



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2025 – 08:48 pm GMT

PDB ID : 9HKF / pdb\_00009hkf  
Title : X-Ray crystal structure of a photoswitchable HaloTag bound to JF635  
Authors : Weidenhausen, J.; Ugarte-Uribe, B.; Walterspiel, F.; Mueller, C.W.; Deo, C.  
Deposited on : 2024-12-03  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

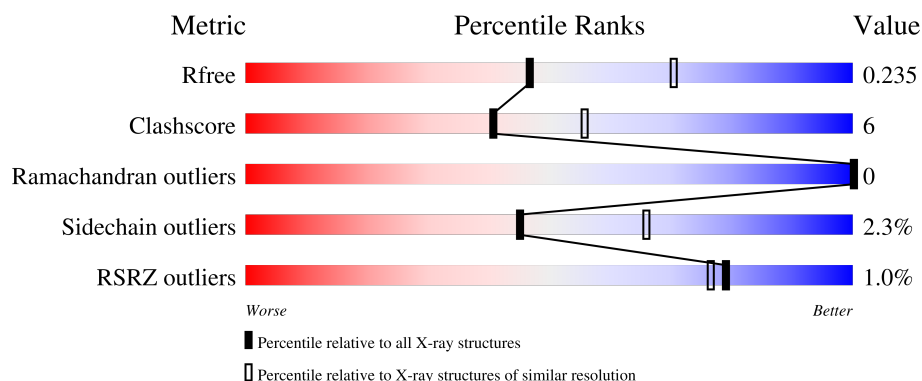
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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	439	 85% 13% 2% 2% 2%
1	B	439	 85% 12% 2% 2% 2%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	509	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7598 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 Haloalkane dehalogenase, non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	432	Total	C	N	O	S	0	0	0
			3496	2254	597	633	12			
1	A	432	Total	C	N	O	S	0	0	0
			3496	2254	597	633	12			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P0A3G2
B	0	PRO	-	expression tag	UNP P0A3G2
B	1	MET	-	expression tag	UNP P0A3G2
B	2	ALA	-	expression tag	UNP P0A3G2
B	47	VAL	LEU	engineered mutation	UNP P0A3G2
B	58	THR	SER	engineered mutation	UNP P0A3G2
B	78	GLY	ASP	engineered mutation	UNP P0A3G2
B	87	PHE	TYR	engineered mutation	UNP P0A3G2
B	88	MET	LEU	engineered mutation	UNP P0A3G2
B	128	PHE	CYS	engineered mutation	UNP P0A3G2
B	143	TRP	GLU	engineered mutation	UNP P0A3G2
B	144	PHE	-	linker	UNP P0A3G2
B	145	ALA	-	linker	UNP P0A3G2
B	146	GLY	-	linker	UNP P0A3G2
B	155	ILE	VAL	engineered mutation	UNP A0A453KFI0
B	200	ALA	ASP	engineered mutation	UNP A0A453KFI0
B	265	ARG	LYS	engineered mutation	UNP A0A453KFI0
B	283	PRO	-	linker	UNP A0A453KFI0
B	285	TRP	ALA	engineered mutation	UNP P0A3G2
B	295	THR	ALA	engineered mutation	UNP P0A3G2
B	300	LYS	GLU	engineered mutation	UNP P0A3G2
B	307	VAL	ALA	engineered mutation	UNP P0A3G2
B	312	THR	ALA	engineered mutation	UNP P0A3G2
B	315	MET	LYS	engineered mutation	UNP P0A3G2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	316	GLY	CYS	engineered mutation	UNP P0A3G2
B	335	ASN	LYS	engineered mutation	UNP P0A3G2
B	364	GLU	ALA	engineered mutation	UNP P0A3G2
B	367	ASP	ASN	engineered mutation	UNP P0A3G2
B	397	LYS	GLU	engineered mutation	UNP P0A3G2
B	404	ALA	THR	engineered mutation	UNP P0A3G2
B	412	ASN	HIS	engineered mutation	UNP P0A3G2
B	413	LEU	TYR	engineered mutation	UNP P0A3G2
B	431	SER	-	expression tag	UNP P0A3G2
B	432	THR	-	expression tag	UNP P0A3G2
B	433	LEU	-	expression tag	UNP P0A3G2
B	434	GLU	-	expression tag	UNP P0A3G2
B	435	ILE	-	expression tag	UNP P0A3G2
B	436	SER	-	expression tag	UNP P0A3G2
B	437	GLY	-	expression tag	UNP P0A3G2
A	-1	GLY	-	expression tag	UNP P0A3G2
A	0	PRO	-	expression tag	UNP P0A3G2
A	1	MET	-	expression tag	UNP P0A3G2
A	2	ALA	-	expression tag	UNP P0A3G2
A	47	VAL	LEU	engineered mutation	UNP P0A3G2
A	58	THR	SER	engineered mutation	UNP P0A3G2
A	78	GLY	ASP	engineered mutation	UNP P0A3G2
A	87	PHE	TYR	engineered mutation	UNP P0A3G2
A	88	MET	LEU	engineered mutation	UNP P0A3G2
A	128	PHE	CYS	engineered mutation	UNP P0A3G2
A	143	TRP	GLU	engineered mutation	UNP P0A3G2
A	144	PHE	-	linker	UNP P0A3G2
A	145	ALA	-	linker	UNP P0A3G2
A	146	GLY	-	linker	UNP P0A3G2
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A	283	PRO	-	linker	UNP A0A453KFI0
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A	307	VAL	ALA	engineered mutation	UNP P0A3G2
A	312	THR	ALA	engineered mutation	UNP P0A3G2
A	315	MET	LYS	engineered mutation	UNP P0A3G2
A	316	GLY	CYS	engineered mutation	UNP P0A3G2
A	335	ASN	LYS	engineered mutation	UNP P0A3G2
A	364	GLU	ALA	engineered mutation	UNP P0A3G2

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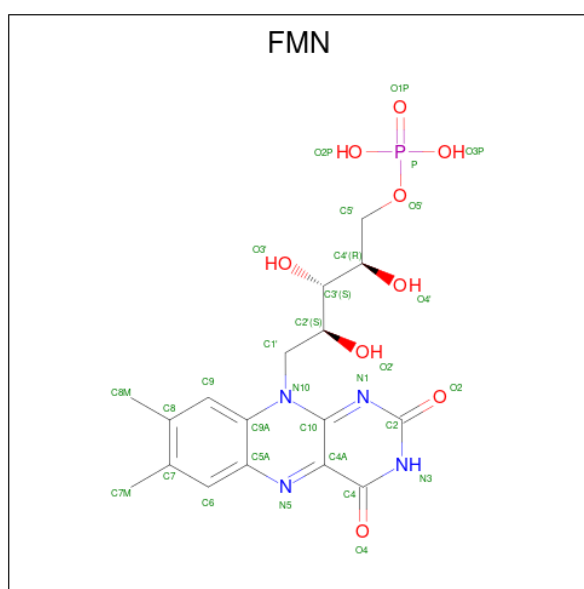
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Chain	Residue	Modelled	Actual	Comment	Reference
A	367	ASP	ASN	engineered mutation	UNP P0A3G2
A	397	LYS	GLU	engineered mutation	UNP P0A3G2
A	404	ALA	THR	engineered mutation	UNP P0A3G2
A	412	ASN	HIS	engineered mutation	UNP P0A3G2
A	413	LEU	TYR	engineered mutation	UNP P0A3G2
A	431	SER	-	expression tag	UNP P0A3G2
A	432	THR	-	expression tag	UNP P0A3G2
A	433	LEU	-	expression tag	UNP P0A3G2
A	434	GLU	-	expression tag	UNP P0A3G2
A	435	ILE	-	expression tag	UNP P0A3G2
A	436	SER	-	expression tag	UNP P0A3G2
A	437	GLY	-	expression tag	UNP P0A3G2

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

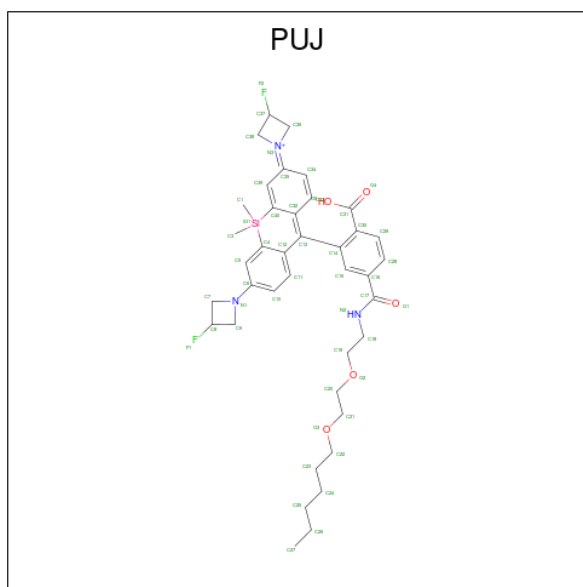
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



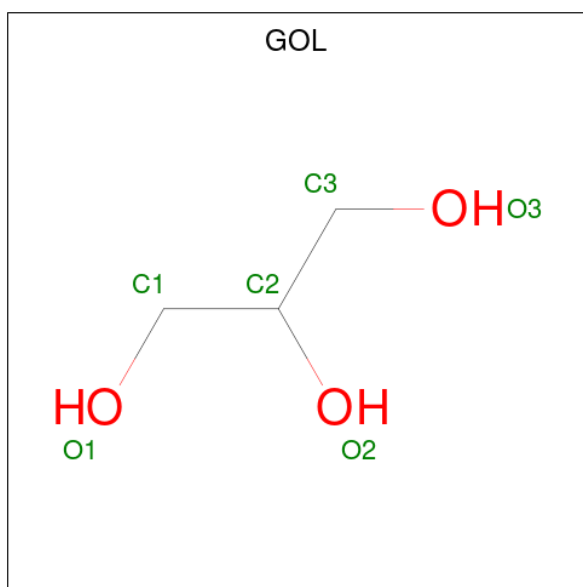
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is (1E,3S)-1-{10-[2-carboxy-5-({2-[2-(hexyloxy)ethoxy]ethyl}carbamoyl)phenyl]-7-(3-fluoroazetidin-1-yl)-5,5-dimethyldibenz o[b,e]silin-3(5H)-ylidene}-3-fluoroazetidin-1-ium (CCD ID: PUJ) (formula: C<sub>39</sub>H<sub>48</sub>F<sub>2</sub>N<sub>3</sub>O<sub>5</sub>Si) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	Si	0	0
			50	39	2	3	5	1		
4	A	1	Total	C	F	N	O	Si	0	0
			50	39	2	3	5	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	169	Total	O	0	0
			169	169		

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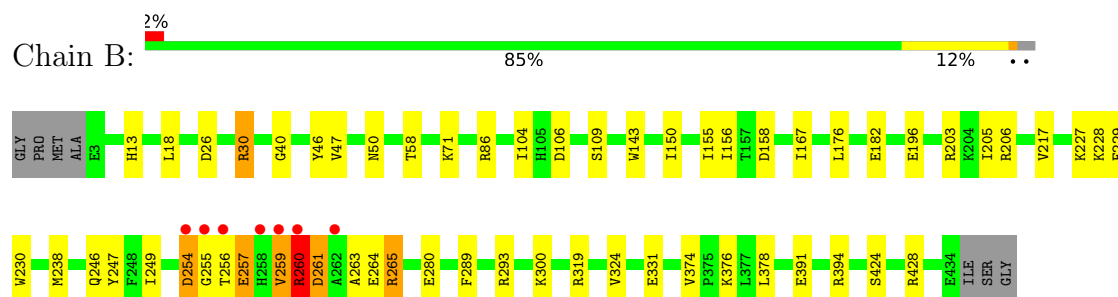
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	207	Total 207	O 207	0	0

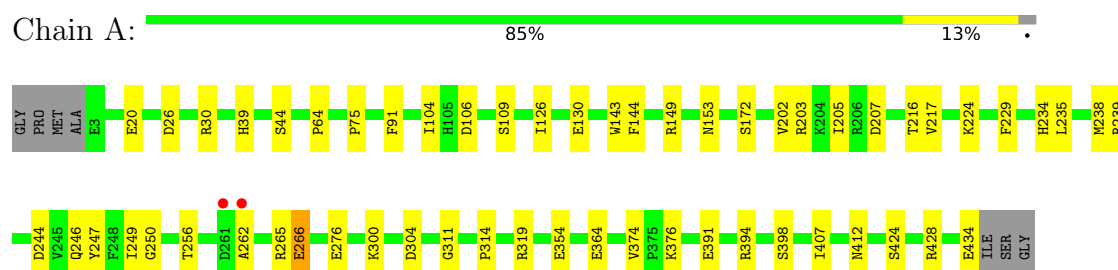
### 3 Residue-property plots

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: Haloalkane dehalogenase,non-specific serine/threonine protein kinase



- Molecule 1: Haloalkane dehalogenase,non-specific serine/threonine protein kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.74Å 78.02Å 81.81Å 90.00° 103.92° 90.00°	Depositor
Resolution (Å)	70.36 – 2.40 70.36 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.36-2.40) 99.6 (70.36-2.40)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487:000)	Depositor
R, $R_{free}$	0.185 , 0.235 0.189 , 0.235	Depositor DCC
$R_{free}$ test set	2040 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PUJ, FMN, GOL, CL

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	0.40	0/3600	0.55	0/4906
1	B	0.39	0/3600	0.60	2/4906 (0.0%)
All	All	0.39	0/7200	0.58	2/9812 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	259	VAL	N-CA-C	-10.01	103.00	111.91
1	B	255	GLY	CA-C-O	-6.12	118.01	122.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	260	ARG	Sidechain
1	B	265	ARG	Sidechain
1	B	293	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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	3496	0	3417	44	0
1	B	3496	0	3417	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	19	0	0
3	B	31	0	19	1	0
4	A	50	0	0	5	0
4	B	50	0	0	3	0
5	A	42	0	56	9	0
5	B	24	0	32	2	0
6	A	207	0	0	9	0
6	B	169	0	0	8	0
All	All	7598	0	6960	91	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 6.

All (91) 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:106:ASP:OD2	4:B:503:PUJ:C27	1.84	1.25
1:B:106:ASP:CG	4:B:503:PUJ:C27	2.27	1.06
1:A:106:ASP:OD1	4:A:503:PUJ:C27	2.01	1.06
1:A:106:ASP:CG	4:A:503:PUJ:C27	2.34	1.00
1:A:276:GLU:OE1	6:A:601:HOH:O	1.82	0.96
1:A:106:ASP:OD2	4:A:503:PUJ:C27	2.12	0.95
1:B:50:ASN:OD1	6:B:601:HOH:O	1.87	0.93
1:A:153:ASN:H	5:A:508:GOL:H11	1.34	0.92
1:B:106:ASP:OD1	4:B:503:PUJ:C27	2.20	0.89
1:A:143:TRP:HZ2	1:A:238:MET:HE1	1.45	0.82
1:A:265:ARG:O	6:A:602:HOH:O	1.97	0.81
1:B:196:GLU:OE1	1:B:228:LYS:NZ	2.16	0.79
1:A:143:TRP:CZ2	1:A:238:MET:HE1	2.19	0.77
1:A:207:ASP:OD2	6:A:603:HOH:O	2.01	0.77
1:B:58:THR:OG1	6:B:602:HOH:O	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG12	5:A:509:GOL:H32	1.69	0.74
1:A:354:GLU:OE1	6:A:604:HOH:O	2.05	0.74
1:B:257:GLU:C	1:B:259:VAL:H	1.97	0.71
1:B:331:GLU:OE2	6:B:604:HOH:O	2.10	0.69
1:B:319:ARG:O	6:B:603:HOH:O	2.09	0.69
1:A:238:MET:HE2	1:A:249:ILE:CG1	2.27	0.64
1:A:238:MET:CG	1:A:249:ILE:HD11	2.28	0.64
1:B:203:ARG:NH1	6:B:608:HOH:O	2.25	0.64
5:A:509:GOL:H31	6:A:694:HOH:O	1.97	0.63
1:B:374:VAL:O	1:B:376:LYS:NZ	2.34	0.60
1:A:238:MET:HE2	1:A:249:ILE:HG12	1.83	0.60
1:A:238:MET:HG3	1:A:249:ILE:HD11	1.83	0.60
1:B:229:PHE:HB2	1:B:256:THR:HA	1.84	0.59
1:B:238:MET:HE2	1:B:249:ILE:HB	1.84	0.59
1:A:319:ARG:O	6:A:606:HOH:O	2.16	0.59
1:A:262:ALA:O	1:A:266:GLU:HG2	2.03	0.58
1:B:182:GLU:OE2	1:B:182:GLU:N	2.29	0.55
1:B:257:GLU:C	1:B:259:VAL:N	2.64	0.55
1:B:46:TYR:HB2	5:B:505:GOL:H12	1.89	0.54
1:A:391:GLU:OE1	1:A:394:ARG:NH2	2.40	0.53
1:A:229:PHE:HB2	1:A:256:THR:HB	1.92	0.52
1:A:104:ILE:HB	1:A:109:SER:HA	1.91	0.51
1:B:71:LYS:HE3	6:B:751:HOH:O	2.10	0.51
1:A:239:ARG:HA	1:A:244:ASP:O	2.11	0.51
1:A:144:PHE:HZ	5:A:507:GOL:H31	1.76	0.51
1:B:156:ILE:HD13	1:B:249:ILE:HD13	1.94	0.50
1:B:280:GLU:OE2	5:A:504:GOL:H31	2.12	0.50
1:A:247:TYR:OH	5:A:507:GOL:H2	2.11	0.50
1:A:26:ASP:CG	1:A:30:ARG:HH22	2.21	0.48
1:B:230:TRP:HB2	1:B:257:GLU:HB2	1.95	0.48
1:B:30:ARG:HE	1:B:30:ARG:HB3	1.46	0.48
1:B:246:GLN:HG3	1:B:247:TYR:CD2	2.49	0.47
1:B:238:MET:CE	1:B:249:ILE:HB	2.45	0.47
1:A:311:GLY:O	1:A:314:PRO:HD2	2.14	0.47
5:B:507:GOL:O3	5:B:507:GOL:O1	2.15	0.47
1:B:176:LEU:HD13	1:B:254:ASP:HA	1.97	0.46
1:B:150:ILE:O	6:B:605:HOH:O	2.20	0.46
1:A:64:PRO:HB3	1:A:91:PHE:CZ	2.50	0.46
1:B:261:ASP:O	1:B:263:ALA:N	2.47	0.46
1:A:202:VAL:CG1	5:A:509:GOL:H32	2.44	0.46
1:B:259:VAL:C	1:B:261:ASP:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLU:OE2	1:A:75:PRO:HB3	2.16	0.46
1:B:424:SER:O	1:B:428:ARG:HG3	2.16	0.46
1:B:230:TRP:HB2	1:B:256:THR:O	2.16	0.44
1:A:130:GLU:HG3	1:A:412:ASN:HA	1.98	0.44
1:A:434:GLU:OE1	6:A:607:HOH:O	2.21	0.44
1:B:18:LEU:HD11	1:B:86:ARG:HG2	1.99	0.43
1:B:260:ARG:C	1:B:264:GLU:HB2	2.42	0.43
1:A:424:SER:O	1:A:428:ARG:HG3	2.17	0.43
1:A:149:ARG:HB2	4:A:503:PUJ:F1	2.08	0.43
1:B:143:TRP:HZ2	1:B:238:MET:HE1	1.84	0.43
1:B:391:GLU:OE1	1:B:394:ARG:NH1	2.52	0.43
1:A:234:HIS:O	1:A:250:GLY:HA2	2.18	0.43
1:B:227:LYS:NZ	1:B:228:LYS:O	2.52	0.42
1:B:254:ASP:OD1	1:B:254:ASP:N	2.49	0.42
1:B:300:LYS:HD3	4:A:503:PUJ:C6	2.49	0.42
1:B:324:VAL:HG23	6:B:730:HOH:O	2.19	0.42
1:B:205:ILE:HD11	1:B:217:VAL:HG21	2.00	0.42
1:A:153:ASN:N	5:A:508:GOL:H11	2.17	0.42
1:B:40:GLY:HA3	1:B:106:ASP:HB3	2.01	0.42
1:A:205:ILE:HD11	1:A:217:VAL:HG21	2.02	0.42
1:A:246:GLN:HG3	1:A:247:TYR:CD2	2.54	0.42
1:B:104:ILE:HD12	1:B:109:SER:HA	2.02	0.42
1:A:30:ARG:HA	1:A:30:ARG:HD2	1.77	0.42
3:B:502:FMN:HM73	3:B:502:FMN:HM81	1.86	0.41
1:A:39:HIS:CD2	1:A:44:SER:HA	2.56	0.41
1:B:158:ASP:HB2	1:B:167:ILE:HD13	2.03	0.41
1:A:374:VAL:O	1:A:376:LYS:NZ	2.54	0.41
1:B:104:ILE:HB	1:B:109:SER:HA	2.01	0.41
1:B:155:ILE:O	1:B:249:ILE:HD12	2.21	0.41
1:A:203:ARG:HA	5:A:509:GOL:O3	2.20	0.41
1:A:224:LYS:NZ	6:A:634:HOH:O	2.53	0.41
1:A:364:GLU:OE2	6:A:609:HOH:O	2.22	0.40
1:B:13:HIS:CD2	1:B:26:ASP:HB3	2.56	0.40
1:A:300:LYS:O	1:A:304:ASP:HB2	2.22	0.40
1:A:374:VAL:O	1:A:376:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/439 (98%)	413 (96%)	17 (4%)	0	100	100
1	B	430/439 (98%)	407 (95%)	23 (5%)	0	100	100
All	All	860/878 (98%)	820 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/380 (99%)	369 (98%)	7 (2%)	52	72
1	B	376/380 (99%)	366 (97%)	10 (3%)	40	60
All	All	752/760 (99%)	735 (98%)	17 (2%)	45	66

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	30	ARG
1	B	47	VAL
1	B	206	ARG
1	B	254	ASP
1	B	257	GLU
1	B	260	ARG
1	B	261	ASP
1	B	265	ARG

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Mol	Chain	Res	Type
1	B	289	PHE
1	B	378	LEU
1	A	126	ILE
1	A	172	SER
1	A	216	THR
1	A	235	LEU
1	A	266	GLU
1	A	398	SER
1	A	407	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	HIS
1	B	246	GLN
1	B	252	GLN
1	B	290	GLN
1	A	211	ASN
1	A	246	GLN
1	A	371	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
5	GOL	B	507	-	5,5,5	0.92	0	5,5,5	1.03	0
4	PUJ	B	503	-	48,55,55	0.93	1 (2%)	60,79,79	2.29	16 (26%)
5	GOL	B	505	-	5,5,5	0.96	0	5,5,5	1.07	0
5	GOL	A	504	-	5,5,5	0.99	0	5,5,5	0.92	0
3	FMN	A	502	-	33,33,33	1.13	2 (6%)	48,50,50	1.30	7 (14%)
5	GOL	A	510	-	5,5,5	0.89	0	5,5,5	0.99	0
5	GOL	A	505	-	5,5,5	0.88	0	5,5,5	1.06	0
5	GOL	B	506	-	5,5,5	0.96	0	5,5,5	1.03	0
5	GOL	A	509	-	5,5,5	0.10	0	5,5,5	0.33	0
5	GOL	B	504	-	5,5,5	0.85	0	5,5,5	1.02	0
5	GOL	A	507	-	5,5,5	1.24	1 (20%)	5,5,5	0.73	0
5	GOL	A	506	-	5,5,5	0.99	0	5,5,5	1.19	1 (20%)
3	FMN	B	502	-	33,33,33	1.04	2 (6%)	48,50,50	1.32	7 (14%)
4	PUJ	A	503	-	48,55,55	0.98	1 (2%)	60,79,79	2.18	14 (23%)
5	GOL	A	508	-	5,5,5	1.01	0	5,5,5	1.01	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
5	GOL	B	507	-	-	2/4/4/4	-
4	PUJ	B	503	-	-	11/31/82/82	0/5/6/6
5	GOL	B	505	-	-	1/4/4/4	-
5	GOL	A	504	-	-	0/4/4/4	-
3	FMN	A	502	-	-	1/18/18/18	0/3/3/3
5	GOL	A	510	-	-	4/4/4/4	-
5	GOL	A	505	-	-	0/4/4/4	-
5	GOL	B	506	-	-	4/4/4/4	-
5	GOL	A	509	-	-	4/4/4/4	-
5	GOL	B	504	-	-	4/4/4/4	-
5	GOL	A	507	-	-	4/4/4/4	-
5	GOL	A	506	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	B	502	-	-	1/18/18/18	0/3/3/3
4	PUJ	A	503	-	-	9/31/82/82	0/5/6/6
5	GOL	A	508	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	FMN	C4A-N5	4.42	1.39	1.30
3	B	502	FMN	C4A-N5	3.84	1.38	1.30
4	A	503	PUJ	C5-C4	-3.54	1.34	1.40
4	B	503	PUJ	C5-C4	-3.33	1.34	1.40
3	A	502	FMN	C10-N1	2.82	1.39	1.33
3	B	502	FMN	C10-N1	2.47	1.38	1.33
5	A	507	GOL	C1-C2	2.07	1.60	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	PUJ	C14-C13-C12	-9.56	108.79	119.94
4	A	503	PUJ	C12-C13-C32	6.58	133.15	119.99
4	B	503	PUJ	C12-C13-C32	6.09	132.18	119.99
4	B	503	PUJ	C14-C13-C12	-5.91	113.04	119.94
4	B	503	PUJ	C5-C4-C12	5.46	124.64	118.23
4	B	503	PUJ	C14-C13-C32	-5.32	114.77	120.45
4	B	503	PUJ	C6-C5-C4	-5.20	117.63	122.68
4	A	503	PUJ	C5-C4-C12	5.05	124.17	118.23
4	B	503	PUJ	C8-C9-N1	-4.88	84.67	87.96
4	B	503	PUJ	C8-C7-N1	-4.57	84.88	87.96
4	B	503	PUJ	C37-C36-N3	4.20	90.78	87.96
4	A	503	PUJ	C6-C5-C4	-3.81	118.98	122.68
4	A	503	PUJ	C37-C38-N3	3.66	90.42	87.96
4	B	503	PUJ	C37-C38-N3	3.61	90.39	87.96
4	A	503	PUJ	C5-C6-N1	-3.45	117.62	121.33
3	B	502	FMN	C4-N3-C2	-3.40	119.37	125.64
4	A	503	PUJ	C37-C36-N3	3.30	90.18	87.96
4	A	503	PUJ	C11-C12-C4	-3.24	115.28	119.28
3	B	502	FMN	C4A-C10-N10	3.22	121.18	116.48
3	A	502	FMN	C4A-C10-N10	3.08	120.99	116.48
3	A	502	FMN	C4-N3-C2	-2.92	120.24	125.64
4	B	503	PUJ	C11-C12-C4	-2.87	115.73	119.28
4	B	503	PUJ	C3-SI1-C4	2.84	115.67	109.54
4	B	503	PUJ	C5-C6-N1	-2.71	118.41	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	FMN	O4-C4-C4A	-2.70	119.44	126.60
4	B	503	PUJ	C1-SI1-C4	-2.60	103.92	109.54
3	A	502	FMN	P-O5'-C5'	2.52	125.23	118.30
3	B	502	FMN	C4A-C4-N3	2.49	119.52	113.19
3	A	502	FMN	C10-C4A-N5	-2.47	119.61	124.86
4	B	503	PUJ	C19-C18-N2	-2.44	106.06	111.83
4	A	503	PUJ	C1-SI1-C4	-2.38	104.39	109.54
3	B	502	FMN	C4A-C10-N1	-2.34	119.30	124.73
3	A	502	FMN	C4A-C4-N3	2.31	119.06	113.19
4	A	503	PUJ	C14-C13-C32	-2.28	118.01	120.45
4	A	503	PUJ	C8-C7-N1	-2.27	86.43	87.96
4	A	503	PUJ	C34-C35-N3	2.26	125.01	121.11
3	B	502	FMN	C10-C4A-N5	-2.24	120.10	124.86
4	A	503	PUJ	C8-C9-N1	-2.22	86.46	87.96
3	A	502	FMN	C4A-C10-N1	-2.20	119.62	124.73
5	A	506	GOL	C3-C2-C1	-2.19	103.20	111.70
4	B	503	PUJ	O5-C31-O4	-2.18	118.52	123.35
3	A	502	FMN	O4-C4-C4A	-2.09	121.06	126.60
3	B	502	FMN	C4-C4A-C10	2.06	120.26	116.79
4	B	503	PUJ	C33-C32-C13	-2.06	119.54	123.96
4	A	503	PUJ	C39-C35-N3	-2.01	117.41	121.49

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	PUJ	C10-C6-N1-C7
4	B	503	PUJ	C11-C12-C13-C14
4	B	503	PUJ	C11-C12-C13-C32
4	A	503	PUJ	C5-C6-N1-C9
4	A	503	PUJ	C10-C6-N1-C9
4	A	503	PUJ	C11-C12-C13-C14
4	A	503	PUJ	C11-C12-C13-C32
5	B	504	GOL	O1-C1-C2-C3
5	B	504	GOL	C1-C2-C3-O3
5	B	506	GOL	C1-C2-C3-O3
5	B	506	GOL	O2-C2-C3-O3
5	B	507	GOL	C1-C2-C3-O3
5	B	507	GOL	O2-C2-C3-O3
5	A	506	GOL	C1-C2-C3-O3
5	A	509	GOL	O1-C1-C2-C3
5	A	510	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	503	PUJ	N2-C18-C19-O2
5	A	509	GOL	O2-C2-C3-O3
4	B	503	PUJ	O3-C22-C23-C24
5	B	506	GOL	O1-C1-C2-C3
5	A	507	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	A	508	GOL	C1-C2-C3-O3
5	A	509	GOL	C1-C2-C3-O3
5	A	510	GOL	O1-C1-C2-C3
4	B	503	PUJ	C23-C24-C25-C26
5	B	504	GOL	O1-C1-C2-O2
5	B	506	GOL	O1-C1-C2-O2
5	A	509	GOL	O1-C1-C2-O2
5	A	510	GOL	O1-C1-C2-O2
5	A	510	GOL	O2-C2-C3-O3
5	B	504	GOL	O2-C2-C3-O3
5	A	506	GOL	O2-C2-C3-O3
5	A	508	GOL	O2-C2-C3-O3
4	A	503	PUJ	C23-C24-C25-C26
3	B	502	FMN	C4'-C5'-O5'-P
4	B	503	PUJ	C21-C20-O2-C19
5	B	505	GOL	O1-C1-C2-O2
5	A	507	GOL	O2-C2-C3-O3
3	A	502	FMN	C4'-C5'-O5'-P
4	B	503	PUJ	C24-C25-C26-C27
4	B	503	PUJ	C5-C6-N1-C9
4	A	503	PUJ	C20-C21-O3-C22
5	A	507	GOL	O1-C1-C2-O2
4	A	503	PUJ	C18-C19-O2-C20
4	A	503	PUJ	O2-C20-C21-O3
4	B	503	PUJ	O2-C20-C21-O3
4	B	503	PUJ	C5-C6-N1-C7
4	B	503	PUJ	C10-C6-N1-C9

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	507	GOL	1	0
4	B	503	PUJ	3	0
5	B	505	GOL	1	0
5	A	504	GOL	1	0

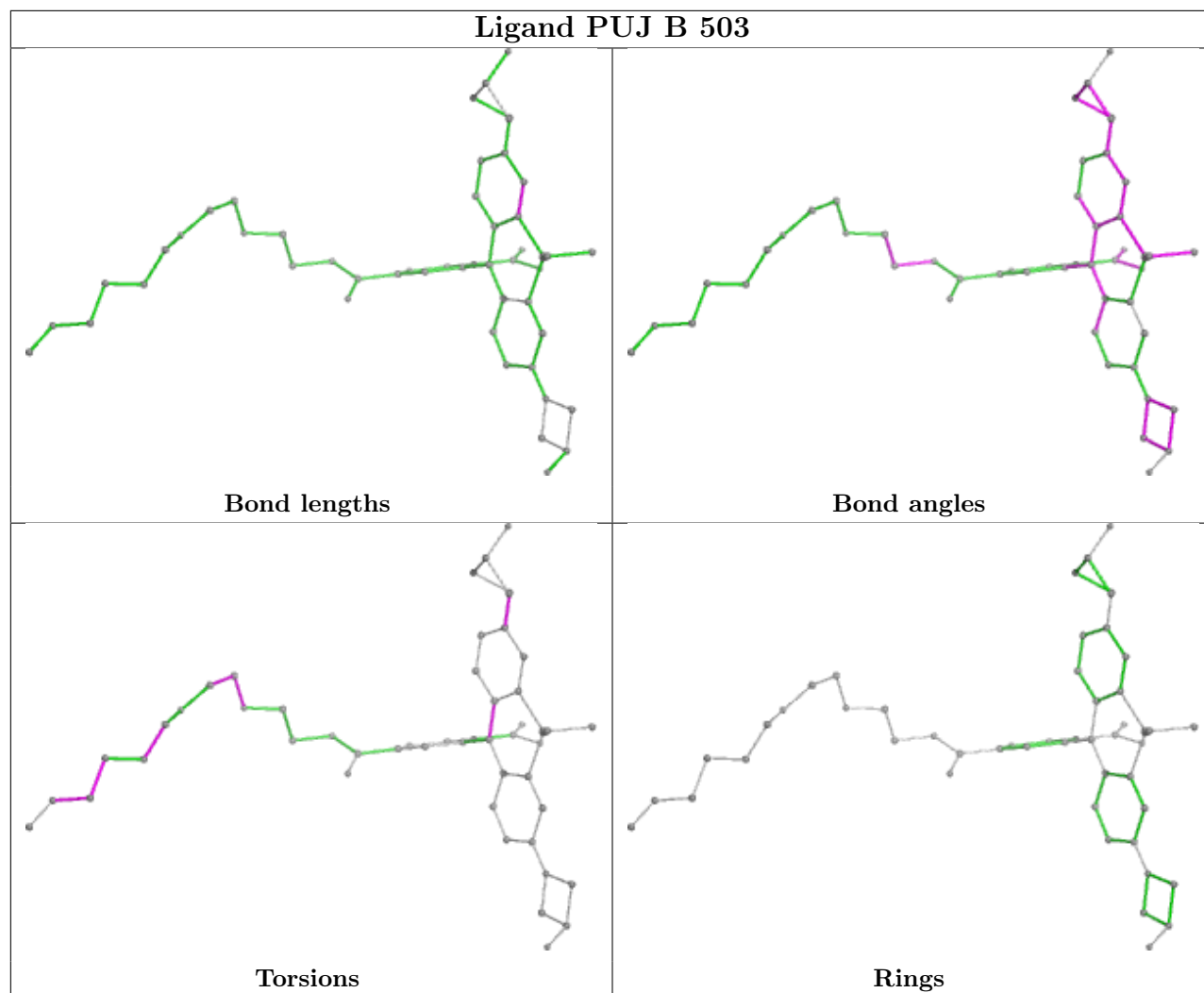
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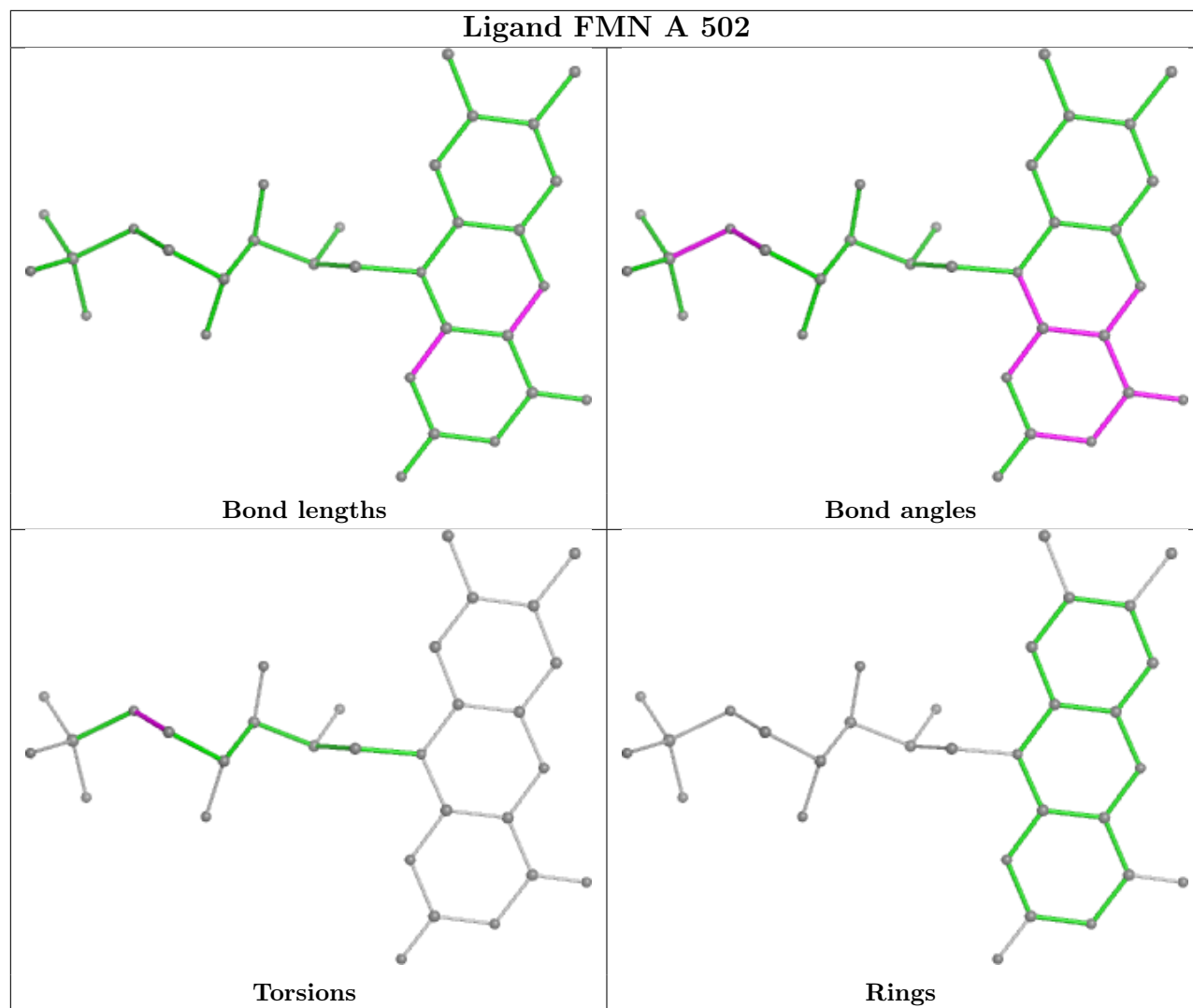
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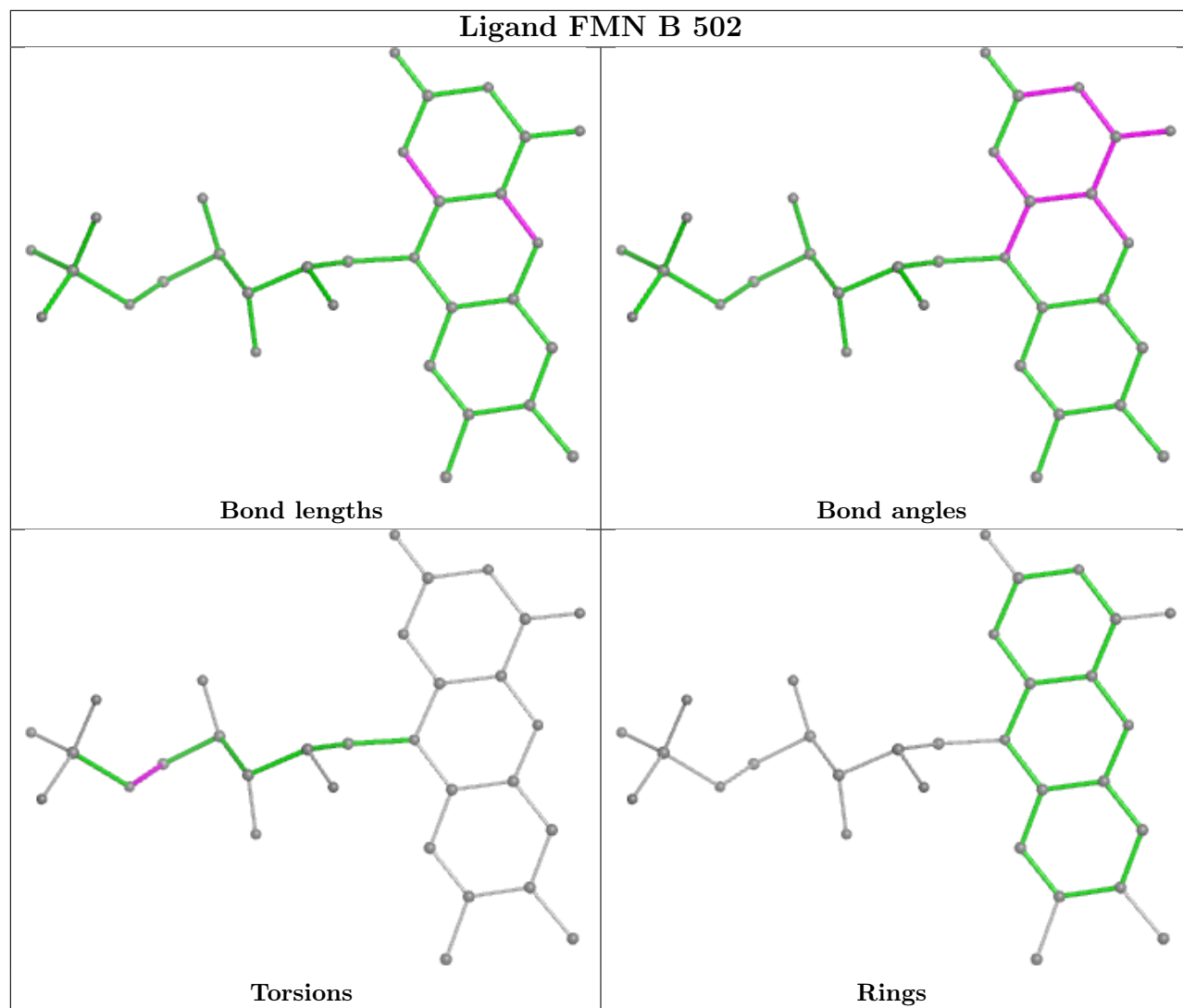
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	GOL	4	0
5	A	507	GOL	2	0
3	B	502	FMN	1	0
4	A	503	PUJ	5	0
5	A	508	GOL	2	0

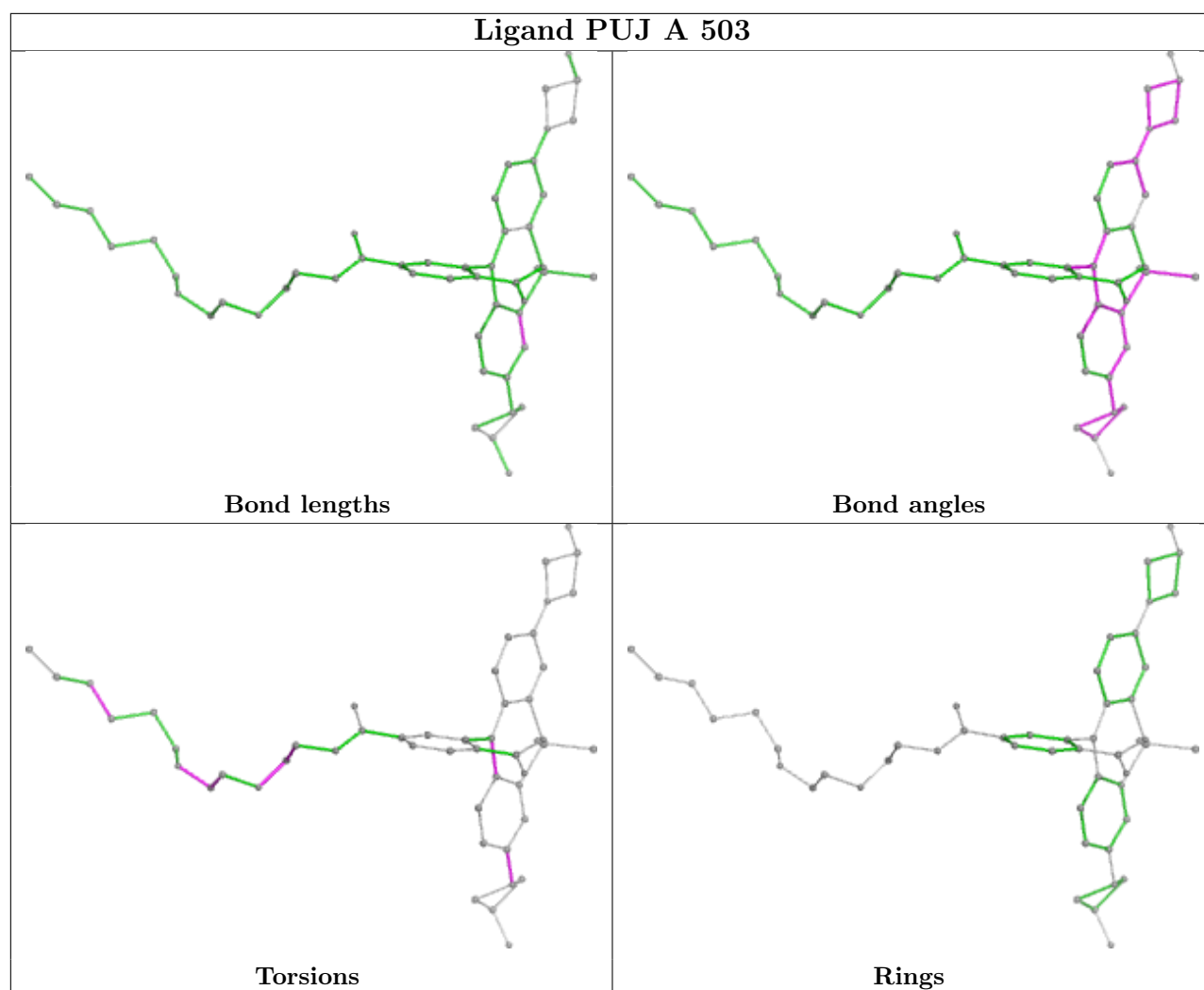
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 PUJ 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 [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, 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	432/439 (98%)	-0.36	2 (0%) 87 85	26, 36, 56, 93	0
1	B	432/439 (98%)	-0.23	7 (1%) 70 67	27, 39, 60, 115	0
All	All	864/878 (98%)	-0.30	9 (1%) 79 76	26, 37, 59, 115	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	THR	5.4
1	B	259	VAL	5.1
1	B	262	ALA	3.9
1	B	258	HIS	3.4
1	B	255	GLY	2.8
1	B	254	ASP	2.4
1	A	261	ASP	2.3
1	A	262	ALA	2.3
1	B	260	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,

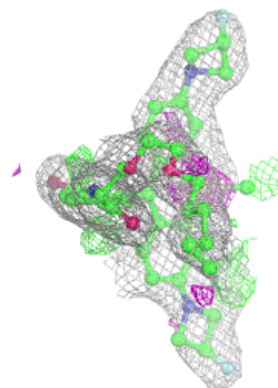
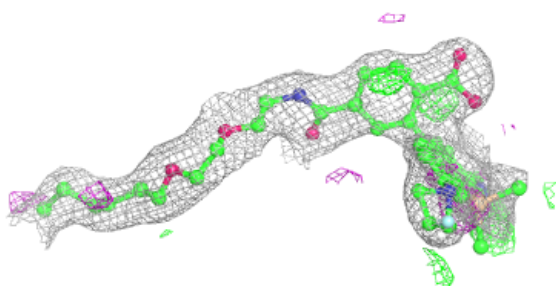
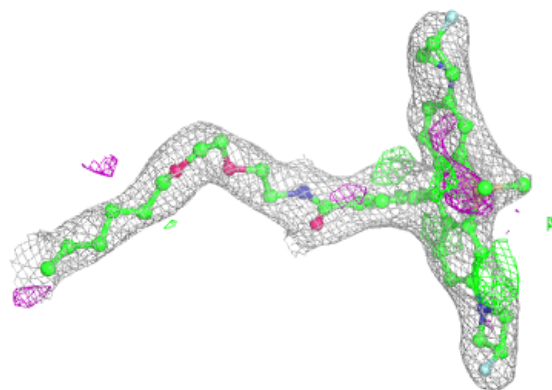
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	509	6/6	0.66	0.22	46,48,50,53	0
5	GOL	B	504	6/6	0.74	0.16	47,48,52,59	0
5	GOL	B	505	6/6	0.76	0.23	42,45,46,48	0
5	GOL	A	507	6/6	0.82	0.22	39,43,45,46	0
5	GOL	A	510	6/6	0.82	0.15	40,46,49,51	0
5	GOL	A	505	6/6	0.84	0.15	41,44,46,47	0
4	PUJ	B	503	50/50	0.85	0.13	29,46,53,68	0
5	GOL	A	504	6/6	0.85	0.13	40,45,47,48	0
4	PUJ	A	503	50/50	0.86	0.13	26,43,52,64	0
5	GOL	B	506	6/6	0.87	0.17	43,47,51,52	0
5	GOL	A	506	6/6	0.88	0.16	39,42,44,45	0
5	GOL	A	508	6/6	0.88	0.13	40,44,49,50	0
5	GOL	B	507	6/6	0.90	0.13	46,53,60,64	0
3	FMN	B	502	31/31	0.93	0.08	35,42,47,48	0
2	CL	B	501	1/1	0.93	0.12	43,43,43,43	0
3	FMN	A	502	31/31	0.94	0.08	36,40,44,45	0
2	CL	A	501	1/1	0.94	0.09	36,36,36,36	0

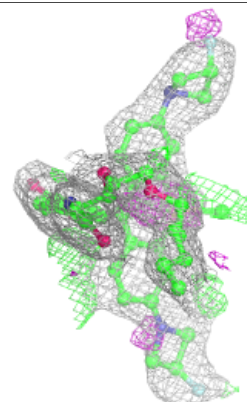
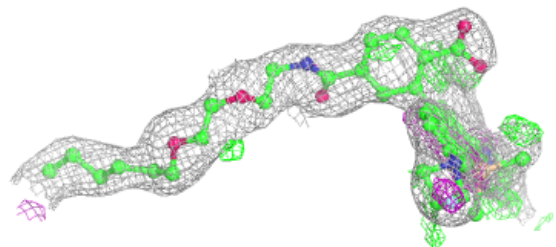
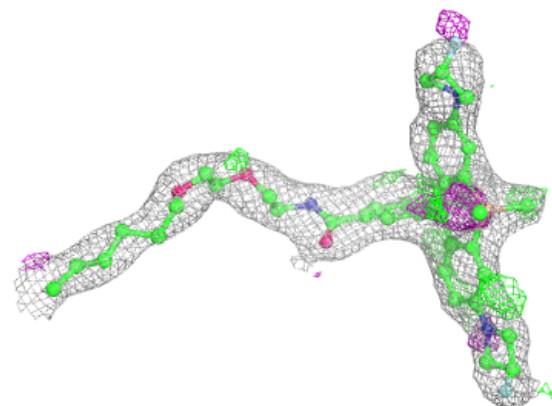
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PUJ 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)

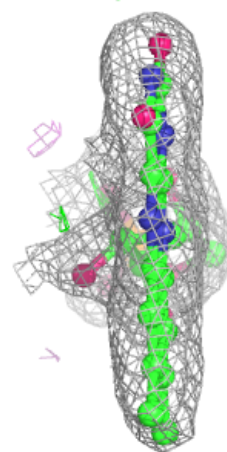
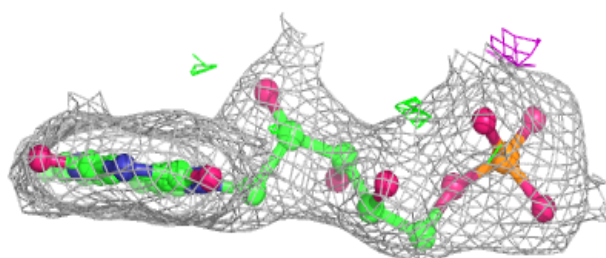
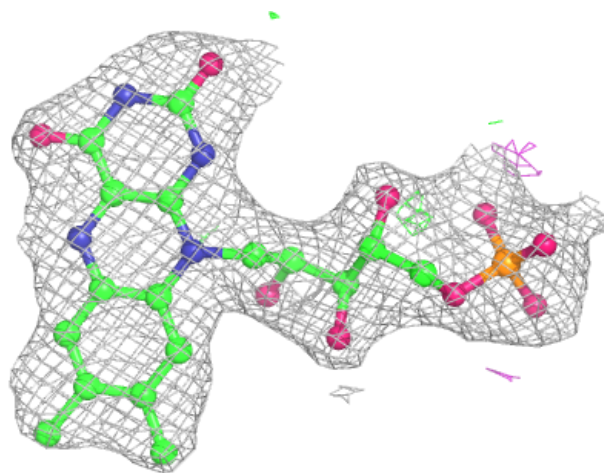
**Electron density around PUJ A 503:**

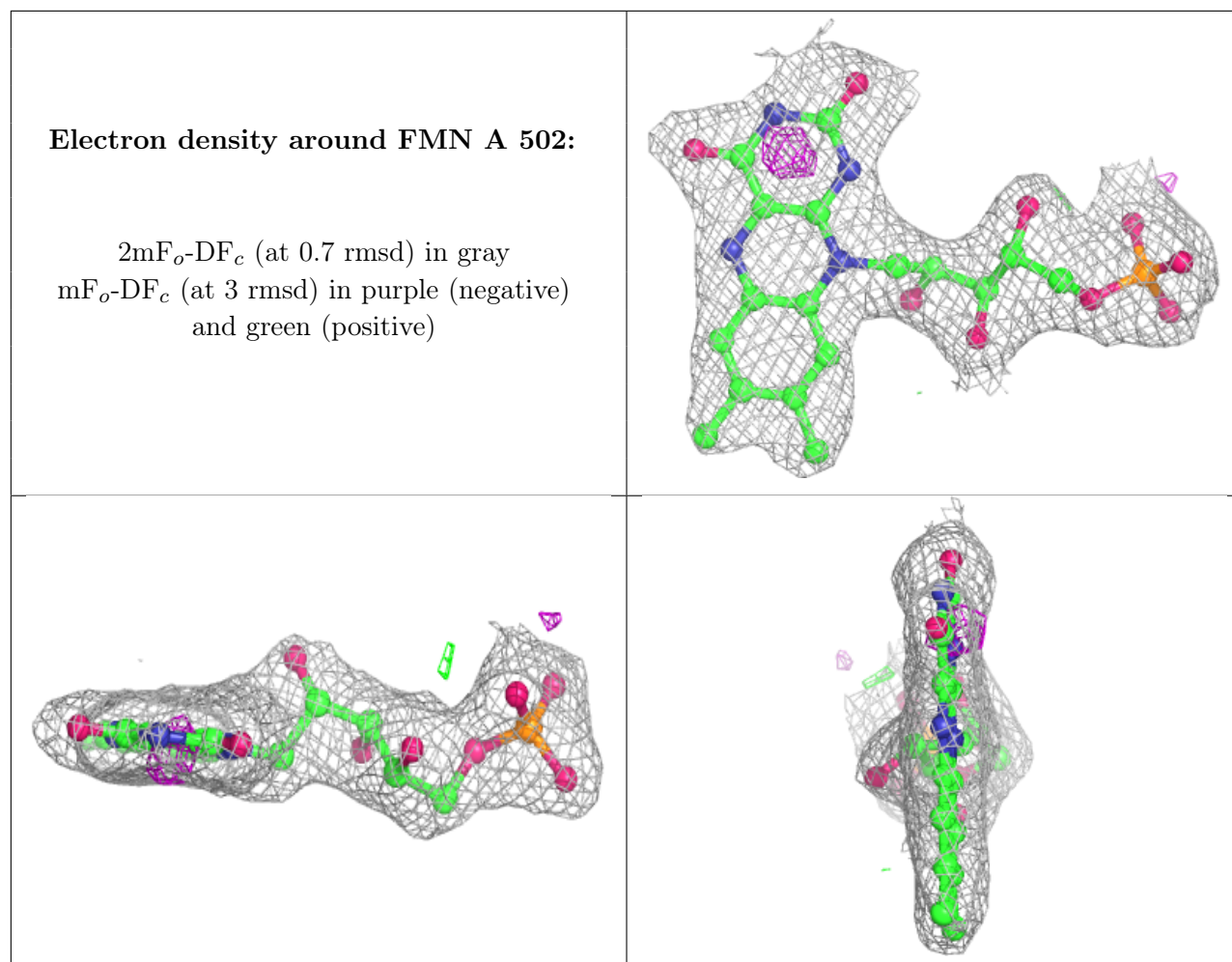
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN B 502:**

$2mF_o-DF_c$  (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.