



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 12:28 PM EDT

PDB ID : 3ICT
Title : Crystal structure of reduced Bacillus anthracis CoADR-RHD
Authors : Wallen, J.R.; Claiborne, A.
Deposited on : 2009-07-18
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

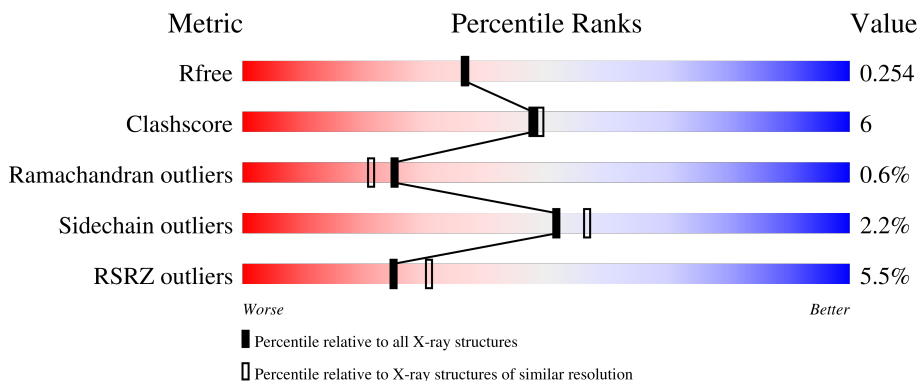
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	588	 7% 83% 11% • 5%
1	B	588	 3% 78% 15% • 6%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9098 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
			Total	C	N	O	S	Se			
1	A	557	Total	C	N	O	S	Se	0	0	0
			4308	2733	735	822	2	16			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4292	2725	731	818	2	16			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MSE	-	expression tag	UNP Q81UT5
A	-32	GLY	-	expression tag	UNP Q81UT5
A	-31	GLY	-	expression tag	UNP Q81UT5
A	-30	SER	-	expression tag	UNP Q81UT5
A	-29	HIS	-	expression tag	UNP Q81UT5
A	-28	HIS	-	expression tag	UNP Q81UT5
A	-27	HIS	-	expression tag	UNP Q81UT5
A	-26	HIS	-	expression tag	UNP Q81UT5
A	-25	HIS	-	expression tag	UNP Q81UT5
A	-24	HIS	-	expression tag	UNP Q81UT5
A	-23	GLY	-	expression tag	UNP Q81UT5
A	-22	MSE	-	expression tag	UNP Q81UT5
A	-21	ALA	-	expression tag	UNP Q81UT5
A	-20	SER	-	expression tag	UNP Q81UT5
A	-19	MSE	-	expression tag	UNP Q81UT5
A	-18	THR	-	expression tag	UNP Q81UT5
A	-17	GLY	-	expression tag	UNP Q81UT5
A	-16	GLY	-	expression tag	UNP Q81UT5
A	-15	GLN	-	expression tag	UNP Q81UT5
A	-14	GLN	-	expression tag	UNP Q81UT5
A	-13	MSE	-	expression tag	UNP Q81UT5
A	-12	GLY	-	expression tag	UNP Q81UT5
A	-11	ARG	-	expression tag	UNP Q81UT5
A	-10	THR	-	expression tag	UNP Q81UT5
A	-9	LEU	-	expression tag	UNP Q81UT5

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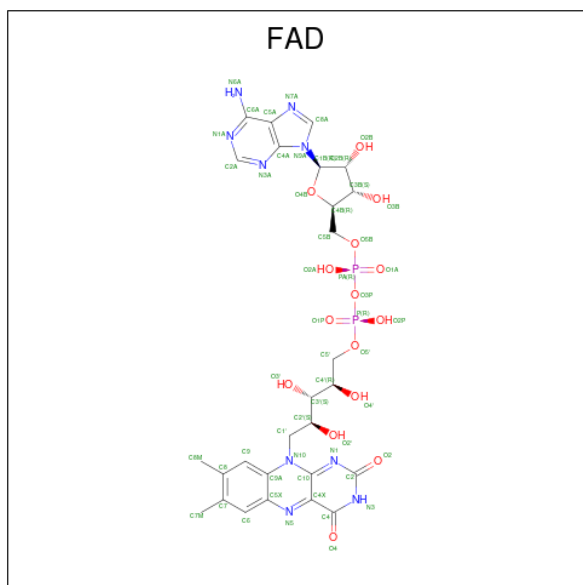
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	TYR	-	expression tag	UNP Q81UT5
A	-7	ASP	-	expression tag	UNP Q81UT5
A	-6	ASP	-	expression tag	UNP Q81UT5
A	-5	ASP	-	expression tag	UNP Q81UT5
A	-4	ASP	-	expression tag	UNP Q81UT5
A	-3	LYS	-	expression tag	UNP Q81UT5
A	-2	ASP	-	expression tag	UNP Q81UT5
A	-1	ARG	-	expression tag	UNP Q81UT5
A	0	TRP	-	expression tag	UNP Q81UT5
A	1	GLY	-	expression tag	UNP Q81UT5
B	-33	MSE	-	expression tag	UNP Q81UT5
B	-32	GLY	-	expression tag	UNP Q81UT5
B	-31	GLY	-	expression tag	UNP Q81UT5
B	-30	SER	-	expression tag	UNP Q81UT5
B	-29	HIS	-	expression tag	UNP Q81UT5
B	-28	HIS	-	expression tag	UNP Q81UT5
B	-27	HIS	-	expression tag	UNP Q81UT5
B	-26	HIS	-	expression tag	UNP Q81UT5
B	-25	HIS	-	expression tag	UNP Q81UT5
B	-24	HIS	-	expression tag	UNP Q81UT5
B	-23	GLY	-	expression tag	UNP Q81UT5
B	-22	MSE	-	expression tag	UNP Q81UT5
B	-21	ALA	-	expression tag	UNP Q81UT5
B	-20	SER	-	expression tag	UNP Q81UT5
B	-19	MSE	-	expression tag	UNP Q81UT5
B	-18	THR	-	expression tag	UNP Q81UT5
B	-17	GLY	-	expression tag	UNP Q81UT5
B	-16	GLY	-	expression tag	UNP Q81UT5
B	-15	GLN	-	expression tag	UNP Q81UT5
B	-14	GLN	-	expression tag	UNP Q81UT5
B	-13	MSE	-	expression tag	UNP Q81UT5
B	-12	GLY	-	expression tag	UNP Q81UT5
B	-11	ARG	-	expression tag	UNP Q81UT5
B	-10	THR	-	expression tag	UNP Q81UT5
B	-9	LEU	-	expression tag	UNP Q81UT5
B	-8	TYR	-	expression tag	UNP Q81UT5
B	-7	ASP	-	expression tag	UNP Q81UT5
B	-6	ASP	-	expression tag	UNP Q81UT5
B	-5	ASP	-	expression tag	UNP Q81UT5
B	-4	ASP	-	expression tag	UNP Q81UT5
B	-3	LYS	-	expression tag	UNP Q81UT5
B	-2	ASP	-	expression tag	UNP Q81UT5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ARG	-	expression tag	UNP Q81UT5
B	0	TRP	-	expression tag	UNP Q81UT5
B	1	GLY	-	expression tag	UNP Q81UT5

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



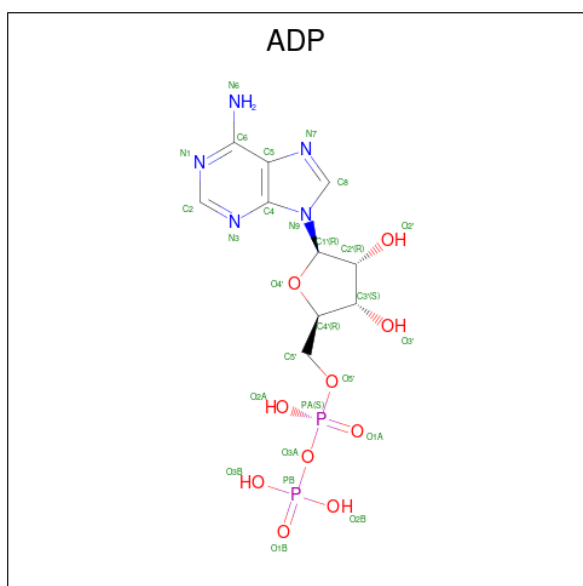
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	48	21	7	16	3	1	0	0
3	B	1	48	21	7	16	3	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	27	10	5	10	2	0	0

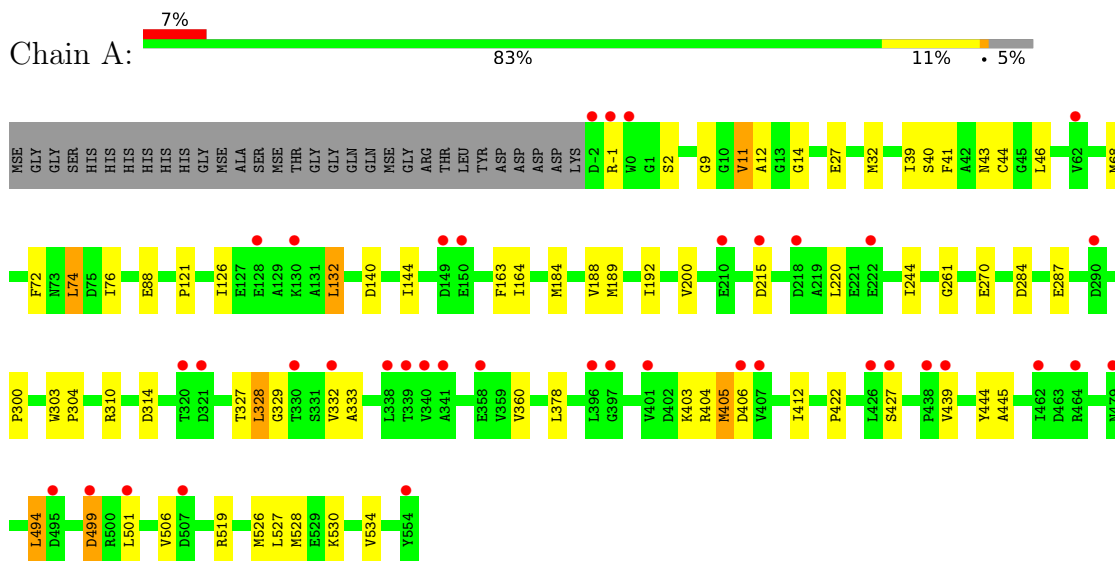
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total 130	O 130	0	0
5	B	139	Total 139	O 139	0	0

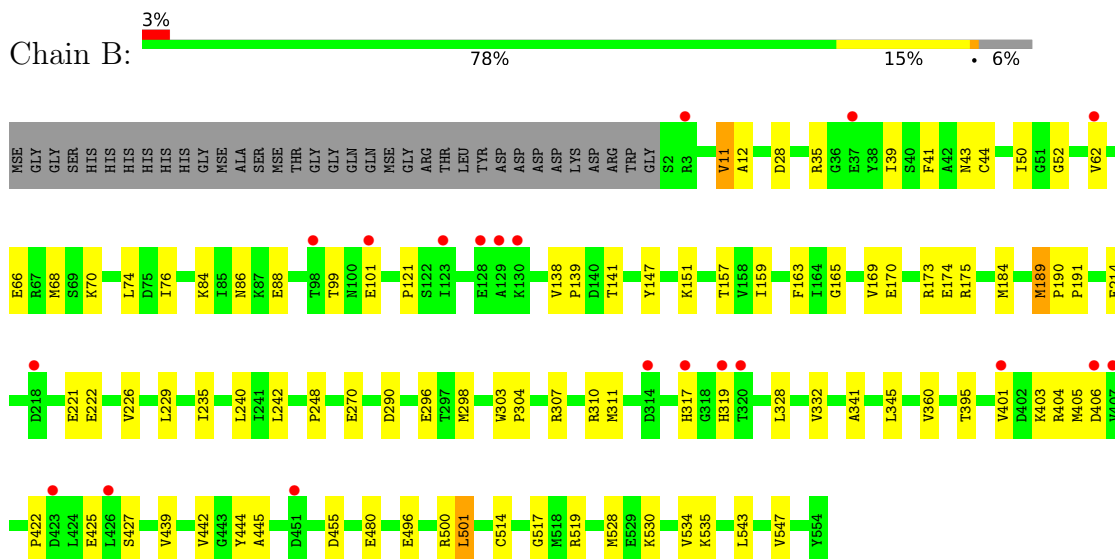
3 Residue-property plots

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	67.62Å 110.55Å 80.08Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	46.13 – 2.10 46.12 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.13-2.10) 99.8 (46.12-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.255 0.211 , 0.254	Depositor DCC
R_{free} test set	3390 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9098	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, FAD, ADP

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	0.53	0/4363	0.64	1/5883 (0.0%)
1	B	0.54	0/4347	0.64	0/5863
All	All	0.54	0/8710	0.64	1/11746 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4308	0	4384	56	0
1	B	4292	0	4375	58	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	48	0	32	6	0
3	B	48	0	32	1	0
4	B	27	0	12	0	0
5	A	130	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	139	0	0	2	0
All	All	9098	0	8897	108	0

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

All (108) 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:44:CYS:SG	3:A:556:COA:H21	2.07	0.95
1:B:455:ASP:OD2	1:B:535:LYS:HE2	1.69	0.93
1:B:395:THR:HG22	1:B:405:MSE:HE2	1.59	0.83
1:B:395:THR:HG22	1:B:405:MSE:CE	2.12	0.79
1:A:189:MSE:HE1	1:A:200:VAL:HG21	1.64	0.78
1:B:395:THR:HG23	1:B:401:VAL:HG13	1.65	0.77
1:B:41:PHE:CE1	1:B:43:ASN:HB3	2.26	0.71
1:A:41:PHE:HE1	1:A:43:ASN:HB3	1.59	0.68
1:A:41:PHE:CE1	1:A:43:ASN:HB3	2.29	0.67
1:B:270:GLU:H	1:B:270:GLU:CD	1.98	0.66
1:A:44:CYS:SG	3:A:556:COA:C2P	2.82	0.66
1:B:395:THR:CG2	1:B:405:MSE:HE2	2.24	0.66
1:A:405:MSE:HA	1:A:405:MSE:CE	2.26	0.65
1:A:310:ARG:HH11	1:A:310:ARG:HG3	1.61	0.65
1:A:528:MSE:HG3	1:A:534:VAL:HG12	1.80	0.64
1:A:189:MSE:HE3	1:A:192:ILE:CD1	2.28	0.64
1:B:39:ILE:HD12	1:B:68:MSE:SE	2.49	0.63
1:A:261:GLY:HA3	1:A:287:GLU:OE1	2.00	0.61
1:A:403:LYS:HD2	1:B:406:ASP:OD2	2.00	0.61
1:B:41:PHE:HE1	1:B:43:ASN:HB3	1.64	0.61
1:A:270:GLU:H	1:A:270:GLU:CD	2.05	0.60
1:B:44:CYS:SG	3:B:556:COA:H21	2.41	0.60
1:B:404:ARG:HG3	1:B:439:VAL:HG23	1.85	0.59
1:A:310:ARG:HG3	1:A:310:ARG:NH1	2.17	0.58
1:A:44:CYS:HG	3:A:556:COA:H21	1.69	0.58
1:A:404:ARG:HG3	1:A:439:VAL:HG23	1.86	0.58
1:B:341:ALA:HB1	1:B:405:MSE:HG2	1.84	0.58
1:A:43:ASN:HA	1:A:46:LEU:HG	1.87	0.57
1:A:303:TRP:HB3	1:A:304:PRO:HD3	1.86	0.57
1:B:480:GLU:OE2	1:B:519:ARG:NH1	2.33	0.57
1:A:405:MSE:HA	1:A:405:MSE:HE3	1.85	0.56
1:B:138:VAL:HB	1:B:139:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:CYS:HG	3:A:556:COA:C2P	2.19	0.56
1:B:229:LEU:HD11	1:B:235:ILE:HD11	1.89	0.54
1:B:159:ILE:HD11	1:B:240:LEU:HD22	1.90	0.54
1:A:72:PHE:HB2	1:A:74:LEU:HD22	1.89	0.53
1:B:84:LYS:HE3	1:B:86:ASN:OD1	2.07	0.53
1:A:11:VAL:HG12	1:A:12:ALA:H	1.72	0.52
1:A:422:PRO:HB3	1:A:444:TYR:CE1	2.45	0.52
1:A:121:PRO:HD3	1:A:244:ILE:HD11	1.93	0.51
1:B:528:MSE:HG3	1:B:534:VAL:CG1	2.41	0.51
1:B:184:MSE:O	1:B:214:GLU:HA	2.10	0.51
1:B:303:TRP:HB3	1:B:304:PRO:HD3	1.92	0.51
1:A:72:PHE:O	1:A:74:LEU:HD13	2.11	0.51
1:B:50:ILE:O	1:B:175:ARG:HD2	2.11	0.51
1:B:296:GLU:H	1:B:296:GLU:CD	2.14	0.50
1:B:501:LEU:HD11	1:B:530:LYS:HD2	1.93	0.50
1:A:189:MSE:HE3	1:A:192:ILE:HD11	1.92	0.50
1:B:28:ASP:OD2	1:B:317:HIS:CE1	2.64	0.50
1:A:140:ASP:O	1:A:144:ILE:HG13	2.11	0.50
1:A:328:LEU:HD21	1:A:412:ILE:HG21	1.93	0.49
1:B:290:ASP:HB2	5:B:673:HOH:O	2.10	0.49
1:A:43:ASN:OD1	3:A:556:COA:H22	2.12	0.49
1:B:163:PHE:CZ	1:B:189:MSE:HE2	2.48	0.49
1:A:528:MSE:HG3	1:A:534:VAL:CG1	2.42	0.49
1:A:499:ASP:OD1	1:B:70:LYS:NZ	2.46	0.48
1:B:39:ILE:HD13	1:B:76:ILE:HD13	1.94	0.48
1:A:163:PHE:CD1	1:A:333:ALA:HB2	2.49	0.48
1:A:494:LEU:HD12	1:A:519:ARG:HG2	1.96	0.48
1:A:499:ASP:OD2	1:A:499:ASP:N	2.47	0.48
1:B:190:PRO:HG2	1:B:191:PRO:HD3	1.95	0.48
1:A:284:ASP:OD1	1:A:300:PRO:HA	2.14	0.47
1:A:427:SER:HB3	1:B:332:VAL:CG1	2.44	0.47
1:B:170:GLU:O	1:B:174:GLU:HG2	2.14	0.47
1:A:189:MSE:HE3	1:A:192:ILE:HD13	1.95	0.47
1:A:2:SER:HB3	1:A:27:GLU:HG2	1.95	0.47
1:A:310:ARG:NH1	1:A:314:ASP:OD2	2.47	0.46
1:A:32:MSE:HE3	1:A:76:ILE:HG12	1.96	0.46
1:A:39:ILE:HD12	1:A:68:MSE:SE	2.65	0.46
1:B:395:THR:CG2	1:B:401:VAL:HG13	2.41	0.46
1:A:332:VAL:HB	1:B:427:SER:HB2	1.96	0.46
1:B:221:GLU:HB2	1:B:226:VAL:HB	1.98	0.46
1:B:422:PRO:HB3	1:B:444:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG23	1:A:189:MSE:HE2	1.98	0.45
1:B:52:GLY:HA2	5:B:650:HOH:O	2.16	0.45
1:A:9:GLY:O	1:A:14:GLY:HA3	2.17	0.45
1:B:43:ASN:ND2	2:B:555:FAD:O2'	2.49	0.45
1:A:88:GLU:H	1:A:88:GLU:CD	2.21	0.44
1:B:147:TYR:CE1	1:B:151:LYS:HG3	2.52	0.44
1:B:496:GLU:HB3	1:B:500:ARG:HD3	2.00	0.44
1:A:39:ILE:HD13	1:A:76:ILE:HD13	2.00	0.44
1:A:40:SER:HB3	3:A:556:COA:O9P	2.18	0.43
1:B:121:PRO:HD2	1:B:242:LEU:HD21	2.00	0.43
1:B:11:VAL:HG12	1:B:12:ALA:N	2.33	0.43
1:B:163:PHE:CE1	1:B:189:MSE:HE2	2.53	0.43
1:B:395:THR:HG22	1:B:405:MSE:HE3	1.93	0.43
1:A:526:MSE:O	1:A:530:LYS:HG2	2.19	0.43
1:B:514:CYS:SG	1:B:517:GLY:N	2.86	0.43
1:B:66:GLU:H	1:B:66:GLU:CD	2.23	0.43
1:B:99:THR:OG1	1:B:101:GLU:HG2	2.19	0.42
1:A:501:LEU:HD21	1:A:527:LEU:HD23	2.02	0.42
1:A:126:ILE:HA	1:A:220:LEU:HD12	2.02	0.41
1:B:311:MSE:HE2	1:B:311:MSE:HB3	2.00	0.41
1:A:11:VAL:HG12	1:A:12:ALA:N	2.35	0.41
1:A:303:TRP:CE3	1:B:425:GLU:HG3	2.55	0.41
1:A:327:THR:HG22	1:A:329:GLY:N	2.34	0.41
1:B:248:PRO:HD3	1:B:298:MSE:SE	2.71	0.41
1:A:163:PHE:CE1	1:A:333:ALA:HB2	2.56	0.41
1:B:165:GLY:O	1:B:169:VAL:HG23	2.21	0.41
1:B:50:ILE:HD11	1:B:141:THR:HG23	2.02	0.41
1:B:157:THR:HB	1:B:240:LEU:HD23	2.03	0.41
1:A:360:VAL:HG21	1:A:445:ALA:HB1	2.02	0.41
1:B:360:VAL:HG21	1:B:445:ALA:HB1	2.03	0.41
1:A:406:ASP:OD2	1:B:403:LYS:HD2	2.21	0.40
1:B:455:ASP:HB3	1:B:535:LYS:HG2	2.02	0.40
1:B:395:THR:HG23	1:B:401:VAL:CG1	2.44	0.40
1:B:543:LEU:O	1:B:547:VAL:HG12	2.21	0.40
1:A:189:MSE:HE3	1:A:189:MSE:HB2	2.01	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	555/588 (94%)	540 (97%)	13 (2%)	2 (0%)	34	32
1	B	551/588 (94%)	533 (97%)	13 (2%)	5 (1%)	17	12
All	All	1106/1176 (94%)	1073 (97%)	26 (2%)	7 (1%)	25	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	B	11	VAL
1	B	319	HIS
1	B	222	GLU
1	A	11	VAL
1	B	62	VAL
1	B	189	MSE

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	467/474 (98%)	456 (98%)	11 (2%)	49	53
1	B	467/474 (98%)	457 (98%)	10 (2%)	53	59
All	All	934/948 (98%)	913 (98%)	21 (2%)	52	57

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

Mol	Chain	Res	Type
1	A	74	LEU
1	A	132	LEU
1	A	164	ILE
1	A	184	MSE
1	A	215	ASP
1	A	328	LEU
1	A	378	LEU
1	A	405	MSE
1	A	494	LEU
1	A	499	ASP
1	A	506	VAL
1	B	35	ARG
1	B	74	LEU
1	B	88	GLU
1	B	173	ARG
1	B	307	ARG
1	B	310	ARG
1	B	328	LEU
1	B	345	LEU
1	B	442	VAL
1	B	501	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	HIS
1	B	319	HIS
1	B	367	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	COA	A	556	-	41,50,50	0.72	0	52,75,75	1.61	11 (21%)
2	FAD	A	555	-	53,58,58	0.92	2 (3%)	68,89,89	1.43	11 (16%)
4	ADP	B	600	-	24,29,29	1.00	1 (4%)	29,45,45	1.31	3 (10%)
2	FAD	B	555	-	53,58,58	0.94	2 (3%)	68,89,89	1.49	13 (19%)
3	COA	B	556	-	41,50,50	0.67	0	52,75,75	1.61	8 (15%)

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	COA	A	556	-	-	7/44/64/64	0/3/3/3
2	FAD	A	555	-	-	2/30/50/50	0/6/6/6
4	ADP	B	600	-	-	2/12/32/32	0/3/3/3
2	FAD	B	555	-	-	3/30/50/50	0/6/6/6
3	COA	B	556	-	-	10/44/64/64	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	555	FAD	C4X-N5	3.18	1.36	1.30
2	B	555	FAD	C4X-N5	2.68	1.36	1.30
4	B	600	ADP	C5-C4	2.56	1.47	1.40
2	A	555	FAD	C10-N10	2.44	1.42	1.37
2	B	555	FAD	C10-N10	2.12	1.42	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	555	FAD	N3A-C2A-N1A	-5.62	119.89	128.68
2	A	555	FAD	N3A-C2A-N1A	-5.41	120.22	128.68
3	A	556	COA	N3A-C2A-N1A	-5.17	120.60	128.68
3	B	556	COA	N3A-C2A-N1A	-4.78	121.21	128.68
3	B	556	COA	C2P-C3P-N4P	-4.09	102.96	112.31
4	B	600	ADP	N3-C2-N1	-3.71	122.88	128.68
3	A	556	COA	C7P-N8P-C9P	3.56	128.94	122.59
3	B	556	COA	C7P-N8P-C9P	3.51	128.85	122.59
3	A	556	COA	C6P-C7P-N8P	-3.47	104.89	111.90
3	B	556	COA	C3P-N4P-C5P	3.39	129.13	122.84
3	B	556	COA	C6P-C7P-N8P	-3.36	105.11	111.90
2	A	555	FAD	C5'-C4'-C3'	-3.34	105.75	112.20
3	A	556	COA	C3P-N4P-C5P	3.26	128.88	122.84
3	A	556	COA	C5B-C4B-C3B	-2.91	104.75	114.40
2	B	555	FAD	C1B-N9A-C4A	-2.91	121.53	126.64
3	A	556	COA	C2P-C3P-N4P	-2.80	105.91	112.31
2	A	555	FAD	C4-N3-C2	-2.70	120.66	125.64
2	B	555	FAD	C5'-C4'-C3'	-2.63	107.12	112.20
4	B	600	ADP	PA-O3A-PB	-2.60	123.92	132.83
2	B	555	FAD	C4-C4X-N5	2.53	121.83	118.23
2	A	555	FAD	O4B-C1B-C2B	-2.50	103.27	106.93
2	A	555	FAD	C10-C4X-N5	-2.44	119.67	124.86
2	A	555	FAD	C4-C4X-N5	2.44	121.70	118.23
3	A	556	COA	O9A-P3B-O8A	2.43	116.91	107.64
2	B	555	FAD	C4-N3-C2	-2.42	121.17	125.64
2	A	555	FAD	C4X-C10-N10	2.42	120.01	116.48
2	B	555	FAD	C4X-C10-N10	2.38	119.96	116.48
3	B	556	COA	O2A-P1A-O1A	2.37	123.97	112.24
2	B	555	FAD	O2A-PA-O1A	2.36	123.91	112.24
2	A	555	FAD	C4X-C10-N1	-2.33	119.33	124.73
2	A	555	FAD	O2-C2-N1	-2.32	117.98	121.83
4	B	600	ADP	C4-C5-N7	-2.32	106.98	109.40
2	B	555	FAD	C4X-C4-N3	2.31	119.06	113.19
3	B	556	COA	P2A-O3A-P1A	-2.29	124.97	132.83
2	A	555	FAD	C4X-C4-N3	2.27	118.96	113.19
3	B	556	COA	CDP-CBP-CAP	2.26	112.75	108.82
2	B	555	FAD	C10-C4X-N5	-2.26	120.06	124.86
2	B	555	FAD	O4-C4-C4X	-2.24	120.65	126.60
2	B	555	FAD	C5X-N5-C4X	2.20	121.73	118.07
3	A	556	COA	O3B-C3B-C4B	-2.19	102.18	110.08
2	B	555	FAD	O2-C2-N1	-2.18	118.21	121.83
3	A	556	COA	CDP-CBP-CAP	2.15	112.55	108.82
2	A	555	FAD	C5X-N5-C4X	2.08	121.54	118.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	556	COA	O2A-P1A-O1A	2.06	122.43	112.24
3	A	556	COA	O5A-P2A-O4A	2.03	122.26	112.24
2	B	555	FAD	C10-N1-C2	2.02	120.95	116.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

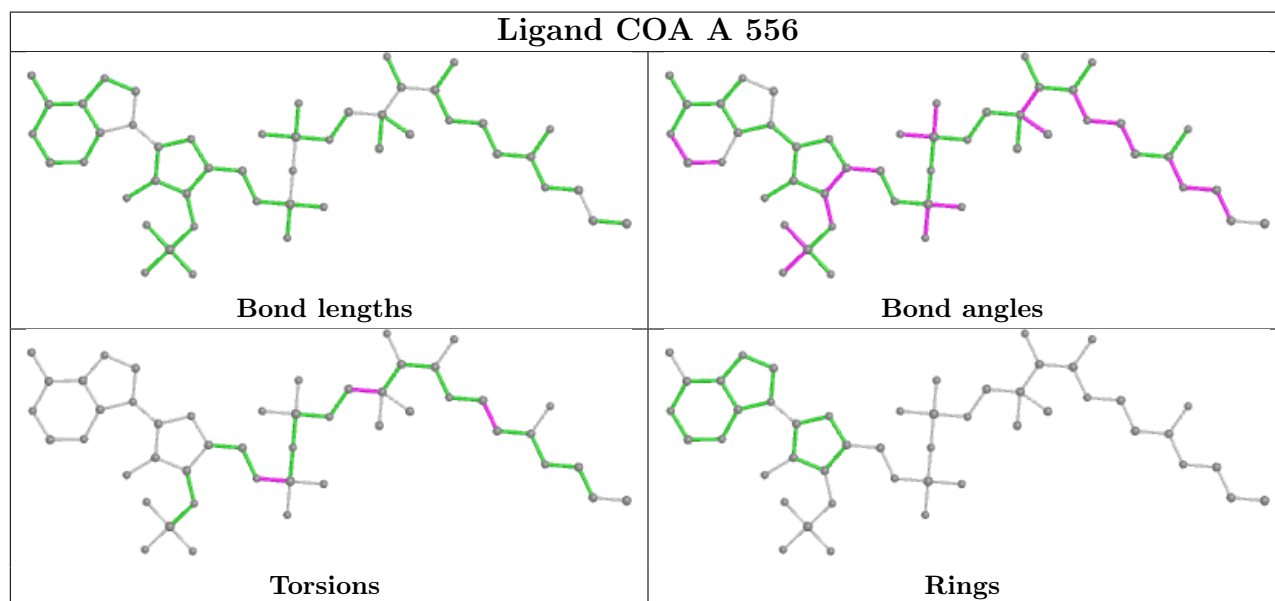
Mol	Chain	Res	Type	Atoms
3	A	556	COA	C5B-O5B-P1A-O1A
3	A	556	COA	C5B-O5B-P1A-O2A
3	A	556	COA	CAP-CBP-CCP-O6A
3	B	556	COA	C5B-O5B-P1A-O2A
3	B	556	COA	CCP-O6A-P2A-O5A
3	B	556	COA	O9P-C9P-CAP-OAP
3	B	556	COA	N8P-C9P-CAP-OAP
3	B	556	COA	C5P-C6P-C7P-N8P
2	A	555	FAD	O4B-C4B-C5B-O5B
2	B	555	FAD	O4B-C4B-C5B-O5B
4	B	600	ADP	O4'-C4'-C5'-O5'
2	A	555	FAD	C3B-C4B-C5B-O5B
2	B	555	FAD	C3B-C4B-C5B-O5B
4	B	600	ADP	C3'-C4'-C5'-O5'
3	A	556	COA	CDP-CBP-CCP-O6A
3	A	556	COA	CEP-CBP-CCP-O6A
3	B	556	COA	CCP-O6A-P2A-O3A
3	B	556	COA	CCP-O6A-P2A-O4A
3	B	556	COA	S1P-C2P-C3P-N4P
3	A	556	COA	C5P-C6P-C7P-N8P
3	A	556	COA	C5B-O5B-P1A-O3A
3	B	556	COA	C3B-O3B-P3B-O9A
2	B	555	FAD	P-O3P-PA-O2A
3	B	556	COA	O4B-C4B-C5B-O5B

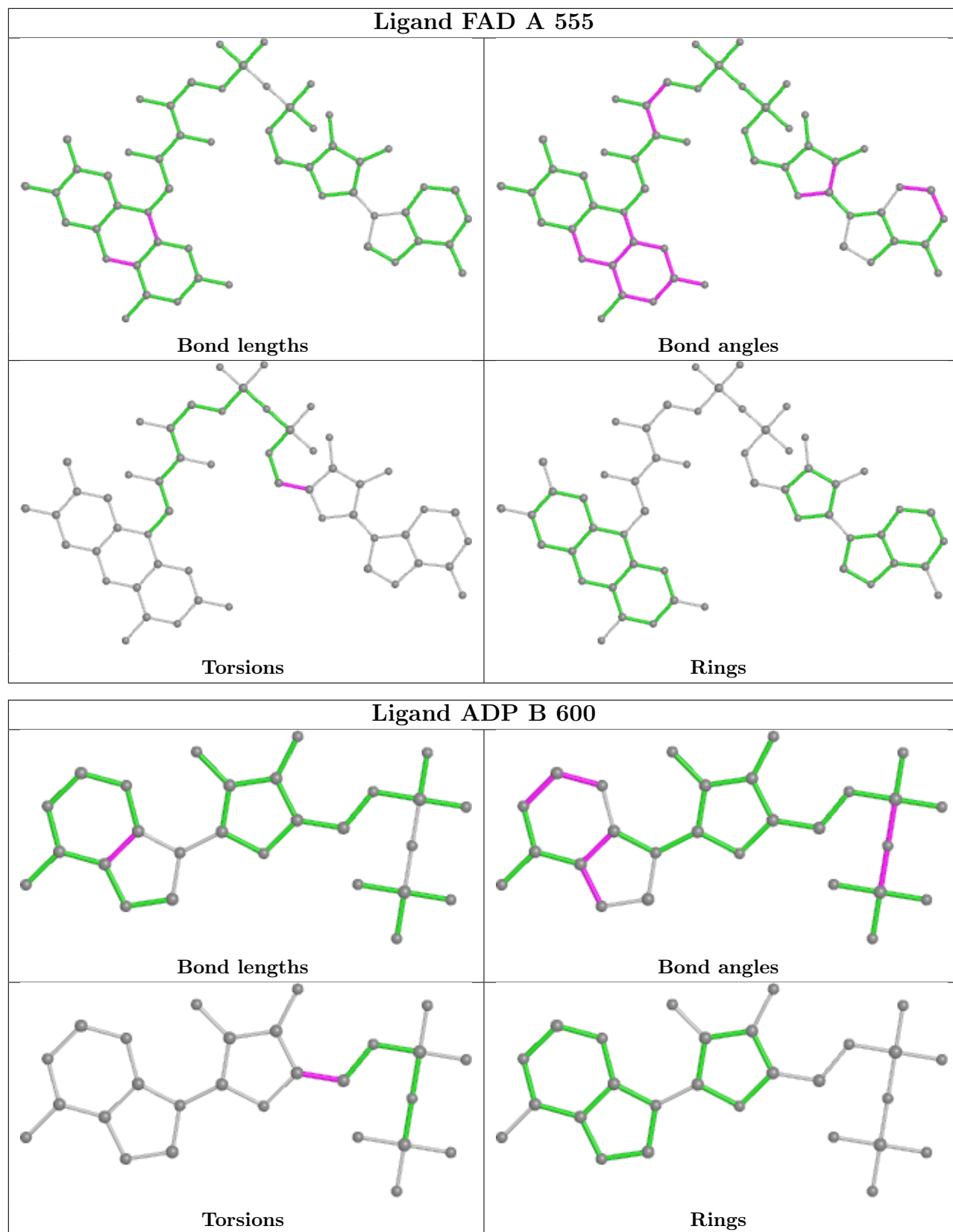
There are no ring outliers.

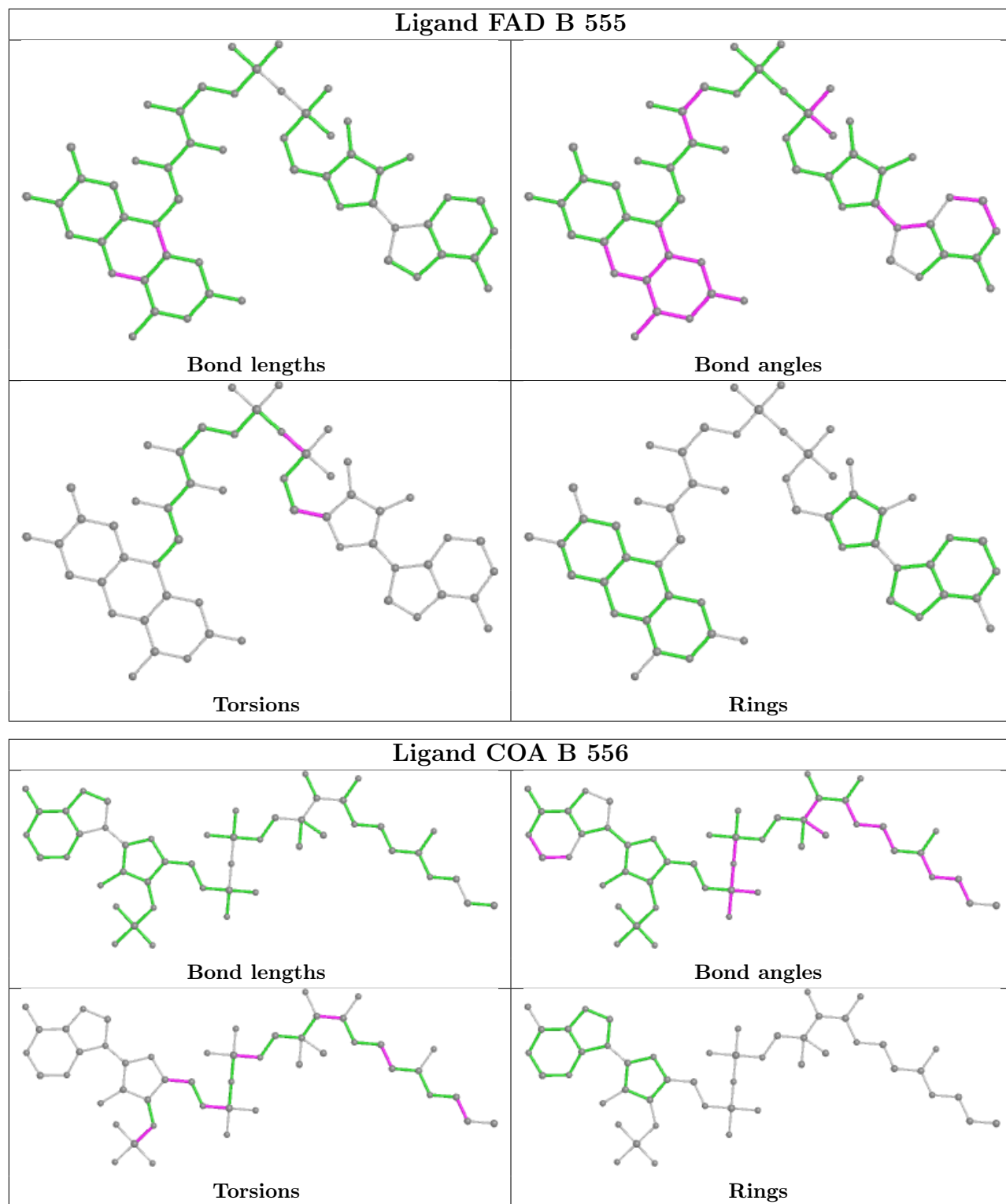
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	COA	6	0
2	B	555	FAD	1	0
3	B	556	COA	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

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	541/588 (92%)	0.54	39 (7%) 15 19	30, 46, 63, 71	0
1	B	537/588 (91%)	0.40	20 (3%) 41 48	28, 45, 64, 74	0
All	All	1078/1176 (91%)	0.47	59 (5%) 25 31	28, 45, 63, 74	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	VAL	4.3
1	A	320	THR	4.2
1	A	218	ASP	4.1
1	A	499	ASP	3.7
1	A	130	LYS	3.6
1	A	427	SER	3.6
1	A	222	GLU	3.5
1	B	101	GLU	3.4
1	A	-2	ASP	3.4
1	A	128	GLU	3.4
1	B	128	GLU	3.4
1	A	62	VAL	3.3
1	A	401	VAL	3.3
1	B	320	THR	3.0
1	A	150	GLU	3.0
1	B	130	LYS	3.0
1	A	149	ASP	2.9
1	B	3	ARG	2.9
1	B	317	HIS	2.9
1	A	0	TRP	2.8
1	A	439	VAL	2.8
1	A	406	ASP	2.8
1	A	332	VAL	2.7
1	A	438	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	215	ASP	2.6
1	B	314	ASP	2.6
1	B	98	THR	2.6
1	A	-1	ARG	2.6
1	A	507	ASP	2.6
1	A	495	ASP	2.5
1	A	397	GLY	2.5
1	A	426	LEU	2.5
1	A	341	ALA	2.5
1	A	210	GLU	2.5
1	A	554	TYR	2.5
1	B	319	HIS	2.4
1	B	129	ALA	2.4
1	A	290	ASP	2.4
1	A	501	LEU	2.3
1	B	401	VAL	2.3
1	A	321	ASP	2.3
1	B	406	ASP	2.3
1	A	330	THR	2.2
1	A	338	LEU	2.2
1	B	407	VAL	2.2
1	B	423	ASP	2.2
1	A	407	VAL	2.2
1	A	464	ARG	2.2
1	A	479	ASN	2.1
1	B	37	GLU	2.1
1	B	123	ILE	2.1
1	A	340	VAL	2.1
1	A	358	GLU	2.1
1	A	396	LEU	2.0
1	B	218	ASP	2.0
1	B	451	ASP	2.0
1	A	339	THR	2.0
1	A	462	ILE	2.0
1	B	426	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

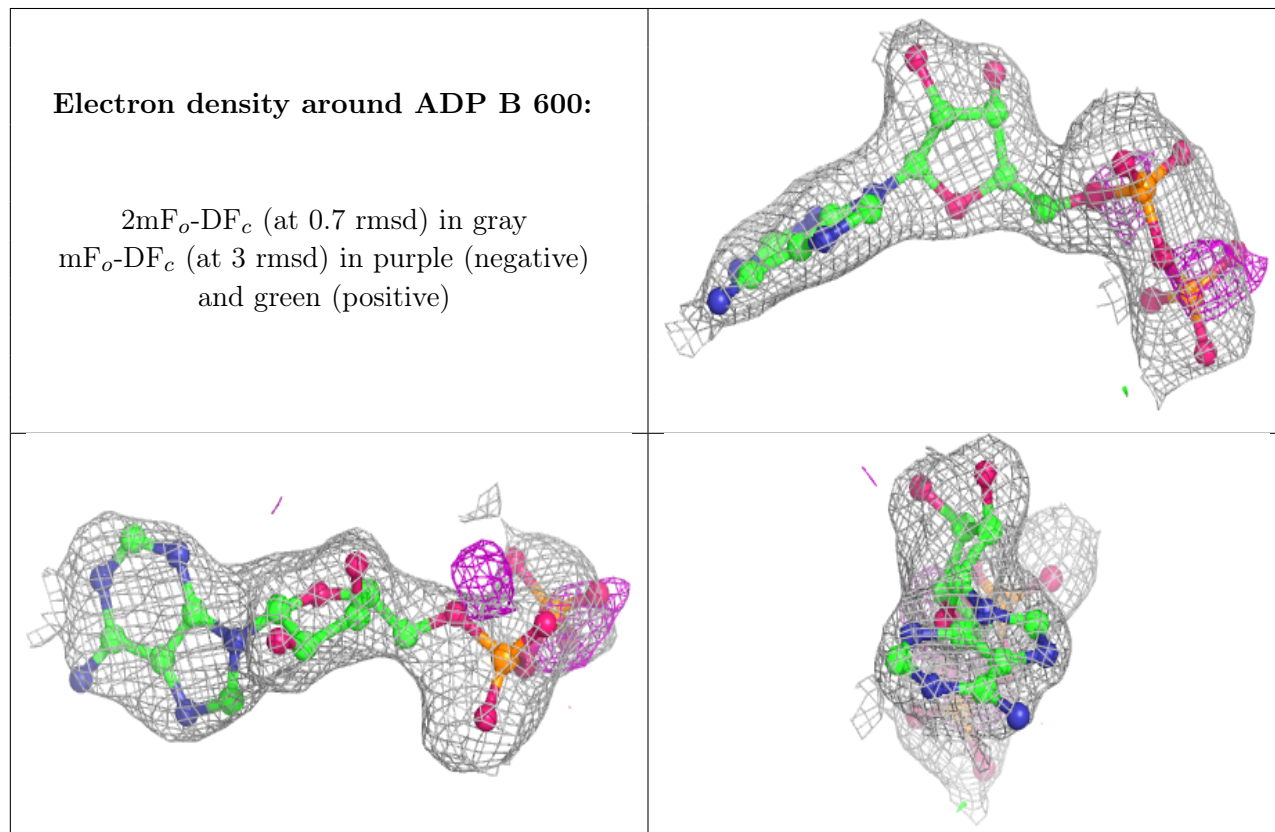
There are no monosaccharides in this entry.

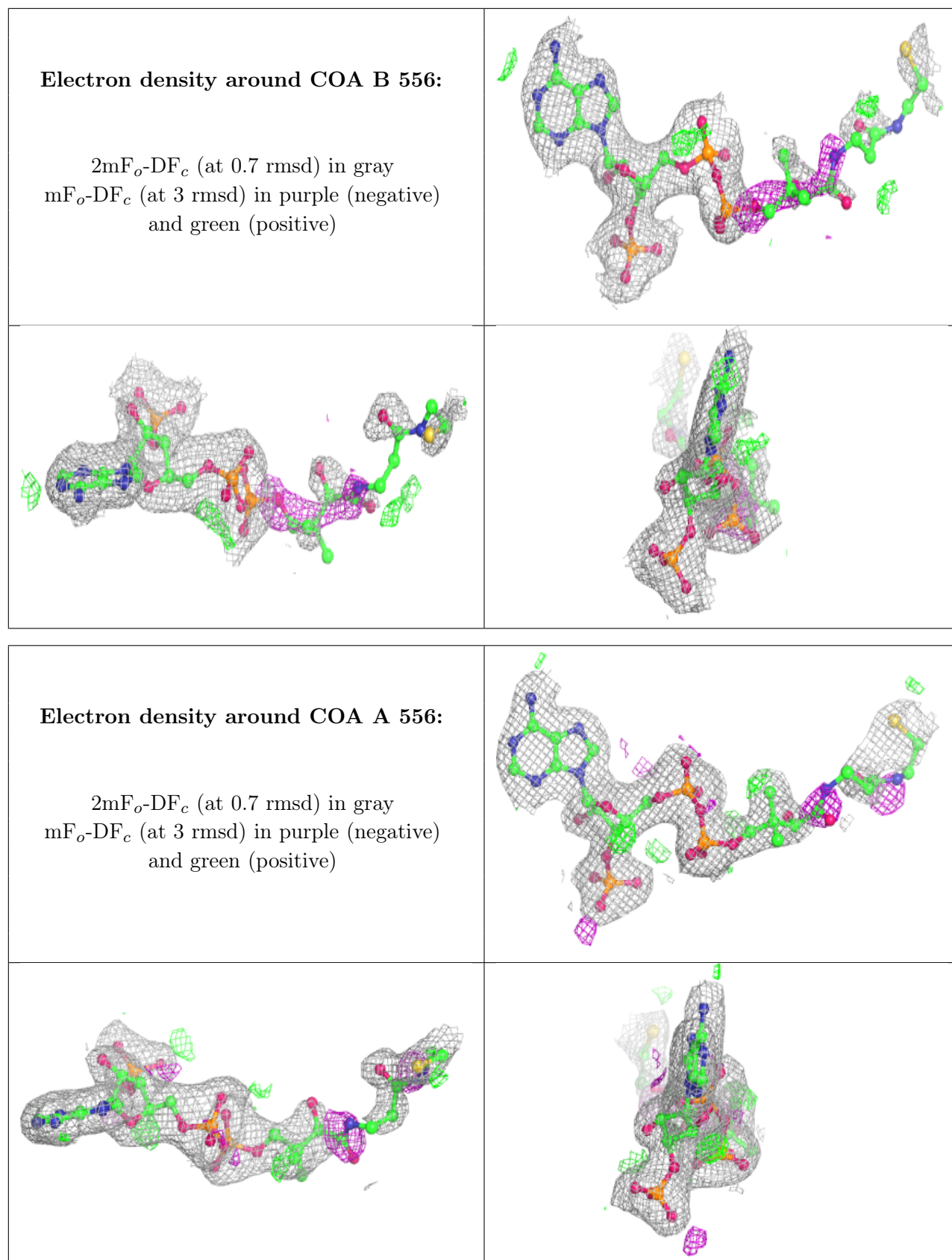
6.4 Ligands [i](#)

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
4	ADP	B	600	27/27	0.91	0.22	68,69,79,79	0
3	COA	B	556	48/48	0.93	0.19	39,64,97,101	0
3	COA	A	556	48/48	0.95	0.13	32,53,81,82	0
2	FAD	B	555	53/53	0.97	0.09	36,40,45,48	0
2	FAD	A	555	53/53	0.97	0.09	32,40,44,47	0

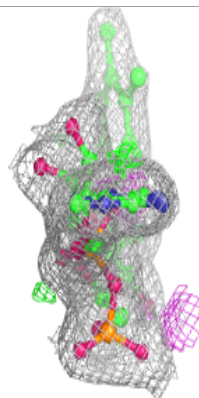
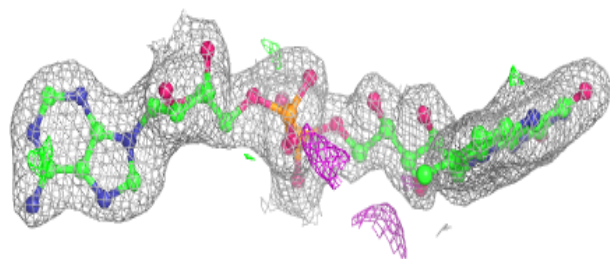
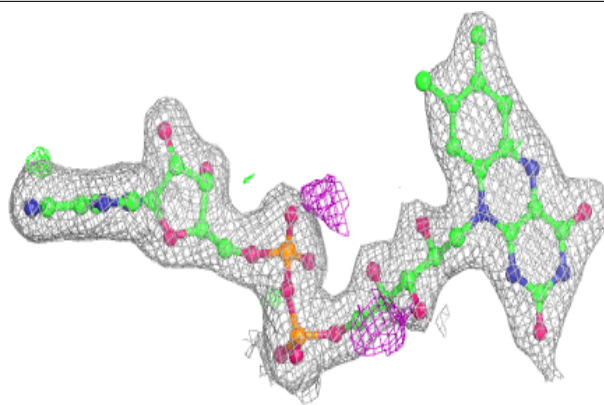
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



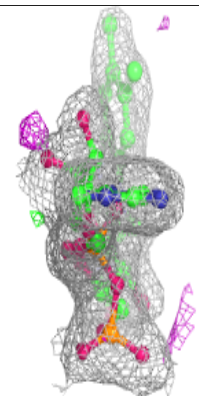
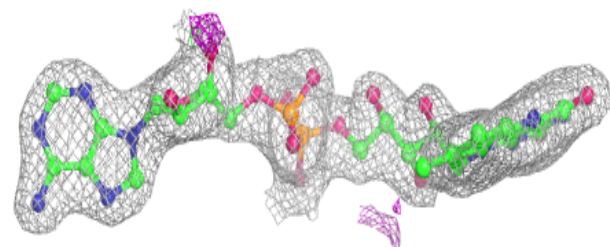
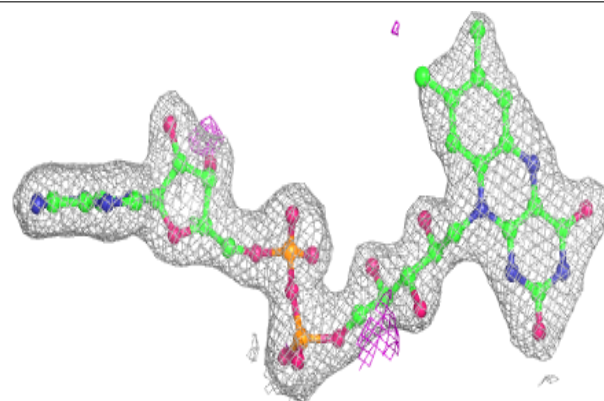


Electron density around FAD B 555:

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

**Electron density around FAD A 555:**

$2mF_o-DF_c$ (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.