



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:25 PM UTC

PDB ID : 8GMI / pdb_00008gmi
Title : Citrate Synthase (CitA) in Mycobacterium tuberculosis modified by Ebselen at C143 residue
Authors : Pathirage, R.; Ronning, D.
Deposited on : 2023-03-25
Resolution : 2.70 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

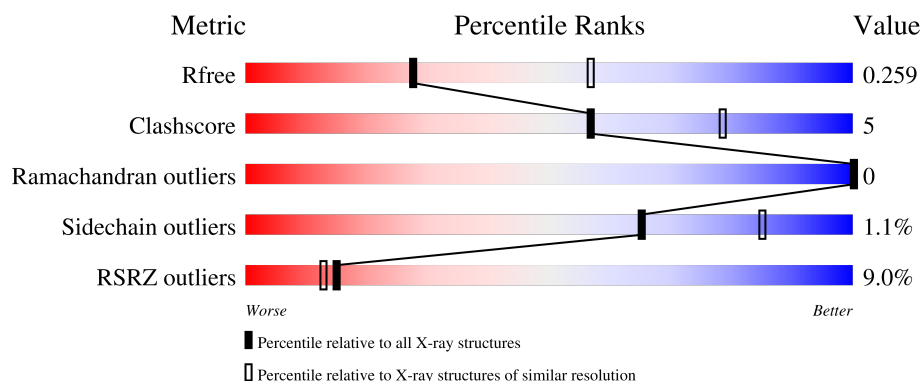
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	379	4% 86% 11% .
1	B	379	3% 92% 6% .
1	C	379	4% 91% 7% .
1	D	379	4% 89% 8% .
1	E	379	4% 89% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	379	8% 86% 12%
1	G	379	22% 79% 14% 6%
1	H	379	20% 76% 18% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22574 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 citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2797	1762	507	515	13			
1	B	373	Total	C	N	O	S	0	0	0
			2824	1778	511	521	14			
1	C	371	Total	C	N	O	S	0	0	0
			2812	1771	509	518	14			
1	D	370	Total	C	N	O	S	0	0	0
			2804	1766	508	517	13			
1	E	367	Total	C	N	O	S	0	0	0
			2783	1752	505	513	13			
1	F	372	Total	C	N	O	S	0	0	0
			2816	1773	510	520	13			
1	G	356	Total	C	N	O	S	0	0	0
			2699	1700	490	496	13			
1	H	360	Total	C	N	O	S	0	0	0
			2728	1718	494	503	13			

There are 48 discrepancies between the modelled and reference sequences:

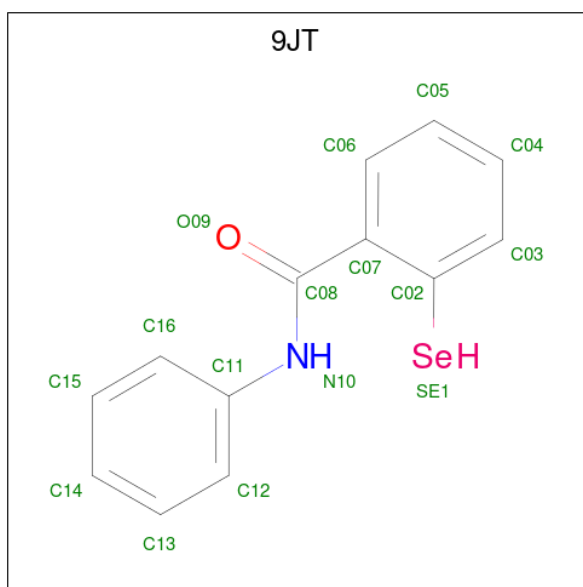
Chain	Residue	Modelled	Actual	Comment	Reference
A	374	HIS	-	expression tag	UNP A0A045JB88
A	375	HIS	-	expression tag	UNP A0A045JB88
A	376	HIS	-	expression tag	UNP A0A045JB88
A	377	HIS	-	expression tag	UNP A0A045JB88
A	378	HIS	-	expression tag	UNP A0A045JB88
A	379	HIS	-	expression tag	UNP A0A045JB88
B	374	HIS	-	expression tag	UNP A0A045JB88
B	375	HIS	-	expression tag	UNP A0A045JB88
B	376	HIS	-	expression tag	UNP A0A045JB88
B	377	HIS	-	expression tag	UNP A0A045JB88
B	378	HIS	-	expression tag	UNP A0A045JB88
B	379	HIS	-	expression tag	UNP A0A045JB88
C	374	HIS	-	expression tag	UNP A0A045JB88

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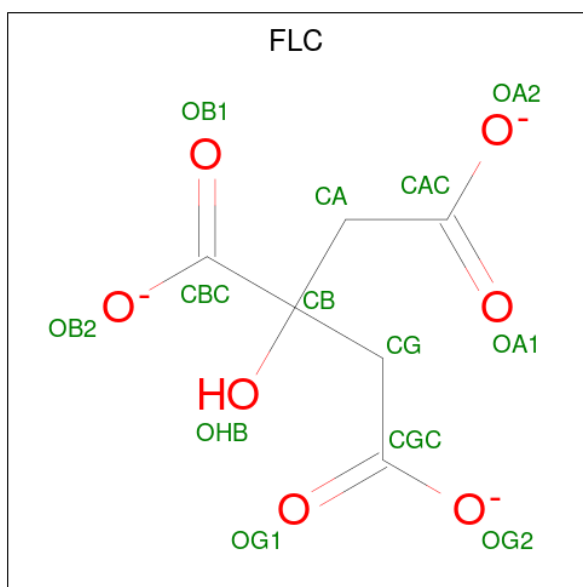
Chain	Residue	Modelled	Actual	Comment	Reference
C	375	HIS	-	expression tag	UNP A0A045JB88
C	376	HIS	-	expression tag	UNP A0A045JB88
C	377	HIS	-	expression tag	UNP A0A045JB88
C	378	HIS	-	expression tag	UNP A0A045JB88
C	379	HIS	-	expression tag	UNP A0A045JB88
D	374	HIS	-	expression tag	UNP A0A045JB88
D	375	HIS	-	expression tag	UNP A0A045JB88
D	376	HIS	-	expression tag	UNP A0A045JB88
D	377	HIS	-	expression tag	UNP A0A045JB88
D	378	HIS	-	expression tag	UNP A0A045JB88
D	379	HIS	-	expression tag	UNP A0A045JB88
E	374	HIS	-	expression tag	UNP A0A045JB88
E	375	HIS	-	expression tag	UNP A0A045JB88
E	376	HIS	-	expression tag	UNP A0A045JB88
E	377	HIS	-	expression tag	UNP A0A045JB88
E	378	HIS	-	expression tag	UNP A0A045JB88
E	379	HIS	-	expression tag	UNP A0A045JB88
F	374	HIS	-	expression tag	UNP A0A045JB88
F	375	HIS	-	expression tag	UNP A0A045JB88
F	376	HIS	-	expression tag	UNP A0A045JB88
F	377	HIS	-	expression tag	UNP A0A045JB88
F	378	HIS	-	expression tag	UNP A0A045JB88
F	379	HIS	-	expression tag	UNP A0A045JB88
G	374	HIS	-	expression tag	UNP A0A045JB88
G	375	HIS	-	expression tag	UNP A0A045JB88
G	376	HIS	-	expression tag	UNP A0A045JB88
G	377	HIS	-	expression tag	UNP A0A045JB88
G	378	HIS	-	expression tag	UNP A0A045JB88
G	379	HIS	-	expression tag	UNP A0A045JB88
H	374	HIS	-	expression tag	UNP A0A045JB88
H	375	HIS	-	expression tag	UNP A0A045JB88
H	376	HIS	-	expression tag	UNP A0A045JB88
H	377	HIS	-	expression tag	UNP A0A045JB88
H	378	HIS	-	expression tag	UNP A0A045JB88
H	379	HIS	-	expression tag	UNP A0A045JB88

- Molecule 2 is N-phenyl-2-selanylbenzamide (CCD ID: 9JT) (formula: C₁₃H₁₁NOS_e) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Se	0	0
			16	13	1	1	1		
2	B	1	Total	C	N	O	Se	0	0
			16	13	1	1	1		
2	C	1	Total	C	N	O	Se	0	0
			16	13	1	1	1		
2	D	1	Total	C	N	O	Se	0	0
			16	13	1	1	1		
2	E	1	Total	C	N	O	Se	0	0
			16	13	1	1	1		
2	F	1	Total	C	N	O	Se	0	0
			16	13	1	1	1		
2	G	1	Total	C	N	O	Se	0	0
			16	13	1	1	1		
2	H	1	Total	C	N	O	Se	0	0
			16	13	1	1	1		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	20	Total	O	0	0
			20	20		
4	C	20	Total	O	0	0
			20	20		
4	D	18	Total	O	0	0
			18	18		
4	E	31	Total	O	0	0
			31	31		
4	F	12	Total	O	0	0
			12	12		
4	G	2	Total	O	0	0
			2	2		

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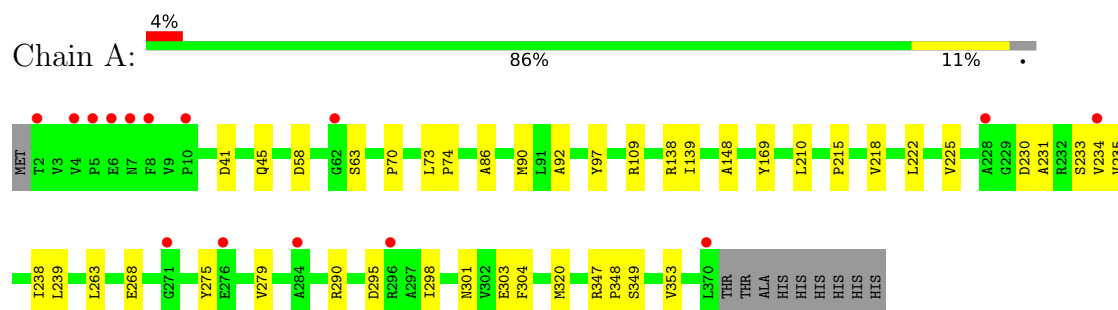
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		

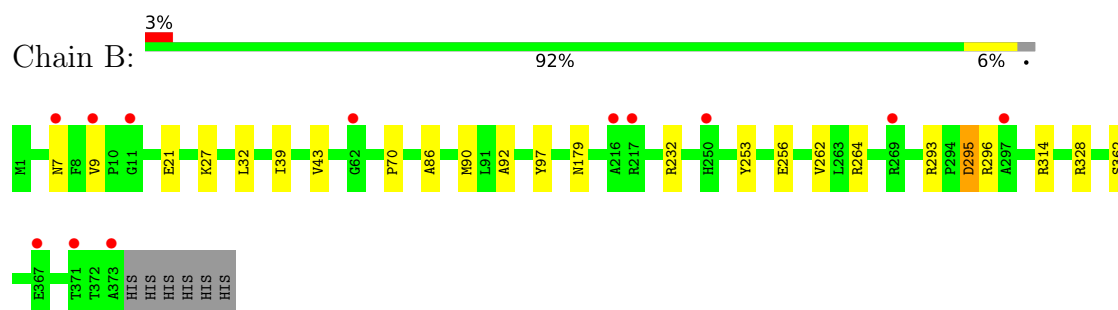
3 Residue-property plots [i](#)

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.

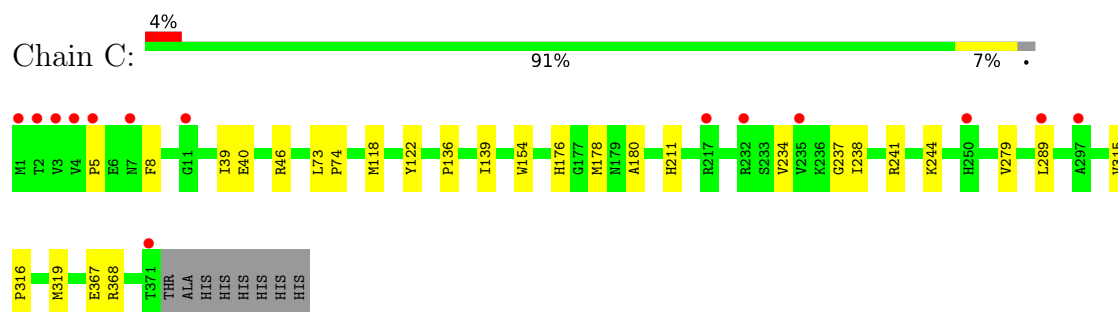
- Molecule 1: citrate synthase



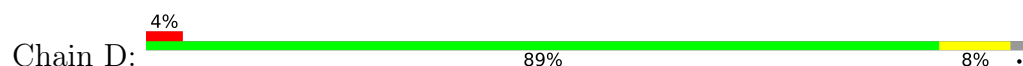
- Molecule 1: citrate synthase

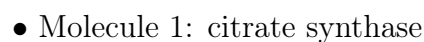


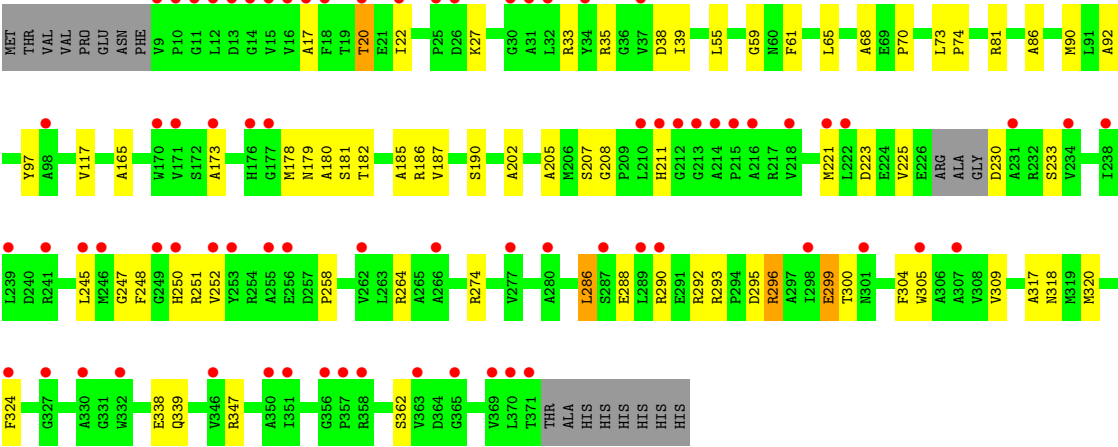
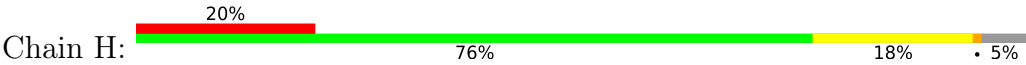
- Molecule 1: citrate synthase



- Molecule 1: citrate synthase







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.02Å 167.49Å 221.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.06 – 2.70 63.06 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.06-2.70) 87.0 (63.06-2.70)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.24 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158:000	Depositor
R, R_{free}	0.214 , 0.253 0.221 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22574	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: FLC, 9JT

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	0.10	0/2861	0.22	0/3898
1	B	0.10	0/2888	0.22	0/3935
1	C	0.11	0/2876	0.23	0/3918
1	D	0.10	0/2868	0.22	0/3908
1	E	0.11	0/2847	0.24	0/3877
1	F	0.13	0/2880	0.26	0/3925
1	G	0.12	0/2759	0.25	0/3755
1	H	0.12	0/2789	0.25	0/3798
All	All	0.11	0/22768	0.24	0/31014

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	2797	0	2771	25	0
1	B	2824	0	2802	17	0
1	C	2812	0	2790	21	0
1	D	2804	0	2778	21	0
1	E	2783	0	2754	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2816	0	2790	28	0
1	G	2699	0	2673	40	0
1	H	2728	0	2703	50	0
2	A	16	0	0	1	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
2	D	16	0	0	0	0
2	E	16	0	0	0	0
2	F	16	0	0	0	0
2	G	16	0	0	0	0
2	H	16	0	0	0	0
3	B	13	0	5	1	0
3	C	13	0	5	1	0
3	D	13	0	5	1	0
3	E	13	0	5	1	0
3	F	13	0	5	3	0
4	A	14	0	0	0	0
4	B	20	0	0	0	0
4	C	20	0	0	0	0
4	D	18	0	0	0	0
4	E	31	0	0	0	0
4	F	12	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
All	All	22574	0	22086	204	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 5.

All (204) 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:G:232:ARG:HH11	1:G:236:LYS:HB2	1.50	0.75
1:G:159:ASP:HB3	1:G:162:HIS:CD2	2.25	0.72
1:G:159:ASP:HB3	1:G:162:HIS:HD2	1.56	0.70
1:A:225:VAL:HG22	1:A:234:VAL:HG11	1.74	0.67
1:F:215:PRO:O	1:F:217:ARG:NH1	2.27	0.67
1:F:328:ARG:NH2	3:F:401:FLC:OB2	2.28	0.65
1:A:138:ARG:HG3	1:A:139:ILE:HD12	1.77	0.65
1:C:315:VAL:HG13	1:C:319:MET:HE3	1.78	0.65
1:B:70:PRO:HB2	1:H:70:PRO:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:345:LEU:HD22	1:G:347:ARG:HB2	1.81	0.62
1:E:226:GLU:CD	1:E:227:ARG:H	2.09	0.61
1:E:288:GLU:OE2	1:E:292:ARG:NH1	2.34	0.60
1:G:43:VAL:HG11	1:G:262:VAL:HB	1.83	0.60
1:B:92:ALA:HA	1:B:97:TYR:HB2	1.85	0.59
1:H:185:ALA:HB2	1:H:202:ALA:HB2	1.84	0.59
1:D:58:ASP:OD2	1:D:109:ARG:NH2	2.36	0.59
1:H:33:ARG:HG2	1:H:38:ASP:HA	1.85	0.59
1:D:259:ARG:NH1	3:D:401:FLC:OB2	2.32	0.58
1:D:235:VAL:HG13	1:D:245:LEU:HD11	1.84	0.58
1:B:179:ASN:HB3	3:B:401:FLC:HG2	1.86	0.57
1:H:68:ALA:HB2	1:H:117:VAL:HG22	1.85	0.57
1:H:295:ASP:N	1:H:295:ASP:OD1	2.38	0.57
1:F:154:TRP:CZ2	1:F:319:MET:HE1	2.39	0.57
1:H:250:HIS:CG	1:H:296:ARG:HH21	2.23	0.56
1:E:226:GLU:O	1:E:227:ARG:NE	2.39	0.56
1:F:293:ARG:HH11	1:F:296:ARG:HH21	1.52	0.56
1:H:264:ARG:HG3	1:H:305:TRP:CE2	2.41	0.56
1:B:256:GLU:OE2	1:B:264:ARG:NH1	2.34	0.55
1:C:316:PRO:HD2	1:C:319:MET:HE2	1.88	0.55
1:G:254:ARG:NE	1:G:254:ARG:HA	2.20	0.55
1:B:295:ASP:OD1	1:B:295:ASP:N	2.33	0.55
1:D:71:PHE:HB3	1:D:118:MET:HE1	1.89	0.55
1:G:191:THR:HG23	1:H:208:GLY:HA3	1.89	0.55
1:C:73:LEU:HD12	1:C:74:PRO:HD2	1.88	0.54
1:E:352:TYR:CG	1:F:24:GLU:HB2	2.43	0.54
1:A:58:ASP:OD2	1:A:109:ARG:NH2	2.37	0.54
1:A:231:ALA:O	1:A:235:VAL:HG22	2.08	0.54
1:C:238:ILE:HA	1:C:241:ARG:HE	1.73	0.54
1:H:317:ALA:HA	1:H:320:MET:HG3	1.89	0.54
1:A:70:PRO:HB2	1:G:70:PRO:HB2	1.90	0.53
1:C:5:PRO:HB2	1:C:8:PHE:HB2	1.89	0.53
1:C:178:MET:O	1:D:347:ARG:NH2	2.41	0.53
1:A:215:PRO:HG2	1:A:320:MET:HB3	1.90	0.53
1:C:238:ILE:H	1:C:238:ILE:HD12	1.73	0.53
1:G:49:PHE:CD1	1:G:170:TRP:HB3	2.44	0.53
1:G:100:LEU:HD23	1:G:103:ILE:HD11	1.90	0.53
1:H:179:ASN:ND2	1:H:182:THR:H	2.07	0.53
1:A:92:ALA:HA	1:A:97:TYR:HB2	1.89	0.53
1:G:185:ALA:HB1	1:G:336:ILE:HD11	1.91	0.53
1:H:187:VAL:O	1:H:190:SER:OG	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:ARG:HD2	1:H:59:GLY:HA2	1.90	0.52
1:H:178:MET:HE1	1:H:186:ARG:HD2	1.90	0.52
1:C:367:GLU:CD	1:C:367:GLU:H	2.17	0.52
1:G:12:LEU:HD21	1:H:17:ALA:HA	1.91	0.52
1:F:73:LEU:HD12	1:F:74:PRO:HD2	1.92	0.52
1:F:92:ALA:HA	1:F:97:TYR:HB2	1.91	0.52
1:H:92:ALA:HA	1:H:97:TYR:HB2	1.91	0.52
1:F:259:ARG:NH2	3:F:401:FLC:OB1	2.30	0.51
1:H:221:MET:SD	1:H:221:MET:N	2.81	0.51
1:G:35:ARG:HD2	1:G:59:GLY:HA2	1.93	0.51
1:G:73:LEU:HD12	1:G:74:PRO:HD2	1.91	0.51
1:G:234:VAL:O	1:G:237:GLY:N	2.43	0.51
1:D:46:ARG:HH22	1:D:269:ARG:HD2	1.75	0.51
1:E:92:ALA:HA	1:E:97:TYR:HB2	1.93	0.51
1:G:287:SER:O	1:G:291:GLU:HG2	2.11	0.51
1:A:268:GLU:HB3	1:A:275:TYR:CZ	2.46	0.51
1:F:279:VAL:HA	1:F:282:GLU:HB3	1.92	0.51
1:F:238:ILE:H	1:F:238:ILE:HD12	1.75	0.51
1:F:249:GLY:H	1:F:301:ASN:ND2	2.09	0.50
1:D:92:ALA:HA	1:D:97:TYR:HB2	1.94	0.50
1:G:181:SER:H	1:G:211:HIS:CD2	2.30	0.50
1:H:247:GLY:HA3	1:H:304:PHE:HB2	1.93	0.50
1:G:52:VAL:HG11	1:G:171:VAL:HG23	1.94	0.49
1:A:73:LEU:HD12	1:A:74:PRO:HD2	1.95	0.49
1:H:179:ASN:ND2	1:H:181:SER:OG	2.45	0.49
1:D:310:LEU:HD13	1:D:320:MET:HG2	1.94	0.49
1:H:225:VAL:HG23	1:H:225:VAL:O	2.12	0.49
1:G:347:ARG:NH2	1:H:178:MET:O	2.45	0.49
1:H:290:ARG:NH2	1:H:299:GLU:OE1	2.45	0.49
1:A:86:ALA:O	1:A:90:MET:HG3	2.13	0.49
1:B:27:LYS:HA	1:B:253:TYR:CD2	2.48	0.49
1:A:235:VAL:O	1:A:239:LEU:HD12	2.12	0.49
1:C:136:PRO:HD2	1:C:139:ILE:HD12	1.95	0.49
1:E:68:ALA:HB2	1:E:117:VAL:HG22	1.95	0.48
1:F:231:ALA:O	1:F:235:VAL:HG23	2.13	0.48
1:C:234:VAL:O	1:C:237:GLY:N	2.46	0.48
1:E:360:PRO:HG3	1:F:41:ASP:HB3	1.95	0.48
1:C:154:TRP:CH2	1:C:319:MET:HE1	2.48	0.48
1:G:232:ARG:HA	1:G:235:VAL:HG12	1.95	0.48
1:A:301:ASN:HB3	1:A:303:GLU:OE1	2.14	0.48
1:H:223:ASP:OD1	1:H:274:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ARG:NH1	1:E:243:GLU:OE2	2.47	0.48
1:F:58:ASP:OD2	1:F:109:ARG:NH2	2.47	0.47
1:A:347:ARG:NH1	1:A:348:PRO:O	2.47	0.47
1:G:367:GLU:HG2	1:G:368:ARG:HG3	1.96	0.47
1:B:362:SER:HB3	1:C:5:PRO:HD3	1.96	0.47
1:F:285:ALA:O	1:F:289:LEU:HD12	2.15	0.47
1:G:40:GLU:H	1:G:40:GLU:HG2	1.43	0.47
1:G:188:ILE:HG12	1:H:205:ALA:HB2	1.97	0.47
1:G:347:ARG:NH1	1:G:348:PRO:O	2.48	0.47
1:H:86:ALA:O	1:H:90:MET:HG3	2.15	0.47
1:F:185:ALA:HB2	1:F:202:ALA:HB2	1.97	0.46
1:F:234:VAL:O	1:F:238:ILE:HD12	2.15	0.46
1:H:318:ASN:ND2	1:H:318:ASN:H	2.14	0.46
1:E:301:ASN:HB3	1:E:303:GLU:OE1	2.16	0.46
1:A:41:ASP:O	1:A:45:GLN:HG3	2.15	0.46
1:E:215:PRO:HG2	1:E:320:MET:HB3	1.97	0.46
1:H:293:ARG:HD3	1:H:293:ARG:HA	1.76	0.46
1:D:226:GLU:HG2	1:D:277:VAL:HG21	1.97	0.46
1:H:27:LYS:HB2	1:H:251:ARG:HH12	1.81	0.45
1:H:180:ALA:HB3	1:H:211:HIS:CD2	2.51	0.45
1:D:232:ARG:HG3	1:D:232:ARG:HH11	1.81	0.45
1:G:92:ALA:HA	1:G:97:TYR:HB2	1.98	0.45
1:C:180:ALA:HB3	1:C:211:HIS:HD2	1.82	0.45
1:D:70:PRO:HB2	1:F:70:PRO:HB2	1.99	0.45
1:H:165:ALA:HB1	1:H:309:VAL:HG13	1.98	0.45
1:G:49:PHE:HD1	1:G:170:TRP:HB3	1.82	0.45
1:A:169:TYR:HA	1:A:263:LEU:HD21	1.99	0.45
1:H:286:LEU:HD12	1:H:286:LEU:HA	1.83	0.45
1:H:286:LEU:C	1:H:288:GLU:H	2.25	0.44
1:H:20:THR:OG1	1:H:338:GLU:OE1	2.31	0.44
1:B:314:ARG:HG2	1:B:314:ARG:HH11	1.83	0.44
1:F:264:ARG:NH1	1:F:282:GLU:OE2	2.50	0.44
1:H:39:ILE:HD11	1:H:258:PRO:HB2	1.99	0.44
1:A:353:VAL:HG23	1:B:21:GLU:HG2	2.00	0.44
1:F:250:HIS:HB3	1:F:251:ARG:HD3	1.98	0.44
1:G:24:GLU:OE2	1:G:33:ARG:NE	2.42	0.44
1:G:351:ILE:HD12	1:G:352:TYR:H	1.82	0.44
1:H:20:THR:OG1	1:H:22:ILE:HD12	2.17	0.44
1:D:175:GLU:OE2	1:D:335:HIS:NE2	2.48	0.44
1:E:176:HIS:ND1	3:E:401:FLC:HA1	2.32	0.44
1:B:86:ALA:O	1:B:90:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LYS:HA	1:D:253:TYR:CD2	2.52	0.43
1:D:241:ARG:NH2	1:D:243:GLU:OE1	2.51	0.43
1:B:314:ARG:HG2	1:B:314:ARG:NH1	2.34	0.43
1:C:176:HIS:ND1	3:C:401:FLC:HG2	2.33	0.43
1:G:24:GLU:HG3	1:G:33:ARG:HB2	2.00	0.43
1:D:73:LEU:HD12	1:D:74:PRO:HD2	2.01	0.43
1:F:315:VAL:HG13	1:F:319:MET:HE3	1.99	0.43
1:H:73:LEU:HD12	1:H:74:PRO:HD2	2.00	0.43
1:H:186:ARG:NH2	1:H:338:GLU:OE1	2.52	0.43
1:D:215:PRO:HA	1:D:303:GLU:HB3	1.99	0.43
1:F:27:LYS:HA	1:F:253:TYR:CD2	2.54	0.43
1:G:68:ALA:HB2	1:G:117:VAL:HG22	2.00	0.43
1:C:234:VAL:O	1:C:238:ILE:HD12	2.18	0.43
1:A:218:VAL:HG11	1:A:304:PHE:HD1	1.84	0.43
1:D:251:ARG:HD2	1:D:253:TYR:O	2.18	0.43
1:G:179:ASN:ND2	1:G:328:ARG:HH12	2.16	0.42
1:G:162:HIS:ND1	1:G:313:ALA:HA	2.34	0.42
1:H:81:ARG:HD3	1:H:207:SER:HB3	2.01	0.42
1:H:292:ARG:HA	1:H:292:ARG:HD3	1.89	0.42
1:A:230:ASP:OD2	1:A:233:SER:OG	2.37	0.42
1:B:43:VAL:HG11	1:B:262:VAL:HG13	2.02	0.42
1:B:293:ARG:NH2	1:B:295:ASP:OD2	2.53	0.42
1:A:148:ALA:HB1	2:A:401:9JT:SE1	2.69	0.42
1:C:368:ARG:HE	1:D:62:GLY:HA2	1.85	0.42
1:D:210:LEU:HD23	1:D:210:LEU:HA	1.86	0.42
1:B:232:ARG:HD2	1:B:232:ARG:HA	1.92	0.42
1:C:118:MET:HE2	1:C:122:TYR:CE1	2.54	0.42
1:H:55:LEU:HB2	1:H:61:PHE:CE2	2.55	0.42
1:H:248:PHE:HD1	1:H:300:THR:HA	1.84	0.42
1:H:317:ALA:HA	1:H:320:MET:HE2	2.01	0.42
1:B:293:ARG:HD3	1:B:296:ARG:NH2	2.35	0.42
1:F:68:ALA:HB2	1:F:117:VAL:HG22	2.02	0.42
1:G:34:TYR:O	1:G:55:LEU:HD21	2.20	0.42
1:H:65:LEU:HD12	1:H:65:LEU:HA	1.87	0.42
1:A:138:ARG:H	1:A:138:ARG:HG2	1.67	0.41
1:E:188:ILE:HG12	1:F:205:ALA:HB2	2.01	0.41
1:G:188:ILE:O	1:G:191:THR:HG22	2.20	0.41
1:B:32:LEU:HD23	1:B:39:ILE:HG21	2.01	0.41
1:H:230:ASP:OD1	1:H:233:SER:N	2.52	0.41
1:F:319:MET:HE3	1:F:319:MET:HB3	1.94	0.41
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:LYS:HA	1:G:253:TYR:CD2	2.56	0.41
1:E:347:ARG:NE	3:F:401:FLC:OA2	2.48	0.41
1:C:46:ARG:HD2	1:D:372:THR:HG21	2.02	0.41
1:E:39:ILE:O	1:E:43:VAL:HG22	2.20	0.41
1:E:364:ASP:OD1	1:E:364:ASP:N	2.52	0.41
1:F:227:ARG:CZ	1:F:227:ARG:HB3	2.51	0.41
1:A:275:TYR:O	1:A:279:VAL:HG23	2.21	0.41
1:E:143:CYS:HB2	1:E:149:ARG:HG3	2.02	0.41
1:G:352:TYR:OH	1:G:355:PRO:O	2.30	0.41
1:H:173:ALA:HB1	1:H:324:PHE:HE1	1.85	0.41
1:A:234:VAL:O	1:A:238:ILE:HG13	2.19	0.41
1:G:179:ASN:HB3	1:G:211:HIS:NE2	2.35	0.41
1:G:185:ALA:HB2	1:G:202:ALA:HB2	2.02	0.41
1:G:208:GLY:HA2	1:G:209:PRO:HD3	1.97	0.41
1:H:223:ASP:CG	1:H:274:ARG:HH22	2.28	0.41
1:H:293:ARG:NH1	1:H:296:ARG:HH11	2.19	0.41
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.94	0.41
1:B:328:ARG:HA	1:B:328:ARG:HD3	1.75	0.41
1:C:39:ILE:HG13	1:C:40:GLU:N	2.36	0.41
1:E:217:ARG:O	1:E:220:PRO:HD2	2.21	0.41
1:C:319:MET:HG2	1:C:319:MET:O	2.22	0.40
1:F:139:ILE:O	1:F:142:GLU:HG2	2.21	0.40
1:H:251:ARG:HD2	1:H:251:ARG:HA	1.82	0.40
1:E:344:LYS:HD2	1:E:344:LYS:HA	1.79	0.40
1:G:178:MET:O	1:H:347:ARG:NE	2.53	0.40
1:A:295:ASP:OD1	1:A:295:ASP:N	2.52	0.40
1:H:190:SER:HB3	1:H:339:GLN:NE2	2.37	0.40
1:A:290:ARG:NH1	1:A:298:ILE:O	2.54	0.40
1:H:250:HIS:CD2	1:H:296:ARG:HH21	2.40	0.40
1:D:71:PHE:CB	1:D:118:MET:HE1	2.52	0.40
1:F:221:MET:O	1:F:224:GLU:HG2	2.21	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	367/379 (97%)	360 (98%)	7 (2%)	0	100	100
1	B	371/379 (98%)	361 (97%)	10 (3%)	0	100	100
1	C	369/379 (97%)	361 (98%)	8 (2%)	0	100	100
1	D	368/379 (97%)	358 (97%)	10 (3%)	0	100	100
1	E	365/379 (96%)	356 (98%)	9 (2%)	0	100	100
1	F	370/379 (98%)	357 (96%)	13 (4%)	0	100	100
1	G	350/379 (92%)	343 (98%)	7 (2%)	0	100	100
1	H	356/379 (94%)	350 (98%)	6 (2%)	0	100	100
All	All	2916/3032 (96%)	2846 (98%)	70 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	282/291 (97%)	279 (99%)	3 (1%)	65	85
1	B	285/291 (98%)	282 (99%)	3 (1%)	65	85
1	C	284/291 (98%)	282 (99%)	2 (1%)	76	90
1	D	283/291 (97%)	283 (100%)	0	100	100
1	E	280/291 (96%)	276 (99%)	4 (1%)	59	82
1	F	284/291 (98%)	280 (99%)	4 (1%)	59	82
1	G	272/291 (94%)	270 (99%)	2 (1%)	76	90
1	H	275/291 (94%)	268 (98%)	7 (2%)	42	71
All	All	2245/2328 (96%)	2220 (99%)	25 (1%)	65	85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	210	LEU
1	A	349	SER
1	B	7	ASN
1	B	9	VAL
1	B	295	ASP
1	C	244	LYS
1	C	279	VAL
1	E	39	ILE
1	E	226	GLU
1	E	362	SER
1	E	364	ASP
1	F	2	THR
1	F	88	LEU
1	F	277	VAL
1	F	279	VAL
1	G	40	GLU
1	G	234	VAL
1	H	20	THR
1	H	245	LEU
1	H	252	VAL
1	H	286	LEU
1	H	296	ARG
1	H	299	GLU
1	H	362	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	85	GLN
1	B	76	HIS
1	B	132	GLN
1	C	60	ASN
1	D	60	ASN
1	D	76	HIS
1	D	111	GLN
1	D	283	GLN
1	E	60	ASN
1	E	76	HIS
1	E	137	GLN
1	F	60	ASN
1	F	301	ASN

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Mol	Chain	Res	Type
1	G	179	ASN
1	G	301	ASN
1	G	318	ASN
1	H	179	ASN
1	H	318	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	9JT	G	401	1	16,17,17	1.97	3 (18%)	21,22,22	1.08	1 (4%)
3	FLC	F	401	-	12,12,12	1.10	0	17,17,17	1.34	1 (5%)
2	9JT	E	402	1	16,17,17	1.96	3 (18%)	21,22,22	1.07	1 (4%)
2	9JT	F	402	1	16,17,17	1.97	3 (18%)	21,22,22	1.06	1 (4%)
3	FLC	B	401	-	12,12,12	1.11	0	17,17,17	1.43	1 (5%)
3	FLC	E	401	-	12,12,12	1.08	0	17,17,17	1.32	1 (5%)
2	9JT	D	402	1	16,17,17	1.97	3 (18%)	21,22,22	1.04	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9JT	C	402	1	16,17,17	1.96	3 (18%)	21,22,22	1.04	1 (4%)
2	9JT	A	401	1	16,17,17	1.95	3 (18%)	21,22,22	1.06	1 (4%)
2	9JT	H	401	1	16,17,17	1.99	3 (18%)	21,22,22	1.17	2 (9%)
2	9JT	B	402	1	16,17,17	1.96	3 (18%)	21,22,22	1.03	1 (4%)
3	FLC	D	401	-	12,12,12	1.10	0	17,17,17	1.41	1 (5%)
3	FLC	C	401	-	12,12,12	1.08	0	17,17,17	1.36	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	9JT	G	401	1	-	2/8/8/8	0/2/2/2
3	FLC	F	401	-	-	6/16/16/16	-
2	9JT	E	402	1	-	3/8/8/8	0/2/2/2
2	9JT	F	402	1	-	2/8/8/8	0/2/2/2
3	FLC	B	401	-	-	0/16/16/16	-
3	FLC	E	401	-	-	6/16/16/16	-
2	9JT	D	402	1	-	0/8/8/8	0/2/2/2
2	9JT	C	402	1	-	4/8/8/8	0/2/2/2
2	9JT	A	401	1	-	3/8/8/8	0/2/2/2
2	9JT	H	401	1	-	4/8/8/8	0/2/2/2
2	9JT	B	402	1	-	2/8/8/8	0/2/2/2
3	FLC	D	401	-	-	7/16/16/16	-
3	FLC	C	401	-	-	9/16/16/16	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	9JT	SE1-C02	5.28	1.95	1.89
2	G	401	9JT	SE1-C02	5.21	1.95	1.89
2	D	402	9JT	SE1-C02	5.21	1.95	1.89
2	F	402	9JT	SE1-C02	5.06	1.95	1.89
2	C	402	9JT	SE1-C02	5.05	1.95	1.89
2	B	402	9JT	SE1-C02	5.05	1.95	1.89
2	A	401	9JT	SE1-C02	5.04	1.95	1.89
2	E	402	9JT	SE1-C02	5.02	1.95	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	402	9JT	C08-N10	3.67	1.46	1.35
2	E	402	9JT	C08-N10	3.65	1.46	1.35
2	B	402	9JT	C08-N10	3.65	1.46	1.35
2	C	402	9JT	C08-N10	3.64	1.46	1.35
2	A	401	9JT	C08-N10	3.59	1.46	1.35
2	D	402	9JT	C08-N10	3.55	1.46	1.35
2	G	401	9JT	C08-N10	3.55	1.46	1.35
2	H	401	9JT	C08-N10	3.55	1.46	1.35
2	C	402	9JT	C11-N10	2.32	1.46	1.41
2	F	402	9JT	C11-N10	2.32	1.46	1.41
2	E	402	9JT	C11-N10	2.32	1.46	1.41
2	B	402	9JT	C11-N10	2.31	1.46	1.41
2	A	401	9JT	C11-N10	2.20	1.46	1.41
2	D	402	9JT	C11-N10	2.16	1.46	1.41
2	H	401	9JT	C11-N10	2.11	1.45	1.41
2	G	401	9JT	C11-N10	2.10	1.45	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	FLC	OB2-CBC-CB	3.70	120.24	113.14
3	B	401	FLC	OB2-CBC-CB	3.67	120.19	113.14
2	E	402	9JT	C13-C12-C11	3.67	123.96	119.73
2	F	402	9JT	C13-C12-C11	3.66	123.95	119.73
2	C	402	9JT	C13-C12-C11	3.66	123.95	119.73
3	C	401	FLC	OB2-CBC-CB	3.59	120.04	113.14
2	B	402	9JT	C13-C12-C11	3.59	123.87	119.73
2	A	401	9JT	C13-C12-C11	3.59	123.86	119.73
3	F	401	FLC	OB2-CBC-CB	3.55	119.96	113.14
2	D	402	9JT	C13-C12-C11	3.45	123.70	119.73
3	E	401	FLC	OB2-CBC-CB	3.42	119.70	113.14
2	G	401	9JT	C13-C12-C11	3.41	123.66	119.73
2	H	401	9JT	C13-C12-C11	3.35	123.59	119.73
2	H	401	9JT	C07-C08-N10	2.18	120.55	116.03

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	9JT	C02-C07-C08-O09
2	A	401	9JT	C02-C07-C08-N10
2	C	402	9JT	C02-C07-C08-N10

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Mol	Chain	Res	Type	Atoms
3	C	401	FLC	OHB-CB-CBC-OB1
3	C	401	FLC	OHB-CB-CBC-OB2
3	D	401	FLC	CG-CB-CBC-OB1
3	D	401	FLC	CG-CB-CBC-OB2
3	D	401	FLC	OHB-CB-CBC-OB1
3	D	401	FLC	OHB-CB-CBC-OB2
3	E	401	FLC	CG-CB-CBC-OB1
3	E	401	FLC	CG-CB-CBC-OB2
3	E	401	FLC	OHB-CB-CBC-OB1
3	E	401	FLC	OHB-CB-CBC-OB2
3	C	401	FLC	CA-CB-CG-CGC
3	C	401	FLC	CA-CB-CBC-OB1
3	C	401	FLC	CA-CB-CBC-OB2
3	C	401	FLC	CBC-CB-CG-CGC
2	G	401	9JT	C02-C07-C08-O09
2	G	401	9JT	C02-C07-C08-N10
2	H	401	9JT	C02-C07-C08-O09
2	H	401	9JT	C02-C07-C08-N10
3	C	401	FLC	CG-CB-CBC-OB2
3	F	401	FLC	OHB-CB-CG-CGC
3	D	401	FLC	CAC-CA-CB-CBC
2	F	402	9JT	C06-C07-C08-O09
3	D	401	FLC	CA-CB-CBC-OB2
3	E	401	FLC	CA-CB-CBC-OB1
3	E	401	FLC	CA-CB-CBC-OB2
3	F	401	FLC	CA-CB-CBC-OB1
3	F	401	FLC	CA-CB-CBC-OB2
3	F	401	FLC	CG-CB-CBC-OB1
3	F	401	FLC	CG-CB-CBC-OB2
3	C	401	FLC	OHB-CB-CG-CGC
3	D	401	FLC	CAC-CA-CB-OHB
2	C	402	9JT	C02-C07-C08-O09
2	E	402	9JT	C02-C07-C08-N10
2	H	401	9JT	C12-C11-N10-C08
2	F	402	9JT	C06-C07-C08-N10
2	B	402	9JT	C06-C07-C08-O09
2	H	401	9JT	C16-C11-N10-C08
2	E	402	9JT	C06-C07-C08-O09
3	F	401	FLC	OHB-CB-CBC-OB1
2	B	402	9JT	C06-C07-C08-N10
3	C	401	FLC	CG-CB-CBC-OB1
2	C	402	9JT	C06-C07-C08-O09

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Mol	Chain	Res	Type	Atoms
2	E	402	9JT	C06-C07-C08-N10
2	C	402	9JT	C06-C07-C08-N10
2	A	401	9JT	C06-C07-C08-O09

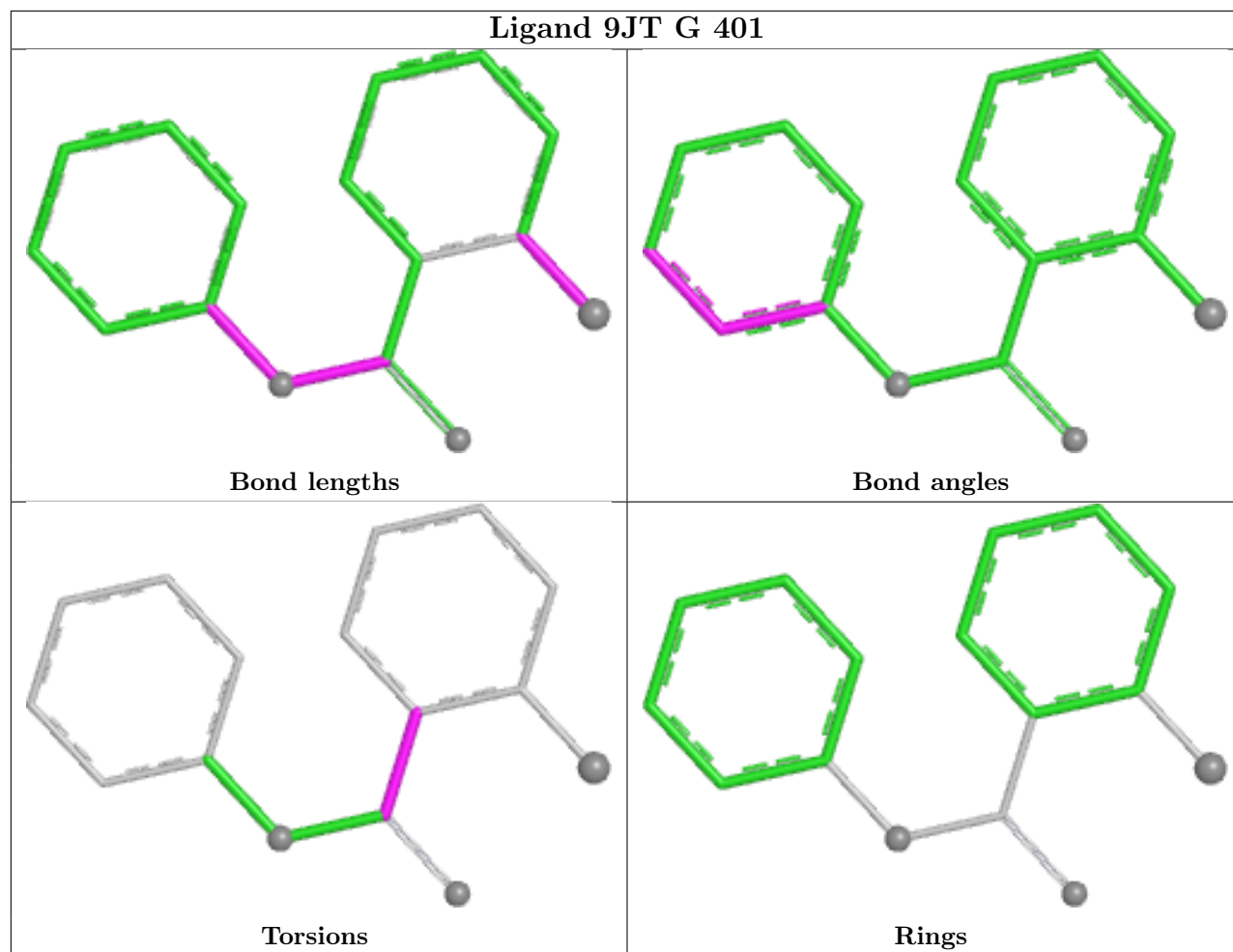
There are no ring outliers.

6 monomers are involved in 8 short contacts:

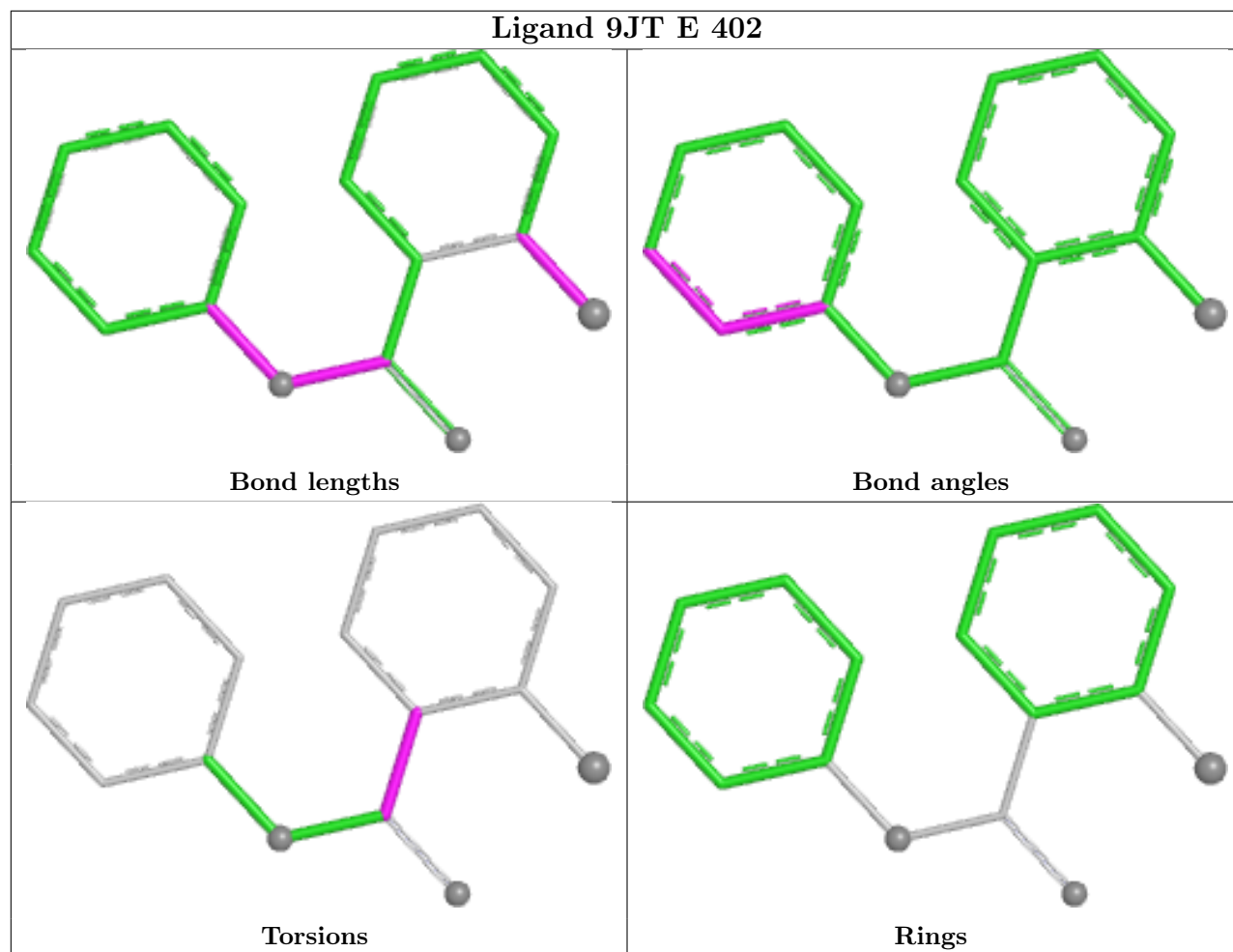
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	FLC	3	0
3	B	401	FLC	1	0
3	E	401	FLC	1	0
2	A	401	9JT	1	0
3	D	401	FLC	1	0
3	C	401	FLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

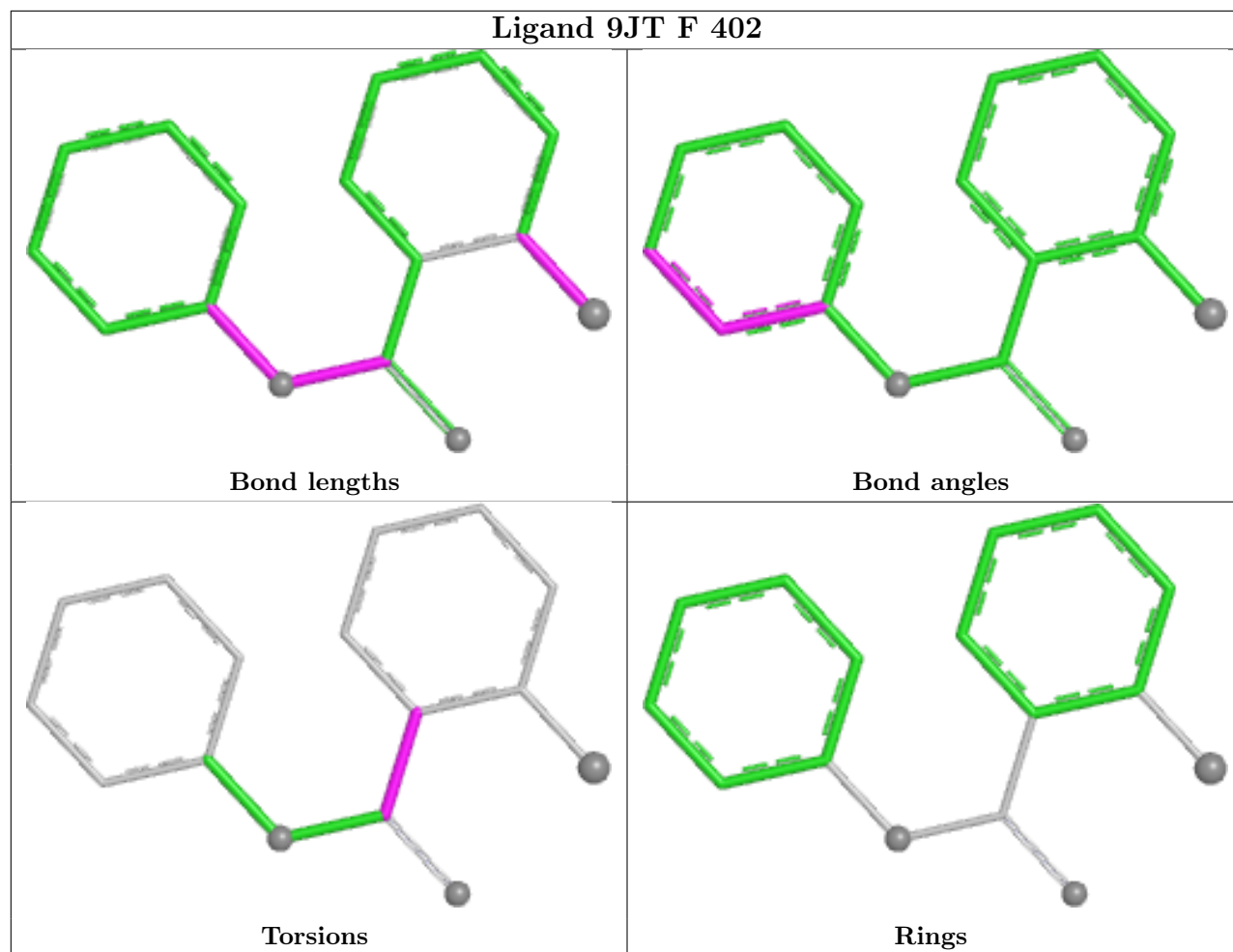
Ligand 9JT G 401



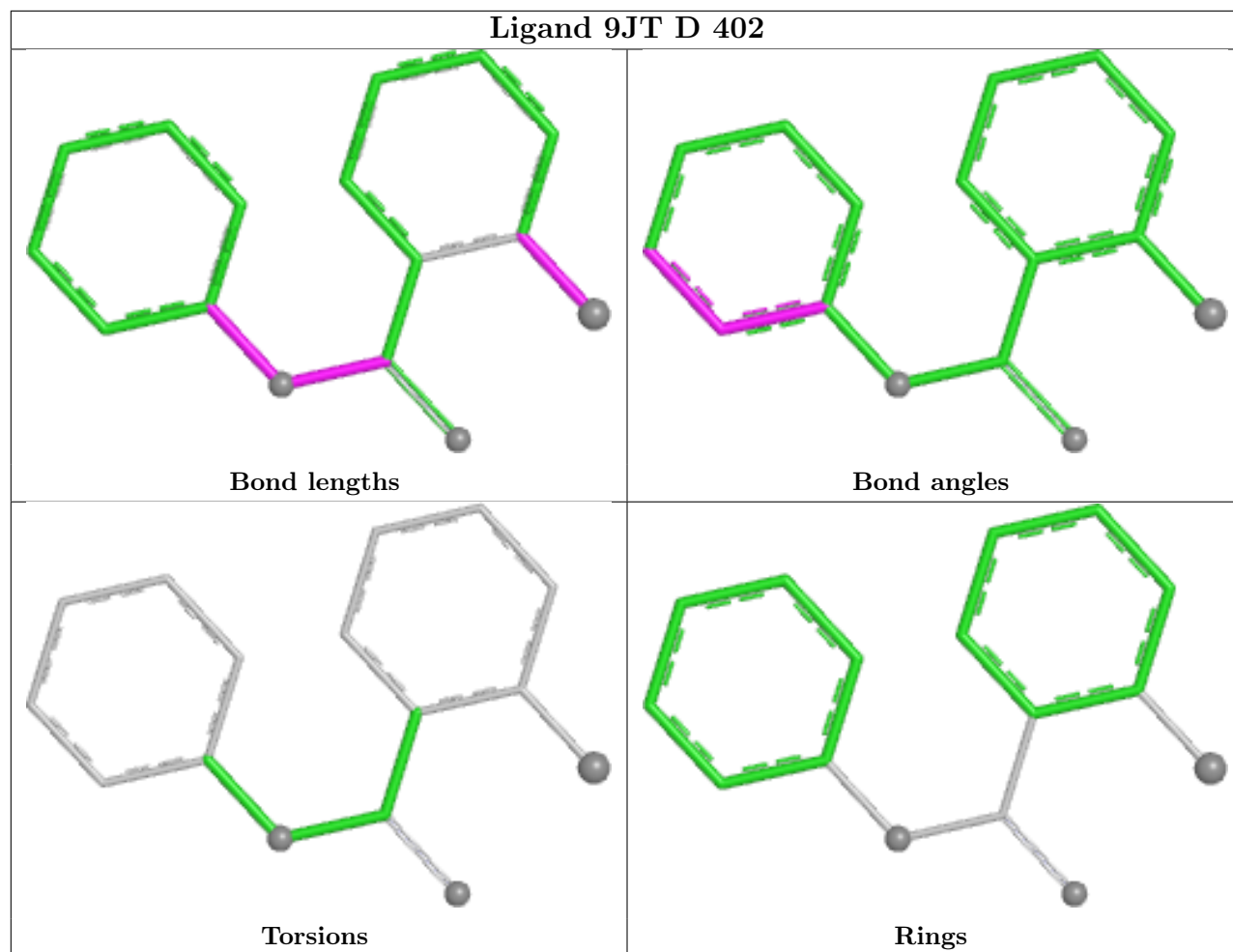
Ligand 9JT E 402



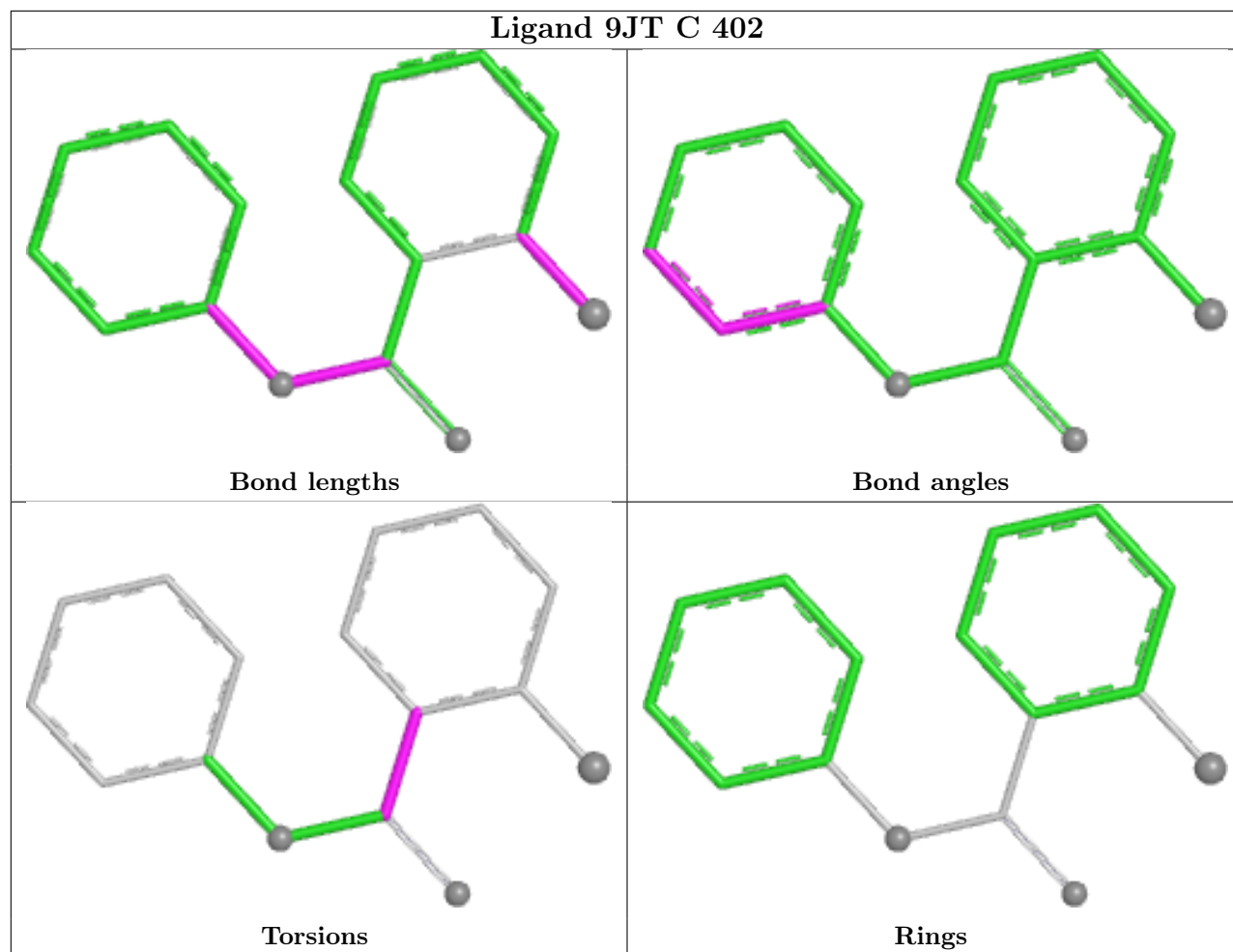
Ligand 9JT F 402



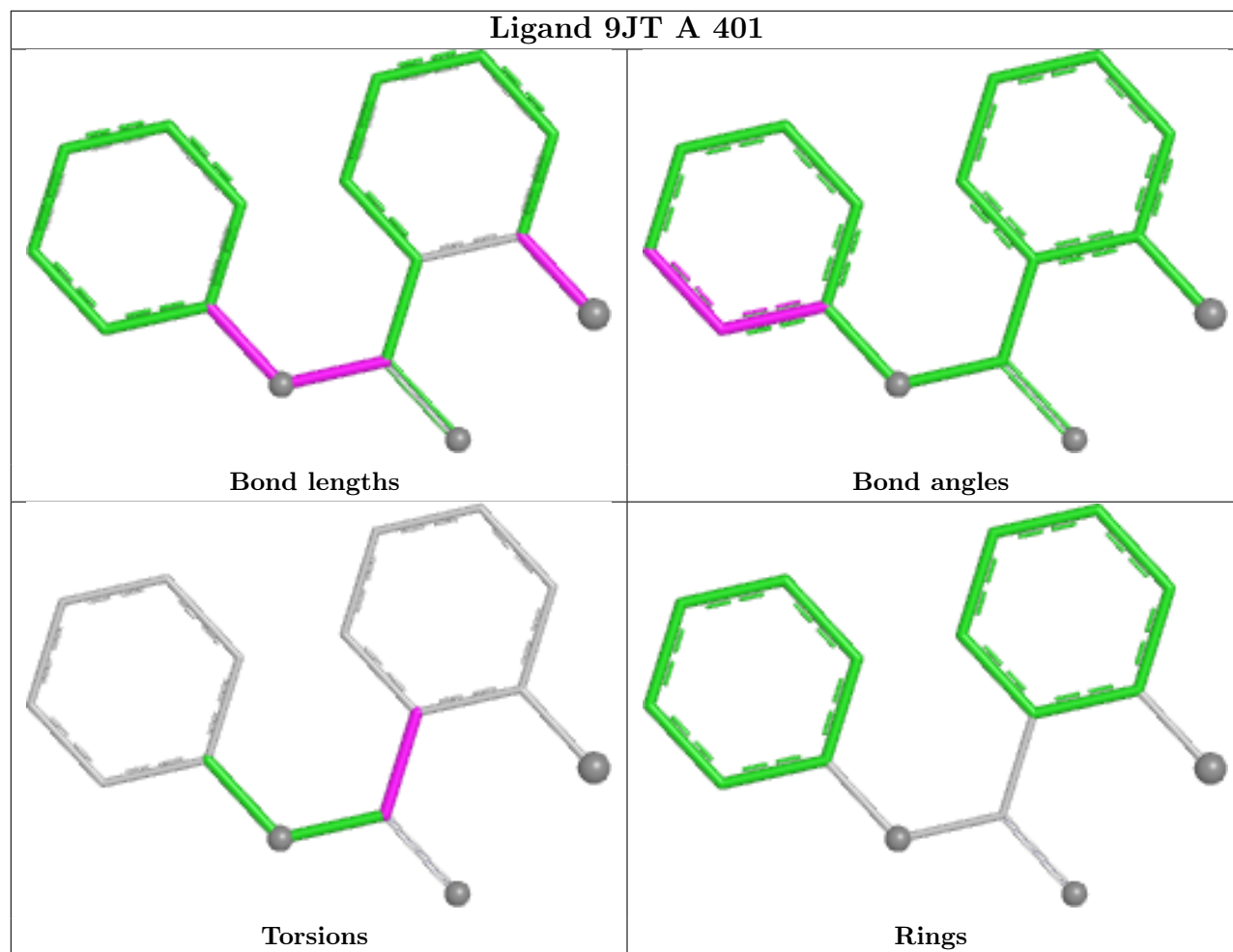
Ligand 9JT D 402



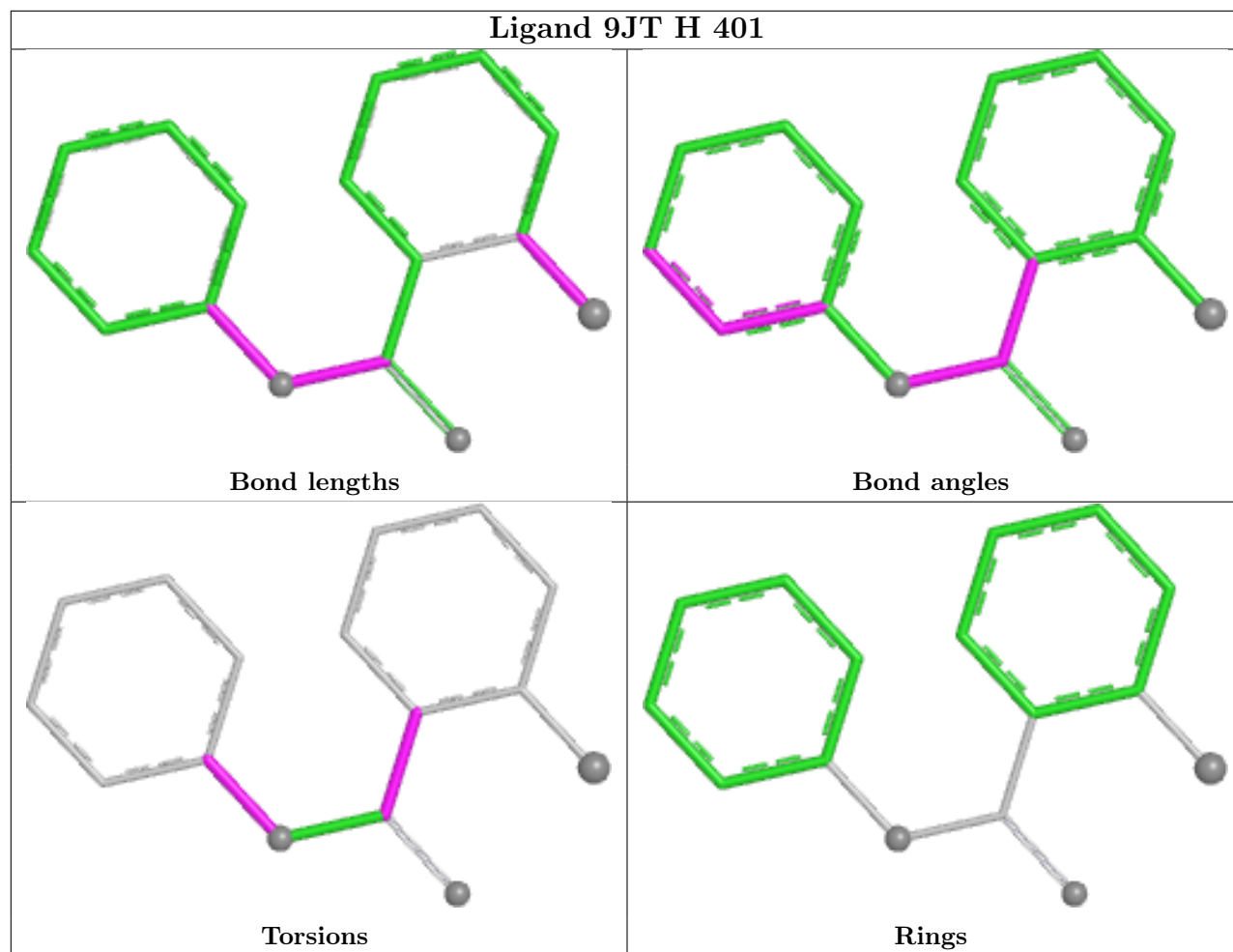
Ligand 9JT C 402

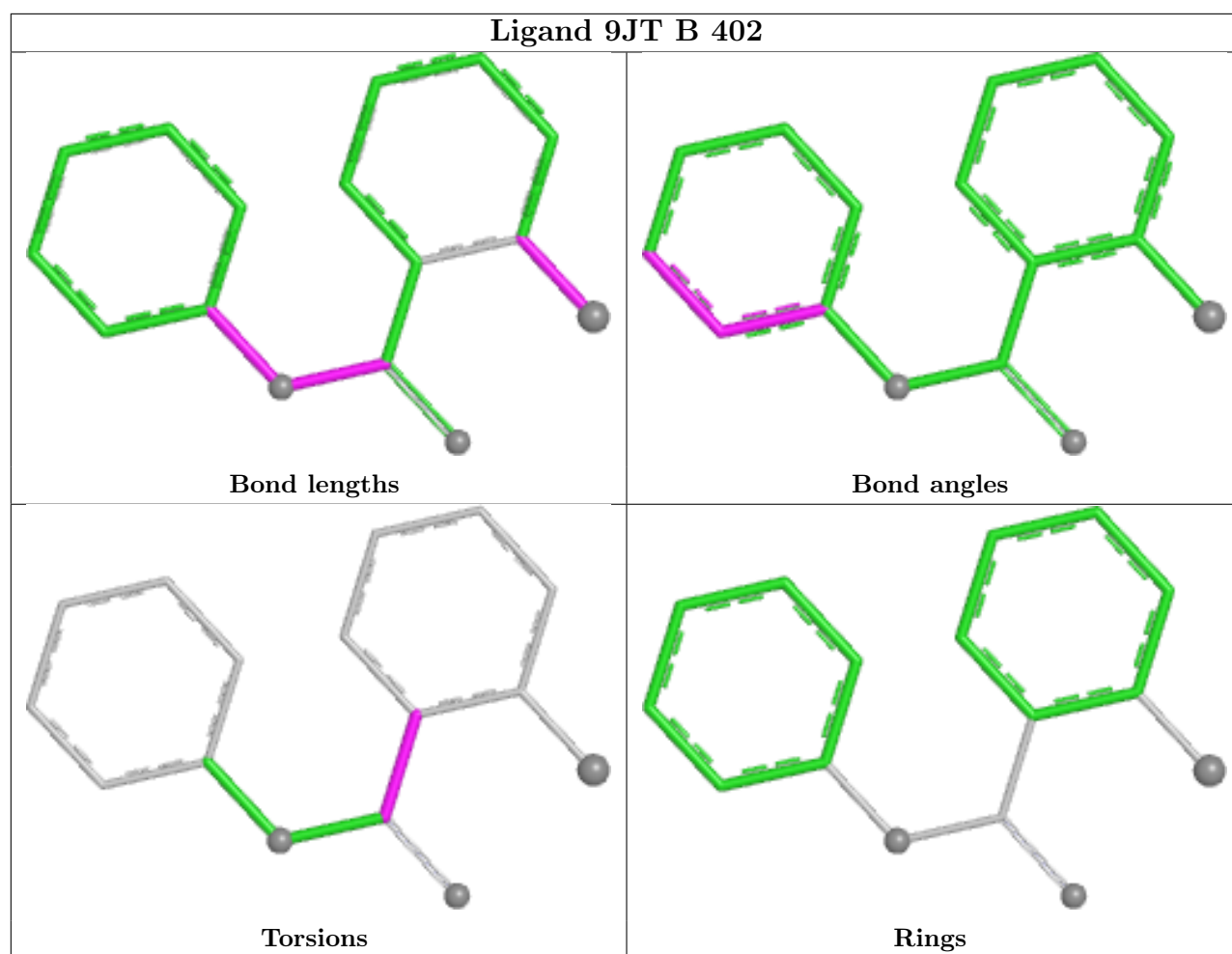


Ligand 9JT A 401



Ligand 9JT H 401





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	369/379 (97%)	0.30	15 (4%)	41	37	36, 56, 104, 122	1 (0%)
1	B	373/379 (98%)	0.17	12 (3%)	50	46	36, 52, 89, 120	1 (0%)
1	C	371/379 (97%)	0.23	14 (3%)	44	40	37, 54, 110, 128	1 (0%)
1	D	370/379 (97%)	0.24	16 (4%)	40	36	37, 52, 98, 145	1 (0%)
1	E	367/379 (96%)	0.17	15 (4%)	41	37	34, 50, 100, 160	0
1	F	372/379 (98%)	0.59	32 (8%)	16	13	37, 63, 119, 143	0
1	G	356/379 (93%)	1.31	85 (23%)	2	1	50, 92, 142, 164	1 (0%)
1	H	360/379 (94%)	1.35	74 (20%)	2	2	46, 92, 139, 170	0
All	All	2938/3032 (96%)	0.54	263 (8%)	15	13	34, 61, 122, 170	5 (0%)

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	370	LEU	6.1
1	D	255	ALA	5.5
1	F	373	ALA	5.5
1	G	235	VAL	5.2
1	E	5	PRO	4.8
1	D	4	VAL	4.8
1	G	305	TRP	4.7
1	H	25	PRO	4.6
1	H	215	PRO	4.6
1	G	9	VAL	4.5
1	H	216	ALA	4.5
1	C	4	VAL	4.5
1	E	371	THR	4.4
1	A	6	GLU	4.4
1	G	231	ALA	4.3
1	D	216	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	14	GLY	4.3
1	G	18	PHE	4.3
1	G	255	ALA	4.2
1	H	255	ALA	4.2
1	G	370	LEU	4.2
1	H	238	ILE	4.1
1	D	8	PHE	3.9
1	G	31	ALA	3.8
1	B	216	ALA	3.8
1	D	5	PRO	3.8
1	B	373	ALA	3.8
1	H	214	ALA	3.7
1	C	1	MET	3.7
1	G	36	GLY	3.7
1	C	5	PRO	3.7
1	H	176	HIS	3.6
1	H	252	VAL	3.6
1	H	31	ALA	3.5
1	H	18	PHE	3.5
1	G	284	ALA	3.5
1	F	372	THR	3.5
1	F	250	HIS	3.5
1	G	281	VAL	3.5
1	F	371	THR	3.4
1	H	11	GLY	3.4
1	H	213	GLY	3.4
1	H	32	LEU	3.4
1	H	289	LEU	3.4
1	H	277	VAL	3.4
1	H	298	ILE	3.4
1	H	371	THR	3.4
1	G	256	GLU	3.4
1	E	255	ALA	3.4
1	G	30	GLY	3.3
1	C	2	THR	3.3
1	H	301	ASN	3.3
1	F	283	GLN	3.3
1	D	256	GLU	3.2
1	A	228	ALA	3.2
1	H	9	VAL	3.2
1	H	231	ALA	3.2
1	G	351	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	14	GLY	3.2
1	G	259	ARG	3.2
1	H	305	TRP	3.2
1	G	352	TYR	3.2
1	B	62	GLY	3.1
1	A	2	THR	3.1
1	G	254	ARG	3.1
1	F	2	THR	3.1
1	E	228	ALA	3.1
1	D	252	VAL	3.1
1	D	3	VAL	3.1
1	H	287	SER	3.0
1	H	239	LEU	3.0
1	G	25	PRO	3.0
1	H	351	ILE	3.0
1	E	9	VAL	3.0
1	H	222	LEU	2.9
1	G	39	ILE	2.9
1	E	227	ARG	2.9
1	D	229	GLY	2.9
1	G	356	GLY	2.9
1	H	173	ALA	2.9
1	H	210	LEU	2.9
1	H	245	LEU	2.9
1	H	250	HIS	2.9
1	H	10	PRO	2.9
1	B	371	THR	2.9
1	G	12	LEU	2.9
1	G	245	LEU	2.9
1	G	246	MET	2.8
1	G	19	THR	2.8
1	G	61	PHE	2.8
1	G	176	HIS	2.8
1	E	226	GLU	2.8
1	F	298	ILE	2.8
1	C	3	VAL	2.8
1	F	214	ALA	2.8
1	F	228	ALA	2.8
1	G	350	ALA	2.8
1	G	173	ALA	2.8
1	D	10	PRO	2.7
1	H	356	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	246	MET	2.7
1	G	20	THR	2.7
1	H	34	TYR	2.7
1	B	11	GLY	2.7
1	H	357	PRO	2.7
1	H	212	GLY	2.7
1	D	7	ASN	2.7
1	H	256	GLU	2.7
1	H	280	ALA	2.7
1	F	242	GLY	2.7
1	G	252	VAL	2.7
1	G	353	VAL	2.7
1	C	11	GLY	2.6
1	F	11	GLY	2.6
1	F	255	ALA	2.6
1	H	12	LEU	2.6
1	C	7	ASN	2.6
1	G	277	VAL	2.6
1	G	10	PRO	2.6
1	F	7	ASN	2.6
1	H	332	TRP	2.6
1	G	286	LEU	2.6
1	E	296	ARG	2.6
1	G	33	ARG	2.6
1	H	177	GLY	2.6
1	D	228	ALA	2.6
1	G	330	ALA	2.6
1	H	171	VAL	2.6
1	F	217	ARG	2.5
1	H	30	GLY	2.5
1	G	23	ALA	2.5
1	C	217	ARG	2.5
1	G	34	TYR	2.5
1	H	234	VAL	2.5
1	F	279	VAL	2.5
1	G	234	VAL	2.5
1	G	278	ALA	2.5
1	G	27	LYS	2.5
1	A	370	LEU	2.5
1	G	289	LEU	2.5
1	G	24	GLU	2.5
1	A	5	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	3	VAL	2.5
1	F	277	VAL	2.5
1	H	358	ARG	2.4
1	G	22	ILE	2.4
1	G	345	LEU	2.4
1	B	250	HIS	2.4
1	G	221	MET	2.4
1	G	253	TYR	2.4
1	H	16	VAL	2.4
1	A	7	ASN	2.4
1	D	250	HIS	2.4
1	G	309	VAL	2.4
1	E	238	ILE	2.4
1	B	367	GLU	2.4
1	F	219	LEU	2.4
1	E	357	PRO	2.4
1	A	62	GLY	2.4
1	C	232	ARG	2.4
1	H	37	VAL	2.4
1	D	297	ALA	2.4
1	G	49	PHE	2.4
1	G	55	LEU	2.3
1	E	250	HIS	2.3
1	B	7	ASN	2.3
1	A	271	GLY	2.3
1	E	356	GLY	2.3
1	B	9	VAL	2.3
1	A	284	ALA	2.3
1	F	319	MET	2.3
1	G	251	ARG	2.3
1	H	327	GLY	2.3
1	F	8	PHE	2.3
1	G	280	ALA	2.3
1	H	20	THR	2.3
1	G	41	ASP	2.3
1	H	15	VAL	2.3
1	G	304	PHE	2.3
1	G	306	ALA	2.3
1	H	98	ALA	2.3
1	H	211	HIS	2.3
1	H	249	GLY	2.3
1	F	222	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	370	LEU	2.3
1	G	239	LEU	2.3
1	H	218	VAL	2.3
1	C	297	ALA	2.2
1	G	307	ALA	2.2
1	H	350	ALA	2.2
1	C	250	HIS	2.2
1	A	10	PRO	2.2
1	E	365	GLY	2.2
1	F	245	LEU	2.2
1	G	32	LEU	2.2
1	H	22	ILE	2.2
1	H	324	PHE	2.2
1	E	214	ALA	2.2
1	H	221	MET	2.2
1	A	296	ARG	2.2
1	G	365	GLY	2.2
1	F	221	MET	2.2
1	G	334	ALA	2.2
1	H	330	ALA	2.2
1	C	371	THR	2.2
1	H	290	ARG	2.2
1	H	253	TYR	2.2
1	G	308	VAL	2.2
1	H	363	VAL	2.2
1	G	285	ALA	2.2
1	G	357	PRO	2.2
1	G	189	ALA	2.1
1	G	216	ALA	2.1
1	F	251	ARG	2.1
1	G	191	THR	2.1
1	D	246	MET	2.1
1	F	239	LEU	2.1
1	G	295	ASP	2.1
1	H	26	ASP	2.1
1	G	175	GLU	2.1
1	G	261	ARG	2.1
1	H	241	ARG	2.1
1	F	30	GLY	2.1
1	G	29	GLY	2.1
1	G	237	GLY	2.1
1	G	250	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	2.1
1	C	235	VAL	2.1
1	G	43	VAL	2.1
1	G	225	VAL	2.1
1	A	276	GLU	2.1
1	B	217	ARG	2.1
1	E	370	LEU	2.1
1	F	212	GLY	2.1
1	F	249	GLY	2.1
1	A	234	VAL	2.1
1	H	13	ASP	2.1
1	G	300	THR	2.1
1	G	56	LEU	2.1
1	H	365	GLY	2.1
1	G	238	ILE	2.1
1	G	346	VAL	2.1
1	B	269	ARG	2.0
1	F	297	ALA	2.0
1	G	44	SER	2.0
1	H	17	ALA	2.0
1	H	266	ALA	2.0
1	G	344	LYS	2.0
1	H	170	TRP	2.0
1	G	37	VAL	2.0
1	A	8	PHE	2.0
1	F	248	PHE	2.0
1	G	40	GLU	2.0
1	B	297	ALA	2.0
1	D	214	ALA	2.0
1	H	307	ALA	2.0
1	G	355	PRO	2.0
1	C	289	LEU	2.0
1	F	235	VAL	2.0
1	G	218	VAL	2.0
1	H	262	VAL	2.0
1	H	346	VAL	2.0
1	H	369	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

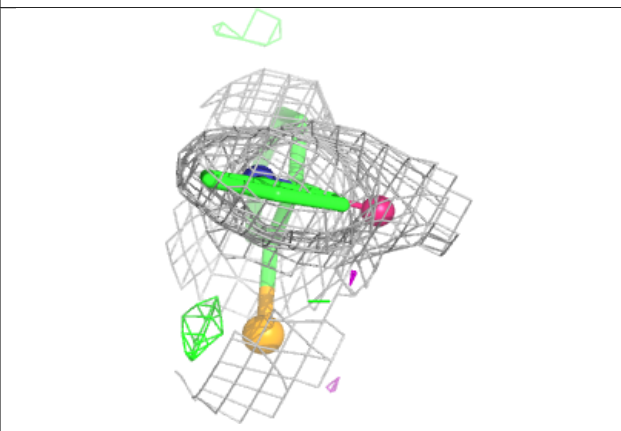
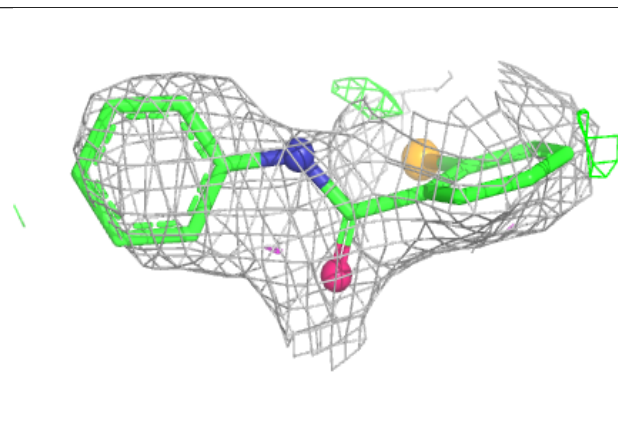
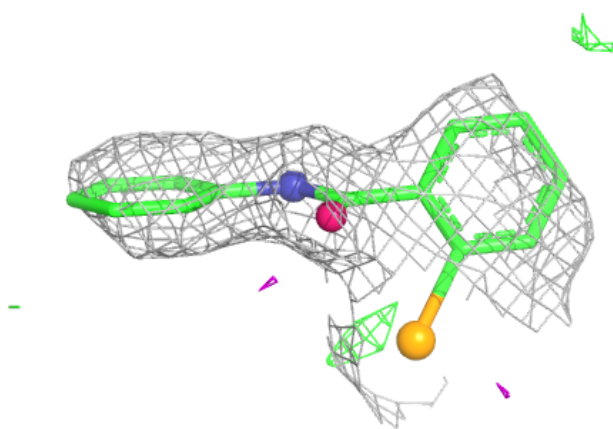
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FLC	F	401	13/13	0.74	0.19	62,75,87,98	0
3	FLC	C	401	13/13	0.75	0.17	72,79,90,96	0
3	FLC	E	401	13/13	0.78	0.15	59,69,83,84	0
2	9JT	F	402	16/16	0.83	0.18	80,99,110,139	0
2	9JT	H	401	16/16	0.83	0.20	98,108,114,164	0
3	FLC	B	401	13/13	0.83	0.14	57,63,75,77	0
2	9JT	G	401	16/16	0.85	0.19	90,94,104,130	16
2	9JT	D	402	16/16	0.87	0.18	68,77,86,115	16
2	9JT	E	402	16/16	0.89	0.15	48,61,68,101	0
3	FLC	D	401	13/13	0.90	0.11	57,60,73,77	0
2	9JT	B	402	16/16	0.92	0.14	53,61,69,94	16
2	9JT	C	402	16/16	0.92	0.15	61,68,75,88	16
2	9JT	A	401	16/16	0.92	0.16	67,73,81,101	16

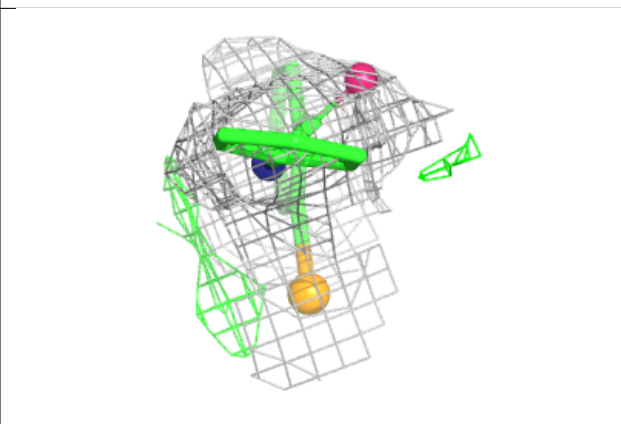
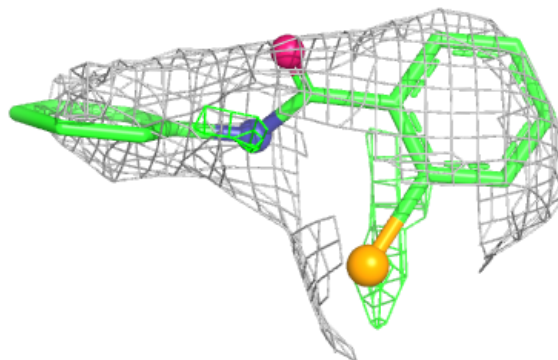
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 9JT F 402:

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

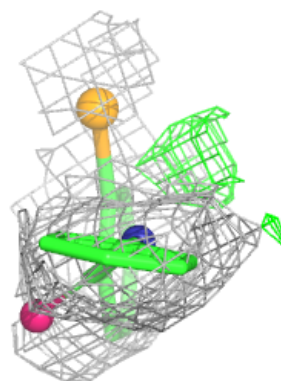
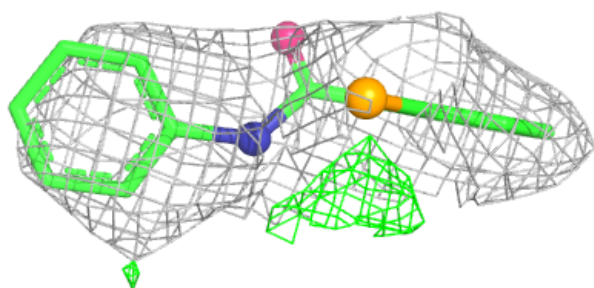
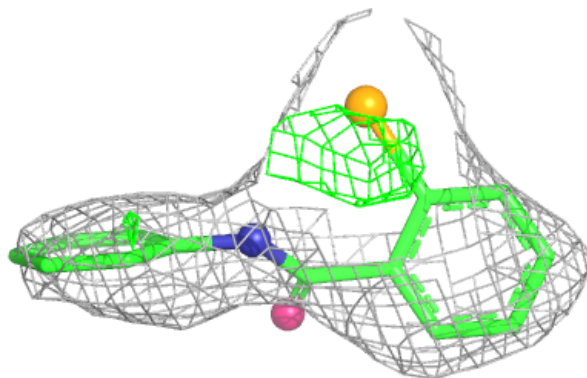
**Electron density around 9JT H 401:**

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

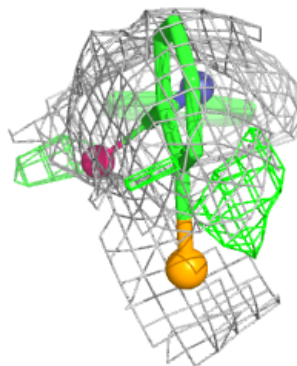
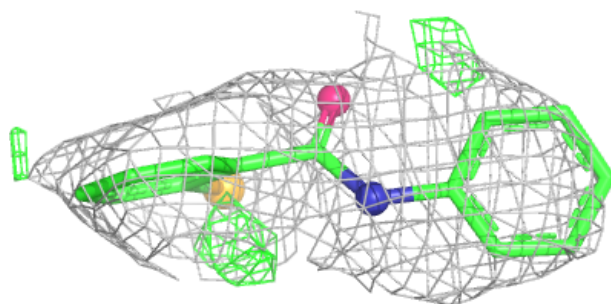
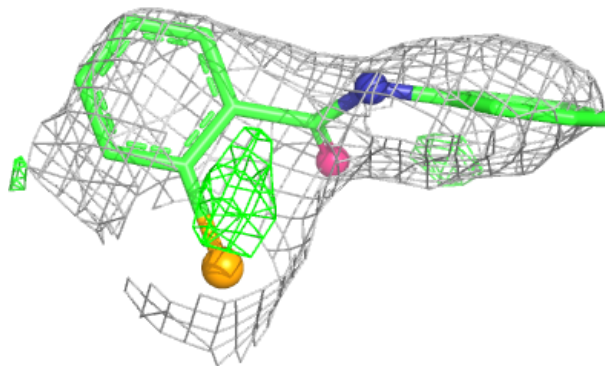


Electron density around 9JT G 401:

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

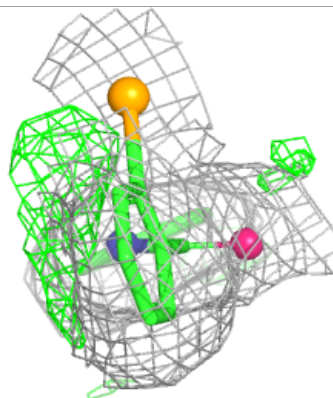
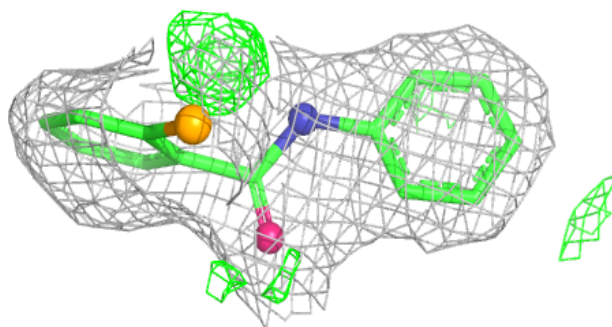
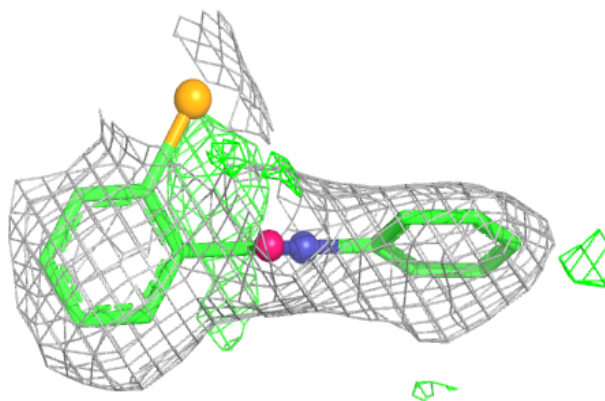
**Electron density around 9JT D 402:**

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

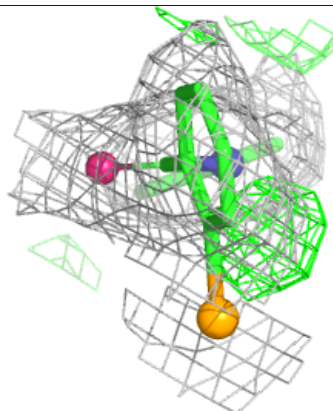
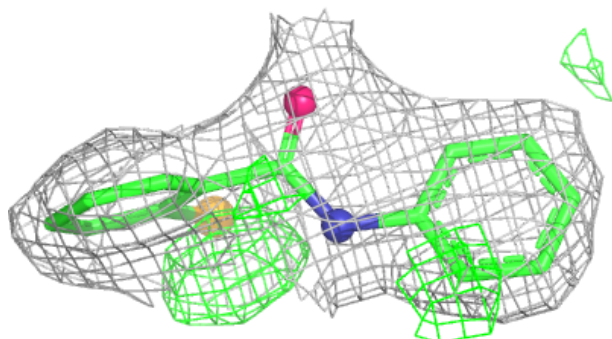
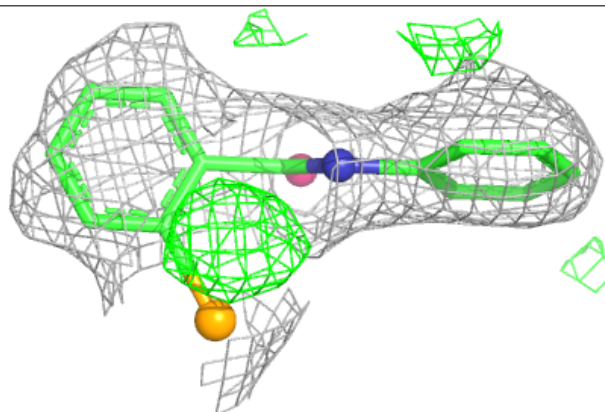


Electron density around 9JT E 402:

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

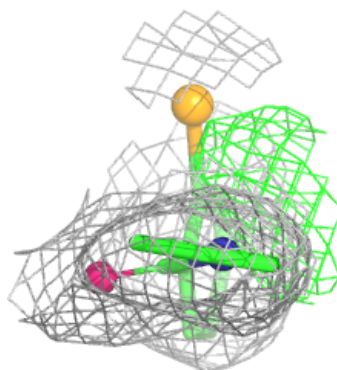
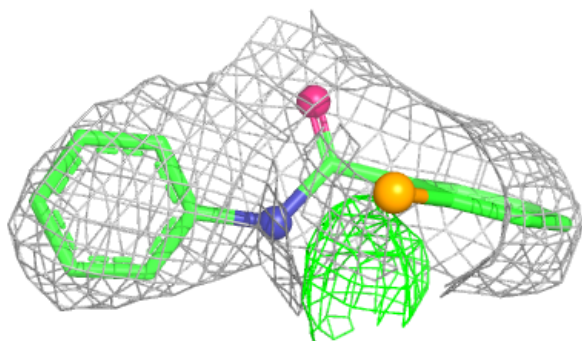
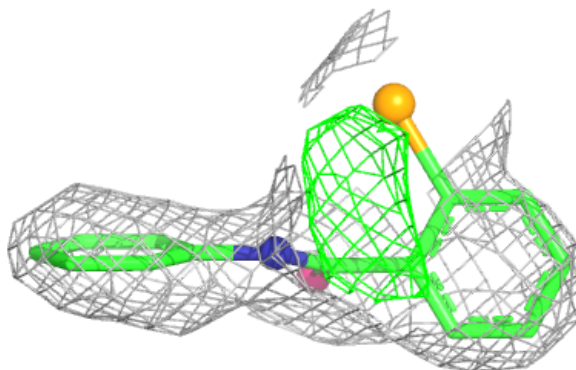
**Electron density around 9JT B 402:**

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

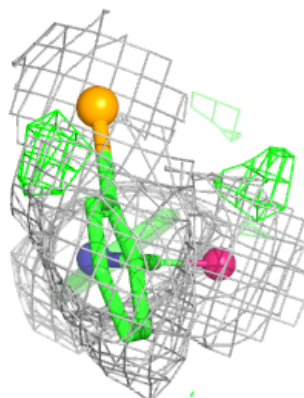
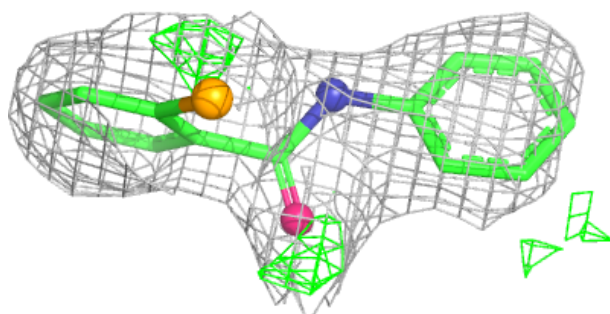
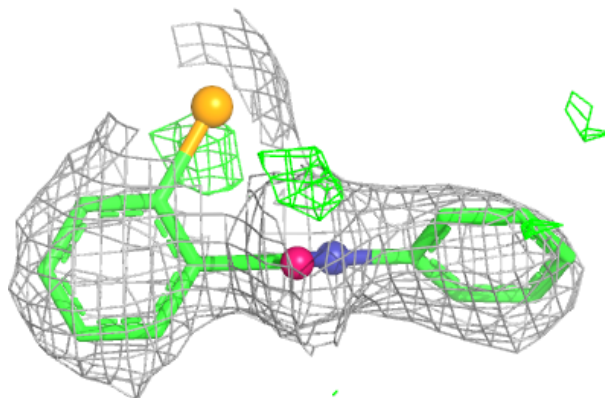


Electron density around 9JT C 402:

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

**Electron density around 9JT A 401:**

$2mF_o-DF_c$ (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.