



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:08 pm BST

PDB ID : 2YDF
Title : HUMAN SERUM ALBUMIN COMPLEXED WITH IOPHENOXIC ACID
Authors : Ryan, A.J.; Curry, S.
Deposited on : 2011-03-18
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

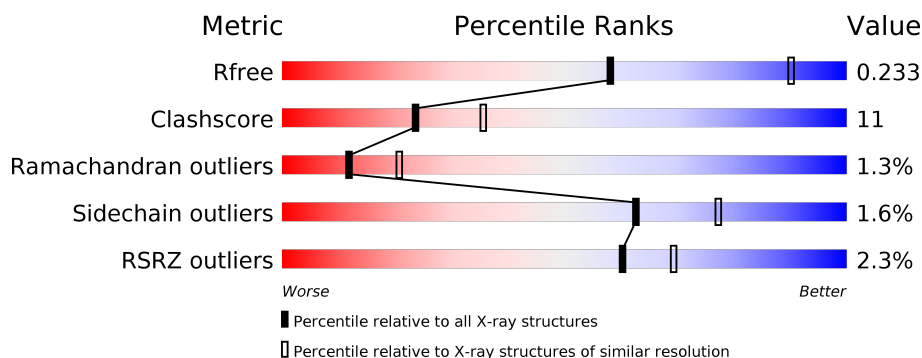
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>••</div> </div> </div>
1	B	585	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <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	IO3	B	2004	-	-	X	-

2 Entry composition [i](#)

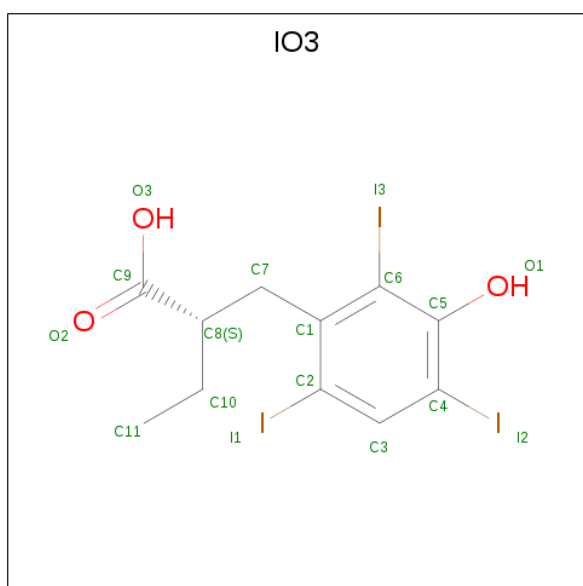
There are 3 unique types of molecules in this entry. The entry contains 8442 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4177	2640	704	794	39			
1	B	566	Total	C	N	O	S	0	0	0
			4106	2590	685	792	39			

- Molecule 2 is IOPHENOXIC ACID (three-letter code: IO3) (formula: C₁₁H₁₁I₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	I	O	0	0
			17	11	3	3		
2	A	1	Total	C	I	O	0	0
			17	11	3	3		
2	A	1	Total	C	I	O	0	0
			17	11	3	3		
2	A	1	Total	C	I	O	0	0
			17	11	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	I	O	0	0
			17	11	3	3		
2	B	1	Total	C	I	O	0	0
			17	11	3	3		
2	B	1	Total	C	I	O	0	0
			17	11	3	3		
2	B	1	Total	C	I	O	0	0
			17	11	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	11	Total	O	0	0
			11	11		

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.

Chain A:

29% 76% 20%

ASP
ALA
HIS
LYS
S5
E6
V7
A8
H9
D13
F19
V23
E27
A28
Q29
Y30
G34
P35
F36
E37
D38
H39
V40
Y41
L42
V43
V46
V54
A55
A59
C62
K73
A78
THR
LEU
ARG
GLU
THR
TYR
GLY
MET
A88
E95
P96
E97
I102

P110
N111
L112
R117
P118
V120
D129
L135
Y138
A143
Y150
A151
P152
C168
A172
A175
L179
P180
R181
L182
R186
A194
K199
L219
R222
F223
K225
T236
C245
H247
R257
Q268
S272
S273
K274
L275

P282
E285
T290
V293
N295
D296
E297
P299
A300
V310
Y319
Y323
K324
R337
E368
C369
Y370
A371
K372
V373
F374
D375
E376
F377
K378
P379
L380
E383
P384
Q385
I388
K389
Q390
E393
L394
L398
L408
V409
R410
K414
T420
P421

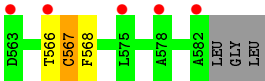
V424
R428
M429
L430
V433
M446
P447
Y452
V455
V456
L463
M483
R484
R495
P496
C497
F498
A504
E505
T508
F509
H510
S517
R521
Q526
L529
V533
T540
Q543
L544
A553
F554
V555
E556
K557
C558
C559
K560
D561
D562
D563

A582
LEU
GLY
LEU

Chain B:

75% 22%

ASP
ALA
HIS
LYS
SLS
E6
V7
A8
H9
R10
F11
K12
D13
E16
V23
L24
F27
A28
Q29
C34
P35
F36
E37
D38
H39
V40
R41
L42
V43
V46
R51
T52
C53
V54
A55
S58
A59
C62
L66
V76
VAL
ALA
THR
LEU
ARG
GLU
THR
TVR
GLY
C111



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.07Å 55.44Å 119.84Å 81.00° 90.83° 64.52°	Depositor
Resolution (Å)	35.12 – 2.75 49.23 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.7 (35.12-2.75) 95.5 (49.23-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.207 , 0.239 0.202 , 0.233	Depositor DCC
R_{free} test set	2505 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8442	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.01% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IO3

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	0.22	0/4257	0.37	0/5798
1	B	0.22	0/4184	0.37	0/5709
All	All	0.22	0/8441	0.37	0/11507

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4177	0	3790	82	0
1	B	4106	0	3652	88	0
2	A	68	0	40	12	0
2	B	68	0	40	10	0
3	A	12	0	0	1	0
3	B	11	0	0	0	0
All	All	8442	0	7522	178	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:HD13	2:A:2002:IO3:H3	1.41	1.02
2:A:2001:IO3:I3	2:A:2001:IO3:H6	2.44	0.87
2:A:2003:IO3:H7	2:A:2003:IO3:I3	2.51	0.80
2:B:2001:IO3:H6	2:B:2001:IO3:I3	2.53	0.79
1:A:95:GLU:CB	1:A:96:PRO:HD2	2.13	0.79
1:B:406:ALA:HB1	2:B:2004:IO3:H7	1.66	0.78
1:A:553:ALA:HA	1:A:556:GLU:HG2	1.68	0.76
1:B:430:LEU:HD12	1:B:456:VAL:HG11	1.70	0.73
1:A:73:LYS:HA	1:A:73:LYS:HE2	1.71	0.71
1:A:117:ARG:HH12	1:A:182:LEU:HB3	1.56	0.71
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.72	0.70
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.73	0.69
1:B:302:LEU:HB3	1:B:337:ARG:HH21	1.57	0.69
1:A:117:ARG:NH1	1:A:182:LEU:HB3	2.10	0.67
1:B:51:LYS:O	1:B:54:VAL:HG22	1.93	0.67
1:B:553:ALA:HA	1:B:556:GLU:HG2	1.77	0.66
1:B:152:PRO:HB2	1:B:257:ARG:HH11	1.61	0.66
1:B:410:ARG:HD3	2:B:2004:IO3:H11	1.77	0.66
1:B:556:GLU:HG3	1:B:556:GLU:O	1.96	0.66
1:B:410:ARG:HH11	2:B:2004:IO3:H11	1.61	0.65
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.79	0.64
1:B:305:LEU:HD13	1:B:334:TYR:CD2	2.32	0.64
1:A:103:LEU:HD21	1:A:247:HIS:HA	1.78	0.64
1:B:430:LEU:HD12	1:B:456:VAL:CG1	2.28	0.63
1:B:95:GLU:CB	1:B:96:PRO:HD2	2.29	0.62
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.83	0.61
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.83	0.61
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.83	0.60
1:A:222:ARG:HD2	1:A:293:VAL:O	2.01	0.60
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.84	0.60
2:B:2004:IO3:H8	2:B:2004:IO3:I3	2.73	0.59
1:B:95:GLU:O	1:B:97:GLU:N	2.35	0.59
1:A:430:LEU:HD12	1:A:456:VAL:HG11	1.85	0.59
1:B:556:GLU:O	1:B:560:LYS:HD3	2.05	0.57
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.87	0.57
1:A:452:TYR:O	1:A:456:VAL:HG23	2.04	0.56
1:B:11:PHE:CZ	1:B:16:GLU:HG2	2.40	0.56
1:A:95:GLU:O	1:A:97:GLU:N	2.38	0.56
1:A:414:LYS:HE3	1:A:488:PHE:O	2.04	0.56
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.86	0.56
1:B:414:LYS:HE3	1:B:488:PHE:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:HIS:O	1:B:43:VAL:HG23	2.06	0.55
2:A:2004:IO3:H6	2:A:2004:IO3:I3	2.76	0.55
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.88	0.55
1:A:30:TYR:HE1	1:A:103:LEU:HD12	1.72	0.55
1:A:95:GLU:CB	1:A:96:PRO:CD	2.83	0.55
1:A:384:PRO:O	1:A:388:ILE:HG12	2.07	0.55
1:A:517:SER:O	1:A:521:ARG:HG3	2.07	0.55
1:B:430:LEU:O	1:B:433:VAL:HG12	2.07	0.55
1:A:540:THR:HG23	1:A:543:GLN:H	1.71	0.54
1:A:540:THR:O	1:A:544:LEU:HD12	2.07	0.54
1:B:492:GLU:HG3	1:B:493:VAL:HG23	1.89	0.54
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.90	0.53
1:A:430:LEU:O	1:A:433:VAL:HG12	2.08	0.53
1:B:452:TYR:O	1:B:456:VAL:HG23	2.09	0.53
1:B:222:ARG:HD2	1:B:293:VAL:O	2.08	0.53
2:A:2004:IO3:C8	2:A:2004:IO3:I3	3.27	0.53
1:A:557:LYS:HG3	1:A:558:CYS:H	1.72	0.53
1:A:556:GLU:O	1:A:556:GLU:HG3	2.08	0.52
1:B:11:PHE:HZ	1:B:16:GLU:HG2	1.72	0.52
1:B:110:PRO:HB2	1:B:112:LEU:HG	1.92	0.52
1:A:35:PRO:HG2	1:A:38:ASP:OD2	2.09	0.52
1:A:290:ILE:O	1:A:293:VAL:HG12	2.10	0.52
1:B:520:GLU:O	1:B:524:LYS:HG2	2.11	0.51
2:B:2003:IO3:I1	2:B:2003:IO3:H7	2.81	0.51
1:B:54:VAL:HG23	1:B:55:ALA:N	2.24	0.51
1:A:376:GLU:O	1:A:380:LEU:HD12	2.11	0.51
1:B:95:GLU:CB	1:B:96:PRO:CD	2.87	0.51
1:A:29:GLN:HG2	1:A:143:ALA:O	2.10	0.51
1:B:153:GLU:HG2	1:B:257:ARG:HH12	1.77	0.51
1:B:557:LYS:HG3	1:B:558:CYS:N	2.26	0.51
1:A:23:VAL:O	1:A:27:PHE:HD1	1.95	0.50
1:A:34:CYS:HB2	1:A:39:HIS:NE2	2.26	0.50
1:A:504:ALA:O	1:A:508:THR:HG23	2.10	0.50
1:B:35:PRO:HG2	1:B:38:ASP:OD2	2.11	0.50
1:A:533:VAL:HG22	1:A:544:LEU:HD21	1.94	0.50
1:A:557:LYS:HG3	1:A:558:CYS:N	2.25	0.50
2:A:2004:IO3:I3	2:A:2004:IO3:H7	2.82	0.50
1:A:219:LEU:HD21	2:A:2001:IO3:H10	1.94	0.50
1:A:390:GLN:O	1:A:393:GLU:HG2	2.12	0.50
1:B:391:ASN:HD21	2:B:2002:IO3:H9	1.77	0.49
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HD12	1:A:456:VAL:CG1	2.42	0.49
1:B:504:ALA:O	1:B:508:THR:HG23	2.13	0.49
1:A:268:GLN:HG3	1:A:275:LEU:HB2	1.95	0.48
1:B:268:GLN:HG3	1:B:275:LEU:HB2	1.95	0.48
1:B:38:ASP:O	1:B:42:LEU:HG	2.12	0.48
1:B:296:ASP:OD1	1:B:297:GLU:N	2.47	0.48
1:B:410:ARG:CD	2:B:2004:IO3:H11	2.44	0.48
1:A:388:ILE:CD1	2:A:2002:IO3:H3	2.28	0.48
1:B:376:GLU:O	1:B:380:LEU:HD12	2.14	0.48
1:B:464:HIS:CG	1:B:473:VAL:HG11	2.49	0.48
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.94	0.47
1:B:299:PRO:HG2	1:B:336:ARG:HH21	1.78	0.47
1:A:296:ASP:OD1	1:A:297:GLU:N	2.47	0.47
1:B:23:VAL:O	1:B:27:PHE:HD1	1.96	0.47
1:B:483:ASN:C	1:B:486:PRO:HD2	2.34	0.47
1:B:305:LEU:HD11	1:B:337:ARG:HD2	1.95	0.47
1:B:420:THR:HB	1:B:421:PRO:HD3	1.97	0.47
1:A:39:HIS:O	1:A:43:VAL:HG23	2.15	0.47
1:A:385:GLN:HG3	1:A:446:MET:CE	2.45	0.47
1:B:135:LEU:O	1:B:138:TYR:HB3	2.14	0.47
1:B:139:LEU:HD23	1:B:154:LEU:HG	1.95	0.47
1:B:290:ILE:O	1:B:293:VAL:HG12	2.15	0.47
1:B:9:HIS:CE1	1:B:13:ASP:OD2	2.68	0.47
1:B:557:LYS:HG3	1:B:558:CYS:H	1.80	0.46
1:A:54:VAL:HG23	1:A:55:ALA:N	2.30	0.46
1:A:319:TYR:CE1	1:A:323:LYS:HG3	2.50	0.46
1:B:29:GLN:HG2	1:B:143:ALA:O	2.15	0.46
1:B:410:ARG:HH11	2:B:2004:IO3:C11	2.29	0.46
1:B:42:LEU:O	1:B:46:VAL:HG23	2.15	0.45
1:B:222:ARG:HA	1:B:295:ASN:OD1	2.16	0.45
1:B:429:ASN:HD22	1:B:429:ASN:N	2.15	0.45
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.57	0.45
1:B:54:VAL:HG23	1:B:55:ALA:H	1.80	0.45
1:B:243:THR:O	1:B:247:HIS:ND1	2.50	0.45
1:B:322:ALA:HB1	1:B:325:VAL:HB	1.97	0.45
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.99	0.44
1:A:135:LEU:O	1:A:138:TYR:HB3	2.17	0.44
1:A:324:ASP:OD1	1:A:324:ASP:N	2.48	0.44
1:A:272:SER:HA	1:A:296:ASP:OD2	2.18	0.44
1:A:446:MET:HB3	1:A:447:PRO:HD3	2.00	0.44
1:B:260:LEU:O	1:B:264:ILE:HG13	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:O	1:A:179:LEU:HG	2.18	0.44
1:A:529:LEU:O	1:A:533:VAL:HG23	2.17	0.44
1:B:127:PHE:CE1	1:B:131:GLU:HG3	2.52	0.44
1:A:42:LEU:O	1:A:46:VAL:HG23	2.17	0.44
1:A:37:GLU:O	1:A:40:VAL:HG22	2.17	0.44
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.47	0.44
1:B:219:LEU:HD11	1:B:238:LEU:HD12	2.00	0.43
1:B:34:CYS:HB2	1:B:39:HIS:NE2	2.33	0.43
1:A:274:LYS:HD3	1:A:294:GLU:HG3	2.00	0.43
1:B:141:GLU:OE1	1:B:144:ARG:HD3	2.18	0.43
1:B:186:ARG:HA	2:B:2003:IO3:C5	2.49	0.43
1:B:415:VAL:O	1:B:415:VAL:HG23	2.19	0.43
1:A:37:GLU:N	1:A:37:GLU:OE1	2.51	0.43
1:A:394:LEU:HG	1:A:398:LEU:CD1	2.49	0.43
1:A:110:PRO:HB2	1:A:112:LEU:HG	2.01	0.43
1:B:446:MET:HB3	1:B:447:PRO:HD3	2.01	0.43
1:A:199:LYS:HE2	3:A:2011:HOH:O	2.20	0.42
1:A:186:ARG:HA	2:A:2003:IO3:C3	2.49	0.42
1:A:186:ARG:CG	2:A:2003:IO3:H11	2.49	0.42
1:B:540:THR:HG23	1:B:543:GLN:H	1.84	0.42
1:A:19:PHE:O	1:A:23:VAL:HG23	2.19	0.42
1:B:153:GLU:HG2	1:B:257:ARG:NH1	2.34	0.42
1:B:94:GLN:O	1:B:95:GLU:O	2.37	0.42
1:B:566:THR:O	1:B:567:CYS:C	2.58	0.42
1:A:9:HIS:CE1	1:A:13:ASP:OD2	2.73	0.42
1:B:222:ARG:HG2	1:B:223:PHE:CE1	2.54	0.42
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.85	0.42
1:A:483:ASN:C	1:A:486:PRO:HD2	2.40	0.42
1:B:324:ASP:OD1	1:B:324:ASP:N	2.53	0.42
1:A:38:ASP:O	1:A:42:LEU:HG	2.20	0.41
1:A:54:VAL:CG2	1:A:55:ALA:N	2.83	0.41
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.55	0.41
1:A:410:ARG:NH2	2:A:2002:IO3:O3	2.53	0.41
1:A:555:VAL:C	1:A:557:LYS:H	2.24	0.41
1:B:376:GLU:O	1:B:379:PRO:HD2	2.21	0.41
1:A:424:VAL:O	1:A:428:ARG:HG3	2.20	0.41
1:B:132:GLU:O	1:B:136:LYS:HG3	2.21	0.41
1:B:472:ARG:NH2	1:B:491:LEU:HD22	2.34	0.41
1:B:190:LYS:HB2	1:B:190:LYS:HZ2	1.85	0.41
1:A:310:VAL:O	1:A:370:TYR:HE1	2.04	0.41
1:B:141:GLU:HA	1:B:141:GLU:OE1	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:HIS:HA	1:B:568:PHE:CB	2.50	0.41
1:A:282:PRO:HB2	1:A:285:GLU:OE1	2.21	0.41
1:A:420:THR:HB	1:A:421:PRO:HD3	2.03	0.41
1:B:370:TYR:HD1	1:B:370:TYR:O	2.04	0.41
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.56	0.41
1:B:540:THR:HG22	1:B:543:GLN:OE1	2.20	0.41
1:A:5:SER:HA	1:A:62:CYS:O	2.20	0.40
1:A:103:LEU:HD11	1:A:247:HIS:O	2.22	0.40
1:A:368:GLU:HA	1:A:371:ALA:HB2	2.03	0.40
1:B:36:PHE:CZ	1:B:40:VAL:HG11	2.56	0.40
1:A:410:ARG:HD2	2:A:2004:IO3:O3	2.21	0.40
1:B:414:LYS:O	1:B:472:ARG:NH1	2.55	0.40
1:B:103:LEU:HD21	1:B:247:HIS:O	2.21	0.40
1:B:66:LEU:HD13	1:B:251:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	565/585 (97%)	525 (93%)	33 (6%)	7 (1%)	13	23
1	B	562/585 (96%)	524 (93%)	30 (5%)	8 (1%)	11	19
All	All	1127/1170 (96%)	1049 (93%)	63 (6%)	15 (1%)	12	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	300	ALA
1	A	517	SER
1	B	96	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	300	ALA
1	B	517	SER
1	A	95	GLU
1	B	95	GLU
1	B	129	ASP
1	A	129	ASP
1	A	150	TYR
1	B	567	CYS
1	B	150	TYR
1	B	118	PRO
1	A	118	PRO

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	401/511 (78%)	392 (98%)	9 (2%)	52	70
1	B	390/511 (76%)	386 (99%)	4 (1%)	76	85
All	All	791/1022 (77%)	778 (98%)	13 (2%)	62	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	103	LEU
1	A	236	THR
1	A	245	CYS
1	A	337	ARG
1	A	380	LEU
1	A	430	LEU
1	A	463	LEU
1	A	559	CYS
1	B	7	VAL
1	B	58	SER
1	B	337	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	559	CYS

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

Mol	Chain	Res	Type
1	A	391	ASN
1	B	391	ASN
1	B	429	ASN

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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IO3	A	2003	-	14,17,17	1.31	1 (7%)	18,24,24	1.48	2 (11%)
2	IO3	B	2002	-	14,17,17	1.31	1 (7%)	18,24,24	1.49	1 (5%)
2	IO3	A	2002	-	14,17,17	1.38	1 (7%)	18,24,24	1.92	2 (11%)
2	IO3	A	2001	-	14,17,17	1.33	1 (7%)	18,24,24	1.61	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IO3	B	2003	-	14,17,17	1.37	1 (7%)	18,24,24	1.83	4 (22%)
2	IO3	B	2004	-	14,17,17	1.33	1 (7%)	18,24,24	1.56	2 (11%)
2	IO3	A	2004	-	14,17,17	1.20	1 (7%)	18,24,24	1.64	2 (11%)
2	IO3	B	2001	-	14,17,17	1.29	1 (7%)	18,24,24	1.45	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IO3	A	2003	-	-	4/6/10/10	0/1/1/1
2	IO3	B	2002	-	-	2/6/10/10	0/1/1/1
2	IO3	A	2002	-	-	2/6/10/10	0/1/1/1
2	IO3	A	2001	-	-	2/6/10/10	0/1/1/1
2	IO3	B	2003	-	-	3/6/10/10	0/1/1/1
2	IO3	B	2004	-	-	0/6/10/10	0/1/1/1
2	IO3	A	2004	-	-	4/6/10/10	0/1/1/1
2	IO3	B	2001	-	-	4/6/10/10	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2003	IO3	C7-C8	-4.25	1.49	1.54
2	A	2002	IO3	C7-C8	-4.20	1.49	1.54
2	B	2004	IO3	C7-C8	-4.12	1.49	1.54
2	A	2001	IO3	C7-C8	-4.02	1.49	1.54
2	B	2001	IO3	C7-C8	-3.86	1.49	1.54
2	A	2003	IO3	C7-C8	-3.85	1.49	1.54
2	A	2004	IO3	C7-C8	-3.73	1.49	1.54
2	B	2002	IO3	C7-C8	-3.73	1.49	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	IO3	C1-C7-C8	6.92	123.82	114.09
2	A	2004	IO3	C1-C7-C8	5.35	121.61	114.09
2	B	2003	IO3	C1-C7-C8	5.23	121.45	114.09
2	B	2004	IO3	C1-C7-C8	4.85	120.91	114.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2002	IO3	C1-C7-C8	4.76	120.78	114.09
2	A	2003	IO3	C1-C7-C8	4.41	120.29	114.09
2	A	2001	IO3	C1-C7-C8	4.10	119.86	114.09
2	B	2001	IO3	C1-C7-C8	4.02	119.74	114.09
2	B	2003	IO3	C6-C1-C2	3.37	120.09	116.30
2	B	2004	IO3	C6-C1-C2	3.32	120.03	116.30
2	A	2003	IO3	C6-C1-C2	2.88	119.53	116.30
2	A	2001	IO3	C1-C6-I3	2.76	123.13	119.59
2	A	2004	IO3	C6-C1-C2	2.65	119.28	116.30
2	B	2003	IO3	C7-C1-C2	-2.57	118.08	123.10
2	B	2003	IO3	C1-C6-I3	2.35	122.61	119.59
2	A	2001	IO3	C5-C6-I3	-2.21	116.39	119.20
2	A	2002	IO3	C6-C1-C2	2.13	118.69	116.30

There are no chirality outliers.

All (21) torsion outliers are listed below:

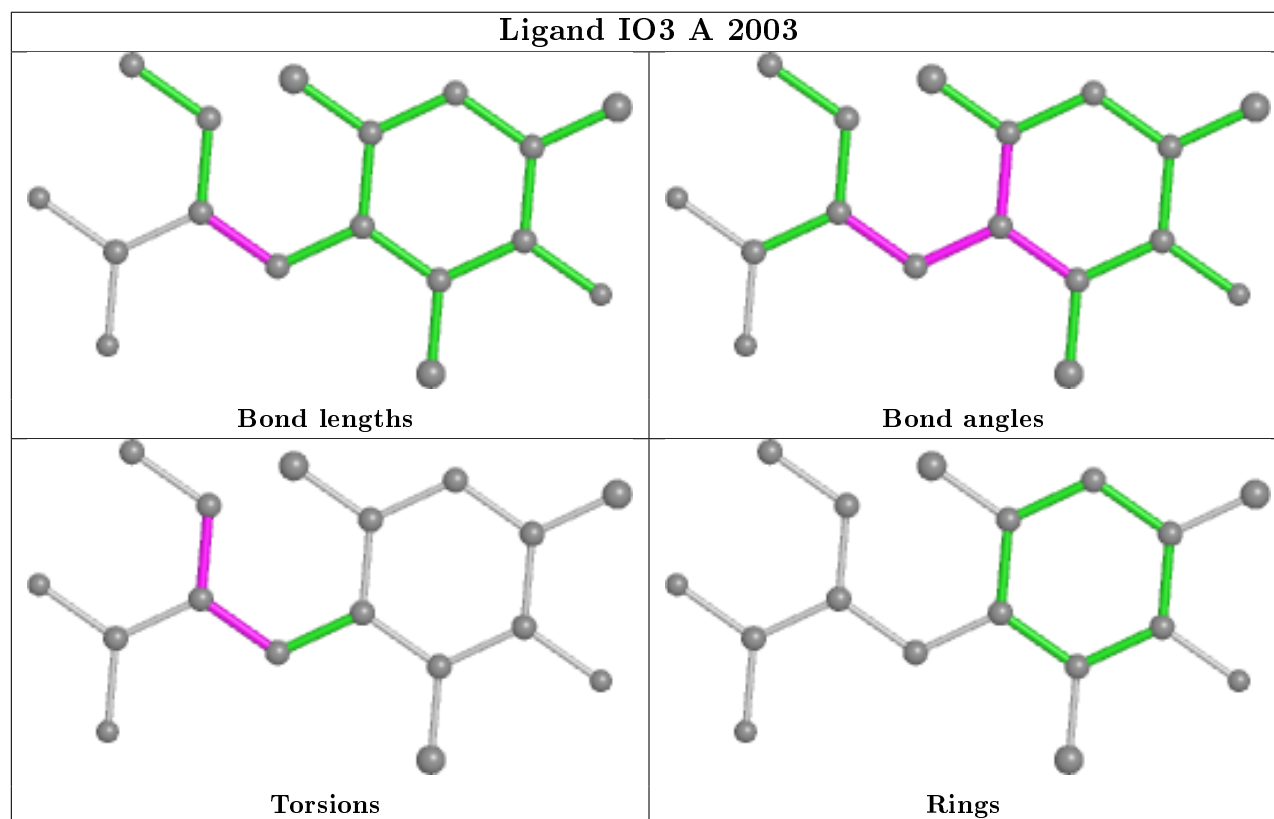
Mol	Chain	Res	Type	Atoms
2	A	2003	IO3	C1-C7-C8-C10
2	A	2003	IO3	C11-C10-C8-C9
2	B	2002	IO3	C1-C7-C8-C10
2	A	2002	IO3	C1-C7-C8-C10
2	A	2001	IO3	C6-C1-C7-C8
2	A	2004	IO3	C1-C7-C8-C9
2	A	2004	IO3	C1-C7-C8-C10
2	B	2001	IO3	C11-C10-C8-C9
2	A	2003	IO3	C11-C10-C8-C7
2	A	2001	IO3	C2-C1-C7-C8
2	B	2001	IO3	C6-C1-C7-C8
2	B	2003	IO3	C1-C7-C8-C10
2	B	2001	IO3	C11-C10-C8-C7
2	B	2003	IO3	C11-C10-C8-C7
2	A	2003	IO3	C1-C7-C8-C9
2	B	2002	IO3	C1-C7-C8-C9
2	A	2002	IO3	C1-C7-C8-C9
2	A	2004	IO3	C2-C1-C7-C8
2	A	2004	IO3	C6-C1-C7-C8
2	B	2001	IO3	C2-C1-C7-C8
2	B	2003	IO3	C11-C10-C8-C9

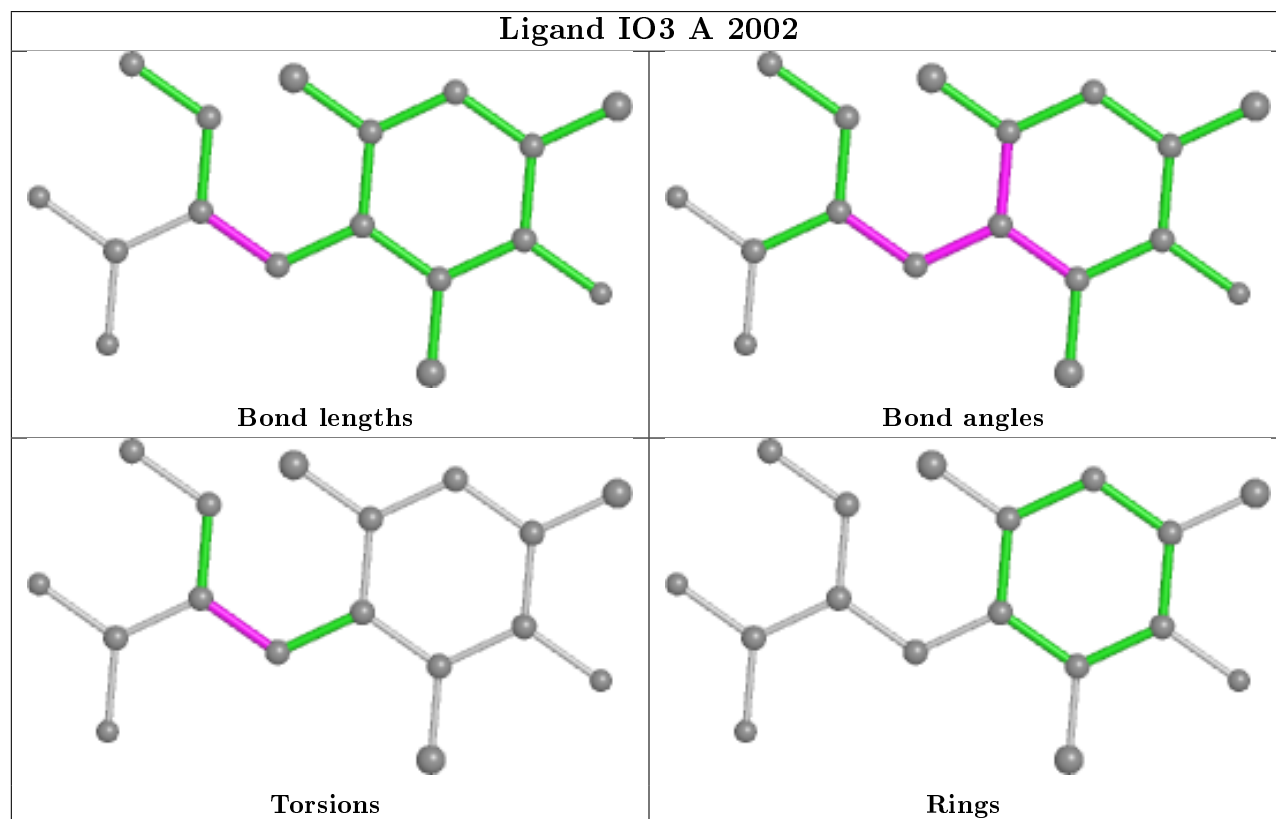
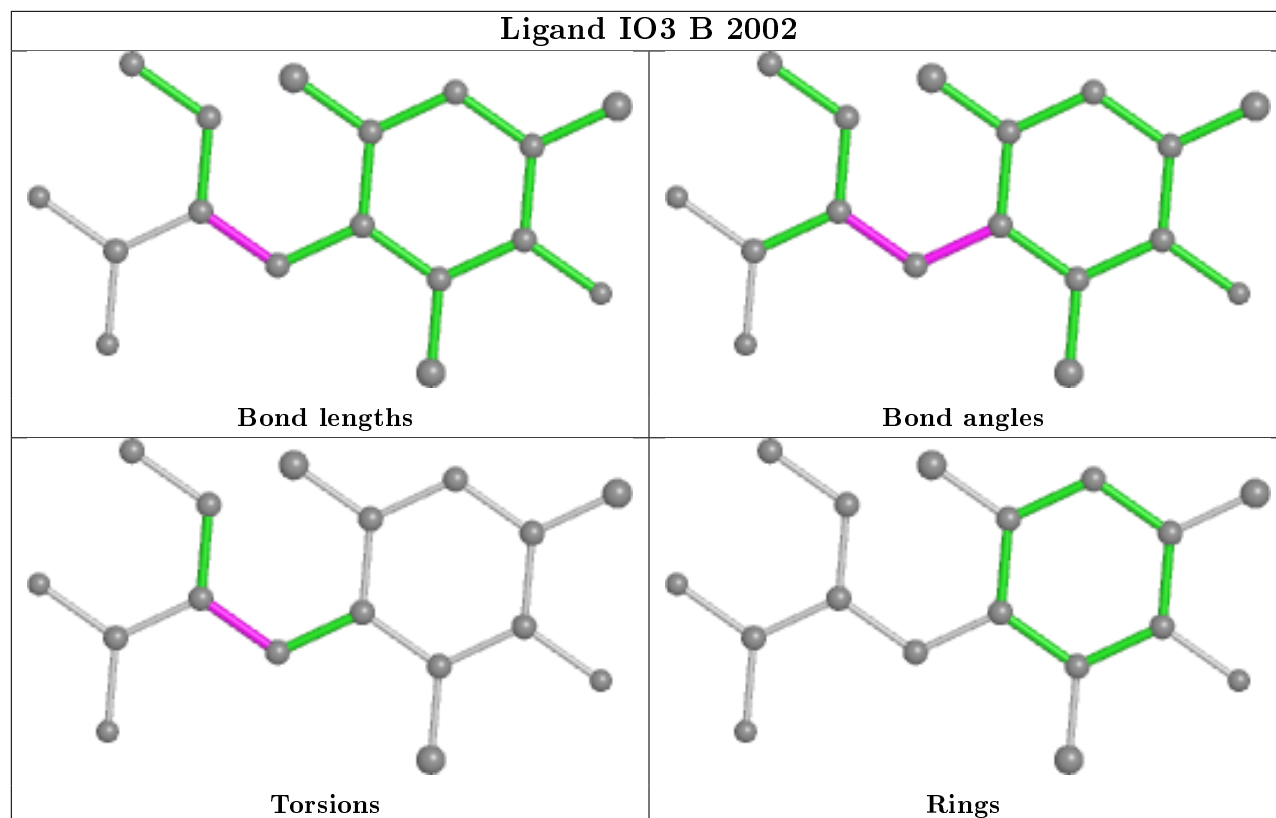
There are no ring outliers.

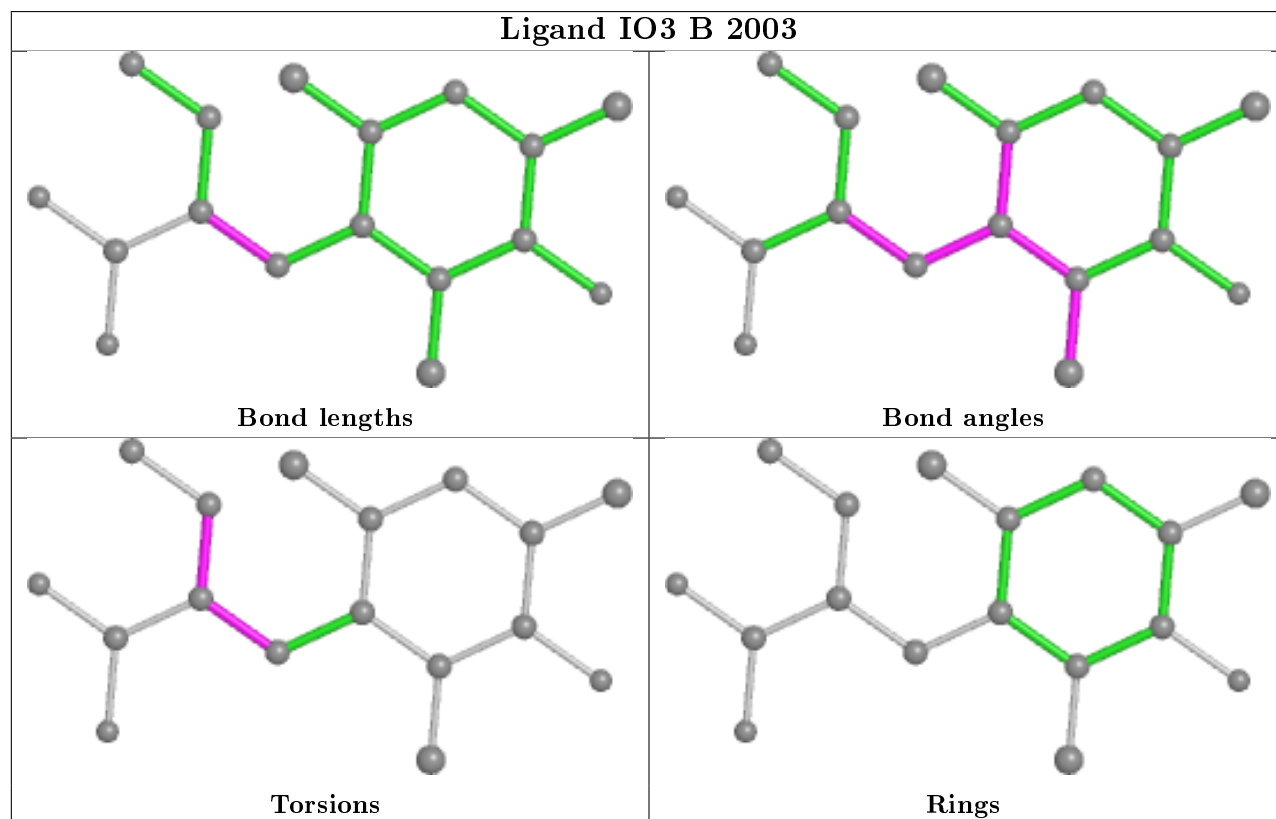
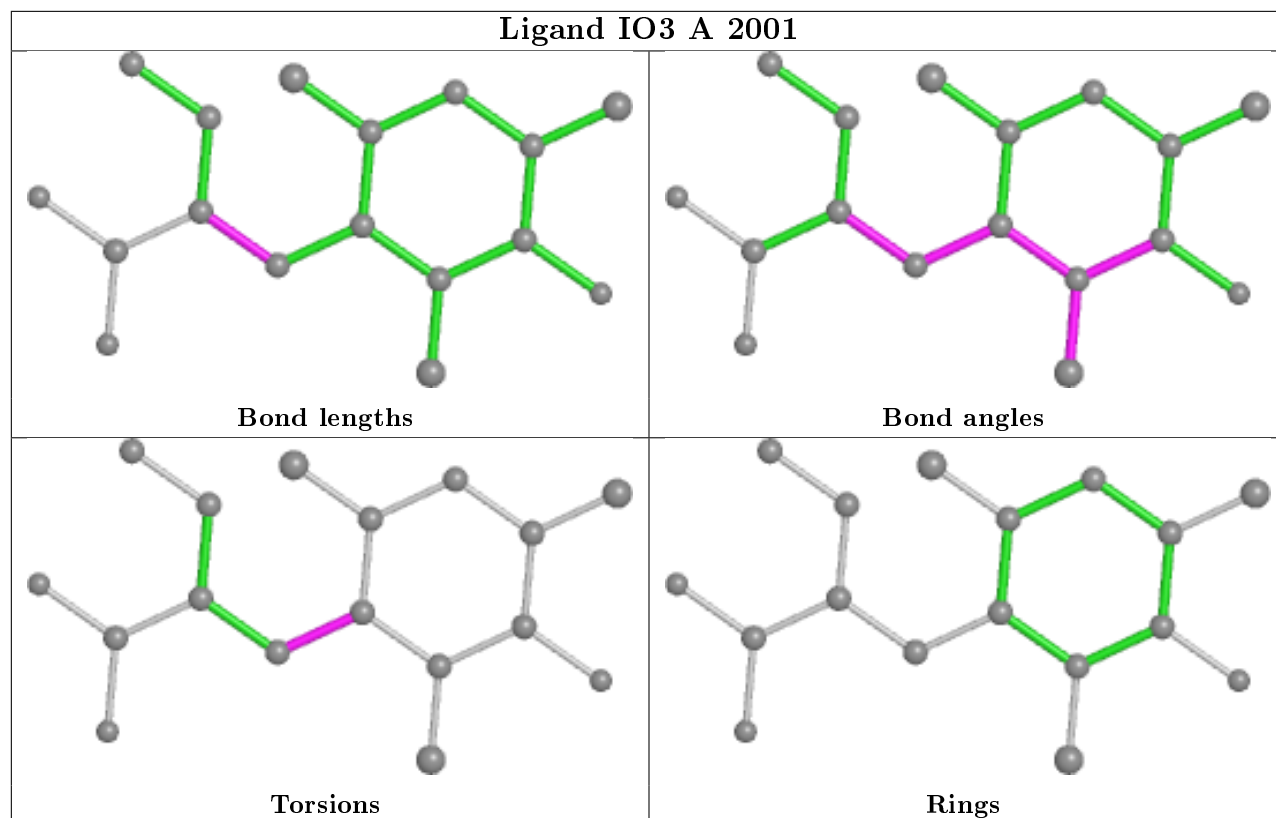
8 monomers are involved in 22 short contacts:

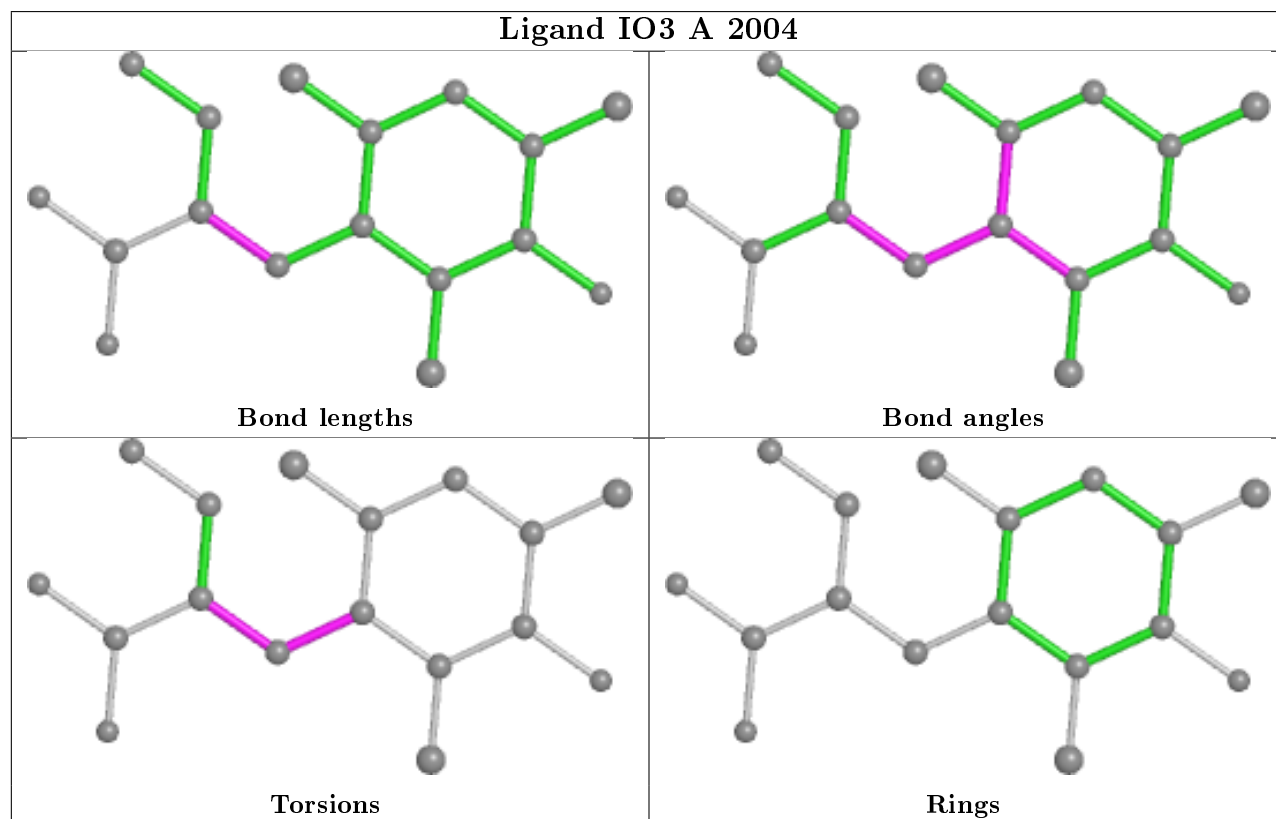
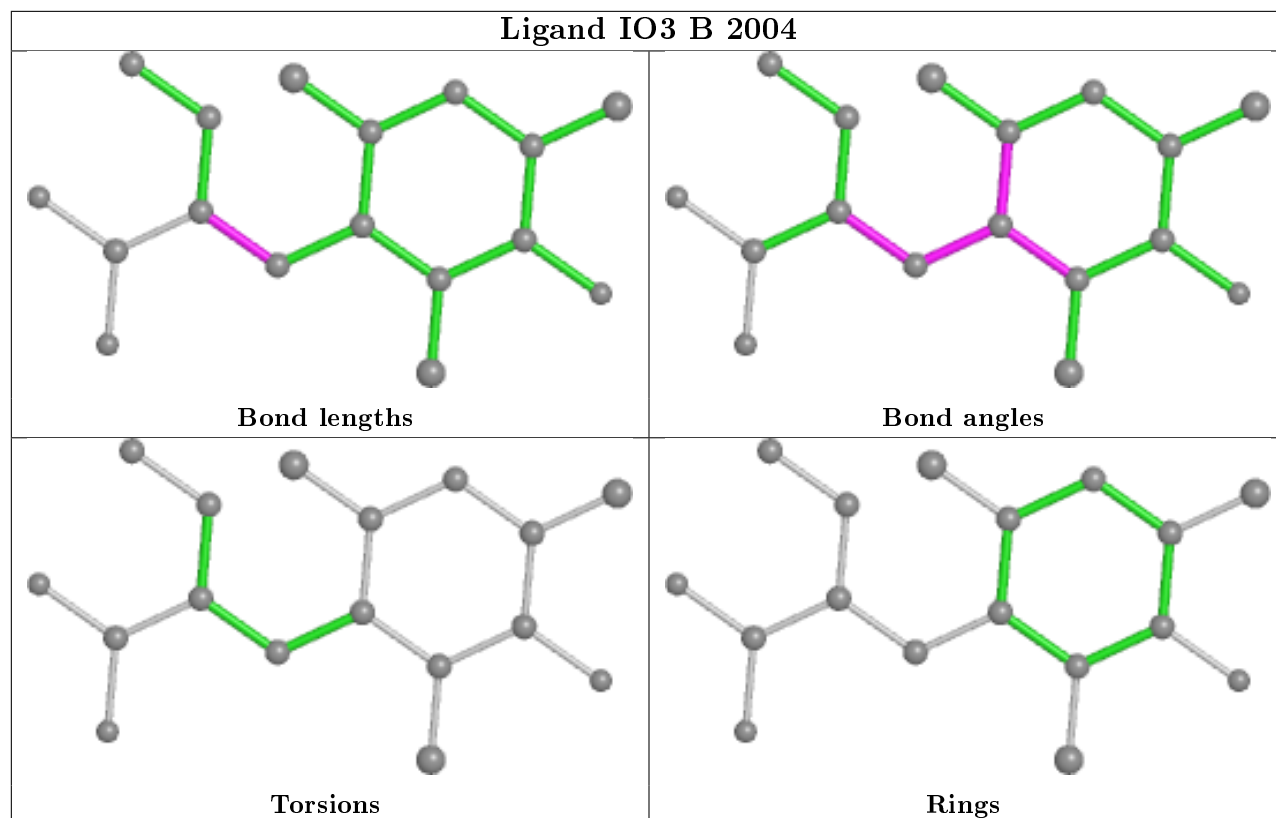
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2003	IO3	3	0
2	B	2002	IO3	1	0
2	A	2002	IO3	3	0
2	A	2001	IO3	2	0
2	B	2003	IO3	2	0
2	B	2004	IO3	6	0
2	A	2004	IO3	4	0
2	B	2001	IO3	1	0

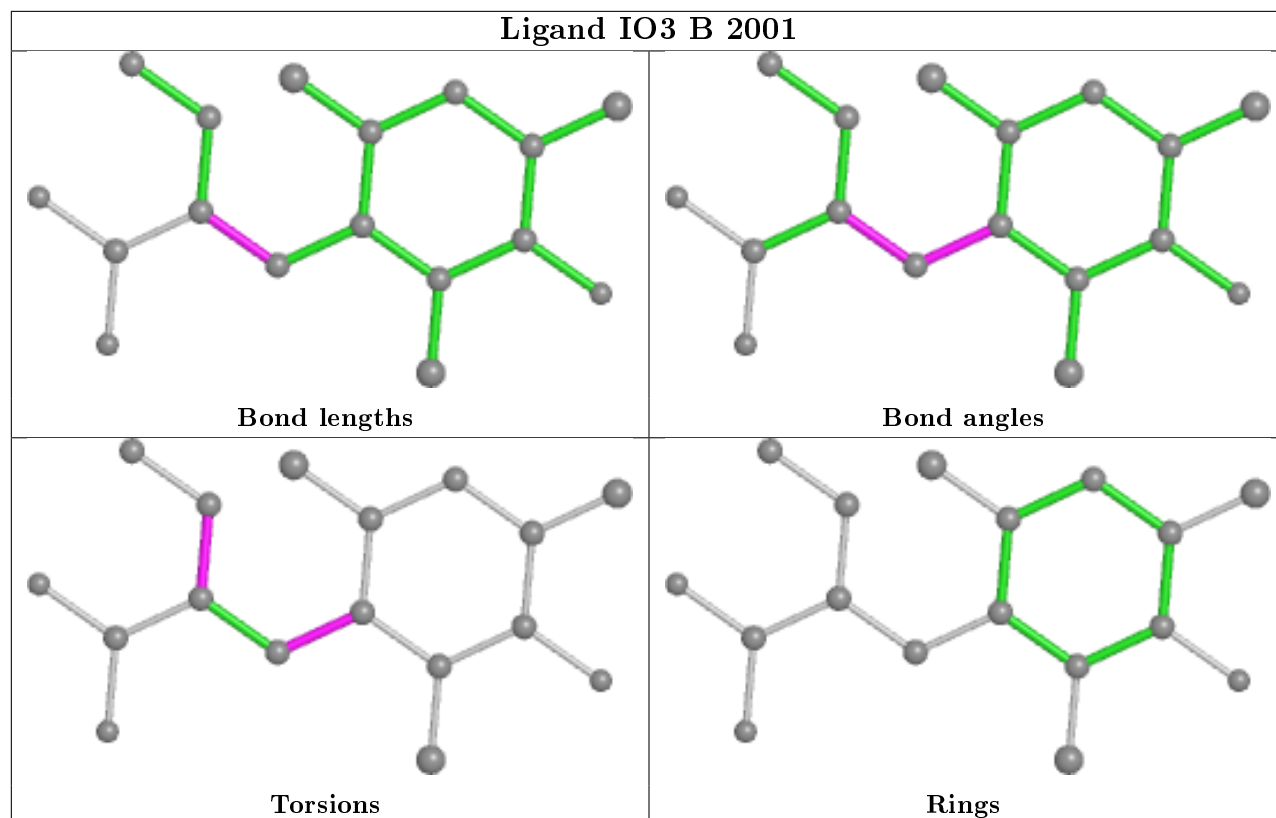
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	569/585 (97%)	-0.25	13 (2%) 60 69	1, 30, 164, 266	0
1	B	566/585 (96%)	-0.23	13 (2%) 60 69	2, 35, 163, 261	0
All	All	1135/1170 (97%)	-0.24	26 (2%) 60 69	1, 32, 165, 266	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	HIS	9.6
1	A	504	ALA	8.4
1	B	562	ASP	7.8
1	B	563	ASP	5.2
1	B	510	HIS	4.8
1	B	504	ALA	4.0
1	B	566	THR	4.0
1	A	505	GLU	3.9
1	A	59	ALA	3.1
1	B	52	THR	3.1
1	B	575	LEU	3.1
1	A	172	ALA	3.1
1	A	509	PHE	3.0
1	A	561	ALA	2.9
1	B	578	ALA	2.9
1	B	59	ALA	2.7
1	A	562	ASP	2.6
1	B	508	THR	2.5
1	A	168	CYS	2.5
1	A	563	ASP	2.5
1	B	582	ALA	2.4
1	B	561	ALA	2.4
1	A	54	VAL	2.2
1	A	138	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	582	ALA	2.1
1	B	24	LEU	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](#)

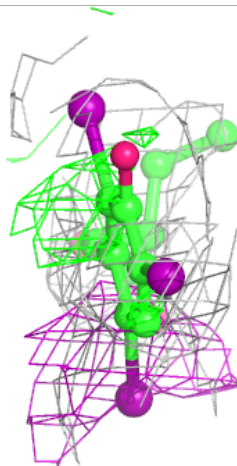
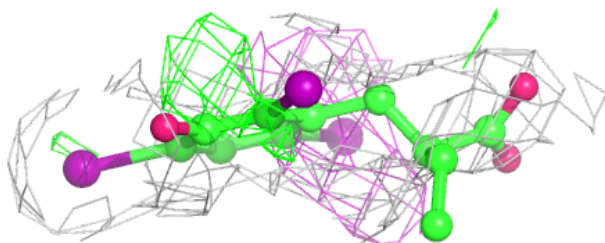
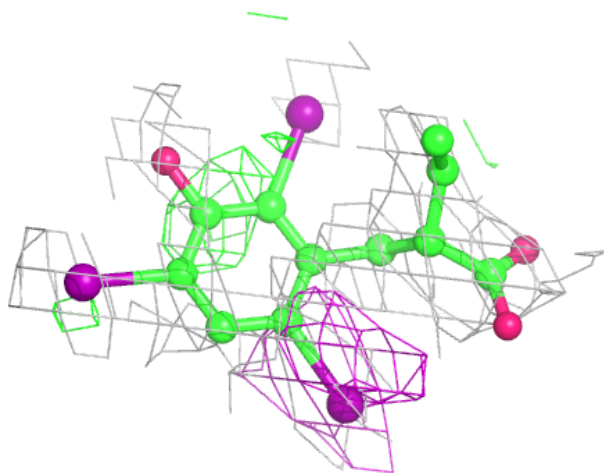
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IO3	A	2003	17/17	0.82	0.19	71,86,184,201	0
2	IO3	B	2004	17/17	0.82	0.40	109,111,171,173	0
2	IO3	A	2004	17/17	0.85	0.29	90,94,120,205	0
2	IO3	B	2003	17/17	0.91	0.17	57,72,102,132	0
2	IO3	A	2002	17/17	0.98	0.14	25,30,41,48	0
2	IO3	B	2002	17/17	0.99	0.16	26,36,52,52	0
2	IO3	B	2001	17/17	0.99	0.15	9,17,27,28	0
2	IO3	A	2001	17/17	1.00	0.16	0,16,27,27	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.

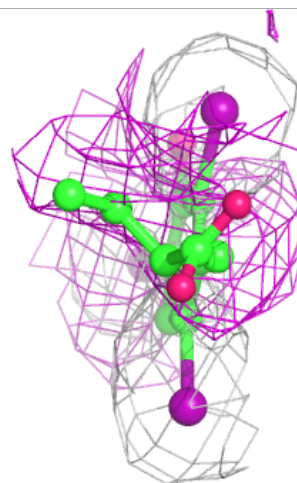
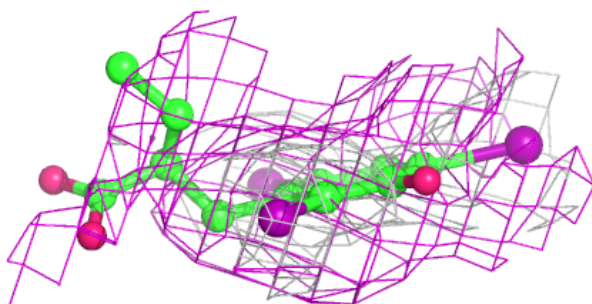
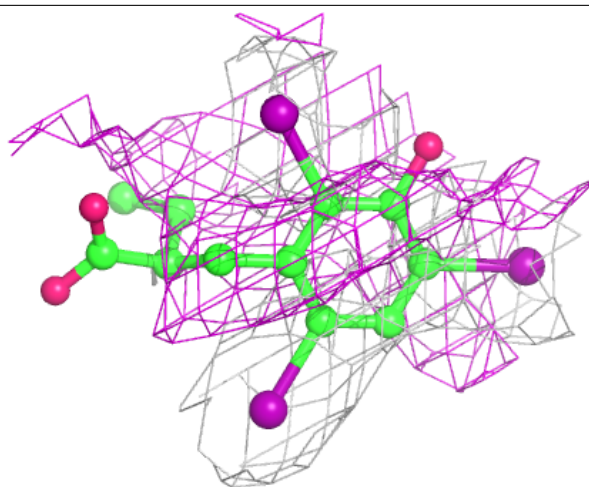
Electron density around IO3 A 2003:

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



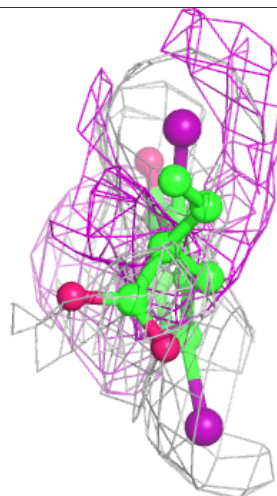
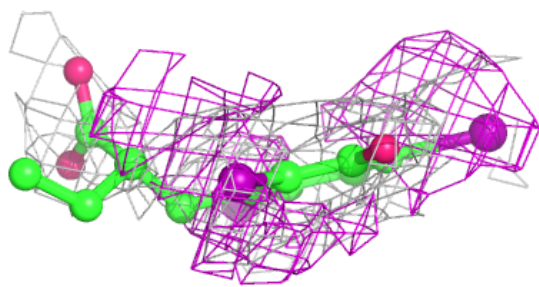
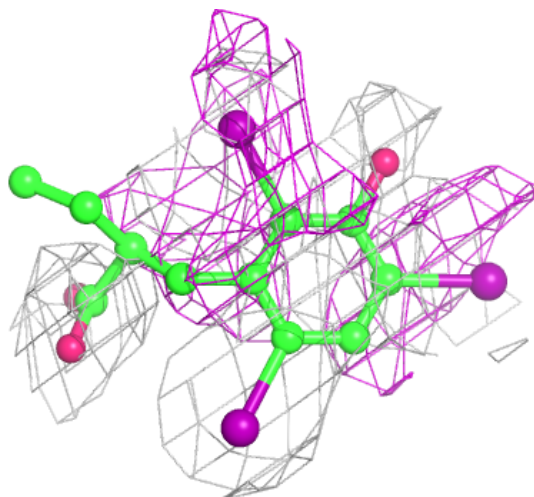
Electron density around IO3 B 2004:

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



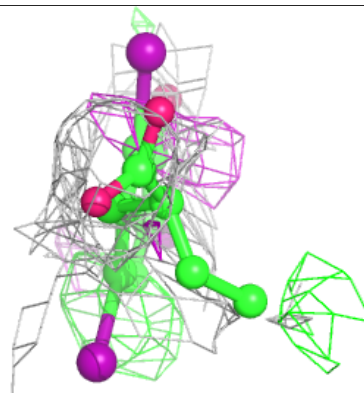
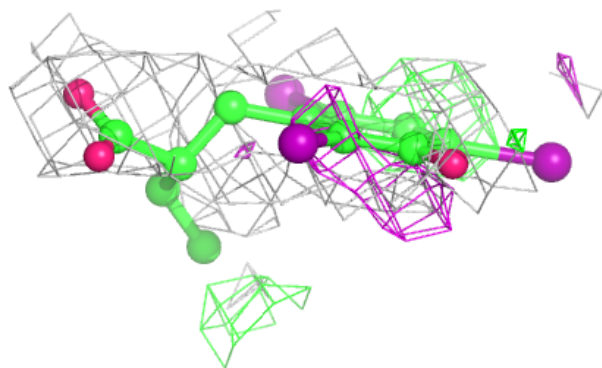
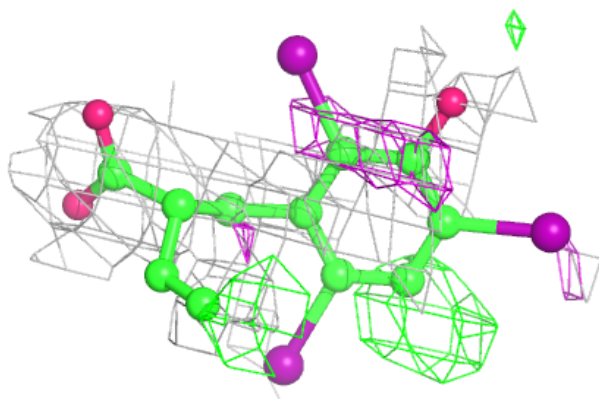
Electron density around IO3 A 2004:

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



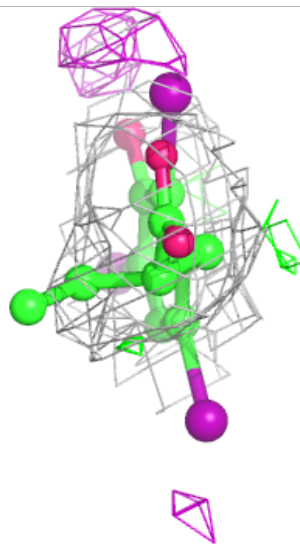
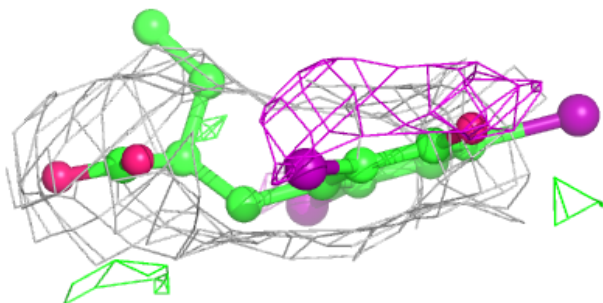
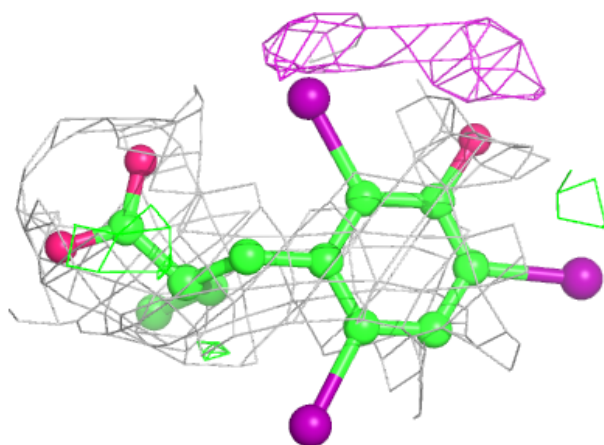
Electron density around IO3 B 2003:

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



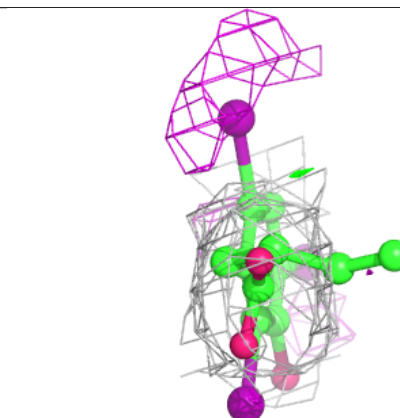
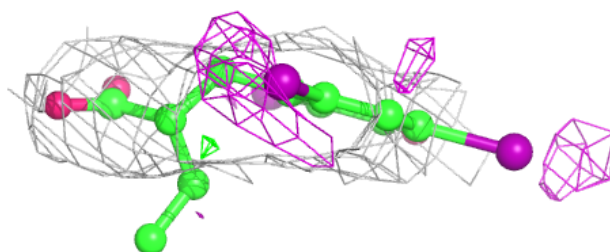
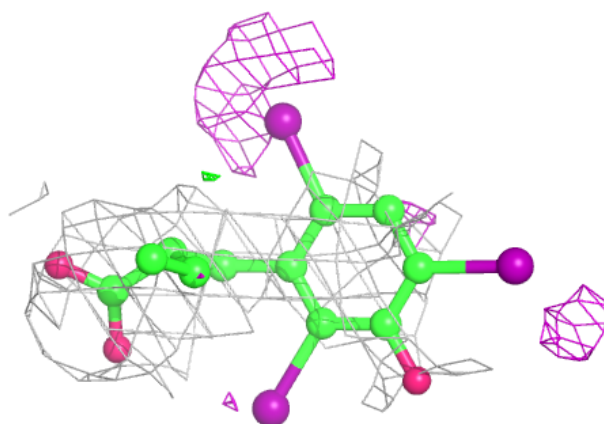
Electron density around IO3 A 2002:

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

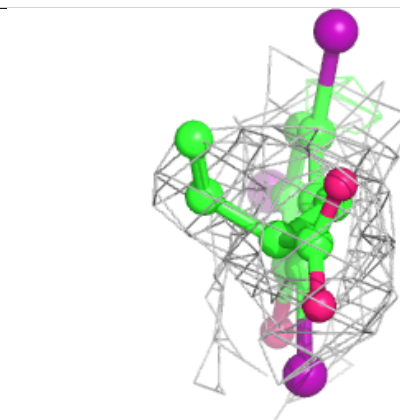
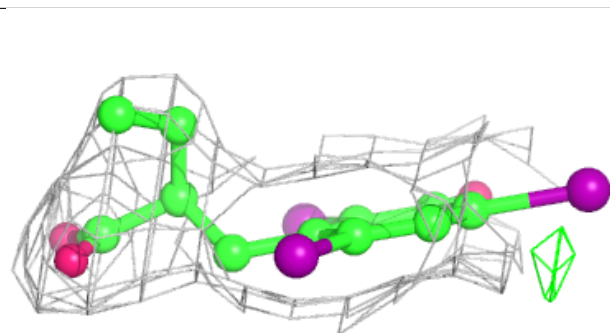
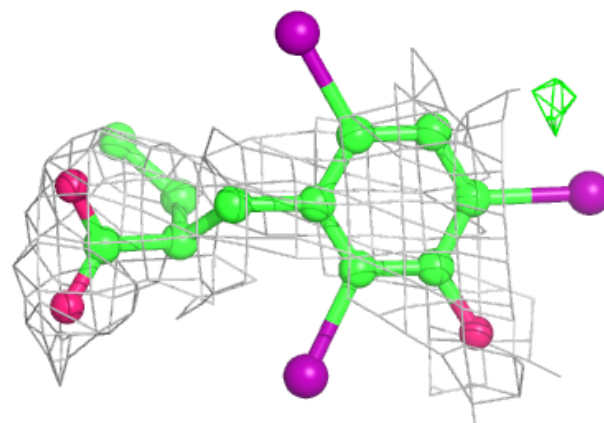


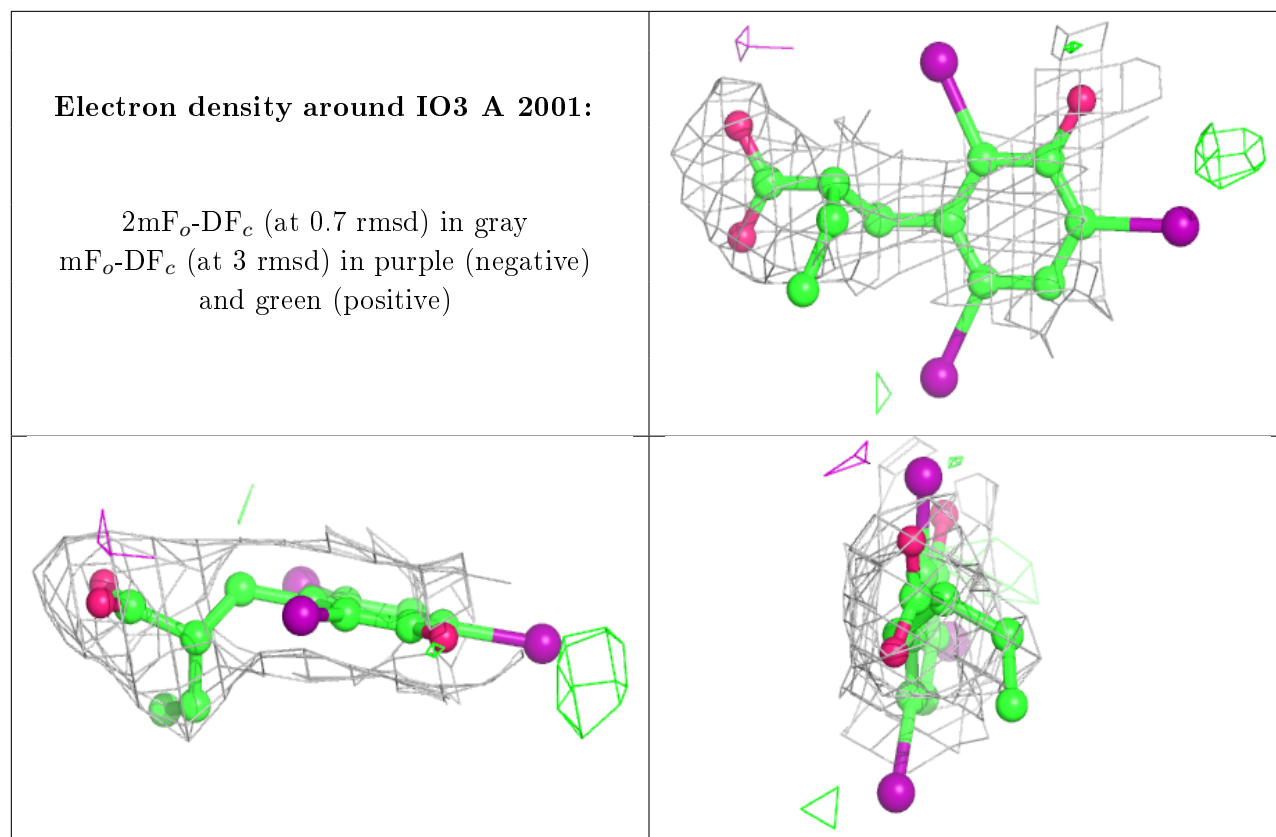
Electron density around IO3 B 2002:

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

**Electron density around IO3 B 2001:**

$2mF_o-DF_c$ (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.