



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:52 am BST

PDB ID : 6E43
Title : Crystal structure of human indoleamine 2,3-dioxygenase 1 (IDO1) in complex with a BMS-978587 analog
Authors : Luo, S.; Tong, L.
Deposited on : 2018-07-16
Resolution : 1.71 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 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 : 2.11
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) : 2.11

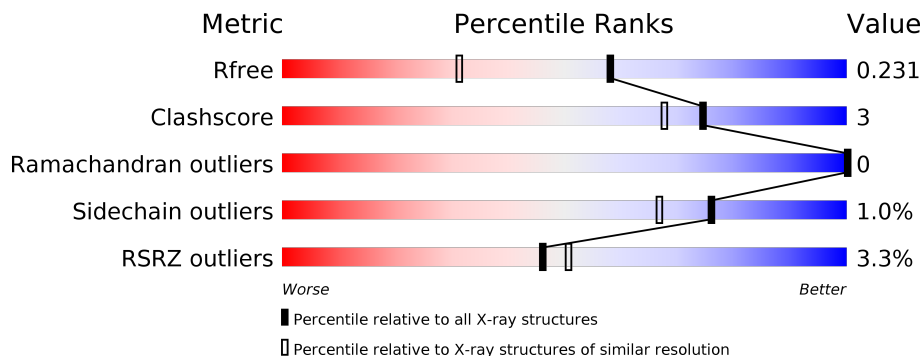
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	405	 3% 84% 8% 8%
1	B	405	 3% 86% 6% 8%
1	C	405	 2% 88% 7% 5%
1	D	405	 4% 85% 7% 7%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 13245 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 Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	372	2943	1893	501	530	19	0	2	0
1	B	373	2951	1898	502	531	20	0	3	0
1	C	375	2964	1905	504	536	19	0	3	0
1	D	375	2962	1903	504	536	19	0	2	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P14902
A	0	GLY	-	expression tag	UNP P14902
A	1	SER	-	expression tag	UNP P14902
A	2	SER	-	expression tag	UNP P14902
A	3	HIS	-	expression tag	UNP P14902
A	4	HIS	-	expression tag	UNP P14902
A	5	HIS	-	expression tag	UNP P14902
A	6	HIS	-	expression tag	UNP P14902
A	7	HIS	-	expression tag	UNP P14902
A	8	HIS	-	expression tag	UNP P14902
A	9	SER	-	expression tag	UNP P14902
A	10	SER	-	expression tag	UNP P14902
A	11	GLY	-	expression tag	UNP P14902
A	12	SER	-	expression tag	UNP P14902
A	13	ALA	-	expression tag	UNP P14902
A	14	ALA	-	expression tag	UNP P14902
A	116	ALA	LYS	engineered mutation	UNP P14902
A	117	ALA	LYS	engineered mutation	UNP P14902
B	-1	MET	-	initiating methionine	UNP P14902
B	0	GLY	-	expression tag	UNP P14902
B	1	SER	-	expression tag	UNP P14902

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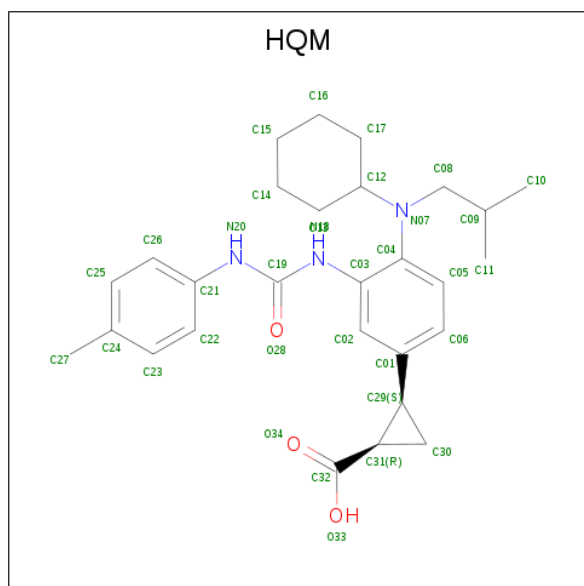
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP P14902
B	3	HIS	-	expression tag	UNP P14902
B	4	HIS	-	expression tag	UNP P14902
B	5	HIS	-	expression tag	UNP P14902
B	6	HIS	-	expression tag	UNP P14902
B	7	HIS	-	expression tag	UNP P14902
B	8	HIS	-	expression tag	UNP P14902
B	9	SER	-	expression tag	UNP P14902
B	10	SER	-	expression tag	UNP P14902
B	11	GLY	-	expression tag	UNP P14902
B	12	SER	-	expression tag	UNP P14902
B	13	ALA	-	expression tag	UNP P14902
B	14	ALA	-	expression tag	UNP P14902
B	116	ALA	LYS	engineered mutation	UNP P14902
B	117	ALA	LYS	engineered mutation	UNP P14902
C	-1	MET	-	initiating methionine	UNP P14902
C	0	GLY	-	expression tag	UNP P14902
C	1	SER	-	expression tag	UNP P14902
C	2	SER	-	expression tag	UNP P14902
C	3	HIS	-	expression tag	UNP P14902
C	4	HIS	-	expression tag	UNP P14902
C	5	HIS	-	expression tag	UNP P14902
C	6	HIS	-	expression tag	UNP P14902
C	7	HIS	-	expression tag	UNP P14902
C	8	HIS	-	expression tag	UNP P14902
C	9	SER	-	expression tag	UNP P14902
C	10	SER	-	expression tag	UNP P14902
C	11	GLY	-	expression tag	UNP P14902
C	12	SER	-	expression tag	UNP P14902
C	13	ALA	-	expression tag	UNP P14902
C	14	ALA	-	expression tag	UNP P14902
C	116	ALA	LYS	engineered mutation	UNP P14902
C	117	ALA	LYS	engineered mutation	UNP P14902
D	-1	MET	-	initiating methionine	UNP P14902
D	0	GLY	-	expression tag	UNP P14902
D	1	SER	-	expression tag	UNP P14902
D	2	SER	-	expression tag	UNP P14902
D	3	HIS	-	expression tag	UNP P14902
D	4	HIS	-	expression tag	UNP P14902
D	5	HIS	-	expression tag	UNP P14902
D	6	HIS	-	expression tag	UNP P14902
D	7	HIS	-	expression tag	UNP P14902

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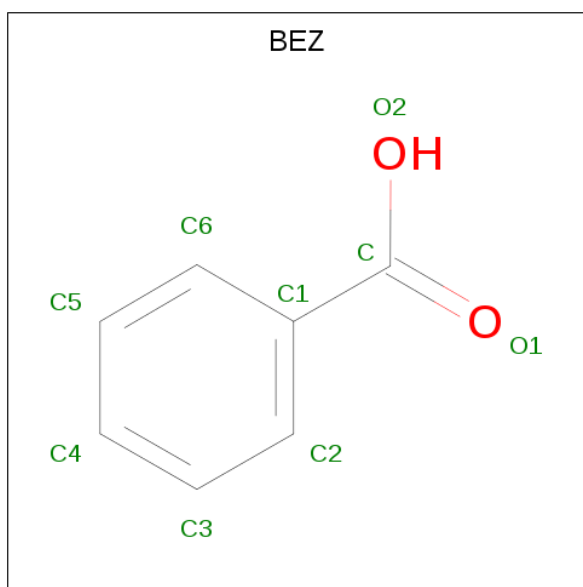
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P14902
D	9	SER	-	expression tag	UNP P14902
D	10	SER	-	expression tag	UNP P14902
D	11	GLY	-	expression tag	UNP P14902
D	12	SER	-	expression tag	UNP P14902
D	13	ALA	-	expression tag	UNP P14902
D	14	ALA	-	expression tag	UNP P14902
D	116	ALA	LYS	engineered mutation	UNP P14902
D	117	ALA	LYS	engineered mutation	UNP P14902

- Molecule 2 is (1R,2S)-2-(4-[cyclohexyl(2-methylpropyl)amino]-3-[(4-methylphenyl)carbamoyl]amino}phenyl)cyclopropane-1-carboxylic acid (three-letter code: HQM) (formula: C₂₈H₃₇N₃O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	N	O	0	0
			34	28	3	3		
2	B	1	Total	C	N	O	0	0
			34	28	3	3		
2	C	1	Total	C	N	O	0	0
			34	28	3	3		
2	D	1	Total	C	N	O	0	0
			34	28	3	3		

- Molecule 3 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0
3	C	1	Total C O 9 7 2	0	0
3	D	1	Total C O 9 7 2	0	0

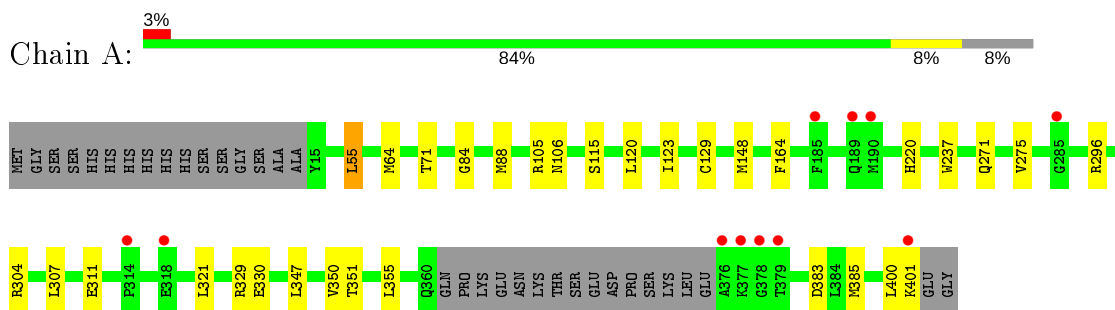
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	272	Total O 272 272	0	0
4	B	271	Total O 271 271	0	0
4	C	338	Total O 338 338	0	0
4	D	372	Total O 372 372	0	0

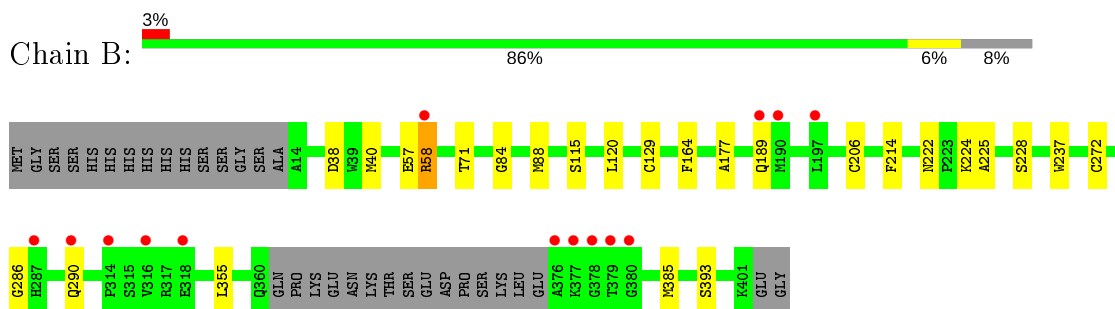
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

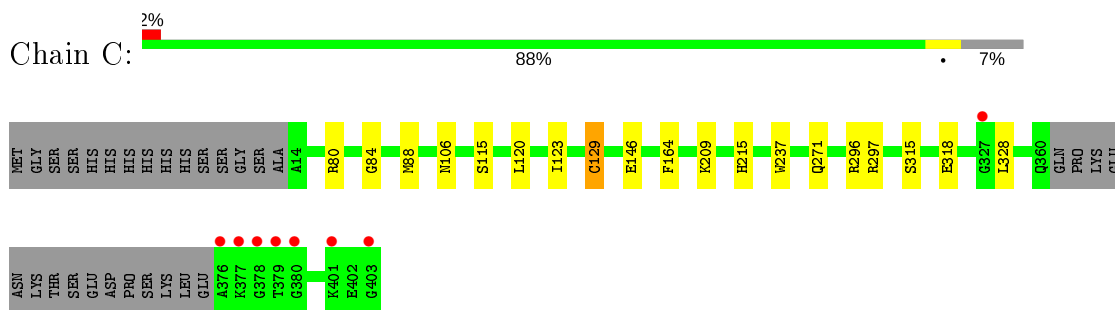
- Molecule 1: Indoleamine 2,3-dioxygenase 1



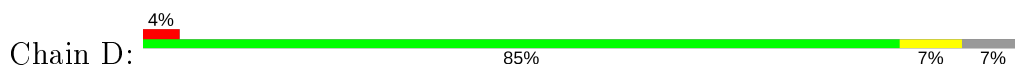
- Molecule 1: Indoleamine 2,3-dioxygenase 1

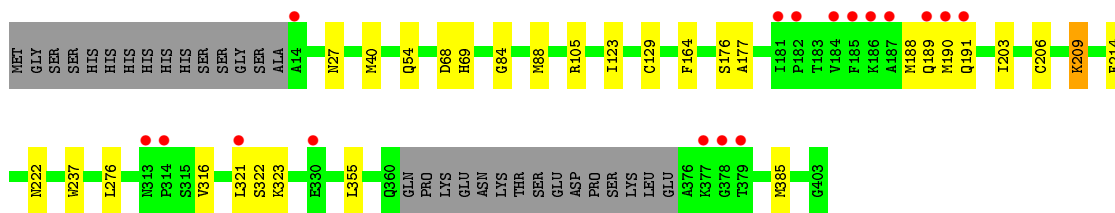


- Molecule 1: Indoleamine 2,3-dioxygenase 1



- Molecule 1: Indoleamine 2,3-dioxygenase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.48Å 195.39Å 118.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 1.71 47.64 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.64-1.71) 99.1 (47.64-1.71)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.71Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.194 , 0.231 0.194 , 0.231	Depositor DCC
R_{free} test set	3011 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtrriage
Anisotropy	0.106	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13245	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 44.22 % 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 1.5745e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: BEZ, HQM

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	0.41	0/3017	0.53	1/4082 (0.0%)
1	B	0.36	0/3028	0.53	1/4097 (0.0%)
1	C	0.46	2/3041 (0.1%)	0.54	0/4114
1	D	0.40	0/3036	0.55	0/4106
All	All	0.41	2/12122 (0.0%)	0.54	2/16399 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129[A]	CYS	CB-SG	-5.05	1.73	1.81
1	C	129[B]	CYS	CB-SG	-5.05	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	LEU	CA-CB-CG	-6.82	99.61	115.30
1	B	58	ARG	NE-CZ-NH1	5.53	123.06	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2943	0	2961	28	0
1	B	2951	0	2971	18	0
1	C	2964	0	2980	14	0
1	D	2962	0	2975	18	0
2	A	34	0	0	0	0
2	B	34	0	0	0	0
2	C	34	0	0	0	0
2	D	34	0	0	0	0
3	A	9	0	5	0	0
3	B	9	0	5	1	0
3	C	9	0	5	0	0
3	D	9	0	5	1	0
4	A	272	0	0	6	0
4	B	271	0	0	7	0
4	C	338	0	0	3	1
4	D	372	0	0	2	1
All	All	13245	0	11907	76	1

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 (76) 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:88[A]:MET:SD	4:B:715:HOH:O	2.35	0.83
1:B:222:ASN:HD22	1:B:225:ALA:H	1.26	0.83
1:B:58:ARG:NH1	4:B:601:HOH:O	2.15	0.79
1:D:189:GLN:NE2	1:D:190:MET:SD	2.57	0.78
1:A:88[B]:MET:HE1	1:A:123:ILE:HG13	1.67	0.75
1:D:88[A]:MET:HE1	1:D:123:ILE:HG13	1.70	0.73
1:C:88[B]:MET:HE1	1:C:123:ILE:HG13	1.73	0.71
1:C:297:ARG:NH1	4:C:602:HOH:O	2.25	0.69
1:A:271:GLN:HE22	1:A:296:ARG:HE	1.41	0.67
1:A:350:VAL:HB	1:A:385:MET:HE2	1.78	0.65
1:A:329:ARG:HE	1:A:401:LYS:HE2	1.62	0.65
1:A:105:ARG:NH1	4:A:605:HOH:O	2.30	0.64
1:B:57:GLU:HG3	4:B:610:HOH:O	1.98	0.63
1:A:296:ARG:O	1:A:304:ARG:HD3	1.99	0.63
1:D:355:LEU:HD11	1:D:385:MET:HG3	1.82	0.62
1:C:129[A]:CYS:SG	1:C:164:PHE:CZ	2.94	0.60
1:A:350:VAL:HB	1:A:385:MET:CE	2.32	0.60
1:B:129[B]:CYS:SG	1:B:164:PHE:CZ	2.95	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASN:ND2	1:B:225:ALA:H	1.97	0.60
1:D:129[B]:CYS:SG	1:D:164:PHE:CZ	2.95	0.60
1:D:68:ASP:OD2	1:D:69:HIS:ND1	2.35	0.59
1:A:355:LEU:HD11	1:A:385:MET:HG3	1.84	0.59
1:B:286:GLY:O	1:B:290:GLN:HG3	2.04	0.58
1:C:271:GLN:HE22	1:C:296:ARG:HE	1.53	0.57
1:A:330:GLU:OE2	4:A:601:HOH:O	2.18	0.56
1:B:71:THR:OG1	4:B:602:HOH:O	2.18	0.56
1:B:355:LEU:HD11	1:B:385:MET:HG3	1.90	0.54
1:C:146:GLU:HG2	1:D:222:ASN:HB2	1.90	0.52
1:B:224:LYS:HE3	1:B:228:SER:HB3	1.91	0.52
1:A:71:THR:HB	1:D:54:GLN:HG2	1.92	0.52
1:A:129[B]:CYS:SG	1:A:164:PHE:CZ	3.03	0.51
1:C:209:LYS:HA	1:C:209:LYS:HE2	1.93	0.51
1:A:220:HIS:HE1	4:A:718:HOH:O	1.92	0.51
1:A:271:GLN:NE2	1:A:296:ARG:HE	2.07	0.50
1:A:55:LEU:HG	1:A:55:LEU:O	2.07	0.50
1:D:84:GLY:O	1:D:88[B]:MET:HG2	2.11	0.50
1:B:84:GLY:O	1:B:88[A]:MET:HG2	2.12	0.50
1:A:329:ARG:HH21	1:A:401:LYS:NZ	2.10	0.49
1:A:115:SER:HB3	1:A:120:LEU:O	2.13	0.48
1:A:84:GLY:O	1:A:88[A]:MET:HG2	2.14	0.48
1:D:322:SER:OG	1:D:323:LYS:NZ	2.39	0.48
1:A:329:ARG:HE	1:A:401:LYS:CE	2.26	0.48
1:C:315:SER:HB3	1:C:318:GLU:HB3	1.96	0.48
1:A:148:MET:HB2	1:A:148:MET:HE3	1.77	0.47
1:B:40:MET:HG3	4:B:721:HOH:O	2.14	0.47
1:D:176:SER:HB2	1:D:206:CYS:SG	2.55	0.47
1:B:214:PHE:HZ	3:B:502:BEZ:H2	1.80	0.46
1:C:84:GLY:O	1:C:88[A]:MET:HG2	2.15	0.46
1:C:271:GLN:NE2	1:C:296:ARG:HE	2.13	0.46
1:A:307:LEU:O	1:A:311:GLU:HG3	2.16	0.46
1:A:106:ASN:HB2	4:A:789:HOH:O	2.15	0.46
1:C:106:ASN:HB2	4:C:760:HOH:O	2.16	0.45
1:C:209:LYS:HE3	4:C:809:HOH:O	2.16	0.45
1:A:275:VAL:HG13	1:A:311:GLU:HG2	1.98	0.45
1:A:64:MET:HB2	1:A:106:ASN:ND2	2.32	0.44
1:D:214:PHE:HZ	3:D:502:BEZ:H6	1.82	0.44
1:D:40:MET:HG3	4:D:789:HOH:O	2.18	0.44
1:A:106:ASN:HB2	4:A:750:HOH:O	2.17	0.43
1:D:188:MET:SD	1:D:316:VAL:HG22	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:O	1:A:385:MET:HE1	2.18	0.43
1:A:351:THR:HA	1:A:355:LEU:HB2	1.98	0.43
1:D:203:ILE:HD13	1:D:276:LEU:HD21	2.00	0.43
1:B:58:ARG:NE	4:B:606:HOH:O	2.37	0.43
1:B:115:SER:HB3	1:B:120:LEU:O	2.18	0.43
1:C:115:SER:HB3	1:C:120:LEU:O	2.19	0.42
1:A:321:LEU:HD21	1:A:400:LEU:HD22	2.01	0.42
1:D:209:LYS:HG3	1:D:209:LYS:O	2.20	0.42
1:D:27:ASN:ND2	4:D:617:HOH:O	2.53	0.42
1:A:355:LEU:O	4:A:602:HOH:O	2.22	0.41
1:B:38:ASP:HA	4:B:601:HOH:O	2.21	0.41
1:C:209:LYS:HE2	1:C:209:LYS:CA	2.50	0.41
1:D:177:ALA:HB2	1:D:206:CYS:HB2	2.02	0.41
1:B:222:ASN:HD21	1:B:224:LYS:HB3	1.85	0.41
1:C:328:LEU:HA	1:C:328:LEU:HD23	1.94	0.41
1:B:177:ALA:HB2	1:B:206:CYS:HB2	2.02	0.40
1:D:321:LEU:HA	1:D:321:LEU:HD23	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:713:HOH:O	4:D:900:HOH:O[1_455]	2.15	0.05

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	370/405 (91%)	363 (98%)	7 (2%)	0	100	100
1	B	372/405 (92%)	365 (98%)	7 (2%)	0	100	100
1	C	374/405 (92%)	366 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	373/405 (92%)	368 (99%)	5 (1%)	0	100	100
All	All	1489/1620 (92%)	1462 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/346 (92%)	318 (99%)	2 (1%)	86	80
1	B	321/346 (93%)	316 (98%)	5 (2%)	62	48
1	C	322/346 (93%)	319 (99%)	3 (1%)	78	70
1	D	321/346 (93%)	317 (99%)	4 (1%)	71	59
All	All	1284/1384 (93%)	1270 (99%)	14 (1%)	76	63

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	TRP
1	A	383	ASP
1	B	189	GLN
1	B	237	TRP
1	B	272[A]	CYS
1	B	272[B]	CYS
1	B	393	SER
1	C	80	ARG
1	C	215	HIS
1	C	237	TRP
1	D	105	ARG
1	D	191	GLN
1	D	209	LYS
1	D	237	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	106	ASN
1	A	140	ASN
1	A	222	ASN
1	A	271	GLN
1	B	191	GLN
1	B	222	ASN
1	B	290	GLN
1	B	360	GLN
1	B	386	ASN
1	C	27	ASN
1	C	29	GLN
1	C	63	ASN
1	C	271	GLN
1	C	348	GLN
1	C	386	ASN
1	D	242	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HQM	C	501	-	33,37,37	1.63	8 (24%)	45,52,52	1.95	8 (17%)
2	HQM	A	501	-	33,37,37	1.80	9 (27%)	45,52,52	1.84	6 (13%)
2	HQM	B	501	-	33,37,37	1.64	8 (24%)	45,52,52	1.73	6 (13%)
2	HQM	D	501	-	33,37,37	1.65	7 (21%)	45,52,52	2.02	8 (17%)
3	BEZ	A	502	-	7,9,9	1.15	1 (14%)	8,11,11	0.83	0
3	BEZ	B	502	-	7,9,9	1.34	1 (14%)	8,11,11	0.60	0
3	BEZ	C	502	-	7,9,9	1.04	1 (14%)	8,11,11	0.77	0
3	BEZ	D	502	-	7,9,9	1.23	1 (14%)	8,11,11	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HQM	C	501	-	-	7/24/41/41	0/4/4/4
2	HQM	A	501	-	-	6/24/41/41	0/4/4/4
2	HQM	B	501	-	-	5/24/41/41	0/4/4/4
2	HQM	D	501	-	-	5/24/41/41	0/4/4/4
3	BEZ	A	502	-	-	0/0/4/4	0/1/1/1
3	BEZ	B	502	-	-	0/0/4/4	0/1/1/1
3	BEZ	C	502	-	-	0/0/4/4	0/1/1/1
3	BEZ	D	502	-	-	0/0/4/4	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HQM	C19-N18	4.96	1.47	1.37
2	D	501	HQM	C19-N18	4.12	1.46	1.37
2	A	501	HQM	C19-N20	4.10	1.46	1.37
2	B	501	HQM	C19-N18	4.07	1.45	1.37
2	C	501	HQM	C19-N20	3.97	1.45	1.37
2	C	501	HQM	C19-N18	3.75	1.45	1.37
2	B	501	HQM	C19-N20	3.72	1.45	1.37
2	D	501	HQM	C19-N20	3.64	1.45	1.37
3	B	502	BEZ	C1-C	3.39	1.50	1.47
2	B	501	HQM	C04-N07	3.22	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HQM	C04-N07	3.10	1.51	1.41
3	D	502	BEZ	C1-C	3.04	1.50	1.47
2	A	501	HQM	C04-N07	3.04	1.51	1.41
2	D	501	HQM	C01-C29	3.00	1.56	1.51
2	A	501	HQM	C21-N20	2.97	1.47	1.41
3	A	502	BEZ	C1-C	2.90	1.50	1.47
2	C	501	HQM	C04-N07	2.85	1.50	1.41
2	A	501	HQM	C03-N18	2.85	1.47	1.41
2	C	501	HQM	C12-N07	2.72	1.52	1.47
2	A	501	HQM	C12-N07	2.70	1.52	1.47
2	A	501	HQM	C01-C29	2.70	1.55	1.51
2	C	501	HQM	C01-C29	2.68	1.55	1.51
2	D	501	HQM	C12-N07	2.64	1.52	1.47
3	C	502	BEZ	C1-C	2.53	1.49	1.47
2	B	501	HQM	C08-N07	2.44	1.51	1.47
2	B	501	HQM	C01-C29	2.40	1.55	1.51
2	B	501	HQM	C12-N07	2.39	1.51	1.47
2	B	501	HQM	C21-N20	2.35	1.46	1.41
2	C	501	HQM	C08-N07	2.29	1.51	1.47
2	C	501	HQM	C21-N20	2.23	1.46	1.41
2	D	501	HQM	C08-N07	2.23	1.51	1.47
2	D	501	HQM	C03-C04	-2.19	1.38	1.40
2	B	501	HQM	C03-C04	-2.15	1.38	1.40
2	A	501	HQM	O28-C19	-2.15	1.18	1.23
2	C	501	HQM	C03-N18	2.15	1.45	1.41
2	A	501	HQM	C08-N07	2.07	1.51	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HQM	C13-C12-N07	-8.22	101.77	112.80
2	C	501	HQM	C17-C12-N07	-7.74	102.42	112.80
2	B	501	HQM	C13-C12-N07	-7.06	103.32	112.80
2	A	501	HQM	C13-C12-N07	-6.12	104.58	112.80
2	D	501	HQM	C30-C29-C01	5.86	133.53	122.24
2	A	501	HQM	C30-C29-C01	5.81	133.41	122.24
2	C	501	HQM	C30-C29-C01	5.16	132.16	122.24
2	B	501	HQM	C30-C29-C01	4.86	131.59	122.24
2	D	501	HQM	C21-N20-C19	-3.98	118.47	126.61
2	C	501	HQM	C21-N20-C19	-3.90	118.64	126.61
2	C	501	HQM	C01-C29-C31	3.82	127.16	121.31
2	A	501	HQM	C01-C29-C31	3.81	127.14	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HQM	C21-N20-C19	-3.52	119.41	126.61
2	B	501	HQM	C21-N20-C19	-3.39	119.68	126.61
2	D	501	HQM	C26-C21-C22	3.26	123.50	119.03
2	D	501	HQM	C23-C22-C21	-3.10	116.72	120.30
2	B	501	HQM	C26-C21-C22	2.92	123.03	119.03
2	D	501	HQM	C26-C25-C24	-2.70	117.77	121.38
2	C	501	HQM	C26-C21-C22	2.64	122.64	119.03
2	C	501	HQM	C22-C23-C24	-2.63	117.85	121.38
2	C	501	HQM	C25-C26-C21	-2.25	117.70	120.30
2	B	501	HQM	C01-C29-C31	2.17	124.64	121.31
2	D	501	HQM	C30-C31-C32	-2.16	115.81	120.02
2	B	501	HQM	C23-C22-C21	-2.12	117.85	120.30
2	C	501	HQM	C05-C06-C01	-2.11	119.08	121.20
2	D	501	HQM	C25-C24-C23	2.08	122.67	118.11
2	A	501	HQM	C26-C21-C22	2.05	121.83	119.03
2	A	501	HQM	N20-C19-N18	2.00	115.99	112.49

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	HQM	C09-C08-N07-C04
2	A	501	HQM	C09-C08-N07-C04
2	B	501	HQM	C09-C08-N07-C04
2	D	501	HQM	C09-C08-N07-C04
2	A	501	HQM	N07-C08-C09-C11
2	A	501	HQM	N07-C08-C09-C10
2	A	501	HQM	C03-C04-N07-C08
2	C	501	HQM	C03-C04-N07-C08
2	B	501	HQM	C03-C04-N07-C08
2	D	501	HQM	C03-C04-N07-C08
2	C	501	HQM	N07-C08-C09-C11
2	A	501	HQM	C05-C04-N07-C08
2	A	501	HQM	C17-C12-N07-C08
2	B	501	HQM	C05-C04-N07-C08
2	C	501	HQM	C05-C04-N07-C08
2	D	501	HQM	C05-C04-N07-C08
2	C	501	HQM	C13-C12-N07-C08
2	B	501	HQM	C17-C12-N07-C08
2	C	501	HQM	C05-C04-N07-C12
2	B	501	HQM	C05-C04-N07-C12
2	D	501	HQM	C05-C04-N07-C12

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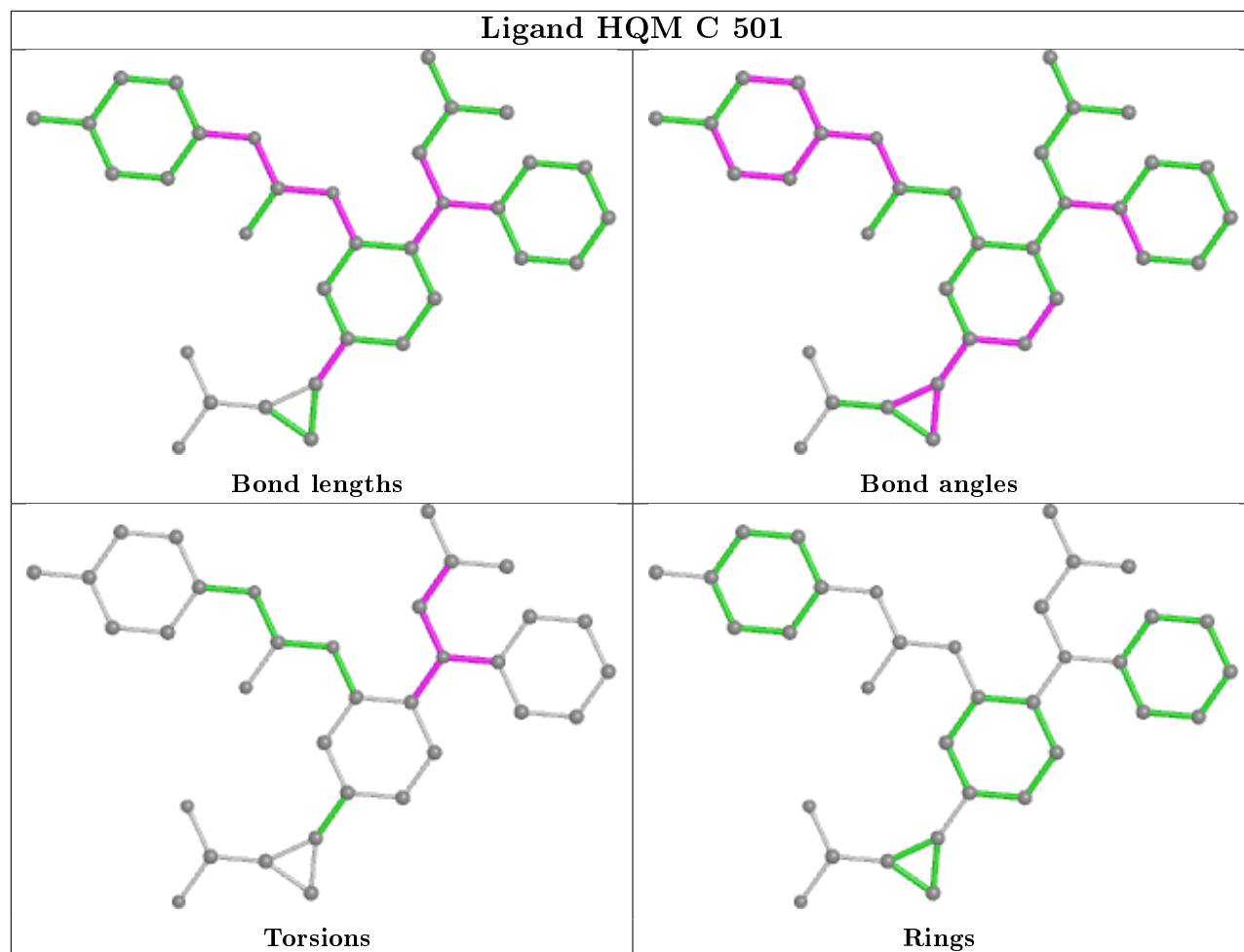
Mol	Chain	Res	Type	Atoms
2	C	501	HQM	N07-C08-C09-C10
2	D	501	HQM	C26-C21-N20-C19

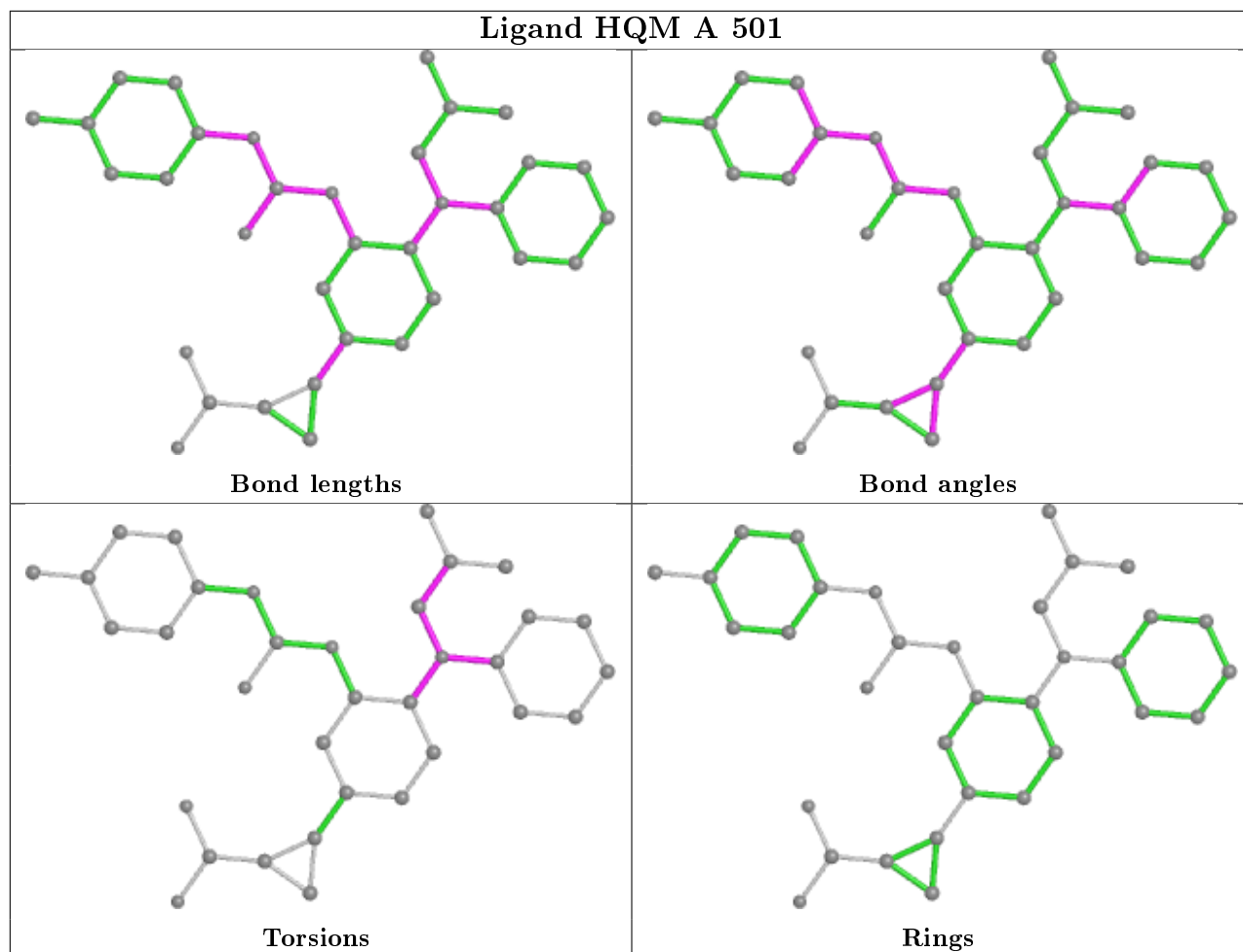
There are no ring outliers.

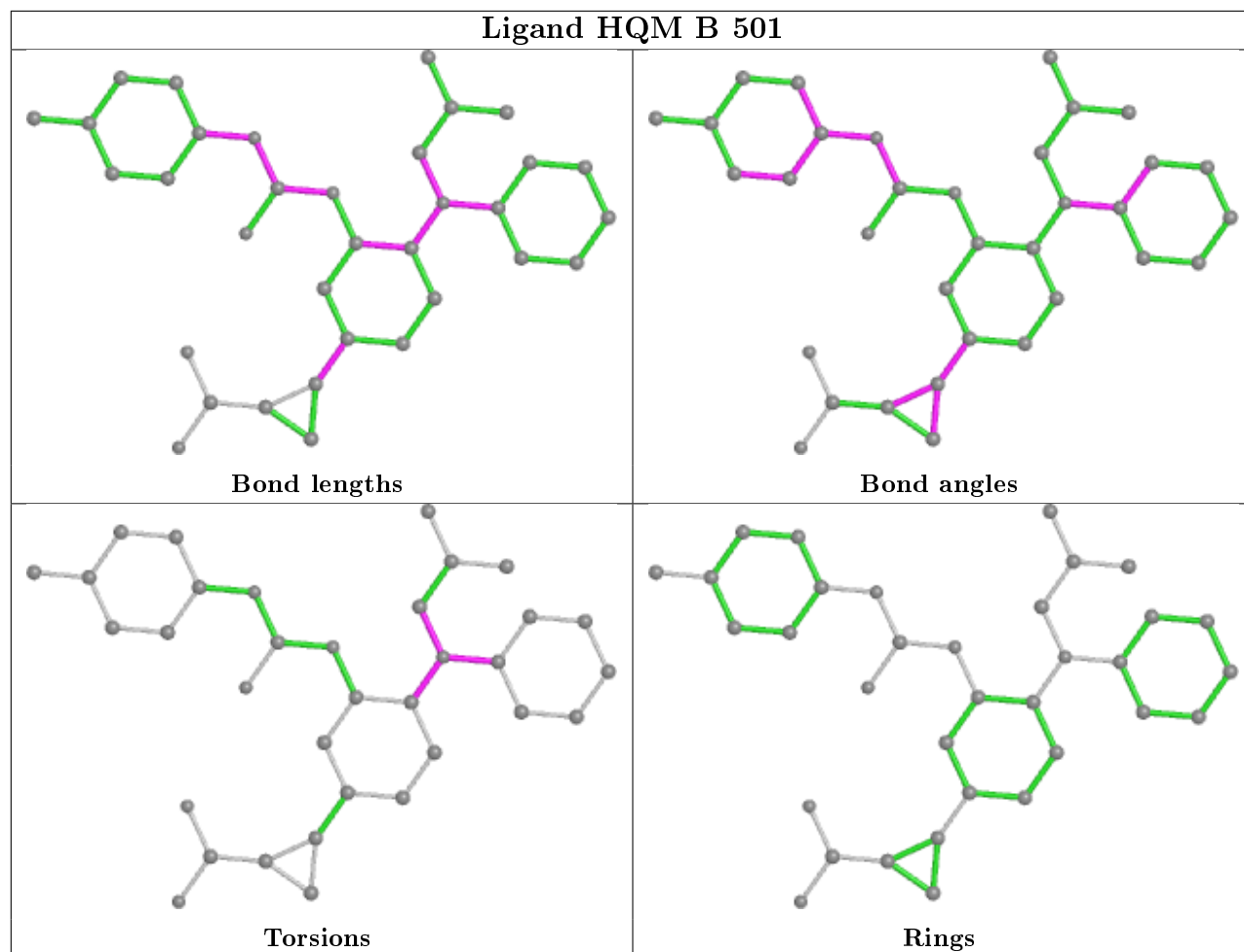
2 monomers are involved in 2 short contacts:

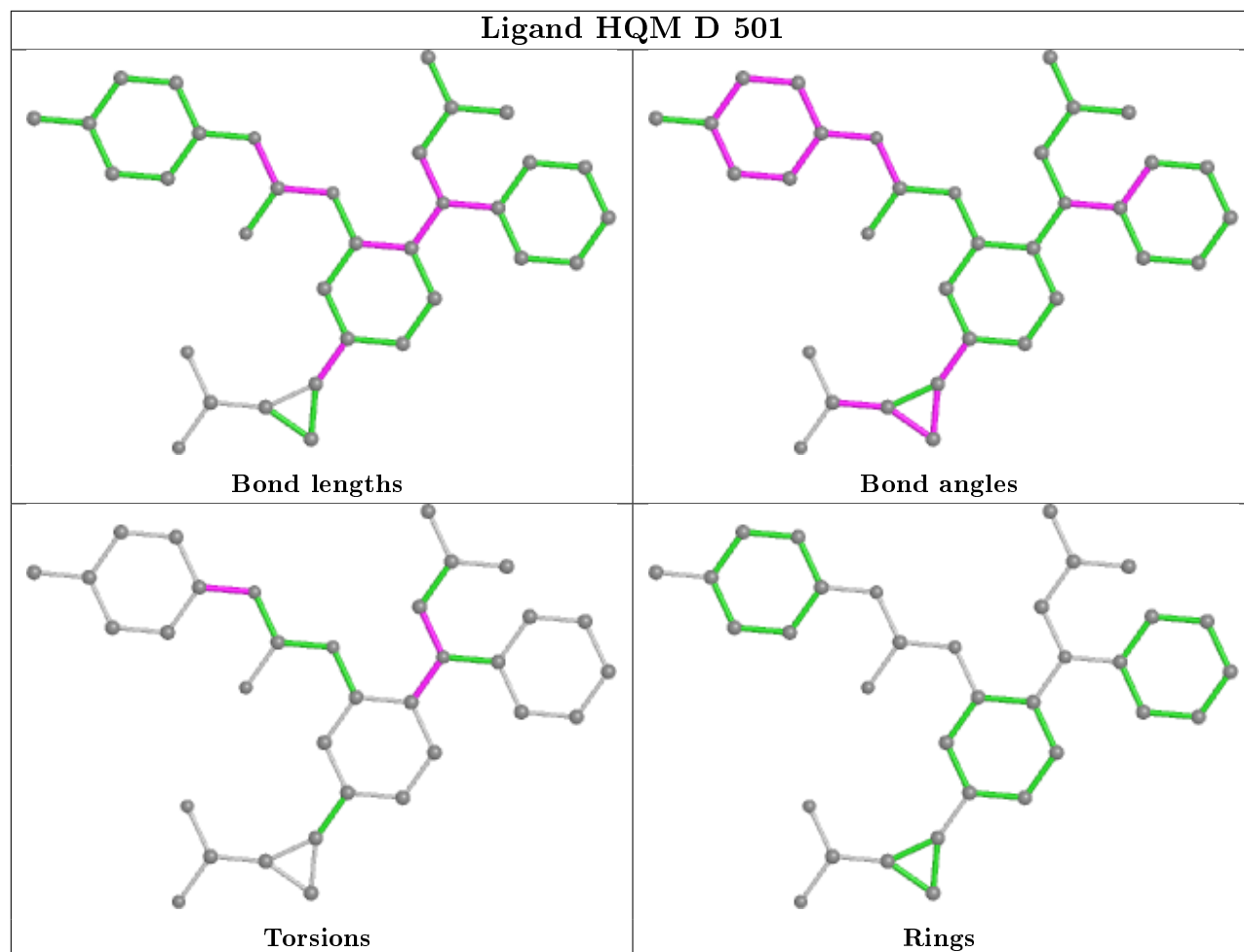
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	BEZ	1	0
3	D	502	BEZ	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	372/405 (91%)	0.18	11 (2%) 50 54	20, 34, 50, 60	0
1	B	373/405 (92%)	0.25	14 (3%) 40 45	19, 33, 51, 62	0
1	C	375/405 (92%)	0.11	8 (2%) 63 67	19, 30, 48, 65	0
1	D	375/405 (92%)	0.18	17 (4%) 33 37	17, 28, 45, 57	0
All	All	1495/1620 (92%)	0.18	50 (3%) 46 51	17, 32, 49, 65	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	379	THR	6.9
1	A	379	THR	6.6
1	B	379	THR	5.9
1	D	189	GLN	4.9
1	C	378	GLY	4.5
1	C	377	LYS	4.4
1	D	191	GLN	4.3
1	B	189	GLN	4.3
1	A	377	LYS	4.0
1	D	185	PHE	3.9
1	D	379	THR	3.8
1	C	403	GLY	3.7
1	D	190	MET	3.6
1	B	377	LYS	3.5
1	B	318	GLU	3.5
1	A	189	GLN	3.5
1	B	316	VAL	3.4
1	B	378	GLY	3.4
1	B	190	MET	3.3
1	B	380	GLY	3.2
1	B	314	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	378	GLY	3.1
1	C	380	GLY	3.0
1	A	378	GLY	3.0
1	C	376	ALA	3.0
1	D	181	ILE	2.9
1	D	314	PRO	2.9
1	B	376	ALA	2.8
1	D	377	LYS	2.8
1	A	285	GLY	2.7
1	D	184	VAL	2.7
1	A	314	PRO	2.6
1	C	327	GLY	2.5
1	D	14	ALA	2.5
1	C	401	LYS	2.4
1	D	313	ASN	2.4
1	A	190	MET	2.3
1	B	287	HIS	2.3
1	D	182	PRO	2.3
1	A	318	GLU	2.2
1	D	186	LYS	2.2
1	B	197	LEU	2.2
1	A	185	PHE	2.2
1	D	321	LEU	2.2
1	A	401	LYS	2.1
1	B	290	GLN	2.1
1	A	376	ALA	2.1
1	B	58	ARG	2.1
1	D	330	GLU	2.0
1	D	187	ALA	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 carbohydrates in this entry.

6.4 Ligands

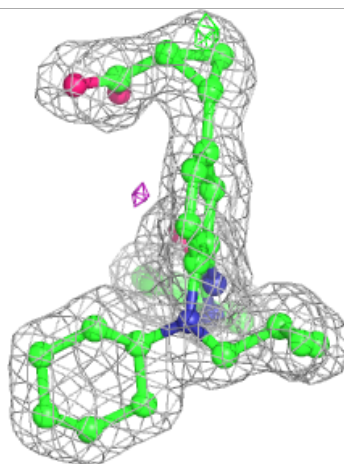
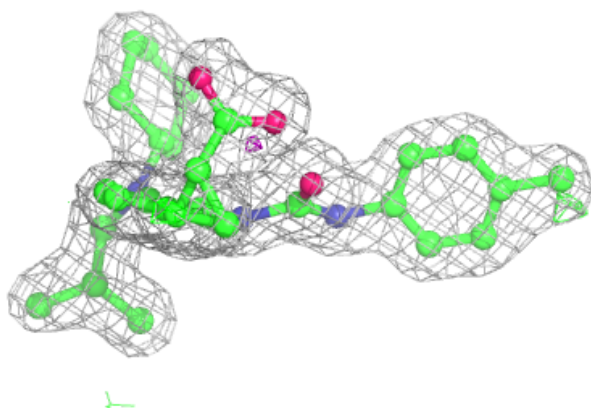
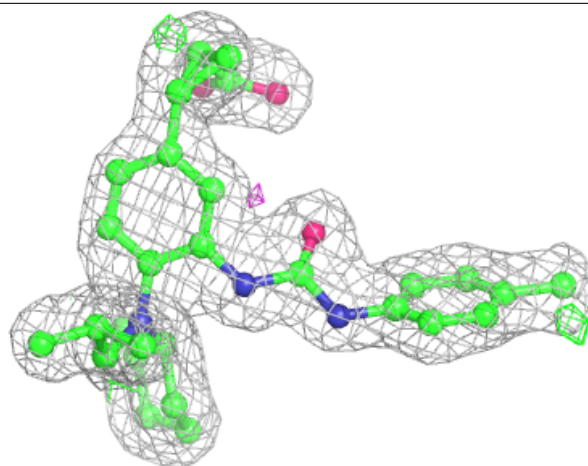
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

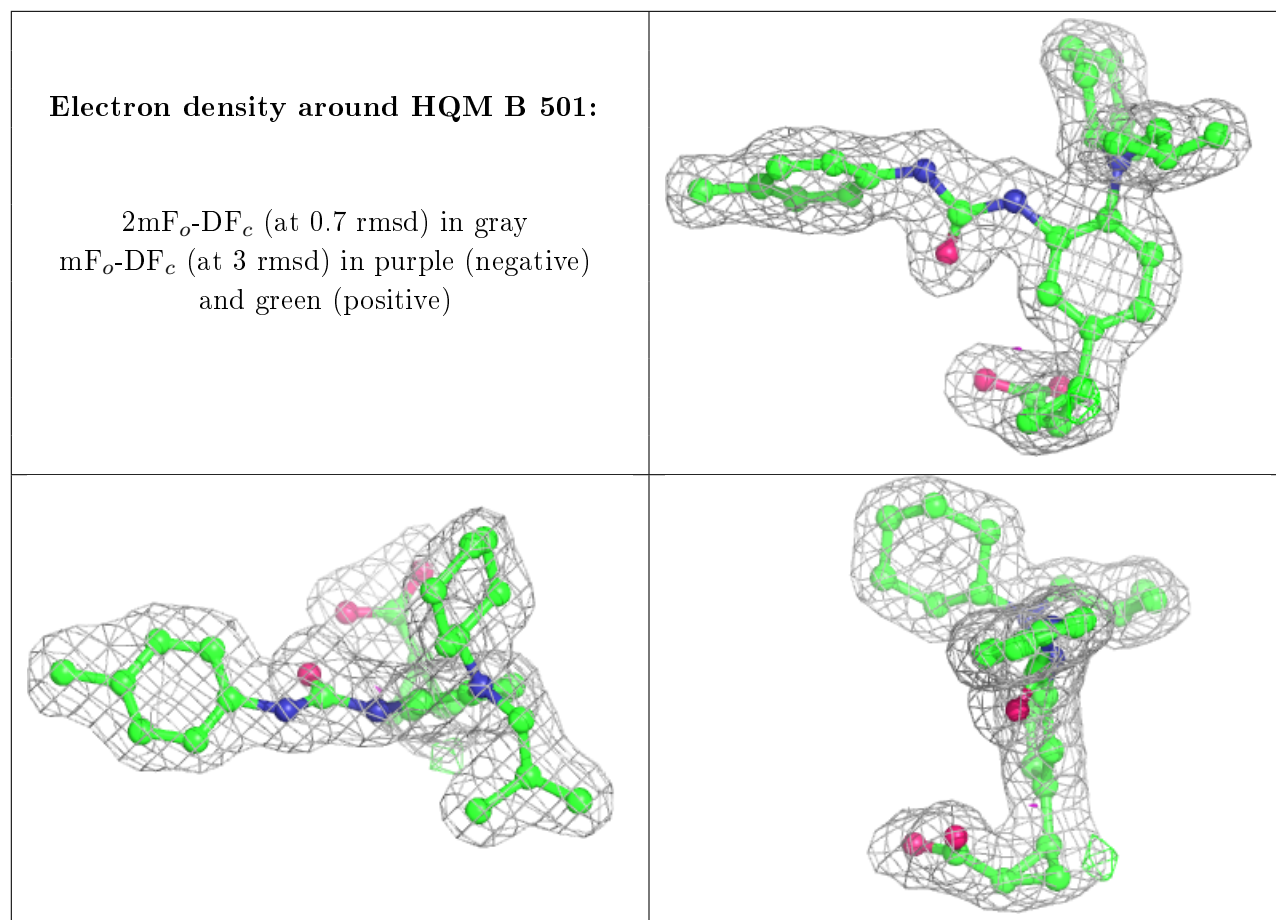
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BEZ	B	502	9/9	0.92	0.18	31,34,35,36	0
3	BEZ	A	502	9/9	0.93	0.11	33,34,37,38	0
2	HQM	A	501	34/34	0.93	0.10	25,29,40,42	0
3	BEZ	D	502	9/9	0.93	0.09	27,28,29,29	0
3	BEZ	C	502	9/9	0.94	0.14	28,30,31,32	0
2	HQM	B	501	34/34	0.95	0.10	22,26,35,39	0
2	HQM	D	501	34/34	0.95	0.12	19,23,33,35	0
2	HQM	C	501	34/34	0.96	0.10	20,24,36,37	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 HQM A 501:

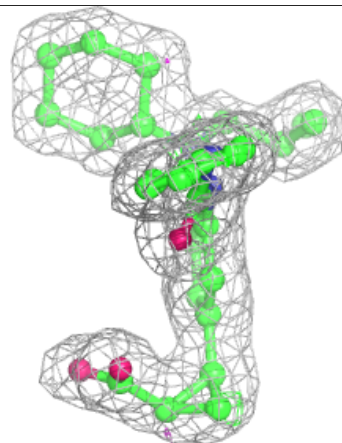
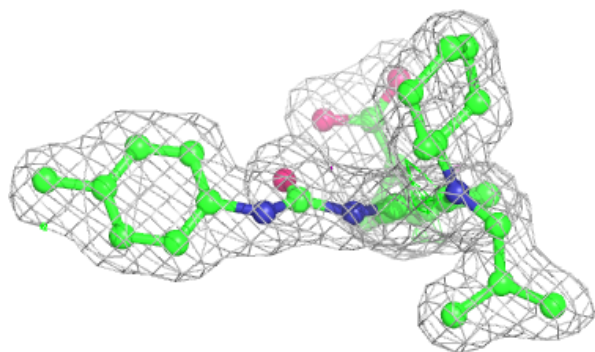
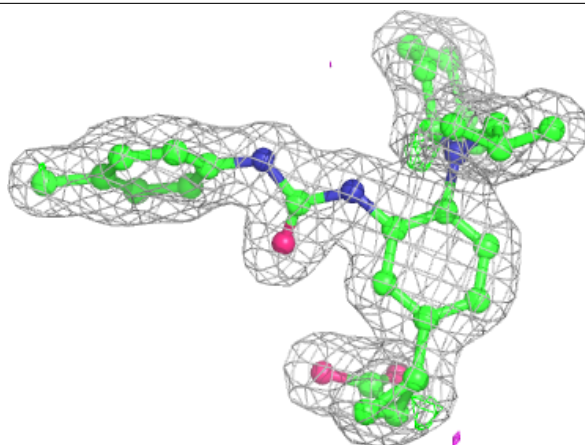
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

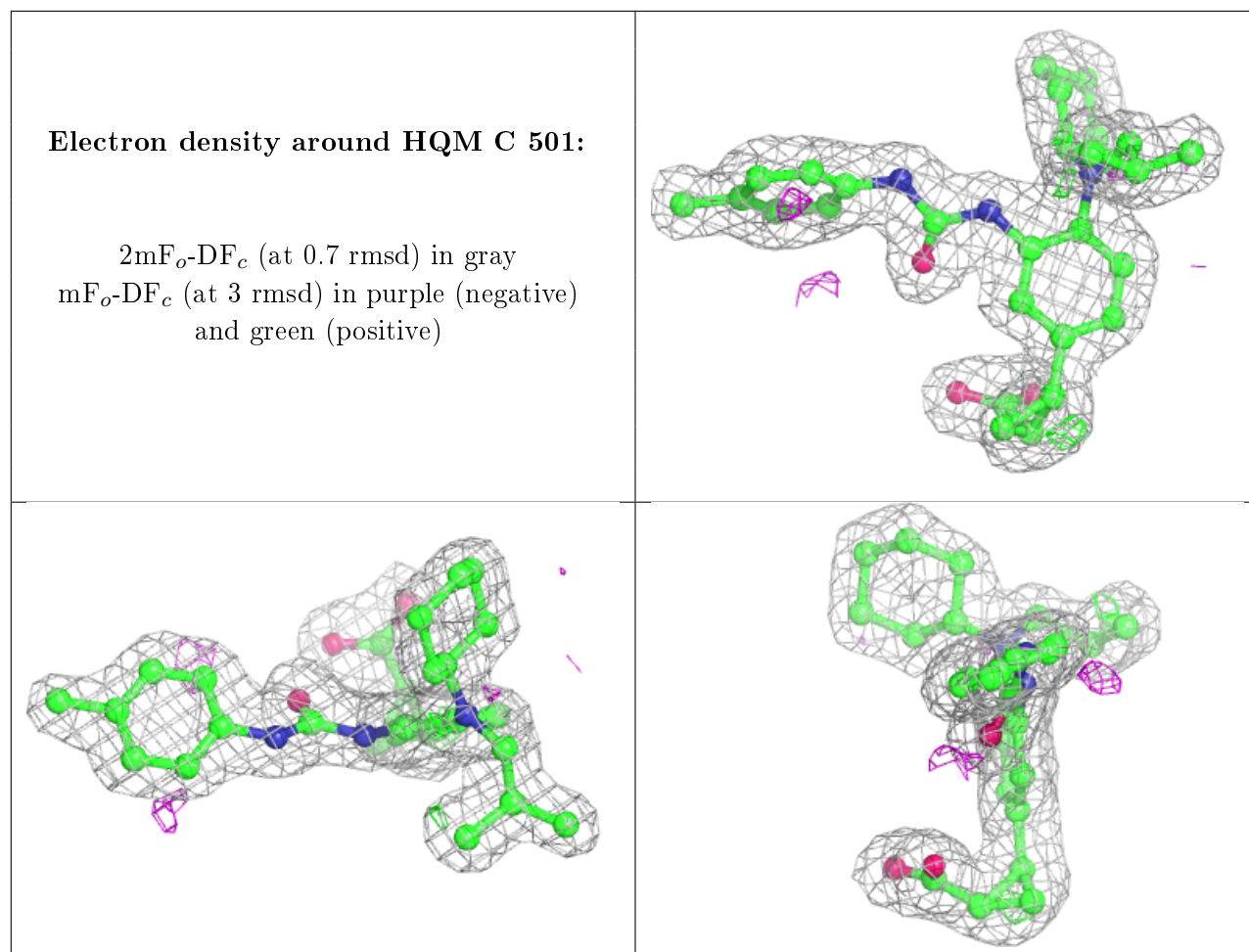




Electron density around HQM D 501:

$2mF_o-DF_c$ (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.