



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:19 pm BST

PDB ID : 3CNS  
Title : Crystal structure of fms1 in complex with S-Bz-MeSpermidine  
Authors : Huang, Q.; Hao, H.  
Deposited on : 2008-03-26  
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.

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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

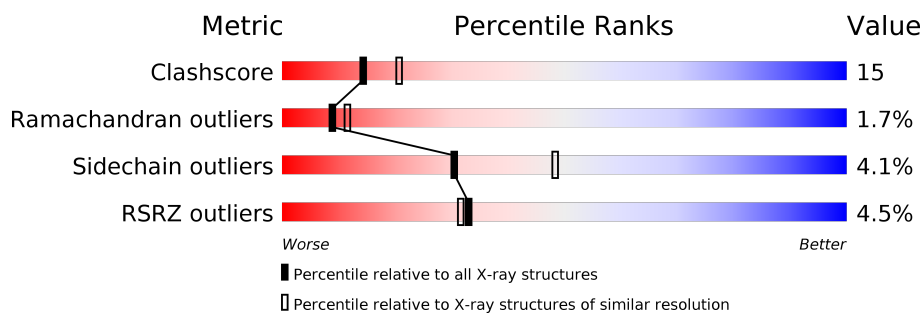
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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	516	
1	B	516	

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	SP8	A	518	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8090 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 fms1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3935	2489	684	740	22			
1	B	487	Total	C	N	O	S	0	0	0
			3896	2462	676	736	22			

There are 16 discrepancies between the modelled and reference sequences:

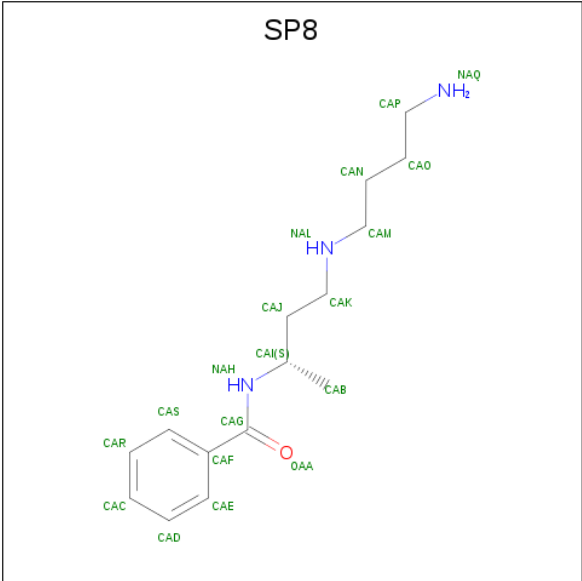
Chain	Residue	Modelled	Actual	Comment	Reference
A	509	LEU	-	EXPRESSION TAG	UNP P50264
A	510	GLU	-	EXPRESSION TAG	UNP P50264
A	511	HIS	-	EXPRESSION TAG	UNP P50264
A	512	HIS	-	EXPRESSION TAG	UNP P50264
A	513	HIS	-	EXPRESSION TAG	UNP P50264
A	514	HIS	-	EXPRESSION TAG	UNP P50264
A	515	HIS	-	EXPRESSION TAG	UNP P50264
A	516	HIS	-	EXPRESSION TAG	UNP P50264
B	509	LEU	-	EXPRESSION TAG	UNP P50264
B	510	GLU	-	EXPRESSION TAG	UNP P50264
B	511	HIS	-	EXPRESSION TAG	UNP P50264
B	512	HIS	-	EXPRESSION TAG	UNP P50264
B	513	HIS	-	EXPRESSION TAG	UNP P50264
B	514	HIS	-	EXPRESSION TAG	UNP P50264
B	515	HIS	-	EXPRESSION TAG	UNP P50264
B	516	HIS	-	EXPRESSION TAG	UNP P50264

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is N-{(1S)-3-[(4-aminobutyl)amino]-1-methylpropyl}benzamide (three-letter code: SP8) (formula: C<sub>15</sub>H<sub>25</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	15	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			19	15	3	1		

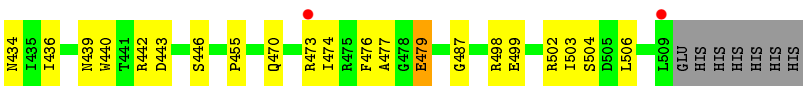
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	52	Total	O	0	0
			52	52		

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 ( $\text{RSRZ} > 2$ ). 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.

- [illegible]

- Chain B:
- 
- 64% 28% 6%
- | Amino Acid | Frequency (%) |
|------------|---------------|
| Met        | 6%            |
| Asn        | 6%            |
| Thr        | 6%            |
| Val        | 6%            |
| Ser        | 6%            |
| Pro        | 6%            |
| Ala        | 6%            |
| Lys        | 6%            |
| Phe        | 6%            |
| Glu        | 64%           |
| His        | 6%            |
| Leu        | 6%            |
| Ile        | 6%            |
| Tyr        | 6%            |
| Trp        | 6%            |
| Arg        | 6%            |
| Pro        | 6%            |
| Ser        | 6%            |
| Val        | 6%            |
| Thr        | 6%            |
| Asn        | 6%            |
| Met        | 6%            |



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.28Å 215.13Å 117.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 39.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.40) 98.0 (39.66-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.223 , 0.272 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: SP8, FAD

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	0.38	0/4016	0.62	0/5429
1	B	0.36	0/3973	0.59	0/5370
All	All	0.37	0/7989	0.61	0/10799

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	3935	0	3862	112	0
1	B	3896	0	3811	128	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
3	A	19	0	25	11	0
3	B	19	0	25	4	0
4	A	63	0	0	1	0
4	B	52	0	0	1	0
All	All	8090	0	7785	244	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 15.

All (244) 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:A:173:LEU:O	3:A:518:SP8:HAB	1.50	1.07
1:A:67:HIS:HE2	3:A:518:SP8:HNAL	0.98	0.94
1:B:382:ASN:HD22	1:B:382:ASN:H	1.10	0.93
1:A:132:GLN:HG2	1:A:134:LEU:HD13	1.53	0.90
1:A:385:GLU:O	1:A:388:ARG:HG2	1.70	0.90
1:A:342:ARG:HH11	1:A:342:ARG:HG3	1.38	0.88
1:B:382:ASN:ND2	1:B:382:ASN:H	1.65	0.85
1:A:377:GLN:NE2	1:A:377:GLN:H	1.75	0.84
1:A:377:GLN:HE21	1:A:377:GLN:H	1.23	0.84
1:A:463:VAL:HG21	1:A:483:MET:HE2	1.60	0.84
1:B:228:ARG:HH21	1:B:473:ARG:HD2	1.42	0.83
1:B:341:GLU:O	1:B:342:ARG:HG3	1.80	0.81
1:B:122:MET:HE1	1:B:145:VAL:HG13	1.62	0.81
1:A:136:VAL:O	1:A:137:SER:HB3	1.80	0.80
1:A:104:ARG:HB2	1:A:104:ARG:HH11	1.47	0.80
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.64	0.80
1:A:133:HIS:O	1:A:134:LEU:HD12	1.82	0.79
1:A:173:LEU:O	3:A:518:SP8:CAB	2.28	0.79
1:A:264:PRO:O	1:A:265:GLU:HB2	1.80	0.79
1:A:104:ARG:HB2	1:A:104:ARG:NH1	1.98	0.78
1:A:376:MET:HE1	1:A:384:ILE:HB	1.63	0.77
1:B:333:LEU:HD12	1:B:333:LEU:H	1.50	0.76
1:A:104:ARG:HG3	1:A:104:ARG:O	1.86	0.75
1:B:423:ASN:ND2	1:B:433:ARG:HH12	1.85	0.75
1:A:127:GLU:O	1:A:131:HIS:HB2	1.88	0.74
1:B:228:ARG:HG2	1:B:234:VAL:HG22	1.72	0.72
3:A:518:SP8:HABB	3:A:518:SP8:OAA	1.89	0.71
1:B:228:ARG:NH2	1:B:473:ARG:HD2	2.05	0.70
1:A:463:VAL:HG21	1:A:483:MET:CE	2.21	0.69
1:B:247:ASP:O	1:B:473:ARG:HD3	1.92	0.69
1:B:420:PRO:O	1:B:422:GLU:HG2	1.92	0.69
1:B:240:ASP:OD2	1:B:242:THR:HG23	1.92	0.68
1:B:68:ASP:HB3	1:B:192:GLN:HB2	1.76	0.68
1:B:279:LYS:HG3	1:B:281:VAL:HG12	1.77	0.66
1:B:418:MET:O	1:B:420:PRO:HD3	1.95	0.66
1:A:189:PHE:HE2	1:A:191:HIS:NE2	1.95	0.65
1:B:377:GLN:NE2	1:B:377:GLN:H	1.95	0.65
1:B:212:PHE:HB2	1:B:213:PRO:HD2	1.78	0.65
1:B:278:LEU:HA	1:B:470:GLN:HE22	1.62	0.65
1:A:189:PHE:HE2	1:A:191:HIS:CE1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ALA:O	1:B:289:ILE:HG22	1.97	0.64
1:B:141:PHE:O	1:B:145:VAL:HG23	1.97	0.64
1:A:224:LYS:HD3	1:A:239:GLU:HB3	1.79	0.63
1:A:342:ARG:NH1	1:A:342:ARG:HG3	2.08	0.63
1:B:322:GLU:O	1:B:326:ILE:HG13	1.99	0.62
1:B:382:ASN:ND2	1:B:382:ASN:N	2.45	0.62
1:A:278:LEU:HA	1:A:470:GLN:NE2	2.15	0.62
1:B:67:HIS:ND1	1:B:195:ASN:ND2	2.48	0.62
1:A:290:HIS:HD2	1:A:457:ASP:OD2	1.83	0.62
1:A:189:PHE:N	1:A:189:PHE:CD1	2.68	0.61
1:A:164:LEU:N	1:A:165:PRO:HD2	2.15	0.61
1:A:150:LEU:O	1:A:153:ARG:HD2	2.01	0.61
1:A:376:MET:CE	1:A:380:LEU:HG	2.31	0.60
1:A:376:MET:CE	1:A:381:THR:HA	2.31	0.60
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.32	0.60
1:A:213:PRO:O	1:A:216:TRP:HB2	2.03	0.59
1:A:278:LEU:HA	1:A:470:GLN:HE22	1.66	0.59
1:B:14:ILE:CD1	1:B:226:ILE:HD11	2.32	0.59
1:A:225:SER:HB3	1:A:273:GLU:HB3	1.83	0.59
1:A:479:GLU:OE1	1:A:487:GLY:HA2	2.01	0.59
1:A:389:GLU:OE1	1:A:389:GLU:HA	2.03	0.58
1:A:122:MET:HG2	1:A:148:TYR:CG	2.38	0.58
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.33	0.58
1:A:234:VAL:O	1:A:245:ASN:HA	2.03	0.58
1:B:279:LYS:HB2	1:B:280:PRO:HD2	1.85	0.58
3:A:518:SP8:HAC	4:A:556:HOH:O	2.03	0.58
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.33	0.57
1:B:391:LYS:N	1:B:391:LYS:HD2	2.20	0.57
1:B:418:MET:HE3	1:B:434:ASN:HA	1.86	0.57
1:A:218:LYS:HD2	1:A:221:CYS:HB3	1.86	0.57
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.04	0.57
1:A:174:TRP:CZ2	3:A:518:SP8:HAP	2.40	0.57
1:A:12:ILE:HB	1:A:249:VAL:HG12	1.87	0.56
1:A:210:GLN:HE21	1:A:210:GLN:CA	2.18	0.56
1:B:14:ILE:HD12	1:B:251:ILE:HG12	1.87	0.56
1:B:255:GLN:HE22	1:B:289:ILE:HG13	1.71	0.56
1:B:399:GLN:HB3	1:B:400:PRO:HD3	1.86	0.56
1:A:376:MET:HG3	1:A:381:THR:OG1	2.04	0.56
1:B:202:ASP:O	1:B:206:GLN:HG2	2.05	0.56
1:B:333:LEU:N	1:B:333:LEU:HD12	2.19	0.56
1:B:41:ARG:HH21	1:B:46:GLY:HA2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HA	1:B:470:GLN:NE2	2.21	0.56
1:B:382:ASN:HD22	1:B:382:ASN:N	1.93	0.56
1:B:420:PRO:C	1:B:422:GLU:HG2	2.26	0.56
1:A:101:ASP:OD2	1:A:103:GLU:HB3	2.07	0.55
1:B:502:ARG:HG2	1:B:502:ARG:HH11	1.71	0.55
1:B:63:ALA:HA	2:B:517:FAD:N5	2.22	0.55
1:A:306:TRP:HE1	1:A:362:ASN:HD21	1.55	0.54
1:A:377:GLN:N	1:A:377:GLN:NE2	2.51	0.54
1:B:122:MET:HG2	1:B:148:TYR:CD2	2.42	0.54
1:A:41:ARG:NH1	1:A:443:ASP:OD2	2.41	0.54
1:B:116:GLU:N	1:B:116:GLU:OE1	2.38	0.54
1:B:72:ASN:C	1:B:72:ASN:HD22	2.11	0.54
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.72	0.54
1:A:381:THR:O	1:A:385:GLU:HG3	2.09	0.53
1:B:122:MET:CE	1:B:145:VAL:HG22	2.39	0.53
1:A:189:PHE:CE2	1:A:191:HIS:NE2	2.77	0.53
1:B:141:PHE:CD1	1:B:187:THR:HG21	2.44	0.53
1:B:165:PRO:O	1:B:169:ARG:HG3	2.09	0.53
1:B:228:ARG:NH1	1:B:232:LYS:HA	2.23	0.53
1:B:332:ASN:ND2	1:B:334:ASP:H	2.07	0.53
1:A:132:GLN:HG2	1:A:134:LEU:CD1	2.35	0.53
1:A:122:MET:CE	1:A:145:VAL:HG22	2.39	0.52
1:A:311:SER:HA	1:A:362:ASN:HB3	1.91	0.52
1:A:279:LYS:HG3	1:A:470:GLN:OE1	2.09	0.52
1:B:226:ILE:HG12	1:B:236:VAL:HG22	1.90	0.52
1:A:112:GLU:HG3	1:A:113:LEU:N	2.24	0.52
1:A:64:SER:OG	1:A:296:LYS:NZ	2.42	0.52
1:A:157:THR:OG1	1:A:160:GLN:HG3	2.10	0.51
1:A:167:LEU:O	1:A:170:TYR:HD2	1.92	0.51
1:A:376:MET:HE1	1:A:384:ILE:CB	2.39	0.51
1:A:136:VAL:O	1:A:137:SER:CB	2.56	0.51
1:B:122:MET:HE3	1:B:145:VAL:HG22	1.92	0.51
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.25	0.51
1:B:228:ARG:HH12	1:B:232:LYS:HA	1.75	0.51
1:B:332:ASN:OD1	1:B:335:GLU:HG3	2.11	0.51
1:A:63:ALA:HA	2:A:517:FAD:N5	2.26	0.51
1:B:67:HIS:HE2	3:B:518:SP8:HNAL	1.56	0.51
1:B:35:CYS:HB2	1:B:216:TRP:CZ2	2.46	0.51
3:A:518:SP8:OAA	3:A:518:SP8:CAB	2.56	0.51
1:B:110:ASP:O	1:B:114:LEU:HD23	2.11	0.51
1:A:398:PHE:O	1:A:402:LEU:HG	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.91	0.50
1:B:227:THR:HG23	1:B:275:GLN:HB3	1.94	0.50
1:A:44:VAL:CG1	1:A:217:LEU:HD21	2.41	0.50
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.52	0.50
1:B:213:PRO:HG2	1:B:216:TRP:CG	2.47	0.50
1:A:191:HIS:O	1:B:124:LYS:HE3	2.12	0.49
1:B:423:ASN:HB3	1:B:426:ASN:OD1	2.12	0.49
1:B:9:LYS:HE2	1:B:36:LEU:HD11	1.94	0.49
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.47	0.49
1:A:57:ARG:HD3	1:A:369:VAL:CG1	2.42	0.49
1:A:122:MET:HG2	1:A:148:TYR:CD2	2.48	0.49
1:B:502:ARG:HG2	1:B:502:ARG:NH1	2.25	0.49
1:A:415:ILE:HB	1:A:431:VAL:HG22	1.93	0.49
1:B:54:TYR:O	1:B:57:ARG:HG3	2.13	0.49
1:B:177:LEU:CD1	1:B:292:GLY:HA2	2.42	0.48
2:A:517:FAD:N5	3:A:518:SP8:HAKA	2.29	0.48
1:B:502:ARG:O	1:B:506:LEU:HG	2.13	0.48
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.96	0.48
1:B:423:ASN:HD21	1:B:433:ARG:HH12	1.62	0.48
1:B:332:ASN:HD21	1:B:334:ASP:HB2	1.79	0.48
1:A:218:LYS:HD2	1:A:221:CYS:CB	2.43	0.48
1:B:189:PHE:CE1	1:B:191:HIS:CE1	3.02	0.48
1:A:14:ILE:HD12	1:A:14:ILE:N	2.29	0.47
1:B:104:ARG:NH2	1:B:113:LEU:HD21	2.29	0.47
1:B:311:SER:HA	1:B:362:ASN:HB3	1.96	0.47
1:A:395:PHE:CZ	1:A:399:GLN:HG3	2.50	0.47
1:A:67:HIS:CE1	3:A:518:SP8:HNAL	2.30	0.47
1:B:237:ASN:HB3	1:B:243:VAL:HA	1.96	0.47
1:B:30:ASN:HD22	1:B:504:SER:HB3	1.79	0.47
1:B:137:SER:O	1:B:138:ASP:HB3	2.14	0.47
1:A:463:VAL:HG11	1:A:483:MET:HG2	1.96	0.47
1:B:67:HIS:CD2	3:B:518:SP8:HNAL	2.33	0.46
1:A:399:GLN:HB3	1:A:400:PRO:HD3	1.98	0.46
1:B:164:LEU:N	1:B:165:PRO:HD2	2.30	0.46
1:A:228:ARG:HH21	1:A:232:LYS:HA	1.81	0.46
1:A:259:ASN:O	1:A:262:VAL:HG22	2.15	0.46
1:A:174:TRP:CE2	3:A:518:SP8:HAP	2.50	0.46
1:B:174:TRP:HD1	3:B:518:SP8:CAS	2.28	0.46
1:A:212:PHE:HB2	1:A:213:PRO:CD	2.45	0.46
1:A:483:MET:HA	1:A:483:MET:CE	2.45	0.46
1:B:213:PRO:O	1:B:216:TRP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASN:HD21	1:B:364:SER:HB3	1.79	0.46
1:B:391:LYS:HG3	1:B:418:MET:HE1	1.98	0.46
1:A:376:MET:HE3	1:A:380:LEU:HG	1.98	0.46
1:A:335:GLU:HG2	1:A:339:MET:SD	2.56	0.45
1:A:342:ARG:NH1	1:A:342:ARG:CG	2.74	0.45
1:A:173:LEU:N	1:A:173:LEU:HD22	2.31	0.45
1:B:232:LYS:O	1:B:473:ARG:NH1	2.49	0.45
1:A:116:GLU:OE2	1:A:116:GLU:N	2.37	0.45
1:A:134:LEU:C	1:A:136:VAL:H	2.19	0.45
1:B:440:TRP:HB2	4:B:525:HOH:O	2.17	0.45
1:B:340:LEU:C	1:B:342:ARG:H	2.20	0.45
1:B:167:LEU:HD23	1:B:167:LEU:C	2.37	0.45
1:B:13:ILE:O	1:B:37:VAL:HA	2.15	0.45
1:B:174:TRP:HE1	3:B:518:SP8:CAD	2.30	0.45
1:B:412:GLU:HG2	1:B:429:LYS:HE2	1.98	0.45
1:B:229:GLU:C	1:B:231:SER:N	2.70	0.45
1:B:323:PHE:O	1:B:327:VAL:HG23	2.17	0.45
1:B:333:LEU:H	1:B:333:LEU:CD1	2.26	0.45
1:B:70:LEU:HB2	1:B:192:GLN:O	2.17	0.44
1:B:281:VAL:HG13	1:B:282:ILE:N	2.33	0.44
1:A:174:TRP:HA	3:A:518:SP8:HAB	2.00	0.44
1:A:113:LEU:CD2	1:A:159:ASP:HB3	2.48	0.44
1:B:380:LEU:HD13	1:B:380:LEU:O	2.18	0.44
1:B:443:ASP:HB3	1:B:446:SER:OG	2.18	0.44
1:B:9:LYS:O	1:B:246:ALA:HA	2.18	0.44
1:A:252:THR:HG22	1:A:477:ALA:HB3	2.00	0.44
1:B:476:PHE:O	1:B:499:GLU:HG3	2.17	0.43
1:A:434:ASN:ND2	1:A:435:ILE:H	2.17	0.43
1:A:169:ARG:O	1:A:172:GLU:HG3	2.17	0.43
1:A:212:PHE:HB2	1:A:213:PRO:HD2	2.00	0.43
1:B:223:VAL:HA	1:B:238:CYS:HA	2.00	0.43
1:B:439:ASN:HD21	1:B:442:ARG:HH11	1.65	0.43
1:B:262:VAL:C	1:B:263:GLN:HG3	2.39	0.43
1:B:229:GLU:C	1:B:231:SER:H	2.21	0.43
1:A:341:GLU:O	1:A:342:ARG:CB	2.66	0.43
1:A:341:GLU:C	1:A:342:ARG:HG2	2.40	0.42
1:B:298:ILE:HB	1:B:436:ILE:HB	2.01	0.42
1:B:139:CYS:O	1:B:455:PRO:HB3	2.18	0.42
1:A:167:LEU:O	1:A:170:TYR:CD2	2.72	0.42
1:A:414:VAL:HA	1:A:430:PRO:HG2	2.01	0.42
1:B:213:PRO:HG2	1:B:216:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLU:O	1:B:231:SER:N	2.53	0.42
1:B:261:SER:C	1:B:263:GLN:H	2.23	0.42
1:B:293:ALA:HB3	1:B:378:ALA:HB2	2.01	0.42
1:B:141:PHE:CE1	1:B:187:THR:HG21	2.55	0.42
1:B:254:PRO:HG3	2:B:517:FAD:O1A	2.19	0.42
1:A:362:ASN:HD21	1:A:364:SER:HB3	1.84	0.42
2:A:517:FAD:H9	2:A:517:FAD:H1'1	1.86	0.42
1:A:67:HIS:ND1	1:A:195:ASN:ND2	2.67	0.42
1:A:336:LEU:O	1:A:340:LEU:HG	2.20	0.42
1:B:248:TYR:HB3	1:B:503:ILE:HD13	2.02	0.42
1:A:124:LYS:O	1:A:128:LEU:HG	2.19	0.42
1:A:483:MET:HA	1:A:483:MET:HE2	2.02	0.42
1:A:341:GLU:O	1:A:342:ARG:HB2	2.19	0.41
1:A:12:ILE:HG12	1:A:246:ALA:HB2	2.01	0.41
1:A:54:TYR:CD2	1:A:55:GLN:HG3	2.55	0.41
1:B:111:LYS:HG3	1:B:112:GLU:HG3	2.01	0.41
1:A:376:MET:HE2	1:A:381:THR:HA	1.99	0.41
1:B:35:CYS:HB2	1:B:216:TRP:CH2	2.55	0.41
1:A:115:LEU:HB3	1:A:167:LEU:HD13	2.01	0.41
1:B:30:ASN:HD22	1:B:504:SER:CB	2.33	0.41
1:B:362:ASN:C	1:B:362:ASN:ND2	2.73	0.41
1:B:426:ASN:HB2	1:B:427:ALA:H	1.61	0.41
1:A:300:GLU:OE1	1:A:434:ASN:HB3	2.21	0.41
1:B:269:ARG:HG3	1:B:269:ARG:HH11	1.86	0.41
1:A:376:MET:HE1	1:A:381:THR:HA	2.01	0.41
1:A:238:CYS:HB2	1:A:242:THR:HB	2.02	0.41
1:A:268:LEU:HD12	1:A:271:ARG:HD2	2.02	0.41
1:B:110:ASP:HB3	1:B:113:LEU:HB2	2.02	0.41
1:B:113:LEU:O	1:B:114:LEU:C	2.59	0.41
1:B:72:ASN:HD22	1:B:73:PRO:N	2.19	0.41
1:A:470:GLN:HB3	1:A:474:ILE:HB	2.04	0.40
1:A:290:HIS:CD2	1:A:457:ASP:OD2	2.69	0.40
1:B:336:LEU:O	1:B:340:LEU:HG	2.22	0.40
1:A:133:HIS:C	1:A:134:LEU:HD12	2.40	0.40
1:A:165:PRO:O	1:A:169:ARG:HG3	2.22	0.40
1:B:143:GLN:O	1:B:147:LYS:HG3	2.22	0.40
1:B:324:VAL:O	1:B:327:VAL:N	2.52	0.40
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.78	0.40
1:B:59:TYR:OH	1:B:300:GLU:HG2	2.21	0.40
1:B:57:ARG:HD3	1:B:369:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/516 (94%)	453 (93%)	26 (5%)	7 (1%)	11	15
1	B	477/516 (92%)	436 (91%)	32 (7%)	9 (2%)	8	10
All	All	963/1032 (93%)	889 (92%)	58 (6%)	16 (2%)	9	11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	265	GLU
1	B	200	ASN
1	A	104	ARG
1	B	262	VAL
1	B	427	ALA
1	A	241	GLY
1	B	498	ARG
1	A	133	HIS
1	A	137	SER
1	B	350	SER
1	B	423	ASN
1	B	424	ILE
1	B	479	GLU
1	B	31	GLY
1	A	136	VAL

### 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	433/457 (95%)	417 (96%)	16 (4%)	34	53
1	B	429/457 (94%)	410 (96%)	19 (4%)	28	45
All	All	862/914 (94%)	827 (96%)	35 (4%)	30	48

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	112	GLU
1	A	122	MET
1	A	131	HIS
1	A	153	ARG
1	A	179	TRP
1	A	189	PHE
1	A	201	TYR
1	A	210	GLN
1	A	221	CYS
1	A	242	THR
1	A	267	ASN
1	A	291	PHE
1	A	331	GLU
1	A	377	GLN
1	A	388	ARG
1	B	72	ASN
1	B	118	VAL
1	B	122	MET
1	B	173	LEU
1	B	177	LEU
1	B	179	TRP
1	B	201	TYR
1	B	221	CYS
1	B	228	ARG
1	B	239	GLU
1	B	291	PHE
1	B	322	GLU
1	B	337	ASP
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	391	LYS
1	B	412	GLU
1	B	426	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	49	GLN
1	A	80	GLN
1	A	191	HIS
1	A	195	ASN
1	A	210	GLN
1	A	290	HIS
1	A	362	ASN
1	A	377	GLN
1	A	434	ASN
1	B	30	ASN
1	B	33	GLN
1	B	72	ASN
1	B	109	HIS
1	B	195	ASN
1	B	255	GLN
1	B	259	ASN
1	B	283	GLN
1	B	329	ASN
1	B	332	ASN
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	399	GLN
1	B	423	ASN
1	B	434	ASN
1	B	439	ASN
1	B	468	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	FAD	A	517	-	51,58,58	1.62	7 (13%)	60,89,89	1.58	9 (15%)
3	SP8	A	518	-	19,19,19	0.47	0	20,22,22	0.74	0
2	FAD	B	517	-	51,58,58	1.63	6 (11%)	60,89,89	1.56	9 (15%)
3	SP8	B	518	-	19,19,19	0.48	0	20,22,22	0.56	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	FAD	A	517	-	-	1/30/50/50	0/6/6/6
3	SP8	A	518	-	-	2/16/16/16	0/1/1/1
2	FAD	B	517	-	-	2/30/50/50	0/6/6/6
3	SP8	B	518	-	-	2/16/16/16	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	517	FAD	C10-N1	5.61	1.40	1.33
2	B	517	FAD	C10-N1	5.55	1.40	1.33
2	B	517	FAD	C4X-N5	5.03	1.40	1.33
2	A	517	FAD	C4X-N5	4.92	1.40	1.33
2	A	517	FAD	C4-N3	4.25	1.40	1.33
2	B	517	FAD	C4-N3	4.23	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	517	FAD	C5X-N5	3.19	1.40	1.35
2	A	517	FAD	C5X-N5	3.12	1.40	1.35
2	B	517	FAD	PA-O1A	2.98	1.61	1.50
2	A	517	FAD	P-O1P	2.95	1.61	1.50
2	B	517	FAD	P-O1P	2.94	1.61	1.50
2	A	517	FAD	PA-O1A	2.94	1.61	1.50
2	A	517	FAD	O4B-C1B	2.03	1.43	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	517	FAD	C4-N3-C2	5.83	120.06	115.14
2	B	517	FAD	C4-N3-C2	5.78	120.02	115.14
2	A	517	FAD	N3A-C2A-N1A	-4.57	121.54	128.68
2	B	517	FAD	N3A-C2A-N1A	-4.46	121.71	128.68
2	A	517	FAD	O4B-C1B-C2B	-3.99	101.10	106.93
2	B	517	FAD	O4B-C1B-C2B	-3.71	101.51	106.93
2	B	517	FAD	C4X-N5-C5X	3.69	120.46	116.77
2	A	517	FAD	P-O3P-PA	-3.33	121.39	132.83
2	B	517	FAD	P-O3P-PA	-3.28	121.57	132.83
2	A	517	FAD	C4X-N5-C5X	3.24	120.01	116.77
2	A	517	FAD	C5X-C9A-N10	3.02	119.90	117.72
2	B	517	FAD	C5X-C9A-N10	2.97	119.87	117.72
2	A	517	FAD	C1'-N10-C9A	2.87	120.55	118.29
2	B	517	FAD	C4X-C4-N3	-2.37	120.19	123.43
2	B	517	FAD	C10-C4X-N5	-2.36	119.63	121.26
2	A	517	FAD	C4X-C4-N3	-2.35	120.22	123.43
2	B	517	FAD	C1'-N10-C9A	2.10	119.95	118.29
2	A	517	FAD	C5'-C4'-C3'	-2.10	108.16	112.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

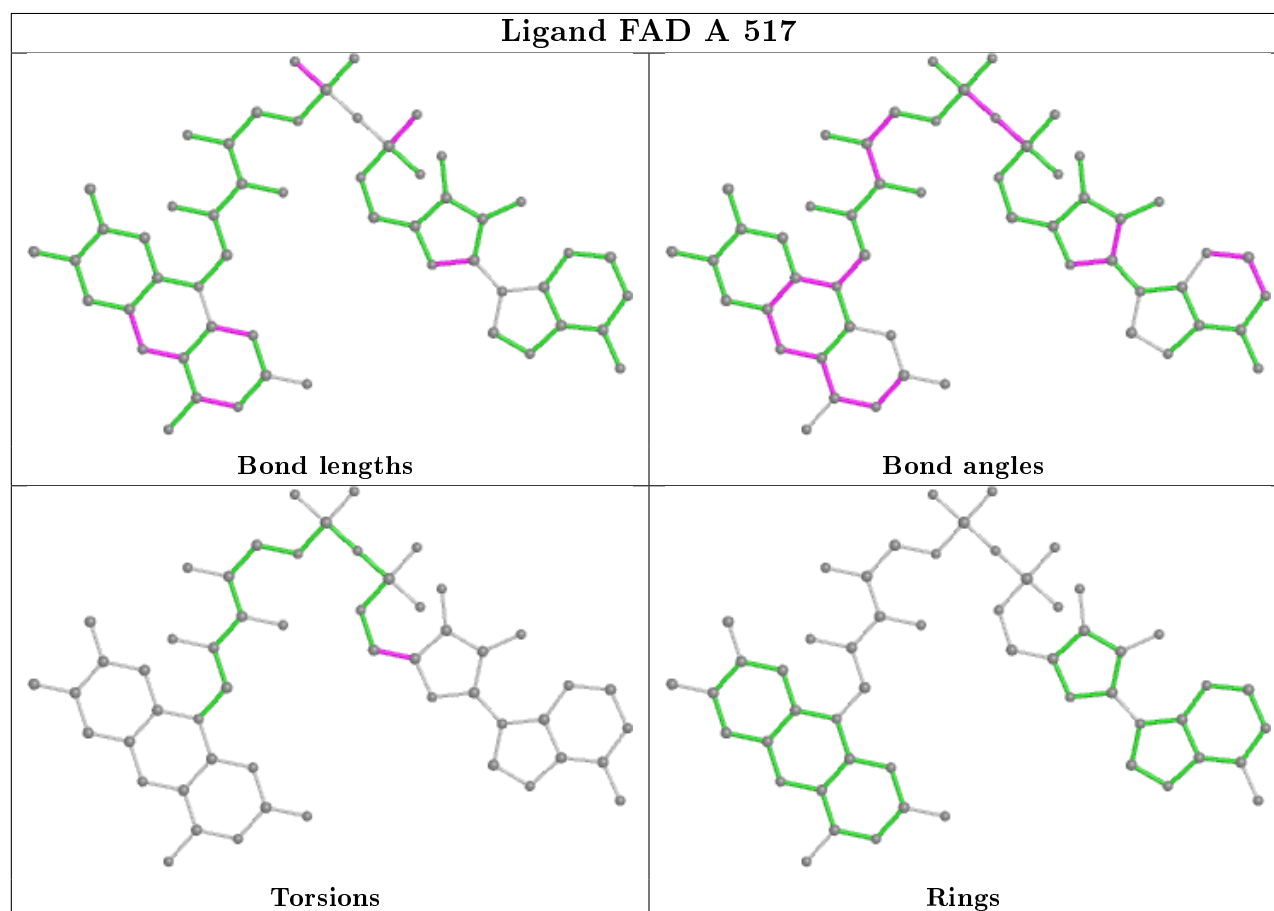
Mol	Chain	Res	Type	Atoms
3	A	518	SP8	CAB-CAI-NAH-CAG
3	B	518	SP8	CAJ-CAK-NAL-CAM
3	B	518	SP8	CAJ-CAI-NAH-CAG
2	A	517	FAD	O4B-C4B-C5B-O5B
2	B	517	FAD	O4B-C4B-C5B-O5B
2	B	517	FAD	C5B-O5B-PA-O2A
3	A	518	SP8	CAJ-CAK-NAL-CAM

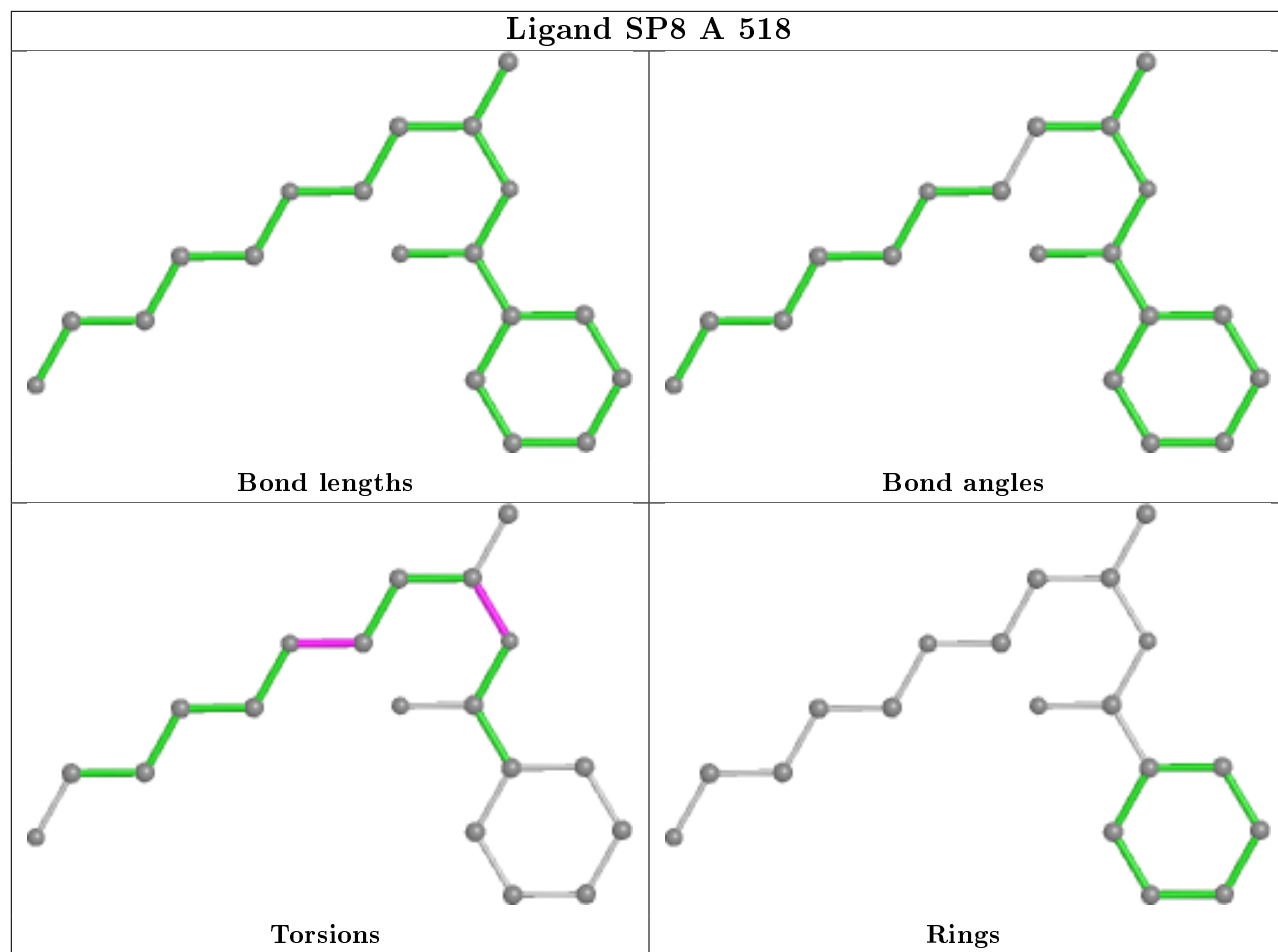
There are no ring outliers.

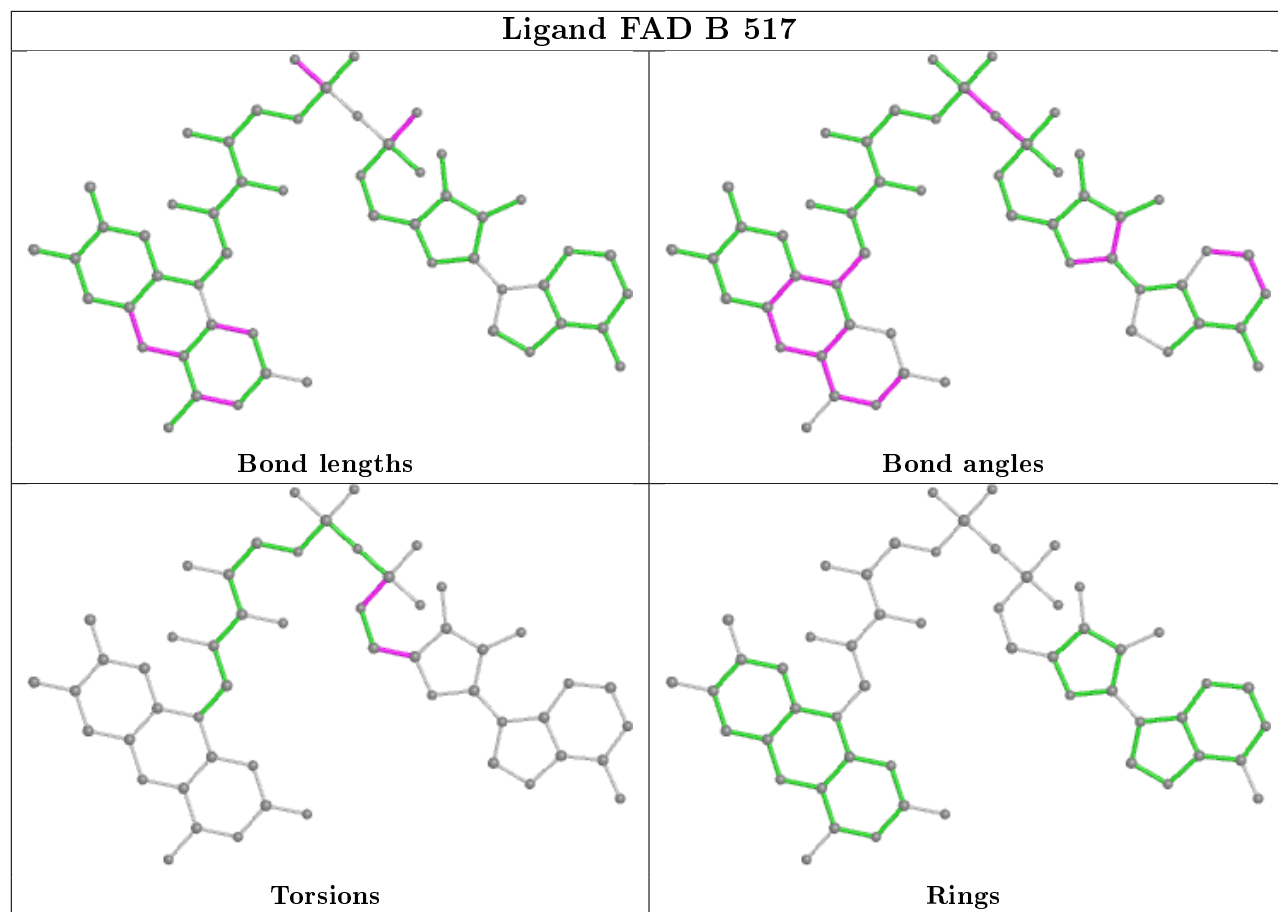
4 monomers are involved in 19 short contacts:

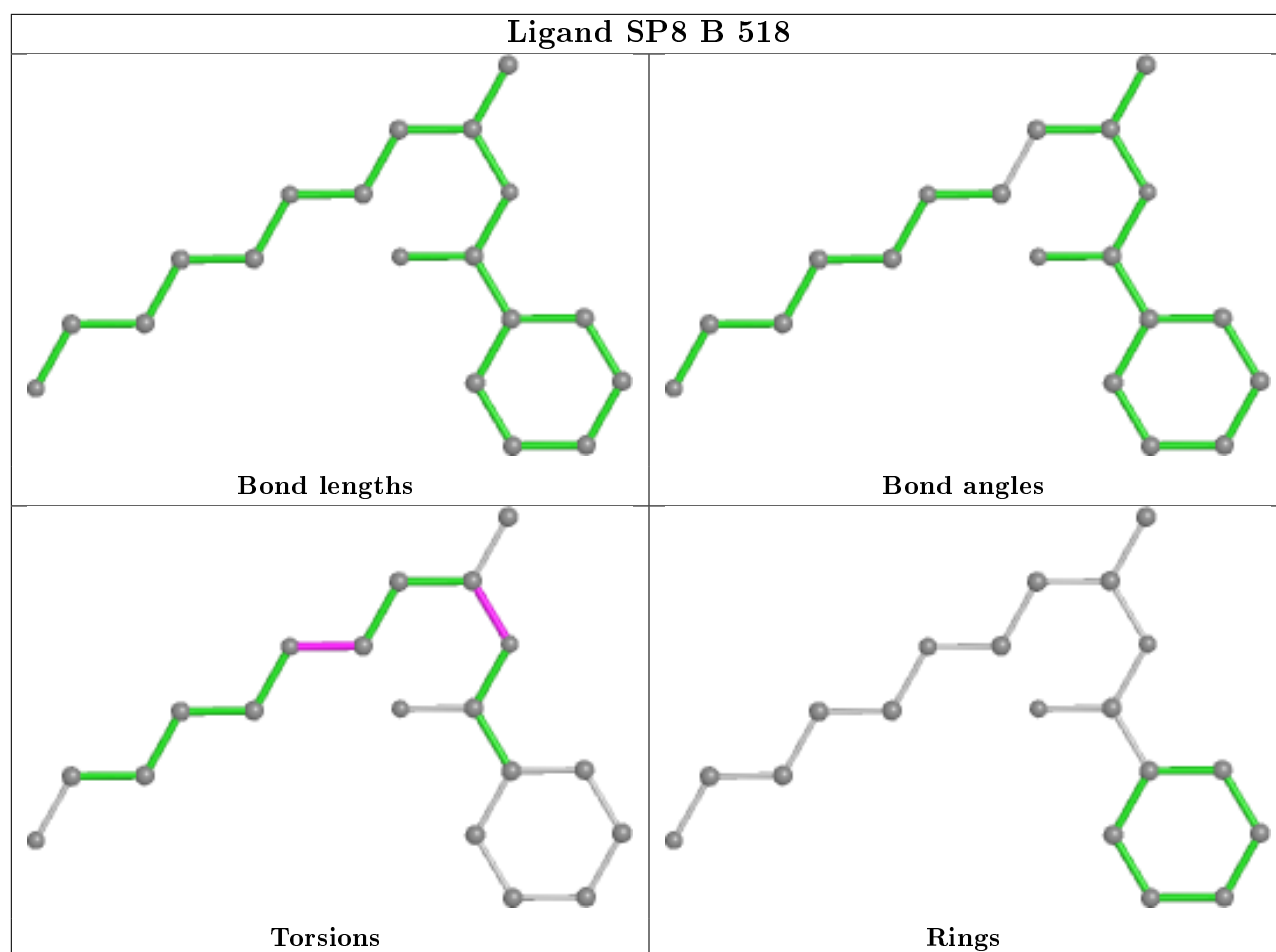
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	517	FAD	3	0
3	A	518	SP8	11	0
2	B	517	FAD	2	0
3	B	518	SP8	4	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	492/516 (95%)	-0.10	19 (3%)	39 38	27, 43, 69, 86	0
1	B	487/516 (94%)	-0.06	25 (5%)	28 26	28, 45, 83, 109	0
All	All	979/1032 (94%)	-0.08	44 (4%)	33 31	27, 44, 77, 109	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	ALA	7.1
1	B	424	ILE	6.9
1	A	428	ASN	5.6
1	A	420	PRO	4.8
1	B	426	ASN	4.6
1	A	7	ALA	4.1
1	B	427	ALA	4.1
1	A	230	PRO	4.1
1	B	423	ASN	4.1
1	A	133	HIS	4.0
1	B	428	ASN	3.9
1	A	6	PRO	3.8
1	B	230	PRO	3.8
1	A	136	VAL	3.8
1	B	420	PRO	3.2
1	A	427	ALA	3.1
1	B	232	LYS	2.9
1	B	349	THR	2.9
1	B	422	GLU	2.8
1	A	131	HIS	2.8
1	A	231	SER	2.8
1	B	137	SER	2.8
1	B	238	CYS	2.7
1	A	508	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	264	PRO	2.5
1	B	35	CYS	2.5
1	B	419	ARG	2.4
1	B	31	GLY	2.4
1	A	338	SER	2.4
1	B	333	LEU	2.4
1	A	233	ASN	2.3
1	A	191	HIS	2.3
1	A	232	LYS	2.3
1	B	231	SER	2.3
1	B	509	LEU	2.3
1	B	473	ARG	2.3
1	B	267	ASN	2.3
1	A	419	ARG	2.2
1	B	235	THR	2.1
1	B	341	GLU	2.1
1	B	332	ASN	2.0
1	A	31	GLY	2.0
1	A	410	ASP	2.0
1	A	331	GLU	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( $\text{\AA}^2$ )	Q<0.9
3	SP8	B	518	19/19	0.69	0.30	58,65,70,70	0
3	SP8	A	518	19/19	0.71	0.30	58,67,71,71	0
2	FAD	B	517	53/53	0.96	0.14	25,34,39,40	0

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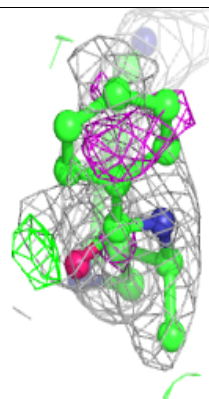
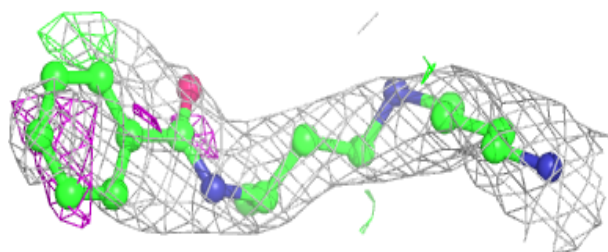
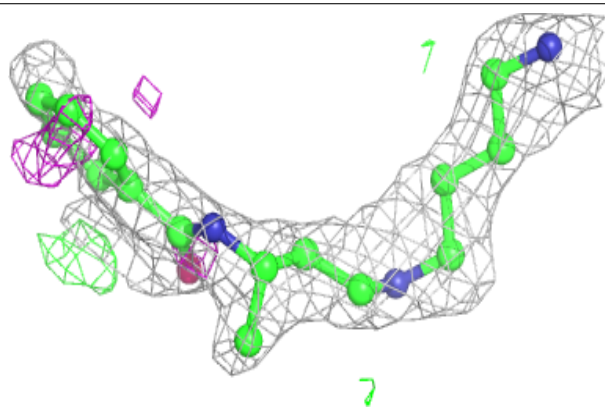
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	517	53/53	0.96	0.16	24,29,33,34	0

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.

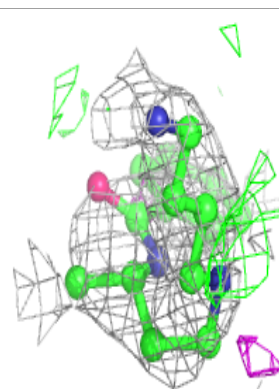
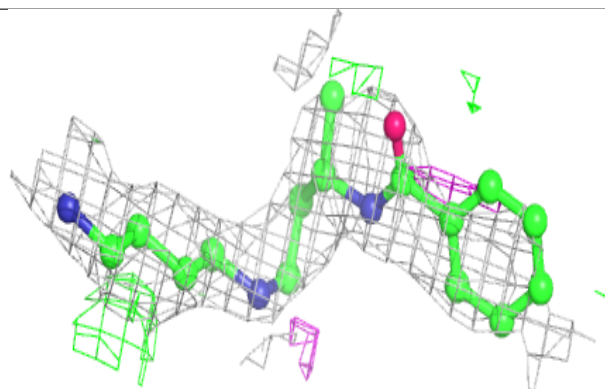
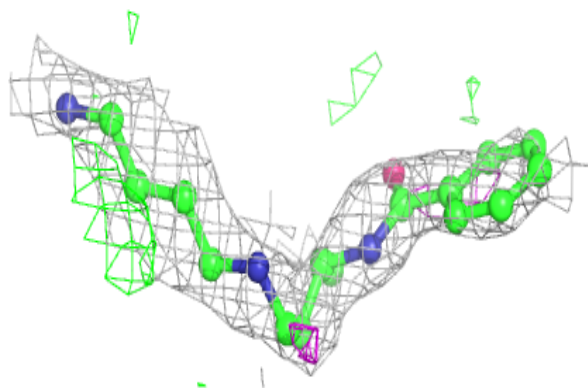
**Electron density around SP8 B 518:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

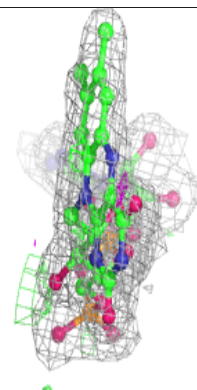
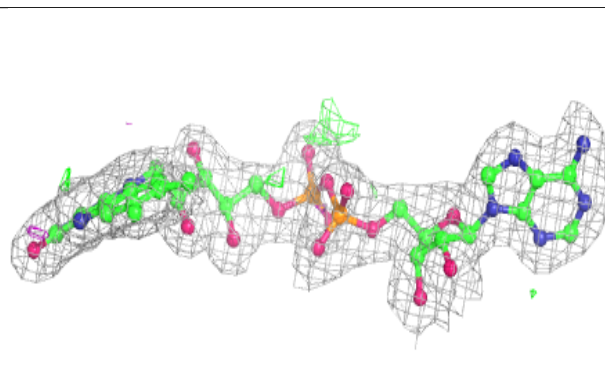
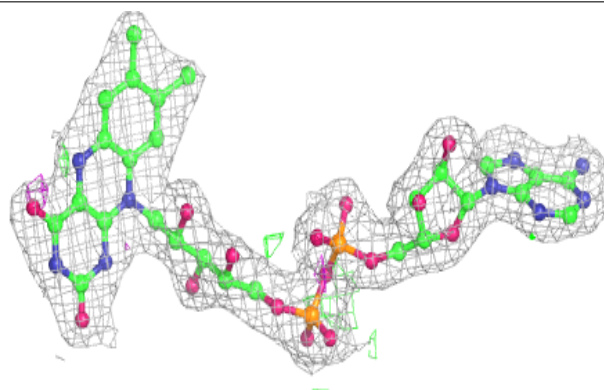


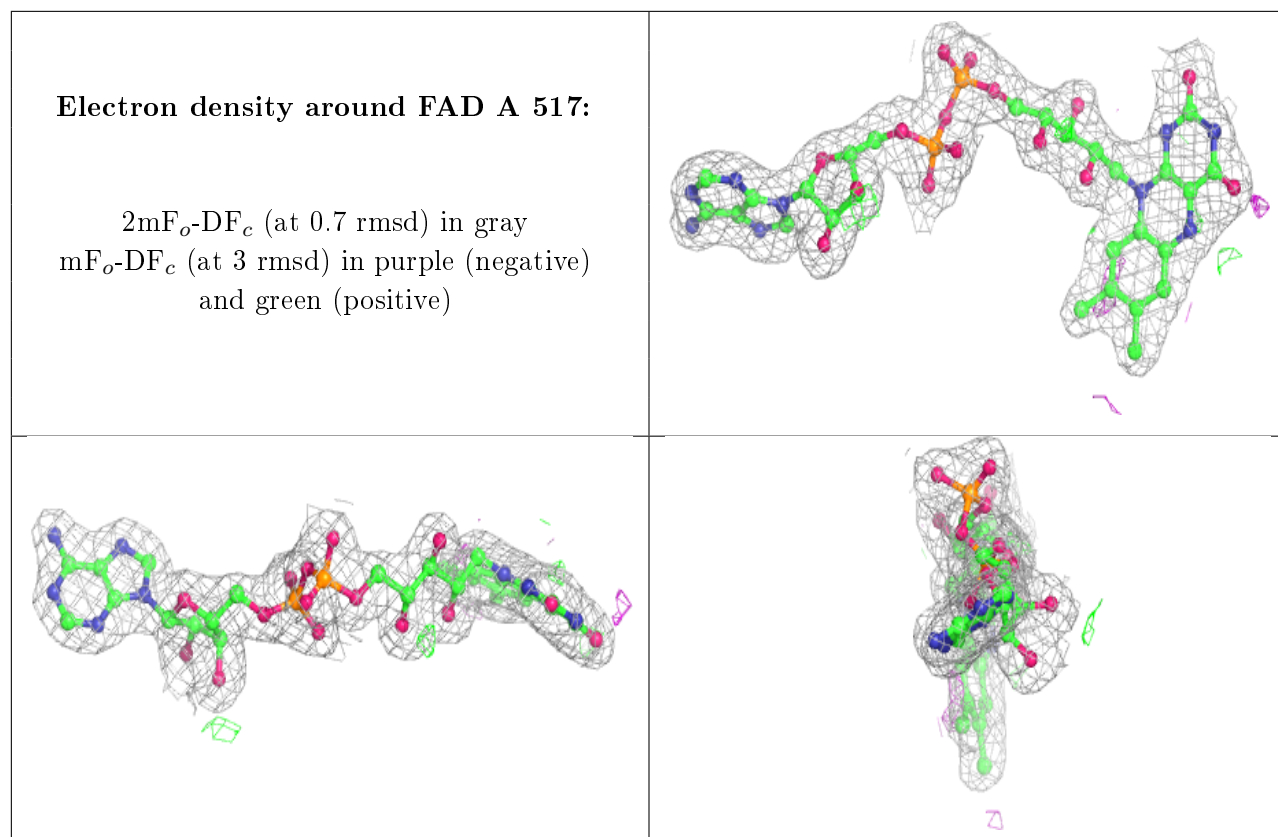
**Electron density around SP8 A 518:**

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

**Electron density around FAD B 517:**

$2mF_o-DF_c$  (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.