



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:34 AM UTC

PDB ID : 3MSS / pdb_00003mss
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

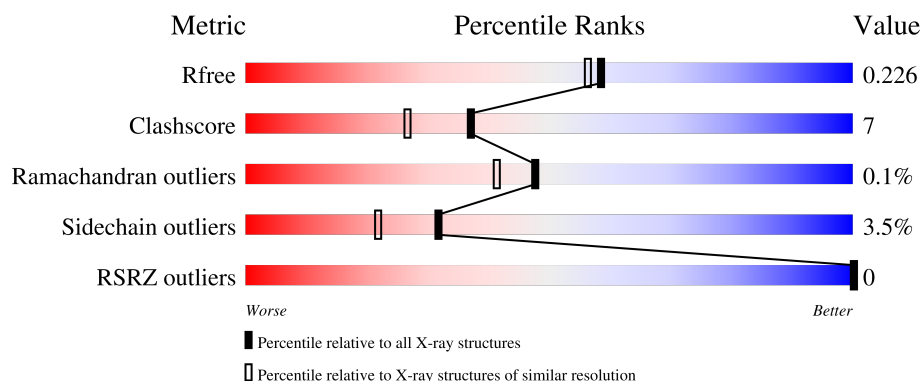
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	293	
1	B	293	
1	C	293	
1	D	293	

2 Entry composition

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
1	A	264	Total	C	N	O	S	0	0	0
			2151	1390	350	394	17			
1	B	264	Total	C	N	O	S	0	0	0
			2151	1390	350	394	17			
1	C	264	Total	C	N	O	S	0	0	0
			2151	1390	350	394	17			
1	D	264	Total	C	N	O	S	0	0	0
			2151	1390	350	394	17			

There are 24 discrepancies between the modelled and reference sequences:

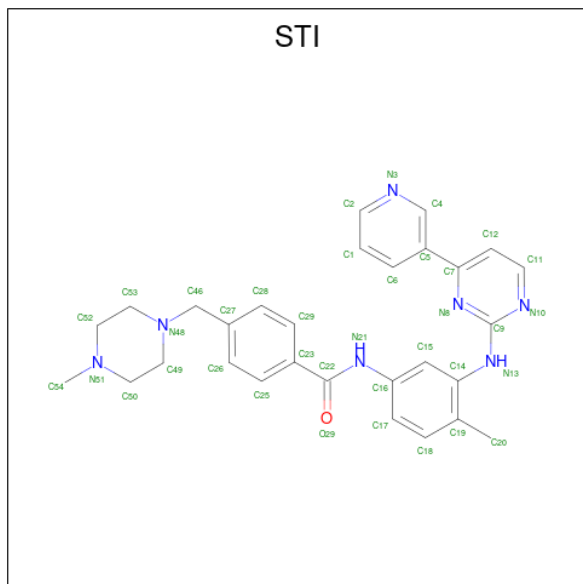
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLY	-	expression tag	UNP P00520
A	224	ALA	-	expression tag	UNP P00520
A	225	MET	-	expression tag	UNP P00520
A	226	ASP	-	expression tag	UNP P00520
A	227	PRO	-	expression tag	UNP P00520
A	228	SER	-	expression tag	UNP P00520
B	223	GLY	-	expression tag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

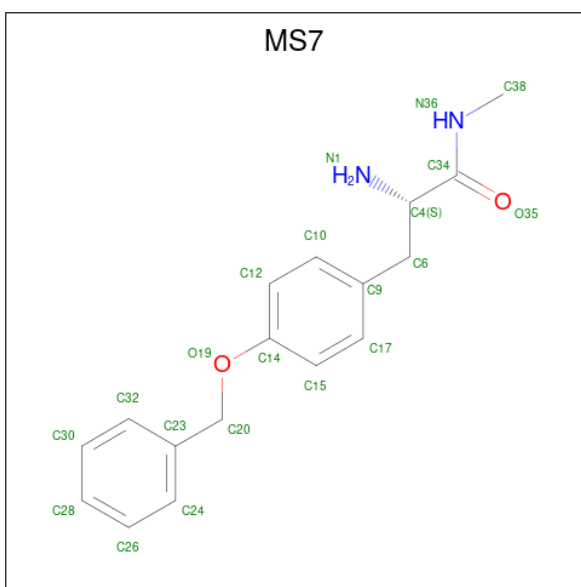
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Chain	Residue	Modelled	Actual	Comment	Reference
D	226	ASP	-	expression tag	UNP P00520
D	227	PRO	-	expression tag	UNP P00520
D	228	SER	-	expression tag	UNP P00520

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





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

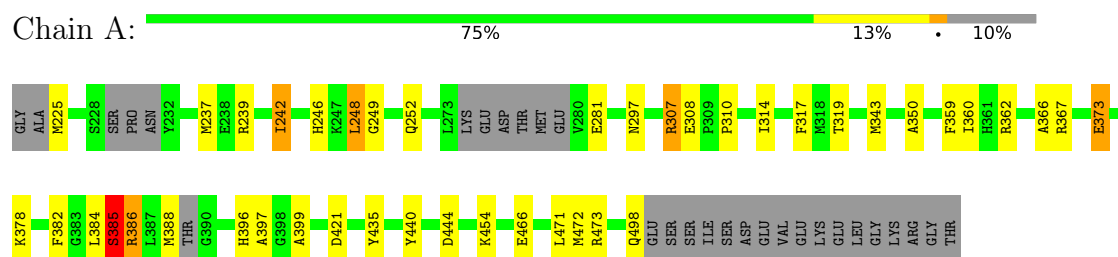
- Molecule 4 is water.

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

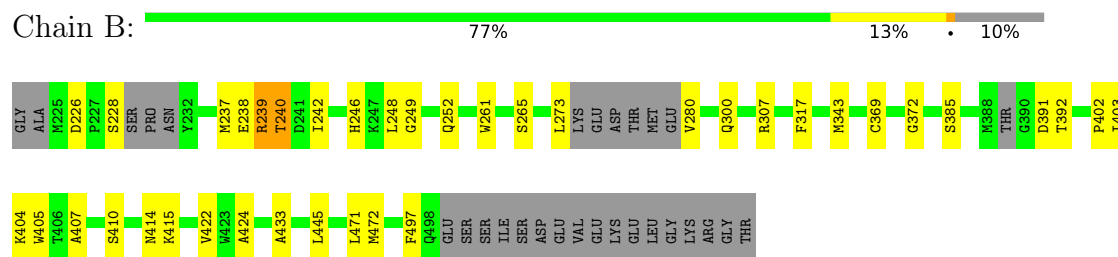
3 Residue-property plots

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.

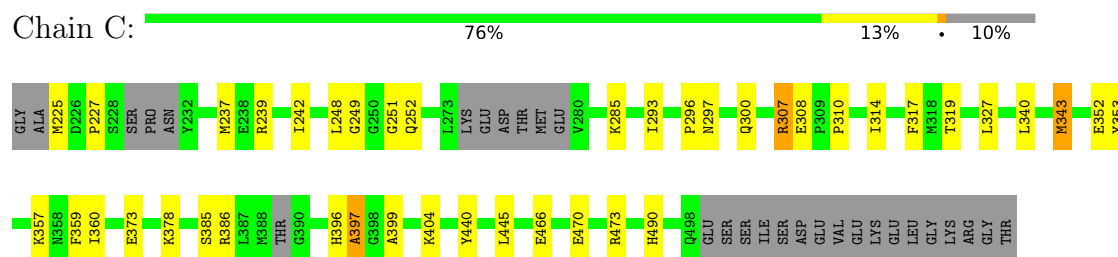
• Molecule 1: Tyrosine-protein kinase ABL1



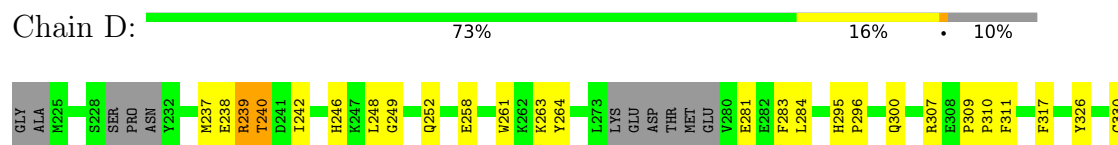
• Molecule 1: Tyrosine-protein kinase ABL1

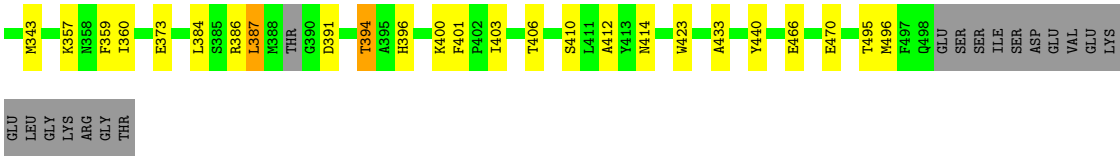


• Molecule 1: Tyrosine-protein kinase ABL1



• Molecule 1: Tyrosine-protein kinase ABL1





4 Data and refinement statistics

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 52.93 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.6 (52.93-1.95) 96.2 (52.93-1.96)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.37 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-h-2*1,1/2*h-1/2*k 0.025 for -h,h+2*1,1/2*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.*

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: MS7, STI

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	1.32	6/2206 (0.3%)	1.17	7/2982 (0.2%)
1	B	1.32	7/2206 (0.3%)	1.12	3/2982 (0.1%)
1	C	1.30	4/2206 (0.2%)	1.14	6/2982 (0.2%)
1	D	1.31	4/2206 (0.2%)	1.12	3/2982 (0.1%)
All	All	1.31	21/8824 (0.2%)	1.14	19/11928 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	343	MET	SD-CE	-8.48	1.58	1.79
1	C	343	MET	SD-CE	-7.95	1.59	1.79
1	B	372	GLY	N-CA	7.82	1.50	1.44
1	B	343	MET	SD-CE	-7.13	1.61	1.79
1	A	440	TYR	N-CA	6.33	1.50	1.46
1	C	297	ASN	N-CA	6.31	1.53	1.46
1	D	440	TYR	N-CA	6.19	1.50	1.46
1	A	435	TYR	CA-C	5.88	1.60	1.53
1	C	440	TYR	N-CA	5.82	1.50	1.46
1	D	309	PRO	CA-C	5.64	1.57	1.52
1	B	422	VAL	CA-CB	5.55	1.61	1.54
1	B	369	CYS	N-CA	5.38	1.52	1.45
1	A	366	ALA	CA-CB	5.26	1.61	1.53
1	A	297	ASN	N-CA	5.25	1.52	1.46
1	C	440	TYR	CA-C	-5.18	1.49	1.53
1	A	421	ASP	N-CA	5.15	1.52	1.46
1	A	350	ALA	CA-CB	5.13	1.61	1.53
1	D	300	GLN	N-CA	5.13	1.52	1.46
1	B	405	TRP	N-CA	5.09	1.52	1.46
1	B	300	GLN	N-CA	5.08	1.52	1.46
1	B	424	ALA	CA-CB	5.02	1.61	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	385	SER	CB-CA-C	-7.72	97.93	110.74
1	D	387	LEU	N-CA-C	6.62	118.15	111.07
1	A	343	MET	CG-SD-CE	-6.48	86.64	100.90
1	A	373	GLU	N-CA-C	6.27	118.39	110.24
1	C	473	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	A	473	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	A	385	SER	CB-CA-C	-5.85	98.77	110.42
1	A	319	THR	N-CA-C	5.63	118.14	111.33
1	A	242	ILE	N-CA-C	5.54	115.83	107.80
1	C	227	PRO	N-CA-C	-5.51	106.97	113.86
1	A	472	MET	CB-CA-C	-5.28	102.36	110.81
1	C	440	TYR	CA-C-N	-5.17	114.59	119.76
1	C	440	TYR	C-N-CA	-5.17	114.59	119.76
1	B	472	MET	CB-CA-C	-5.11	102.86	110.88
1	D	394	THR	CB-CA-C	5.11	119.06	109.71
1	D	412	ALA	N-CA-C	5.09	117.72	111.82
1	C	319	THR	N-CA-C	5.06	117.45	111.33
1	B	407	ALA	CA-C-N	5.01	125.03	119.32
1	B	407	ALA	C-N-CA	5.01	125.03	119.32

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	32	1
1	B	2151	0	2105	19	0
1	C	2151	0	2105	36	0
1	D	2151	0	2105	32	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

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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	14	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	124	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 (124) 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:CD	1:A:388:MET:HE1	1.79	1.13
1:A:367:ARG:HD2	1:A:388:MET:CE	1.78	1.12
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: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
1:A:367:ARG:HD2	1:A:388:MET:HE1	0.86	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:359:PHE:C	1:C:360:ILE:HD12	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:ILE:HD12	1:D:360:ILE:N	2.11	0.66
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: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:237:MET:HE1	1:B:261:TRP:CE2	2.36	0.61
1:D:495:THR:C	4:D:754:HOH:O	2.46	0.58
1:D:359:PHE:C	1:D:360:ILE:HD12	2.29	0.57
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:340:LEU:HA	1:C:343:MET:HE2	1.88	0.56
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:B:497:PHE:HD1	4:B:548:HOH:O	1.92	0.53
1:A:397:ALA:C	1:A:399:ALA:H	2.17	0.52
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:A:444:ASP:CG	4:A:773:HOH:O	2.54	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:HIS:CE1	4:D:575:HOH:O	2.63	0.49
1:C:237:MET:HB3	4:C:593:HOH:O	2.13	0.48
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:237:MET:HE1	1:D:261:TRP:CE2	2.49	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: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:C:327:LEU:HD21	1:C:343:MET:HE1	1.97	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:C:396:HIS:O	1:C:397:ALA:C	2.58	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:378:LYS:NZ	4:A:579:HOH:O	2.51	0.44
1:D:423:TRP:C	1:D:423:TRP:CD1	2.96	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:SER:CB	4:A:559:HOH:O	2.68	0.42
1:A:359:PHE:C	1:A:360:ILE:HD12	2.45	0.42
1:A:396:HIS:O	1:A:397:ALA:C	2.62	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
1:B:237:MET:CE	1:B:261:TRP:CE2	3.04	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%)	30	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	256/293 (87%)	245 (96%)	11 (4%)	0	100	100
All	All	1024/1172 (87%)	981 (96%)	42 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	397	ALA

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	230/255 (90%)	221 (96%)	9 (4%)	28	18
1	B	230/255 (90%)	222 (96%)	8 (4%)	32	22
1	C	230/255 (90%)	226 (98%)	4 (2%)	53	49
1	D	230/255 (90%)	219 (95%)	11 (5%)	23	12
All	All	920/1020 (90%)	888 (96%)	32 (4%)	32	22

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	LEU
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	A	454	LYS
1	A	471	LEU
1	B	226	ASP
1	B	228	SER
1	B	239	ARG
1	B	240	THR

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Mol	Chain	Res	Type
1	B	242	ILE
1	B	265	SER
1	B	307	ARG
1	B	471	LEU
1	C	293	ILE
1	C	307	ARG
1	C	308	GLU
1	C	373	GLU
1	D	239	ARG
1	D	240	THR
1	D	242	ILE
1	D	281	GLU
1	D	284	LEU
1	D	307	ARG
1	D	357	LYS
1	D	373	GLU
1	D	386	ARG
1	D	391	ASP
1	D	400	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	498	GLN
1	B	246	HIS
1	B	374	ASN
1	C	374	ASN
1	C	490	HIS
1	C	498	GLN
1	D	246	HIS
1	D	396	HIS
1	D	491	GLN

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 [i](#)

There are no oligosaccharides 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
2	STI	D	1	-	41,41,41	1.18	3 (7%)	56,56,56	2.18	16 (28%)
3	MS7	A	516	-	22,22,22	1.33	1 (4%)	28,28,28	1.35	4 (14%)
3	MS7	C	516	-	22,22,22	1.23	1 (4%)	28,28,28	1.16	3 (10%)
3	MS7	D	516	-	22,22,22	1.25	1 (4%)	28,28,28	1.16	2 (7%)
2	STI	B	1	-	41,41,41	1.30	4 (9%)	56,56,56	1.90	15 (26%)
2	STI	A	1	-	41,41,41	1.39	7 (17%)	56,56,56	2.36	15 (26%)
2	STI	C	1	-	41,41,41	1.25	4 (9%)	56,56,56	2.23	11 (19%)
3	MS7	B	516	-	22,22,22	1.16	1 (4%)	28,28,28	1.09	1 (3%)

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	STI	D	1	-	-	3/20/30/30	0/5/5/5
3	MS7	A	516	-	-	0/15/15/15	0/2/2/2
3	MS7	C	516	-	-	4/15/15/15	0/2/2/2
3	MS7	D	516	-	-	4/15/15/15	0/2/2/2
2	STI	B	1	-	-	2/20/30/30	0/5/5/5
2	STI	A	1	-	-	2/20/30/30	0/5/5/5
2	STI	C	1	-	-	2/20/30/30	0/5/5/5
3	MS7	B	516	-	-	3/15/15/15	0/2/2/2

All (22) 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	3.94	1.38	1.33
2	B	1	STI	C20-C19	3.92	1.58	1.51
3	B	516	MS7	C34-N36	3.78	1.38	1.33
3	C	516	MS7	C34-N36	3.72	1.38	1.33
2	A	1	STI	C46-C27	3.72	1.58	1.51
2	D	1	STI	C20-C19	3.67	1.57	1.51
2	C	1	STI	C46-N48	2.75	1.52	1.47
2	C	1	STI	C46-C27	2.67	1.56	1.51
2	A	1	STI	C49-N48	2.59	1.53	1.46
2	B	1	STI	C17-C16	2.54	1.43	1.39
2	A	1	STI	C29-C28	2.50	1.42	1.38
2	B	1	STI	C15-C14	2.48	1.43	1.39
2	C	1	STI	C4-C5	2.41	1.43	1.39
2	A	1	STI	C20-C19	2.37	1.55	1.51
2	A	1	STI	C46-N48	2.32	1.52	1.47
2	A	1	STI	C2-N3	2.29	1.40	1.33
2	D	1	STI	C17-C16	2.29	1.43	1.39
2	A	1	STI	C4-C5	2.29	1.43	1.39
2	C	1	STI	C49-N48	2.18	1.52	1.46
2	D	1	STI	C54-N51	2.11	1.52	1.46
2	B	1	STI	C2-N3	2.00	1.39	1.33

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	STI	C7-N8-C9	7.93	122.92	116.81
2	A	1	STI	C7-N8-C9	7.16	122.32	116.81
2	A	1	STI	C11-N10-C9	7.10	121.35	115.42
2	D	1	STI	N10-C9-N8	-6.76	119.88	126.42
2	C	1	STI	C11-N10-C9	6.50	120.85	115.42
2	A	1	STI	N10-C9-N8	-6.31	120.32	126.42
2	C	1	STI	N10-C9-N8	-6.24	120.39	126.42
2	D	1	STI	C7-N8-C9	5.82	121.29	116.81
2	D	1	STI	C11-N10-C9	5.76	120.23	115.42
2	A	1	STI	C12-C11-N10	-4.85	118.03	123.97
2	B	1	STI	C11-N10-C9	4.83	119.45	115.42
2	D	1	STI	C18-C19-C14	4.46	121.68	117.50
2	B	1	STI	N10-C9-N8	-4.40	122.17	126.42
2	B	1	STI	C12-C11-N10	-4.32	118.67	123.97
3	A	516	MS7	C4-C34-N36	4.31	121.88	116.18
2	C	1	STI	C12-C11-N10	-4.25	118.76	123.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	STI	C12-C7-N8	-3.86	116.89	121.97
2	A	1	STI	C11-C12-C7	3.85	120.91	117.20
2	D	1	STI	C46-N48-C53	3.80	119.24	111.07
3	C	516	MS7	C4-C34-N36	3.75	121.13	116.18
2	A	1	STI	C12-C7-N8	-3.72	117.06	121.97
2	B	1	STI	C7-N8-C9	3.71	119.67	116.81
2	B	1	STI	C18-C19-C14	3.65	120.92	117.50
2	A	1	STI	C54-N51-C52	-3.57	103.83	110.63
2	A	1	STI	C46-N48-C53	3.49	118.58	111.07
2	D	1	STI	C2-N3-C4	3.11	122.29	116.85
2	D	1	STI	C50-N51-C52	3.09	114.46	109.54
2	C	1	STI	C11-C12-C7	3.07	120.16	117.20
3	D	516	MS7	C20-O19-C14	3.03	124.85	117.62
2	D	1	STI	C49-N48-C53	3.01	115.33	108.84
2	B	1	STI	C11-C12-C7	2.99	120.09	117.20
2	B	1	STI	C50-N51-C52	2.96	114.25	109.54
2	D	1	STI	C25-C26-C27	-2.95	117.12	121.00
2	B	1	STI	C49-N48-C53	2.86	115.01	108.84
2	A	1	STI	C26-C25-C23	-2.86	117.74	120.80
2	C	1	STI	C46-N48-C53	2.81	117.12	111.07
3	A	516	MS7	C20-O19-C14	2.81	124.30	117.62
2	C	1	STI	C29-C28-C27	-2.64	117.52	121.00
3	A	516	MS7	O35-C34-C4	-2.64	114.71	120.28
2	B	1	STI	C25-C26-C27	-2.63	117.55	121.00
3	D	516	MS7	C4-C34-N36	2.60	119.61	116.18
3	B	516	MS7	C28-C30-C32	2.56	123.40	120.24
2	A	1	STI	C14-N13-C9	-2.56	121.41	129.22
2	C	1	STI	C54-N51-C52	-2.52	105.84	110.63
2	D	1	STI	C28-C27-C26	2.52	121.97	118.23
2	A	1	STI	C49-C50-N51	-2.50	106.83	110.86
2	A	1	STI	C29-C23-C25	2.48	121.73	118.57
2	D	1	STI	C28-C29-C23	-2.47	118.16	120.80
2	A	1	STI	C2-N3-C4	2.45	121.14	116.85
2	C	1	STI	C28-C27-C26	2.44	121.86	118.23
2	B	1	STI	C28-C27-C26	2.38	121.77	118.23
2	B	1	STI	C46-N48-C53	2.37	116.16	111.07
2	D	1	STI	C12-C11-N10	-2.35	121.09	123.97
2	D	1	STI	C54-N51-C52	2.33	115.08	110.63
2	B	1	STI	C52-C53-N48	-2.32	105.98	110.65
2	A	1	STI	O29-C22-C23	-2.28	116.37	120.90
2	B	1	STI	C46-C27-C26	-2.26	116.58	120.75
3	A	516	MS7	C32-C23-C24	2.25	121.58	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	516	MS7	O35-C34-C4	-2.24	115.55	120.28
2	D	1	STI	C5-C4-N3	-2.24	118.08	123.59
2	B	1	STI	C2-N3-C4	2.21	120.73	116.85
2	D	1	STI	C52-C53-N48	-2.20	106.22	110.65
3	C	516	MS7	C20-O19-C14	2.13	122.70	117.62
2	D	1	STI	C20-C19-C14	-2.09	118.86	121.23
2	B	1	STI	C12-C7-C5	2.08	125.84	121.97
2	A	1	STI	C6-C1-C2	-2.06	115.95	118.92
2	C	1	STI	C19-C14-N13	2.04	122.21	118.68

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	STI	C19-C14-N13-C9
2	A	1	STI	C15-C14-N13-C9
2	B	1	STI	C19-C14-N13-C9
2	B	1	STI	C15-C14-N13-C9
2	C	1	STI	C19-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
2	D	1	STI	C19-C14-N13-C9
3	B	516	MS7	C15-C14-O19-C20
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:

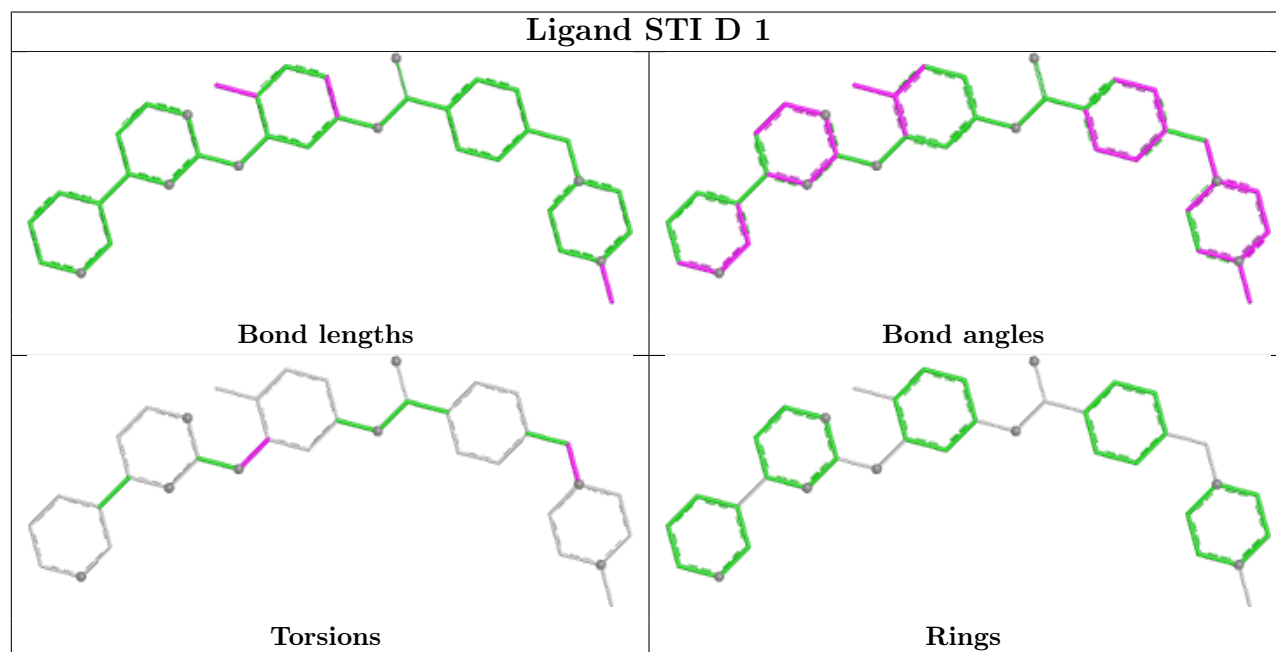
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	STI	1	0
3	A	516	MS7	1	0

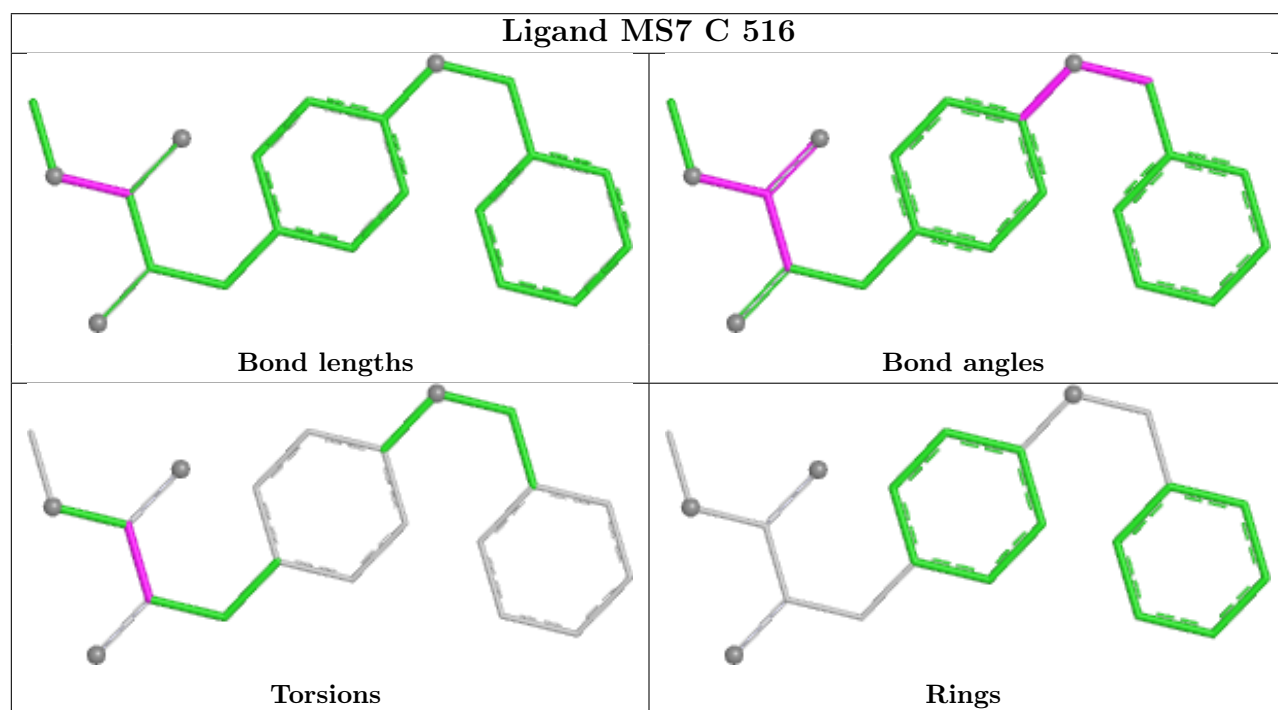
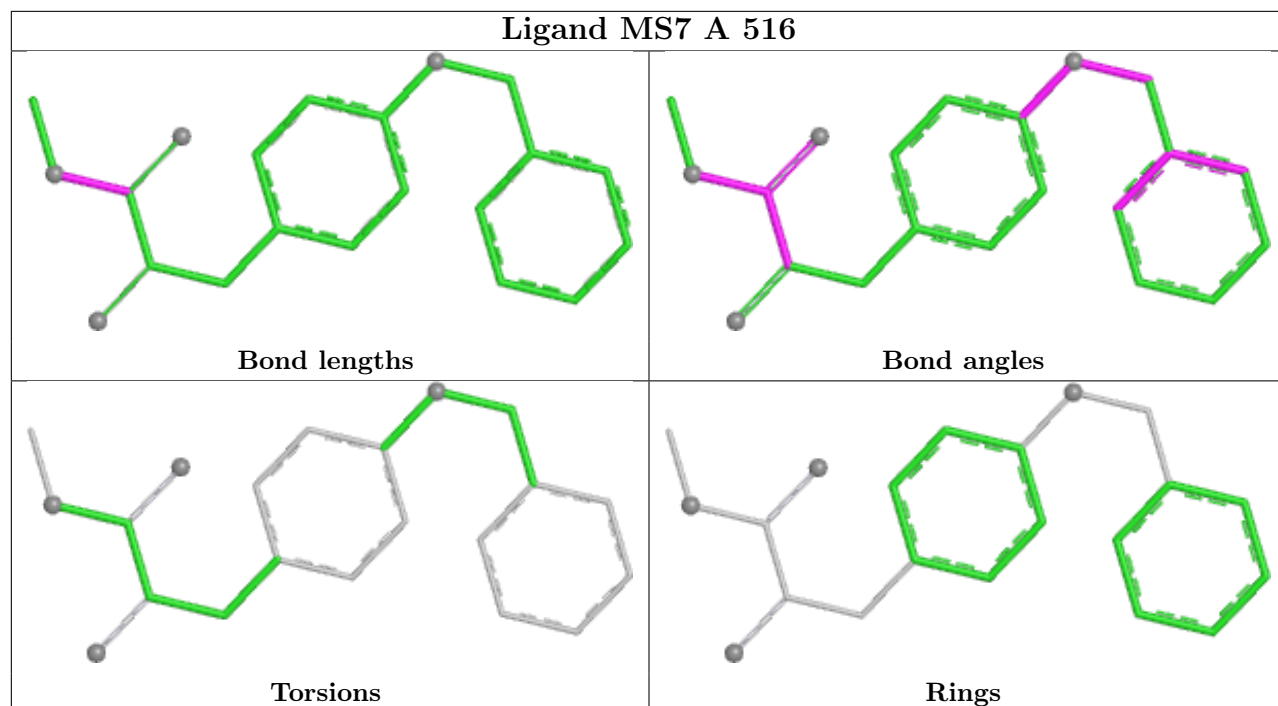
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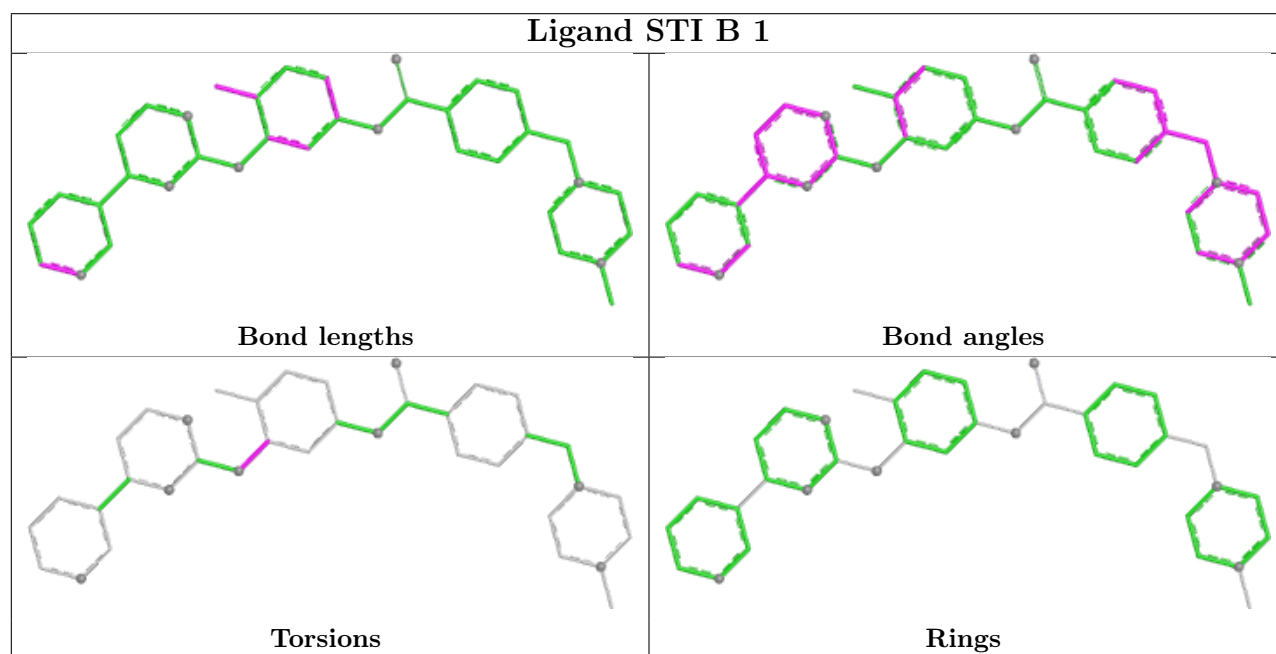
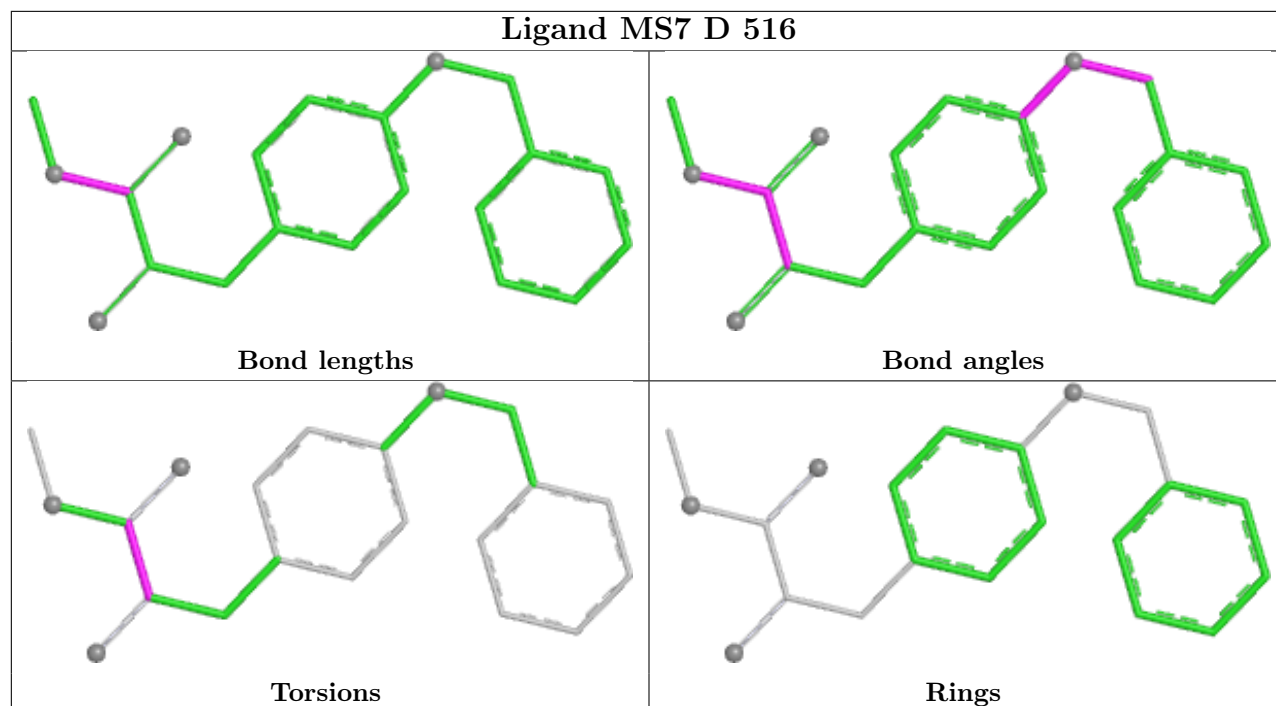
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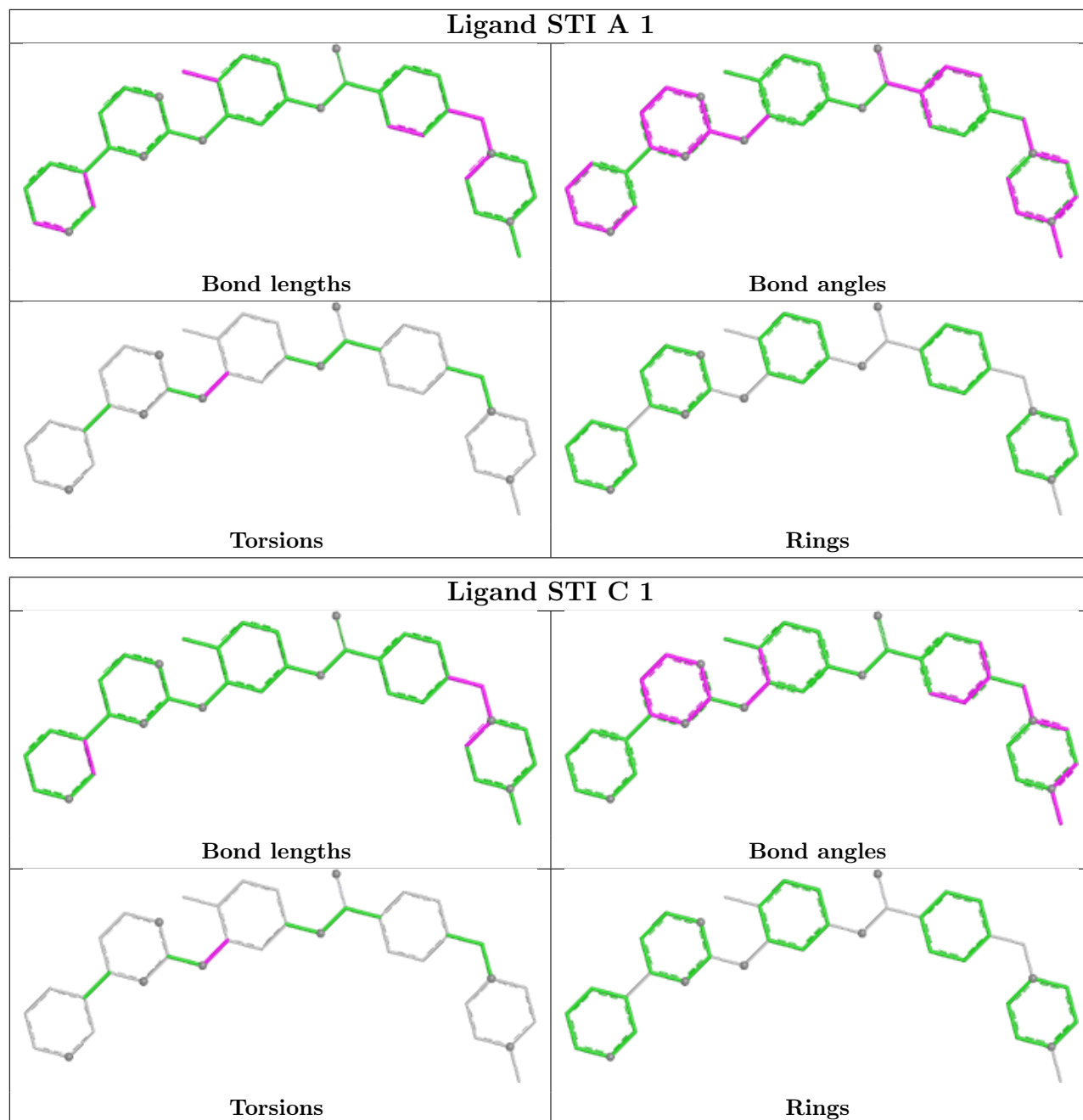
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	516	MS7	1	0
3	D	516	MS7	1	0
2	A	1	STI	1	0
2	C	1	STI	1	0
3	B	516	MS7	1	0

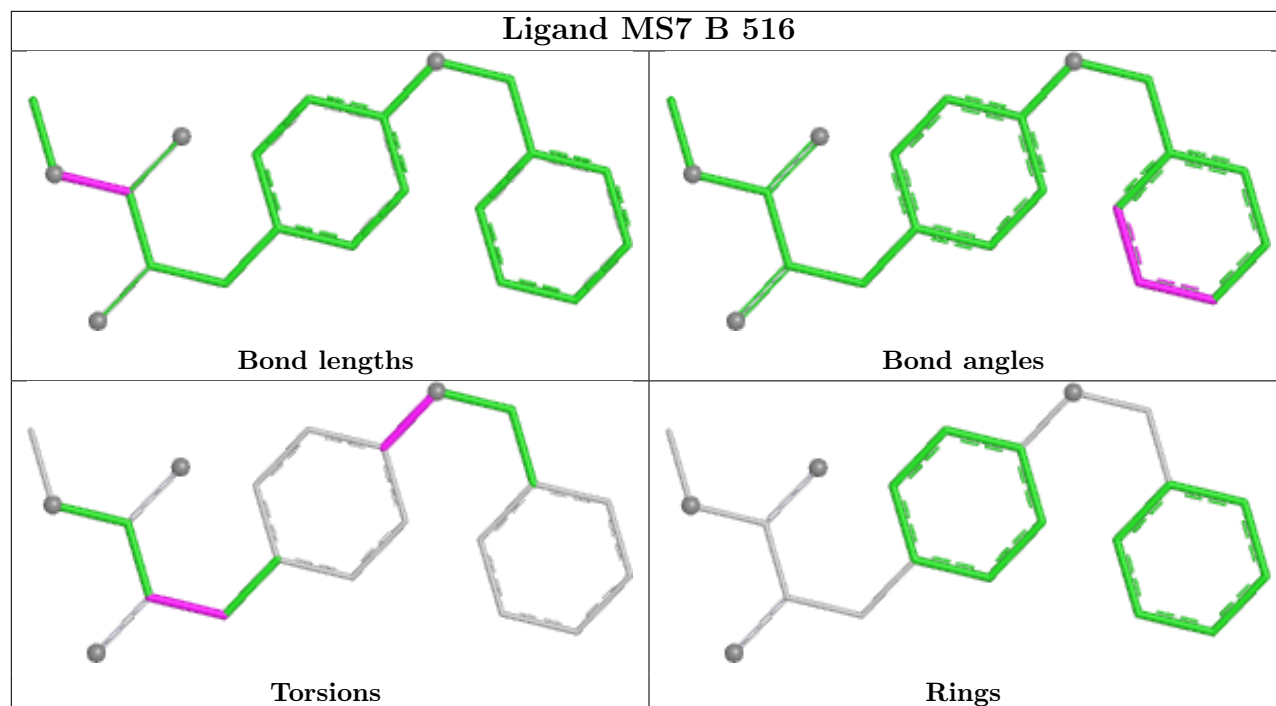
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [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%)	-1.23	0 100 100	15, 25, 45, 54	0
1	B	264/293 (90%)	-1.21	0 100 100	15, 24, 45, 58	0
1	C	264/293 (90%)	-1.22	0 100 100	16, 25, 45, 53	0
1	D	264/293 (90%)	-1.22	0 100 100	16, 25, 45, 56	0
All	All	1056/1172 (90%)	-1.22	0 100 100	15, 25, 46, 58	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MS7	C	516	21/21	0.98	0.06	29,35,59,60	0
2	STI	B	1	37/37	0.99	0.03	18,22,27,28	0
2	STI	C	1	37/37	0.99	0.03	17,22,30,31	0
2	STI	D	1	37/37	0.99	0.02	17,22,27,27	0

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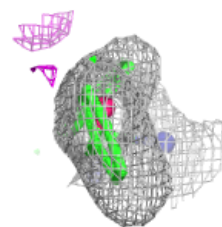
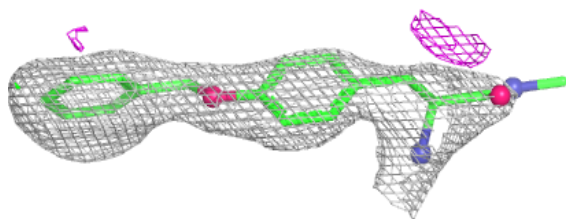
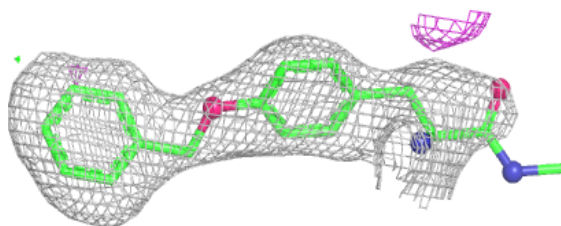
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MS7	A	516	21/21	0.99	0.04	26,34,57,58	0
3	MS7	B	516	21/21	0.99	0.05	29,35,62,63	0
2	STI	A	1	37/37	0.99	0.03	19,22,26,27	0
3	MS7	D	516	21/21	0.99	0.05	30,37,61,62	0

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.

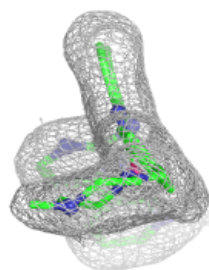
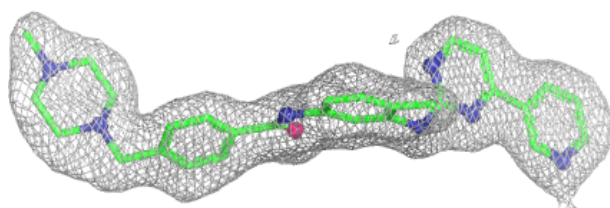
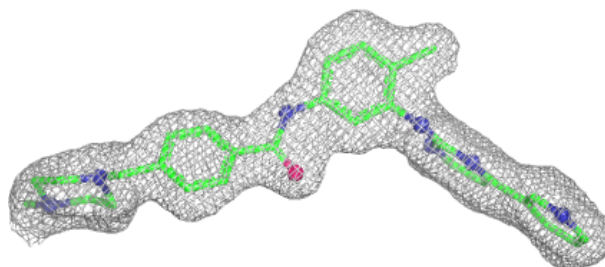
Electron density around MS7 C 516:

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

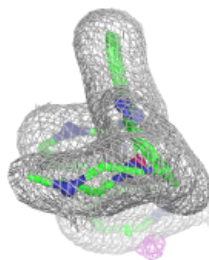
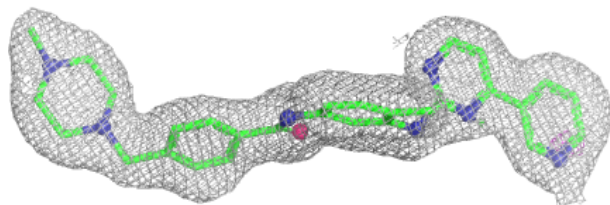
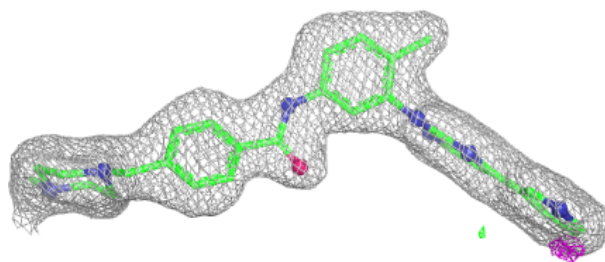


Electron density around STI B 1:

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

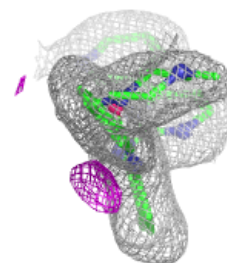
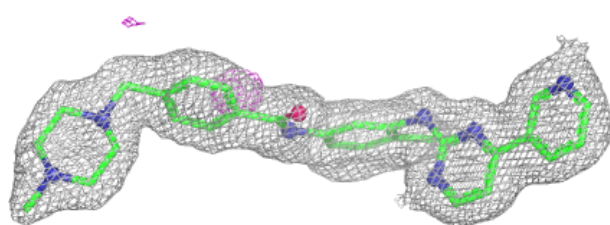
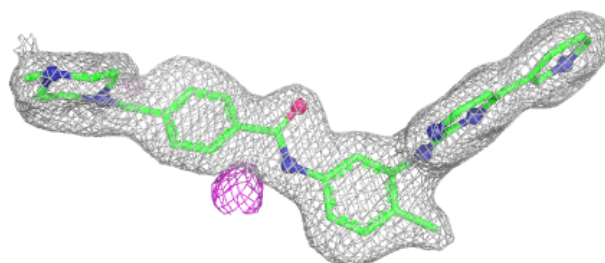
**Electron density around STI C 1:**

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

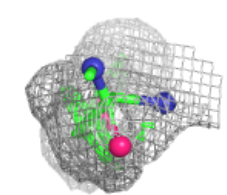
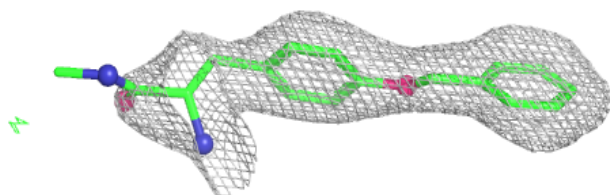
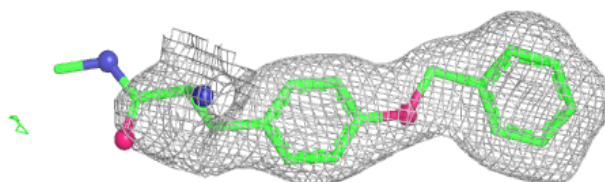


Electron density around STI D 1:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

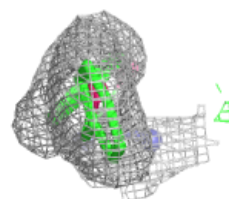
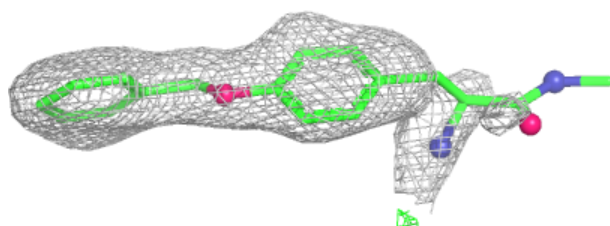
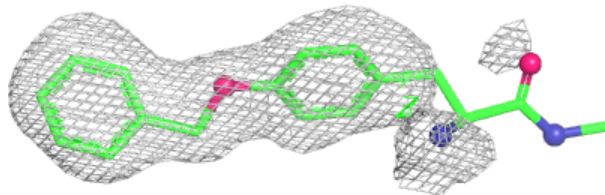
**Electron density around MS7 A 516:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

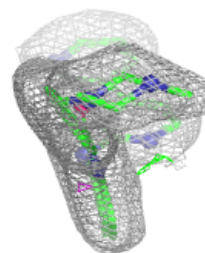
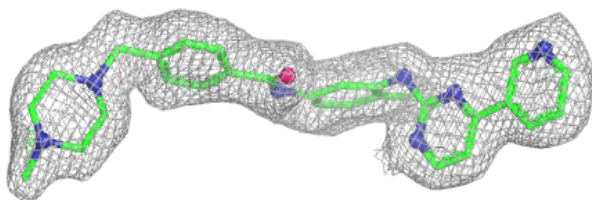
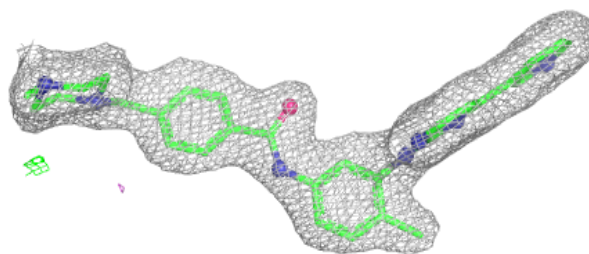


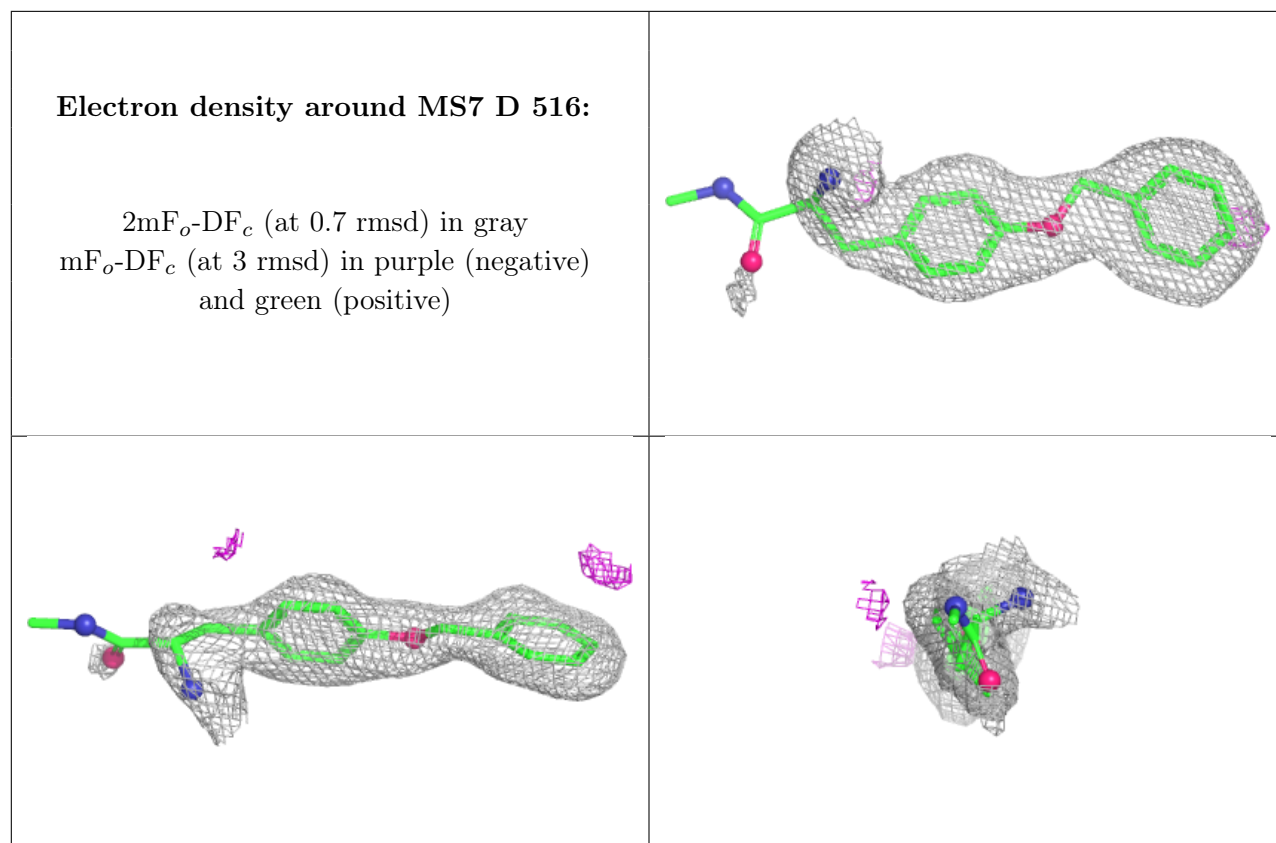
Electron density around MS7 B 516:

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

**Electron density around 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.