Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 07:53 AM EDT

PDB ID	:	3MSS
Title	:	Abl kinase in complex with imatinib and fragment (FRAG2) in the myristate site
Authors	:	Cowan-Jacob, S.W.; Rummel, G.; Fendrich, G.
Deposited on	:	2010-04-29
Resolution	:	1.95 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 (i) 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 (i)) were used in the production of this report:

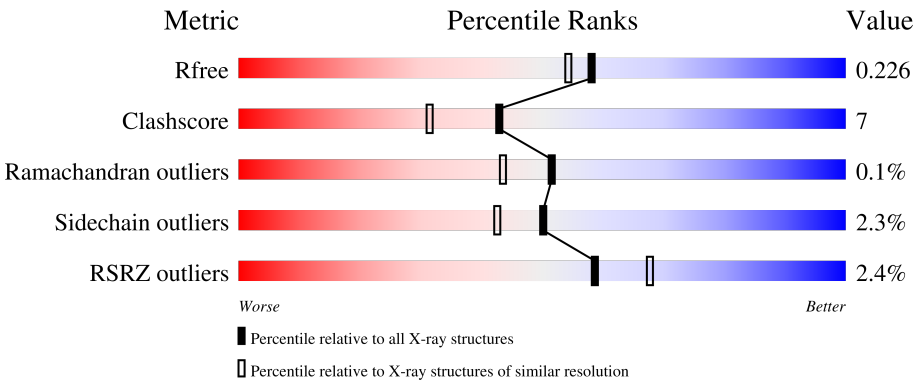
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	293	2% 77% 11% • 10%
1	B	293	3% 78% 11% • 10%
1	C	293	2% 76% 13% • 10%
1	D	293	% 75% 14% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9563 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 Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2151	1390	350	394	17	0	0	0
1	B	264	2151	1390	350	394	17	0	0	0
1	C	264	2151	1390	350	394	17	0	0	0
1	D	264	2151	1390	350	394	17	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

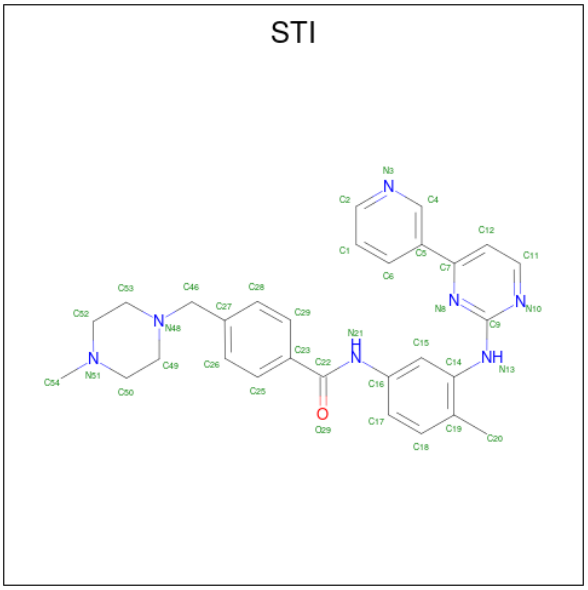
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLY	-	expression tag	UNP P00520
A	224	ALA	-	expression tag	UNP P00520
A	225	MET	-	expression tag	UNP P00520
A	226	ASP	-	expression tag	UNP P00520
A	227	PRO	-	expression tag	UNP P00520
A	228	SER	-	expression tag	UNP P00520
B	223	GLY	-	expression tag	UNP P00520
B	224	ALA	-	expression tag	UNP P00520
B	225	MET	-	expression tag	UNP P00520
B	226	ASP	-	expression tag	UNP P00520
B	227	PRO	-	expression tag	UNP P00520
B	228	SER	-	expression tag	UNP P00520
C	223	GLY	-	expression tag	UNP P00520
C	224	ALA	-	expression tag	UNP P00520
C	225	MET	-	expression tag	UNP P00520
C	226	ASP	-	expression tag	UNP P00520
C	227	PRO	-	expression tag	UNP P00520
C	228	SER	-	expression tag	UNP P00520
D	223	GLY	-	expression tag	UNP P00520
D	224	ALA	-	expression tag	UNP P00520
D	225	MET	-	expression tag	UNP P00520

Continued on next page...

Continued from previous page...

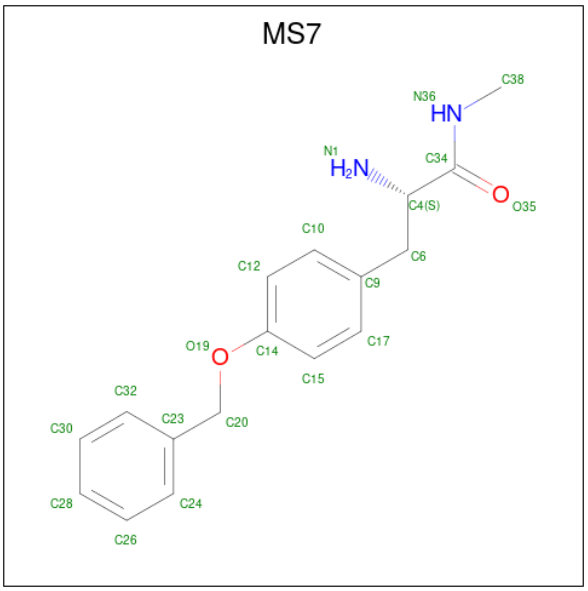
Chain	Residue	Modelled	Actual	Comment	Reference
D	226	ASP	-	expression tag	UNP P00520
D	227	PRO	-	expression tag	UNP P00520
D	228	SER	-	expression tag	UNP P00520

- Molecule 2 is 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE (three-letter code: STI) (formula: $C_{29}H_{31}N_7O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	37	29	7	1	0	0
2	B	1	37	29	7	1	0	0
2	C	1	37	29	7	1	0	0
2	D	1	37	29	7	1	0	0

- Molecule 3 is O-benzyl-N-methyl-L-tyrosinamide (three-letter code: MS7) (formula: $C_{17}H_{20}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	21	17	2	2	0	0
3	B	1	21	17	2	2	0	0
3	C	1	21	17	2	2	0	0
3	D	1	21	17	2	2	0	0

- Molecule 4 is water.

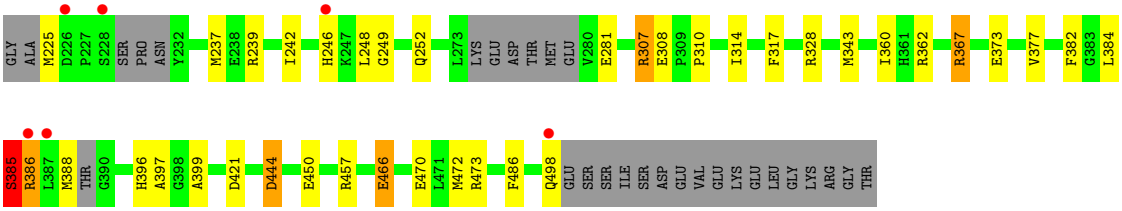
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	184	184	184	0	0
4	B	177	177	177	0	0
4	C	180	180	180	0	0
4	D	186	186	186	0	0

3 Residue-property plots (i)

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

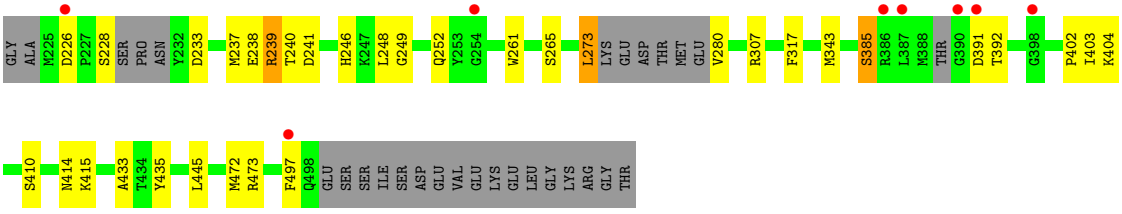
• Molecule 1: Tyrosine-protein kinase ABL1

Chain A: 2% 77% 11% 10%



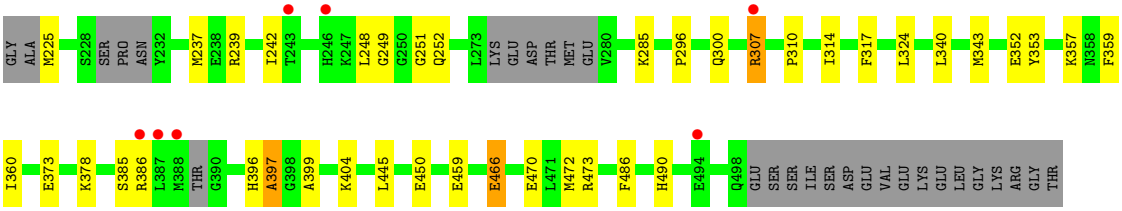
• Molecule 1: Tyrosine-protein kinase ABL1

Chain B: 3% 78% 11% 10%



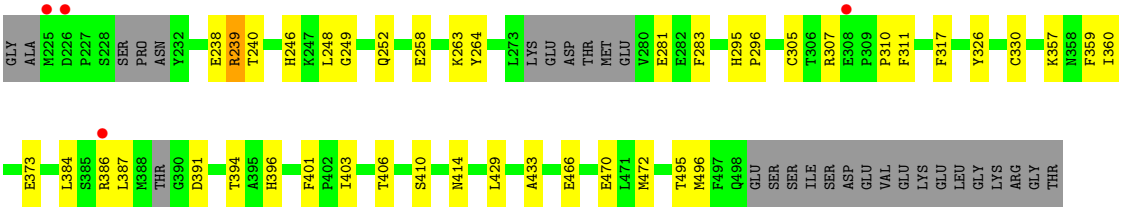
• Molecule 1: Tyrosine-protein kinase ABL1

Chain C: 2% 76% 13% 10%



• Molecule 1: Tyrosine-protein kinase ABL1

Chain D: % 75% 14% 10%


GLY
ALA
M225
D226
P227
S228
SER
PRO
ASN
Y232
E238
R239
T240
H246
K247
L248
G249
Q252
E258
K263
Y264
L273
LYS
GLU
ASP
THR
MET
GLU
V280
E281
E282
F283
H295
P296
C305
T306
R307
E308
P309
P310
F311
F317
Y326
C330
K357
N358
F359
I360
E373
L384
S385
R386
L387
M388
THR
G390
D391
T394
A395
H396
F401
P402
I403
T406
S410
N414
L429
A433
E466
E470
L471
M472
T495
M496
F497
Q498
GLU
SER
SER
ILE
SER
ASP
GLU
VAL
GLU
LYS
GLU
LEU
GLY
LYS
ARG
GLY
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.22Å 146.78Å 95.81Å 90.00° 127.07° 90.00°	Depositor
Resolution (Å)	52.93 – 1.95 36.34 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.6 (52.93-1.95) 96.2 (36.34-1.96)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.169 , 0.220 0.175 , 0.226	Depositor DCC
R_{free} test set	4461 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 31.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-h-2*l,1/2*h-1/2*k 0.025 for -h,h+2*l,1/2*h+1/2*k 0.457 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9563	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: STI, MS7

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.19	6/2206 (0.3%)	1.01	10/2982 (0.3%)
1	B	1.15	2/2206 (0.1%)	0.96	6/2982 (0.2%)
1	C	1.15	5/2206 (0.2%)	0.96	5/2982 (0.2%)
1	D	1.13	1/2206 (0.0%)	0.93	2/2982 (0.1%)
All	All	1.16	14/8824 (0.2%)	0.97	23/11928 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	GLU	CG-CD	6.88	1.62	1.51
1	A	450	GLU	CG-CD	6.24	1.61	1.51
1	B	385	SER	CB-OG	-6.18	1.34	1.42
1	C	385	SER	CB-OG	-5.86	1.34	1.42
1	C	459	GLU	CG-CD	5.81	1.60	1.51
1	C	450	GLU	CG-CD	5.58	1.60	1.51
1	C	486	PHE	CD1-CE1	5.39	1.50	1.39
1	A	470	GLU	CG-CD	5.36	1.59	1.51
1	A	486	PHE	CD1-CE1	5.23	1.49	1.39
1	D	305	CYS	CB-SG	-5.21	1.73	1.81
1	C	466	GLU	CG-CD	5.19	1.59	1.51
1	A	486	PHE	CE1-CZ	5.16	1.47	1.37
1	A	377	VAL	CB-CG1	5.08	1.63	1.52
1	B	435	TYR	CE1-CZ	5.01	1.45	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	473	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	A	473	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	B	473	ARG	NE-CZ-NH2	-10.44	115.08	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	473	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	A	343	MET	CG-SD-CE	-8.48	86.64	100.20
1	A	444	ASP	CB-CG-OD1	-7.54	111.51	118.30
1	B	473	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	C	385	SER	CB-CA-C	-6.41	97.93	110.10
1	A	457	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	472	MET	CG-SD-CE	-6.38	89.99	100.20
1	A	473	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	385	SER	CB-CA-C	-5.96	98.77	110.10
1	B	472	MET	CG-SD-CE	-5.86	90.83	100.20
1	A	367	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	343	MET	CG-SD-CE	-5.49	91.42	100.20
1	A	421	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	472	MET	CG-SD-CE	-5.36	91.63	100.20
1	A	472	MET	CG-SD-CE	-5.33	91.67	100.20
1	B	273	LEU	CB-CG-CD2	-5.20	102.17	111.00
1	B	233	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	C	324	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	A	328	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	D	429	LEU	CA-CB-CG	5.08	126.98	115.30

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	2151	0	2105	30	1
1	B	2151	0	2105	19	0
1	C	2151	0	2105	35	0
1	D	2151	0	2105	30	0
2	A	37	0	31	1	0
2	B	37	0	31	0	0
2	C	37	0	31	1	0
2	D	37	0	31	1	0
3	A	21	0	20	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	20	1	0
3	C	21	0	20	1	0
3	D	21	0	20	1	0
4	A	184	0	0	13	0
4	B	177	0	0	7	0
4	C	180	0	0	12	1
4	D	186	0	0	7	2
All	All	9563	0	8624	119	2

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 (119) 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:367:ARG:HD2	1:A:388:MET:CE	1.78	1.12
1:A:367:ARG:HD2	1:A:388:MET:HE3	1.40	0.98
3:A:516:MS7:H4	4:A:690:HOH:O	1.69	0.92
1:A:498:GLN:O	4:A:785:HOH:O	1.88	0.91
1:A:367:ARG:HD2	1:A:388:MET:HE1	1.51	0.91
1:D:238:GLU:HG3	1:D:240:THR:HB	1.54	0.87
1:B:415:LYS:HE2	4:B:58:HOH:O	1.76	0.84
1:A:239:ARG:NH1	1:A:310:PRO:O	2.13	0.81
1:D:249:GLY:O	1:D:252:GLN:HG2	1.82	0.80
1:A:225:MET:HB2	4:A:544:HOH:O	1.82	0.78
1:C:239:ARG:NH1	1:C:310:PRO:O	2.13	0.78
1:C:300:GLN:HG3	4:C:595:HOH:O	1.86	0.76
1:A:386:ARG:HD2	4:A:648:HOH:O	1.87	0.73
1:A:237:MET:HB3	4:A:656:HOH:O	1.89	0.73
1:C:490:HIS:HE1	4:C:542:HOH:O	1.72	0.72
1:C:404:LYS:HE3	4:C:799:HOH:O	1.89	0.72
1:B:249:GLY:O	1:B:252:GLN:HG2	1.91	0.71
1:C:242:ILE:CD1	1:C:314:ILE:HD13	2.19	0.71
3:C:516:MS7:H4	4:C:577:HOH:O	1.90	0.71
1:B:385:SER:HB2	4:B:164:HOH:O	1.91	0.70
1:C:249:GLY:O	1:C:252:GLN:HG2	1.92	0.69
1:A:242:ILE:CD1	1:A:314:ILE:HD13	2.24	0.68
1:C:307:ARG:NE	1:C:307:ARG:HA	2.08	0.68
1:D:495:THR:O	4:D:754:HOH:O	2.10	0.68
1:B:391:ASP:OD1	4:B:697:HOH:O	2.14	0.66
1:D:360:ILE:HD12	1:D:360:ILE:N	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:HIS:H	1:B:246:HIS:CD2	2.14	0.66
1:D:310:PRO:HA	4:D:767:HOH:O	1.95	0.66
1:A:249:GLY:O	1:A:252:GLN:HG2	1.97	0.65
1:C:359:PHE:C	1:C:360:ILE:HD12	2.17	0.65
1:A:444:ASP:HB2	4:A:773:HOH:O	1.95	0.65
1:A:225:MET:N	4:A:126:HOH:O	2.29	0.64
1:A:444:ASP:OD2	4:A:773:HOH:O	2.14	0.64
1:C:225:MET:N	4:C:184:HOH:O	2.31	0.64
1:A:242:ILE:HD13	1:A:314:ILE:HD13	1.80	0.63
1:D:239:ARG:HG3	1:D:239:ARG:HH11	1.64	0.63
1:C:242:ILE:HD11	1:C:314:ILE:HD13	1.80	0.61
1:B:415:LYS:HE3	4:B:626:HOH:O	2.04	0.57
1:D:396:HIS:HE1	4:D:575:HOH:O	1.86	0.57
1:C:242:ILE:HD13	1:C:314:ILE:HD13	1.86	0.57
1:B:238:GLU:HG3	1:B:240:THR:HB	1.86	0.57
1:C:242:ILE:CD1	1:C:314:ILE:CD1	2.84	0.56
1:C:352:GLU:OE2	1:C:490:HIS:CD2	2.58	0.56
1:D:248:LEU:HD11	1:D:317:PHE:HE1	1.70	0.56
1:C:360:ILE:CD1	4:C:674:HOH:O	2.53	0.55
1:C:307:ARG:HA	1:C:307:ARG:HE	1.72	0.55
1:C:396:HIS:N	1:C:399:ALA:O	2.40	0.54
1:C:248:LEU:HD11	1:C:317:PHE:HE1	1.70	0.54
1:A:396:HIS:N	1:A:399:ALA:O	2.33	0.54
1:D:495:THR:C	4:D:754:HOH:O	2.46	0.53
1:B:497:PHE:HD1	4:B:548:HOH:O	1.92	0.53
1:D:359:PHE:C	1:D:360:ILE:HD12	2.29	0.53
1:C:353:TYR:CZ	1:C:357:LYS:HD2	2.45	0.52
1:C:360:ILE:HD12	1:C:360:ILE:N	2.24	0.52
1:D:414:ASN:O	1:D:414:ASN:ND2	2.42	0.52
1:D:263:LYS:HE2	1:D:264:TYR:CE1	2.45	0.52
1:D:263:LYS:HE2	1:D:264:TYR:CZ	2.45	0.52
1:B:403:ILE:HD11	4:B:671:HOH:O	2.10	0.51
1:D:246:HIS:CD2	1:D:246:HIS:H	2.27	0.51
1:C:242:ILE:HD13	1:C:314:ILE:CD1	2.40	0.51
1:C:404:LYS:HE2	1:C:445:LEU:CD2	2.41	0.51
1:A:307:ARG:NE	1:A:307:ARG:HA	2.25	0.51
1:C:360:ILE:HD11	4:C:674:HOH:O	2.09	0.51
1:D:396:HIS:CE1	4:D:575:HOH:O	2.63	0.49
1:A:367:ARG:CD	1:A:388:MET:HE3	2.27	0.49
1:C:237:MET:HB3	4:C:593:HOH:O	2.13	0.48
1:A:397:ALA:C	1:A:399:ALA:H	2.17	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD13	1:A:388:MET:CE	2.44	0.48
1:C:386:ARG:NH2	4:C:676:HOH:O	2.47	0.48
1:C:237:MET:SD	1:C:314:ILE:HD12	2.53	0.48
1:A:382:PHE:HB2	1:A:384:LEU:HG	1.97	0.47
1:D:433:ALA:HA	3:D:516:MS7:H30	1.97	0.47
1:C:251:GLY:HA2	4:C:121:HOH:O	2.14	0.47
2:C:1:STI:H151	2:C:1:STI:O29	2.14	0.47
1:C:285:LYS:HE3	4:C:590:HOH:O	2.14	0.47
1:C:296:PRO:O	1:C:378:LYS:HE2	2.14	0.47
1:A:444:ASP:CG	4:A:773:HOH:O	2.54	0.47
1:C:340:LEU:HA	1:C:343:MET:HE2	1.97	0.47
1:A:386:ARG:HB2	4:A:538:HOH:O	2.14	0.46
1:D:384:LEU:HD23	1:D:387:LEU:HD12	1.96	0.46
1:B:239:ARG:HG2	1:B:240:THR:N	2.29	0.46
1:B:237:MET:HE1	1:B:261:TRP:CE2	2.51	0.46
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.76	0.46
1:B:273:LEU:HD21	1:B:280:VAL:HA	1.98	0.46
1:A:246:HIS:HB2	4:A:525:HOH:O	2.15	0.46
1:A:444:ASP:CB	4:A:773:HOH:O	2.58	0.45
2:D:1:STI:O29	2:D:1:STI:H151	2.17	0.45
1:A:396:HIS:O	1:A:399:ALA:N	2.49	0.45
1:D:410:SER:O	1:D:414:ASN:HA	2.17	0.45
1:D:248:LEU:HD13	1:D:258:GLU:HB2	2.00	0.44
1:D:295:HIS:CE1	1:D:296:PRO:HD2	2.53	0.44
1:D:387:LEU:H	1:D:387:LEU:HG	1.58	0.44
1:D:401:PHE:HB2	1:D:403:ILE:HD13	2.00	0.44
1:C:404:LYS:HE2	1:C:445:LEU:HD23	2.00	0.44
1:A:248:LEU:HD11	1:A:317:PHE:HE1	1.83	0.43
1:B:404:LYS:HE3	1:B:445:LEU:HD12	1.99	0.43
1:B:410:SER:O	1:B:414:ASN:HA	2.18	0.43
2:A:1:STI:O29	2:A:1:STI:H151	2.20	0.42
1:D:496:MET:HA	4:D:754:HOH:O	2.20	0.42
1:A:237:MET:SD	1:A:314:ILE:HD12	2.60	0.42
1:A:360:ILE:HG22	1:A:362:ARG:HG3	2.01	0.42
1:B:445:LEU:HD11	4:B:517:HOH:O	2.19	0.42
1:D:326:TYR:O	1:D:330:CYS:HB3	2.20	0.42
1:C:466:GLU:O	1:C:470:GLU:HG3	2.20	0.42
1:A:385:SER:CB	4:A:559:HOH:O	2.68	0.42
1:B:392:THR:O	1:B:402:PRO:HA	2.21	0.41
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.76	0.41
1:D:406:THR:HG22	1:D:410:SER:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:MET:CE	1:B:261:TRP:CE2	3.04	0.41
1:C:396:HIS:O	1:C:397:ALA:C	2.58	0.41
1:C:386:ARG:HB2	4:C:591:HOH:O	2.21	0.41
1:D:283:PHE:CE2	1:D:311:PHE:HB3	2.55	0.41
1:B:248:LEU:HD11	1:B:317:PHE:HE1	1.85	0.41
1:C:307:ARG:NE	1:C:307:ARG:CA	2.81	0.41
1:D:239:ARG:HH11	1:D:239:ARG:CG	2.32	0.41
1:B:433:ALA:HA	3:B:516:MS7:H30	2.02	0.40
1:C:404:LYS:HE2	1:C:445:LEU:HD21	2.02	0.40
1:D:394:THR:HG22	4:D:678:HOH:O	2.22	0.40
1:D:466:GLU:O	1:D:470:GLU:HG3	2.22	0.40

All (2) 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:A:466:GLU:OE2	4:D:523:HOH:O[4_454]	2.08	0.12
4:C:211:HOH:O	4:D:572:HOH:O[4_454]	2.18	0.02

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	256/293 (87%)	245 (96%)	11 (4%)	0	100	100
1	B	256/293 (87%)	246 (96%)	10 (4%)	0	100	100
1	C	256/293 (87%)	245 (96%)	10 (4%)	1 (0%)	34	22
1	D	256/293 (87%)	245 (96%)	11 (4%)	0	100	100
All	All	1024/1172 (87%)	981 (96%)	42 (4%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	397	ALA

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	230/255 (90%)	224 (97%)	6 (3%)	46	36
1	B	230/255 (90%)	224 (97%)	6 (3%)	46	36
1	C	230/255 (90%)	228 (99%)	2 (1%)	78	77
1	D	230/255 (90%)	223 (97%)	7 (3%)	41	30
All	All	920/1020 (90%)	899 (98%)	21 (2%)	50	42

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	GLU
1	A	307	ARG
1	A	308	GLU
1	A	373	GLU
1	A	385	SER
1	A	386	ARG
1	B	226	ASP
1	B	228	SER
1	B	239	ARG
1	B	241	ASP
1	B	265	SER
1	B	307	ARG
1	C	307	ARG
1	C	373	GLU
1	D	239	ARG
1	D	281	GLU
1	D	307	ARG
1	D	357	LYS
1	D	373	GLU
1	D	386	ARG
1	D	391	ASP

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

Mol	Chain	Res	Type
1	B	246	HIS
1	B	374	ASN
1	C	447	GLN
1	C	490	HIS
1	D	246	HIS
1	D	396	HIS
1	D	477	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	MS7	A	516	-	22,22,22	1.29	1 (4%)	28,28,28	1.30	4 (14%)
3	MS7	B	516	-	22,22,22	1.13	1 (4%)	28,28,28	1.00	1 (3%)
2	STI	C	1	-	40,41,41	1.38	6 (15%)	51,56,56	2.09	11 (21%)
3	MS7	C	516	-	22,22,22	1.19	1 (4%)	28,28,28	1.11	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	STI	D	1	-	40,41,41	1.23	3 (7%)	51,56,56	2.21	18 (35%)
2	STI	B	1	-	40,41,41	1.34	4 (10%)	51,56,56	1.90	13 (25%)
2	STI	A	1	-	40,41,41	1.52	10 (25%)	51,56,56	2.32	13 (25%)
3	MS7	D	516	-	22,22,22	1.23	1 (4%)	28,28,28	1.11	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MS7	A	516	-	-	0/15/15/15	0/2/2/2
3	MS7	B	516	-	-	3/15/15/15	0/2/2/2
2	STI	C	1	-	-	1/16/30/30	0/5/5/5
3	MS7	C	516	-	-	4/15/15/15	0/2/2/2
2	STI	D	1	-	-	3/16/30/30	0/5/5/5
2	STI	B	1	-	-	2/16/30/30	0/5/5/5
2	STI	A	1	-	-	1/16/30/30	0/5/5/5
3	MS7	D	516	-	-	4/15/15/15	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	516	MS7	C34-N36	4.19	1.39	1.33
3	A	516	MS7	C34-N36	3.95	1.38	1.33
3	B	516	MS7	C34-N36	3.79	1.38	1.33
3	C	516	MS7	C34-N36	3.73	1.38	1.33
2	A	1	STI	C46-C27	3.73	1.58	1.51
2	B	1	STI	C20-C19	3.66	1.58	1.51
2	D	1	STI	C20-C19	3.43	1.57	1.51
2	A	1	STI	C12-C11	3.23	1.41	1.36
2	C	1	STI	C12-C11	3.15	1.40	1.36
2	C	1	STI	C46-N48	2.74	1.52	1.47
2	C	1	STI	C46-C27	2.67	1.56	1.51
2	A	1	STI	C4-N3	2.56	1.37	1.32
2	B	1	STI	C17-C16	2.55	1.43	1.39
2	A	1	STI	C49-N48	2.53	1.53	1.46
2	B	1	STI	C15-C14	2.51	1.43	1.39
2	A	1	STI	C46-N48	2.32	1.52	1.47
2	D	1	STI	C17-C16	2.30	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	STI	C29-C28	2.26	1.42	1.38
2	A	1	STI	C12-C7	-2.24	1.38	1.41
2	B	1	STI	C7-N8	-2.24	1.33	1.37
2	D	1	STI	C54-N51	2.22	1.52	1.46
2	A	1	STI	C20-C19	2.21	1.55	1.51
2	A	1	STI	C2-N3	2.20	1.40	1.33
2	A	1	STI	C1-C6	2.19	1.41	1.36
2	C	1	STI	C1-C6	2.12	1.41	1.36
2	C	1	STI	C49-N48	2.12	1.52	1.46
2	C	1	STI	C7-N8	-2.10	1.34	1.37

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	STI	N10-C9-N8	-6.87	119.88	126.52
2	A	1	STI	C11-N10-C9	6.65	121.35	115.45
2	A	1	STI	N10-C9-N8	-6.42	120.32	126.52
2	C	1	STI	N10-C9-N8	-6.35	120.39	126.52
2	C	1	STI	C11-N10-C9	6.09	120.85	115.45
2	A	1	STI	C12-C11-N10	-5.87	118.03	123.81
2	D	1	STI	C11-N10-C9	5.39	120.23	115.45
2	B	1	STI	C12-C11-N10	-5.21	118.67	123.81
2	C	1	STI	C12-C11-N10	-5.12	118.76	123.81
2	A	1	STI	C54-N51-C52	-4.56	103.83	110.66
2	B	1	STI	C11-N10-C9	4.52	119.45	115.45
2	B	1	STI	N10-C9-N8	-4.51	122.17	126.52
2	D	1	STI	C18-C19-C14	4.50	121.68	117.44
2	C	1	STI	C9-N8-C7	4.49	122.92	115.60
3	A	516	MS7	C4-C34-N36	4.17	121.88	116.18
2	A	1	STI	C9-N8-C7	4.12	122.32	115.60
2	B	1	STI	C18-C19-C14	3.70	120.92	117.44
2	D	1	STI	C46-N48-C53	3.67	119.24	111.06
3	C	516	MS7	C4-C34-N36	3.62	121.13	116.18
2	D	1	STI	C50-N51-C52	3.53	114.46	109.52
2	A	1	STI	C49-C50-N51	-3.52	106.83	110.80
2	D	1	STI	C9-N8-C7	3.49	121.29	115.60
2	C	1	STI	C12-C7-N8	-3.48	116.89	121.46
2	B	1	STI	C50-N51-C52	3.38	114.25	109.52
2	A	1	STI	C46-N48-C53	3.38	118.58	111.06
2	D	1	STI	C11-C12-C7	-3.37	116.43	119.31
2	A	1	STI	C12-C7-N8	-3.35	117.06	121.46
2	C	1	STI	C54-N51-C52	-3.22	105.84	110.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	STI	C54-N51-C52	2.95	115.08	110.66
3	D	516	MS7	C20-O19-C14	2.91	124.85	117.65
2	D	1	STI	C49-N48-C53	2.89	115.33	108.83
2	D	1	STI	C25-C26-C27	-2.84	117.12	121.03
2	D	1	STI	C12-C11-N10	-2.76	121.09	123.81
2	B	1	STI	C49-N48-C53	2.75	115.01	108.83
2	C	1	STI	C46-N48-C53	2.72	117.12	111.06
2	A	1	STI	C14-N13-C9	-2.72	121.41	129.60
3	A	516	MS7	C20-O19-C14	2.69	124.30	117.65
2	A	1	STI	C26-C25-C23	-2.61	117.74	120.78
3	A	516	MS7	O35-C34-C4	-2.58	114.71	120.18
2	A	1	STI	O29-C22-C23	-2.56	116.37	120.94
2	C	1	STI	C29-C28-C27	-2.55	117.52	121.03
2	B	1	STI	C25-C26-C27	-2.53	117.55	121.03
3	D	516	MS7	C4-C34-N36	2.51	119.61	116.18
2	B	1	STI	C9-N8-C7	2.49	119.67	115.60
2	D	1	STI	C28-C27-C26	2.42	121.97	118.17
2	D	1	STI	C2-N3-C4	2.36	122.29	117.25
2	C	1	STI	C28-C27-C26	2.35	121.86	118.17
2	A	1	STI	C6-C1-C2	-2.32	115.95	118.93
2	B	1	STI	C28-C27-C26	2.30	121.77	118.17
2	B	1	STI	C46-N48-C53	2.29	116.16	111.06
2	B	1	STI	C52-C53-N48	-2.27	105.98	110.64
2	D	1	STI	C28-C29-C23	-2.25	118.16	120.78
2	B	1	STI	C46-C27-C26	-2.23	116.58	120.77
2	A	1	STI	C29-C23-C25	2.20	121.73	118.59
3	C	516	MS7	O35-C34-C4	-2.19	115.55	120.18
3	A	516	MS7	C32-C23-C24	2.17	121.58	118.17
2	D	1	STI	C52-C53-N48	-2.15	106.22	110.64
2	B	1	STI	C14-N13-C9	-2.13	123.19	129.60
2	D	1	STI	C20-C19-C14	-2.12	118.86	121.25
3	B	516	MS7	C28-C30-C32	2.11	123.40	120.19
2	D	1	STI	C5-C4-N3	-2.11	118.08	123.86
2	C	1	STI	C14-N13-C9	-2.09	123.30	129.60
2	D	1	STI	C14-N13-C9	-2.08	123.32	129.60
2	C	1	STI	C53-C52-N51	2.05	113.12	110.80
3	C	516	MS7	C20-O19-C14	2.05	122.70	117.65

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	STI	C15-C14-N13-C9
2	B	1	STI	C15-C14-N13-C9
2	C	1	STI	C15-C14-N13-C9
2	D	1	STI	C15-C14-N13-C9
3	C	516	MS7	O35-C34-C4-N1
3	C	516	MS7	N36-C34-C4-N1
3	D	516	MS7	O35-C34-C4-N1
3	D	516	MS7	N36-C34-C4-N1
3	B	516	MS7	N1-C4-C6-C9
3	D	516	MS7	N36-C34-C4-C6
3	B	516	MS7	C15-C14-O19-C20
2	B	1	STI	C19-C14-N13-C9
2	D	1	STI	C19-C14-N13-C9
3	B	516	MS7	C12-C14-O19-C20
3	C	516	MS7	O35-C34-C4-C6
3	D	516	MS7	O35-C34-C4-C6
3	C	516	MS7	N36-C34-C4-C6
2	D	1	STI	C27-C46-N48-C53

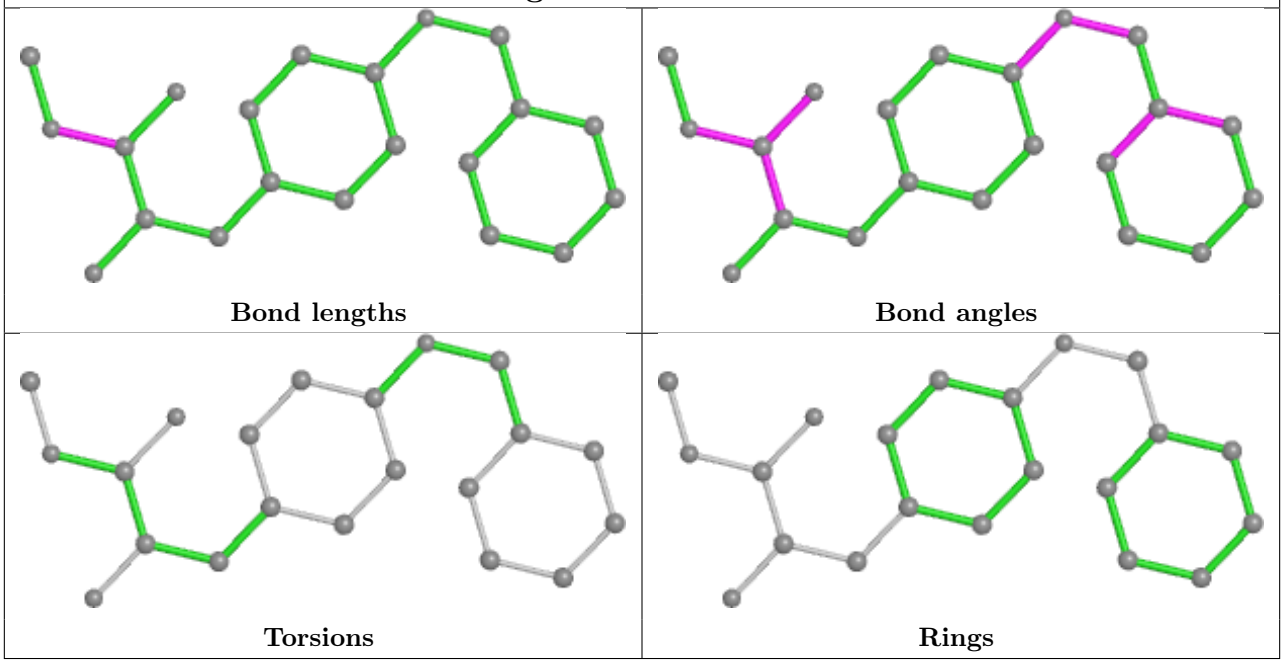
There are no ring outliers.

7 monomers are involved in 7 short contacts:

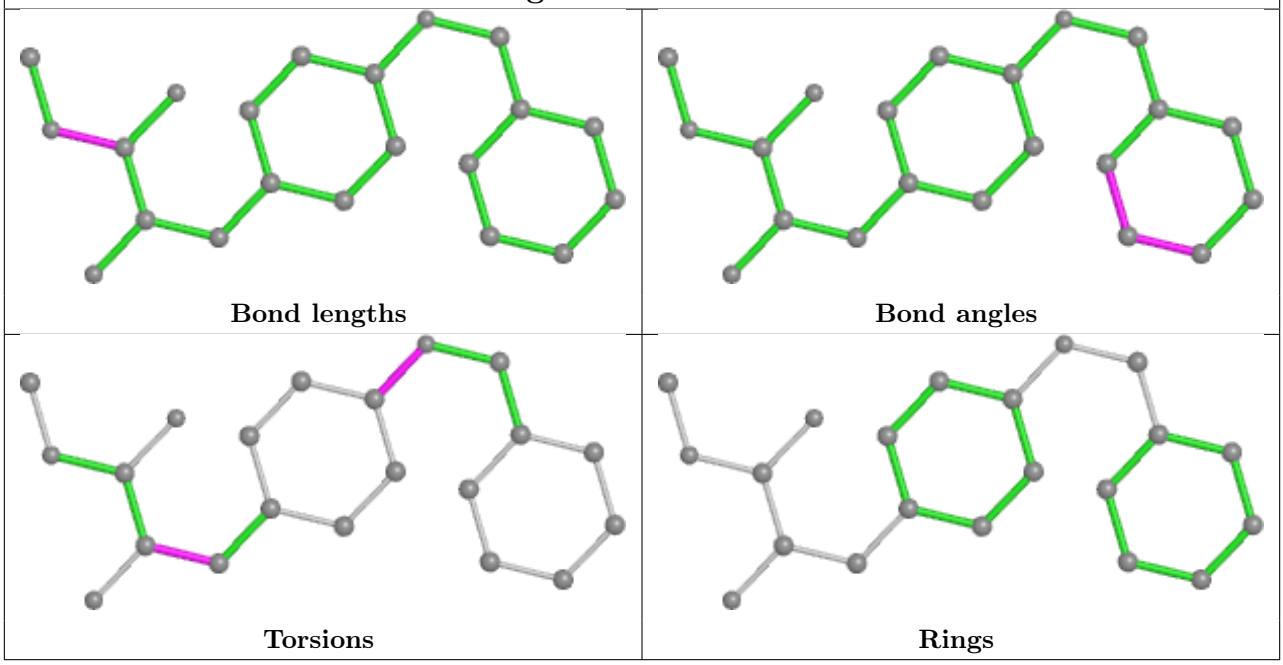
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	516	MS7	1	0
3	B	516	MS7	1	0
2	C	1	STI	1	0
3	C	516	MS7	1	0
2	D	1	STI	1	0
2	A	1	STI	1	0
3	D	516	MS7	1	0

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 then 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.

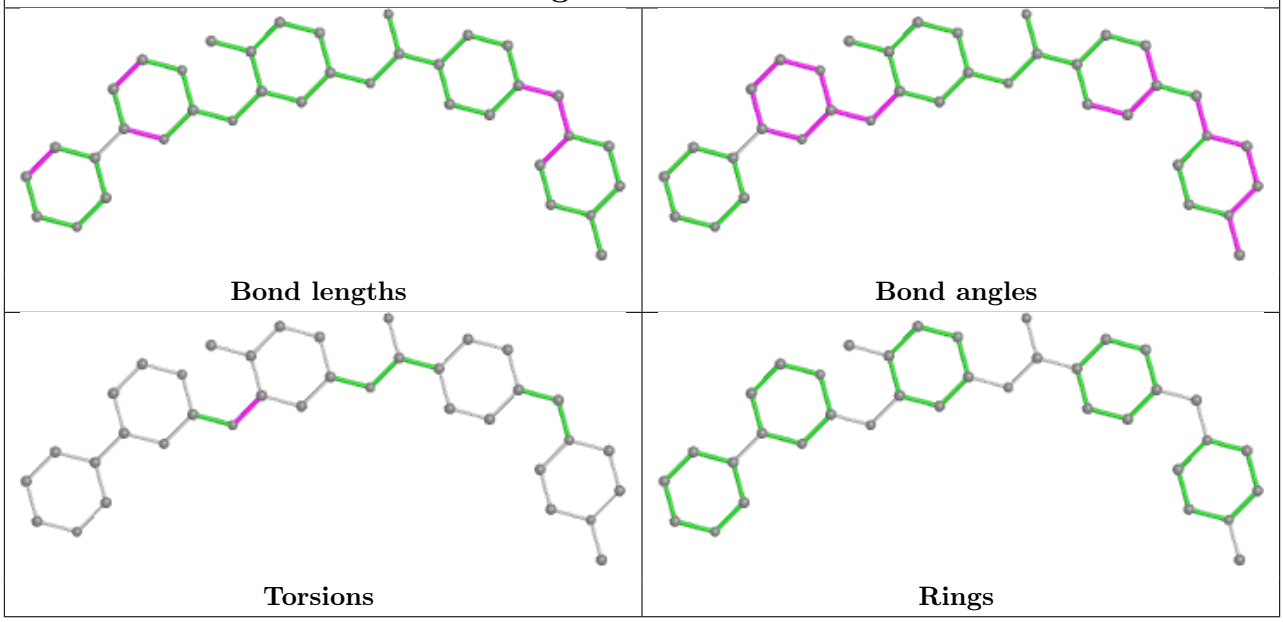
Ligand MS7 A 516



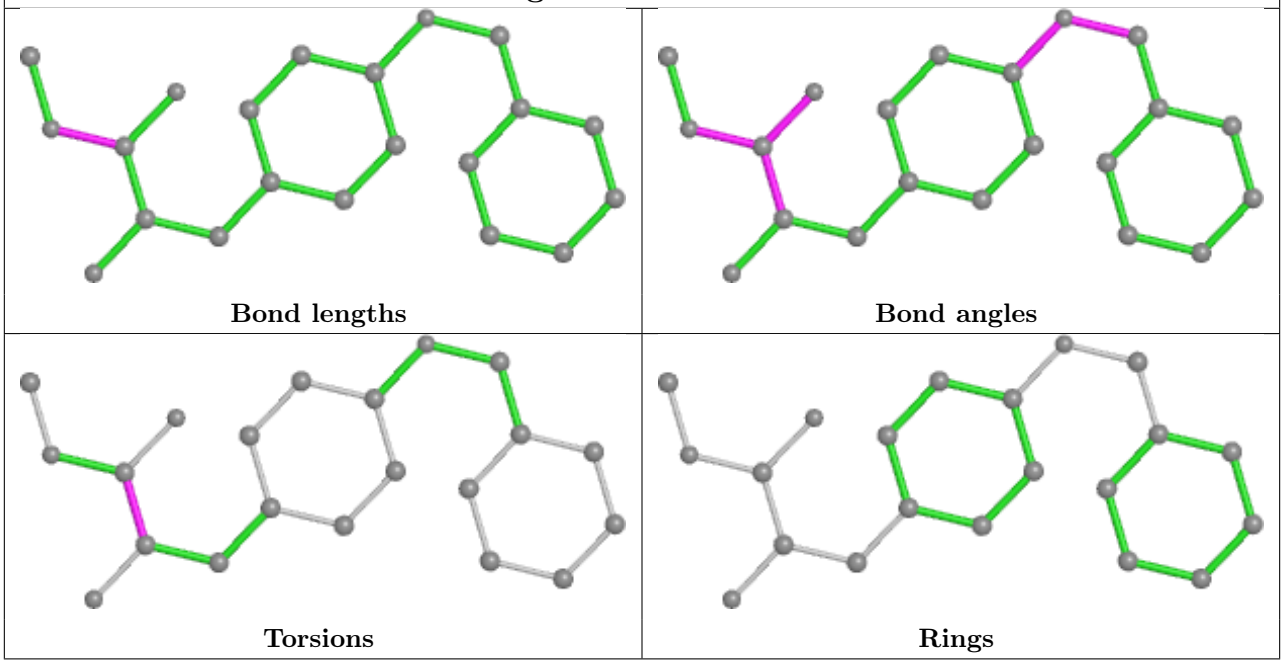
Ligand MS7 B 516



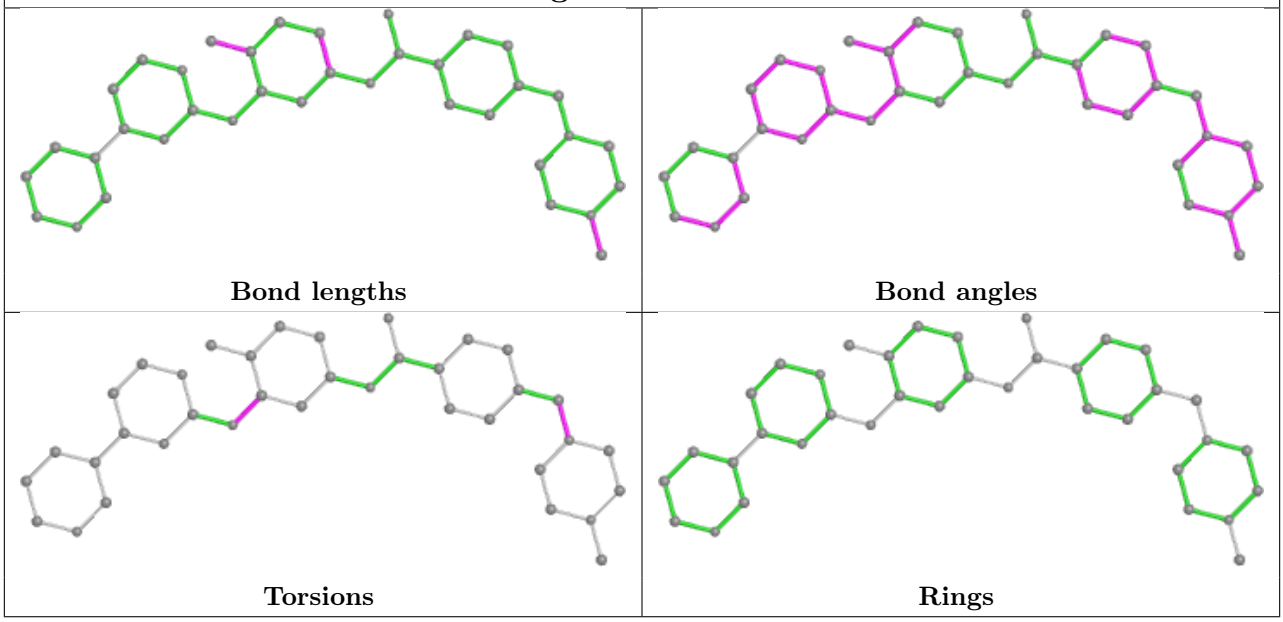
Ligand STI C 1



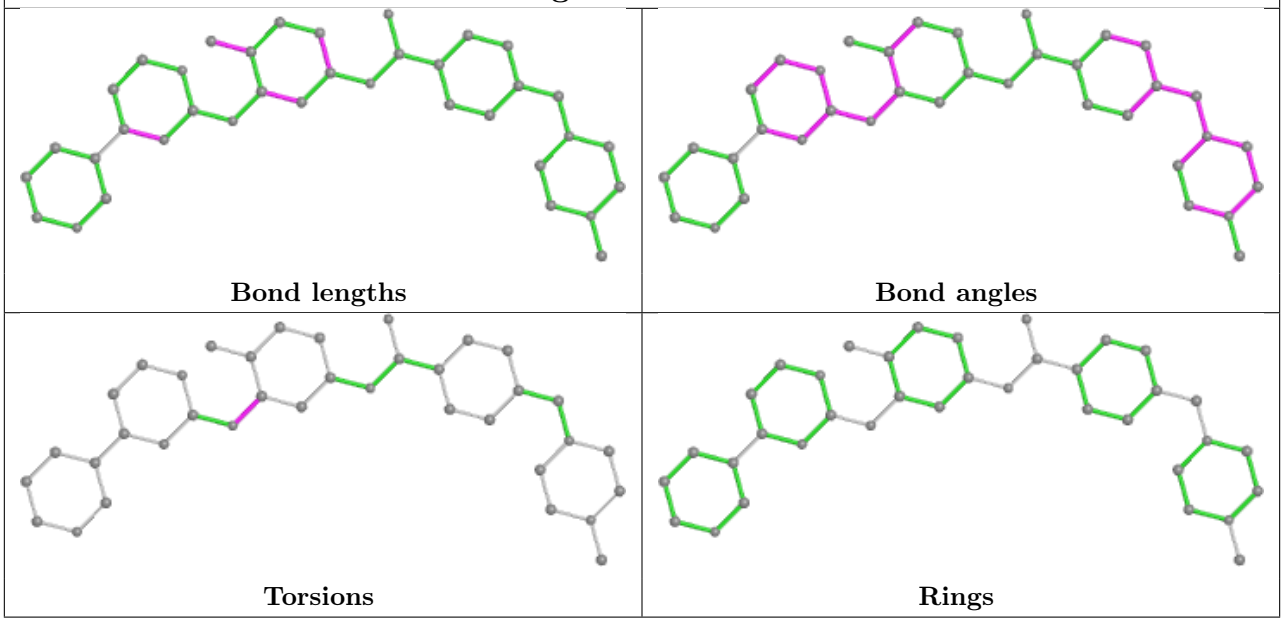
Ligand MS7 C 516



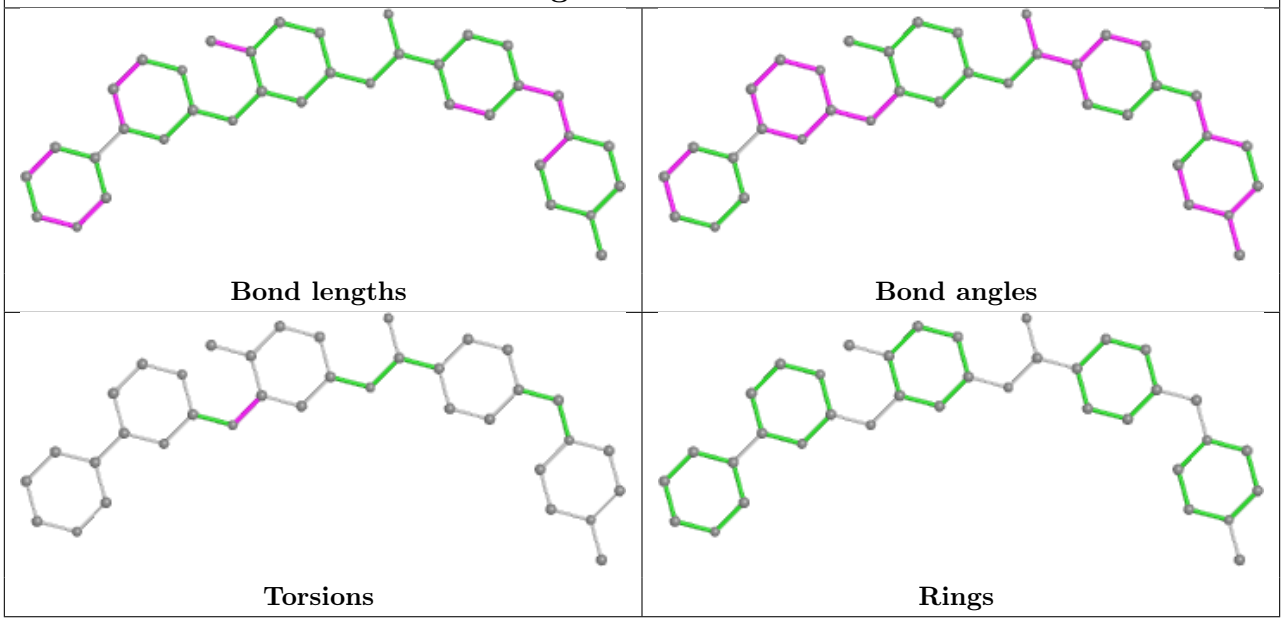
Ligand STI D 1



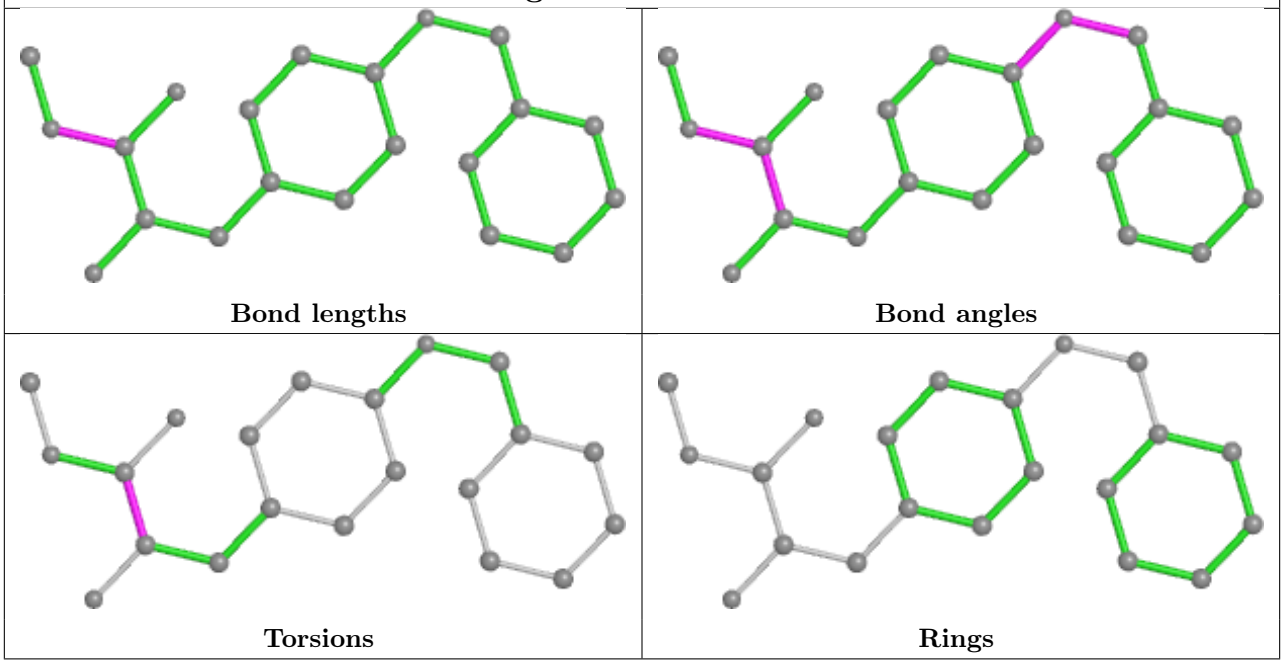
Ligand STI B 1



Ligand STI A 1



Ligand MS7 D 516



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	264/293 (90%)	0.09	6 (2%)	60	69	15, 25, 45, 54	0
1	B	264/293 (90%)	0.19	8 (3%)	50	59	15, 24, 45, 58	0
1	C	264/293 (90%)	0.11	7 (2%)	54	63	16, 25, 45, 53	0
1	D	264/293 (90%)	0.13	4 (1%)	73	81	16, 25, 45, 56	0
All	All	1056/1172 (90%)	0.13	25 (2%)	59	68	15, 25, 46, 58	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	246	HIS	4.4
1	B	391	ASP	3.7
1	C	388	MET	3.6
1	D	308	GLU	3.2
1	A	246	HIS	3.2
1	C	387	LEU	3.1
1	B	398	GLY	3.0
1	B	386	ARG	2.7
1	A	386	ARG	2.5
1	B	387	LEU	2.4
1	A	498	GLN	2.4
1	C	386	ARG	2.4
1	C	243	THR	2.3
1	D	386	ARG	2.3
1	A	387	LEU	2.3
1	D	226	ASP	2.2
1	D	225	MET	2.2
1	B	390	GLY	2.2
1	A	226	ASP	2.1
1	B	254	GLY	2.1
1	A	228	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	307	ARG	2.0
1	B	497	PHE	2.0
1	C	494	GLU	2.0
1	B	226	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

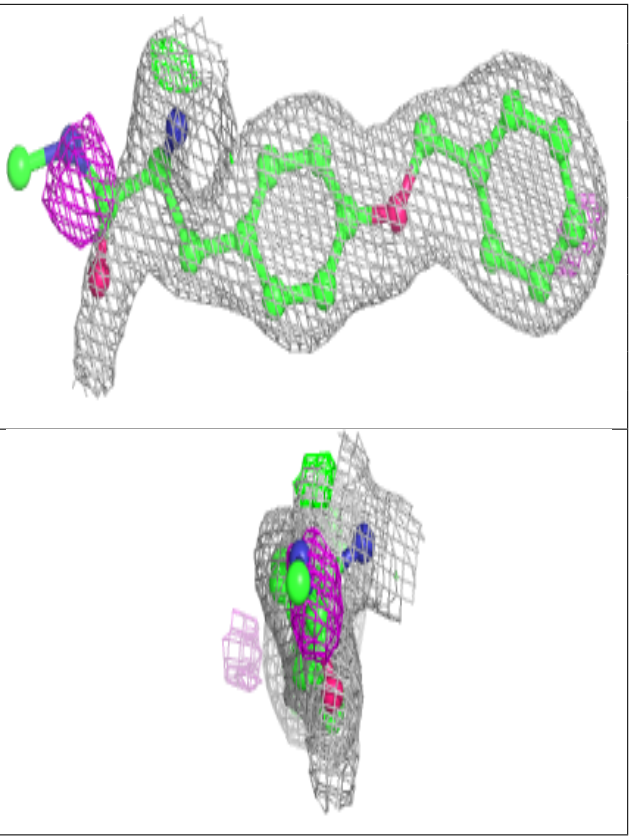
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MS7	D	516	21/21	0.85	0.21	30,37,61,62	0
3	MS7	C	516	21/21	0.86	0.20	29,35,59,60	0
3	MS7	B	516	21/21	0.86	0.18	29,35,62,63	0
3	MS7	A	516	21/21	0.89	0.16	26,34,57,58	0
2	STI	B	1	37/37	0.93	0.10	18,22,27,28	0
2	STI	C	1	37/37	0.96	0.09	17,22,30,31	0
2	STI	D	1	37/37	0.96	0.09	17,22,27,27	0
2	STI	A	1	37/37	0.96	0.12	19,22,26,27	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.

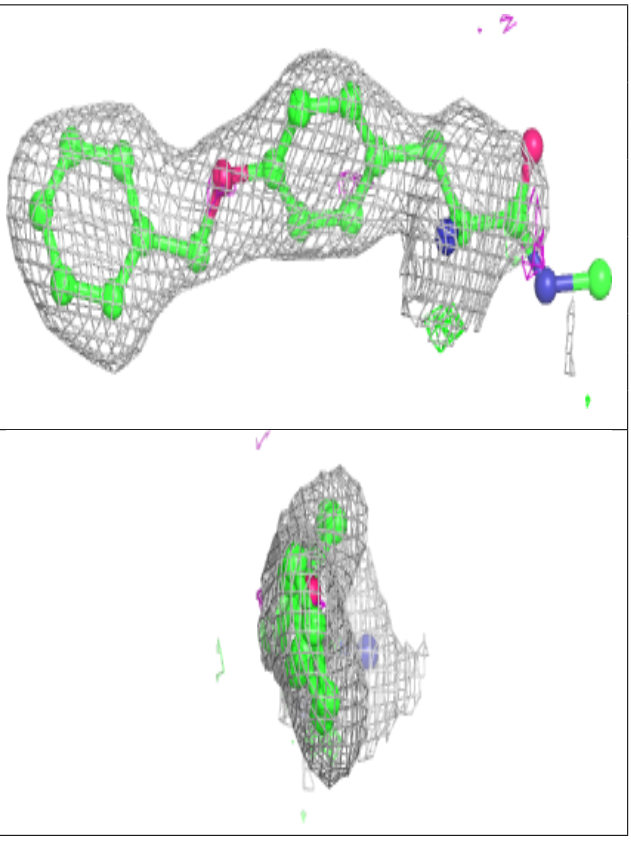
Electron density around MS7 D 516:

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



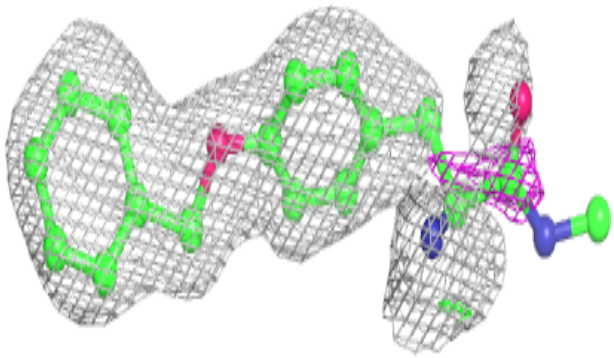
Electron density around MS7 C 516:

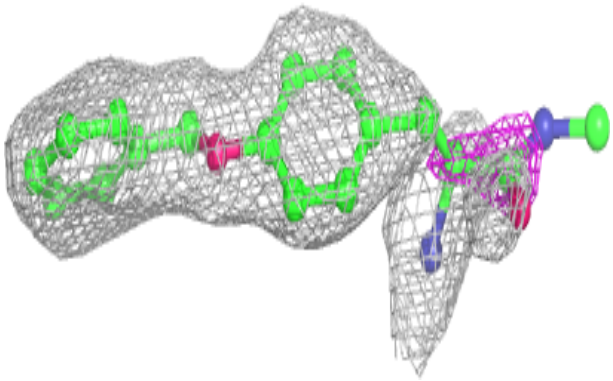
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

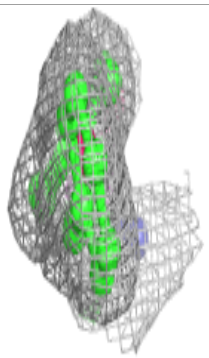


Electron density around MS7 B 516:

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

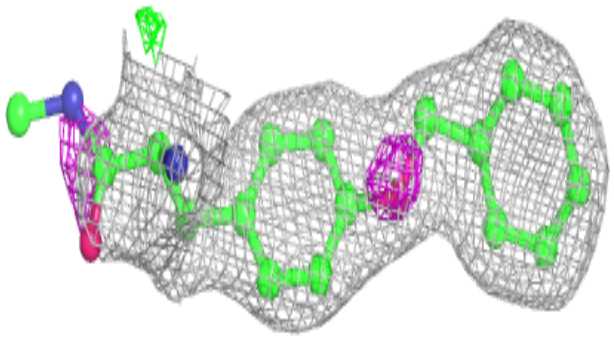


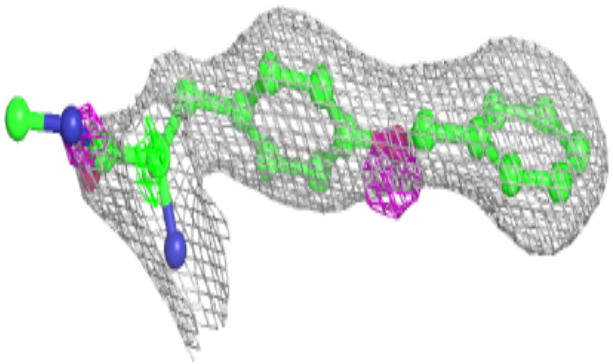


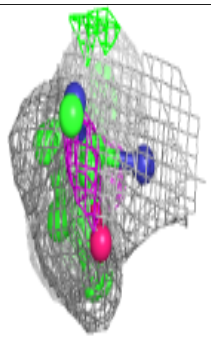


Electron density around MS7 A 516:

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

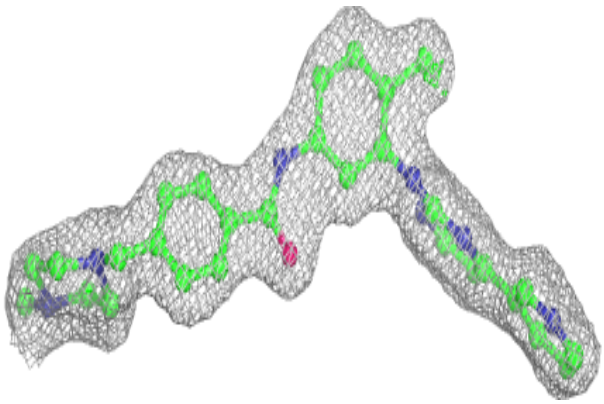


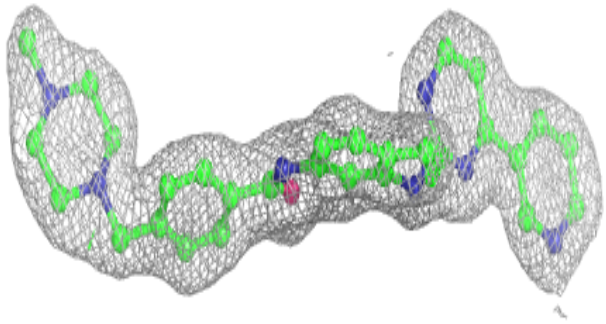


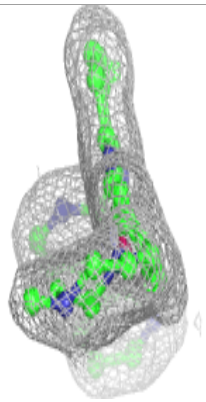


Electron density around STI B 1:

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

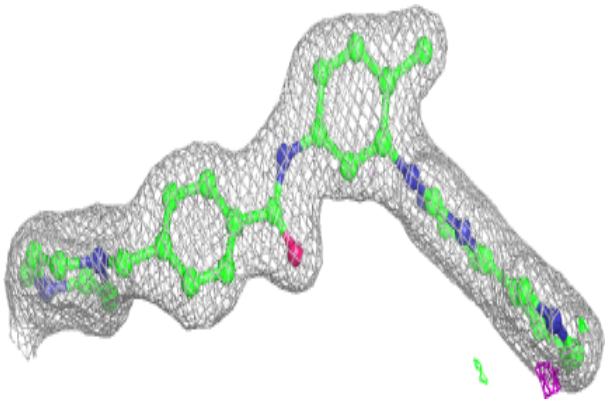


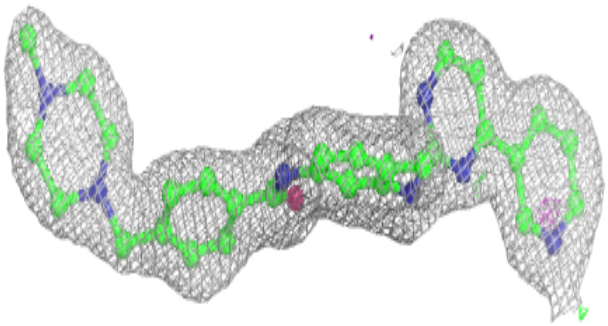


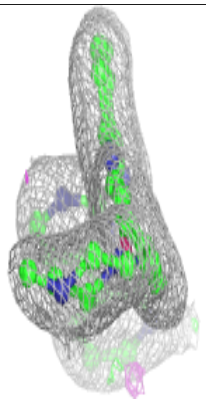


Electron density around STI C 1:

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

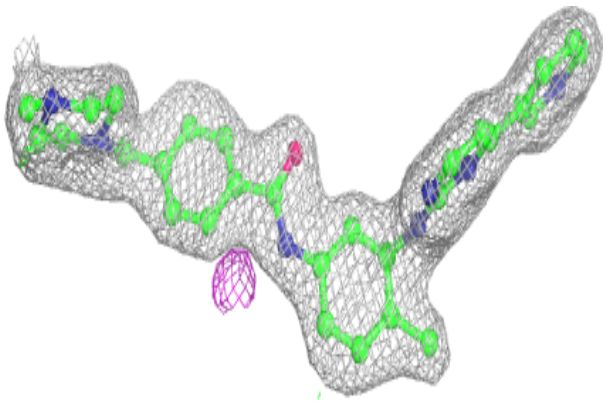


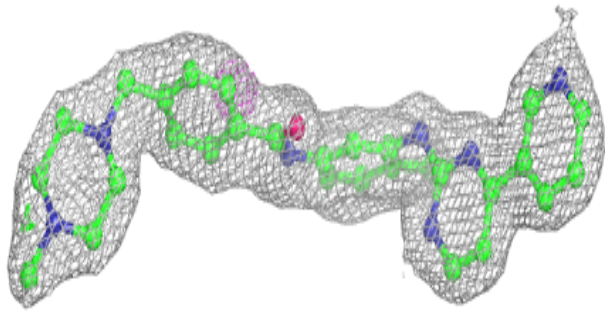


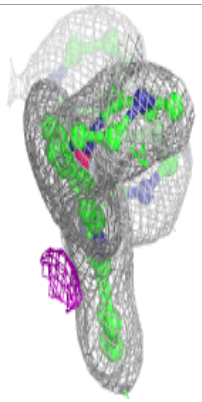


Electron density around STI D 1:

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

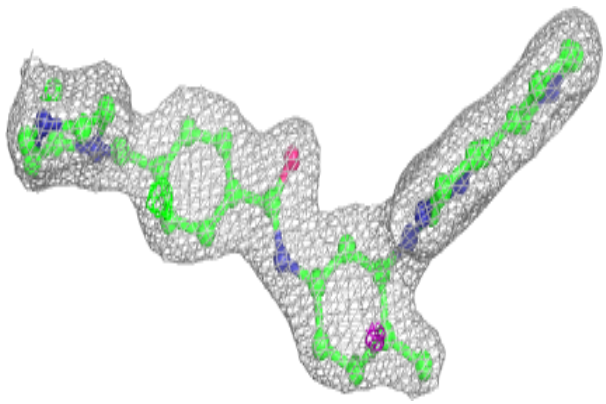


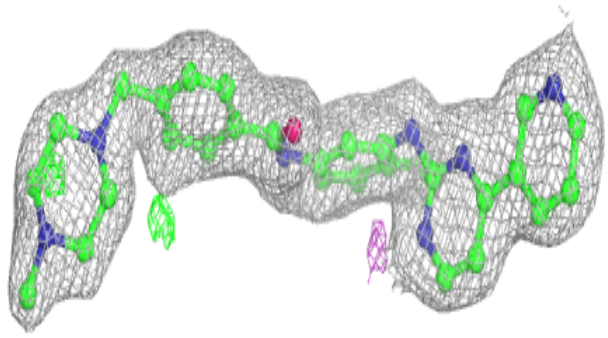


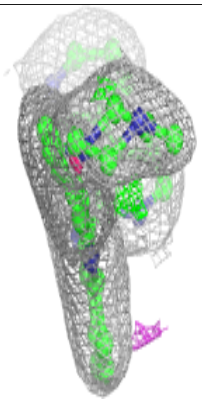


Electron density around STI A 1:

$2mF_o$-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.