



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:57 PM UTC

PDB ID : 4EM4 / pdb_00004em4
Title : Crystal Structure of Staphylococcus aureus bound with the covalent inhibitor Pethyl-VS-CoA
Authors : Wallace, B.D.; Edwards, J.S.; Claiborne, A.; Redinbo, M.R.
Deposited on : 2012-04-11
Resolution : 1.82 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

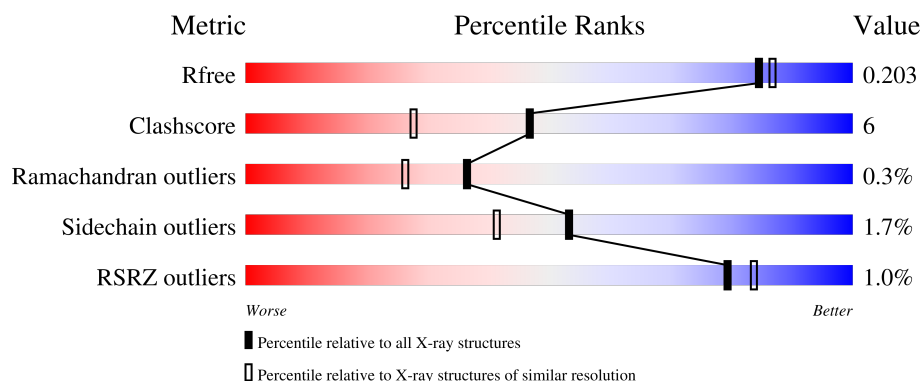
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

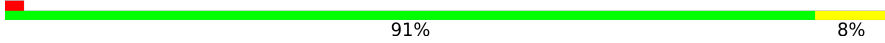
The reported resolution of this entry is 1.82 Å.

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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	437	 89% 10%
1	B	437	 2% 91% 8%

2 Entry composition [i](#)

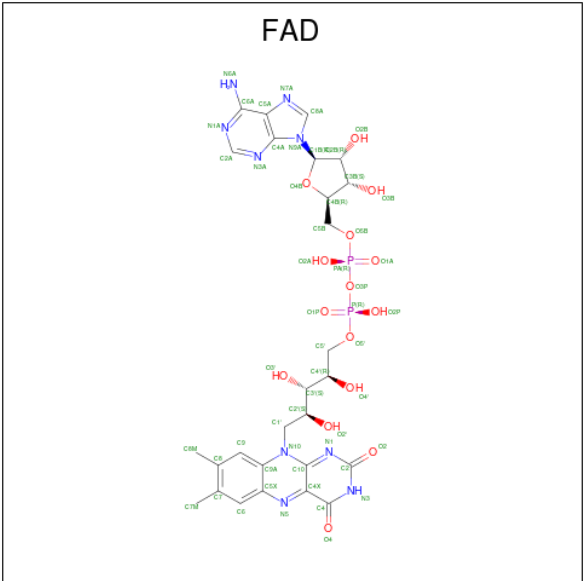
There are 6 unique types of molecules in this entry. The entry contains 8365 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coenzyme A disulfide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	13	0
			3522	2240	597	672	13			
1	B	437	Total	C	N	O	S	0	13	0
			3531	2243	598	677	13			

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



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

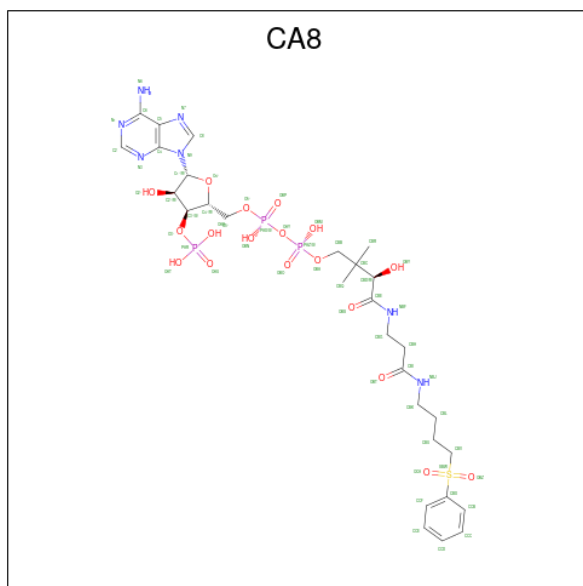
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Cl	0	0
			4	4		
4	B	3	Total	Cl	0	0
			3	3		

- Molecule 5 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(3R)-2,2-dimethyl-3-oxidanyl-4-oxidanylidene-4-[[3-oxidanylidene-3-[4-(phenylsulfonyl)butylamino]propyl]amino]butyl] hydrogen phosphate (CCD ID: CA8) (formula: C₂₉H₄₄N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			58	29	7	18	3	1		
5	B	1	Total	C	N	O	P	S	0	0
			58	29	7	18	3	1		

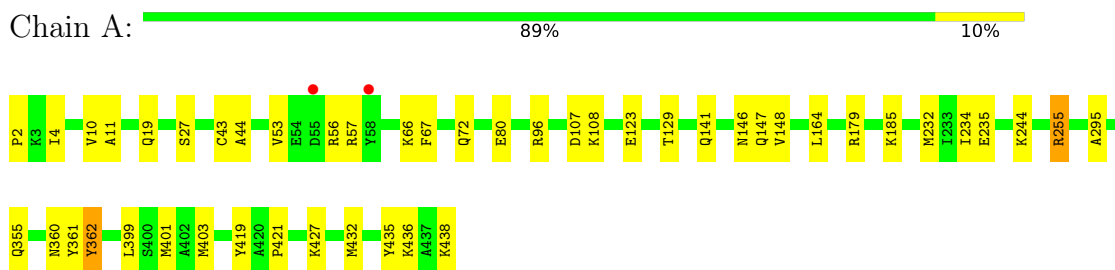
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	564	Total 564	O 564	0	0
6	B	516	Total 516	O 516	0	0

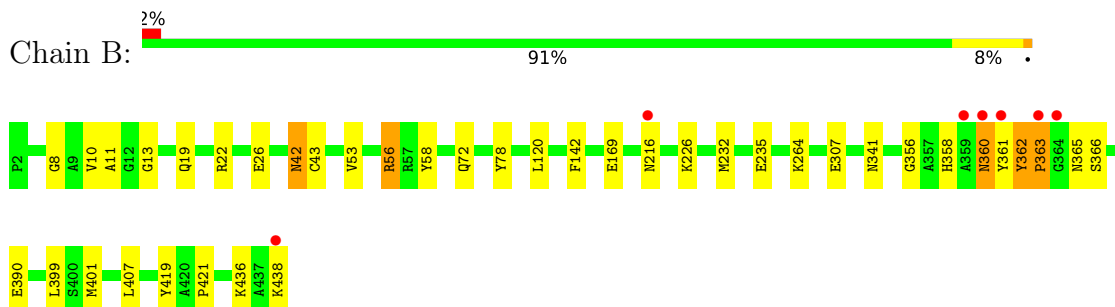
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Coenzyme A disulfide reductase



- Molecule 1: Coenzyme A disulfide reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.14Å 64.91Å 94.44Å 90.00° 104.62° 90.00°	Depositor
Resolution (Å)	32.45 – 1.82 32.45 – 1.82	Depositor EDS
% Data completeness (in resolution range)	95.8 (32.45-1.82) 95.7 (32.45-1.82)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.77 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.8_1057	Depositor
R, R_{free}	0.153 , 0.202 0.154 , 0.203	Depositor DCC
R_{free} test set	3828 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8365	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: MG, CL, CA8, 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	0.52	0/3637	0.88	3/4920 (0.1%)
1	B	0.51	0/3645	0.90	4/4931 (0.1%)
All	All	0.52	0/7282	0.89	7/9851 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	TYR	CA-C-N	7.44	129.14	119.84
1	B	362	TYR	C-N-CA	7.44	129.14	119.84
1	B	362	TYR	N-CA-C	-7.12	100.79	109.83
1	A	362	TYR	CA-C-N	6.22	126.24	119.89
1	A	362	TYR	C-N-CA	6.22	126.24	119.89
1	A	421	PRO	N-CA-C	6.11	118.15	110.70
1	B	421	PRO	N-CA-C	5.09	116.91	110.70

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	3522	0	3507	41	0
1	B	3531	0	3510	37	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	1	0
2	B	53	0	31	4	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	3	0	0	1	0
5	A	58	0	39	8	0
5	B	58	0	38	9	0
6	A	564	0	0	21	2
6	B	516	0	0	16	1
All	All	8365	0	7156	82	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (82) 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)
5:A:508:CA8:OBO	6:A:1161:HOH:O	1.52	1.25
1:A:355:GLN:NE2	1:A:432[B]:MET:SD	2.33	1.00
5:A:508:CA8:HBQA	6:A:1160:HOH:O	1.61	0.99
4:B:505:CL:CL	6:B:1030:HOH:O	2.27	0.89
1:B:360:ASN:OD1	6:B:1106:HOH:O	1.96	0.82
1:B:360:ASN:OD1	1:B:360:ASN:N	2.14	0.76
1:B:419:TYR:OH	6:B:1108:HOH:O	2.03	0.74
1:B:53:VAL:O	6:B:809:HOH:O	2.11	0.68
1:A:179:ARG:NH1	6:A:840:HOH:O	2.27	0.68
1:B:307:GLU:OE2	6:B:854:HOH:O	2.11	0.68
1:B:72:GLN:OE1	6:B:816:HOH:O	2.11	0.67
1:A:362:TYR:OH	6:A:1110:HOH:O	2.11	0.67
1:A:360:ASN:OD1	6:A:1123:HOH:O	2.12	0.67
1:A:436:LYS:NZ	6:A:1061:HOH:O	2.17	0.66
1:B:120:LEU:O	6:B:949:HOH:O	2.13	0.65
1:A:148:VAL:HG11	1:A:232[A]:MET:HE2	1.79	0.64
5:A:508:CA8:OCA	1:B:361:TYR:OH	2.15	0.64
1:B:436:LYS:NZ	6:B:885:HOH:O	2.33	0.61
5:A:508:CA8:HCE	6:B:1113:HOH:O	2.02	0.59
1:A:2:PRO:N	1:A:27:SER:HG	2.01	0.59
1:A:123:GLU:O	6:A:931:HOH:O	2.17	0.59
6:A:1150:HOH:O	5:B:506:CA8:HCC	2.02	0.58
1:B:43:CYS:SG	2:B:501:FAD:C4X	2.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:OE1	6:A:1089:HOH:O	2.17	0.58
1:A:147:GLN:O	6:A:1143:HOH:O	2.18	0.56
1:B:22:ARG:HD2	6:B:980:HOH:O	2.06	0.56
1:B:142:PHE:CD1	1:B:232[B]:MET:HE3	2.41	0.56
1:A:129:THR:HG22	1:A:235[A]:GLU:HG3	1.88	0.55
1:A:419:TYR:CE2	5:B:506:CA8:HBV	2.42	0.55
1:A:438:LYS:HE2	6:A:753:HOH:O	2.06	0.54
1:A:295:ALA:HB2	5:A:508:CA8:HBL	1.90	0.53
1:A:53:VAL:HG22	1:B:361:TYR:HB2	1.89	0.53
1:A:361:TYR:HB3	1:B:58:TYR:CG	2.45	0.51
1:A:419:TYR:HE2	5:B:506:CA8:CBV	2.23	0.51
1:A:427[B]:LYS:NZ	6:A:998:HOH:O	2.44	0.51
1:B:11:ALA:HB3	2:B:501:FAD:O5'	2.12	0.50
1:A:80:GLU:OE1	1:A:96[B]:ARG:NH2	2.46	0.49
1:B:78:TYR:OH	6:B:829:HOH:O	2.19	0.49
1:A:419:TYR:CE2	5:B:506:CA8:CBV	2.95	0.49
1:B:356:GLY:HA3	1:B:365:ASN:HD21	1.78	0.48
1:B:72:GLN:HG3	6:B:1024:HOH:O	2.13	0.48
1:A:66:LYS:NZ	6:A:973:HOH:O	2.47	0.47
1:B:42:ASN:OD1	5:B:506:CA8:HBHA	2.14	0.47
1:A:185:LYS:HG2	6:A:662:HOH:O	2.13	0.47
1:A:355:GLN:HG3	6:A:1120:HOH:O	2.14	0.47
1:B:264:LYS:NZ	6:B:888:HOH:O	2.46	0.47
1:A:53:VAL:CG2	1:B:361:TYR:HB2	2.46	0.46
1:B:19:GLN:NE2	6:B:980:HOH:O	2.48	0.46
1:A:255:ARG:CZ	1:A:255:ARG:HB2	2.46	0.46
1:A:244:LYS:NZ	6:A:855:HOH:O	2.15	0.45
1:B:366:SER:OG	6:B:1105:HOH:O	2.20	0.45
1:A:419:TYR:HE2	5:B:506:CA8:HBV	1.82	0.45
1:A:44:ALA:HB2	1:B:361:TYR:CZ	2.52	0.45
1:B:142:PHE:HD1	1:B:232[B]:MET:HE3	1.81	0.44
1:A:107:ASP:O	1:A:108:LYS:HD3	2.18	0.44
5:A:508:CA8:HBVA	1:B:419:TYR:CE2	2.53	0.43
1:B:358:HIS:HD2	1:B:390:GLU:OE1	2.01	0.43
1:A:419:TYR:OH	5:B:506:CA8:HBVA	2.18	0.43
2:B:501:FAD:H9	2:B:501:FAD:H1'1	1.82	0.43
1:A:19:GLN:NE2	6:A:1161:HOH:O	2.48	0.43
6:A:1150:HOH:O	5:B:506:CA8:HCB	2.18	0.43
1:A:2:PRO:HG2	1:A:4[B]:ILE:HD11	2.01	0.43
1:A:11:ALA:HB3	2:A:501:FAD:O5'	2.20	0.42
1:B:226:LYS:HE2	1:B:226:LYS:HB2	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:HH12	5:B:506:CA8:H2'	1.84	0.42
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.90	0.42
1:A:43:CYS:H	5:A:508:CA8:HBUA	1.85	0.42
1:A:123:GLU:O	1:A:123:GLU:HG3	2.18	0.42
1:A:438:LYS:O	6:A:746:HOH:O	2.21	0.42
1:B:8:GLY:O	1:B:13:GLY:HA3	2.20	0.41
5:A:508:CA8:HBK	5:A:508:CA8:HBV	1.86	0.41
1:A:399:LEU:O	1:A:403:MET:HG3	2.21	0.41
1:B:169:GLU:HG3	6:B:1082:HOH:O	2.21	0.41
1:A:427[B]:LYS:HE2	1:A:435:TYR:CE2	2.56	0.41
1:B:362:TYR:HA	1:B:363:PRO:HD2	1.66	0.41
1:B:407:LEU:HA	1:B:407:LEU:HD12	1.86	0.41
1:A:164:LEU:C	1:A:164:LEU:HD23	2.46	0.40
1:A:146:ASN:ND2	6:A:1134:HOH:O	2.38	0.40
1:A:401:MET:HG3	1:B:401:MET:HG3	2.04	0.40
1:B:43:CYS:SG	2:B:501:FAD:C4	3.10	0.40

All (3) 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)
6:A:973:HOH:O	6:A:1121:HOH:O[2_646]	2.00	0.20
1:B:26[B]:GLU:OE1	6:A:890:HOH:O[2_556]	2.03	0.17
6:B:1021:HOH:O	6:B:1104:HOH:O[2_647]	2.16	0.04

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	448/437 (102%)	437 (98%)	10 (2%)	1 (0%)	43	33
1	B	448/437 (102%)	434 (97%)	12 (3%)	2 (0%)	30	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	896/874 (102%)	871 (97%)	22 (2%)	3 (0%)	36	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	B	363	PRO
1	B	10	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	388/376 (103%)	382 (98%)	6 (2%)	57	46
1	B	389/376 (104%)	380 (98%)	9 (2%)	44	28
All	All	777/752 (103%)	762 (98%)	15 (2%)	53	37

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	57	ARG
1	A	67	PHE
1	A	141	GLN
1	A	234	ILE
1	A	255	ARG
1	B	42	ASN
1	B	56[A]	ARG
1	B	56[B]	ARG
1	B	216	ASN
1	B	235[A]	GLU
1	B	235[B]	GLU
1	B	341	ASN
1	B	360	ASN
1	B	438	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	B	85	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 10 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	CA8	A	508	1	59,61,61	2.08	21 (35%)	86,91,91	2.55	31 (36%)
2	FAD	A	501	-	58,58,58	1.23	7 (12%)	85,89,89	1.59	19 (22%)
5	CA8	B	506	1	59,61,61	3.64	28 (47%)	86,91,91	2.97	34 (39%)
2	FAD	B	501	-	58,58,58	1.22	6 (10%)	85,89,89	1.52	18 (21%)

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	CA8	A	508	1	-	11/59/75/75	0/4/4/4
2	FAD	A	501	-	-	2/34/50/50	0/6/6/6
5	CA8	B	506	1	-	12/59/75/75	0/4/4/4
2	FAD	B	501	-	-	2/34/50/50	0/6/6/6

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	506	CA8	PAR-O3'	-15.38	1.32	1.59
5	B	506	CA8	CBX-SBW	9.53	1.91	1.76
5	B	506	CA8	PAX-OAY	-9.39	1.49	1.59
5	B	506	CA8	PAX-O5'	-8.44	1.26	1.59
5	A	508	CA8	CBX-SBW	-6.58	1.66	1.76
5	B	506	CA8	CBV-SBW	6.43	1.89	1.77
5	B	506	CA8	C3'-C4'	4.84	1.65	1.52
5	B	506	CA8	CBU-CBL	-4.58	1.29	1.51
5	B	506	CA8	O5'-C5'	-4.42	1.27	1.44
5	A	508	CA8	C5'-C4'	4.08	1.63	1.51
5	B	506	CA8	CBB-CBC	4.01	1.59	1.52
5	A	508	CA8	PAX-OBP	3.94	1.64	1.50
5	A	508	CA8	PAZ-OAY	3.89	1.63	1.59
5	B	506	CA8	PAZ-OB0	3.82	1.64	1.50
5	B	506	CA8	C5'-C4'	3.64	1.62	1.51
5	A	508	CA8	C2'-C3'	-3.63	1.45	1.53
5	A	508	CA8	C8-N9	-3.56	1.31	1.37
2	B	501	FAD	C4X-N5	3.55	1.38	1.30
2	A	501	FAD	C4X-N5	3.53	1.38	1.30
5	A	508	CA8	OBZ-SBW	3.49	1.48	1.44
5	A	508	CA8	CBB-CBC	3.41	1.58	1.52
5	A	508	CA8	C5-C4	-3.35	1.33	1.39
2	A	501	FAD	PA-O3P	3.34	1.63	1.59
5	B	506	CA8	O4'-C1'	3.28	1.49	1.42
5	B	506	CA8	C5-N7	-3.10	1.33	1.39
2	B	501	FAD	P-O3P	3.08	1.62	1.59
5	A	508	CA8	C5-N7	-3.06	1.33	1.39
2	B	501	FAD	PA-O3P	3.01	1.62	1.59
2	B	501	FAD	C2A-N1A	3.01	1.39	1.33
5	B	506	CA8	O2'-C2'	2.99	1.50	1.43
2	A	501	FAD	P-O3P	2.96	1.62	1.59
5	A	508	CA8	C3'-C4'	2.84	1.60	1.52
5	B	506	CA8	C2-N3	2.83	1.39	1.33
5	A	508	CA8	PAR-O3'	2.79	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C2A-N1A	2.75	1.38	1.33
5	B	506	CA8	C2-N1	2.74	1.38	1.33
2	B	501	FAD	C2A-N3A	2.71	1.38	1.33
5	A	508	CA8	C4-N9	-2.69	1.32	1.37
5	A	508	CA8	OCA-SBW	2.64	1.47	1.44
5	B	506	CA8	PAR-OAS	2.64	1.64	1.54
5	B	506	CA8	C4-N9	-2.64	1.32	1.37
5	B	506	CA8	PAR-OAU	2.63	1.58	1.50
5	A	508	CA8	PAX-OBN	-2.62	1.43	1.55
2	A	501	FAD	C2A-N3A	2.61	1.38	1.33
5	A	508	CA8	PAR-OAU	2.58	1.58	1.50
5	A	508	CA8	CBH-CBI	2.55	1.56	1.51
5	B	506	CA8	CBG-NBF	2.52	1.51	1.46
5	B	506	CA8	C8-N9	-2.48	1.33	1.37
2	B	501	FAD	C8A-N7A	2.39	1.36	1.31
5	A	508	CA8	PAR-OAT	-2.36	1.46	1.54
5	B	506	CA8	CBH-CBI	2.33	1.56	1.51
5	B	506	CA8	C2'-C3'	-2.31	1.47	1.53
5	B	506	CA8	C5-C6	-2.30	1.34	1.41
5	B	506	CA8	C5-C4	-2.28	1.35	1.39
5	B	506	CA8	PAZ-OBM	-2.26	1.44	1.55
2	A	501	FAD	C8A-N7A	2.21	1.35	1.31
5	B	506	CA8	PAX-OBN	-2.19	1.45	1.55
2	A	501	FAD	C10-N1	2.10	1.37	1.33
5	B	506	CA8	PAX-OBP	2.09	1.58	1.50
5	A	508	CA8	C2-N1	2.07	1.37	1.33
5	A	508	CA8	CBQ-CBC	2.04	1.58	1.53
5	A	508	CA8	C5-C6	-2.01	1.35	1.41

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	506	CA8	PAR-O3'-C3'	9.35	148.40	123.43
5	B	506	CA8	OCA-SBW-OBZ	-9.28	108.51	118.45
5	A	508	CA8	C5'-C4'-C3'	-8.36	86.54	114.38
5	B	506	CA8	O3'-PAR-OAU	7.54	136.22	109.33
5	B	506	CA8	CBV-SBW-CBX	7.13	114.74	105.09
5	B	506	CA8	CBL-CBU-CBV	7.11	135.24	112.25
5	A	508	CA8	OCA-SBW-OBZ	-6.85	111.11	118.45
5	A	508	CA8	N3-C2-N1	-6.40	118.89	128.58
5	B	506	CA8	C5'-C4'-C3'	-6.32	93.32	114.38
5	B	506	CA8	N3-C2-N1	-6.08	119.38	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	508	CA8	OBA-CBB-CBC	5.56	119.49	110.55
5	A	508	CA8	O3'-PAR-OAU	5.49	128.90	109.33
2	A	501	FAD	N3A-C2A-N1A	-5.47	120.30	128.58
2	B	501	FAD	N3A-C2A-N1A	-5.45	120.34	128.58
5	B	506	CA8	PAX-O5'-C5'	5.37	152.12	121.35
5	B	506	CA8	OBZ-SBW-CBV	5.29	116.84	108.18
5	A	508	CA8	CBR-CBC-CBQ	5.28	119.73	109.20
5	B	506	CA8	OAS-PAR-O3'	-4.98	86.45	105.85
5	A	508	CA8	C3'-C2'-C1'	4.84	110.53	99.89
5	A	508	CA8	C5-C4-N3	-4.45	120.59	126.72
5	B	506	CA8	O3'-C3'-C2'	4.25	126.91	111.68
2	A	501	FAD	N9A-C8A-N7A	-4.15	108.06	113.94
2	B	501	FAD	N9A-C8A-N7A	-3.93	108.37	113.94
5	A	508	CA8	N9-C8-N7	-3.88	108.43	113.94
5	B	506	CA8	C5-C4-N3	-3.86	121.40	126.72
5	B	506	CA8	CBK-NBJ-CBI	3.82	129.93	122.82
5	A	508	CA8	OAT-PAR-O3'	-3.81	91.02	105.85
5	B	506	CA8	OBA-CBB-CBC	3.72	116.53	110.55
5	B	506	CA8	OBZ-SBW-CBX	-3.66	104.83	108.33
5	A	508	CA8	C4-C5-N7	-3.65	106.41	110.58
5	B	506	CA8	C3'-C2'-C1'	3.63	107.87	99.89
5	A	508	CA8	O5'-C5'-C4'	3.62	121.31	108.99
5	A	508	CA8	CBQ-CBC-CBD	3.59	114.89	108.77
2	A	501	FAD	C5A-C4A-N3A	-3.53	121.86	126.72
5	B	506	CA8	N9-C8-N7	-3.44	109.05	113.94
5	A	508	CA8	C2-N3-C4	3.44	120.24	111.83
5	B	506	CA8	O4'-C1'-C2'	-3.41	99.33	106.62
5	A	508	CA8	CBQ-CBC-CBB	-3.30	102.78	108.22
5	A	508	CA8	CBV-SBW-CBX	3.28	109.53	105.09
2	B	501	FAD	C5A-C4A-N3A	-3.20	122.31	126.72
5	A	508	CA8	PAR-O3'-C3'	3.18	131.93	123.43
2	A	501	FAD	C4-N3-C2	-3.10	120.13	125.64
5	B	506	CA8	C4-C5-N7	-3.10	107.04	110.58
5	A	508	CA8	C5-C4-N9	3.08	109.17	105.81
5	A	508	CA8	C5-N7-C8	3.08	108.28	103.45
2	B	501	FAD	C4X-C10-N10	3.06	120.86	116.48
5	A	508	CA8	OAT-PAR-OAS	3.05	119.22	107.80
5	B	506	CA8	OCA-SBW-CBX	-2.98	105.48	108.33
2	A	501	FAD	C5A-N7A-C8A	2.95	108.09	103.45
2	B	501	FAD	C4-N3-C2	-2.94	120.42	125.64
5	A	508	CA8	OBZ-SBW-CBV	-2.94	103.37	108.18
5	A	508	CA8	CBH-CBI-NBJ	-2.93	111.01	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C2A-N3A-C4A	2.92	118.97	111.83
5	A	508	CA8	OCA-SBW-CBX	2.92	111.13	108.33
5	B	506	CA8	C5-N7-C8	2.92	108.04	103.45
2	B	501	FAD	C4'-C3'-C2'	-2.88	108.77	113.57
2	B	501	FAD	C5A-N7A-C8A	2.87	107.95	103.45
2	A	501	FAD	C4X-C10-N10	2.78	120.46	116.48
2	A	501	FAD	C4A-N9A-C8A	2.74	108.61	105.74
2	B	501	FAD	C5X-C9A-N10	2.74	120.44	117.97
2	B	501	FAD	C2A-N3A-C4A	2.73	118.50	111.83
5	B	506	CA8	CCC-CCB-CBX	2.73	121.74	118.95
5	B	506	CA8	C2-N3-C4	2.72	118.48	111.83
2	A	501	FAD	N3A-C4A-N9A	2.65	131.67	127.17
2	A	501	FAD	C10-C4X-N5	-2.57	119.55	124.81
2	A	501	FAD	C4'-C3'-C2'	-2.50	109.41	113.57
5	A	508	CA8	OBZ-SBW-CBX	2.50	110.72	108.33
5	A	508	CA8	OBM-PAZ-OAY	-2.47	100.59	107.27
5	B	506	CA8	C5-C4-N9	2.46	108.49	105.81
2	A	501	FAD	C9A-C5X-N5	-2.45	119.86	122.45
5	A	508	CA8	O2'-C2'-C3'	2.43	117.98	111.19
2	B	501	FAD	O4-C4-C4X	-2.40	120.19	126.53
5	A	508	CA8	O4'-C1'-C2'	-2.39	101.49	106.62
2	A	501	FAD	C4X-C4-N3	2.39	119.33	113.25
2	A	501	FAD	C9-C9A-N10	-2.38	118.65	121.85
2	A	501	FAD	C5X-C9A-N10	2.32	120.07	117.97
2	B	501	FAD	C9-C9A-N10	-2.32	118.74	121.85
5	B	506	CA8	CBG-CBH-CBI	2.31	116.23	112.39
5	B	506	CA8	OBT-CBI-NBJ	2.29	127.53	123.03
2	A	501	FAD	O4-C4-C4X	-2.28	120.52	126.53
2	B	501	FAD	O2P-P-O3P	2.26	113.39	107.27
2	B	501	FAD	O3P-PA-O1A	-2.25	103.93	110.70
5	A	508	CA8	C6-C5-C4	2.24	120.23	117.18
2	B	501	FAD	C4A-N9A-C8A	2.21	108.06	105.74
2	B	501	FAD	C4X-C4-N3	2.20	118.84	113.25
5	B	506	CA8	CCF-CBX-SBW	2.18	121.75	119.50
5	B	506	CA8	C6-C5-C4	2.18	120.15	117.18
5	B	506	CA8	O2'-C2'-C3'	-2.18	105.09	111.19
5	B	506	CA8	CBH-CBI-NBJ	-2.17	112.39	116.34
5	A	508	CA8	OBT-CBI-NBJ	2.13	127.21	123.03
2	A	501	FAD	O3P-PA-O1A	-2.13	104.30	110.70
2	A	501	FAD	C5'-C4'-C3'	-2.13	108.21	112.22
5	B	506	CA8	C1'-N9-C8	-2.12	122.39	127.09
5	A	508	CA8	CBK-NBJ-CBI	2.12	126.76	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	O2-C2-N1	-2.11	118.29	121.80
5	A	508	CA8	O4'-C4'-C5'	2.11	116.10	109.33
5	B	506	CA8	CBG-NBF-CBE	2.09	126.30	122.55
2	B	501	FAD	N3A-C4A-N9A	2.08	130.70	127.17
5	B	506	CA8	CCE-CCF-CBX	2.08	121.07	118.95
2	A	501	FAD	O2P-P-O3P	2.07	112.88	107.27
2	B	501	FAD	O2A-PA-O3P	2.03	112.77	107.27
5	B	506	CA8	CCF-CBX-CCB	-2.02	117.83	120.47

There are no chirality outliers.

All (27) torsion outliers are listed below:

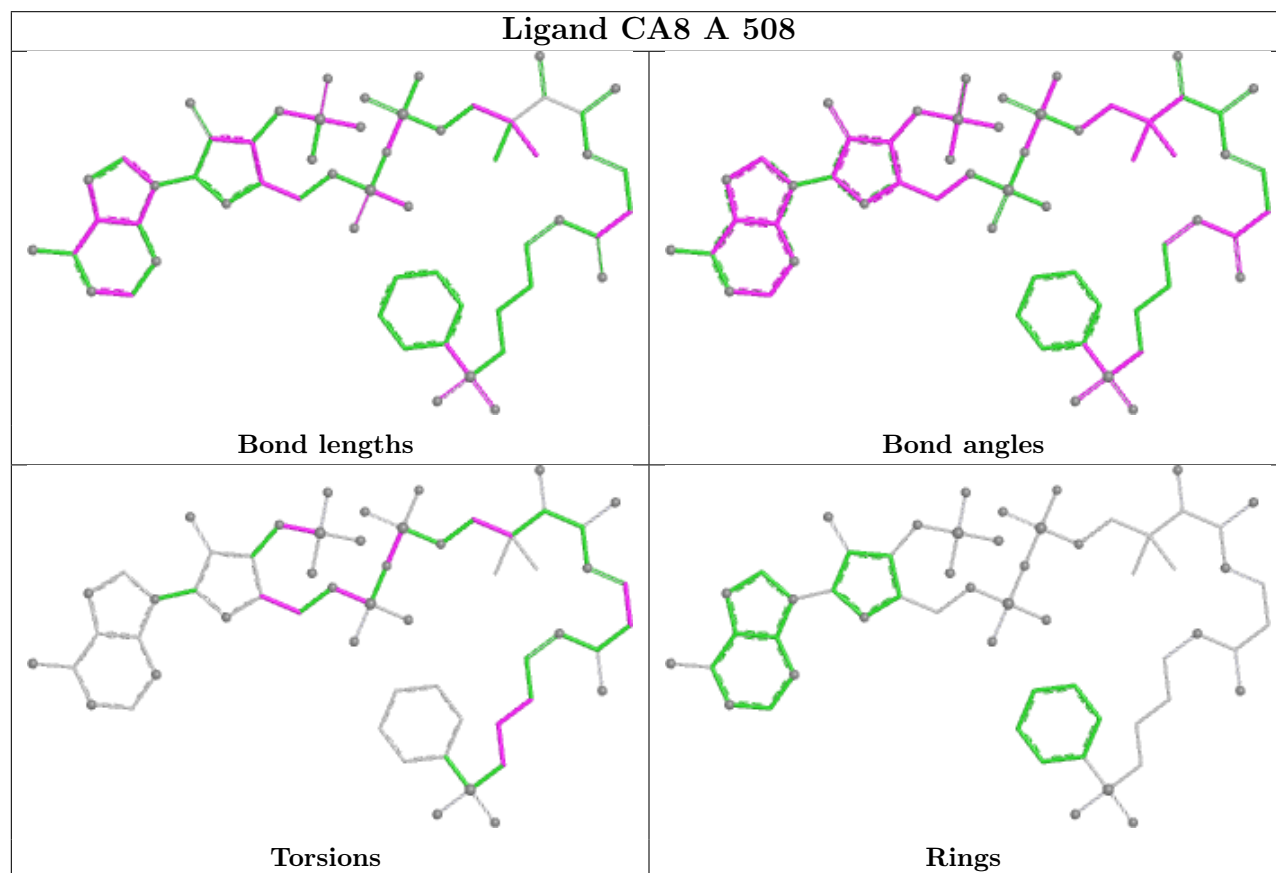
Mol	Chain	Res	Type	Atoms
5	A	508	CA8	O4'-C4'-C5'-O5'
5	A	508	CA8	C5'-O5'-PAX-OAY
5	A	508	CA8	C5'-O5'-PAX-OBN
5	A	508	CA8	CBL-CBU-CBV-SBW
5	B	506	CA8	C3'-C4'-C5'-O5'
5	B	506	CA8	O4'-C4'-C5'-O5'
5	B	506	CA8	C5'-O5'-PAX-OAY
5	B	506	CA8	C5'-O5'-PAX-OBN
5	B	506	CA8	CBB-CBC-CBD-OBY
5	B	506	CA8	CBQ-CBC-CBD-OBY
5	B	506	CA8	CBK-CBL-CBU-CBV
5	B	506	CA8	NBJ-CBK-CBL-CBU
5	B	506	CA8	CBU-CBV-SBW-OBZ
5	B	506	CA8	CBU-CBV-SBW-OCA
2	A	501	FAD	O4B-C4B-C5B-O5B
5	A	508	CA8	C3'-C4'-C5'-O5'
2	A	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B
5	A	508	CA8	PAX-OAY-PAZ-OBA
5	B	506	CA8	CBU-CBV-SBW-CBX
5	A	508	CA8	CBK-CBL-CBU-CBV
5	A	508	CA8	C5'-O5'-PAX-OBP
5	B	506	CA8	C5'-O5'-PAX-OBP
5	A	508	CA8	C3'-O3'-PAR-OAS
5	A	508	CA8	OBA-CBB-CBC-CBR
5	A	508	CA8	NBF-CBG-CBH-CBI

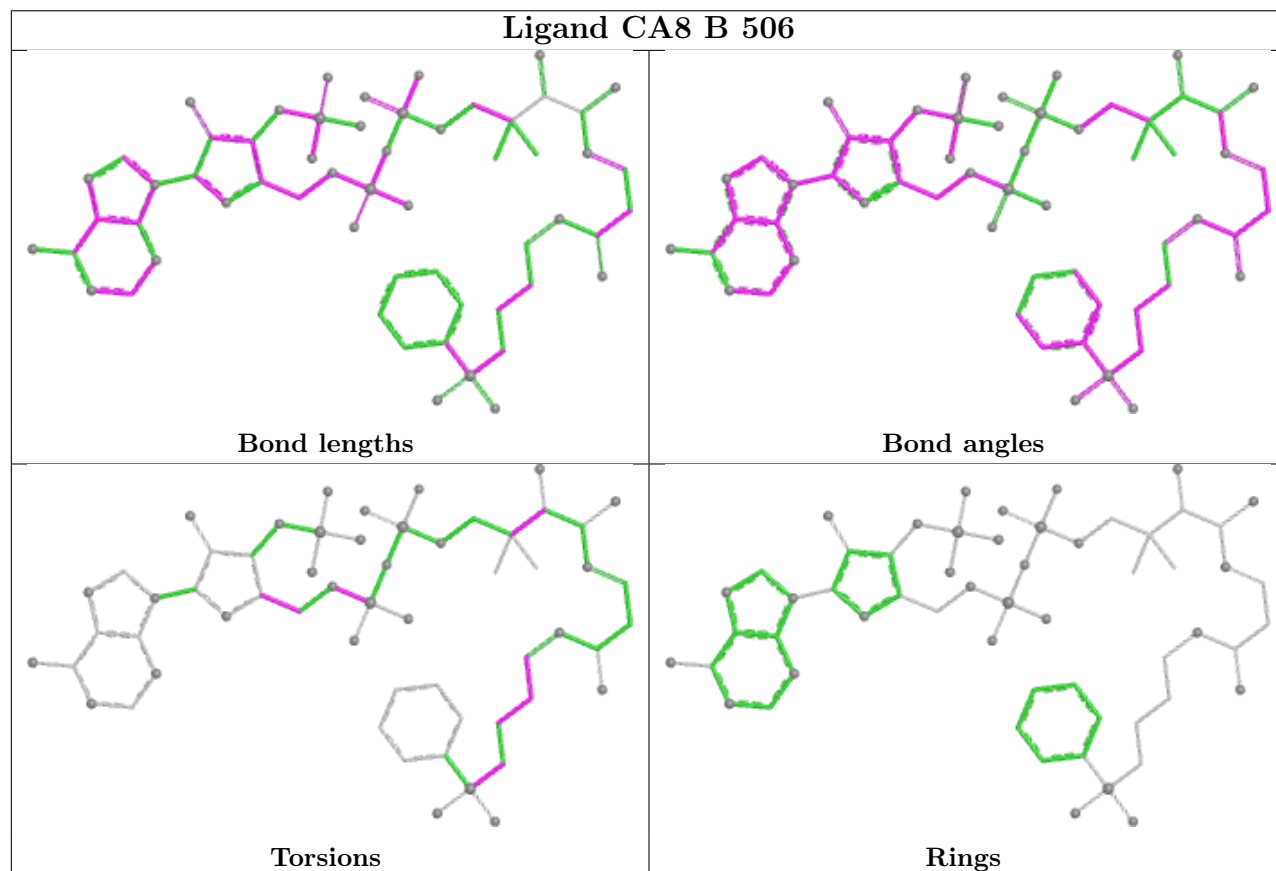
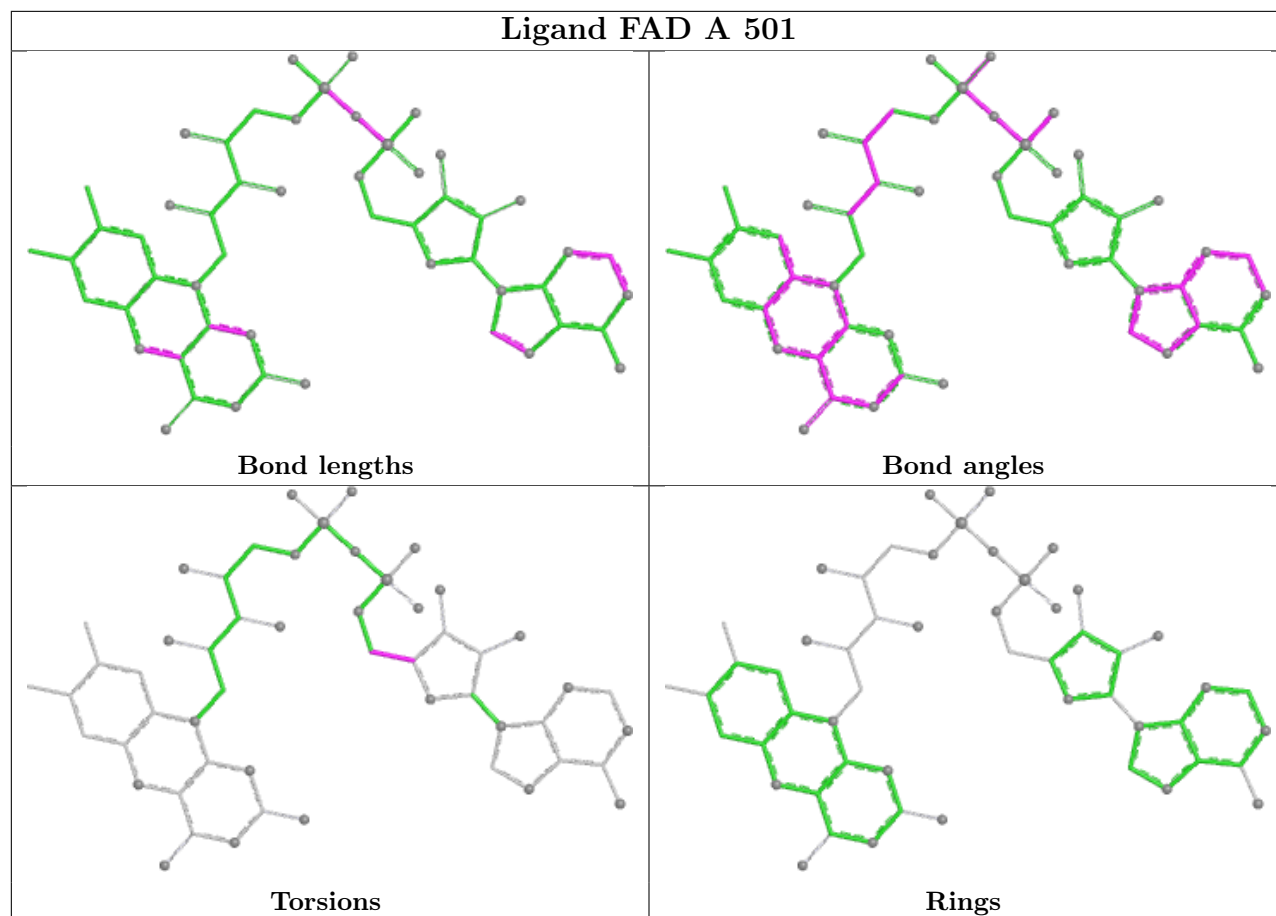
There are no ring outliers.

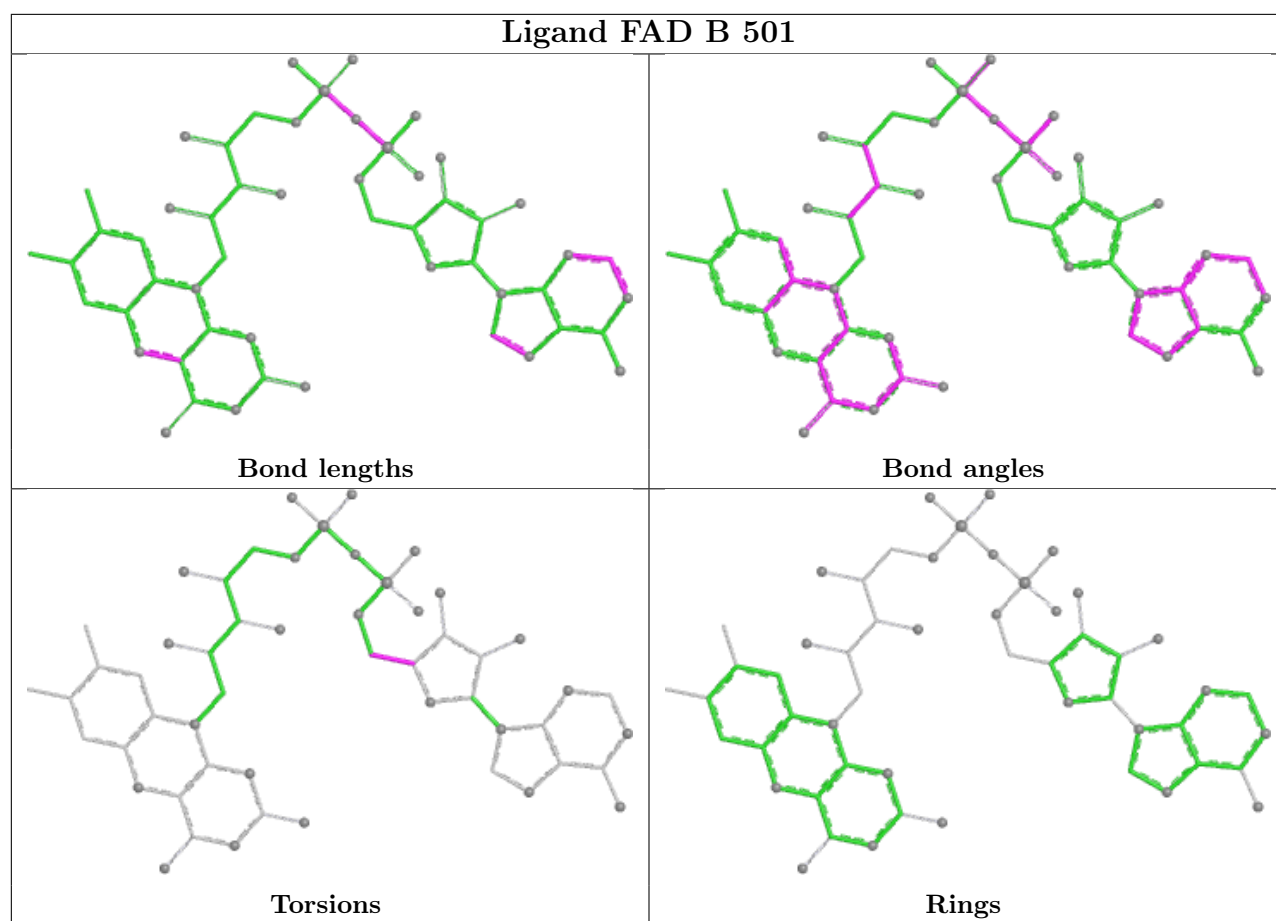
4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	CA8	8	0
2	A	501	FAD	1	0
5	B	506	CA8	9	0
2	B	501	FAD	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/437 (100%)	-0.38	2 (0%) 87 90	14, 23, 43, 68	13 (2%)
1	B	437/437 (100%)	-0.27	7 (1%) 70 77	14, 25, 44, 75	13 (2%)
All	All	874/874 (100%)	-0.33	9 (1%) 79 84	14, 24, 43, 75	26 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	PRO	3.4
1	B	360	ASN	2.6
1	A	58	TYR	2.5
1	B	364	GLY	2.3
1	B	361	TYR	2.2
1	B	359	ALA	2.2
1	A	55	ASP	2.1
1	B	216	ASN	2.0
1	B	438	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

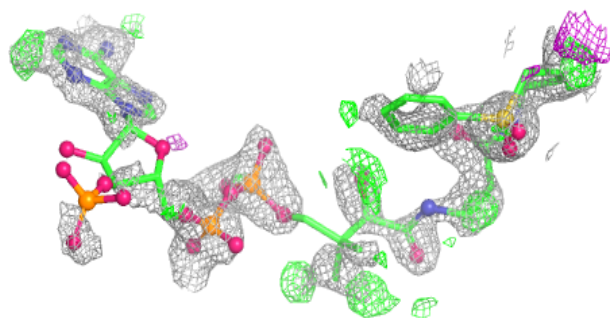
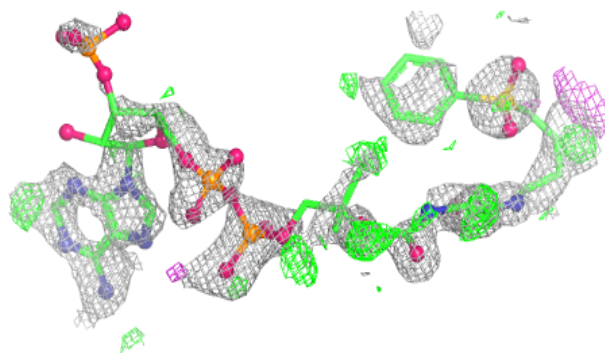
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	503	1/1	0.52	0.15	71,71,71,71	0
4	CL	A	507	1/1	0.65	0.18	86,86,86,86	0
5	CA8	B	506	58/58	0.77	0.17	23,45,70,85	58
4	CL	B	505	1/1	0.83	0.09	79,79,79,79	0
5	CA8	A	508	58/58	0.88	0.12	17,36,54,66	58
4	CL	A	506	1/1	0.90	0.15	61,61,61,61	0
4	CL	A	505	1/1	0.90	0.19	63,63,63,63	0
4	CL	B	503	1/1	0.90	0.09	68,68,68,68	0
4	CL	B	504	1/1	0.92	0.09	76,76,76,76	0
4	CL	A	504	1/1	0.92	0.10	69,69,69,69	0
2	FAD	B	501	53/53	0.97	0.05	14,19,25,28	0
3	MG	A	502	1/1	0.98	0.07	37,37,37,37	0
2	FAD	A	501	53/53	0.98	0.05	11,17,20,23	0
3	MG	B	502	1/1	0.98	0.09	52,52,52,52	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.

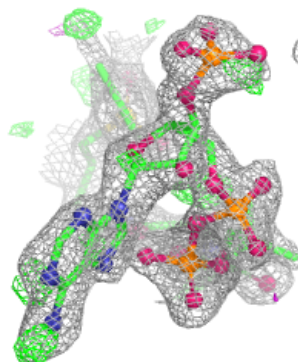
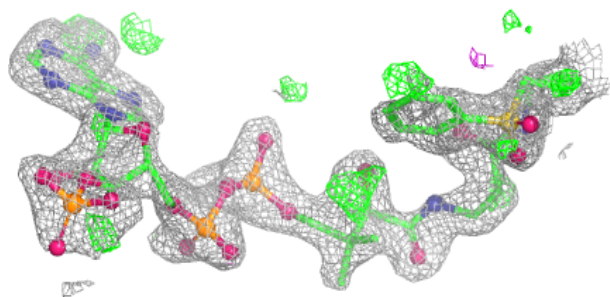
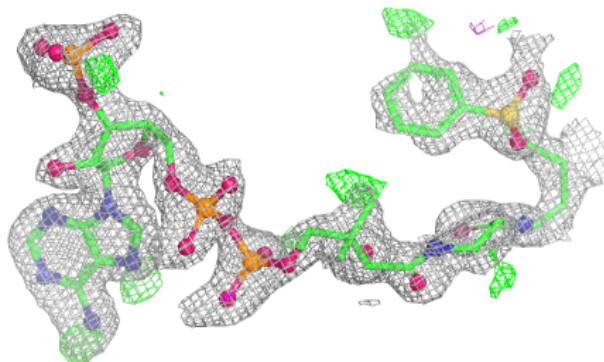
Electron density around CA8 B 506:

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

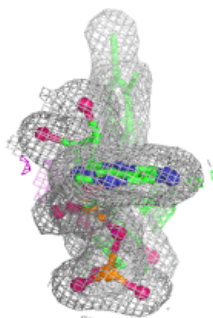
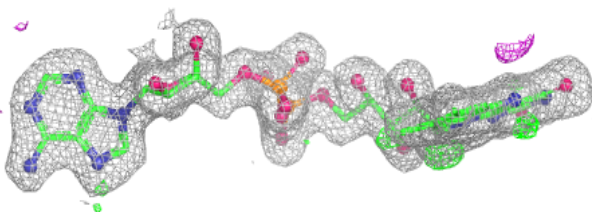
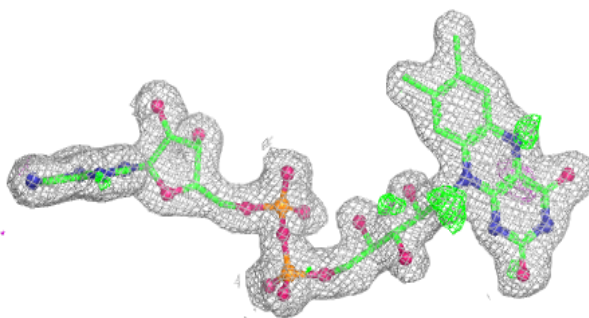


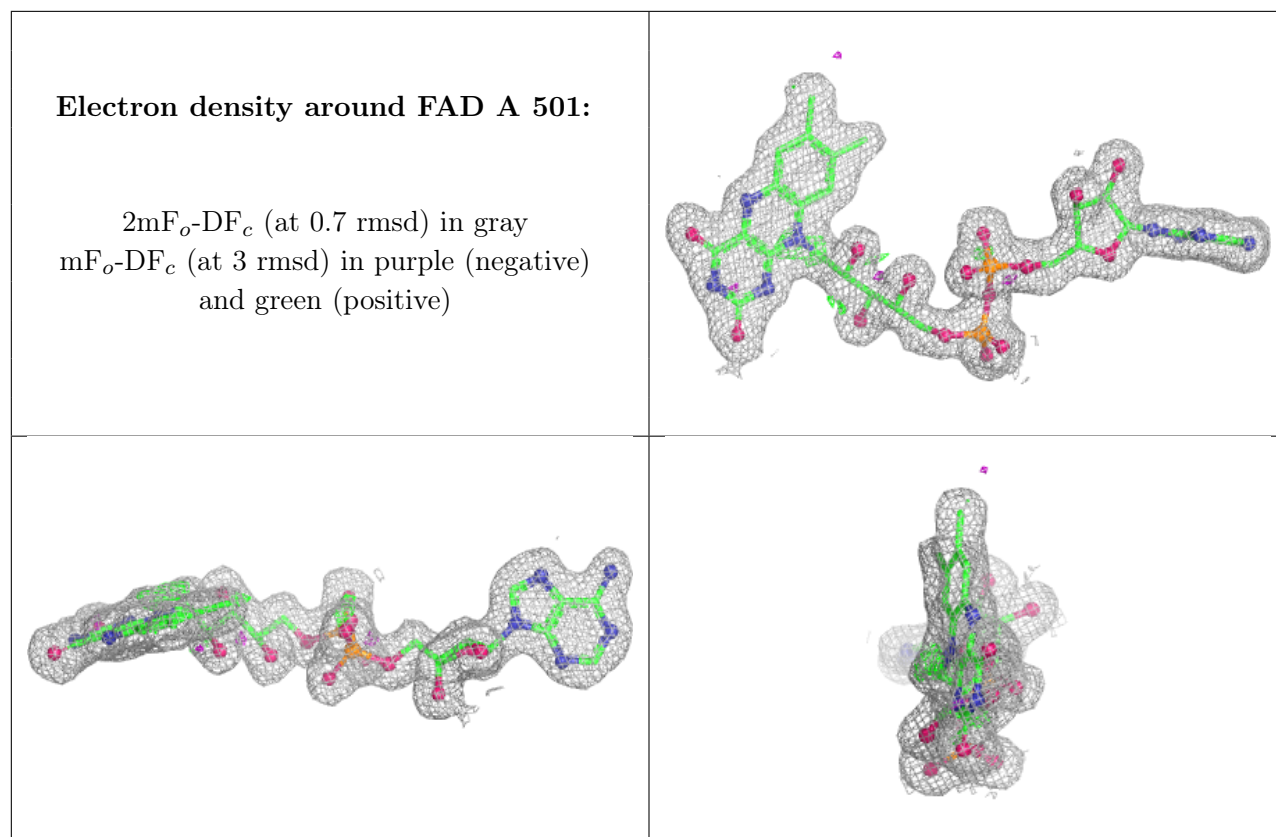
Electron density around CA8 A 508:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.