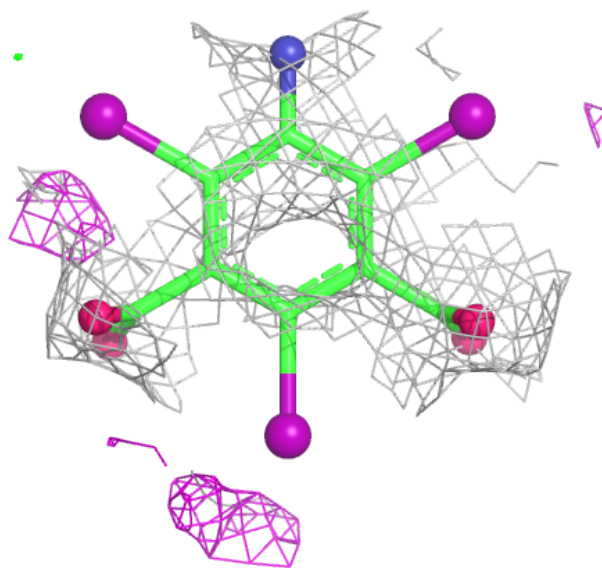
Electron density around I3C A 307:

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



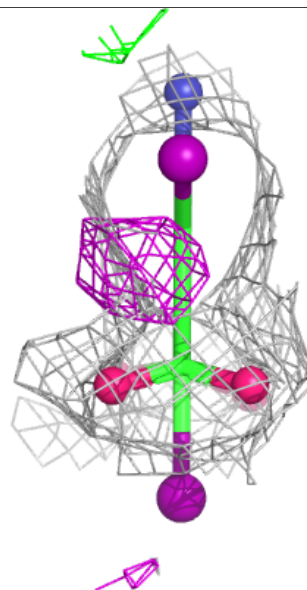
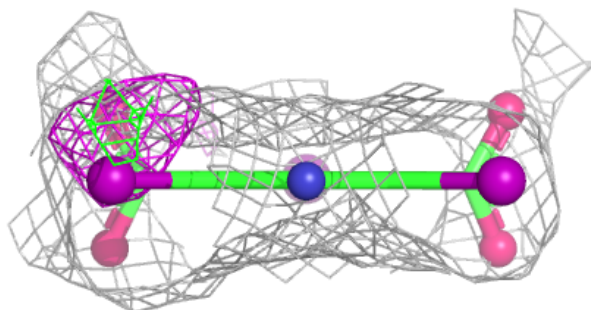
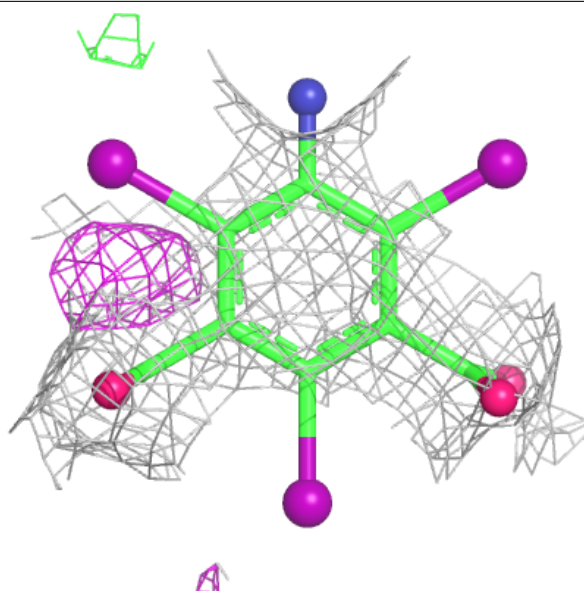
Electron density around I3C A 306:

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



Electron density around I3C B 303:

$2mF_o-DF_c$ (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.