



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:00 am BST

PDB ID : 6VEB  
Title : Precorrin-2-bound S128A *S. typhimurium* siroheme synthase  
Authors : Pennington, J.M.; Stroupe, M.E.  
Deposited on : 2019-12-31  
Resolution : 2.55 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 : 2.11  
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

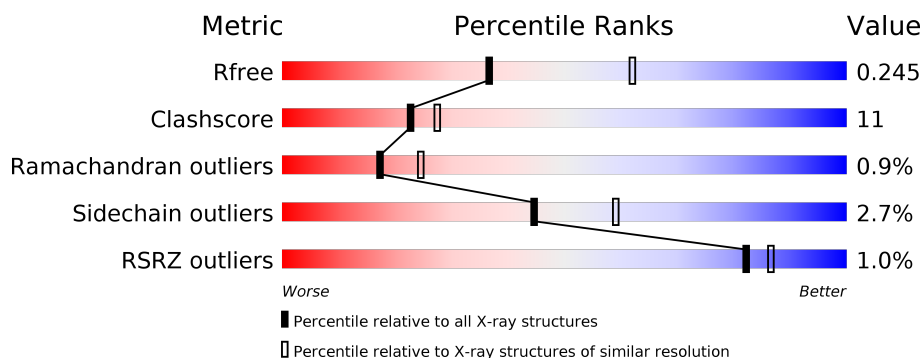
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	457	
1	B	457	

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
3	NAD	A	502	-	-	-	X
4	CL	A	503	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7493 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.

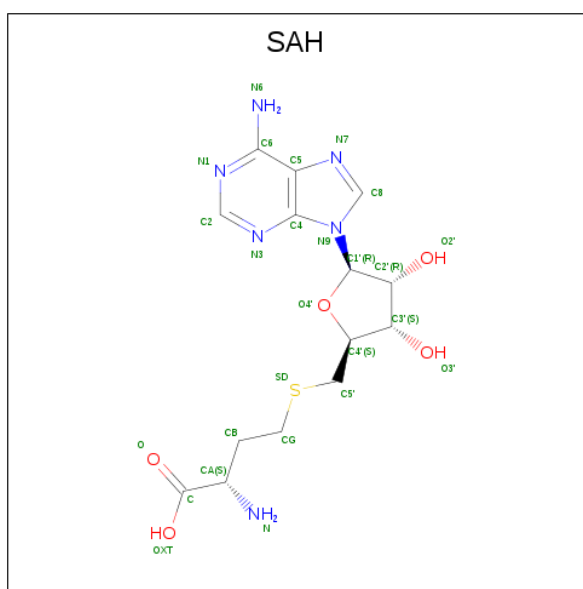
- Molecule 1 is a protein called Siroheme synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	13	0
			3581	2256	655	654	16			
1	B	449	Total	C	N	O	S	0	11	0
			3540	2230	645	648	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	SER	engineered mutation	UNP A0A3U8X2F7
B	128	ALA	SER	engineered mutation	UNP A0A3U8X2F7

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



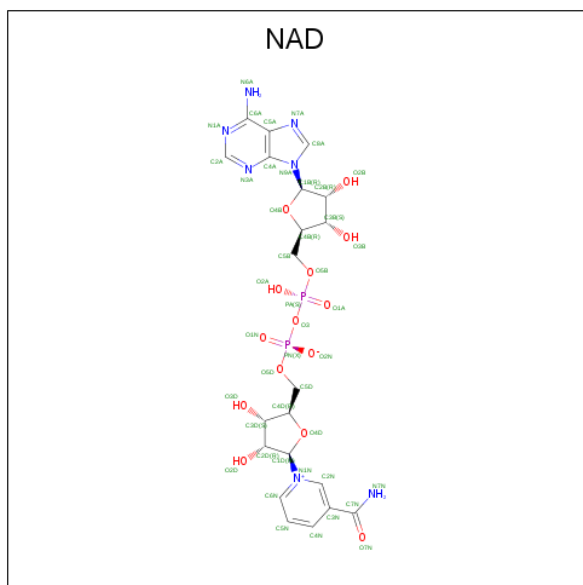
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).

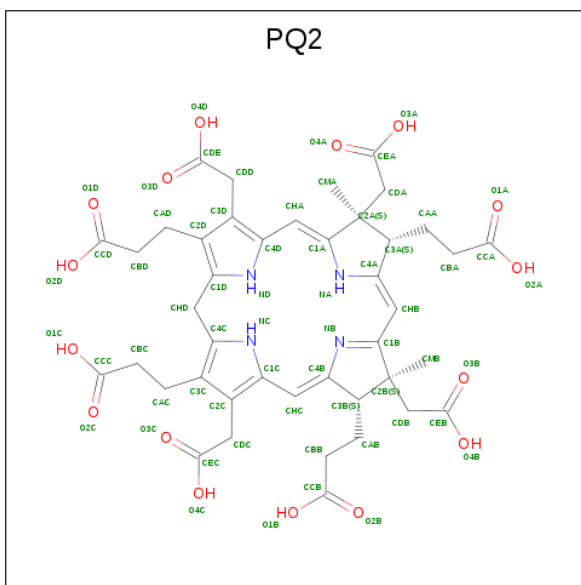


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Cl 2 2	0	0
4	A	5	Total Cl 5 5	0	0

- Molecule 5 is 3,3',3'',3'''-[(7S,8S,12S,13S)-3,8,13,17-tetrakis(carboxymethyl)-8,13-dimethyl-7,8,12,13,20,24-hexahydroporphyrin-2,7,12,18-tetrayl]tetrapropanoic acid (three-letter code: PQ2) (formula:  $C_{42}H_{48}N_4O_{16}$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			62	42	4	16		

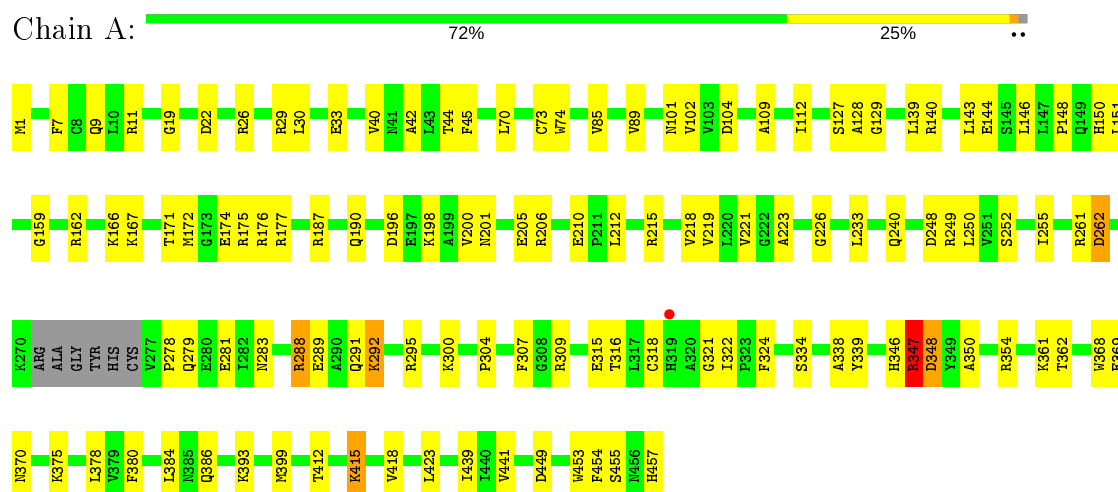
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	105	Total O 105 105	0	0
6	B	102	Total O 102 102	0	0

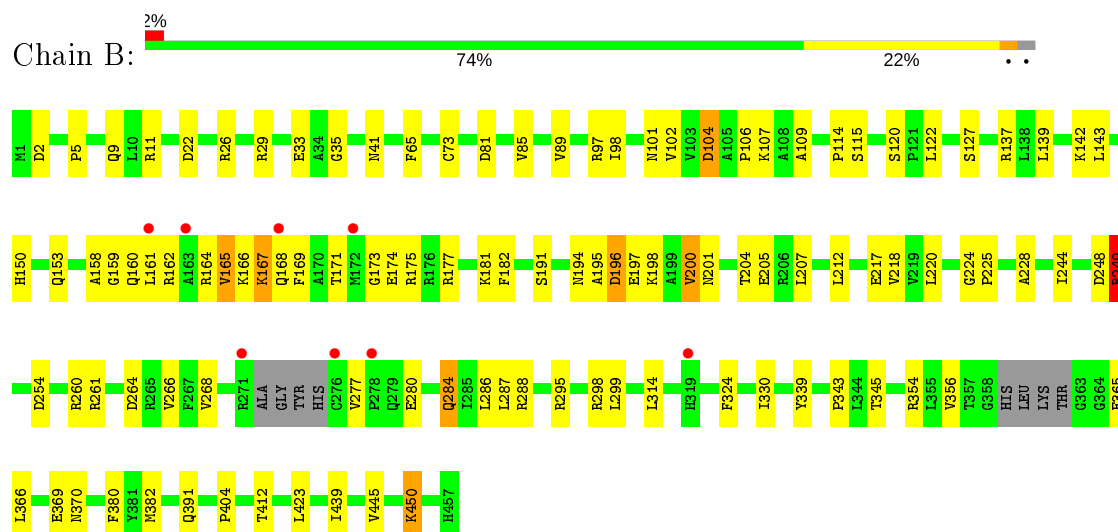
### 3 Residue-property plots

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: Siroheme synthase



#### • Molecule 1: Siroheme synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.68 Å 99.49 Å 146.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.55 49.74 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.74-2.55) 71.7 (49.74-2.16)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.03 (at 2.16 Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.164 , 0.245 0.164 , 0.245	Depositor DCC
$R_{free}$ test set	1547 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PQ2, SAH, NAD, 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	0.47	0/3659	0.62	0/4944
1	B	0.44	0/3615	0.63	0/4886
All	All	0.45	0/7274	0.63	0/9830

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	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347[A]	ARG	Peptide
1	A	348	ASP	Peptide
1	B	161	LEU	Peptide

### 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	3581	0	3660	103	1
1	B	3540	0	3617	84	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
3	A	44	0	26	7	0
4	A	5	0	0	4	0
4	B	2	0	0	0	0
5	B	62	0	0	3	0
6	A	105	0	0	16	0
6	B	102	0	0	3	1
All	All	7493	0	7341	168	2

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 11.

All (168) 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:248:ASP:HB3	1:B:298:ARG:HH12	1.35	0.90
1:B:244:ILE:HD11	1:B:266:VAL:HG23	1.59	0.84
1:A:283:ASN:HB3	1:A:316:THR:HG21	1.62	0.81
1:A:295[A]:ARG:NH2	6:A:603:HOH:O	2.13	0.81
1:A:104:ASP:OD2	6:A:601:HOH:O	1.99	0.79
1:A:190:GLN:OE1	6:A:602:HOH:O	2.01	0.79
1:A:278:PRO:HD2	1:A:281:GLU:HG3	1.66	0.78
1:A:348:ASP:OD2	1:A:375:LYS:HD2	1.86	0.76
1:A:215:ARG:HD2	6:A:606:HOH:O	1.86	0.75
1:B:171:THR:HG22	1:B:173:GLY:H	1.52	0.74
1:B:217:GLU:OE2	1:B:295:ARG:NH1	2.22	0.72
1:B:162[A]:ARG:NH1	6:B:601:HOH:O	2.22	0.71
1:A:171:THR:OG1	1:A:174:GLU:HB2	1.92	0.69
1:A:291[B]:GLN:HG3	1:A:322:ILE:HD11	1.73	0.69
3:A:502:NAD:H2A	6:A:614:HOH:O	1.93	0.68
1:B:29:ARG:NH2	6:B:602:HOH:O	2.25	0.68
1:B:107:LYS:HE2	1:B:107:LYS:HA	1.74	0.68
1:A:354:ARG:HD2	1:B:354:ARG:HG3	1.75	0.68
1:B:166:LYS:O	1:B:169:PHE:N	2.27	0.67
1:B:181:LYS:HD2	1:B:207:LEU:HD23	1.76	0.66
1:B:171:THR:HB	1:B:174:GLU:H	1.59	0.66
1:A:261[B]:ARG:NH2	1:B:115:SER:HA	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:OG	6:A:605:HOH:O	2.15	0.65
1:B:380:PHE:HB2	1:B:439:ILE:HB	1.78	0.64
1:B:159:GLY:HA2	1:B:162[A]:ARG:NH2	2.13	0.64
1:B:177:ARG:HH21	1:B:212:LEU:HD23	1.64	0.62
1:B:201:ASN:HA	1:B:204:THR:HB	1.81	0.62
1:A:346:HIS:N	4:A:503:CL:CL	2.66	0.61
1:B:248:ASP:O	1:B:249:ARG:HB3	2.02	0.60
1:B:41:ASN:OD1	1:B:65:PHE:HA	2.01	0.60
1:A:146:LEU:HD21	1:B:142:LYS:HD3	1.83	0.60
1:A:139:LEU:HD11	1:B:122:LEU:HD21	1.84	0.59
1:A:26:ARG:NH1	6:A:609:HOH:O	2.36	0.59
1:B:150:HIS:HB3	1:B:153:GLN:HG3	1.86	0.58
1:A:162:ARG:HH22	5:B:502:PQ2:CDD	2.17	0.58
1:A:187[B]:ARG:NH1	6:A:602:HOH:O	2.37	0.57
1:A:223:ALA:HB1	1:A:255:ILE:HD13	1.85	0.57
1:A:315:GLU:HA	1:A:318:CYS:SG	2.44	0.57
1:A:140:ARG:NH1	1:A:144:GLU:OE1	2.37	0.57
1:A:42:ALA:HB3	1:A:45:PHE:CE1	2.40	0.56
1:A:288:ARG:O	1:A:292:LYS:HG3	2.06	0.56
1:A:128:ALA:HB3	4:A:506:CL:CL	2.42	0.56
1:B:73[A]:CYS:HB3	1:B:98:ILE:HD13	1.88	0.56
1:B:169:PHE:HD1	1:B:174:GLU:HG2	1.71	0.55
1:A:240:GLN:O	1:B:137:ARG:HD2	2.07	0.55
1:B:391:GLN:HG3	1:B:423:LEU:O	2.06	0.55
1:A:386:GLN:NE2	6:A:604:HOH:O	2.14	0.55
1:A:176[A]:ARG:NH1	6:A:603:HOH:O	2.40	0.55
1:B:29:ARG:HG2	1:B:29:ARG:HH11	1.71	0.54
1:B:249:ARG:HB3	1:B:249:ARG:CZ	2.38	0.54
1:A:159:GLY:HA2	1:A:162:ARG:HG3	1.90	0.54
1:B:268:VAL:HG22	1:B:277:VAL:HG11	1.89	0.54
1:A:172:MET:HA	1:A:175:ARG:HD2	1.90	0.54
1:A:19:GLY:HA2	3:A:502:NAD:H1B	1.91	0.53
1:B:220:LEU:HG	1:B:314:LEU:HD21	1.89	0.53
1:B:365:GLU:HG3	1:B:366:LEU:N	2.23	0.53
1:A:338:ALA:O	1:A:453:TRP:NE1	2.41	0.52
1:A:139:LEU:HD12	1:B:122:LEU:HD11	1.91	0.52
1:A:101:ASN:HA	1:A:109:ALA:HB1	1.92	0.52
1:B:11[A]:ARG:HD3	1:B:35:GLY:HA3	1.92	0.52
1:A:418:VAL:H	1:A:457:HIS:CE1	2.28	0.51
1:A:9:GLN:HE21	1:B:107:LYS:NZ	2.08	0.51
1:B:225:PRO:HG2	1:B:412:THR:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ARG:HH12	1:B:205:GLU:CD	2.13	0.51
1:A:22:ASP:HB2	3:A:502:NAD:O1N	2.11	0.51
1:B:404:PRO:HB2	1:B:445:VAL:HB	1.93	0.51
1:A:307:PHE:CE1	1:B:345:THR:HG21	2.46	0.50
1:B:280:GLU:OE1	1:B:280:GLU:N	2.42	0.50
1:A:339:TYR:CD2	1:A:412:THR:HA	2.45	0.50
1:A:455:SER:HB3	1:B:194[B]:ASN:HD22	1.76	0.50
1:A:174:GLU:HG2	1:A:212:LEU:HD12	1.94	0.50
1:A:250:LEU:HB3	6:A:643:HOH:O	2.12	0.50
1:A:150[B]:HIS:HE1	6:A:688:HOH:O	1.94	0.49
1:A:261[B]:ARG:HH22	1:B:115:SER:HA	1.78	0.49
1:B:22:ASP:O	1:B:26:ARG:HG3	2.13	0.49
1:A:1:MET:N	1:B:33:GLU:O	2.44	0.49
1:A:318:CYS:SG	1:B:450:LYS:HG2	2.53	0.48
1:A:226:GLY:HA2	1:A:252:SER:HB3	1.96	0.48
1:A:454:PHE:O	1:A:455:SER:HB3	2.13	0.48
1:A:1:MET:O	1:B:11[A]:ARG:NH2	2.47	0.48
1:A:112:ILE:CD1	1:A:129:GLY:HA2	2.44	0.47
1:A:128:ALA:HA	1:B:122:LEU:HA	1.97	0.47
1:B:102:VAL:HG12	1:B:104[B]:ASP:OD1	2.14	0.47
1:A:262[A]:ASP:OD2	5:B:502:PQ2:NC	2.48	0.47
1:A:139:LEU:CD1	1:B:122:LEU:HD21	2.45	0.47
1:B:228:ALA:HB2	1:B:254:ASP:HB3	1.97	0.47
1:A:415:LYS:O	6:A:607:HOH:O	2.20	0.46
1:A:44:THR:O	3:A:502:NAD:O2B	2.27	0.46
1:B:114:PRO:HB3	1:B:127:SER:HB2	1.97	0.46
1:A:150[B]:HIS:CE1	6:A:688:HOH:O	2.67	0.46
1:B:9:GLN:OE1	1:B:11[A]:ARG:HG2	2.16	0.46
1:B:85:VAL:O	1:B:89:VAL:HG23	2.15	0.46
1:B:166:LYS:HB3	1:B:175:ARG:NH1	2.30	0.46
1:A:346:HIS:O	1:A:347[A]:ARG:C	2.54	0.46
1:A:399:MET:HG2	1:A:423:LEU:HD22	1.98	0.46
1:A:140:ARG:O	1:A:144:GLU:HG2	2.16	0.46
1:A:22:ASP:O	1:A:26:ARG:HG2	2.16	0.46
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.62	0.46
1:A:378:LEU:HB2	1:A:441:VAL:HB	1.97	0.46
1:A:171:THR:HG1	1:A:174:GLU:H	1.62	0.46
1:A:206:ARG:O	1:A:210:GLU:HG3	2.16	0.45
1:B:164:ARG:HB3	1:B:167:LYS:HG2	1.98	0.45
1:A:70:LEU:O	1:A:73:CYS:HB2	2.17	0.45
1:A:278:PRO:O	1:A:281:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:HD3	1:A:304:PRO:HB3	1.98	0.45
1:A:219:VAL:HG12	1:A:221:VAL:HG23	1.98	0.45
1:A:384:LEU:HD12	1:A:384:LEU:HA	1.76	0.45
1:B:101:ASN:HA	1:B:109:ALA:HB1	1.99	0.45
1:A:295[B]:ARG:CZ	6:A:603:HOH:O	2.64	0.45
1:B:164:ARG:HA	1:B:167:LYS:HB2	1.98	0.44
1:A:85:VAL:HG21	3:A:502:NAD:N6A	2.32	0.44
1:B:169:PHE:HB2	1:B:175:ARG:HG2	2.00	0.44
1:A:350:ALA:O	4:A:503:CL:CL	2.72	0.44
1:A:11:ARG:NH1	1:B:2:ASP:OD1	2.50	0.44
1:B:354:ARG:HG2	1:B:356:VAL:HG22	2.00	0.44
1:B:218:VAL:O	1:B:324:PHE:HA	2.17	0.44
1:A:368:TRP:CE2	1:A:393:LYS:HG3	2.53	0.44
1:A:40:VAL:HG12	1:A:45:PHE:HE1	1.83	0.44
1:B:343:PRO:HB2	1:B:345:THR:O	2.18	0.44
1:A:321:GLY:O	6:A:606:HOH:O	2.20	0.43
1:A:174:GLU:HA	1:A:177:ARG:HD2	2.00	0.43
1:A:7:PHE:CZ	1:B:5:PRO:HB3	2.53	0.43
3:A:502:NAD:H2D	3:A:502:NAD:H6N	1.61	0.43
1:B:158:ALA:HB2	1:B:182:PHE:HE2	1.83	0.43
1:B:244:ILE:HD12	1:B:264:ASP:O	2.18	0.43
1:B:224:GLY:HA2	1:B:330:ILE:O	2.18	0.43
1:A:380:PHE:HB2	1:A:439:ILE:HB	2.01	0.43
1:B:286:LEU:HD21	1:B:298:ARG:HB2	2.00	0.43
1:B:288:ARG:NH2	6:B:607:HOH:O	2.40	0.42
1:B:106:PRO:HB3	5:B:502:PQ2:CMA	2.49	0.42
1:A:279:GLN:HB2	1:A:309:ARG:NH1	2.34	0.42
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.80	0.42
1:A:74:TRP:CE2	1:B:97:ARG:HG2	2.55	0.42
1:B:284:GLN:HA	1:B:287:LEU:HB3	2.02	0.42
1:A:289:GLU:OE2	1:A:292:LYS:HD2	2.20	0.42
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.89	0.42
1:B:382:MET:HG3	2:B:501:SAH:H4'	2.02	0.42
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.81	0.41
1:A:370:ASN:HD21	1:B:370:ASN:HA	1.84	0.41
1:B:197:GLU:HA	1:B:200:VAL:HG23	2.02	0.41
1:B:204:THR:O	1:B:207:LEU:HB2	2.20	0.41
1:A:201:ASN:O	1:A:205:GLU:HG2	2.21	0.41
1:A:218:VAL:O	1:A:324:PHE:HA	2.20	0.41
1:A:74:TRP:CH2	1:B:97:ARG:HA	2.54	0.41
1:B:102:VAL:H	1:B:109:ALA:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASP:OD1	1:A:104:ASP:N	2.46	0.41
1:B:139:LEU:O	1:B:143:LEU:HG	2.20	0.41
1:A:146:LEU:O	1:A:148:PRO:HD3	2.20	0.41
1:B:195:ALA:O	1:B:197:GLU:N	2.54	0.41
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.79	0.41
1:A:146:LEU:HD11	1:B:142:LYS:CE	2.51	0.41
1:A:418:VAL:HB	1:A:457:HIS:CE1	2.56	0.41
1:B:339:TYR:CD2	1:B:412:THR:HA	2.55	0.41
1:A:29:ARG:HG2	1:A:33:GLU:OE2	2.21	0.41
1:A:42:ALA:HB1	3:A:502:NAD:O2B	2.21	0.41
1:A:346:HIS:O	4:A:503:CL:CL	2.77	0.41
1:B:299:LEU:HA	1:B:299:LEU:HD23	1.94	0.41
1:A:102:VAL:H	1:A:109:ALA:HB2	1.86	0.40
1:A:177:ARG:CZ	1:A:295[B]:ARG:HH22	2.35	0.40
1:A:196:ASP:O	1:A:200:VAL:HG23	2.22	0.40
1:A:361:LYS:HG3	1:A:362:THR:N	2.37	0.40
1:A:85:VAL:O	1:A:89:VAL:HG23	2.21	0.40
1:B:159:GLY:HA2	1:B:162[A]:ARG:HH21	1.84	0.40
1:B:166:LYS:O	1:B:168:GLN:N	2.54	0.40

All (2) 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)
1:A:167:LYS:NZ	1:A:369:GLU:OE2[2_755]	2.12	0.08
6:B:607:HOH:O	6:B:684:HOH:O[3_745]	2.14	0.06

## 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	460/457 (101%)	444 (96%)	13 (3%)	3 (1%)	22 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	454/457 (99%)	425 (94%)	22 (5%)	7 (2%)	10	14
All	All	914/914 (100%)	869 (95%)	35 (4%)	10 (1%)	17	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104[A]	ASP
1	B	104[B]	ASP
1	B	165	VAL
1	B	167	LYS
1	B	196	ASP
1	A	292	LYS
1	A	347[A]	ARG
1	A	347[B]	ARG
1	B	249	ARG
1	B	200	VAL

### 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	381/372 (102%)	371 (97%)	10 (3%)	46	61
1	B	377/372 (101%)	366 (97%)	11 (3%)	42	57
All	All	758/744 (102%)	737 (97%)	21 (3%)	44	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LYS
1	A	198	LYS
1	A	248	ASP
1	A	249	ARG
1	A	262[A]	ASP
1	A	262[B]	ASP

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Mol	Chain	Res	Type
1	A	288	ARG
1	A	334	SER
1	A	415	LYS
1	A	449	ASP
1	B	81	ASP
1	B	120	SER
1	B	191	SER
1	B	196	ASP
1	B	198	LYS
1	B	249	ARG
1	B	260	ARG
1	B	261	ARG
1	B	284	GLN
1	B	369	GLU
1	B	450	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	HIS

### 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](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	PQ2	B	502	1	36,66,66	3.00	13 (36%)	41,98,98	3.16	13 (31%)
2	SAH	A	501	-	21,28,28	1.32	2 (9%)	20,40,40	1.54	2 (10%)
2	SAH	B	501	-	21,28,28	1.31	2 (9%)	20,40,40	1.52	1 (5%)
3	NAD	A	502	-	42,48,48	1.51	4 (9%)	50,73,73	1.66	7 (14%)

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	PQ2	B	502	1	-	12/34/94/94	0/4/5/5
2	SAH	A	501	-	-	1/7/31/31	0/3/3/3
2	SAH	B	501	-	-	1/7/31/31	0/3/3/3
3	NAD	A	502	-	-	18/26/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	PQ2	C2B-C1B	9.68	1.60	1.52
5	B	502	PQ2	C1B-NB	8.14	1.48	1.32
3	A	502	NAD	C4N-C3N	7.14	1.51	1.39
5	B	502	PQ2	CDB-C2B	-5.78	1.47	1.56
5	B	502	PQ2	C1A-NA	5.19	1.45	1.38
5	B	502	PQ2	C4A-NA	4.52	1.46	1.37
2	B	501	SAH	C2-N3	4.49	1.39	1.32
2	A	501	SAH	C2-N3	4.10	1.38	1.32
5	B	502	PQ2	CHB-C1B	3.92	1.53	1.42
5	B	502	PQ2	C1C-CHC	3.53	1.54	1.41
5	B	502	PQ2	C3B-C4B	-3.39	1.45	1.51
3	A	502	NAD	C5N-C4N	3.19	1.45	1.38
5	B	502	PQ2	C4D-CHA	3.15	1.53	1.41
3	A	502	NAD	O4D-C1D	2.67	1.44	1.41
3	A	502	NAD	C5A-C4A	2.50	1.47	1.40
2	B	501	SAH	C2-N1	2.44	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	PQ2	CHA-C1A	-2.29	1.32	1.38
5	B	502	PQ2	CHB-C4A	-2.18	1.32	1.36
5	B	502	PQ2	CDA-C2A	-2.12	1.52	1.56
2	A	501	SAH	C2-N1	2.07	1.37	1.33
5	B	502	PQ2	CHD-C1D	2.06	1.53	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	PQ2	C4A-NA-C1A	-12.32	105.96	110.77
5	B	502	PQ2	C2B-C1B-NB	-8.49	103.62	113.67
5	B	502	PQ2	C1C-CHC-C4B	-7.64	118.70	128.57
3	A	502	NAD	C5N-C4N-C3N	-7.20	111.82	120.34
2	B	501	SAH	N3-C2-N1	-5.27	120.44	128.68
5	B	502	PQ2	CAD-C2D-C1D	-4.92	123.84	127.30
2	A	501	SAH	N3-C2-N1	-4.79	121.19	128.68
5	B	502	PQ2	CHB-C1B-NB	-3.92	118.56	124.22
5	B	502	PQ2	CAD-CBD-CCD	-3.59	106.66	112.67
5	B	502	PQ2	CBD-CAD-C2D	3.36	118.69	112.49
3	A	502	NAD	C4A-C5A-N7A	-3.34	105.92	109.40
3	A	502	NAD	C3B-C2B-C1B	3.17	105.75	100.98
3	A	502	NAD	C3D-C2D-C1D	3.06	105.58	100.98
5	B	502	PQ2	C2B-C1B-CHB	-2.86	118.71	122.47
5	B	502	PQ2	CEC-CDC-C2C	-2.81	110.48	115.96
2	A	501	SAH	C5'-SD-CG	-2.80	93.86	102.27
3	A	502	NAD	C2N-C3N-C4N	2.72	121.35	118.26
5	B	502	PQ2	CAC-CBC-CCC	2.62	117.07	112.67
5	B	502	PQ2	CDB-C2B-C3B	2.38	114.77	108.39
3	A	502	NAD	O4D-C4D-C5D	2.37	117.18	109.37
5	B	502	PQ2	CBA-CAA-C3A	2.08	120.70	114.69
3	A	502	NAD	C5N-C6N-N1N	2.05	123.34	120.40
5	B	502	PQ2	CBC-CAC-C3C	-2.01	108.77	112.49

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	502	PQ2	C2A-C1A-CHA-C4D
5	B	502	PQ2	NB-C1B-CHB-C4A
5	B	502	PQ2	C1D-C2D-CAD-CBD
5	B	502	PQ2	C3D-C2D-CAD-CBD
5	B	502	PQ2	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	B	502	PQ2	C4A-C3A-CAA-CBA
5	B	502	PQ2	C2B-C3B-CAB-CBB
5	B	502	PQ2	C4B-C3B-CAB-CBB
5	B	502	PQ2	C3A-C4A-CHB-C1B
5	B	502	PQ2	NA-C4A-CHB-C1B
5	B	502	PQ2	ND-C4D-CHA-C1A
5	B	502	PQ2	C3D-C4D-CHA-C1A
3	A	502	NAD	C5D-O5D-PN-O1N
3	A	502	NAD	O4D-C1D-N1N-C2N
3	A	502	NAD	O4D-C1D-N1N-C6N
3	A	502	NAD	C2D-C1D-N1N-C2N
3	A	502	NAD	C2D-C1D-N1N-C6N
3	A	502	NAD	C2N-C3N-C7N-O7N
3	A	502	NAD	C2N-C3N-C7N-N7N
3	A	502	NAD	O4B-C4B-C5B-O5B
3	A	502	NAD	C3B-C4B-C5B-O5B
3	A	502	NAD	C4N-C3N-C7N-N7N
3	A	502	NAD	C4N-C3N-C7N-O7N
3	A	502	NAD	PN-O3-PA-O5B
3	A	502	NAD	O4D-C4D-C5D-O5D
3	A	502	NAD	C5B-O5B-PA-O3
2	A	501	SAH	C3'-C4'-C5'-SD
3	A	502	NAD	C5B-O5B-PA-O2A
3	A	502	NAD	C4D-C5D-O5D-PN
2	B	501	SAH	C3'-C4'-C5'-SD
3	A	502	NAD	C4B-C5B-O5B-PA
3	A	502	NAD	C3D-C4D-C5D-O5D

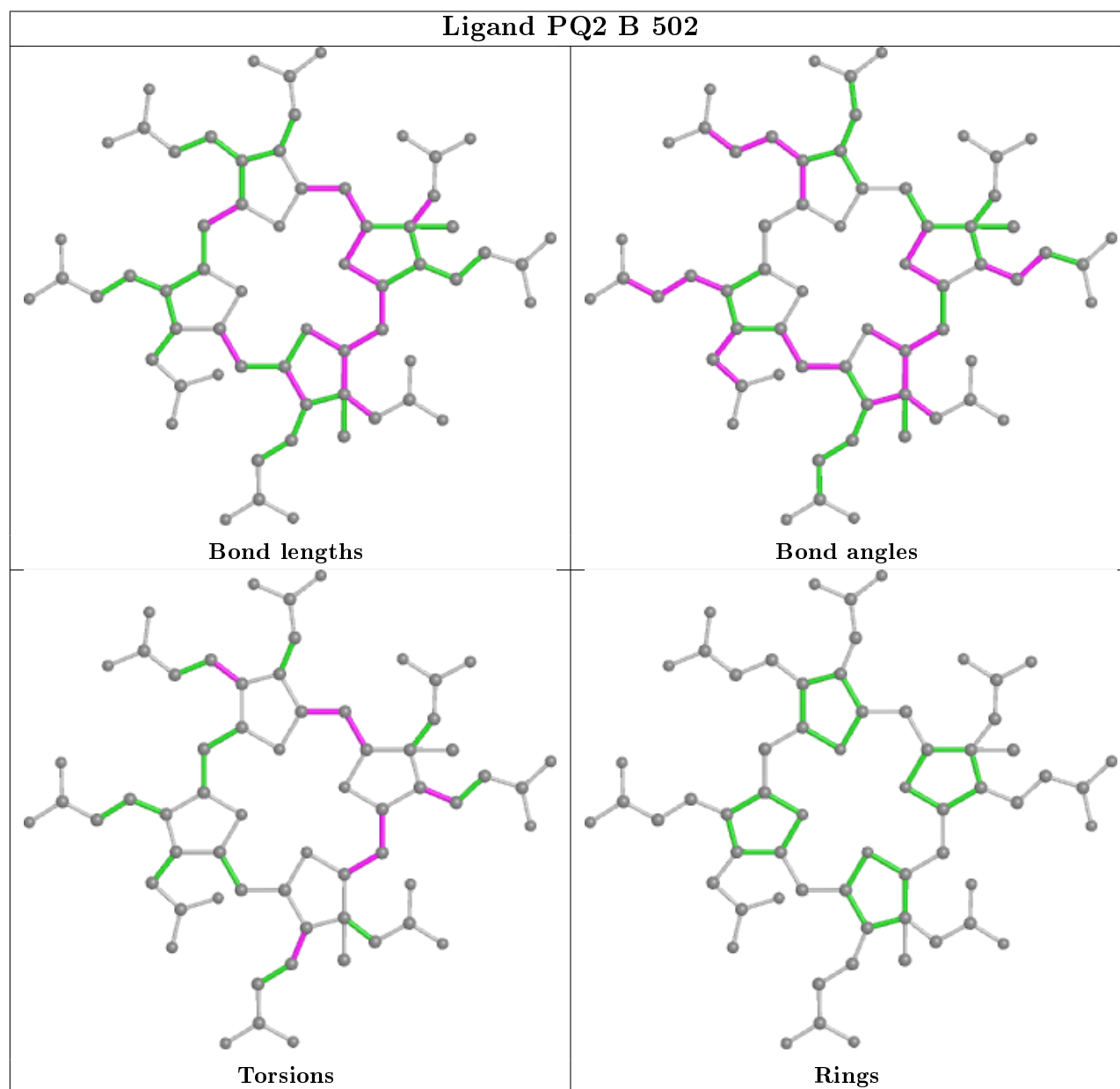
There are no ring outliers.

3 monomers are involved in 11 short contacts:

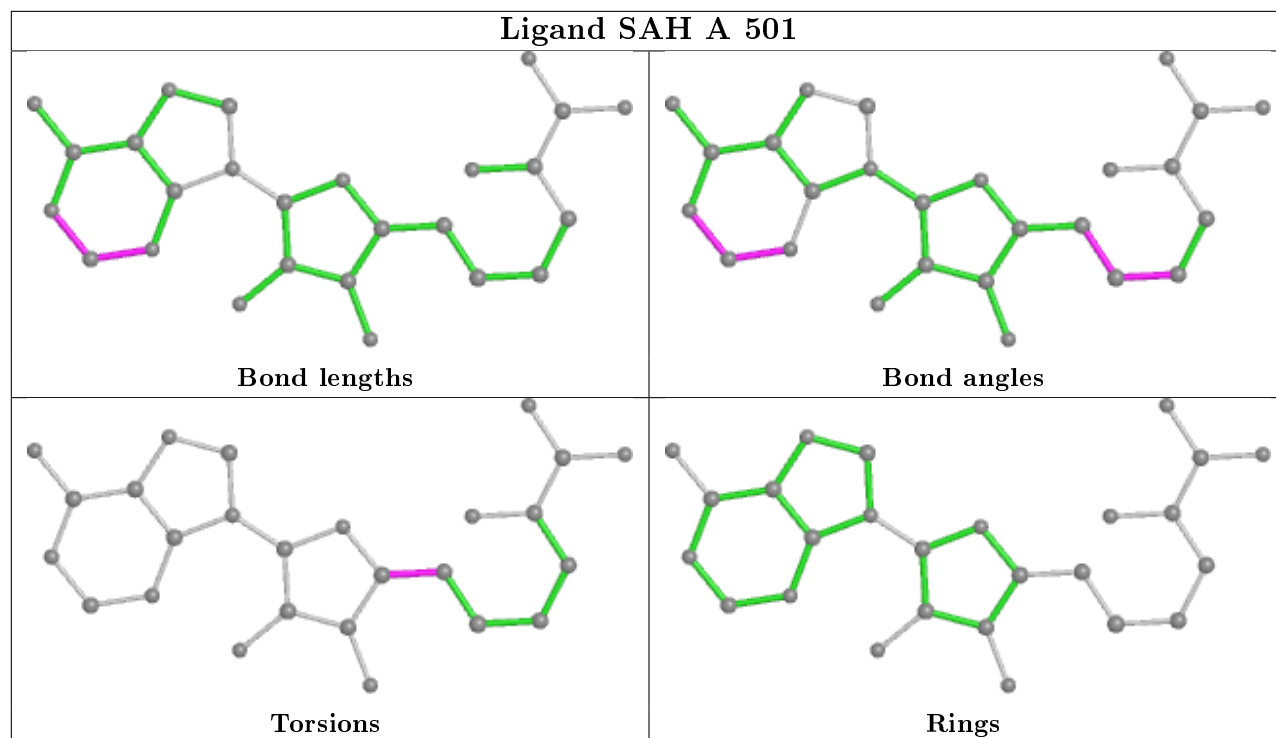
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	PQ2	3	0
2	B	501	SAH	1	0
3	A	502	NAD	7	0

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

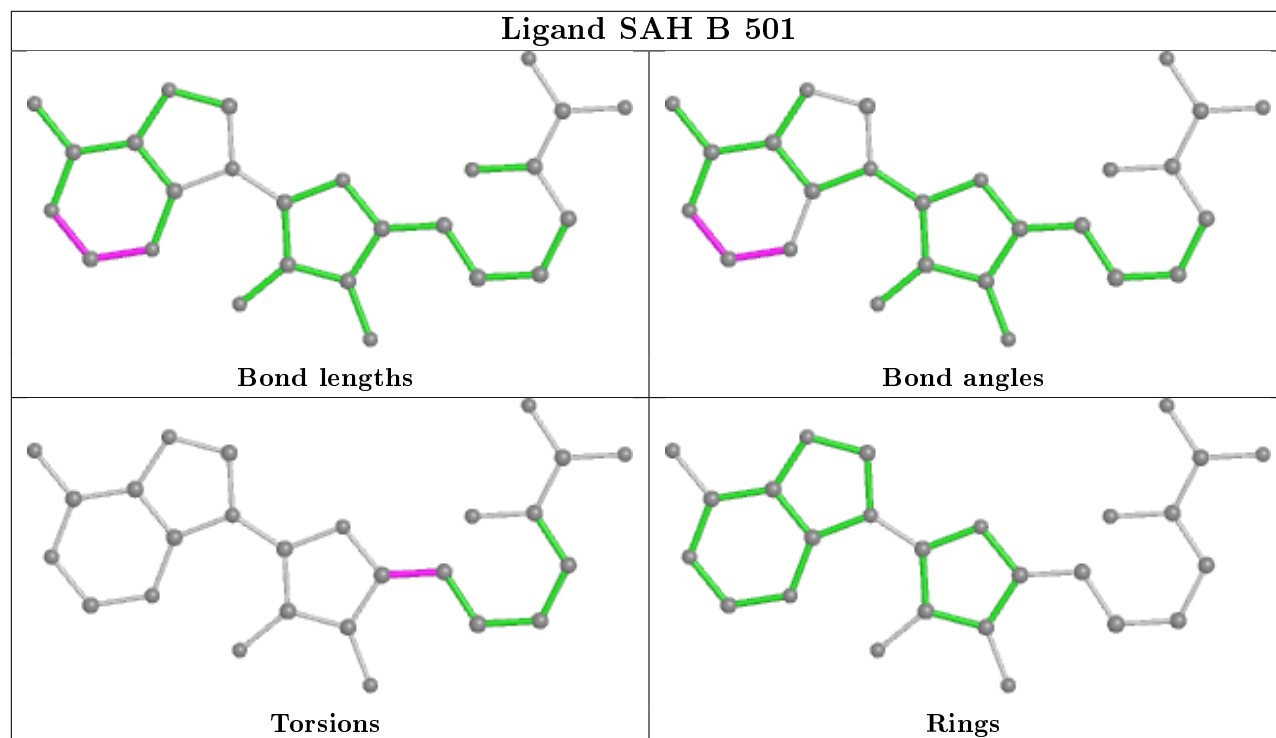
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

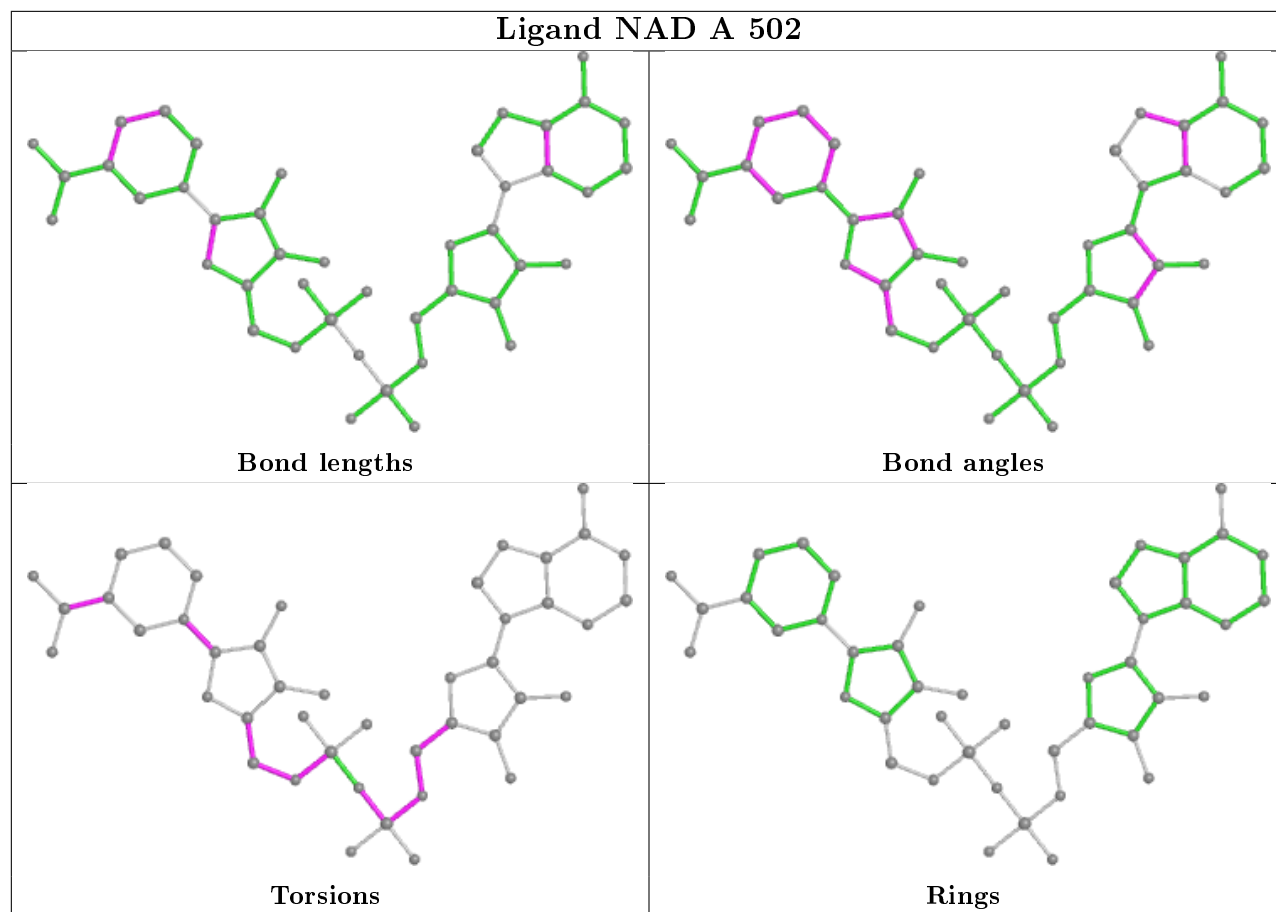


## Ligand SAH A 501



## Ligand SAH B 501





## 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	451/457 (98%)	-0.73	1 (0%) 95 97	24, 43, 87, 136	0
1	B	449/457 (98%)	-0.64	8 (1%) 68 74	23, 45, 96, 142	0
All	All	900/914 (98%)	-0.68	9 (1%) 82 86	23, 44, 94, 142	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	ALA	6.3
1	B	276	CYS	3.7
1	B	271	ARG	3.3
1	B	168	GLN	3.2
1	B	319	HIS	2.8
1	B	278	PRO	2.4
1	B	161	LEU	2.2
1	A	319	HIS	2.1
1	B	172	MET	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.

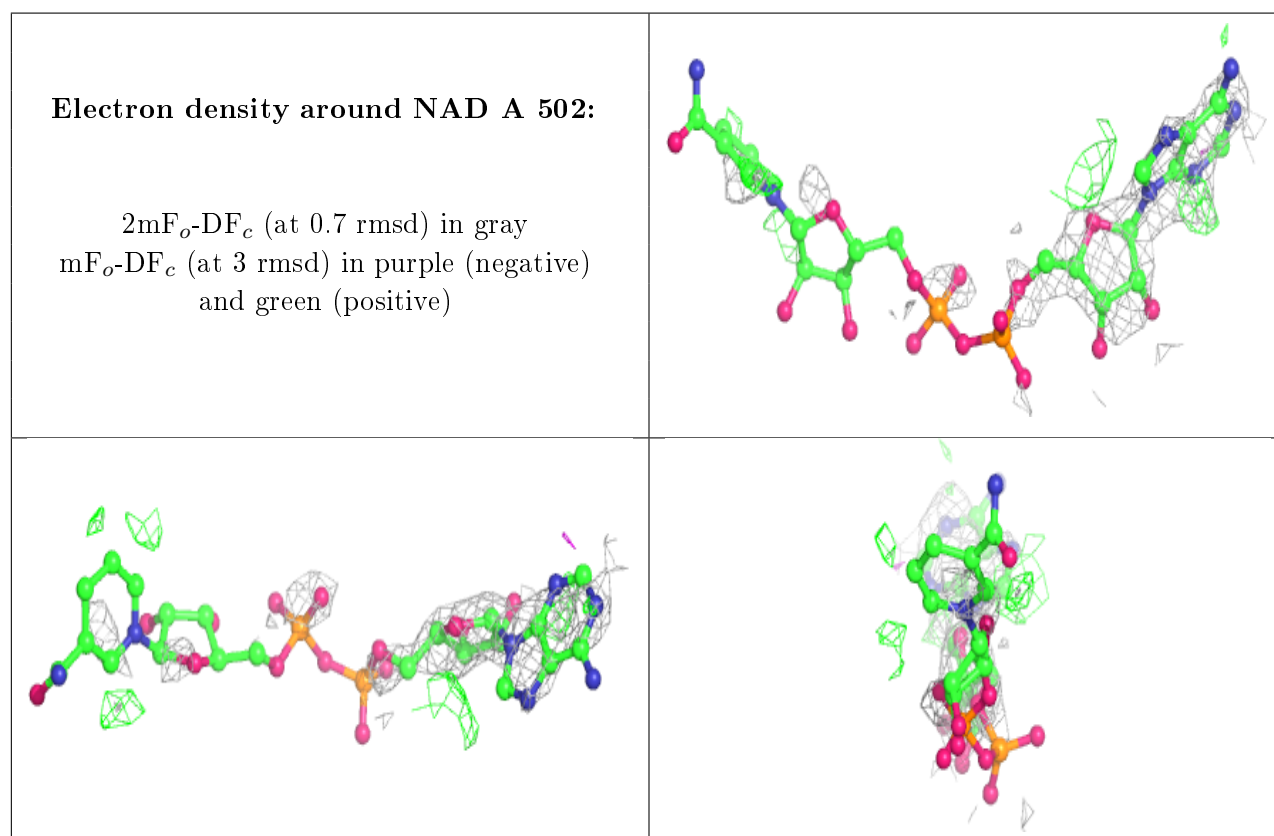
### 6.4 Ligands [i](#)

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	NAD	A	502	44/44	0.66	0.47	50,73,98,101	44
5	PQ2	B	502	62/62	0.76	0.37	20,57,69,74	62
4	CL	A	505	1/1	0.87	0.08	84,84,84,84	0
4	CL	A	503	1/1	0.88	0.13	85,85,85,85	0
4	CL	A	506	1/1	0.90	0.09	77,77,77,77	0
4	CL	B	504	1/1	0.91	0.09	66,66,66,66	0
2	SAH	B	501	26/26	0.96	0.10	23,33,42,47	0
2	SAH	A	501	26/26	0.96	0.09	22,30,42,50	0
4	CL	A	507	1/1	0.96	0.10	58,58,58,58	0
4	CL	B	503	1/1	0.97	0.05	60,60,60,60	0
4	CL	A	504	1/1	0.97	0.11	61,61,61,61	0

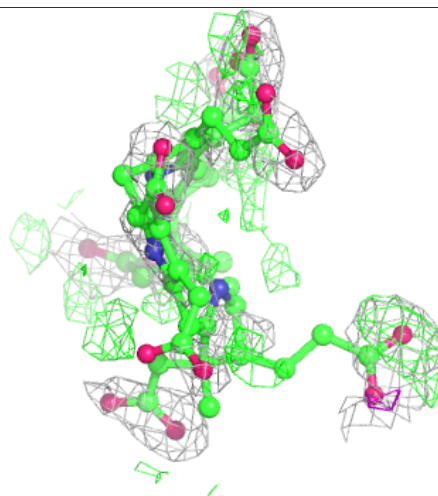
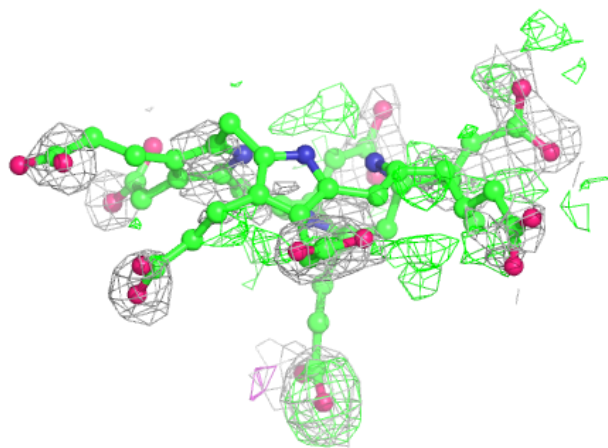
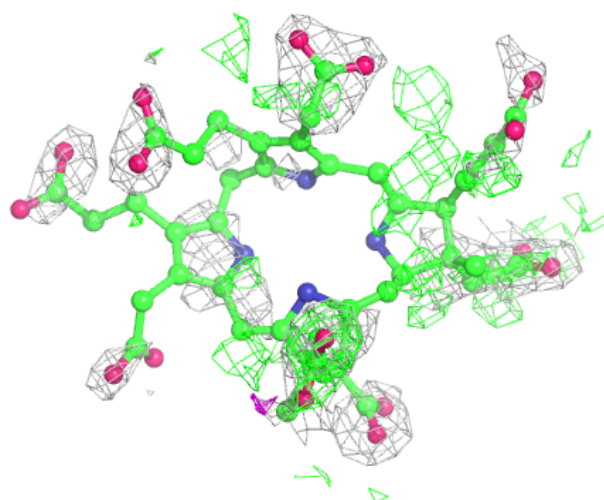
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





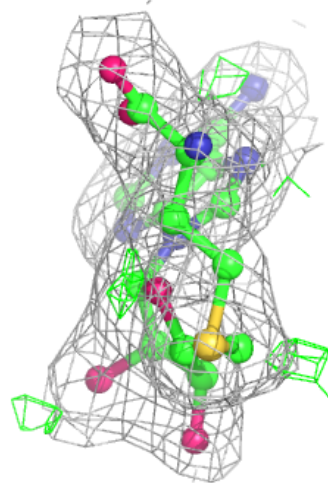
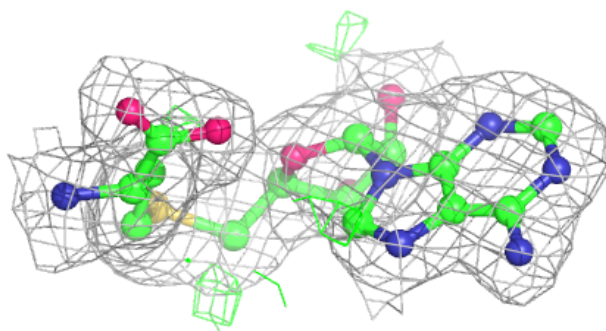
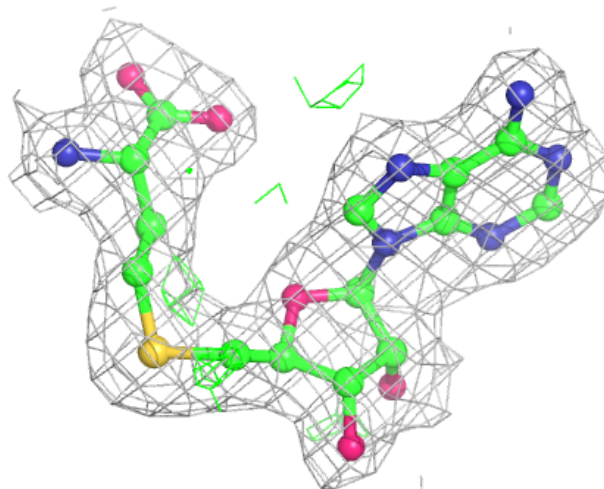
**Electron density around PQ2 B 502:**

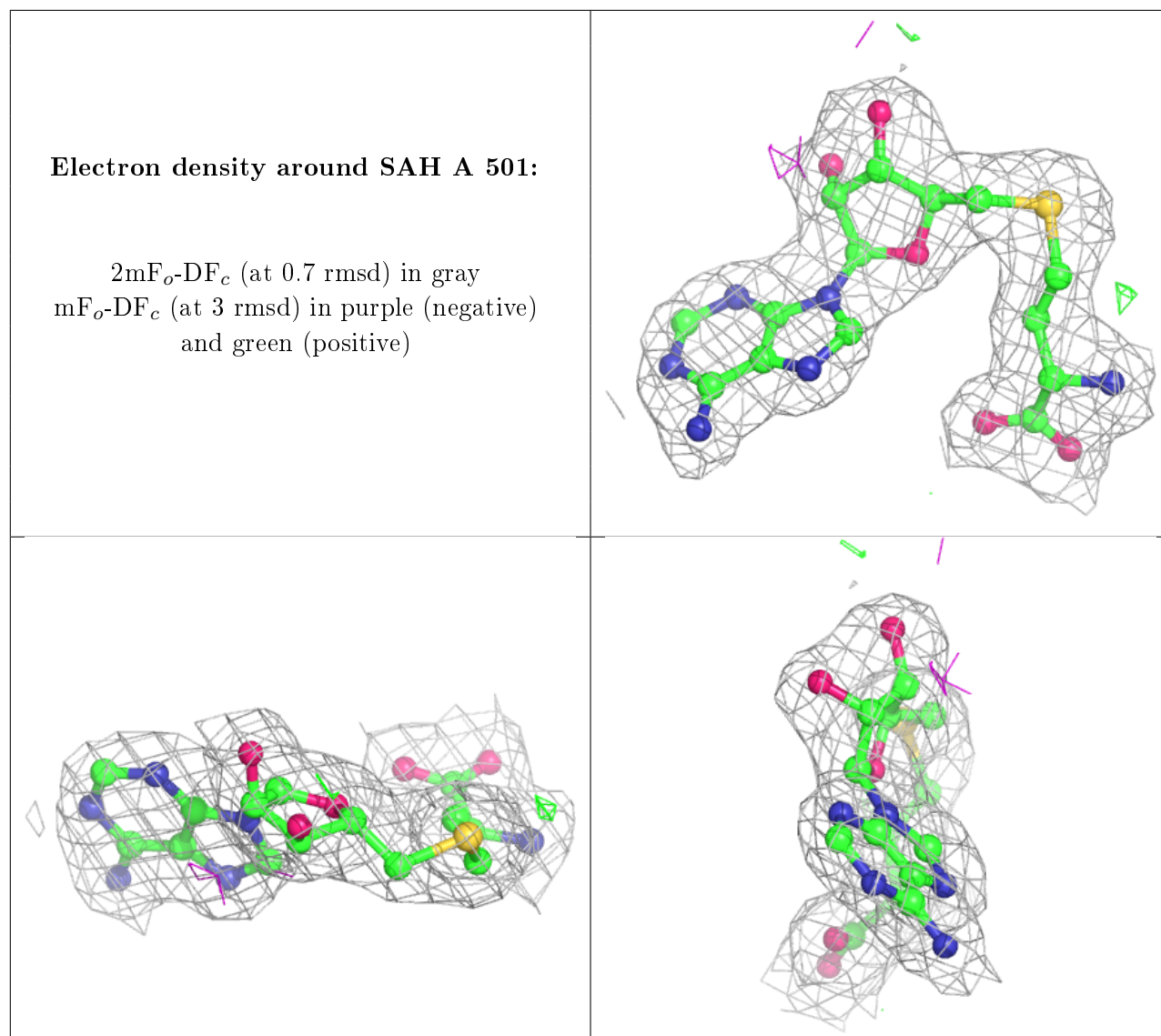
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SAH B 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.