



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:35 am BST

PDB ID : 1NP7
Title : Crystal Structure Analysis of Synechocystis sp. PCC6803 cryptochrome
Authors : Brudler, R.; Hitomi, K.; Daiyasu, H.; Toh, H.; Kucho, K.; Ishiura, M.; Kanehisa, M.; Roberts, V.A.; Todo, T.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2003-01-17
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

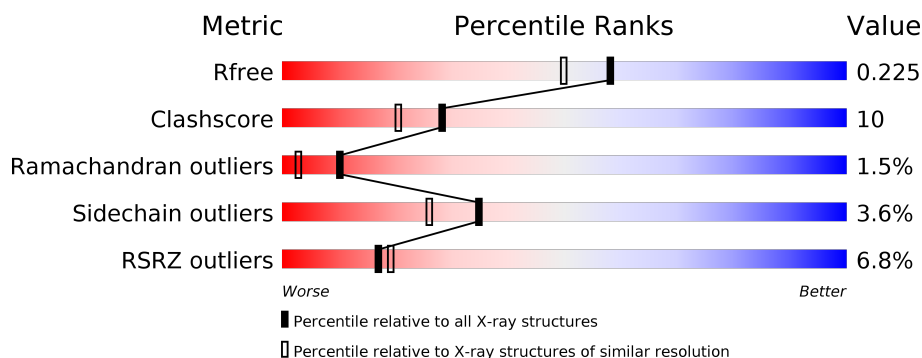
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	489	<div> <div>7%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
1	B	489	<div> <div>7%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>

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	FAD	A	500	X	-	-	-
3	FAD	B	501	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8467 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 DNA photolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3999	2573	706	708	12			
1	B	483	Total	C	N	O	S	0	0	0
			3999	2573	706	708	12			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CONFLICT	UNP P77967
A	2	LYS	-	CONFLICT	UNP P77967
A	3	HIS	-	CONFLICT	UNP P77967
A	4	VAL	-	CONFLICT	UNP P77967
A	5	PRO	-	CONFLICT	UNP P77967
A	6	PRO	-	CONFLICT	UNP P77967
A	7	THR	-	CONFLICT	UNP P77967
A	8	VAL	-	CONFLICT	UNP P77967
A	9	LEU	-	CONFLICT	UNP P77967
A	10	VAL	-	CONFLICT	UNP P77967
A	11	TRP	-	CONFLICT	UNP P77967
A	12	PHE	-	CONFLICT	UNP P77967
A	13	ARG	-	CONFLICT	UNP P77967
A	14	ASN	-	CONFLICT	UNP P77967
A	15	ASP	-	CONFLICT	UNP P77967
A	16	LEU	-	CONFLICT	UNP P77967
A	17	ARG	-	CONFLICT	UNP P77967
A	18	LEU	-	CONFLICT	UNP P77967
A	19	HIS	-	CONFLICT	UNP P77967
A	20	ASP	-	CONFLICT	UNP P77967
A	21	HIS	-	CONFLICT	UNP P77967
A	22	GLU	-	CONFLICT	UNP P77967
A	23	PRO	-	CONFLICT	UNP P77967
A	24	LEU	-	CONFLICT	UNP P77967
A	25	HIS	-	CONFLICT	UNP P77967

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ARG	-	CONFLICT	UNP P77967
A	27	ALA	-	CONFLICT	UNP P77967
A	28	LEU	-	CONFLICT	UNP P77967
A	29	LYS	-	CONFLICT	UNP P77967
A	30	SER	-	CONFLICT	UNP P77967
A	31	GLY	-	CONFLICT	UNP P77967
A	32	LEU	-	CONFLICT	UNP P77967
A	33	ALA	-	CONFLICT	UNP P77967
A	34	ILE	-	CONFLICT	UNP P77967
A	35	THR	-	CONFLICT	UNP P77967
A	36	ALA	-	CONFLICT	UNP P77967
A	37	VAL	-	CONFLICT	UNP P77967
B	1	MET	-	CONFLICT	UNP P77967
B	2	LYS	-	CONFLICT	UNP P77967
B	3	HIS	-	CONFLICT	UNP P77967
B	4	VAL	-	CONFLICT	UNP P77967
B	5	PRO	-	CONFLICT	UNP P77967
B	6	PRO	-	CONFLICT	UNP P77967
B	7	THR	-	CONFLICT	UNP P77967
B	8	VAL	-	CONFLICT	UNP P77967
B	9	LEU	-	CONFLICT	UNP P77967
B	10	VAL	-	CONFLICT	UNP P77967
B	11	TRP	-	CONFLICT	UNP P77967
B	12	PHE	-	CONFLICT	UNP P77967
B	13	ARG	-	CONFLICT	UNP P77967
B	14	ASN	-	CONFLICT	UNP P77967
B	15	ASP	-	CONFLICT	UNP P77967
B	16	LEU	-	CONFLICT	UNP P77967
B	17	ARG	-	CONFLICT	UNP P77967
B	18	LEU	-	CONFLICT	UNP P77967
B	19	HIS	-	CONFLICT	UNP P77967
B	20	ASP	-	CONFLICT	UNP P77967
B	21	HIS	-	CONFLICT	UNP P77967
B	22	GLU	-	CONFLICT	UNP P77967
B	23	PRO	-	CONFLICT	UNP P77967
B	24	LEU	-	CONFLICT	UNP P77967
B	25	HIS	-	CONFLICT	UNP P77967
B	26	ARG	-	CONFLICT	UNP P77967
B	27	ALA	-	CONFLICT	UNP P77967
B	28	LEU	-	CONFLICT	UNP P77967
B	29	LYS	-	CONFLICT	UNP P77967
B	30	SER	-	CONFLICT	UNP P77967

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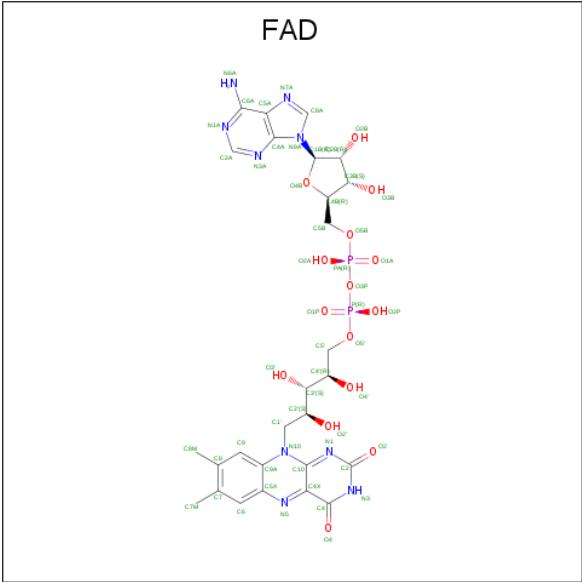
Chain	Residue	Modelled	Actual	Comment	Reference
B	31	GLY	-	CONFLICT	UNP P77967
B	32	LEU	-	CONFLICT	UNP P77967
B	33	ALA	-	CONFLICT	UNP P77967
B	34	ILE	-	CONFLICT	UNP P77967
B	35	THR	-	CONFLICT	UNP P77967
B	36	ALA	-	CONFLICT	UNP P77967
B	37	VAL	-	CONFLICT	UNP P77967

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

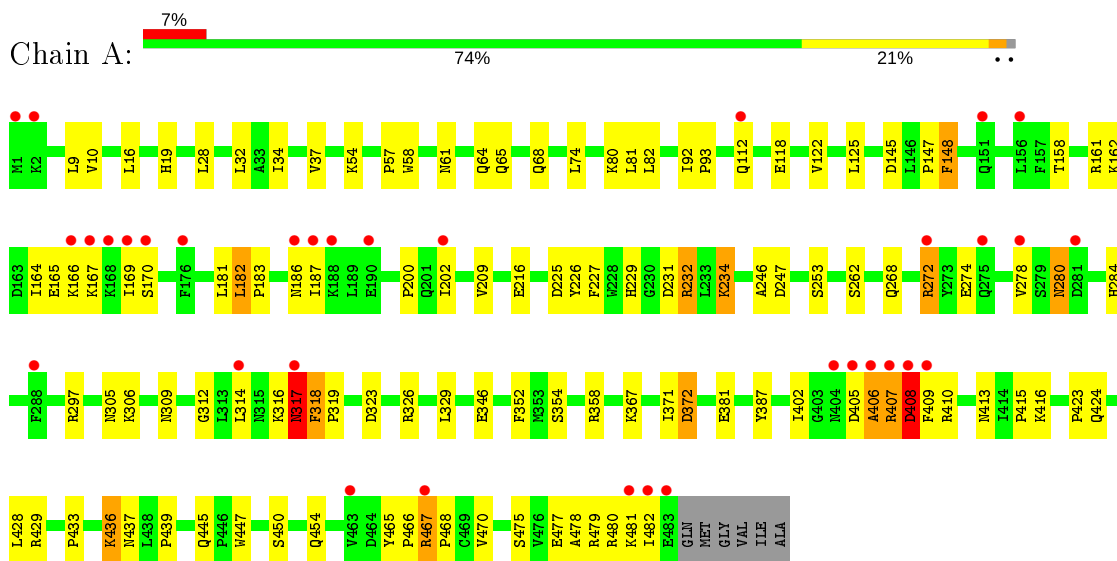
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	0
			201	201		
4	B	147	Total	O	0	0
			147	147		

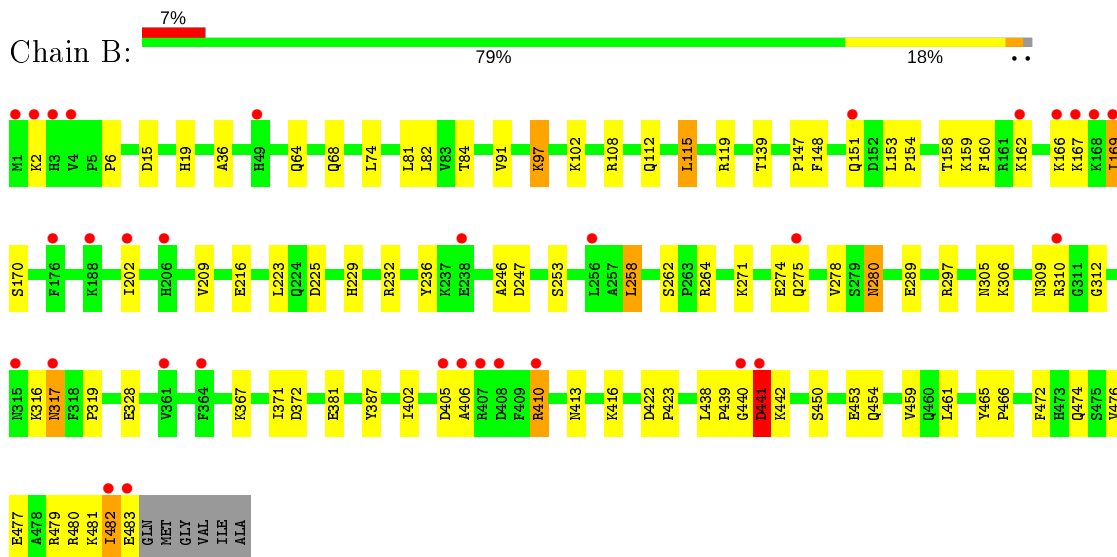
3 Residue-property plots

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

- Molecule 1: DNA photolyase



- Molecule 1: DNA photolyase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.28 Å 89.48 Å 121.69 Å 90.00° 120.46° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.85 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.90) 92.6 (29.85-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.91 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.233 0.200 , 0.225	Depositor DCC
R_{free} test set	4466 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8467	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, 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	0.33	0/4121	0.55	0/5593
1	B	0.33	0/4121	0.55	0/5593
All	All	0.33	0/8242	0.55	0/11186

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	3999	0	3895	92	0
1	B	3999	0	3895	64	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	53	0	29	1	0
3	B	53	0	29	1	0
4	A	201	0	0	3	0
4	B	147	0	0	1	0
All	All	8467	0	7848	156	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 10.

All (156) 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:162:LYS:HE3	1:A:166:LYS:HD2	1.62	0.81
1:A:57:PRO:HB2	1:A:202:ILE:HD11	1.69	0.73
1:A:467:ARG:HD3	1:A:468:PRO:HD2	1.73	0.70
1:B:112:GLN:HB2	1:B:305:ASN:HD21	1.58	0.69
1:B:477:GLU:HG3	1:B:481:LYS:HE3	1.74	0.67
1:A:80:LYS:HE3	1:A:82:LEU:HD21	1.76	0.66
1:A:323:ASP:OD1	1:A:326:ARG:HD3	1.94	0.66
1:A:467:ARG:HD3	1:A:468:PRO:CD	2.26	0.65
1:A:209:VAL:O	1:A:246:ALA:HB2	1.98	0.64
1:A:112:GLN:HB2	1:A:305:ASN:HD21	1.62	0.64
1:B:319:PRO:HD2	1:B:482:ILE:HG12	1.78	0.64
1:A:319:PRO:HD2	1:A:482:ILE:HG21	1.81	0.63
1:A:32:LEU:N	1:A:32:LEU:HD12	2.14	0.62
1:A:429:ARG:HD3	1:A:436:LYS:HE2	1.82	0.62
1:B:19:HIS:HD2	1:B:216:GLU:OE2	1.82	0.62
1:A:319:PRO:HG2	1:A:482:ILE:HD13	1.81	0.62
1:B:158:THR:O	1:B:162:LYS:HG2	1.99	0.61
1:A:182:LEU:HD23	1:A:183:PRO:HD2	1.83	0.61
1:B:19:HIS:HE1	1:B:262:SER:H	1.48	0.60
1:B:202:ILE:O	1:B:202:ILE:HD12	2.01	0.60
1:B:169:ILE:HD13	1:B:169:ILE:O	2.02	0.60
1:B:413:ASN:HB3	1:B:416:LYS:HE2	1.82	0.60
1:B:442:LYS:HE2	1:B:453:GLU:OE1	2.02	0.60
1:A:92:ILE:HB	1:A:93:PRO:HD3	1.83	0.60
1:B:64:GLN:O	1:B:68:GLN:HG3	2.02	0.59
1:A:406:ALA:O	1:A:408:ASP:N	2.35	0.58
1:B:232:ARG:HE	1:B:247:ASP:HB3	1.68	0.58
1:B:97:LYS:O	1:B:97:LYS:HD2	2.03	0.58
1:B:154:PRO:HB3	1:B:159:LYS:HD3	1.86	0.58
1:A:317:ASN:ND2	1:A:318:PHE:H	2.02	0.57
1:A:413:ASN:HB3	1:A:416:LYS:HE2	1.84	0.57
1:A:64:GLN:O	1:A:68:GLN:HG3	2.05	0.57
1:A:19:HIS:HE1	1:A:262:SER:H	1.51	0.57
1:B:108:ARG:HD2	4:B:1136:HOH:O	2.04	0.57
1:A:164:ILE:O	1:A:169:ILE:HG12	2.05	0.57
1:A:28:LEU:HA	1:A:34:ILE:HD11	1.87	0.56
1:A:367:LYS:HA	1:A:479:ARG:HG2	1.87	0.55
1:A:447:TRP:CE3	1:A:468:PRO:HG3	2.41	0.55
1:A:314:LEU:HB3	1:A:316:LYS:HG3	1.88	0.55
1:A:161:ARG:O	1:A:165:GLU:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:PRO:HG2	1:B:160:PHE:HB2	1.90	0.54
1:A:232:ARG:HD3	1:A:247:ASP:HB3	1.89	0.54
1:A:158:THR:O	1:A:162:LYS:HG2	2.06	0.54
1:A:19:HIS:HD2	1:A:216:GLU:OE2	1.90	0.54
1:A:437:ASN:O	1:A:439:PRO:HD3	2.07	0.54
1:A:226:TYR:CD1	1:A:232:ARG:HG3	2.43	0.54
1:B:162:LYS:HE3	1:B:166:LYS:HE3	1.90	0.53
1:A:34:ILE:HD12	1:A:181:LEU:HD22	1.91	0.53
1:A:317:ASN:N	1:A:317:ASN:HD22	2.04	0.53
1:A:478:ALA:HA	1:A:481:LYS:HZ3	1.73	0.53
1:B:439:PRO:O	1:B:441:ASP:N	2.42	0.53
1:A:186:ASN:O	1:A:187:ILE:HD13	2.10	0.52
1:A:317:ASN:O	1:A:318:PHE:HB2	2.07	0.52
1:A:162:LYS:HD2	1:A:165:GLU:OE1	2.11	0.51
1:A:317:ASN:N	1:A:317:ASN:ND2	2.58	0.51
1:A:409:PHE:CD2	1:A:480:ARG:HD3	2.45	0.51
1:B:209:VAL:O	1:B:246:ALA:HB2	2.11	0.50
1:A:9:LEU:HD23	1:A:10:VAL:N	2.26	0.50
1:B:450:SER:O	1:B:454:GLN:HG3	2.11	0.50
1:B:147:PRO:HG2	1:B:148:PHE:CD2	2.47	0.50
1:B:479:ARG:HA	1:B:482:ILE:HG22	1.94	0.50
1:B:367:LYS:HE2	1:B:410:ARG:O	2.12	0.50
1:B:19:HIS:CD2	1:B:216:GLU:OE2	2.65	0.49
1:B:19:HIS:CE1	1:B:262:SER:H	2.28	0.49
1:B:316:LYS:HG3	1:B:402:ILE:HG22	1.94	0.49
1:A:19:HIS:CE1	1:A:262:SER:H	2.29	0.49
1:B:312:GLY:HA3	1:B:402:ILE:HD12	1.95	0.49
1:A:280:ASN:C	1:A:280:ASN:HD22	2.16	0.49
1:A:306:LYS:HA	1:A:309:ASN:ND2	2.27	0.48
1:B:280:ASN:C	1:B:280:ASN:HD22	2.16	0.48
1:A:253:SER:HB3	3:A:500:FAD:H5'1	1.94	0.48
1:B:306:LYS:HA	1:B:309:ASN:ND2	2.29	0.48
1:B:225:ASP:HA	1:B:229:HIS:HB2	1.96	0.48
1:A:118:GLU:O	1:A:122:VAL:HG23	2.13	0.48
1:A:169:ILE:O	1:A:170:SER:HB3	2.14	0.47
1:B:153:LEU:HD12	1:B:154:PRO:HD2	1.95	0.47
1:B:472:PHE:O	1:B:476:VAL:HG23	2.14	0.47
1:A:32:LEU:CD1	1:A:32:LEU:N	2.77	0.47
1:A:450:SER:O	1:A:454:GLN:HG3	2.14	0.47
1:B:381:GLU:HA	1:B:387:TYR:CD2	2.50	0.47
1:B:82:LEU:HD22	1:B:82:LEU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD11	4:A:1182:HOH:O	2.13	0.47
1:B:454:GLN:NE2	1:B:461:LEU:H	2.13	0.47
1:A:57:PRO:HB3	1:A:200:PRO:HG2	1.97	0.47
1:B:465:TYR:CD1	1:B:466:PRO:HD2	2.50	0.47
1:A:346:GLU:HG2	1:A:352:PHE:O	2.16	0.46
1:B:169:ILE:HD13	1:B:169:ILE:C	2.36	0.46
1:A:477:GLU:CD	1:A:480:ARG:HH21	2.19	0.46
1:B:97:LYS:C	1:B:97:LYS:HD2	2.36	0.46
1:B:253:SER:HB3	3:B:501:FAD:H5'1	1.98	0.46
1:A:74:LEU:HD12	1:A:81:LEU:HB2	1.96	0.46
1:B:317:ASN:C	1:B:317:ASN:HD22	2.17	0.46
1:B:441:ASP:OD1	1:B:441:ASP:C	2.54	0.46
1:B:84:THR:HG21	1:B:91:VAL:HG11	1.97	0.45
1:A:297:ARG:HG2	4:A:1097:HOH:O	2.16	0.45
1:A:317:ASN:ND2	1:A:318:PHE:N	2.64	0.45
1:A:367:LYS:HE2	1:A:410:ARG:O	2.16	0.45
1:A:162:LYS:HB3	1:A:166:LYS:HD3	1.99	0.45
1:B:274:GLU:HA	1:B:278:VAL:O	2.17	0.45
1:A:354:SER:O	1:A:358:ARG:HG3	2.16	0.45
1:A:182:LEU:HD23	1:A:183:PRO:CD	2.46	0.45
1:B:6:PRO:HB3	1:B:102:LYS:HE2	1.98	0.44
1:B:454:GLN:HB3	1:B:459:VAL:O	2.17	0.44
1:B:36:ALA:O	1:B:82:LEU:HD23	2.18	0.44
1:A:274:GLU:OE1	1:A:284:HIS:HD2	2.00	0.44
1:A:227:PHE:O	1:A:231:ASP:HA	2.17	0.44
1:B:413:ASN:HB3	1:B:416:LYS:HB3	1.99	0.44
1:A:409:PHE:CE2	1:A:480:ARG:HB2	2.53	0.44
1:B:317:ASN:C	1:B:317:ASN:ND2	2.72	0.43
1:A:433:PRO:O	1:A:436:LYS:HB2	2.18	0.43
1:A:319:PRO:CG	1:A:482:ILE:HD13	2.48	0.43
1:A:407:ARG:O	1:A:407:ARG:HG3	2.19	0.43
1:B:236:TYR:OH	1:B:289:GLU:HG3	2.18	0.43
1:B:482:ILE:HG23	1:B:482:ILE:O	2.18	0.42
1:A:231:ASP:OD2	1:A:234:LYS:HE2	2.18	0.42
1:A:381:GLU:HA	1:A:387:TYR:CD2	2.54	0.42
1:B:154:PRO:CB	1:B:159:LYS:HD3	2.49	0.42
1:A:225:ASP:HA	1:A:229:HIS:HB2	2.00	0.42
1:B:481:LYS:O	1:B:483:GLU:N	2.52	0.42
1:A:268:GLN:O	1:A:272:ARG:HD2	2.18	0.42
1:A:145:ASP:O	1:A:169:ILE:HG23	2.20	0.42
1:A:58:TRP:CZ3	1:A:202:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:THR:HG23	1:B:297:ARG:HD2	2.01	0.42
1:B:441:ASP:OD1	1:B:442:LYS:N	2.52	0.42
1:A:182:LEU:HD22	1:A:183:PRO:O	2.20	0.42
1:B:477:GLU:O	1:B:481:LYS:HG3	2.19	0.42
1:A:147:PRO:HG2	1:A:148:PHE:CD2	2.55	0.42
1:A:371:ILE:O	1:A:372:ASP:C	2.58	0.42
1:A:9:LEU:C	1:A:9:LEU:HD23	2.40	0.42
1:A:54:LYS:HG2	4:A:1174:HOH:O	2.20	0.41
1:A:317:ASN:CG	1:A:318:PHE:H	2.22	0.41
1:A:234:LYS:HZ2	1:A:278:VAL:HG11	1.85	0.41
1:A:470:VAL:CG2	1:A:475:SER:HB3	2.50	0.41
1:B:115:LEU:O	1:B:119:ARG:HG2	2.20	0.41
1:A:61:ASN:O	1:A:65:GLN:HG3	2.21	0.41
1:B:74:LEU:HD12	1:B:81:LEU:HB2	2.02	0.41
1:A:19:HIS:CD2	1:A:216:GLU:OE2	2.71	0.41
1:A:28:LEU:CA	1:A:34:ILE:HD11	2.51	0.41
1:A:37:VAL:HG22	1:A:82:LEU:HB2	2.02	0.41
1:A:413:ASN:HB3	1:A:416:LYS:HB3	2.02	0.41
1:A:445:GLN:HB3	1:A:447:TRP:CE2	2.56	0.41
1:B:258:LEU:HA	1:B:258:LEU:HD12	1.92	0.41
1:B:271:LYS:HA	1:B:271:LYS:HD3	1.83	0.41
1:A:465:TYR:CD1	1:A:466:PRO:HD2	2.56	0.41
1:B:422:ASP:N	1:B:423:PRO:CD	2.84	0.41
1:B:371:ILE:O	1:B:372:ASP:C	2.58	0.41
1:A:423:PRO:HG2	1:A:424:GLN:NE2	2.35	0.41
1:A:445:GLN:HB3	1:A:447:TRP:CZ2	2.56	0.41
1:A:165:GLU:C	1:A:167:LYS:H	2.25	0.41
1:A:226:TYR:CE1	1:A:232:ARG:HG3	2.56	0.41
1:B:15:ASP:OD2	1:B:15:ASP:N	2.53	0.41
1:B:162:LYS:CE	1:B:166:LYS:HE3	2.50	0.41
1:A:413:ASN:OD1	1:A:415:PRO:HG2	2.21	0.40
1:B:223:LEU:HD23	1:B:223:LEU:C	2.42	0.40
1:A:312:GLY:HA3	1:A:402:ILE:HD12	2.02	0.40
1:A:479:ARG:O	1:A:479:ARG:HD3	2.22	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	481/489 (98%)	453 (94%)	21 (4%)	7 (2%)	10	3
1	B	481/489 (98%)	457 (95%)	17 (4%)	7 (2%)	10	3
All	All	962/978 (98%)	910 (95%)	38 (4%)	14 (2%)	10	3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	407	ARG
1	B	167	LYS
1	B	405	ASP
1	B	441	ASP
1	A	405	ASP
1	A	406	ALA
1	B	440	GLY
1	B	406	ALA
1	A	318	PHE
1	B	170	SER
1	A	372	ASP
1	B	482	ILE
1	A	408	ASP

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	428/432 (99%)	414 (97%)	14 (3%)	38	29
1	B	428/432 (99%)	411 (96%)	17 (4%)	31	22
All	All	856/864 (99%)	825 (96%)	31 (4%)	35	26

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	125	LEU
1	A	148	PHE
1	A	182	LEU
1	A	232	ARG
1	A	234	LYS
1	A	272	ARG
1	A	280	ASN
1	A	317	ASN
1	A	329	LEU
1	A	408	ASP
1	A	428	LEU
1	A	436	LYS
1	A	467	ARG
1	B	2	LYS
1	B	97	LYS
1	B	115	LEU
1	B	151	GLN
1	B	169	ILE
1	B	258	LEU
1	B	264	ARG
1	B	275	GLN
1	B	280	ASN
1	B	310	ARG
1	B	317	ASN
1	B	328	GLU
1	B	410	ARG
1	B	438	LEU
1	B	441	ASP
1	B	474	GLN
1	B	480	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	25	HIS
1	A	64	GLN
1	A	203	ASN
1	A	224	GLN
1	A	280	ASN
1	A	284	HIS
1	A	301	GLN
1	A	305	ASN
1	A	317	ASN
1	A	355	ASN
1	A	420	GLN
1	A	424	GLN
1	A	430	HIS
1	A	454	GLN
1	A	456	GLN
1	A	460	GLN
1	A	474	GLN
1	B	19	HIS
1	B	25	HIS
1	B	44	GLN
1	B	64	GLN
1	B	90	GLN
1	B	120	ASN
1	B	124	GLN
1	B	151	GLN
1	B	186	ASN
1	B	213	GLN
1	B	224	GLN
1	B	280	ASN
1	B	301	GLN
1	B	305	ASN
1	B	309	ASN
1	B	317	ASN
1	B	355	ASN
1	B	437	ASN
1	B	454	GLN
1	B	460	GLN
1	B	474	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
3	FAD	B	501	-	51,58,58	3.19	23 (45%)	60,89,89	2.60	14 (23%)
2	SO4	A	1401	-	4,4,4	1.87	2 (50%)	6,6,6	0.91	0
3	FAD	A	500	-	51,58,58	3.18	20 (39%)	60,89,89	2.61	13 (21%)
2	SO4	A	1403	-	4,4,4	1.85	2 (50%)	6,6,6	0.94	0
2	SO4	B	1402	-	4,4,4	1.88	2 (50%)	6,6,6	0.88	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
3	FAD	B	501	-	2/2/9/9	12/30/50/50	0/6/6/6
3	FAD	A	500	-	2/2/9/9	10/30/50/50	0/6/6/6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	FAD	C10-N1	8.45	1.44	1.33
3	A	500	FAD	C10-N1	8.12	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	FAD	C1'-N10	-7.80	1.40	1.48
3	A	500	FAD	C4X-C10	7.32	1.46	1.38
3	A	500	FAD	C1'-N10	-7.08	1.40	1.48
3	B	501	FAD	C9A-N10	6.85	1.47	1.38
3	A	500	FAD	C9A-N10	6.83	1.47	1.38
3	B	501	FAD	C4X-C10	6.58	1.45	1.38
3	B	501	FAD	C4X-N5	6.50	1.42	1.33
3	A	500	FAD	C4X-N5	6.48	1.42	1.33
3	A	500	FAD	C5'-C4'	-5.64	1.43	1.51
3	B	501	FAD	C4-C4X	5.58	1.51	1.41
3	A	500	FAD	C4-C4X	5.52	1.50	1.41
3	A	500	FAD	C5X-N5	5.02	1.43	1.35
3	B	501	FAD	C7M-C7	4.92	1.60	1.51
3	B	501	FAD	C5X-N5	4.85	1.43	1.35
3	B	501	FAD	C5'-C4'	-4.68	1.45	1.51
3	A	500	FAD	C7M-C7	4.44	1.59	1.51
3	A	500	FAD	O2'-C2'	-4.38	1.34	1.43
3	B	501	FAD	O2'-C2'	-4.25	1.34	1.43
3	A	500	FAD	C4-N3	4.25	1.40	1.33
3	B	501	FAD	C4-N3	4.20	1.40	1.33
3	A	500	FAD	C2B-C3B	-3.60	1.43	1.53
3	B	501	FAD	C2B-C3B	-3.38	1.44	1.53
3	B	501	FAD	C4'-C3'	-3.18	1.47	1.53
2	B	1402	SO4	O1-S	3.12	1.62	1.46
3	B	501	FAD	O3'-C3'	-3.11	1.35	1.43
2	A	1403	SO4	O1-S	3.08	1.62	1.46
3	B	501	FAD	PA-O2A	-3.08	1.40	1.55
2	A	1401	SO4	O1-S	3.07	1.62	1.46
3	A	500	FAD	O3'-C3'	-3.02	1.35	1.43
3	A	500	FAD	PA-O2A	-3.01	1.41	1.55
3	A	500	FAD	C4'-C3'	-3.00	1.47	1.53
3	B	501	FAD	C9A-C5X	2.86	1.48	1.42
3	A	500	FAD	C9A-C5X	2.85	1.48	1.42
3	A	500	FAD	C2-N3	2.79	1.43	1.38
3	A	500	FAD	C8-C7	2.68	1.47	1.40
3	B	501	FAD	O4B-C1B	2.63	1.44	1.41
3	B	501	FAD	C8-C7	2.51	1.47	1.40
3	B	501	FAD	C2-N3	2.49	1.43	1.38
3	A	500	FAD	C6-C7	2.25	1.43	1.37
3	B	501	FAD	C6-C7	2.23	1.43	1.37
3	B	501	FAD	C8A-N7A	-2.22	1.30	1.34
3	B	501	FAD	P-O2P	-2.20	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	SO4	O3-S	-2.10	1.30	1.47
3	B	501	FAD	P-O5'	2.08	1.67	1.59
3	A	500	FAD	P-O2P	-2.05	1.45	1.55
2	B	1402	SO4	O3-S	-2.03	1.31	1.47
2	A	1403	SO4	O3-S	-2.00	1.31	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	FAD	C4-N3-C2	13.06	126.17	115.14
3	A	500	FAD	C4-N3-C2	13.00	126.12	115.14
3	A	500	FAD	C1'-N10-C9A	7.76	124.40	118.29
3	B	501	FAD	C1'-N10-C9A	7.51	124.20	118.29
3	A	500	FAD	C4X-C4-N3	-5.42	116.01	123.43
3	B	501	FAD	C4X-C4-N3	-5.38	116.07	123.43
3	B	501	FAD	C4'-C3'-C2'	5.30	124.39	113.36
3	A	500	FAD	C4'-C3'-C2'	4.99	123.73	113.36
3	B	501	FAD	C9A-N10-C10	-4.59	115.89	121.91
3	A	500	FAD	C9A-N10-C10	-4.58	115.91	121.91
3	A	500	FAD	C1'-C2'-C3'	3.76	120.29	109.79
3	B	501	FAD	C1'-C2'-C3'	3.55	119.69	109.79
3	A	500	FAD	C5X-C9A-N10	3.37	120.16	117.72
3	B	501	FAD	C5X-C9A-N10	3.18	120.02	117.72
3	A	500	FAD	C4X-C10-N10	2.92	123.30	120.30
3	B	501	FAD	C4X-C10-N10	2.92	123.30	120.30
3	B	501	FAD	O5B-PA-O1A	2.77	119.89	109.07
3	A	500	FAD	O5B-PA-O1A	2.59	119.20	109.07
3	A	500	FAD	N3A-C2A-N1A	-2.47	124.82	128.68
3	A	500	FAD	C8M-C8-C7	2.42	125.69	120.74
3	A	500	FAD	C8M-C8-C9	-2.39	114.62	120.34
3	B	501	FAD	C8M-C8-C7	2.35	125.54	120.74
3	B	501	FAD	N3A-C2A-N1A	-2.34	125.03	128.68
3	B	501	FAD	C8M-C8-C9	-2.33	114.77	120.34
3	A	500	FAD	C4-C4X-C10	2.03	121.29	119.95
3	B	501	FAD	O5'-C5'-C4'	2.02	114.76	109.36
3	B	501	FAD	C4-C4X-C10	2.00	121.28	119.95

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	501	FAD	C4'
3	B	501	FAD	C2'

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Mol	Chain	Res	Type	Atom
3	A	500	FAD	C4'
3	A	500	FAD	C2'

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	FAD	N10-C1'-C2'-O2'
3	B	501	FAD	N10-C1'-C2'-C3'
3	B	501	FAD	C1'-C2'-C3'-O3'
3	B	501	FAD	C1'-C2'-C3'-C4'
3	B	501	FAD	O2'-C2'-C3'-O3'
3	B	501	FAD	O3'-C3'-C4'-C5'
3	A	500	FAD	N10-C1'-C2'-O2'
3	A	500	FAD	N10-C1'-C2'-C3'
3	A	500	FAD	C1'-C2'-C3'-O3'
3	A	500	FAD	C2'-C3'-C4'-O4'
3	A	500	FAD	O3'-C3'-C4'-O4'
3	A	500	FAD	O3'-C3'-C4'-C5'
3	B	501	FAD	O3'-C3'-C4'-O4'
3	A	500	FAD	O2'-C2'-C3'-O3'
3	B	501	FAD	O2'-C2'-C3'-C4'
3	B	501	FAD	C2'-C3'-C4'-O4'
3	A	500	FAD	C2'-C3'-C4'-C5'
3	A	500	FAD	O2'-C2'-C3'-C4'
3	B	501	FAD	C2'-C3'-C4'-C5'
3	B	501	FAD	P-O3P-PA-O1A
3	A	500	FAD	P-O3P-PA-O1A
3	B	501	FAD	C5B-O5B-PA-O3P

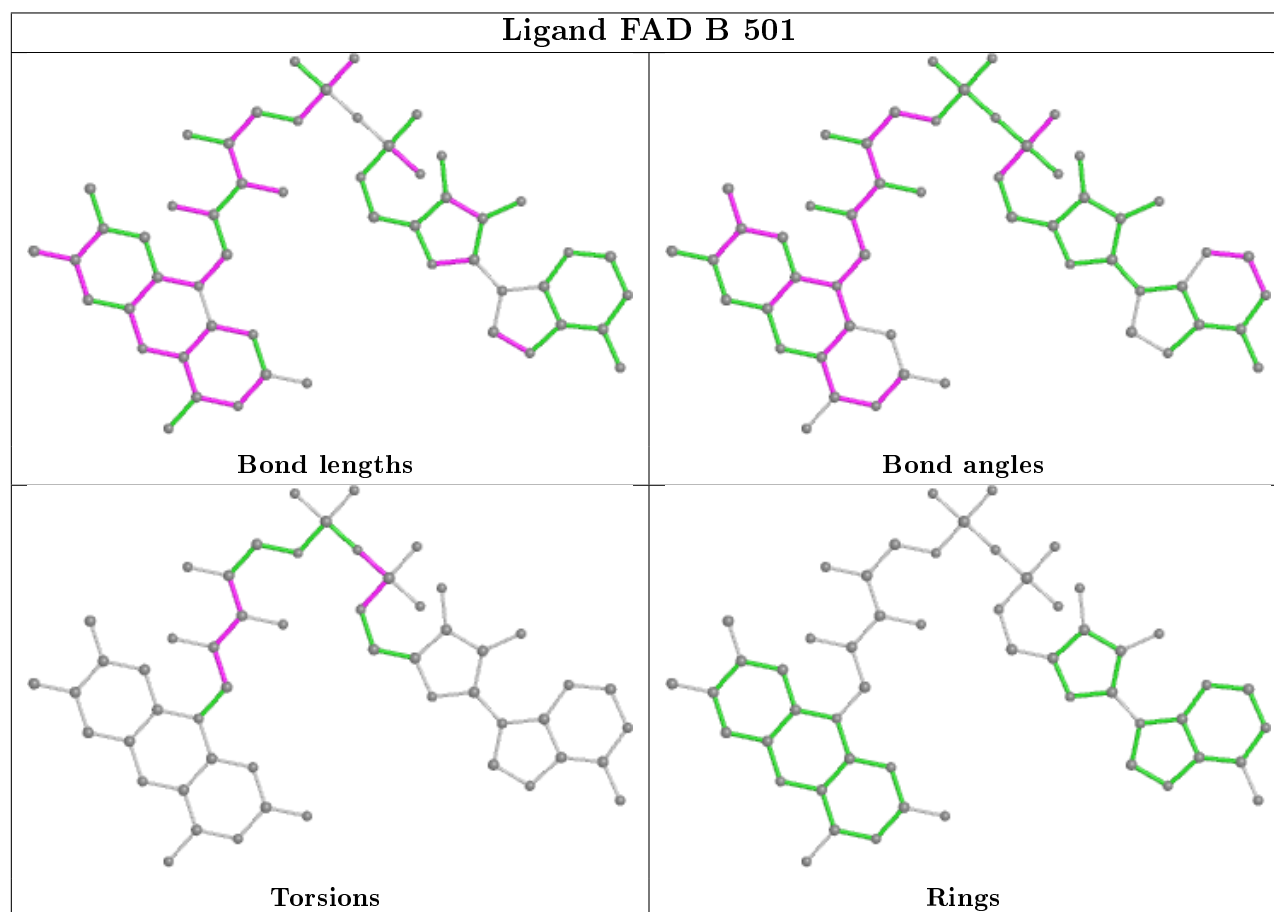
There are no ring outliers.

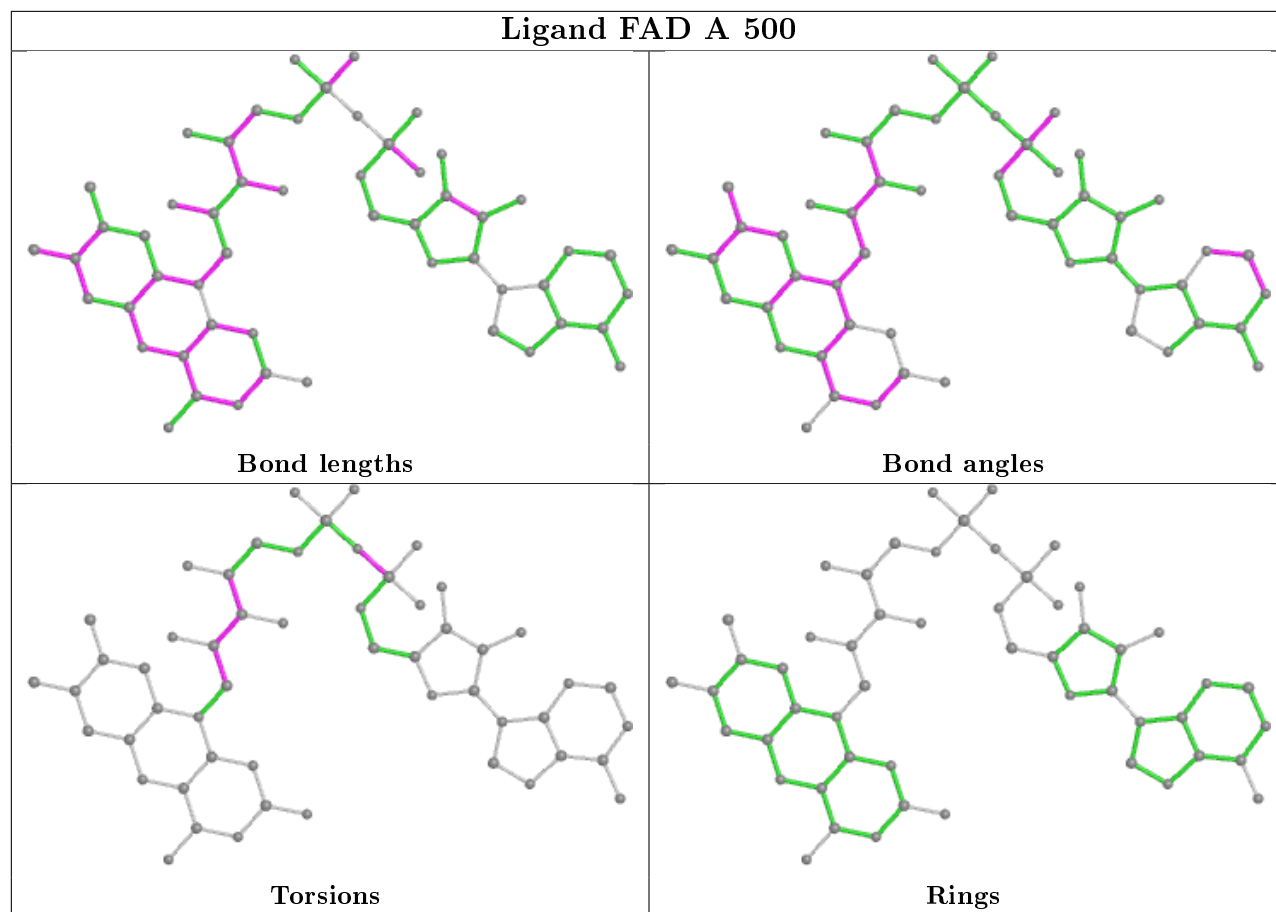
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	FAD	1	0
3	A	500	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	483/489 (98%)	0.33	34 (7%) 16 18	12, 21, 42, 59	0
1	B	483/489 (98%)	0.32	32 (6%) 18 20	12, 22, 42, 62	0
All	All	966/978 (98%)	0.32	66 (6%) 17 19	12, 22, 42, 62	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	12.0
1	A	169	ILE	10.1
1	A	407	ARG	7.9
1	A	1	MET	7.8
1	A	406	ALA	7.0
1	B	407	ARG	6.7
1	A	405	ASP	6.5
1	B	3	HIS	6.5
1	B	2	LYS	5.6
1	A	408	ASP	5.5
1	B	408	ASP	5.4
1	B	169	ILE	5.3
1	B	406	ALA	5.1
1	A	317	ASN	5.0
1	A	404	ASN	4.8
1	A	166	LYS	4.8
1	B	405	ASP	4.6
1	B	440	GLY	4.3
1	A	483	GLU	4.0
1	B	188	LYS	3.9
1	B	166	LYS	3.8
1	B	317	ASN	3.8
1	A	481	LYS	3.6
1	A	482	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	409	PHE	3.3
1	A	187	ILE	3.3
1	B	167	LYS	3.2
1	A	202	ILE	3.2
1	A	188	LYS	3.1
1	A	156	LEU	3.0
1	B	49	HIS	2.9
1	B	176	PHE	2.9
1	B	162	LYS	2.8
1	B	483	GLU	2.8
1	A	190	GLU	2.8
1	A	278	VAL	2.8
1	A	151	GLN	2.8
1	A	168	LYS	2.7
1	A	167	LYS	2.7
1	A	288	PHE	2.7
1	B	482	ILE	2.7
1	A	275	GLN	2.6
1	A	186	ASN	2.6
1	B	275	GLN	2.6
1	A	170	SER	2.6
1	A	112	GLN	2.5
1	B	315	ASN	2.5
1	B	206	HIS	2.5
1	B	238	GLU	2.4
1	A	281	ASP	2.4
1	A	314	LEU	2.4
1	B	151	GLN	2.4
1	B	202	ILE	2.4
1	B	310	ARG	2.3
1	B	441	ASP	2.3
1	B	364	PHE	2.2
1	B	256	LEU	2.2
1	B	361	VAL	2.2
1	A	463	VAL	2.1
1	B	4	VAL	2.1
1	A	272	ARG	2.1
1	A	467	ARG	2.1
1	A	2	LYS	2.1
1	B	168	LYS	2.1
1	A	176	PHE	2.1
1	B	410	ARG	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](#)

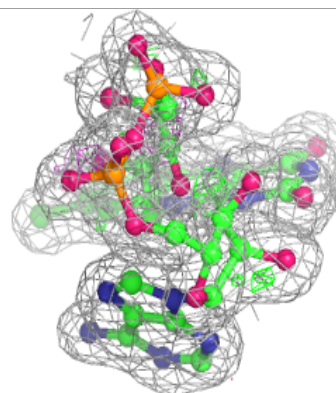
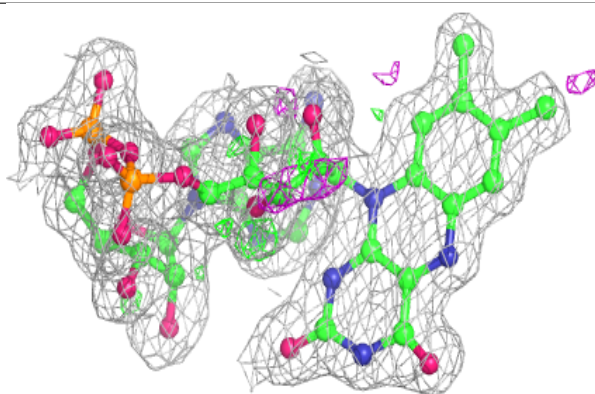
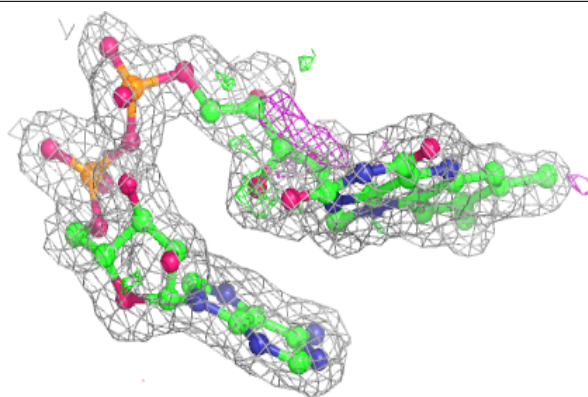
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	1402	5/5	0.94	0.14	35,36,37,37	0
3	FAD	A	500	53/53	0.96	0.16	12,15,19,20	0
3	FAD	B	501	53/53	0.96	0.14	11,16,19,20	0
2	SO4	A	1403	5/5	0.97	0.16	34,34,35,35	0
2	SO4	A	1401	5/5	0.98	0.10	35,35,35,35	0

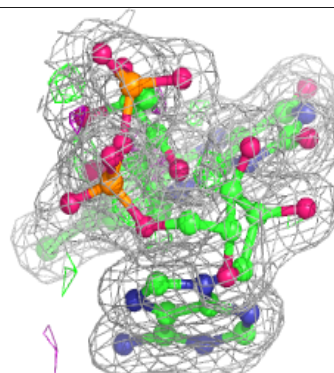
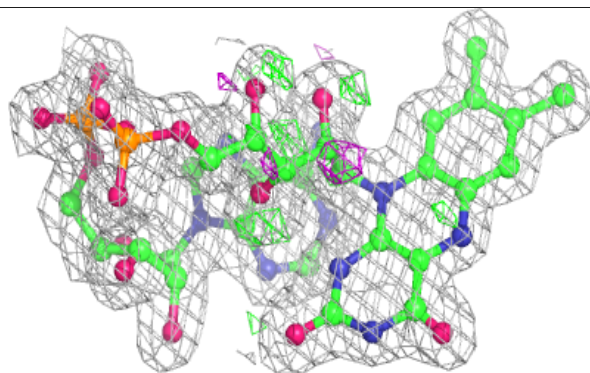
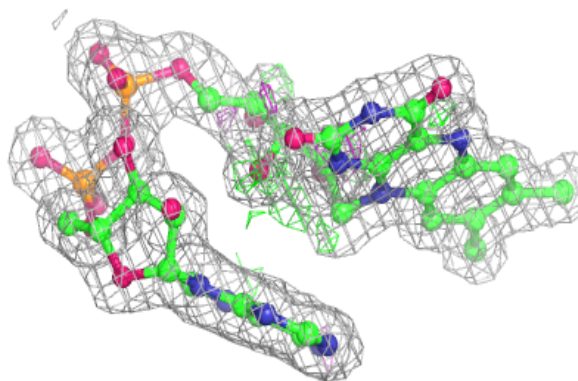
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 500:

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

**Electron density around FAD B 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 ⓘ

There are no such residues in this entry.