



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:27 PM BST

PDB ID : 6OB0  
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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

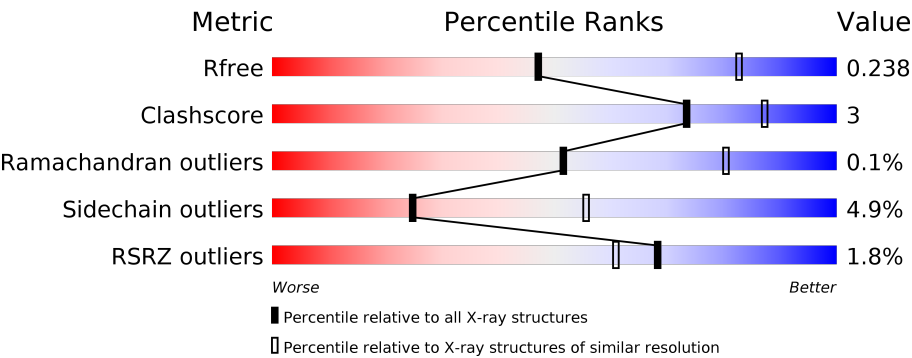
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div><div>%</div><div><div></div><div>88%</div><div>10%</div><div>.</div></div></div>
1	B	448	<div><div>%</div><div><div></div><div>88%</div><div>10%</div><div>.</div></div></div>
1	C	448	<div><div>%</div><div><div></div><div>89%</div><div>10%</div><div>.</div></div></div>
1	D	448	<div><div></div><div><div></div><div>89%</div><div>9%</div><div>..</div></div></div>
2	E	131	<div><div>3%</div><div><div></div><div>53%</div><div>10%</div><div>.</div><div>37%</div></div></div>
2	F	131	<div><div>8%</div><div><div></div><div>46%</div><div>15%</div><div>.</div><div>38%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	131	<div><div><div></div><div></div><div></div><div></div></div><div>8%48%13%38%</div></div>
2	H	131	<div><div><div></div><div></div><div></div><div></div></div><div>%53%8%38%</div></div>

## 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			

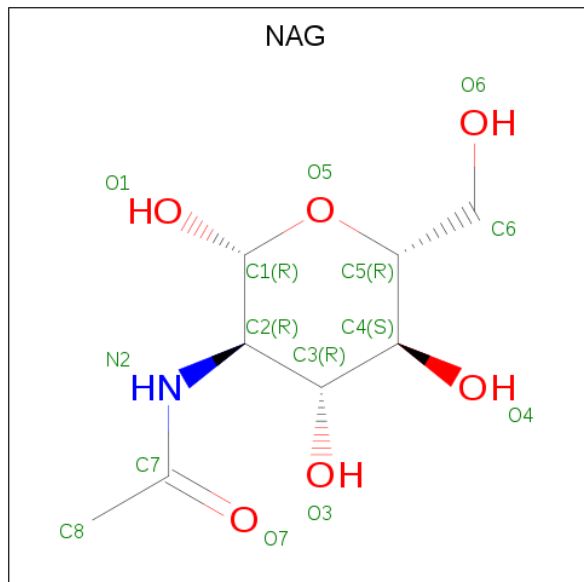
- Molecule 2 is a protein called Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1.

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:

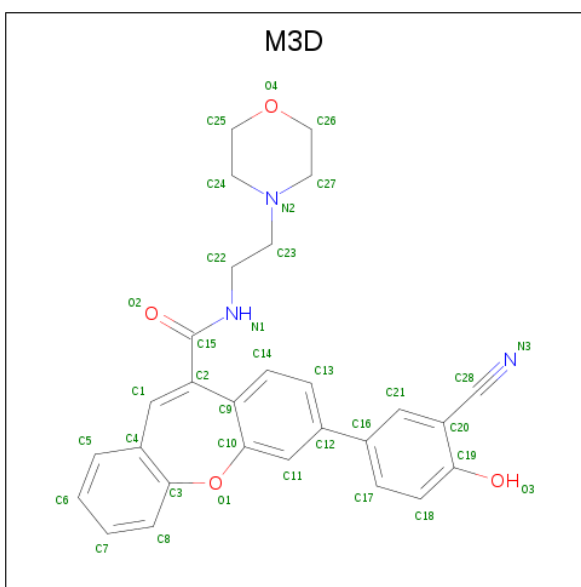
Chain	Residue	Modelled	Actual	Comment	Reference
E	78	ASP	ASN	engineered mutation	UNP Q8IV16
E	82	ASP	ASN	engineered mutation	UNP Q8IV16
F	78	ASP	ASN	engineered mutation	UNP Q8IV16
F	82	ASP	ASN	engineered mutation	UNP Q8IV16
G	78	ASP	ASN	engineered mutation	UNP Q8IV16
G	82	ASP	ASN	engineered mutation	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 (three-letter code: 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 (three-letter code: M3D) (formula:  $C_{28}H_{25}N_3O_4$ ) (labeled as "Ligand of Interest" by author).



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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

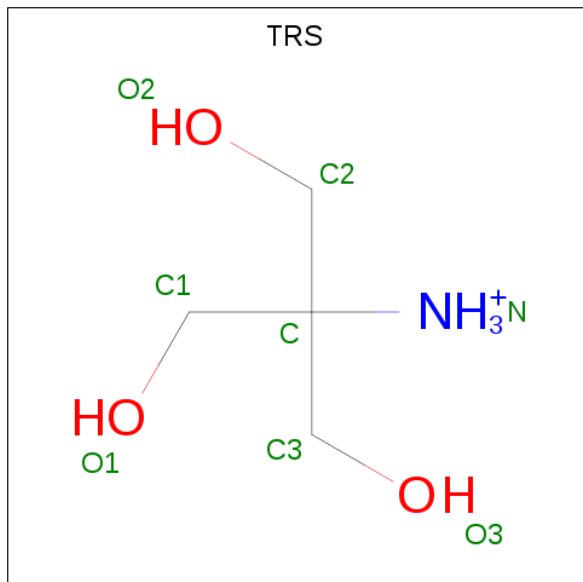


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



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

- Molecule 8 is water.

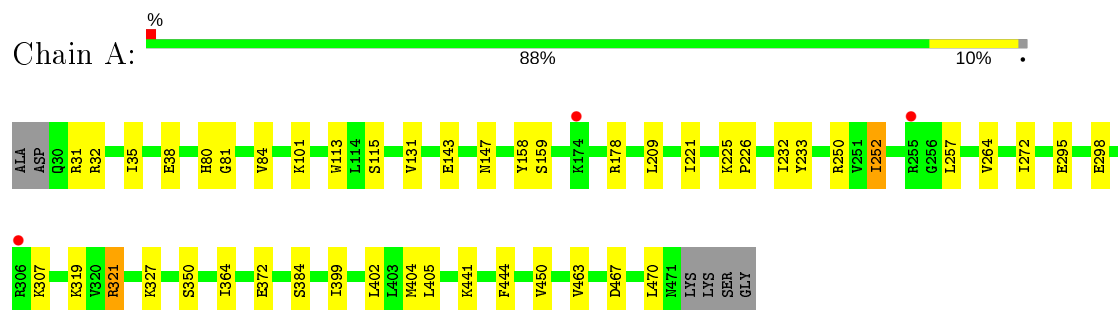
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	63	Total	O	0	0
			63	63		
8	B	50	Total	O	0	0
			50	50		
8	C	48	Total	O	0	0
			48	48		
8	D	58	Total	O	0	0
			58	58		
8	E	2	Total	O	0	0
			2	2		
8	F	2	Total	O	0	0
			2	2		
8	G	2	Total	O	0	0
			2	2		
8	H	1	Total	O	0	0
			1	1		



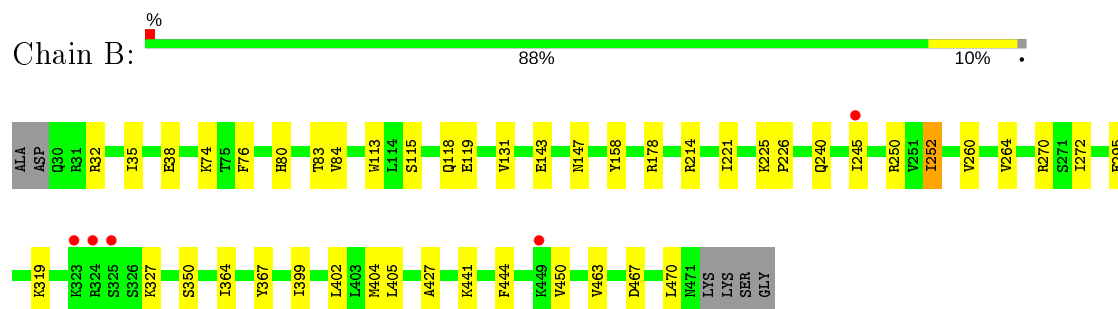
### 3 Residue-property plots [i](#)

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.

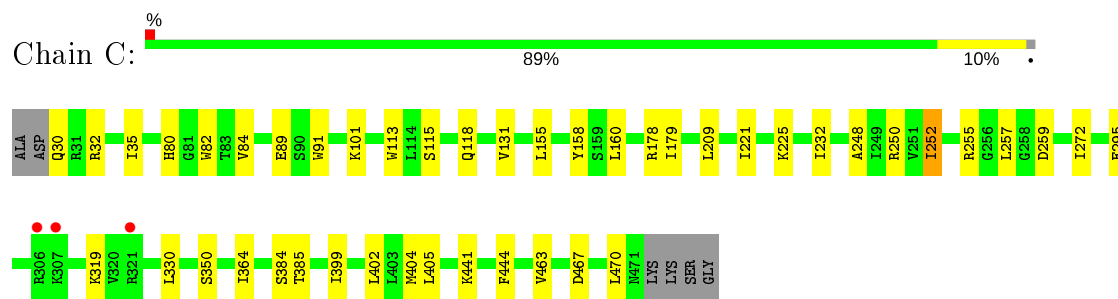
#### • Molecule 1: Lipoprotein lipase



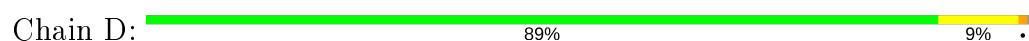
#### • Molecule 1: Lipoprotein lipase

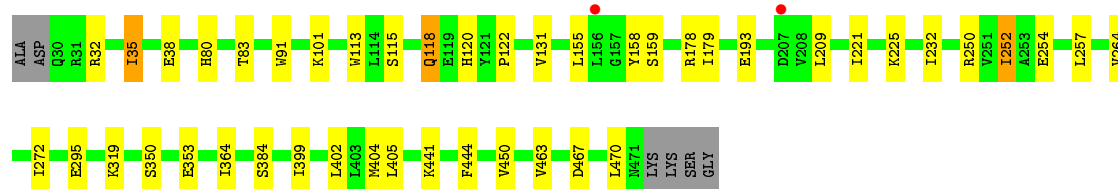


#### • Molecule 1: Lipoprotein lipase

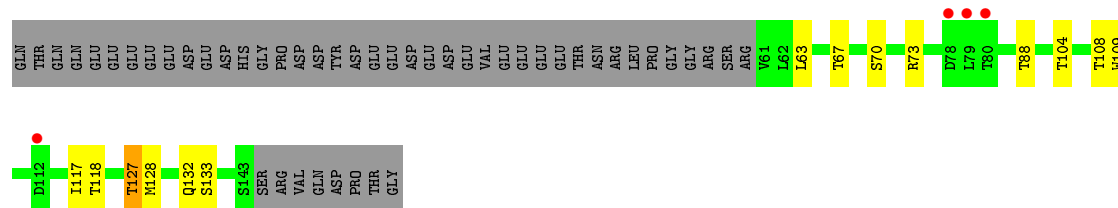


#### • Molecule 1: Lipoprotein lipase

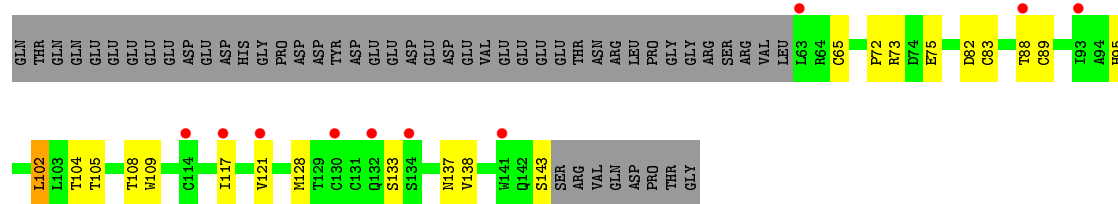




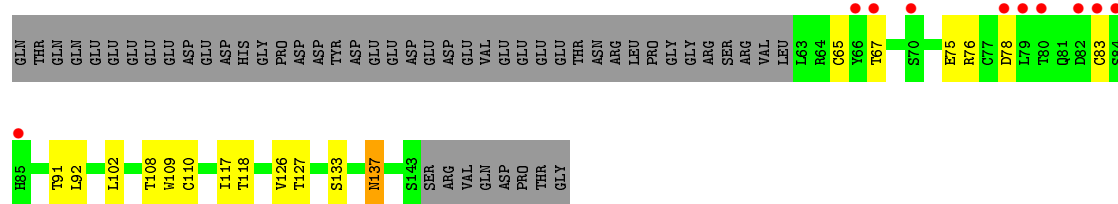
- Molecule 2: Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1



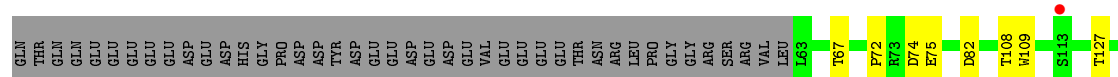
- Molecule 2: Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1



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



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



Q132	S133	C136	S143	SER
				ARG
				VAL
				GLN
				ASP
				PRO
				THR
				GLY

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.43 Å   191.42 Å   97.18 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	37.15 – 2.81 119.72 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.15-2.81) 99.1 (119.72-2.81)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.82 Å)	Xtriage
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 (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: TRS, CA, M3D, NAG, EDO

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	0.52	0/3611	0.70	0/4889
1	B	0.52	0/3600	0.69	0/4874
1	C	0.52	0/3611	0.69	0/4889
1	D	0.52	0/3611	0.68	0/4889
2	E	0.47	0/639	0.71	0/873
2	F	0.49	0/624	0.66	0/852
2	G	0.50	0/624	0.70	0/852
2	H	0.48	0/624	0.70	0/852
All	All	0.51	0/16944	0.69	0/22970

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:402:LEU:HB3	1:A:444:PHE:HZ	1.72	0.54
1:A:80:HIS:HB2	5:A:505:EDO:H12	1.88	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:364:ILE:HD11	1:C:405:LEU:HD21	1.92	0.51
1:C:252:ILE:HD13	1:D:252:ILE:HD13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:TRP:CE3	1:A:131:VAL:HG21	2.53	0.43
1:A:81:GLY:HA3	1:A:159:SER:HB3	1.99	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:N1	4:C:504:M3D:C14	2.81	0.43
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:HH21	1:A:321:ARG:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG13	1:A:35:ILE:H	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:HG13	1:D:35:ILE:H	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%)	47 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	13	37
2	F	79/131 (60%)	71 (90%)	8 (10%)	0	100	100
2	G	79/131 (60%)	68 (86%)	10 (13%)	1 (1%)	12	34
2	H	79/131 (60%)	73 (92%)	6 (8%)	0	100	100
All	All	2081/2316 (90%)	1970 (95%)	108 (5%)	3 (0%)	51	80

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%)	368 (95%)	18 (5%)	26	57
1	B	385/389 (99%)	371 (96%)	14 (4%)	35	67
1	C	386/389 (99%)	371 (96%)	15 (4%)	32	64
1	D	386/389 (99%)	367 (95%)	19 (5%)	25	55
2	E	78/122 (64%)	73 (94%)	5 (6%)	17	44
2	F	76/122 (62%)	69 (91%)	7 (9%)	9	26
2	G	76/122 (62%)	69 (91%)	7 (9%)	9	26
2	H	76/122 (62%)	71 (93%)	5 (7%)	16	42
All	All	1849/2044 (90%)	1759 (95%)	90 (5%)	25	55

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	38	GLU
1	A	84	VAL
1	A	101	LYS
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	295	GLU
1	A	298	GLU
1	A	321	ARG
1	A	350	SER
1	A	372	GLU
1	A	384	SER
1	A	450	VAL
1	B	32	ARG
1	B	35	ILE
1	B	38	GLU
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	350	SER
1	C	30	GLN
1	C	32	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

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Mol	Chain	Res	Type
1	C	295	GLU
1	C	330	LEU
1	C	350	SER
1	C	384	SER
1	C	385	THR
1	D	32	ARG
1	D	35	ILE
1	D	38	GLU
1	D	101	LYS
1	D	115	SER
1	D	118	GLN
1	D	159	SER
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
1	D	295	GLU
1	D	350	SER
1	D	353	GLU
1	D	384	SER
1	D	450	VAL
2	E	88	THR
2	E	108	THR
2	E	127	THR
2	E	128	MET
2	E	133	SER
2	F	82	ASP
2	F	88	THR
2	F	102	LEU
2	F	105	THR
2	F	117	ILE
2	F	128	MET
2	F	133	SER
2	G	75	GLU
2	G	76	ARG
2	G	78	ASP
2	G	91	THR
2	G	102	LEU
2	G	127	THR

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Mol	Chain	Res	Type
2	G	133	SER
2	H	74	ASP
2	H	82	ASP
2	H	127	THR
2	H	132	GLN
2	H	133	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	429	GLN
1	A	454	GLN
1	B	152	ASN
1	B	177	ASN
1	B	429	GLN
1	C	177	ASN
1	C	429	GLN
1	D	177	ASN
1	D	429	GLN
2	E	125	GLN
2	E	142	GLN
2	F	125	GLN
2	H	106	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

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	A	504	-	39,39,39	1.30	6 (15%)	48,54,54	1.37	10 (20%)
4	M3D	B	503	-	39,39,39	1.38	6 (15%)	48,54,54	1.17	6 (12%)
5	EDO	A	505	-	3,3,3	0.64	0	2,2,2	0.55	0
4	M3D	D	503	-	39,39,39	1.34	6 (15%)	48,54,54	1.19	4 (8%)
3	NAG	B	502	1	14,14,15	0.51	0	17,19,21	1.25	1 (5%)
3	NAG	D	501	1	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
3	NAG	A	501	1	14,14,15	0.31	0	17,19,21	0.77	1 (5%)
5	EDO	D	505	-	3,3,3	0.70	0	2,2,2	0.21	0
5	EDO	D	506	-	3,3,3	0.76	0	2,2,2	0.28	0
5	EDO	A	506	-	3,3,3	0.46	0	2,2,2	0.69	0
5	EDO	B	506	-	3,3,3	0.63	0	2,2,2	0.32	0
3	NAG	B	501	1	14,14,15	0.28	0	17,19,21	0.67	0
4	M3D	C	503	-	39,39,39	1.13	2 (5%)	48,54,54	1.33	8 (16%)
5	EDO	B	505	-	3,3,3	0.61	0	2,2,2	0.40	0
5	EDO	C	505	-	3,3,3	1.01	0	2,2,2	0.52	0
5	EDO	C	506	-	3,3,3	0.50	0	2,2,2	0.52	0
3	NAG	D	502	1	14,14,15	0.46	0	17,19,21	1.14	2 (11%)
7	TRS	B	507	-	7,7,7	0.35	0	9,9,9	0.35	0
4	M3D	B	504	-	39,39,39	1.39	4 (10%)	48,54,54	2.11	13 (27%)
3	NAG	C	502	1	14,14,15	0.47	0	17,19,21	1.36	2 (11%)
4	M3D	C	504	-	39,39,39	1.38	7 (17%)	48,54,54	1.79	14 (29%)
3	NAG	C	501	1	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
3	NAG	A	502	1	14,14,15	0.45	0	17,19,21	1.23	2 (11%)
4	M3D	A	503	-	39,39,39	1.24	6 (15%)	48,54,54	1.08	3 (6%)
4	M3D	D	504	-	39,39,39	1.24	3 (7%)	48,54,54	1.59	12 (25%)

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	A	504	-	-	0/14/36/36	0/4/5/5
4	M3D	B	503	-	-	0/14/36/36	0/4/5/5
5	EDO	A	505	-	-	0/1/1/1	-
4	M3D	D	503	-	-	1/14/36/36	0/4/5/5
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
3	NAG	D	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	EDO	D	505	-	-	0/1/1/1	-
5	EDO	D	506	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	B	506	-	-	0/1/1/1	-
3	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	M3D	C	503	-	-	4/14/36/36	0/4/5/5
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	C	505	-	-	1/1/1/1	-
5	EDO	C	506	-	-	0/1/1/1	-
3	NAG	D	502	1	-	0/6/23/26	0/1/1/1
7	TRS	B	507	-	-	0/9/9/9	-
4	M3D	B	504	-	-	4/14/36/36	0/4/5/5
3	NAG	C	502	1	-	0/6/23/26	0/1/1/1
4	M3D	C	504	-	-	4/14/36/36	0/4/5/5
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	M3D	A	503	-	-	0/14/36/36	0/4/5/5
4	M3D	D	504	-	-	3/14/36/36	0/4/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	M3D	C9-C2	3.37	1.52	1.48
4	B	504	M3D	C21-C20	3.20	1.44	1.39
4	C	504	M3D	O1-C10	-3.07	1.34	1.39
4	D	503	M3D	O1-C3	-2.92	1.35	1.39
4	D	504	M3D	C9-C2	2.85	1.51	1.48
4	D	504	M3D	C21-C16	2.71	1.44	1.39
4	B	503	M3D	O1-C10	-2.67	1.35	1.39
4	A	504	M3D	C14-C9	2.67	1.44	1.39
4	A	504	M3D	O1-C10	-2.58	1.35	1.39
4	D	503	M3D	C18-C19	2.54	1.44	1.39
4	C	504	M3D	C21-C20	2.53	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	503	M3D	C21-C16	2.49	1.44	1.39
4	B	503	M3D	O1-C3	-2.46	1.35	1.39
4	C	503	M3D	C21-C16	2.46	1.44	1.39
4	C	504	M3D	C9-C2	2.42	1.51	1.48
4	B	503	M3D	C13-C12	2.40	1.44	1.39
4	D	503	M3D	C17-C16	2.35	1.44	1.39
4	B	504	M3D	C21-C16	2.30	1.43	1.39
4	A	503	M3D	C20-C28	2.30	1.47	1.44
4	C	504	M3D	C21-C16	2.29	1.43	1.39
4	C	504	M3D	C14-C13	2.27	1.42	1.38
4	B	503	M3D	C14-C13	2.26	1.42	1.38
4	A	504	M3D	C14-C13	2.26	1.42	1.38
4	A	504	M3D	C13-C12	2.25	1.44	1.39
4	A	504	M3D	O1-C3	-2.25	1.36	1.39
4	C	504	M3D	C14-C9	2.24	1.43	1.39
4	B	503	M3D	C21-C16	2.24	1.43	1.39
4	B	503	M3D	C14-C9	2.23	1.43	1.39
4	A	503	M3D	O1-C3	-2.22	1.36	1.39
4	C	503	M3D	O1-C3	-2.19	1.36	1.39
4	A	503	M3D	C18-C17	2.19	1.42	1.38
4	C	504	M3D	C6-C5	2.18	1.43	1.38
4	A	504	M3D	C9-C2	2.17	1.50	1.48
4	B	504	M3D	C6-C5	2.11	1.43	1.38
4	D	503	M3D	C18-C17	2.11	1.42	1.38
4	A	503	M3D	C21-C16	2.09	1.43	1.39
4	A	503	M3D	C14-C13	2.08	1.42	1.38
4	A	503	M3D	O1-C10	-2.07	1.36	1.39
4	D	503	M3D	C14-C13	2.06	1.42	1.38
4	D	504	M3D	O1-C3	-2.01	1.36	1.39

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	M3D	C17-C16-C12	-5.65	111.57	121.36
4	B	504	M3D	C21-C16-C12	5.05	129.21	120.86
4	C	504	M3D	C22-N1-C15	4.87	133.47	122.47
3	C	502	NAG	C1-O5-C5	4.16	117.83	112.19
4	B	504	M3D	C27-N2-C24	4.03	117.89	108.83
4	D	503	M3D	C19-C20-C28	3.98	123.28	119.53
4	C	504	M3D	C26-C27-N2	3.95	116.09	110.10
3	B	502	NAG	C1-O5-C5	3.90	117.48	112.19
4	B	504	M3D	C23-N2-C27	3.83	121.02	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	M3D	C23-C22-N1	3.82	118.92	111.60
4	C	503	M3D	C25-C24-N2	3.75	115.79	110.10
4	D	504	M3D	C22-N1-C15	3.69	130.80	122.47
3	A	502	NAG	C1-O5-C5	3.55	117.00	112.19
4	B	504	M3D	C22-N1-C15	3.54	130.46	122.47
4	B	504	M3D	O2-C15-C2	3.44	126.92	121.91
4	B	504	M3D	O1-C10-C9	3.30	123.27	120.22
4	C	504	M3D	C23-C22-N1	3.30	117.92	111.60
3	D	502	NAG	C1-O5-C5	3.23	116.57	112.19
4	D	504	M3D	C17-C16-C12	-3.21	115.79	121.36
4	C	504	M3D	O1-C10-C9	3.18	123.16	120.22
4	C	504	M3D	C17-C16-C12	-3.05	116.07	121.36
4	B	504	M3D	C16-C21-C20	-3.03	118.81	121.53
4	D	503	M3D	O1-C10-C9	2.90	122.89	120.22
4	B	504	M3D	O2-C15-N1	-2.89	118.00	123.30
4	C	504	M3D	C16-C21-C20	-2.84	118.98	121.53
4	C	504	M3D	C25-C24-N2	2.79	114.34	110.10
4	C	504	M3D	C21-C16-C12	2.79	125.47	120.86
4	A	503	M3D	O4-C26-C27	-2.75	105.73	111.80
4	C	503	M3D	C27-N2-C24	2.70	114.92	108.83
3	C	502	NAG	C1-C2-N2	-2.68	105.91	110.49
4	D	504	M3D	C26-C27-N2	2.66	114.14	110.10
4	A	503	M3D	C26-C27-N2	-2.56	106.23	110.10
4	C	503	M3D	O4-C26-C27	-2.54	106.19	111.80
4	A	504	M3D	C22-N1-C15	2.54	128.21	122.47
4	D	504	M3D	C22-C23-N2	2.54	119.19	112.88
4	B	503	M3D	C22-N1-C15	2.50	128.11	122.47
4	A	504	M3D	C25-C24-N2	2.47	113.85	110.10
4	B	504	M3D	C14-C9-C10	-2.46	114.97	118.21
4	C	503	M3D	O4-C25-C24	-2.42	106.47	111.80
4	C	504	M3D	C17-C18-C19	-2.40	118.04	120.50
4	C	503	M3D	C19-C20-C28	2.35	121.75	119.53
4	D	504	M3D	O2-C15-C2	2.34	125.32	121.91
4	B	504	M3D	O3-C19-C20	2.33	125.50	119.37
4	C	503	M3D	O1-C10-C9	2.31	122.36	120.22
3	D	501	NAG	C1-O5-C5	2.31	115.32	112.19
4	A	504	M3D	C8-C3-C4	2.30	122.18	118.17
4	B	504	M3D	C26-O4-C25	2.28	117.49	109.89
3	A	501	NAG	C1-O5-C5	2.27	115.26	112.19
4	D	504	M3D	O1-C10-C9	2.26	122.31	120.22
4	B	503	M3D	C10-O1-C3	2.26	122.96	114.38
4	D	504	M3D	O2-C15-N1	-2.25	119.18	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	M3D	C8-C3-C4	2.25	122.10	118.17
4	C	503	M3D	C22-N1-C15	2.23	127.50	122.47
4	C	503	M3D	C26-C27-N2	2.22	113.46	110.10
4	D	504	M3D	C27-N2-C24	2.21	113.81	108.83
4	A	504	M3D	C17-C18-C19	-2.21	118.23	120.50
4	C	504	M3D	C14-C9-C10	-2.20	115.32	118.21
4	C	504	M3D	C27-N2-C24	2.18	113.74	108.83
4	A	504	M3D	C17-C16-C12	-2.18	117.58	121.36
4	D	504	M3D	C21-C16-C12	2.18	124.47	120.86
4	A	504	M3D	C11-C12-C16	-2.17	117.27	120.86
4	A	504	M3D	O4-C25-C24	-2.17	107.01	111.80
4	B	503	M3D	C26-C27-N2	-2.16	106.83	110.10
4	D	504	M3D	C9-C2-C15	2.16	121.69	114.62
4	C	504	M3D	O1-C10-C11	-2.15	113.70	117.59
4	B	503	M3D	C19-C20-C28	2.14	121.55	119.53
4	B	504	M3D	C22-C23-N2	2.14	118.19	112.88
4	D	504	M3D	C26-O4-C25	2.11	116.94	109.89
4	A	504	M3D	C23-N2-C27	2.11	116.62	111.23
4	B	503	M3D	O4-C26-C27	-2.08	107.22	111.80
4	C	504	M3D	C22-C23-N2	2.07	118.02	112.88
3	C	501	NAG	C1-O5-C5	2.07	114.99	112.19
3	A	502	NAG	C1-C2-N2	-2.06	106.97	110.49
4	A	504	M3D	O4-C26-C27	-2.06	107.27	111.80
4	D	503	M3D	C26-O4-C25	2.05	116.74	109.89
3	D	502	NAG	O4-C4-C5	2.05	114.38	109.30
4	D	503	M3D	O2-C15-C2	2.04	124.89	121.91
4	C	504	M3D	C9-C2-C15	2.03	121.27	114.62
4	A	503	M3D	C22-N1-C15	2.01	127.01	122.47
4	A	504	M3D	C27-N2-C24	2.01	113.34	108.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	503	M3D	C19-C20-C28-N3
4	C	503	M3D	O2-C15-C2-C1
4	C	503	M3D	C22-C23-N2-C27
4	B	504	M3D	C19-C20-C28-N3
4	B	504	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

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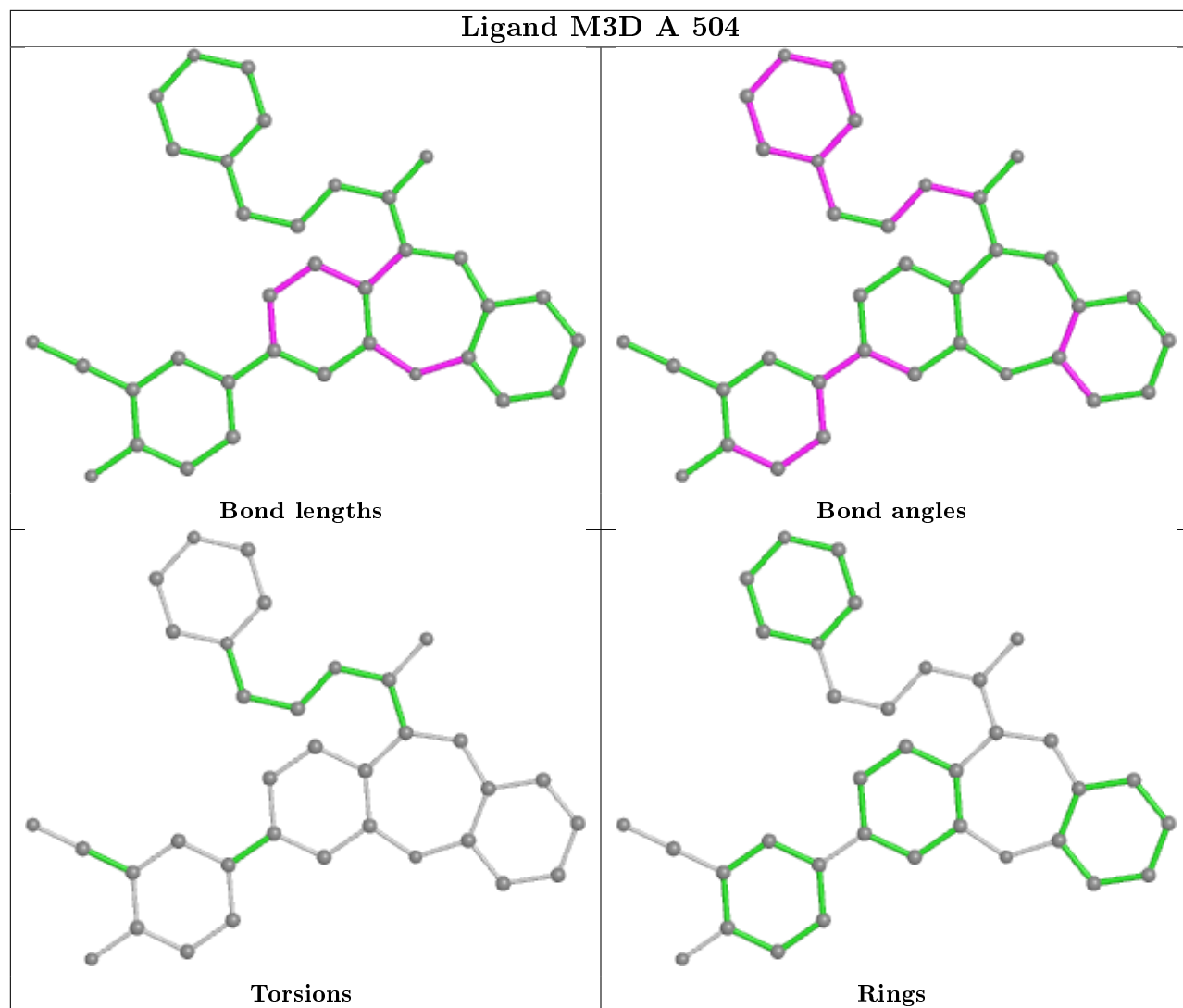
Mol	Chain	Res	Type	Atoms
4	B	504	M3D	C23-C22-N1-C15
4	B	504	M3D	C22-C23-N2-C24
5	C	505	EDO	O1-C1-C2-O2
4	C	503	M3D	N1-C22-C23-N2
4	D	504	M3D	C19-C20-C28-N3
4	C	503	M3D	N1-C15-C2-C1
4	C	504	M3D	N1-C15-C2-C1
4	D	504	M3D	N1-C15-C2-C1
4	C	504	M3D	C22-C23-N2-C24

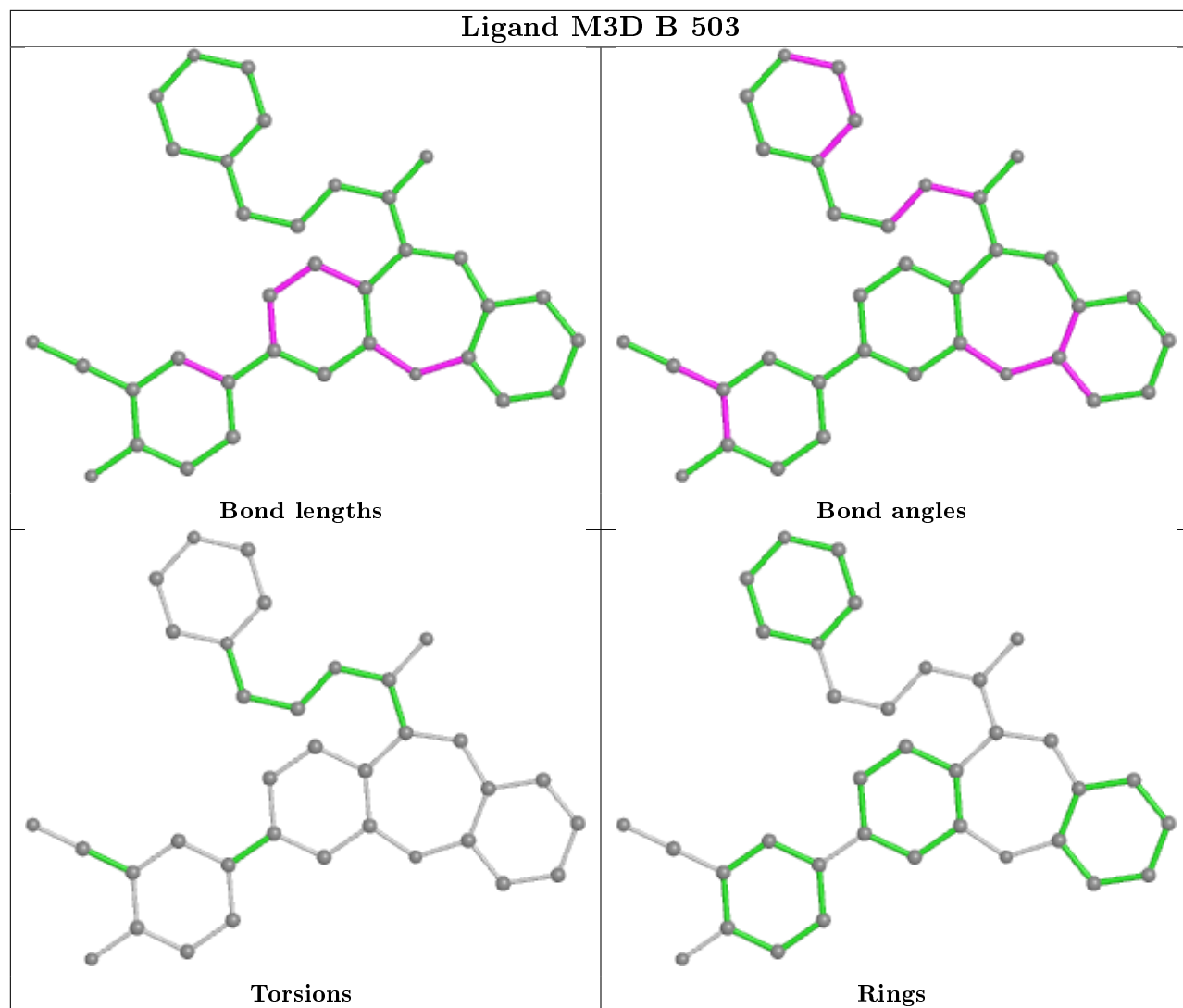
There are no ring outliers.

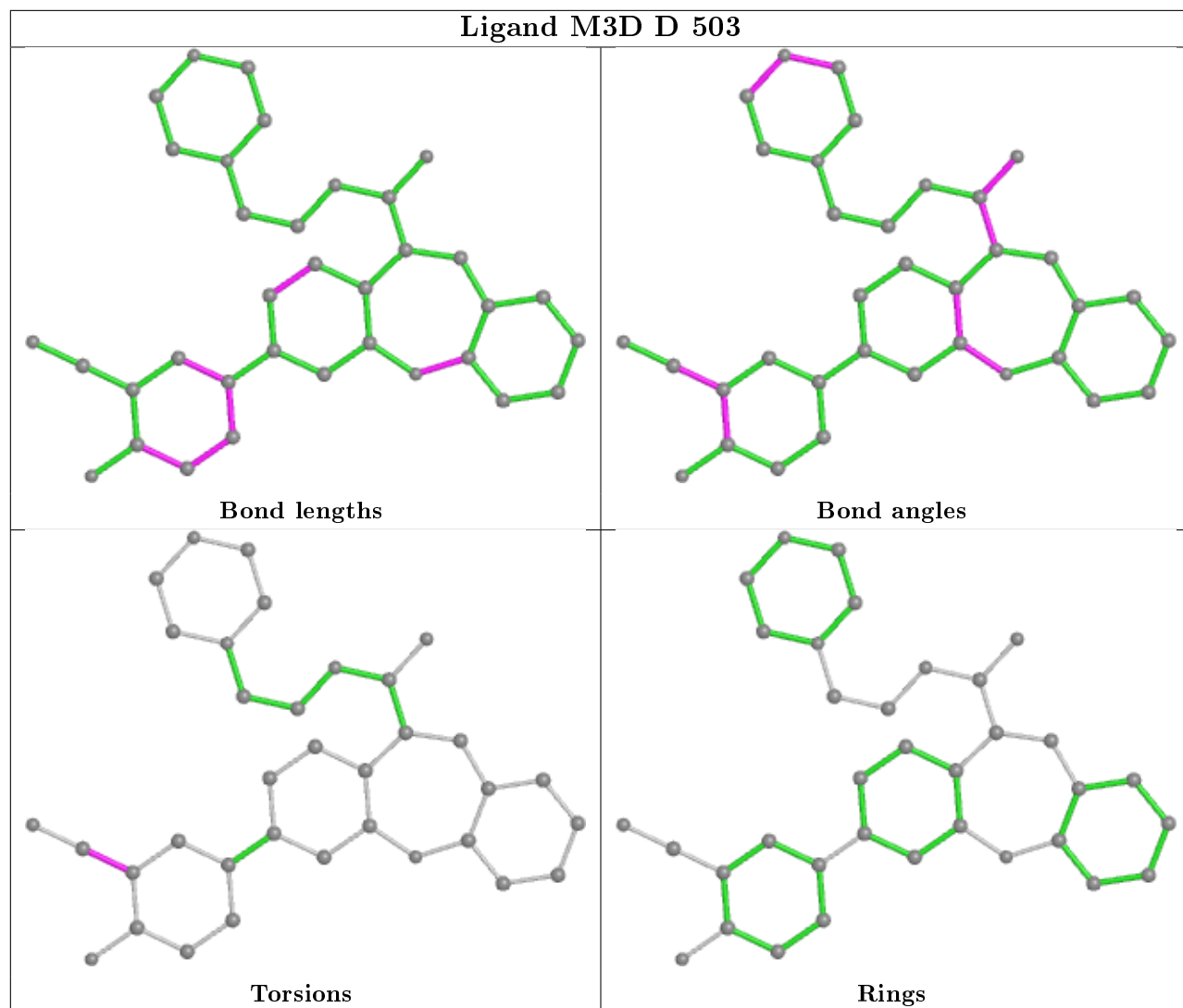
7 monomers are involved in 11 short contacts:

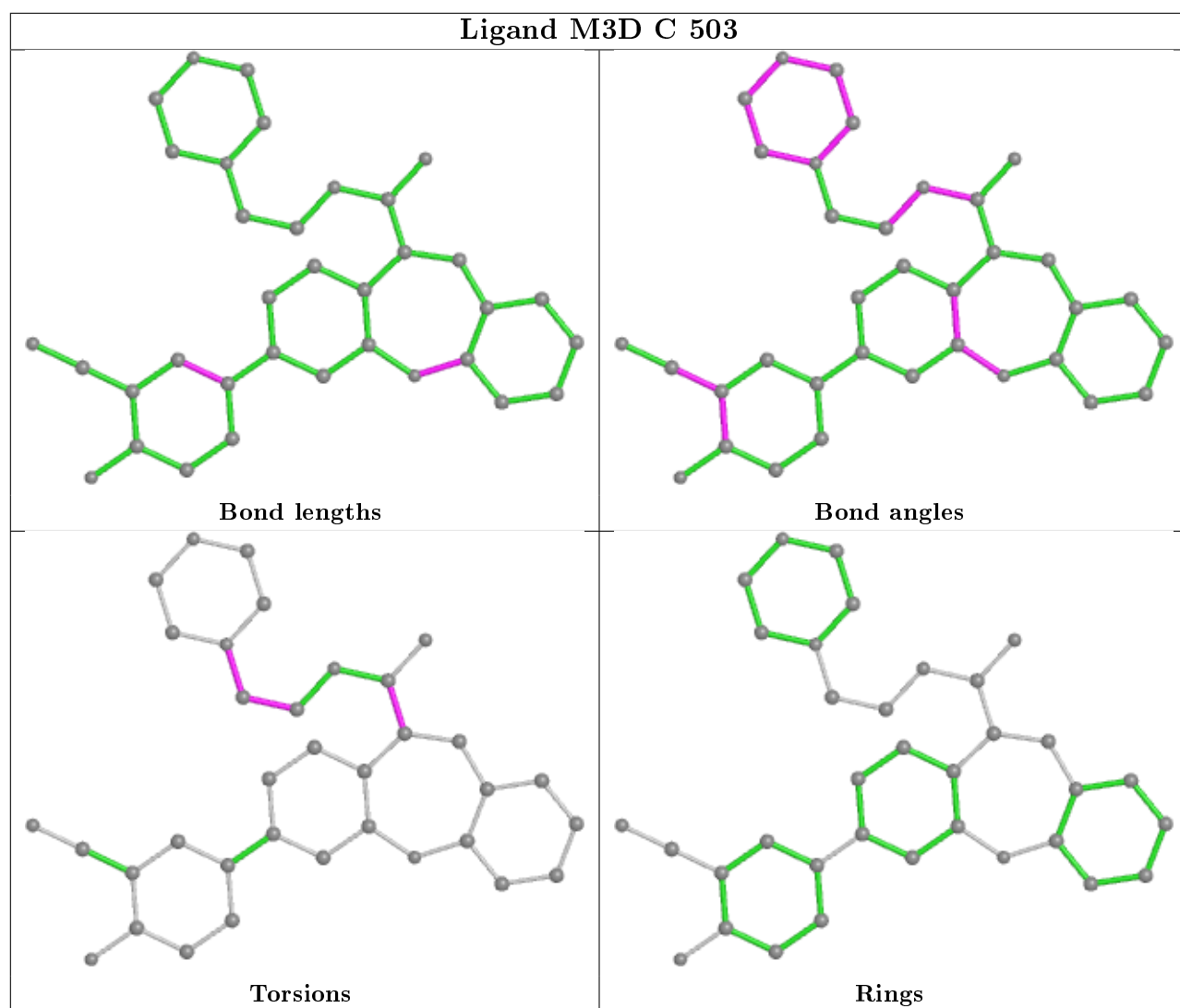
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	EDO	1	0
5	D	505	EDO	2	0
5	B	505	EDO	2	0
5	C	505	EDO	3	0
4	B	504	M3D	1	0
4	C	504	M3D	1	0
4	D	504	M3D	1	0

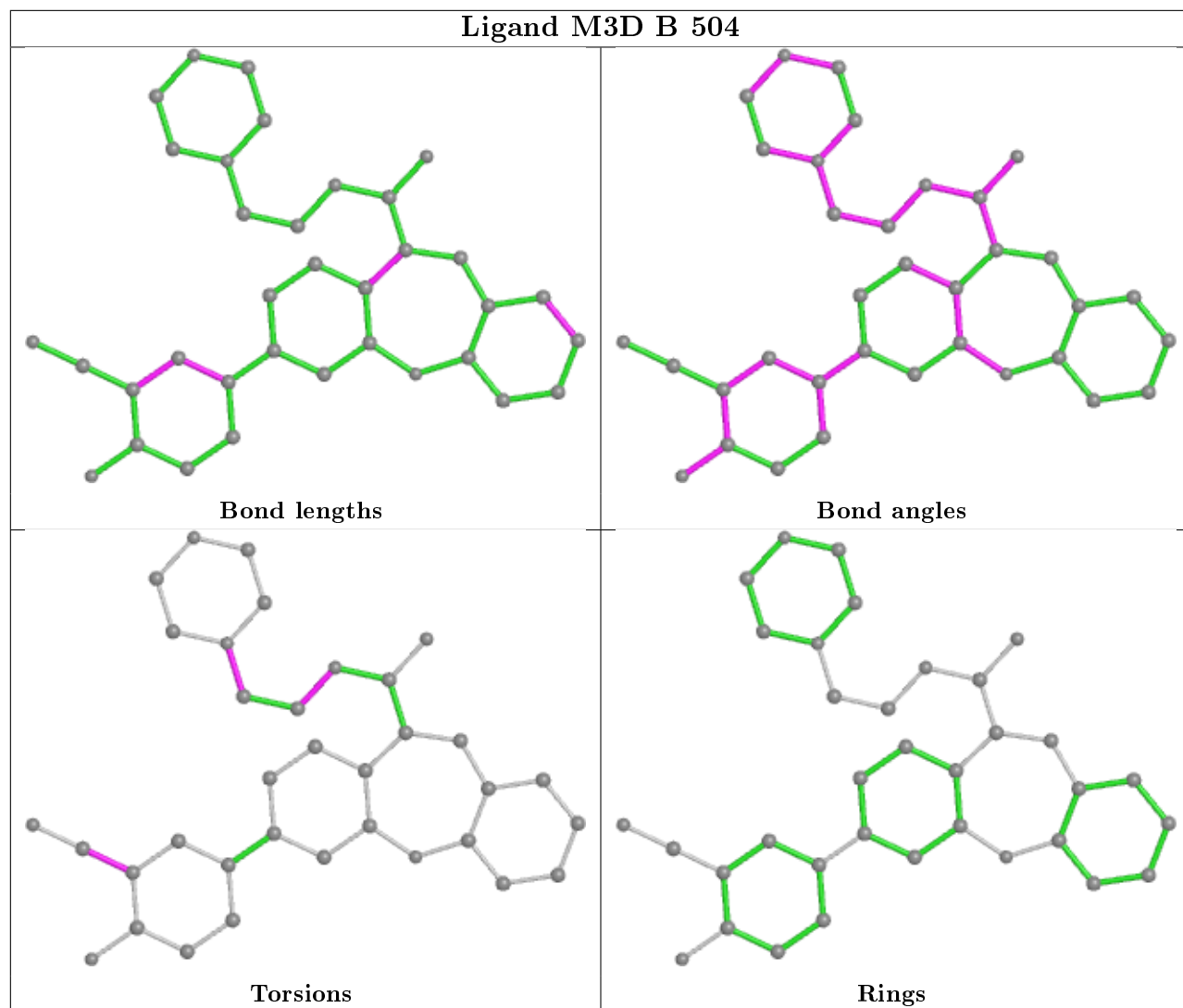
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



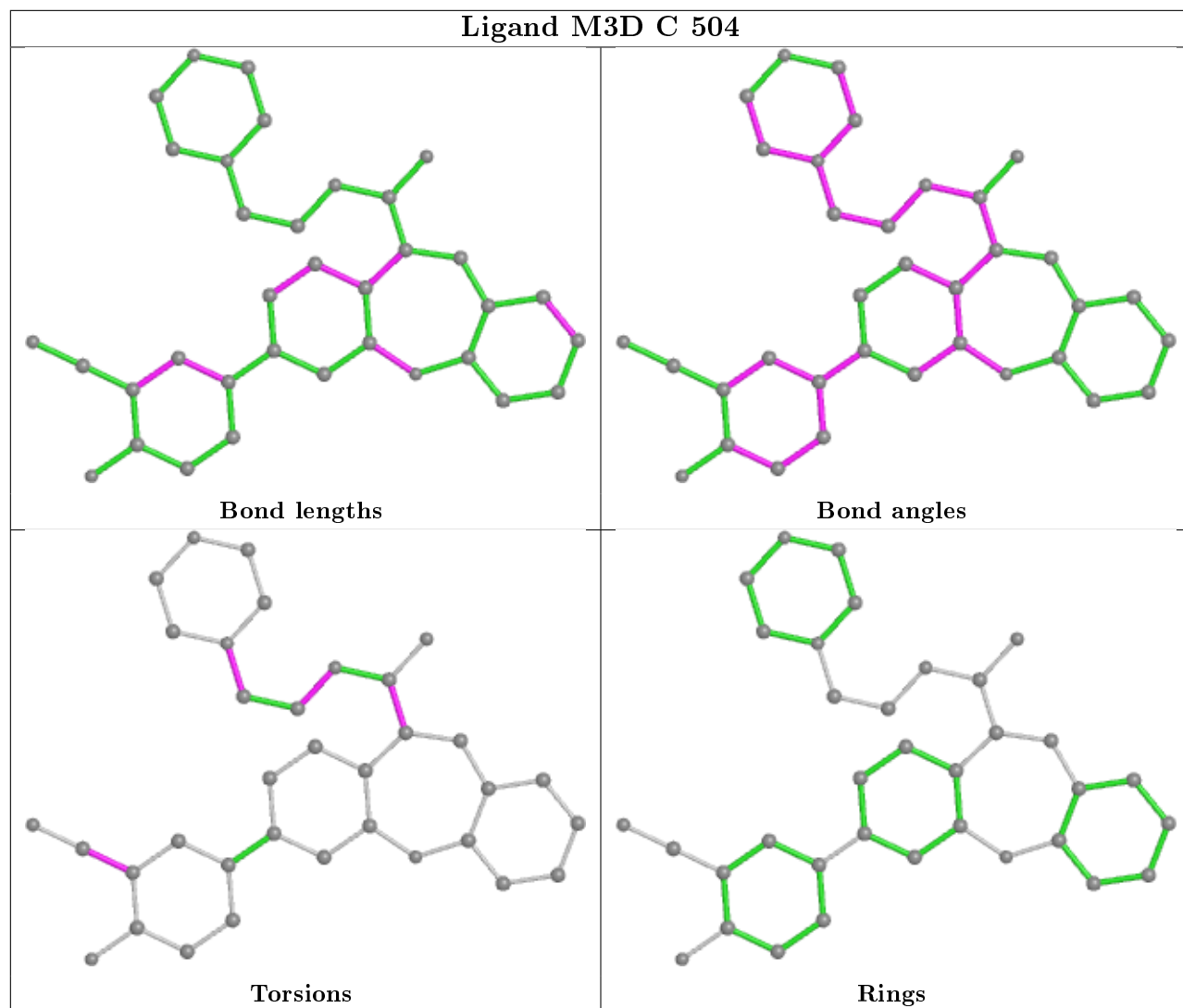


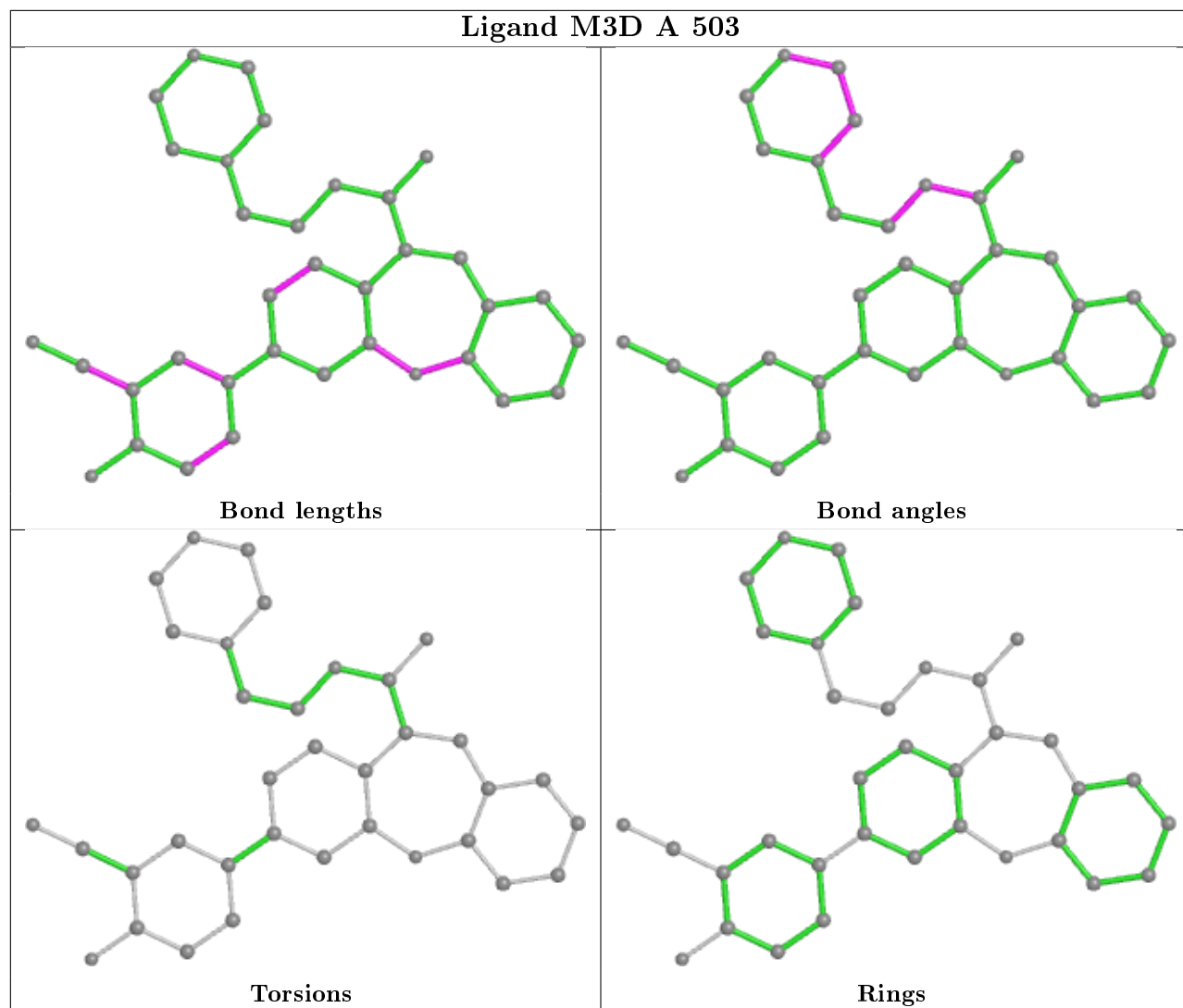


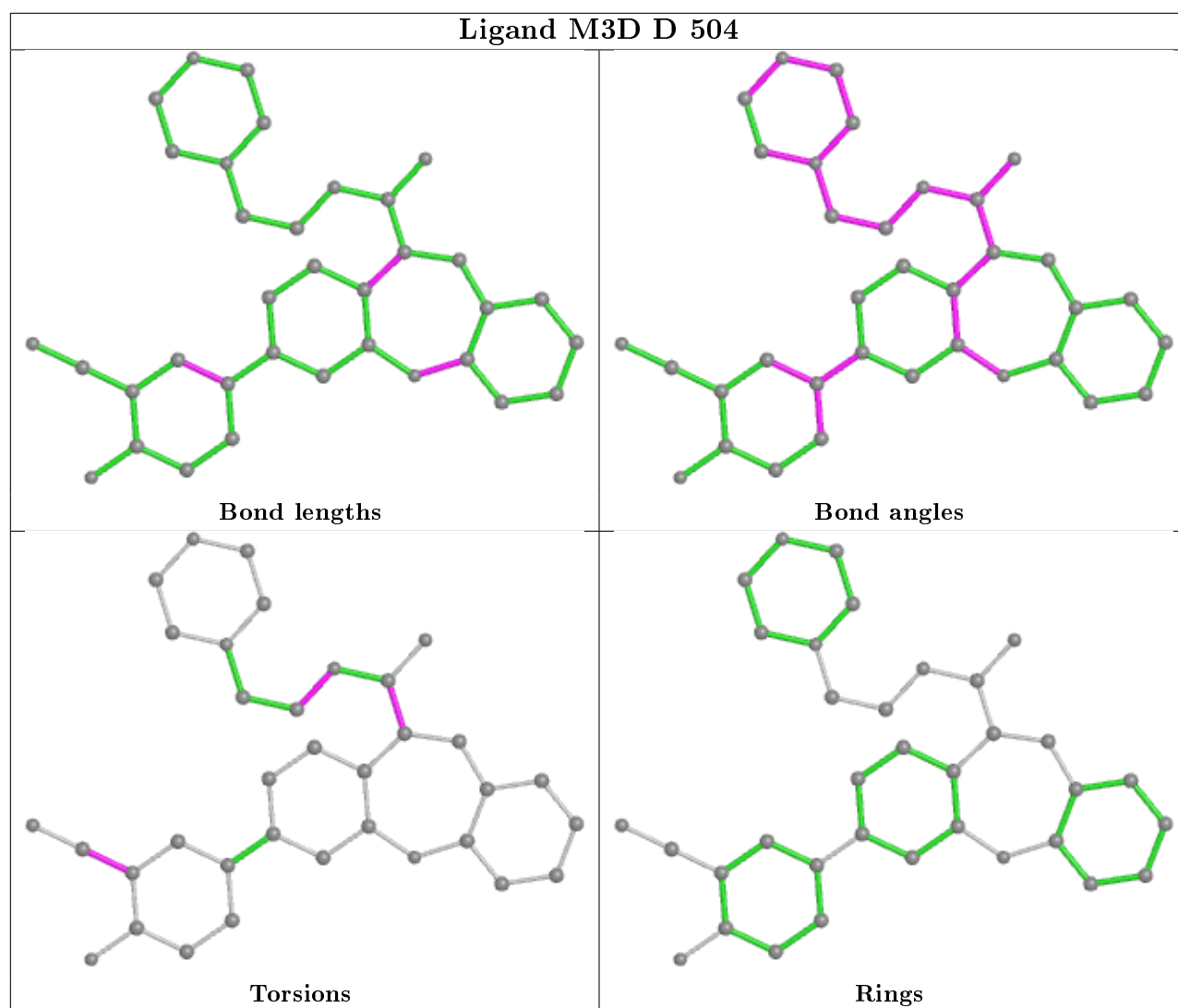












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	442/448 (98%)	0.11	3 (0%) 87 84	39, 60, 94, 128	0
1	B	442/448 (98%)	0.15	5 (1%) 80 75	42, 61, 94, 125	0
1	C	442/448 (98%)	0.13	3 (0%) 87 84	39, 60, 94, 122	0
1	D	442/448 (98%)	0.10	2 (0%) 91 88	40, 59, 93, 131	0
2	E	83/131 (63%)	0.31	4 (4%) 30 21	58, 86, 106, 118	0
2	F	81/131 (61%)	0.84	10 (12%) 4 2	78, 101, 122, 133	0
2	G	81/131 (61%)	0.53	10 (12%) 4 2	66, 97, 121, 126	0
2	H	81/131 (61%)	0.28	1 (1%) 79 73	57, 88, 109, 116	0
All	All	2094/2316 (90%)	0.18	38 (1%) 68 61	39, 63, 106, 133	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	85	HIS	4.9
2	E	79	LEU	4.5
1	B	449	LYS	4.1
2	F	117	ILE	3.5
2	G	80	THR	3.5
2	G	70	SER	3.0
2	F	63	LEU	2.9
2	F	114	CYS	2.8
2	E	80	THR	2.8
1	B	323	LYS	2.7
2	G	79	LEU	2.6
1	A	174	LYS	2.6
2	F	93	ILE	2.6
2	F	132	GLN	2.6
2	G	82	ASP	2.6
2	F	134	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	83	CYS	2.5
2	F	141	TRP	2.5
2	G	78	ASP	2.5
1	A	306	ARG	2.5
2	G	67	THR	2.4
2	G	66	TYR	2.4
1	B	245	ILE	2.4
1	D	207	ASP	2.4
2	F	130	CYS	2.3
1	A	255	ARG	2.3
1	C	321	ARG	2.3
2	E	78	ASP	2.3
2	F	88	THR	2.3
1	C	307	LYS	2.3
1	B	324	ARG	2.2
1	C	306	ARG	2.2
1	D	156	LEU	2.1
1	B	325	SER	2.1
2	F	121	VAL	2.1
2	G	84	SER	2.1
2	E	112	ASP	2.0
2	H	113	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	502	14/15	0.76	0.22	66,85,97,101	0

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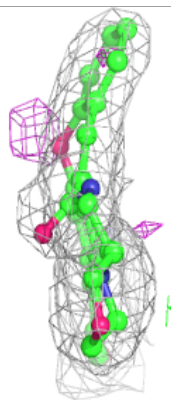
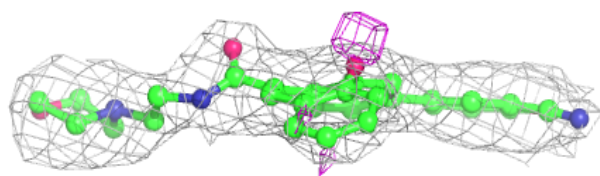
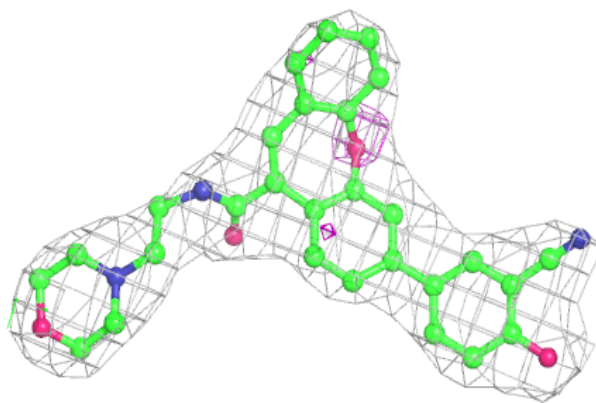
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	502	14/15	0.76	0.22	65,78,88,90	0
3	NAG	D	501	14/15	0.77	0.20	87,90,95,97	0
3	NAG	C	502	14/15	0.79	0.22	65,78,94,97	0
7	TRS	B	507	8/8	0.81	0.16	81,88,95,95	0
3	NAG	C	501	14/15	0.84	0.18	96,104,107,107	0
3	NAG	B	501	14/15	0.84	0.15	96,100,104,104	0
3	NAG	D	502	14/15	0.85	0.21	62,66,74,79	0
3	NAG	A	501	14/15	0.87	0.19	109,112,116,116	0
5	EDO	A	506	4/4	0.89	0.29	57,59,59,59	0
5	EDO	D	506	4/4	0.90	0.39	58,63,64,64	0
5	EDO	A	505	4/4	0.92	0.52	53,54,55,58	0
5	EDO	D	505	4/4	0.94	0.45	60,65,70,72	0
5	EDO	B	506	4/4	0.95	0.39	53,55,56,59	0
4	M3D	B	503	35/35	0.95	0.24	33,44,56,66	0
4	M3D	B	504	35/35	0.95	0.30	45,53,60,65	0
4	M3D	D	504	35/35	0.95	0.24	43,53,63,63	0
5	EDO	C	505	4/4	0.96	0.29	44,48,57,61	0
4	M3D	A	504	35/35	0.96	0.21	47,53,60,62	0
4	M3D	D	503	35/35	0.96	0.25	34,43,59,67	0
5	EDO	B	505	4/4	0.96	0.44	54,57,58,58	0
4	M3D	C	503	35/35	0.97	0.27	38,46,56,59	0
5	EDO	C	506	4/4	0.97	0.51	59,62,63,66	0
4	M3D	A	503	35/35	0.97	0.23	37,45,59,60	0
4	M3D	C	504	35/35	0.97	0.24	38,50,58,66	0
6	CA	C	507	1/1	0.99	0.14	60,60,60,60	0
6	CA	B	508	1/1	0.99	0.16	57,57,57,57	0
6	CA	D	507	1/1	0.99	0.13	52,52,52,52	0
6	CA	A	507	1/1	0.99	0.17	62,62,62,62	0

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

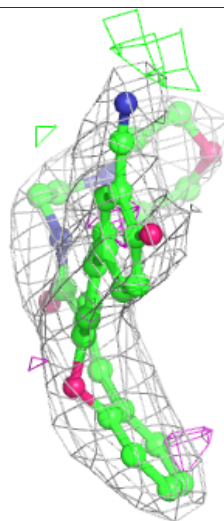
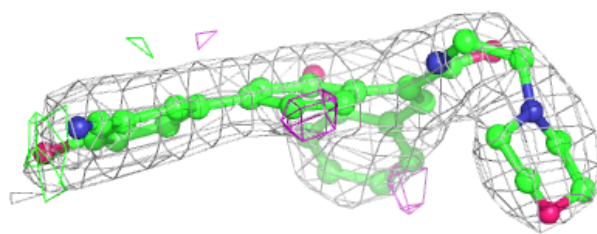
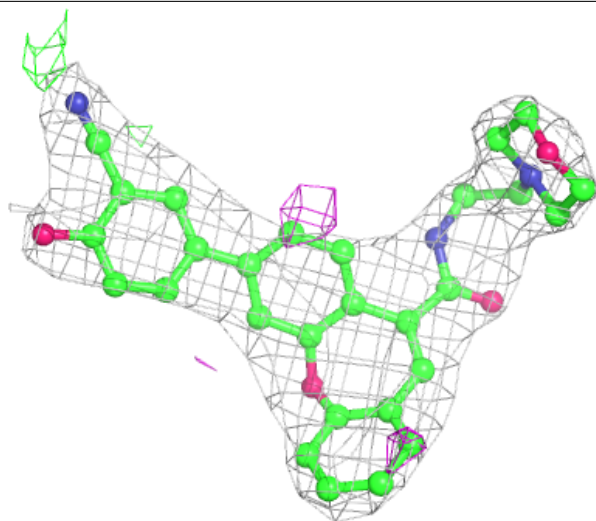
**Electron density around M3D B 503:**

$2mF_o - DF_c$  (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:**

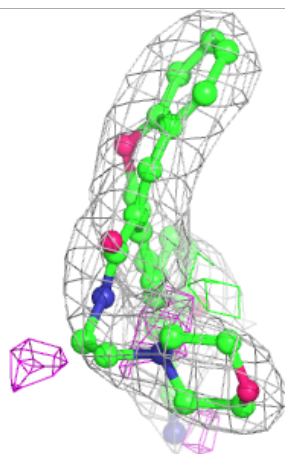
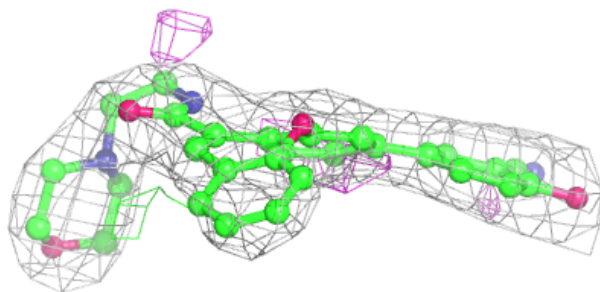
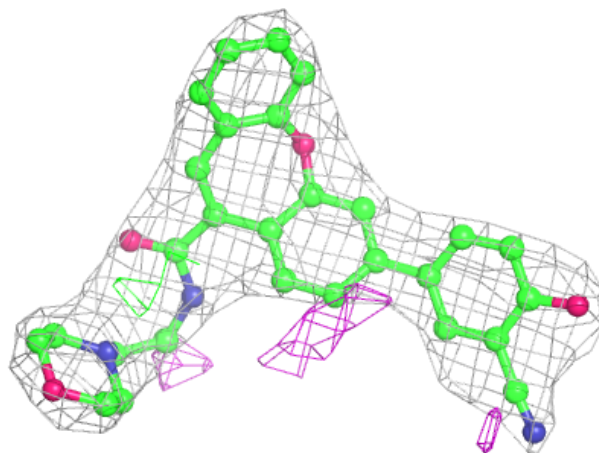
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





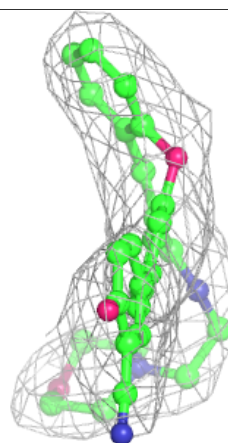
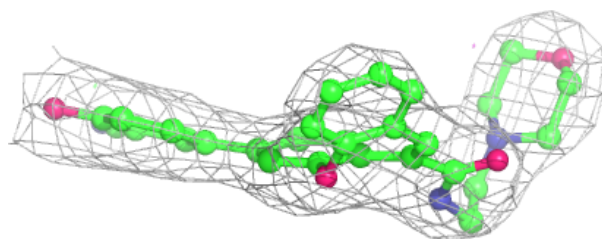
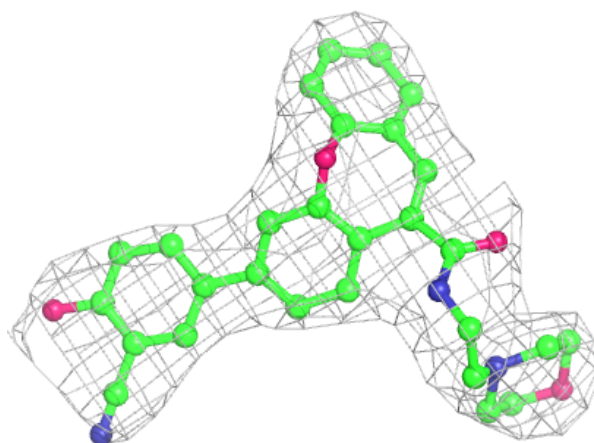
**Electron density around M3D D 504:**

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



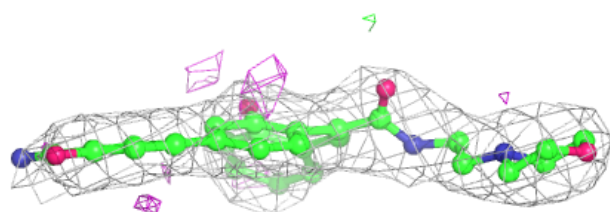
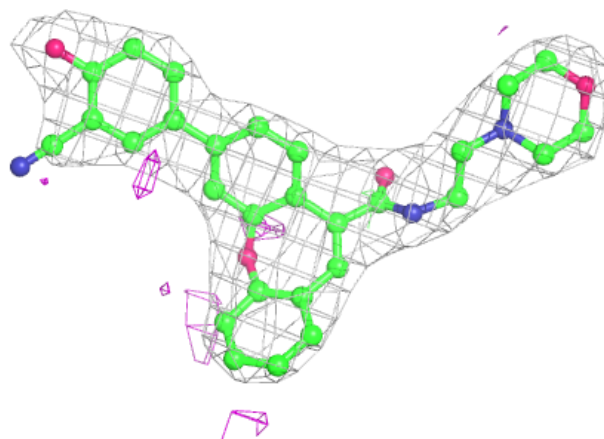
**Electron density around M3D A 504:**

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and green (positive)

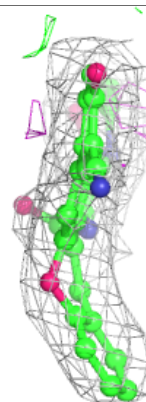
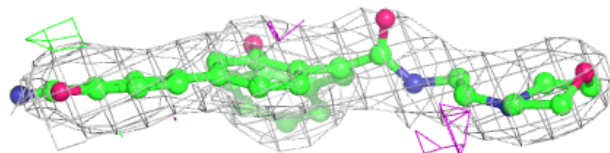
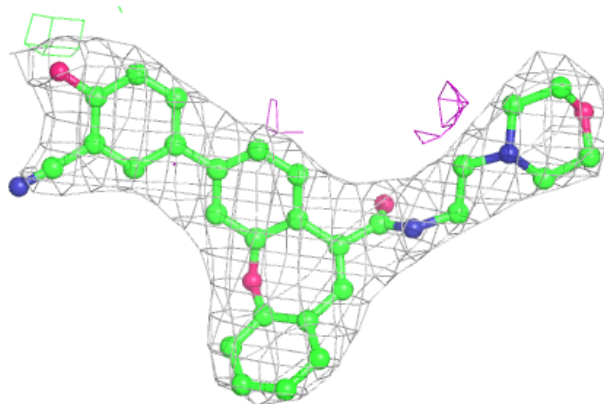


**Electron density around M3D D 503:**

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

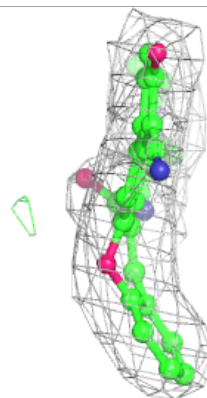
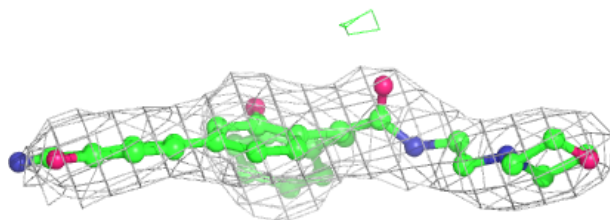
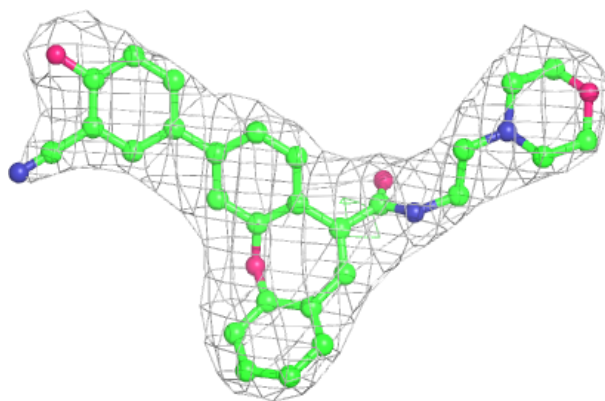
**Electron density around M3D C 503:**

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and green (positive)

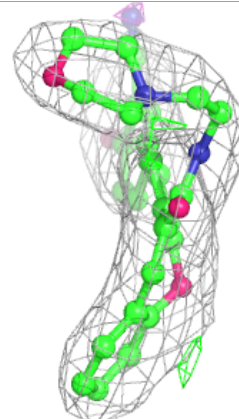
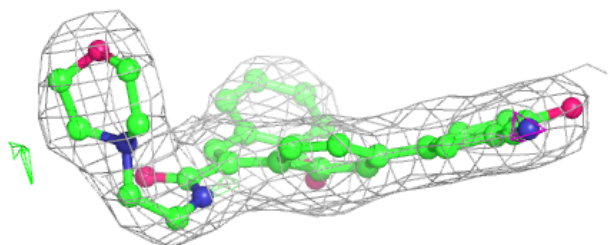
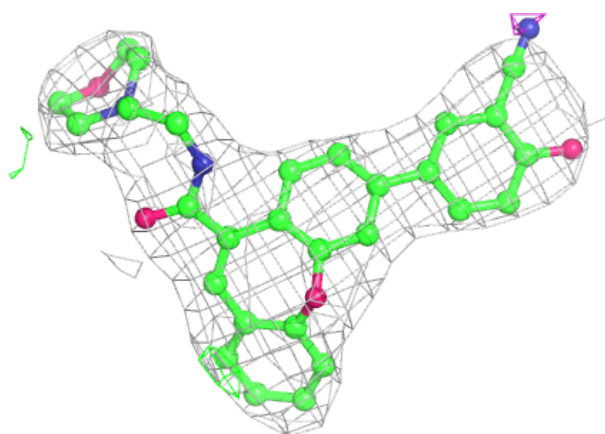


**Electron density around M3D A 503:**

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

**Electron density around M3D C 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 [i](#)

There are no such residues in this entry.