



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:10 AM UTC

PDB ID : 6OB0 / pdb_00006ob0
Title : Compound 2 bound structure of WT Lipoprotein Lipase in Complex with GPIHBP1 Mutant N78D N82D produced in HEK293-F cells
Authors : Arora, R.; Horton, P.A.; Benson, T.E.; Romanowski, M.J.
Deposited on : 2019-03-19
Resolution : 2.81 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

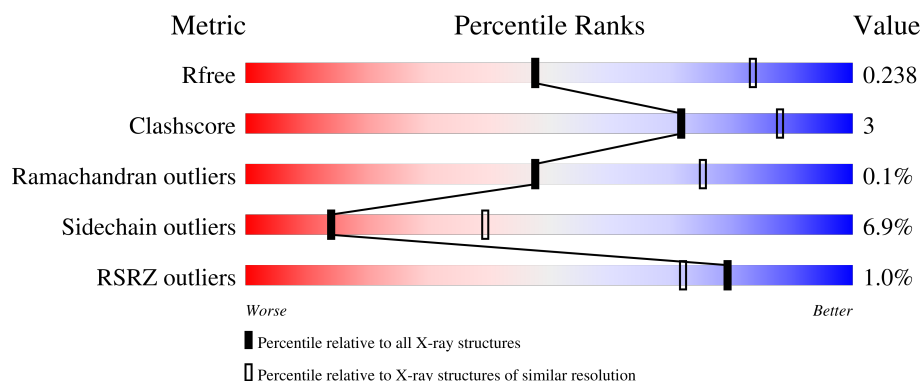
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	448	 86% 12% ..
1	B	448	 86% 11% ..
1	C	448	 85% 13% ..
1	D	448	 86% 11% ..
2	E	131	 50% 12% 37%

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Mol	Chain	Length	Quality of chain
2	F	131	% 45% 15% • 38%
2	G	131	3% 46% 15% • 38%
2	H	131	51% 10% • 38%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17194 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 Lipoprotein lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	1	0
			3518	2236	611	655	16			
1	B	442	Total	C	N	O	S	0	0	0
			3511	2231	609	655	16			
1	C	442	Total	C	N	O	S	0	1	0
			3518	2236	611	655	16			
1	D	442	Total	C	N	O	S	0	1	0
			3518	2236	611	655	16			

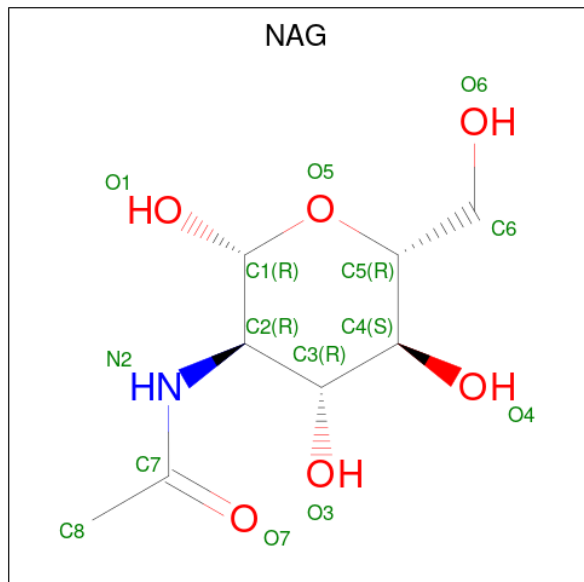
- Molecule 2 is a protein called Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	83	Total	C	N	O	S	0	0	0
			628	378	110	129	11			
2	F	81	Total	C	N	O	S	0	0	0
			613	367	108	127	11			
2	G	81	Total	C	N	O	S	0	0	0
			613	367	108	127	11			
2	H	81	Total	C	N	O	S	0	0	0
			613	367	108	127	11			

There are 8 discrepancies between the modelled and reference sequences:

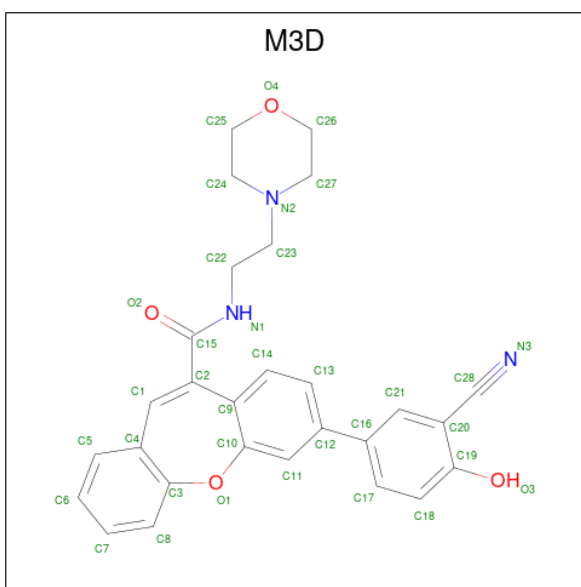
Chain	Residue	Modelled	Actual	Comment	Reference
E	78	ASP	ASN	engineered mutation	UNP Q8IV16
E	82	ASP	ASN	engineered mutation	UNP Q8IV16
F	78	ASP	ASN	engineered mutation	UNP Q8IV16
F	82	ASP	ASN	engineered mutation	UNP Q8IV16
G	78	ASP	ASN	engineered mutation	UNP Q8IV16
G	82	ASP	ASN	engineered mutation	UNP Q8IV16
H	78	ASP	ASN	engineered mutation	UNP Q8IV16
H	82	ASP	ASN	engineered mutation	UNP Q8IV16

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



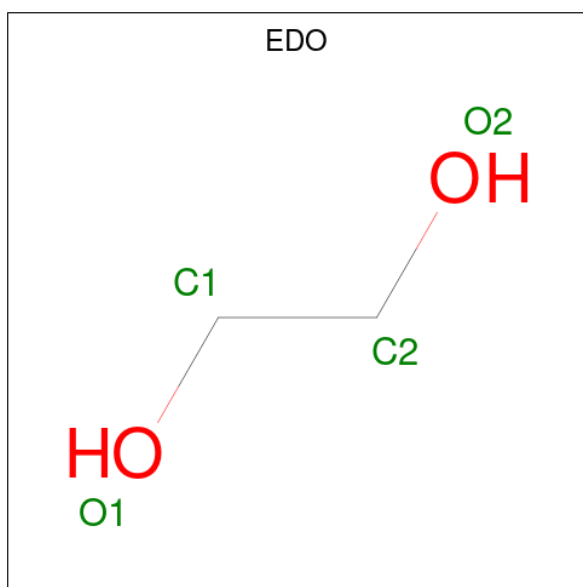
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 7-(3-cyano-4-hydroxyphenyl)-N-[2-(morpholin-4-yl)ethyl]dibenzo[b,f]oxepine-10-carboxamide (CCD ID: M3D) (formula: $C_{28}H_{25}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	3	4		
4	A	1	Total	C	N	O	0	0
			35	28	3	4		
4	B	1	Total	C	N	O	0	0
			35	28	3	4		
4	B	1	Total	C	N	O	0	0
			35	28	3	4		
4	C	1	Total	C	N	O	0	0
			35	28	3	4		
4	C	1	Total	C	N	O	0	0
			35	28	3	4		
4	D	1	Total	C	N	O	0	0
			35	28	3	4		
4	D	1	Total	C	N	O	0	0
			35	28	3	4		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

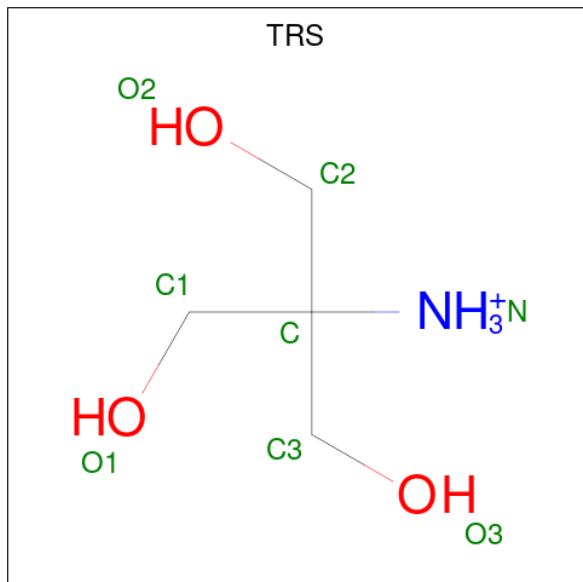


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

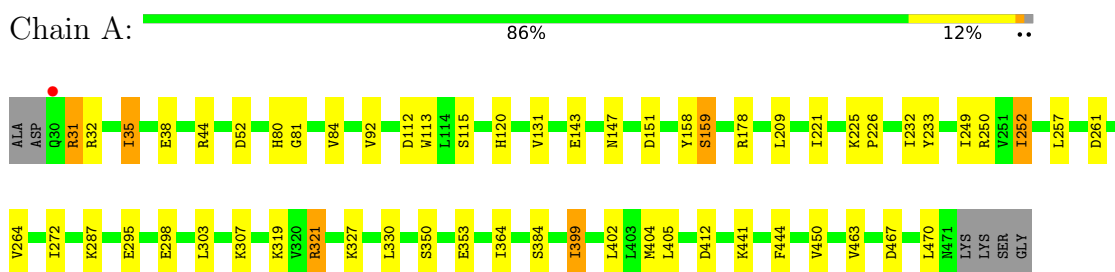
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	63	Total	O	0	0
			63	63		
8	B	50	Total	O	0	0
			50	50		
8	C	48	Total	O	0	0
			48	48		
8	D	58	Total	O	0	0
			58	58		
8	E	2	Total	O	0	0
			2	2		
8	F	2	Total	O	0	0
			2	2		
8	G	2	Total	O	0	0
			2	2		
8	H	1	Total	O	0	0
			1	1		

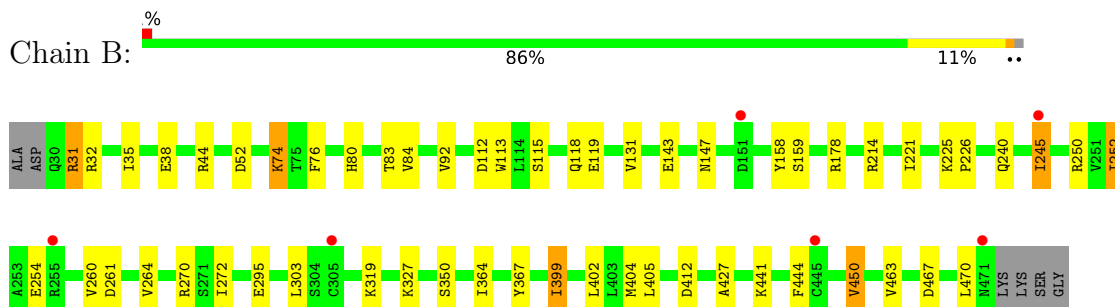
3 Residue-property plots

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.

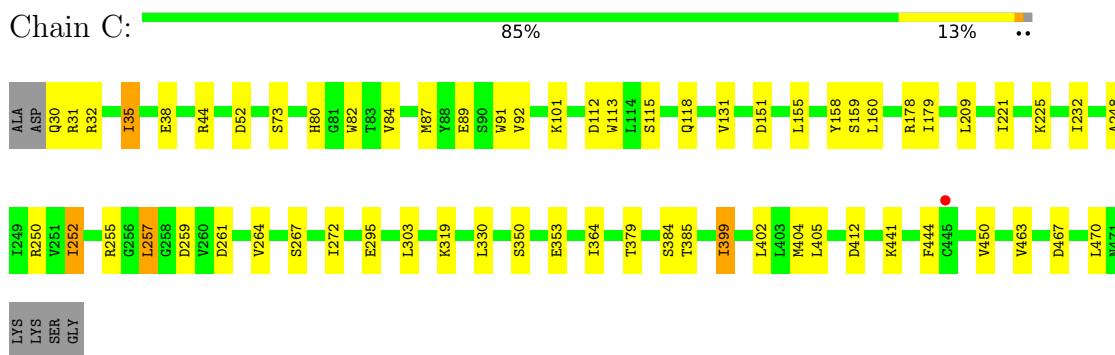
• Molecule 1: Lipoprotein lipase



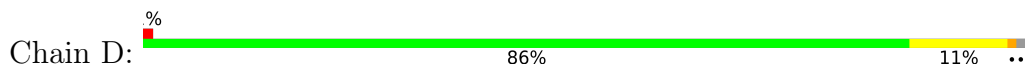
• Molecule 1: Lipoprotein lipase

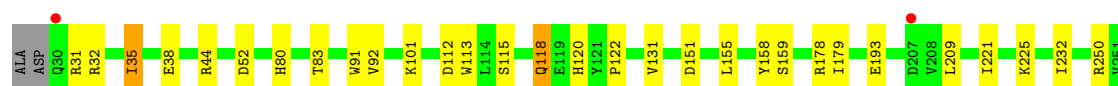


• Molecule 1: Lipoprotein lipase

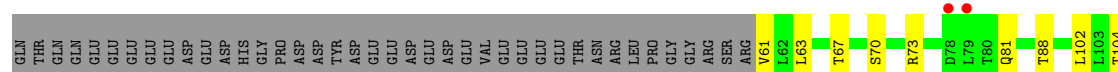


• Molecule 1: Lipoprotein lipase

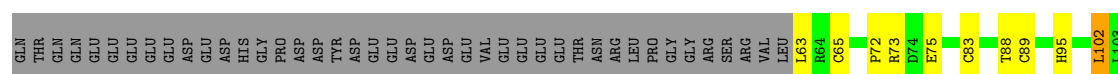




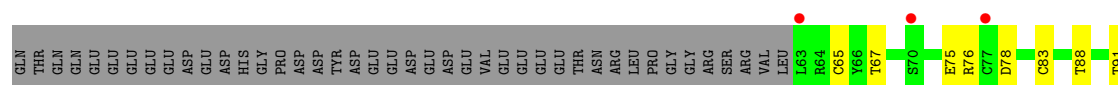
- Molecule 2: Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1



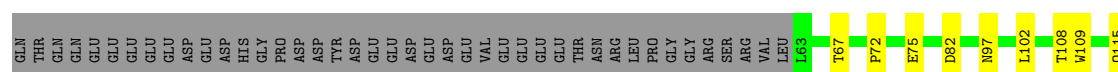
- Molecule 2: Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1



- Molecule 2: Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1



- Molecule 2: Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1



T127	M128	Q132	S133	C136	S143	SER	ARG	VAL	GLN	ASP	PRO	THR	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.43Å 191.42Å 97.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.15 – 2.81 37.15 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.15-2.81) 99.1 (37.15-2.81)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.82Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.198 , 0.233 0.202 , 0.238	Depositor DCC
R_{free} test set	3466 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtrriage
Anisotropy	0.722	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17194	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9706e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: M3D, EDO, CA, NAG, TRS

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	0.88	1/3611 (0.0%)	1.27	9/4889 (0.2%)
1	B	0.88	1/3600 (0.0%)	1.26	10/4874 (0.2%)
1	C	0.86	2/3611 (0.1%)	1.26	9/4889 (0.2%)
1	D	0.86	1/3611 (0.0%)	1.26	9/4889 (0.2%)
2	E	0.81	0/639	1.22	0/873
2	F	0.90	1/624 (0.2%)	1.18	1/852 (0.1%)
2	G	0.85	0/624	1.26	0/852
2	H	0.84	0/624	1.23	1/852 (0.1%)
All	All	0.87	6/16944 (0.0%)	1.26	39/22970 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	MET	SD-CE	6.45	1.95	1.79
1	A	159	SER	CA-C	6.29	1.58	1.52
1	C	159	SER	CA-C	6.06	1.58	1.52
1	B	159	SER	CA-C	5.98	1.58	1.52
1	D	159	SER	CA-C	5.97	1.60	1.52
2	F	139	PRO	CA-C	5.03	1.54	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97	ASN	CA-CB-CG	7.50	120.10	112.60
2	F	139	PRO	N-CA-C	7.24	117.42	110.47
1	D	151	ASP	CA-CB-CG	6.97	119.57	112.60
1	C	261	ASP	CA-CB-CG	6.88	119.47	112.60
1	D	261	ASP	CA-CB-CG	6.75	119.35	112.60
1	C	92	VAL	N-CA-CB	6.48	115.50	110.45
1	A	249	ILE	CA-C-N	6.45	128.93	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ILE	C-N-CA	6.45	128.93	120.28
1	A	92	VAL	N-CA-CB	6.35	115.40	110.45
1	B	92	VAL	N-CA-CB	6.20	115.28	110.45
1	B	112	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	52	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	254	GLU	CB-CA-C	-6.04	109.59	116.54
1	C	412	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	261	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	412	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	92	VAL	N-CA-CB	5.80	114.98	110.45
1	B	254	GLU	CA-C-N	5.69	128.17	120.38
1	B	254	GLU	C-N-CA	5.69	128.17	120.38
1	B	245	ILE	CB-CG1-CD1	5.62	125.59	113.80
1	D	31	ARG	CA-C-N	5.50	127.92	120.38
1	D	31	ARG	C-N-CA	5.50	127.92	120.38
1	D	112	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	151	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	52	ASP	CA-CB-CG	5.41	118.01	112.60
1	C	151	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	261	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	267	SER	CA-C-N	5.38	127.44	120.44
1	C	267	SER	C-N-CA	5.38	127.44	120.44
1	B	52	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	52	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	120	HIS	N-CA-C	-5.27	102.48	110.28
1	B	412	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	112	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	112	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	73	SER	N-CA-C	5.04	117.04	110.53
1	A	412	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	31	ARG	CA-C-N	5.02	127.26	120.38
1	B	31	ARG	C-N-CA	5.02	127.26	120.38

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	3518	0	3438	20	0
1	B	3511	0	3431	24	0
1	C	3518	0	3438	23	0
1	D	3518	0	3438	21	0
2	E	628	0	593	7	0
2	F	613	0	573	12	0
2	G	613	0	573	9	0
2	H	613	0	573	6	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	70	0	0	0	0
4	B	70	0	0	1	0
4	C	70	0	0	1	0
4	D	70	0	0	1	0
5	A	8	0	12	1	0
5	B	8	0	12	2	0
5	C	8	0	12	3	0
5	D	8	0	12	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	8	0	12	0	0
8	A	63	0	0	0	0
8	B	50	0	0	0	0
8	C	48	0	0	0	0
8	D	58	0	0	0	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
8	G	2	0	0	0	0
8	H	1	0	0	0	0
All	All	17194	0	16221	111	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 3.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:HB2	5:B:505:EDO:H21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ASP:HB2	2:H:109:TRP:HE1	1.51	0.75
1:B:467:ASP:HB2	2:F:109:TRP:HE1	1.55	0.70
2:H:72:PRO:HD2	2:H:75:GLU:HB2	1.75	0.68
1:D:80:HIS:HB2	5:D:505:EDO:H12	1.77	0.66
2:G:92:LEU:HD21	2:G:126:VAL:HG13	1.78	0.66
1:D:467:ASP:HB2	2:H:109:TRP:NE1	2.12	0.64
1:B:83:THR:O	1:B:118:GLN:HA	1.98	0.63
1:C:467:ASP:HB2	2:G:109:TRP:HE1	1.64	0.62
2:F:89:CYS:HB3	2:F:137:ASN:HB3	1.83	0.61
1:D:441:LYS:HG3	1:D:470:LEU:HD11	1.85	0.58
1:B:402:LEU:HB3	1:B:444:PHE:HZ	1.71	0.56
1:B:178:ARG:HD2	1:B:319:LYS:HE2	1.87	0.56
1:C:402:LEU:HB3	1:C:444:PHE:HZ	1.71	0.55
1:B:427:ALA:HB1	1:B:450:VAL:HG11	1.89	0.55
2:E:63:LEU:HD21	2:E:132:GLN:O	2.07	0.55
1:A:467:ASP:HB2	2:E:109:TRP:NE1	2.21	0.55
1:A:178:ARG:HD2	1:A:319:LYS:HE2	1.89	0.54
1:B:467:ASP:HB2	2:F:109:TRP:NE1	2.22	0.54
1:C:178:ARG:HD2	1:C:319:LYS:HE2	1.89	0.54
1:D:178:ARG:HD2	1:D:319:LYS:HE2	1.89	0.54
1:D:402:LEU:HB3	1:D:444:PHE:HZ	1.71	0.54
1:A:226:PRO:HG3	1:A:327:LYS:HD3	1.89	0.54
1:C:467:ASP:HB2	2:G:109:TRP:NE1	2.21	0.54
2:H:67:THR:HG22	2:H:109:TRP:HA	1.90	0.54
1:A:80:HIS:HB2	5:A:505:EDO:H12	1.88	0.54
1:A:402:LEU:HB3	1:A:444:PHE:HZ	1.72	0.54
4:B:504:M3D:N1	4:B:504:M3D:C14	2.71	0.53
1:A:252:ILE:HD13	1:B:252:ILE:HD13	1.89	0.53
1:C:399:ILE:HD11	1:C:402:LEU:HG	1.90	0.53
2:G:67:THR:HG22	2:G:109:TRP:HA	1.91	0.53
1:A:399:ILE:HD11	1:A:402:LEU:HG	1.90	0.53
1:A:364:ILE:HD11	1:A:405:LEU:HD21	1.91	0.52
1:C:441:LYS:HG3	1:C:470:LEU:HD11	1.91	0.52
1:B:364:ILE:HD11	1:B:405:LEU:HD21	1.91	0.52
1:B:80:HIS:HB2	5:B:505:EDO:C2	2.36	0.52
1:A:158:TYR:CD1	1:A:272:ILE:HD11	2.45	0.52
1:D:364:ILE:HD11	1:D:405:LEU:HD21	1.92	0.52
1:C:252:ILE:HD13	1:D:252:ILE:HD13	1.92	0.51
1:C:364:ILE:HD11	1:C:405:LEU:HD21	1.92	0.51
1:C:158:TYR:CG	1:C:272:ILE:HD11	2.46	0.51
1:A:307:LYS:HG2	1:A:307:LYS:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:TRP:HB2	1:C:160:LEU:HD12	1.93	0.50
1:D:399:ILE:HD11	1:D:402:LEU:HG	1.93	0.50
1:A:467:ASP:HB2	2:E:109:TRP:HE1	1.76	0.50
1:C:80:HIS:HB2	5:C:505:EDO:H11	1.94	0.50
1:B:399:ILE:HD11	1:B:402:LEU:HG	1.94	0.49
1:B:441:LYS:HG3	1:B:470:LEU:HD11	1.94	0.49
2:H:133:SER:O	2:H:136:CYS:SG	2.70	0.49
2:G:108:THR:HB	2:G:137:ASN:ND2	2.28	0.49
1:A:233:TYR:CE1	1:A:327:LYS:HD2	2.48	0.48
1:C:209:LEU:HD23	1:C:232:ILE:HB	1.95	0.48
2:H:67:THR:HA	2:H:108:THR:O	2.13	0.48
1:D:80:HIS:HB2	5:D:505:EDO:C1	2.44	0.48
1:C:89:GLU:H	5:C:505:EDO:H22	1.78	0.47
1:B:158:TYR:CG	1:B:272:ILE:HD11	2.49	0.47
1:D:91:TRP:CD2	1:D:272:ILE:HD13	2.49	0.47
1:B:404:MET:HG3	1:B:463:VAL:HG22	1.96	0.47
4:D:504:M3D:C14	4:D:504:M3D:N1	2.77	0.47
2:F:65:CYS:SG	2:F:83:CYS:SG	3.13	0.47
1:C:257:LEU:HD23	1:C:257:LEU:HA	1.76	0.47
2:E:67:THR:HG22	2:E:109:TRP:HA	1.97	0.46
1:B:240:GLN:HG3	1:B:270:ARG:HG2	1.98	0.46
1:D:158:TYR:CD1	1:D:272:ILE:HD11	2.51	0.46
2:F:95:HIS:CE1	2:F:102:LEU:HD12	2.51	0.45
1:D:113:TRP:CE3	1:D:131:VAL:HG21	2.50	0.45
1:B:158:TYR:CD1	1:B:272:ILE:HD11	2.51	0.45
1:B:245:ILE:HD11	1:B:260:VAL:HB	1.98	0.45
2:E:118:THR:HB	2:E:127:THR:HG23	1.98	0.45
2:G:65:CYS:HB2	2:G:83:CYS:SG	2.56	0.45
1:A:143:GLU:O	1:A:147:ASN:HA	2.17	0.45
1:B:143:GLU:O	1:B:147:ASN:HA	2.16	0.44
2:F:108:THR:HB	2:F:137:ASN:ND2	2.33	0.44
1:B:74:LYS:HE2	1:B:76:PHE:CZ	2.52	0.44
1:C:35:ILE:H	1:C:35:ILE:HG13	1.60	0.44
1:D:209:LEU:HD23	1:D:232:ILE:HB	2.00	0.44
1:D:404:MET:HG3	1:D:463:VAL:HG22	1.99	0.44
1:A:81:GLY:HA3	1:A:159:SER:HB3	1.99	0.43
1:A:113:TRP:CE3	1:A:131:VAL:HG21	2.53	0.43
1:D:120:HIS:CD2	1:D:122:PRO:HD2	2.53	0.43
1:B:367:TYR:HB3	2:F:121:VAL:HG21	2.01	0.43
1:C:113:TRP:CE3	1:C:131:VAL:HG21	2.52	0.43
4:C:504:M3D:C14	4:C:504:M3D:N1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:TYR:CB	2:F:121:VAL:HG21	2.49	0.43
1:C:91:TRP:CD2	1:C:272:ILE:HD13	2.54	0.43
1:C:91:TRP:HZ2	5:C:505:EDO:H11	1.84	0.43
1:A:321:ARG:CB	1:A:321:ARG:HH21	2.32	0.43
1:A:35:ILE:H	1:A:35:ILE:HG13	1.61	0.43
1:B:113:TRP:CE3	1:B:131:VAL:HG21	2.54	0.42
2:G:117:ILE:HG13	2:G:118:THR:N	2.34	0.42
1:A:441:LYS:HG3	1:A:470:LEU:HD11	2.01	0.42
1:C:404:MET:HG3	1:C:463:VAL:HG22	2.00	0.42
2:F:72:PRO:HG2	2:F:75:GLU:HB2	2.01	0.42
1:C:250:ARG:NH2	1:C:259:ASP:HA	2.34	0.42
2:E:117:ILE:HG13	2:E:118:THR:N	2.35	0.42
2:G:65:CYS:HB3	2:G:110:CYS:SG	2.60	0.42
1:B:226:PRO:HG3	1:B:327:LYS:HD3	2.02	0.42
2:G:117:ILE:HG13	2:G:118:THR:H	1.84	0.42
1:A:404:MET:HG3	1:A:463:VAL:HG22	2.02	0.42
1:D:83:THR:O	1:D:118:GLN:HA	2.20	0.41
2:E:73:ARG:HB2	2:E:104:THR:HB	2.02	0.41
1:C:248:ALA:HB1	1:D:252:ILE:HD12	2.02	0.41
2:F:73:ARG:HB2	2:F:104:THR:HB	2.02	0.41
1:A:209:LEU:HD23	1:A:232:ILE:HB	2.02	0.41
1:D:155:LEU:HB2	1:D:179:ILE:HG12	2.01	0.41
2:F:138:VAL:HG13	2:F:143:SER:HB2	2.02	0.41
1:C:158:TYR:CD1	1:C:272:ILE:HD11	2.56	0.41
1:D:257:LEU:HD23	1:D:257:LEU:HA	1.88	0.41
1:B:367:TYR:HB3	2:F:121:VAL:CG2	2.51	0.40
1:C:155:LEU:HB2	1:C:179:ILE:HG12	2.02	0.40
1:D:35:ILE:H	1:D:35:ILE:HG13	1.61	0.40

There are no symmetry-related clashes.

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	441/448 (98%)	423 (96%)	17 (4%)	1 (0%)	43	71
1	B	440/448 (98%)	420 (96%)	20 (4%)	0	100	100
1	C	441/448 (98%)	423 (96%)	18 (4%)	0	100	100
1	D	441/448 (98%)	419 (95%)	22 (5%)	0	100	100
2	E	81/131 (62%)	73 (90%)	7 (9%)	1 (1%)	10	31
2	F	79/131 (60%)	71 (90%)	8 (10%)	0	100	100
2	G	79/131 (60%)	68 (86%)	10 (13%)	1 (1%)	9	29
2	H	79/131 (60%)	73 (92%)	6 (8%)	0	100	100
All	All	2081/2316 (90%)	1970 (95%)	108 (5%)	3 (0%)	48	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
2	G	137	ASN
2	E	70	SER

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	386/389 (99%)	362 (94%)	24 (6%)	16	44
1	B	385/389 (99%)	365 (95%)	20 (5%)	21	51
1	C	386/389 (99%)	360 (93%)	26 (7%)	15	40
1	D	386/389 (99%)	364 (94%)	22 (6%)	18	47
2	E	78/122 (64%)	68 (87%)	10 (13%)	4	14
2	F	76/122 (62%)	68 (90%)	8 (10%)	6	21
2	G	76/122 (62%)	66 (87%)	10 (13%)	4	13
2	H	76/122 (62%)	69 (91%)	7 (9%)	8	26
All	All	1849/2044 (90%)	1722 (93%)	127 (7%)	14	39

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	32	ARG
1	A	35	ILE
1	A	38	GLU
1	A	44	ARG
1	A	84	VAL
1	A	115	SER
1	A	221	ILE
1	A	225	LYS
1	A	250	ARG
1	A	252	ILE
1	A	257	LEU
1	A	264	VAL
1	A	287	LYS
1	A	295	GLU
1	A	298	GLU
1	A	303	LEU
1	A	321	ARG
1	A	330	LEU
1	A	350	SER
1	A	353	GLU
1	A	384	SER
1	A	399	ILE
1	A	450	VAL
1	B	31	ARG
1	B	32	ARG
1	B	35	ILE
1	B	38	GLU
1	B	44	ARG
1	B	74	LYS
1	B	84	VAL
1	B	115	SER
1	B	119	GLU
1	B	214	ARG
1	B	221	ILE
1	B	225	LYS
1	B	250	ARG
1	B	252	ILE
1	B	264	VAL
1	B	295	GLU
1	B	303	LEU
1	B	350	SER

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Mol	Chain	Res	Type
1	B	399	ILE
1	B	450	VAL
1	C	30	GLN
1	C	31	ARG
1	C	32	ARG
1	C	35	ILE
1	C	38	GLU
1	C	44	ARG
1	C	84	VAL
1	C	101	LYS
1	C	115	SER
1	C	118	GLN
1	C	221	ILE
1	C	225	LYS
1	C	252	ILE
1	C	255	ARG
1	C	257	LEU
1	C	264	VAL
1	C	295	GLU
1	C	303	LEU
1	C	330	LEU
1	C	350	SER
1	C	353	GLU
1	C	379	THR
1	C	384	SER
1	C	385	THR
1	C	399	ILE
1	C	450	VAL
1	D	32	ARG
1	D	35	ILE
1	D	38	GLU
1	D	44	ARG
1	D	101	LYS
1	D	115	SER
1	D	118	GLN
1	D	193	GLU
1	D	221	ILE
1	D	225	LYS
1	D	250	ARG
1	D	252	ILE
1	D	254	GLU
1	D	264	VAL

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Mol	Chain	Res	Type
1	D	295	GLU
1	D	303	LEU
1	D	330	LEU
1	D	350	SER
1	D	353	GLU
1	D	384	SER
1	D	399	ILE
1	D	450	VAL
2	E	61	VAL
2	E	81	GLN
2	E	88	THR
2	E	102	LEU
2	E	108	THR
2	E	115	GLN
2	E	127	THR
2	E	128	MET
2	E	132	GLN
2	E	133	SER
2	F	63	LEU
2	F	88	THR
2	F	102	LEU
2	F	105	THR
2	F	117	ILE
2	F	121	VAL
2	F	128	MET
2	F	133	SER
2	G	75	GLU
2	G	76	ARG
2	G	78	ASP
2	G	88	THR
2	G	91	THR
2	G	102	LEU
2	G	115	GLN
2	G	127	THR
2	G	128	MET
2	G	133	SER
2	H	82	ASP
2	H	102	LEU
2	H	115	GLN
2	H	127	THR
2	H	128	MET
2	H	132	GLN

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Mol	Chain	Res	Type
2	H	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	120	HIS
1	A	177	ASN
1	A	335	GLN
1	A	429	GLN
1	B	177	ASN
1	B	335	GLN
1	B	429	GLN
1	B	454	GLN
1	B	466	HIS
1	C	177	ASN
1	C	281	ASN
1	C	335	GLN
1	C	375	ASN
1	C	429	GLN
1	C	454	GLN
1	C	466	HIS
1	D	177	ASN
1	D	335	GLN
1	D	429	GLN
1	D	454	GLN
1	D	466	HIS
2	E	125	GLN
2	F	125	GLN
2	F	142	GLN
2	G	106	HIS
2	G	125	GLN
2	H	106	HIS
2	H	142	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	M3D	C	503	-	39,39,39	1.19	3 (7%)	49,54,54	1.31	7 (14%)
4	M3D	B	503	-	39,39,39	1.44	7 (17%)	49,54,54	1.19	7 (14%)
5	EDO	D	506	-	3,3,3	0.69	0	2,2,2	0.29	0
4	M3D	A	504	-	39,39,39	1.35	7 (17%)	49,54,54	1.37	10 (20%)
3	NAG	B	502	1	14,14,15	0.51	0	17,19,21	1.28	2 (11%)
3	NAG	A	501	1	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
3	NAG	C	501	1	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
3	NAG	D	501	1	14,14,15	0.36	0	17,19,21	0.71	1 (5%)
5	EDO	C	505	-	3,3,3	0.91	0	2,2,2	0.44	0
4	M3D	D	503	-	39,39,39	1.41	8 (20%)	49,54,54	1.16	3 (6%)
5	EDO	D	505	-	3,3,3	0.64	0	2,2,2	0.26	0
5	EDO	B	505	-	3,3,3	0.54	0	2,2,2	0.44	0
4	M3D	A	503	-	39,39,39	1.31	6 (15%)	49,54,54	1.11	3 (6%)
4	M3D	B	504	-	39,39,39	1.41	6 (15%)	49,54,54	2.05	14 (28%)
4	M3D	D	504	-	39,39,39	1.29	4 (10%)	49,54,54	1.58	11 (22%)
4	M3D	C	504	-	39,39,39	1.45	7 (17%)	49,54,54	1.75	13 (26%)
5	EDO	C	506	-	3,3,3	0.45	0	2,2,2	0.55	0
5	EDO	B	506	-	3,3,3	0.57	0	2,2,2	0.37	0
3	NAG	A	502	1	14,14,15	0.46	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	502	1	14,14,15	0.48	0	17,19,21	1.40	2 (11%)
5	EDO	A	506	-	3,3,3	0.42	0	2,2,2	0.71	0
5	EDO	A	505	-	3,3,3	0.58	0	2,2,2	0.59	0
7	TRS	B	507	-	7,7,7	0.42	0	9,9,9	0.43	0
3	NAG	B	501	1	14,14,15	0.29	0	17,19,21	0.68	0
3	NAG	D	502	1	14,14,15	0.47	0	17,19,21	1.16	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	M3D	C	503	-	-	4/14/36/36	0/5/5/5
4	M3D	B	503	-	-	0/14/36/36	0/5/5/5
5	EDO	D	506	-	-	0/1/1/1	-
4	M3D	A	504	-	-	0/14/36/36	0/5/5/5
3	NAG	B	502	1	-	1/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1
3	NAG	D	501	1	-	0/6/23/26	0/1/1/1
5	EDO	C	505	-	-	1/1/1/1	-
4	M3D	D	503	-	-	1/14/36/36	0/5/5/5
5	EDO	D	505	-	-	0/1/1/1	-
5	EDO	B	505	-	-	0/1/1/1	-
4	M3D	A	503	-	-	0/14/36/36	0/5/5/5
4	M3D	B	504	-	-	4/14/36/36	0/5/5/5
4	M3D	D	504	-	-	3/14/36/36	0/5/5/5
4	M3D	C	504	-	-	4/14/36/36	0/5/5/5
5	EDO	C	506	-	-	0/1/1/1	-
5	EDO	B	506	-	-	0/1/1/1	-
3	NAG	A	502	1	-	1/6/23/26	0/1/1/1
3	NAG	C	502	1	-	0/6/23/26	0/1/1/1
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-
7	TRS	B	507	-	-	1/9/9/9	-
3	NAG	B	501	1	-	0/6/23/26	0/1/1/1
3	NAG	D	502	1	-	0/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	M3D	O1-C10	-3.38	1.34	1.39
4	B	504	M3D	C9-C2	3.25	1.52	1.48
4	D	503	M3D	O1-C3	-3.22	1.35	1.39
4	B	504	M3D	C21-C20	3.01	1.44	1.39
4	B	503	M3D	O1-C10	-2.94	1.35	1.39
4	A	504	M3D	O1-C10	-2.84	1.35	1.39
4	A	504	M3D	C14-C9	2.77	1.44	1.39
4	D	504	M3D	C9-C2	2.76	1.51	1.48
4	B	503	M3D	O1-C3	-2.71	1.35	1.39
4	D	504	M3D	C21-C16	2.70	1.44	1.39
4	C	504	M3D	C6-C5	2.69	1.43	1.38
4	B	504	M3D	C6-C5	2.61	1.43	1.38
4	D	503	M3D	C18-C19	2.60	1.44	1.39
4	B	503	M3D	C13-C12	2.52	1.44	1.39
4	C	504	M3D	C14-C13	2.52	1.42	1.38
4	B	503	M3D	C14-C13	2.51	1.42	1.38
4	A	504	M3D	C14-C13	2.51	1.42	1.38
4	D	503	M3D	C21-C16	2.48	1.44	1.39
4	A	504	M3D	O1-C3	-2.47	1.36	1.39
4	D	503	M3D	C17-C16	2.47	1.44	1.39
4	C	503	M3D	C21-C16	2.45	1.44	1.39
4	A	503	M3D	O1-C3	-2.44	1.36	1.39
4	A	503	M3D	C18-C17	2.43	1.42	1.38
4	C	503	M3D	O1-C3	-2.41	1.36	1.39
4	A	503	M3D	C20-C28	2.40	1.47	1.44
4	C	504	M3D	C21-C20	2.38	1.43	1.39
4	A	504	M3D	C13-C12	2.36	1.44	1.39
4	C	504	M3D	C9-C2	2.35	1.51	1.48
4	A	504	M3D	C6-C5	2.35	1.42	1.38
4	D	503	M3D	C18-C17	2.34	1.42	1.38
4	C	504	M3D	C14-C9	2.32	1.43	1.39
4	B	503	M3D	C6-C5	2.32	1.42	1.38
4	B	503	M3D	C14-C9	2.31	1.43	1.39
4	A	503	M3D	C14-C13	2.31	1.42	1.38
4	B	504	M3D	C21-C16	2.29	1.43	1.39
4	C	504	M3D	C21-C16	2.28	1.43	1.39
4	A	503	M3D	O1-C10	-2.28	1.36	1.39
4	D	503	M3D	C14-C13	2.28	1.42	1.38
4	B	503	M3D	C21-C16	2.23	1.43	1.39
4	D	504	M3D	O1-C3	-2.21	1.36	1.39
4	B	504	M3D	C14-C13	2.14	1.42	1.38
4	A	504	M3D	C9-C2	2.11	1.50	1.48
4	A	503	M3D	C21-C16	2.08	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	M3D	C20-C28	2.07	1.47	1.44
4	D	503	M3D	C6-C5	2.05	1.42	1.38
4	D	504	M3D	C20-C28	2.04	1.47	1.44
4	D	503	M3D	C9-C10	2.03	1.44	1.40
4	B	504	M3D	C9-C10	2.02	1.44	1.40

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	M3D	C17-C16-C12	-5.61	111.57	121.25
4	C	504	M3D	C22-N1-C15	5.02	133.47	122.47
4	B	504	M3D	C21-C16-C12	4.99	129.21	120.84
3	C	502	NAG	C1-O5-C5	4.21	117.83	112.19
4	B	504	M3D	C27-N2-C24	4.20	117.89	108.84
3	B	502	NAG	C1-O5-C5	3.95	117.48	112.19
4	C	504	M3D	C26-C27-N2	3.93	116.09	110.12
4	D	503	M3D	C19-C20-C28	3.92	123.28	119.57
4	D	504	M3D	C23-C22-N1	3.81	118.92	111.56
4	D	504	M3D	C22-N1-C15	3.80	130.80	122.47
4	C	503	M3D	C25-C24-N2	3.73	115.79	110.12
4	B	504	M3D	C23-N2-C27	3.67	121.02	111.24
4	B	504	M3D	C22-N1-C15	3.65	130.46	122.47
3	A	502	NAG	C1-O5-C5	3.60	117.00	112.19
4	B	504	M3D	O2-C15-C2	3.41	126.92	121.61
4	C	504	M3D	C23-C22-N1	3.30	117.92	111.56
3	D	502	NAG	C1-O5-C5	3.27	116.57	112.19
4	D	504	M3D	C17-C16-C12	-3.17	115.79	121.25
4	C	504	M3D	C17-C16-C12	-3.00	116.07	121.25
4	B	504	M3D	O2-C15-N1	-2.96	118.00	123.35
3	C	502	NAG	C1-C2-N2	-2.87	105.91	110.43
4	C	503	M3D	C27-N2-C24	2.82	114.92	108.84
4	A	503	M3D	O4-C26-C27	-2.80	105.73	111.77
4	C	504	M3D	C25-C24-N2	2.78	114.34	110.12
4	C	504	M3D	C21-C16-C12	2.76	125.47	120.84
4	D	504	M3D	C26-C27-N2	2.64	114.14	110.12
4	A	504	M3D	C22-N1-C15	2.62	128.21	122.47
4	D	504	M3D	C22-C23-N2	2.60	119.19	112.84
4	C	503	M3D	O4-C26-C27	-2.59	106.19	111.77
4	B	503	M3D	C22-N1-C15	2.57	128.11	122.47
4	A	503	M3D	C26-C27-N2	-2.56	106.23	110.12
4	B	504	M3D	C14-C9-C10	-2.46	114.97	118.21
4	C	503	M3D	O4-C25-C24	-2.46	106.47	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	504	M3D	C17-C18-C19	-2.46	118.04	120.50
4	A	504	M3D	C25-C24-N2	2.45	113.85	110.12
4	D	504	M3D	O2-C15-C2	2.38	125.32	121.61
4	B	504	M3D	O3-C19-C20	2.38	125.50	119.28
4	B	504	M3D	C26-O4-C25	2.35	117.49	109.88
3	D	501	NAG	C1-O5-C5	2.34	115.32	112.19
4	A	504	M3D	C8-C3-C4	2.33	122.18	118.18
4	D	504	M3D	O2-C15-N1	-2.31	119.18	123.35
4	D	504	M3D	C27-N2-C24	2.31	113.81	108.84
4	C	503	M3D	C19-C20-C28	2.30	121.75	119.57
3	A	501	NAG	C1-O5-C5	2.30	115.26	112.19
4	C	503	M3D	C22-N1-C15	2.29	127.50	122.47
4	B	503	M3D	C8-C3-C4	2.28	122.10	118.18
4	C	504	M3D	C27-N2-C24	2.28	113.74	108.84
4	A	504	M3D	C17-C18-C19	-2.27	118.23	120.50
4	A	504	M3D	O4-C25-C24	-2.21	107.01	111.77
4	B	503	M3D	C10-O1-C3	2.20	122.96	114.11
4	C	504	M3D	C14-C9-C10	-2.20	115.32	118.21
4	C	503	M3D	C26-C27-N2	2.20	113.46	110.12
3	A	502	NAG	C1-C2-N2	-2.20	106.97	110.43
4	B	504	M3D	O1-C10-C9	2.20	123.27	120.39
4	B	504	M3D	C22-C23-N2	2.19	118.19	112.84
4	D	504	M3D	C26-O4-C25	2.18	116.94	109.88
4	D	504	M3D	C9-C2-C15	2.17	121.69	114.63
4	B	503	M3D	C26-C27-N2	-2.17	106.83	110.12
4	D	504	M3D	C21-C16-C12	2.17	124.47	120.84
4	A	504	M3D	C17-C16-C12	-2.13	117.58	121.25
4	A	504	M3D	C11-C12-C16	-2.13	117.27	120.84
4	D	503	M3D	C26-O4-C25	2.12	116.74	109.88
4	C	504	M3D	C22-C23-N2	2.12	118.02	112.84
4	B	503	M3D	O4-C26-C27	-2.11	107.22	111.77
4	C	504	M3D	O1-C10-C9	2.11	123.16	120.39
4	D	503	M3D	O2-C15-C2	2.11	124.89	121.61
3	C	501	NAG	C1-O5-C5	2.09	114.99	112.19
4	A	504	M3D	O4-C26-C27	-2.09	107.27	111.77
4	A	504	M3D	C27-N2-C24	2.09	113.34	108.84
4	B	503	M3D	C19-C20-C28	2.09	121.55	119.57
4	A	503	M3D	C22-N1-C15	2.07	127.01	122.47
3	B	502	NAG	C1-C2-N2	-2.06	107.19	110.43
3	D	502	NAG	O4-C4-C5	2.05	114.38	109.32
4	C	504	M3D	C9-C2-C15	2.04	121.27	114.63
4	C	504	M3D	C6-C7-C8	-2.02	117.74	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	M3D	C5-C4-C1	2.02	121.12	117.53
4	A	504	M3D	C23-N2-C27	2.02	116.62	111.24
4	B	504	M3D	O3-C19-C18	-2.01	113.97	119.36
4	B	504	M3D	C16-C21-C20	-2.01	118.81	121.31

There are no chirality outliers.

All (20) torsion outliers are listed below:

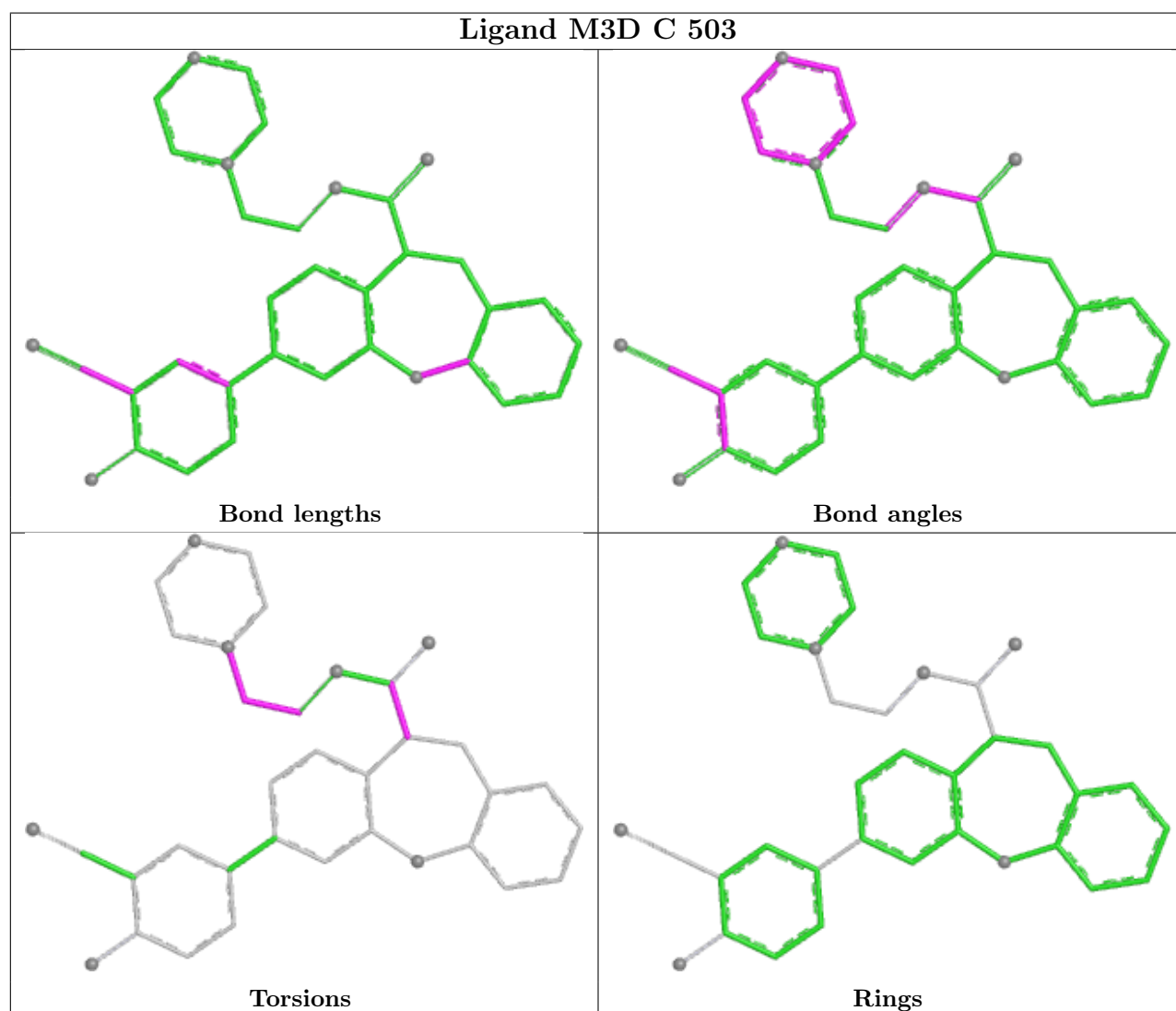
Mol	Chain	Res	Type	Atoms
4	B	504	M3D	C19-C20-C28-N3
4	B	504	M3D	C22-C23-N2-C27
4	C	503	M3D	O2-C15-C2-C1
4	C	503	M3D	C22-C23-N2-C27
4	C	504	M3D	C19-C20-C28-N3
4	C	504	M3D	C23-C22-N1-C15
4	D	504	M3D	C23-C22-N1-C15
4	B	504	M3D	C23-C22-N1-C15
4	B	504	M3D	C22-C23-N2-C24
5	C	505	EDO	O1-C1-C2-O2
4	C	503	M3D	N1-C22-C23-N2
3	A	502	NAG	C1-C2-N2-C7
3	B	502	NAG	C1-C2-N2-C7
4	C	503	M3D	N1-C15-C2-C1
4	C	504	M3D	N1-C15-C2-C1
4	D	503	M3D	C19-C20-C28-N3
4	D	504	M3D	N1-C15-C2-C1
4	D	504	M3D	C19-C20-C28-N3
7	B	507	TRS	C2-C-C3-O3
4	C	504	M3D	C22-C23-N2-C24

There are no ring outliers.

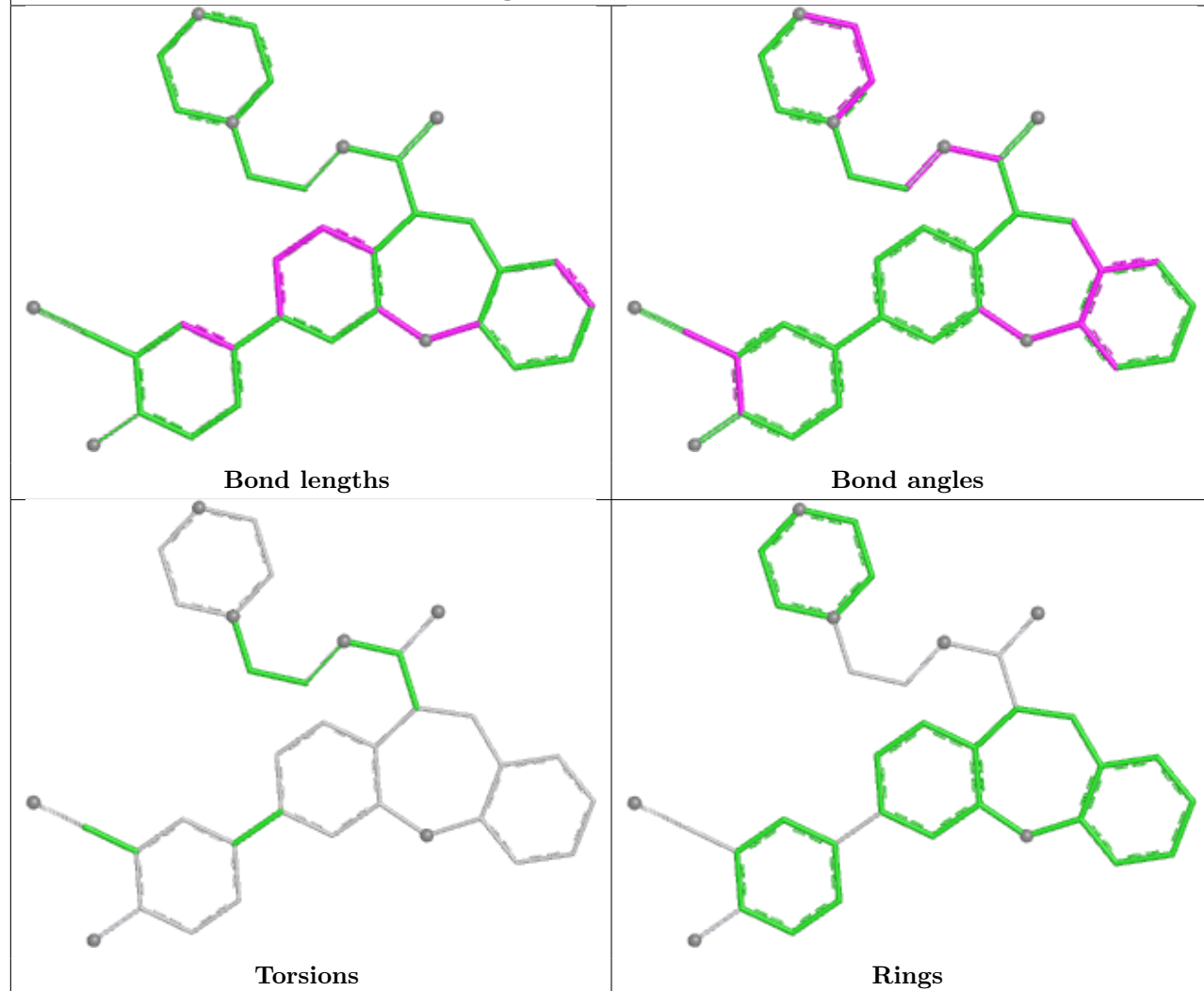
7 monomers are involved in 11 short contacts:

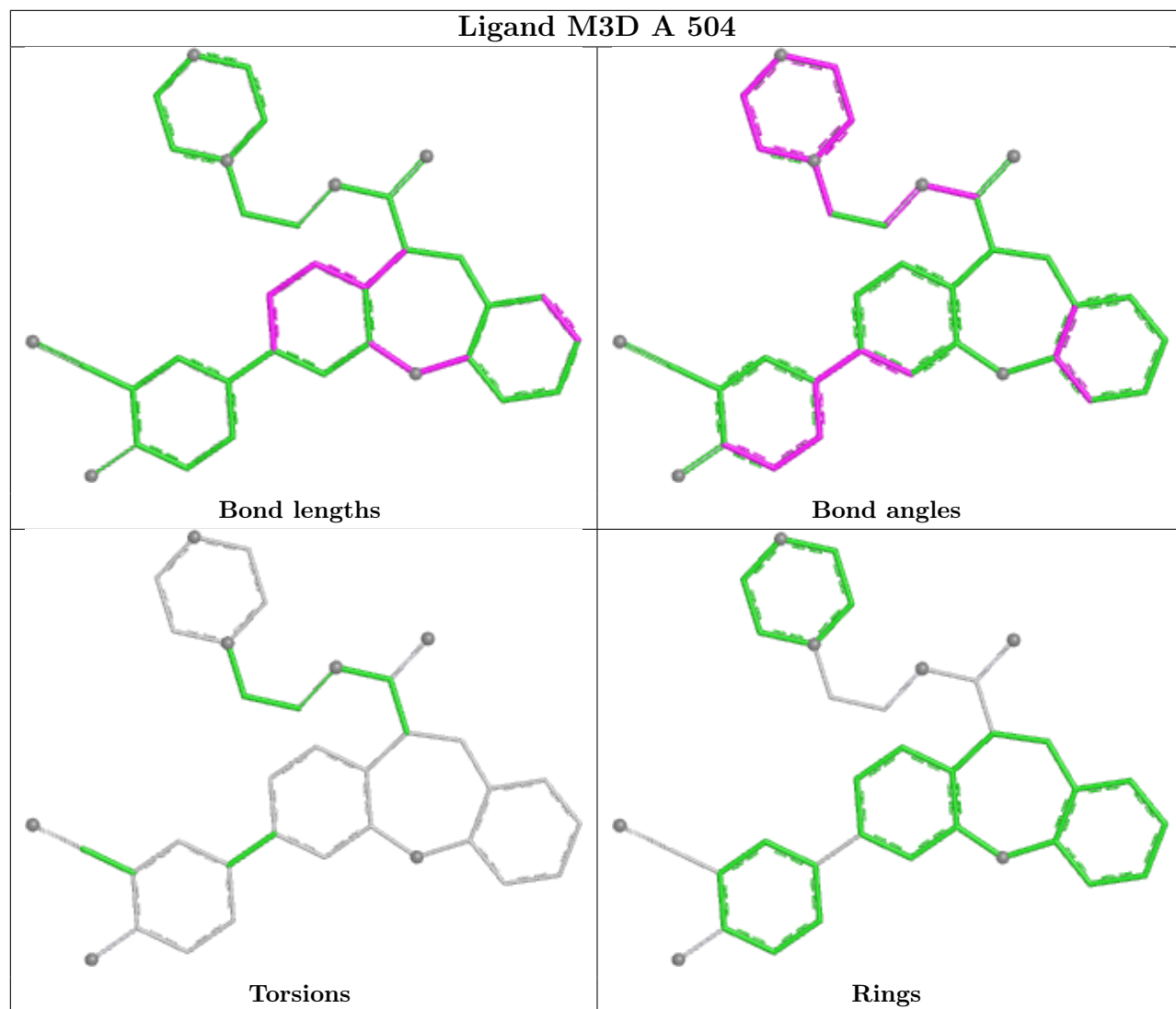
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	505	EDO	3	0
5	D	505	EDO	2	0
5	B	505	EDO	2	0
4	B	504	M3D	1	0
4	D	504	M3D	1	0
4	C	504	M3D	1	0
5	A	505	EDO	1	0

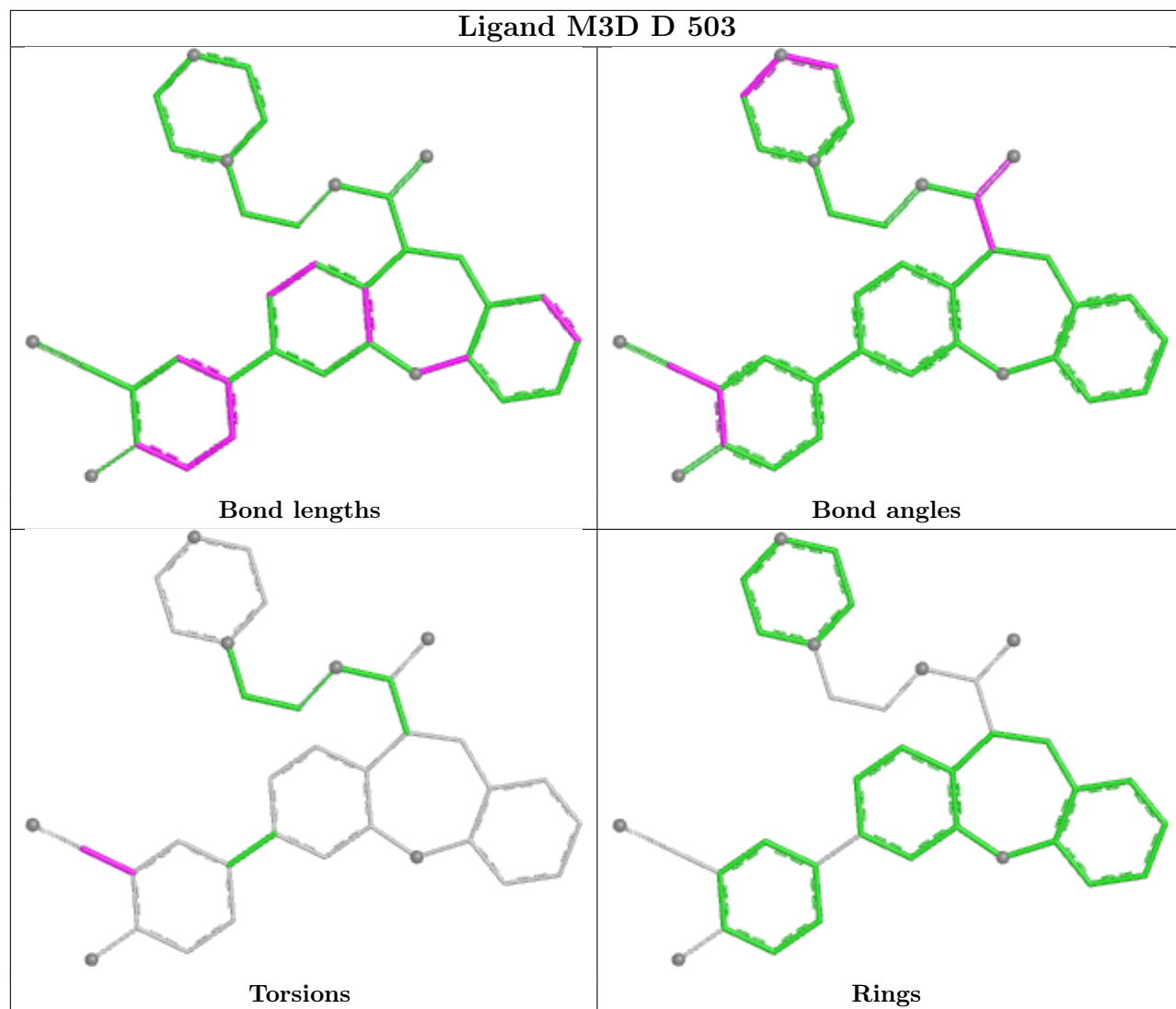
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

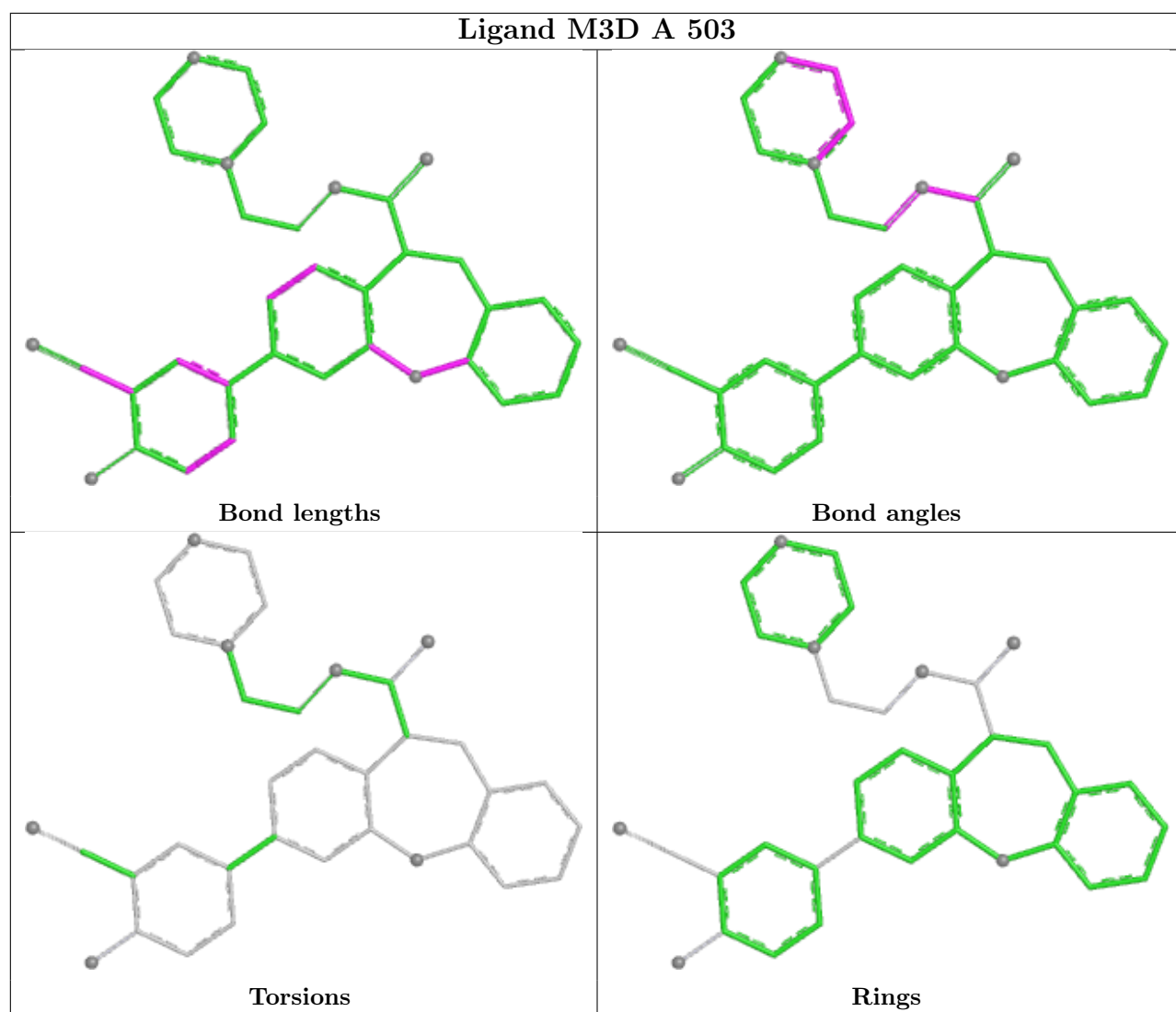


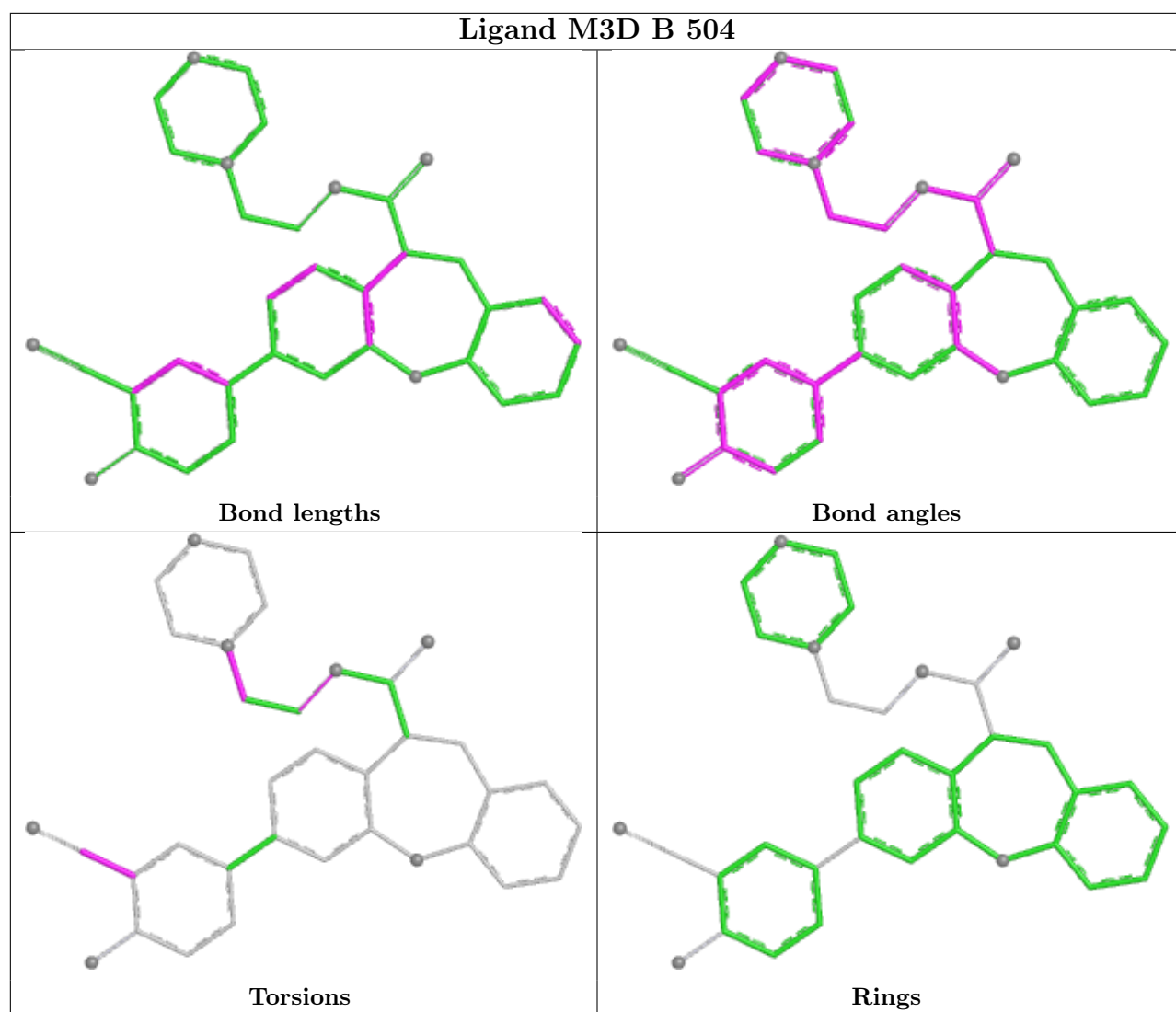
Ligand M3D B 503

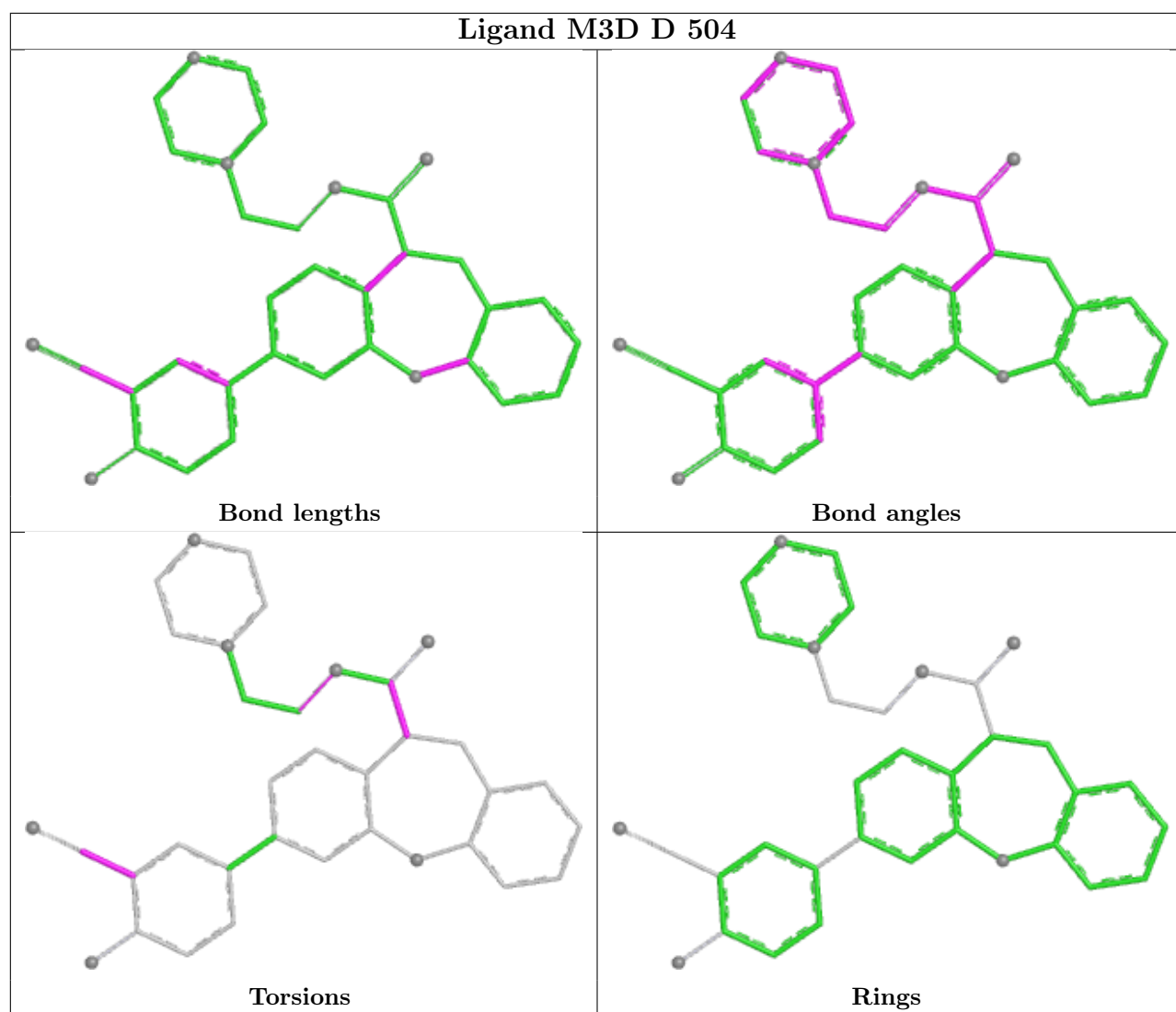


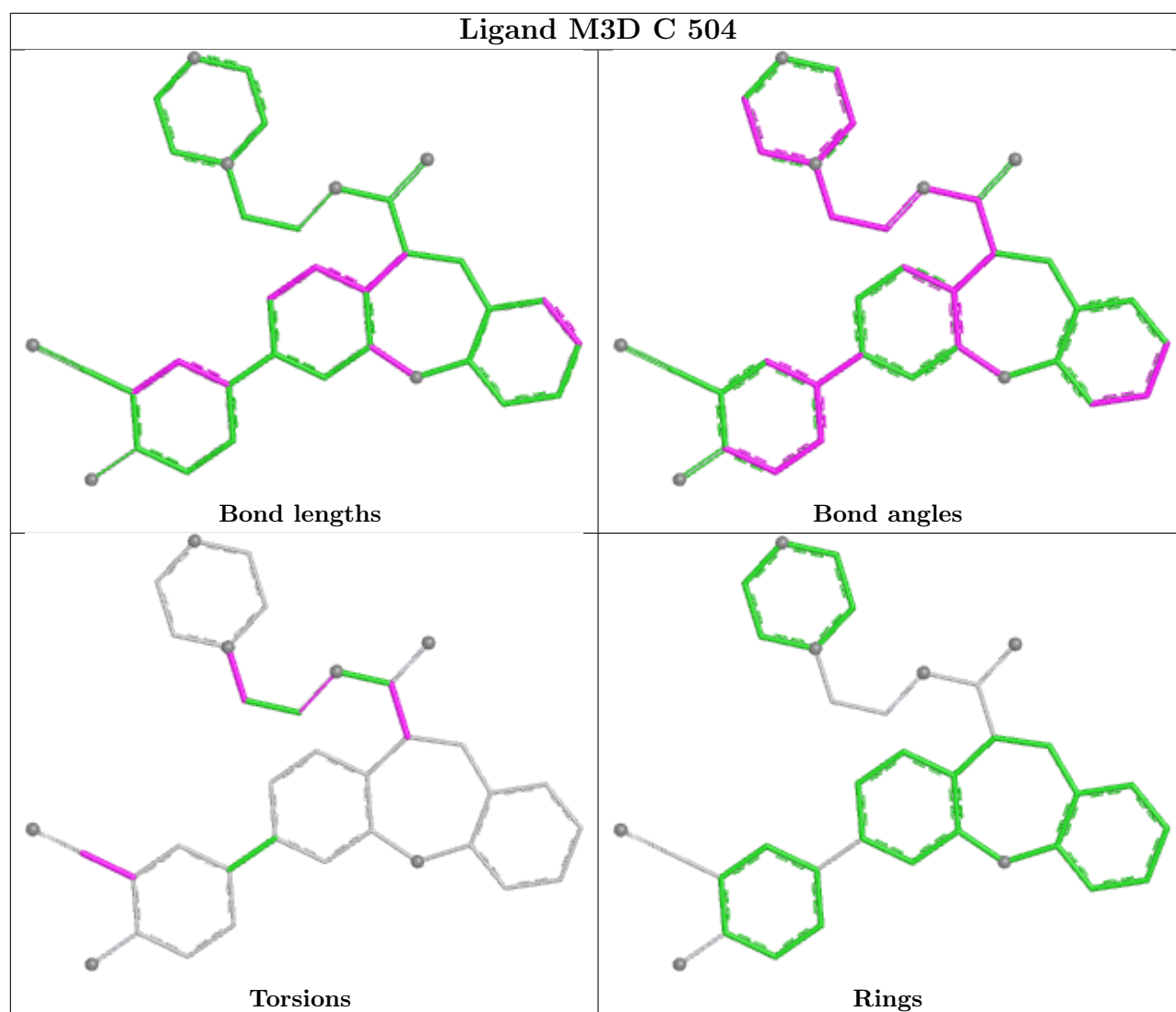












5.7 Other polymers [i](#)

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	442/448 (98%)	-0.15	1 (0%) 91 89	39, 60, 94, 128	1 (0%)
1	B	442/448 (98%)	-0.11	6 (1%) 73 64	42, 61, 94, 124	0
1	C	442/448 (98%)	-0.15	1 (0%) 91 89	39, 60, 94, 122	1 (0%)
1	D	442/448 (98%)	-0.13	4 (0%) 81 74	34, 59, 93, 131	1 (0%)
2	E	83/131 (63%)	0.40	3 (3%) 46 37	58, 86, 106, 118	0
2	F	81/131 (61%)	0.57	1 (1%) 76 68	78, 101, 122, 133	0
2	G	81/131 (61%)	0.54	4 (4%) 35 27	66, 97, 121, 126	0
2	H	81/131 (61%)	0.29	0 100 100	57, 88, 109, 116	0
All	All	2094/2316 (90%)	-0.04	20 (0%) 79 72	34, 63, 106, 133	3 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	143	SER	3.7
1	D	471	ASN	2.7
1	A	30	GLN	2.7
2	G	70	SER	2.7
1	C	445	CYS	2.7
1	D	207	ASP	2.7
1	B	445	CYS	2.4
2	E	143	SER	2.3
1	B	471	ASN	2.3
2	G	77	CYS	2.3
1	D	302	CYS	2.2
2	G	63	LEU	2.2
1	B	245	ILE	2.1
1	B	151	ASP	2.1
1	B	305	CYS	2.1
1	D	30	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	114	CYS	2.1
2	E	78	ASP	2.1
2	E	79	LEU	2.1
1	B	255	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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.

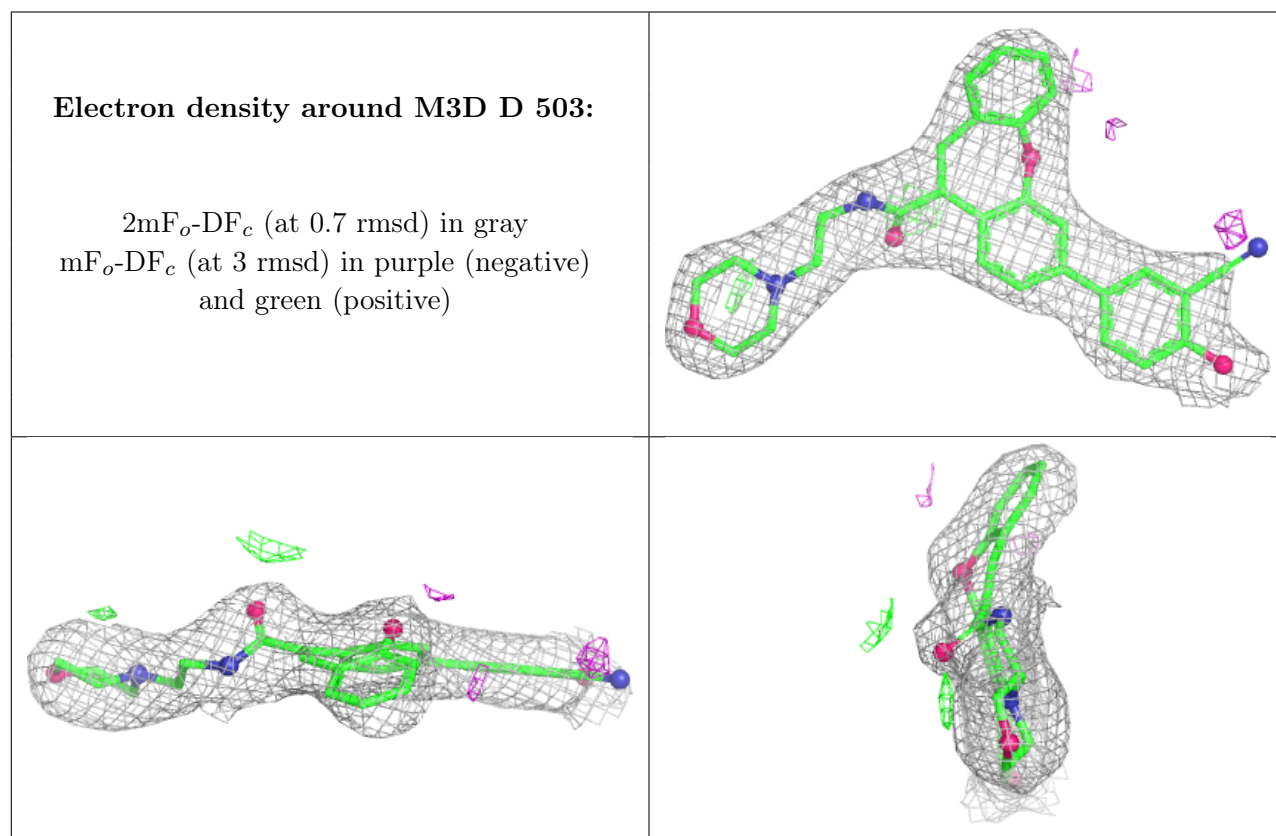
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	501	14/15	0.58	0.16	87,90,95,97	0
7	TRS	B	507	8/8	0.61	0.14	81,88,95,95	0
3	NAG	B	501	14/15	0.65	0.13	96,100,104,104	0
3	NAG	A	501	14/15	0.70	0.14	109,112,116,116	0
3	NAG	C	501	14/15	0.70	0.11	96,104,107,107	0
3	NAG	B	502	14/15	0.72	0.15	66,85,97,101	0
3	NAG	C	502	14/15	0.77	0.13	65,78,94,97	0
3	NAG	D	502	14/15	0.78	0.12	62,66,74,79	0
3	NAG	A	502	14/15	0.78	0.11	65,78,88,90	0
5	EDO	D	506	4/4	0.89	0.12	58,63,64,64	0
5	EDO	A	506	4/4	0.89	0.13	57,59,59,59	0
5	EDO	A	505	4/4	0.91	0.14	53,54,55,58	0
5	EDO	C	505	4/4	0.93	0.09	44,48,57,61	0
5	EDO	C	506	4/4	0.93	0.11	59,62,63,66	0
5	EDO	B	505	4/4	0.94	0.11	54,57,58,58	0
5	EDO	B	506	4/4	0.94	0.11	53,55,56,59	0
4	M3D	D	503	35/35	0.94	0.09	34,43,59,67	0
4	M3D	D	504	35/35	0.94	0.09	43,53,63,63	0
5	EDO	D	505	4/4	0.94	0.12	60,65,70,72	0

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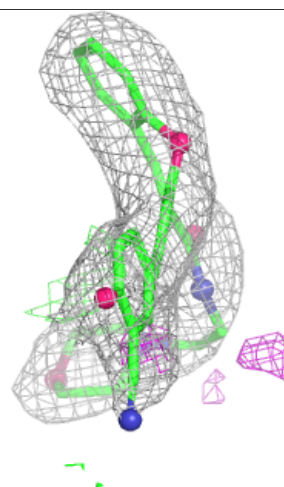
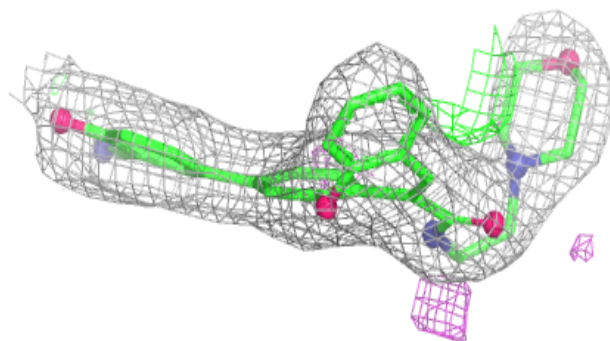
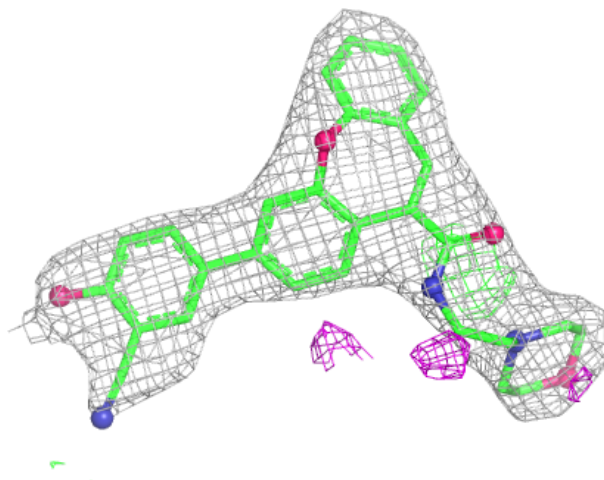
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	M3D	B	503	35/35	0.94	0.09	33,44,56,66	0
4	M3D	B	504	35/35	0.94	0.09	45,53,60,65	0
4	M3D	C	503	35/35	0.95	0.08	38,46,56,59	0
4	M3D	A	503	35/35	0.95	0.09	37,45,59,60	0
4	M3D	A	504	35/35	0.95	0.08	47,53,60,62	0
4	M3D	C	504	35/35	0.96	0.07	38,50,58,66	0
6	CA	A	507	1/1	0.99	0.03	62,62,62,62	0
6	CA	C	507	1/1	1.00	0.02	60,60,60,60	0
6	CA	D	507	1/1	1.00	0.01	52,52,52,52	0
6	CA	B	508	1/1	1.00	0.03	57,57,57,57	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.



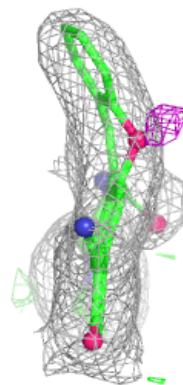
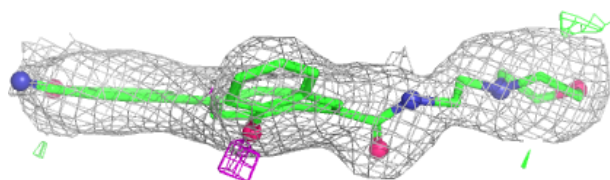
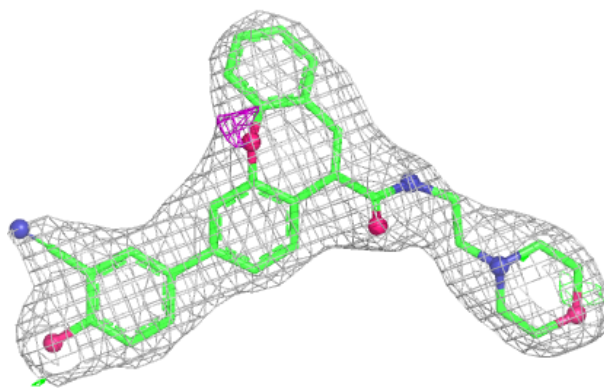
Electron density around M3D D 504:

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



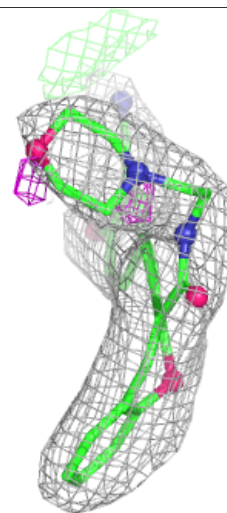
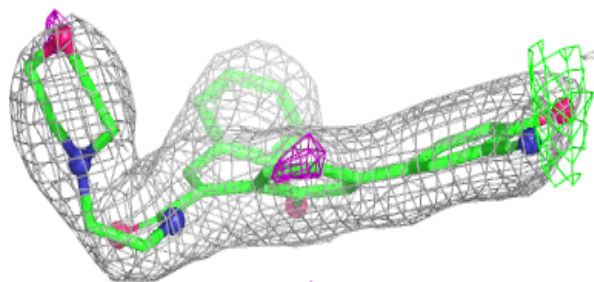
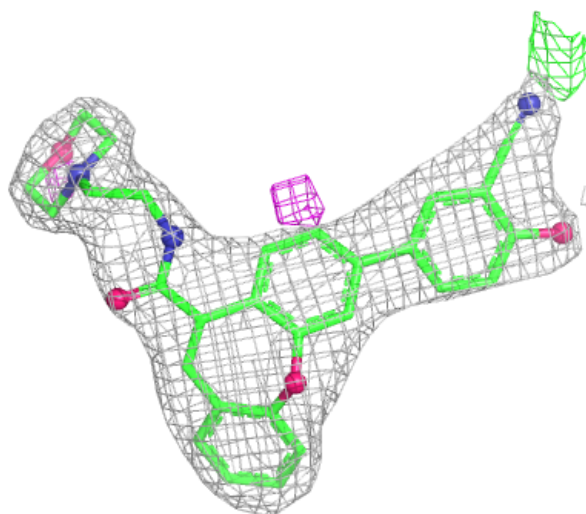
Electron density around M3D B 503:

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



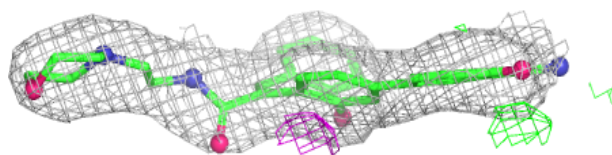
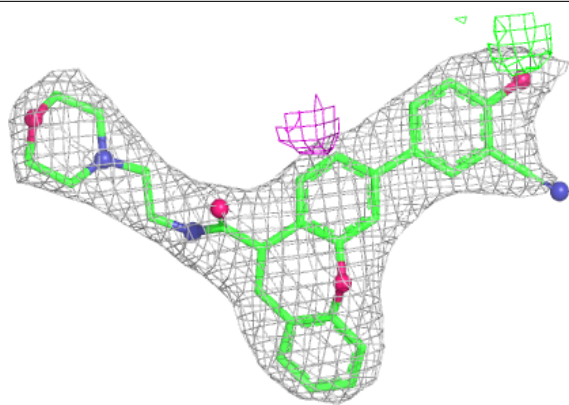
Electron density around M3D B 504:

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

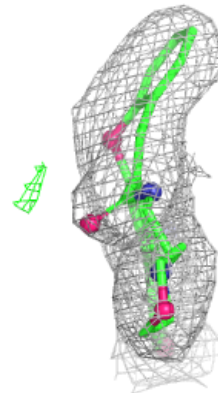
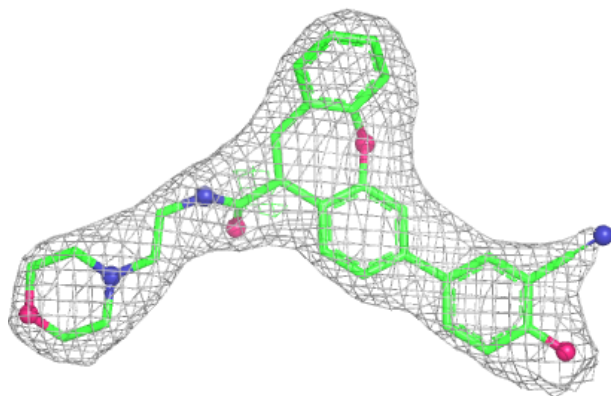


Electron density around M3D C 503:

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

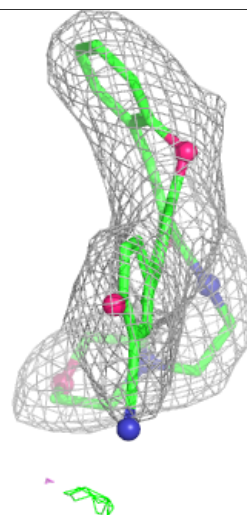
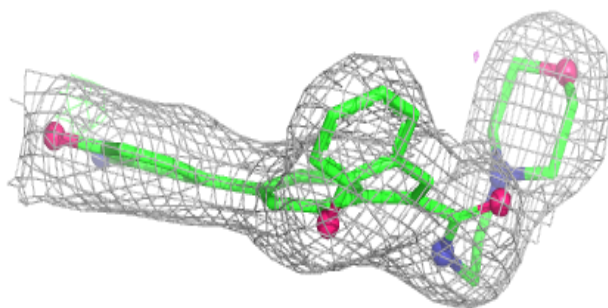
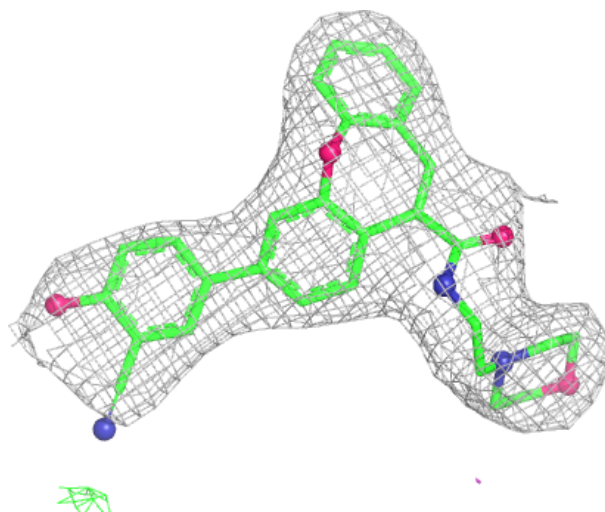
**Electron density around M3D A 503:**

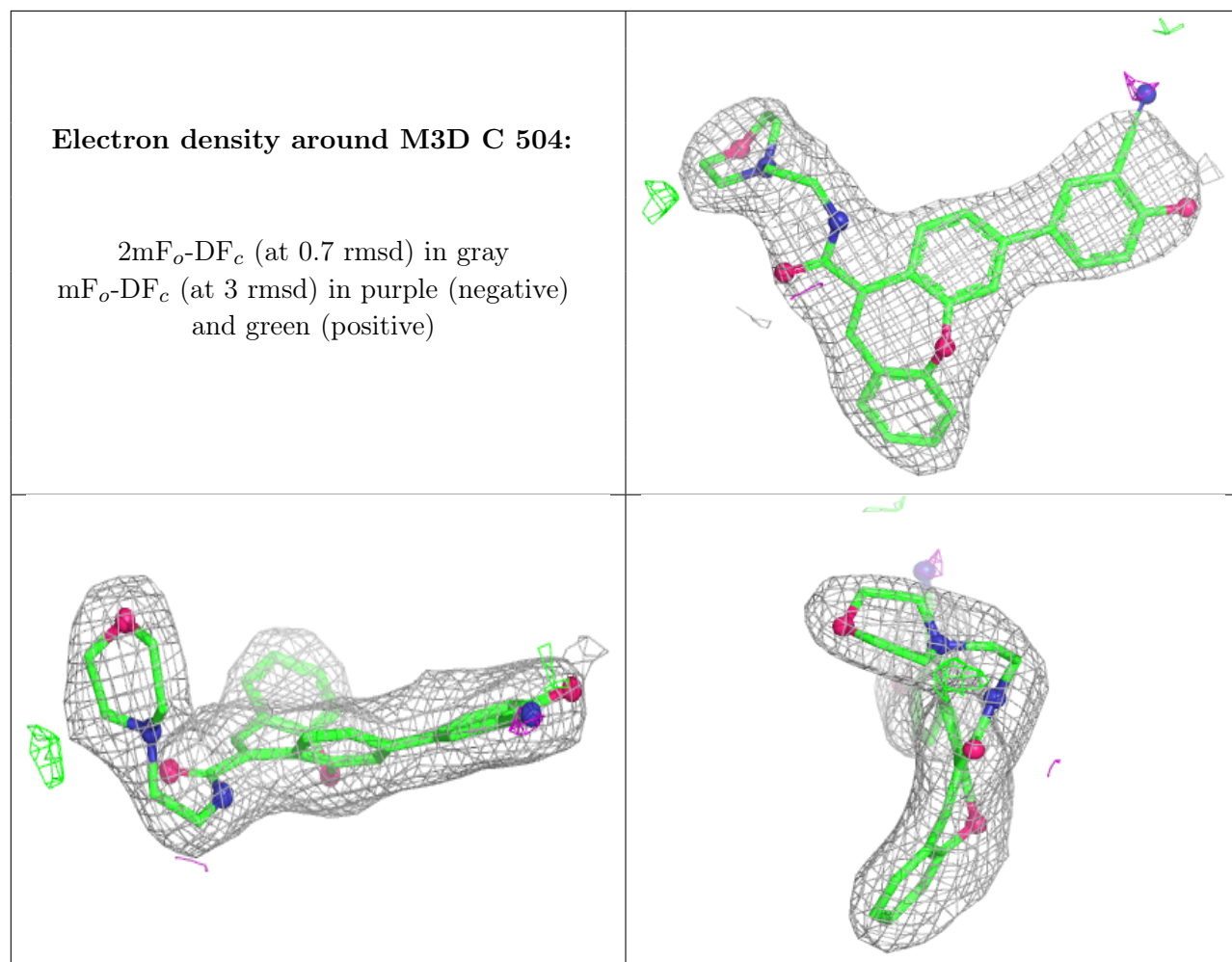
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around M3D A 504:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.