Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2023 – 06:08 pm BST

PDB ID	:	8CP2
Title	:	Structure of Aspartate-N-hydroxylase (FzmM)from Streptomyces sp. V2: complex with NADPH and L-aspartate
Authors	:	Rotilio, L.; Mattevi, A.
Deposited on	:	2023-03-01
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:

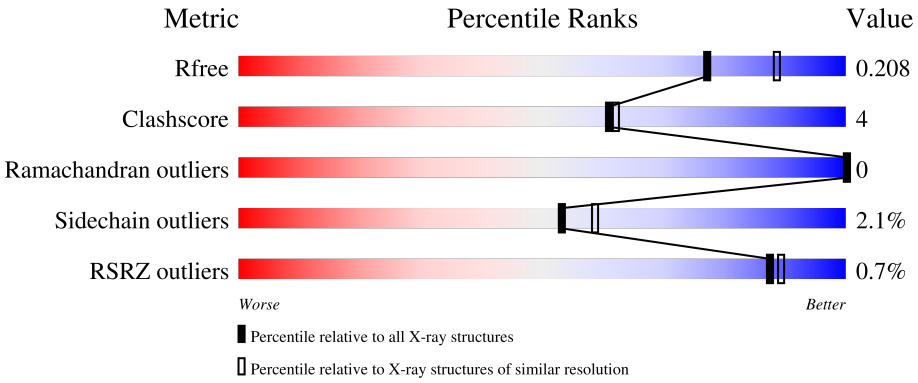
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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 <=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	601	92% 7%
1	B	601	% 90% 9%

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
6	PEG	A	706	-	-	X	-
6	PEG	A	707	-	-	X	-

2 Entry composition

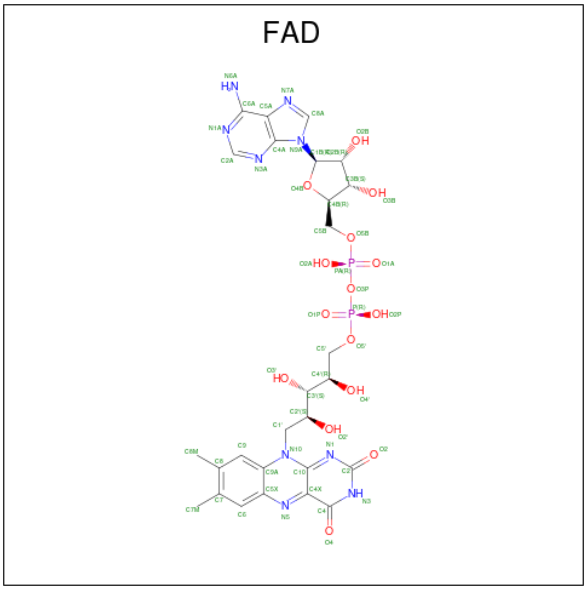
There are 8 unique types of molecules in this entry. The entry contains 10375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FAD-binding protein.

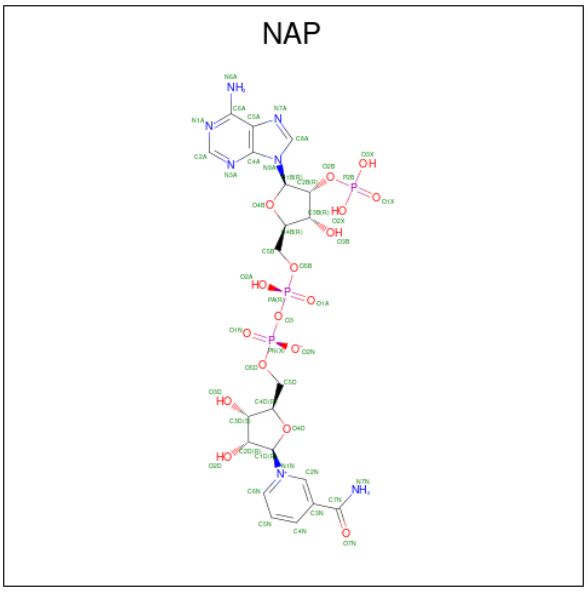
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	1	0
			4648	2915	879	849	5			
1	B	600	Total	C	N	O	S	0	1	0
			4646	2915	876	849	6			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



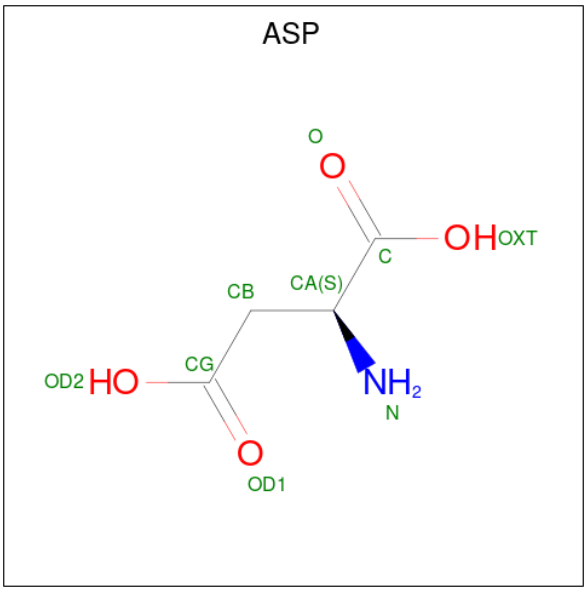
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	4	1	4		

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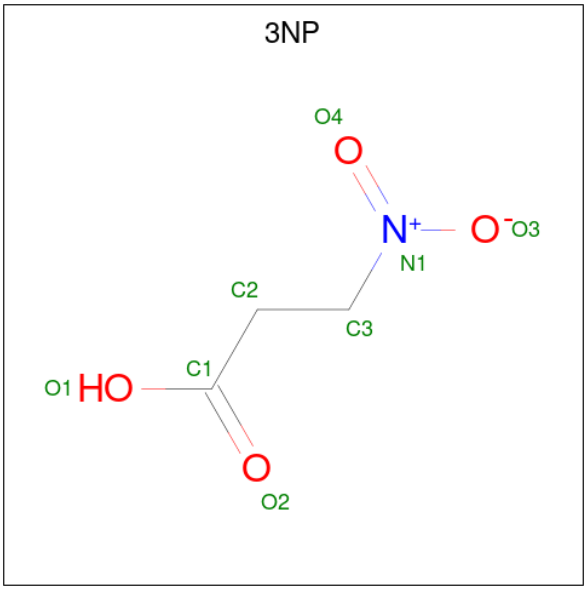
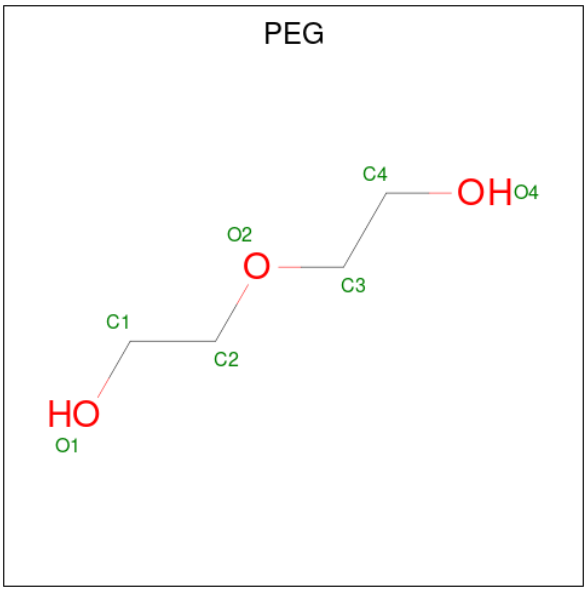
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	4	1	4		
4	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 5 is 3-NITROPROPANOIC ACID (three-letter code: 3NP) (formula: $C_3H_5NO_4$).



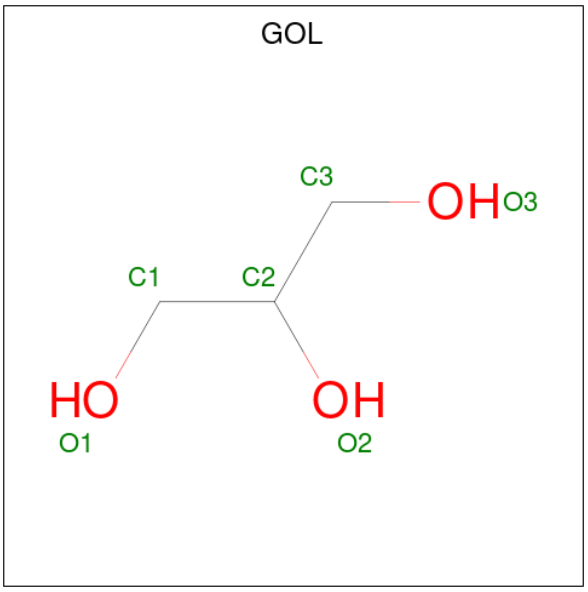
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	3	1	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

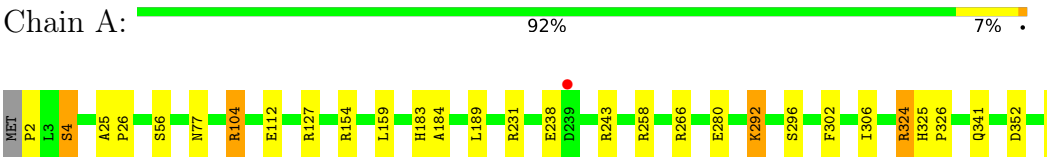
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	497	Total O 497 497	0	0
8	B	299	Total O 299 299	0	0

3 Residue-property plots (i)

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.

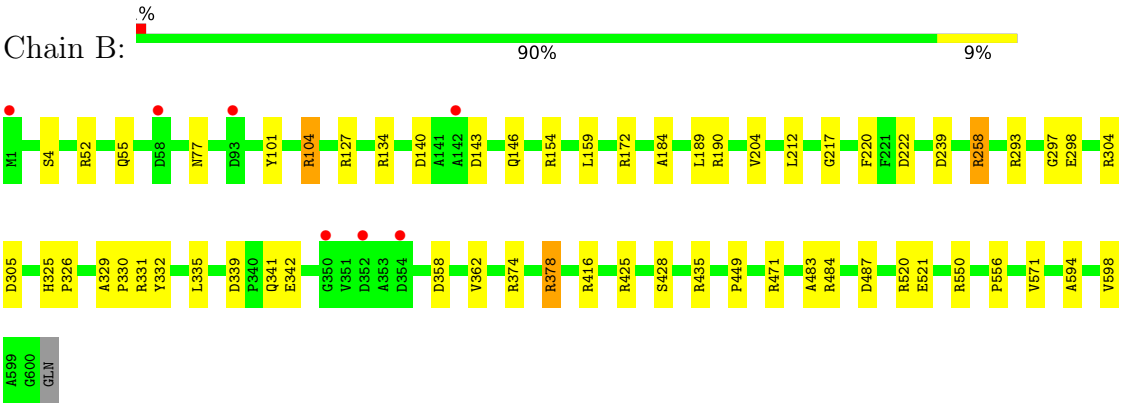
• Molecule 1: FAD-binding protein

Chain A:



• Molecule 1: FAD-binding protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	244.59Å 244.59Å 128.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.30 – 2.10 122.30 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (122.30-2.10) 100.0 (122.30-2.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.179 , 0.202 0.189 , 0.208	Depositor DCC
R_{free} test set	8267 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10375	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 3NP, FAD, GOL, PEG, NAP

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	0.83	1/4768 (0.0%)	1.06	14/6513 (0.2%)
1	B	0.79	0/4763	0.98	9/6508 (0.1%)
All	All	0.81	1/9531 (0.0%)	1.02	23/13021 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	ARG	CD-NE	-5.28	1.37	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	ARG	NE-CZ-NH2	-14.29	113.15	120.30
1	A	412	ARG	NE-CZ-NH2	-13.61	113.50	120.30
1	A	104	ARG	NE-CZ-NH1	11.93	126.26	120.30
1	A	597	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	B	104	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	104	ARG	CG-CD-NE	-7.98	95.05	111.80
1	A	597	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	266	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	231	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	258	ARG	CB-CG-CD	6.35	128.11	111.60
1	B	104	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	374	ARG	CB-CA-C	-6.16	98.08	110.40
1	B	378	ARG	CG-CD-NE	-5.88	99.44	111.80
1	A	412	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	374	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	412	ARG	CG-CD-NE	-5.66	99.91	111.80
1	A	371	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	A	371	PHE	CB-CG-CD2	5.53	124.67	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	429	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	B	52	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	521	GLU	CB-CA-C	-5.41	99.57	110.40
1	B	258	ARG	CG-CD-NE	5.38	123.10	111.80
1	B	520	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	4648	0	4594	29	0
1	B	4646	0	4592	47	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	48	0	25	1	0
3	B	48	0	25	0	0
4	A	18	0	6	4	0
4	B	9	0	3	1	0
5	A	8	0	4	0	0
6	A	21	0	30	6	0
6	B	21	0	30	0	0
7	A	6	0	8	0	0
8	A	497	0	0	18	0
8	B	299	0	0	19	0
All	All	10375	0	9379	85	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 4.

All (85) 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:364:ARG:CD	8:A:801:HOH:O	2.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ARG:HD2	8:B:972:HOH:O	1.64	0.97
1:B:358:ASP:O	1:B:362:VAL:HG23	1.75	0.87
1:B:77:ASN:HB2	8:B:863:HOH:O	1.78	0.82
1:A:364:ARG:CG	8:A:801:HOH:O	2.30	0.80
4:A:704:ASP:HA	8:A:1169:HOH:O	1.89	0.71
1:A:364:ARG:NE	8:A:801:HOH:O	2.21	0.71
1:A:379:GLN:HG2	8:A:1267:HOH:O	1.92	0.70
1:B:521:GLU:HG2	8:B:1005:HOH:O	1.93	0.68
1:B:154:ARG:HD3	8:B:988:HOH:O	1.95	0.67
1:B:594:ALA:O	1:B:598[A]:VAL:HG23	1.95	0.67
1:B:484:ARG:HD2	8:B:1069:HOH:O	1.95	0.66
1:B:416:ARG:HH12	4:B:703:ASP:HA	1.64	0.62
1:B:521:GLU:CG	8:B:1005:HOH:O	2.48	0.61
1:B:329:ALA:HB3	1:B:330:PRO:HD3	1.81	0.60
1:A:378:ARG:NH1	1:A:460:LEU:O	2.34	0.60
1:B:331:ARG:O	1:B:335:LEU:CD1	2.49	0.60
6:A:706:PEG:H12	6:A:707:PEG:C4	2.32	0.58
1:B:598[A]:VAL:HG22	8:B:889:HOH:O	2.03	0.57
1:B:104:ARG:HH22	1:B:222:ASP:CG	2.10	0.55
1:B:339:ASP:OD2	1:B:341:GLN:HB2	2.07	0.54
1:A:4:SER:HB3	1:A:159:LEU:HD23	1.88	0.54
1:A:503:LEU:HD11	2:A:701:FAD:HM83	1.90	0.54
1:A:494:ARG:HD2	8:A:985:HOH:O	2.07	0.54
6:A:706:PEG:C1	6:A:707:PEG:H42	2.37	0.54
1:B:258:ARG:HB3	8:B:1075:HOH:O	2.07	0.54
1:B:143:ASP:N	8:B:805:HOH:O	2.39	0.54
1:A:416:ARG:HH12	4:A:703:ASP:HA	1.74	0.53
1:A:364:ARG:HD2	8:A:801:HOH:O	1.95	0.53
1:B:101:TYR:CE2	1:B:449:PRO:HB3	2.44	0.52
1:B:297:GLY:HA2	8:B:811:HOH:O	2.09	0.52
1:B:332:TYR:CE1	1:B:342:GLU:HG2	2.44	0.52
6:A:706:PEG:H12	6:A:707:PEG:H42	1.93	0.51
1:A:258[A]:ARG:HG2	8:A:933:HOH:O	2.11	0.51
1:B:4:SER:HB3	1:B:159:LEU:HD23	1.93	0.51
1:B:425:ARG:HD2	8:B:1073:HOH:O	2.11	0.51
6:A:706:PEG:C1	6:A:707:PEG:C4	2.89	0.50
1:B:335:LEU:HD12	1:B:335:LEU:N	2.25	0.50
1:A:2:PRO:HB2	8:A:1034:HOH:O	2.11	0.50
1:B:598[B]:VAL:CG1	8:B:831:HOH:O	2.58	0.50
1:A:368:GLN:HA	8:A:1208:HOH:O	2.12	0.49
1:B:425:ARG:HH12	1:B:428:SER:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:HB2	8:A:1207:HOH:O	2.14	0.48
3:A:702:NAP:N3A	8:A:804:HOH:O	2.35	0.48
1:B:471:ARG:NH1	1:B:487:ASP:OD1	2.48	0.47
1:B:304:ARG:HG2	1:B:304:ARG:HH11	1.80	0.47
1:A:154:ARG:HD3	8:A:1147:HOH:O	2.14	0.46
1:B:293:ARG:HB3	1:B:298:GLU:O	2.15	0.46
1:A:184:ALA:HA	1:A:189:LEU:HB2	1.96	0.46
1:A:324:ARG:NH2	8:A:826:HOH:O	2.49	0.46
1:B:184:ALA:HA	1:B:189:LEU:HB2	1.98	0.45
1:A:25:ALA:N	1:A:26:PRO:CD	2.79	0.45
1:A:520:ARG:NH2	8:A:825:HOH:O	2.49	0.45
1:B:598[B]:VAL:HG11	8:B:831:HOH:O	2.15	0.45
1:B:217:GLY:O	1:B:220:PHE:HB3	2.17	0.45
1:B:297:GLY:N	8:B:811:HOH:O	2.44	0.45
1:A:484:ARG:HD2	8:A:1199:HOH:O	2.16	0.44
1:B:297:GLY:CA	8:B:811:HOH:O	2.64	0.44
1:A:510:GLN:OE1	1:A:510:GLN:HA	2.18	0.44
1:B:331:ARG:O	1:B:335:LEU:HD13	2.17	0.44
1:B:140:ASP:OD1	1:B:146:GLN:NE2	2.51	0.44
1:A:302:PHE:HA	1:A:306:ILE:HD12	2.00	0.43
6:A:706:PEG:H22	6:A:706:PEG:H42	1.45	0.43
1:B:212:LEU:HD22	1:B:483:ALA:HB2	2.00	0.43
1:A:292:LYS:HD3	1:A:292:LYS:HA	1.65	0.43
6:A:706:PEG:H11	6:A:707:PEG:H42	1.99	0.43
1:A:597:ARG:HH22	4:A:704:ASP:C	2.22	0.43
1:B:325:HIS:ND1	1:B:326:PRO:HD2	2.33	0.43
1:B:425:ARG:NH1	1:B:428:SER:HB2	2.34	0.43
1:A:183:HIS:HB2	1:A:476:ARG:HD3	2.01	0.42
1:B:304:ARG:NH1	1:B:305:ASP:OD1	2.52	0.42
1:B:258:ARG:HG2	8:B:891:HOH:O	2.19	0.42
1:B:571:VAL:HG12	1:B:571:VAL:O	2.19	0.42
4:A:704:ASP:HB3	8:A:1211:HOH:O	2.20	0.42
1:B:435:ARG:HD2	8:B:1044:HOH:O	2.19	0.42
1:B:104:ARG:HD2	8:B:917:HOH:O	2.19	0.42
1:B:556:PRO:O	1:B:598[B]:VAL:HG11	2.19	0.42
1:A:325:HIS:HA	1:A:326:PRO:HD3	1.96	0.41
1:B:77:ASN:CB	8:B:863:HOH:O	2.54	0.41
1:B:550:ARG:O	1:B:550:ARG:HD2	2.21	0.41
1:A:104:ARG:HD2	8:A:843:HOH:O	2.20	0.41
1:A:543:ARG:HH11	1:A:543:ARG:HD2	1.76	0.40
1:B:190:ARG:HD2	1:B:204:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ARG:CZ	1:B:425:ARG:HB2	2.50	0.40
1:A:238:GLU:OE1	1:A:243:ARG:NH1	2.54	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	599/601 (100%)	584 (98%)	15 (2%)	0	100	100
1	B	599/601 (100%)	573 (96%)	26 (4%)	0	100	100
All	All	1198/1202 (100%)	1157 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	476/476 (100%)	463 (97%)	13 (3%)	44	48
1	B	476/476 (100%)	471 (99%)	5 (1%)	73	79
All	All	952/952 (100%)	934 (98%)	18 (2%)	53	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	56	SER
1	A	112	GLU
1	A	127	ARG
1	A	280	GLU
1	A	292	LYS
1	A	296	SER
1	A	324	ARG
1	A	341	GLN
1	A	352	ASP
1	A	362	VAL
1	A	364	ARG
1	A	370	GLU
1	B	55	GLN
1	B	127	ARG
1	B	134	ARG
1	B	172	ARG
1	B	239	ASP

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

Mol	Chain	Res	Type
1	B	62	ASN

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 (i)

15 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	$\#\|Z\| > 2$
4	ASP	B	703	-	6,8,8	1.06	1 (16%)	8,10,10	1.49	2 (25%)
4	ASP	A	703	-	6,8,8	1.37	1 (16%)	8,10,10	1.50	2 (25%)
2	FAD	B	701	-	53,58,58	0.64	0	68,89,89	0.92	5 (7%)
6	PEG	B	704	-	6,6,6	0.27	0	5,5,5	0.18	0
2	FAD	A	701	-	53,58,58	0.71	0	68,89,89	1.01	6 (8%)
3	NAP	B	702	-	45,52,52	0.77	2 (4%)	56,80,80	1.81	7 (12%)
3	NAP	A	702	-	45,52,52	0.79	0	56,80,80	1.73	7 (12%)
5	3NP	A	705	-	5,7,7	1.12	1 (20%)	4,8,8	0.94	0
7	GOL	A	709	-	5,5,5	0.19	0	5,5,5	0.81	0
6	PEG	B	706	-	6,6,6	0.24	0	5,5,5	0.21	0
6	PEG	A	708	-	6,6,6	0.27	0	5,5,5	0.21	0
4	ASP	A	704	-	6,8,8	1.02	0	8,10,10	2.48	2 (25%)
6	PEG	A	707	-	6,6,6	0.15	0	5,5,5	0.22	0
6	PEG	A	706	-	6,6,6	0.31	0	5,5,5	0.43	0
6	PEG	B	705	-	6,6,6	0.19	0	5,5,5	0.15	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
4	ASP	B	703	-	-	7/8/8/8	-
4	ASP	A	703	-	-	7/8/8/8	-
2	FAD	B	701	-	-	4/30/50/50	0/6/6/6
6	PEG	B	704	-	-	2/4/4/4	-
2	FAD	A	701	-	-	3/30/50/50	0/6/6/6
3	NAP	B	702	-	-	7/31/67/67	0/5/5/5
3	NAP	A	702	-	-	5/31/67/67	0/5/5/5
5	3NP	A	705	-	-	1/4/5/5	-
7	GOL	A	709	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	B	706	-	-	1/4/4/4	-
6	PEG	A	708	-	-	2/4/4/4	-
4	ASP	A	704	-	-	8/8/8/8	-
6	PEG	A	707	-	-	2/4/4/4	-
6	PEG	A	706	-	-	3/4/4/4	-
6	PEG	B	705	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	ASP	OXT-C	-2.59	1.22	1.30
3	B	702	NAP	P2B-O2B	-2.32	1.54	1.59
5	A	705	3NP	O1-C1	-2.29	1.23	1.30
4	B	703	ASP	OXT-C	-2.13	1.23	1.30
3	B	702	NAP	P2B-O2X	-2.09	1.46	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	NAP	O2X-P2B-O2B	6.83	136.61	105.99
3	A	702	NAP	O2B-P2B-O1X	-6.44	84.53	109.39
3	B	702	NAP	O3X-P2B-O2B	-5.98	79.21	105.99
3	B	702	NAP	O2B-C2B-C3B	-5.15	93.02	111.68
3	A	702	NAP	O2X-P2B-O2B	5.08	128.76	105.99
4	A	704	ASP	O-C-CA	-4.92	104.80	122.14
4	A	704	ASP	OXT-C-CA	4.60	129.04	113.38
3	A	702	NAP	O2B-C2B-C3B	-4.59	95.04	111.68
3	A	702	NAP	C6N-N1N-C2N	-3.77	118.54	121.97
3	A	702	NAP	O2B-C2B-C1B	3.31	122.03	110.10
3	B	702	NAP	C6N-N1N-C2N	-3.31	118.96	121.97
3	B	702	NAP	O2B-C2B-C1B	3.18	121.53	110.10
3	B	702	NAP	O2B-P2B-O1X	-3.03	97.69	109.39
2	A	701	FAD	O2'-C2'-C1'	-2.78	103.07	109.80
2	B	701	FAD	O4B-C1B-C2B	-2.48	103.30	106.93
2	A	701	FAD	O2A-PA-O1A	2.47	124.44	112.24
3	A	702	NAP	O2N-PN-O1N	2.44	124.31	112.24
2	B	701	FAD	O2P-P-O1P	2.39	124.06	112.24
3	B	702	NAP	O3X-P2B-O1X	2.39	120.04	110.68
2	A	701	FAD	O2P-P-O1P	2.38	123.99	112.24
4	B	703	ASP	OD1-CG-CB	-2.37	115.22	122.80
2	A	701	FAD	C4A-C5A-N7A	2.36	111.85	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	ASP	OXT-C-O	-2.30	118.87	124.09
2	B	701	FAD	O2A-PA-O1A	2.29	123.57	112.24
4	A	703	ASP	OD1-CG-CB	-2.28	115.50	122.80
2	A	701	FAD	O5'-C5'-C4'	-2.22	103.44	109.36
2	A	701	FAD	C4-N3-C2	-2.19	121.60	125.64
3	A	702	NAP	C4A-C5A-N7A	2.16	111.65	109.40
2	B	701	FAD	C5A-C6A-N6A	2.12	123.58	120.35
4	B	703	ASP	OXT-C-O	-2.08	119.38	124.09
2	B	701	FAD	O2'-C2'-C1'	-2.07	104.80	109.80

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	N10-C1'-C2'-C3'
2	B	701	FAD	N10-C1'-C2'-O2'
2	B	701	FAD	N10-C1'-C2'-C3'
3	A	702	NAP	C2D-C1D-N1N-C6N
4	A	703	ASP	O-C-CA-N
4	A	704	ASP	N-CA-CB-CG
4	B	703	ASP	O-C-CA-N
4	B	703	ASP	N-CA-CB-CG
5	A	705	3NP	C1-C2-C3-N1
7	A	709	GOL	O1-C1-C2-O2
7	A	709	GOL	O1-C1-C2-C3
6	A	706	PEG	C4-C3-O2-C2
3	B	702	NAP	O4B-C4B-C5B-O5B
4	A	703	ASP	CA-CB-CG-OD1
4	B	703	ASP	CA-CB-CG-OD1
6	A	706	PEG	O1-C1-C2-O2
4	B	703	ASP	OXT-C-CA-N
6	B	704	PEG	O1-C1-C2-O2
6	B	705	PEG	O2-C3-C4-O4
4	A	703	ASP	OXT-C-CA-N
4	A	704	ASP	OXT-C-CA-N
4	A	703	ASP	CA-CB-CG-OD2
3	B	702	NAP	C3B-C4B-C5B-O5B
4	A	704	ASP	OXT-C-CA-CB
6	A	706	PEG	O2-C3-C4-O4
6	A	707	PEG	O1-C1-C2-O2
4	A	704	ASP	C-CA-CB-CG
6	A	708	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	704	ASP	CA-CB-CG-OD1
4	A	704	ASP	O-C-CA-CB
3	A	702	NAP	C2N-C3N-C7N-O7N
4	A	704	ASP	CA-CB-CG-OD2
4	B	703	ASP	CA-CB-CG-OD2
4	A	704	ASP	O-C-CA-N
3	B	702	NAP	C2N-C3N-C7N-N7N
4	A	703	ASP	OXT-C-CA-CB
4	B	703	ASP	OXT-C-CA-CB
3	B	702	NAP	C2N-C3N-C7N-O7N
6	B	706	PEG	C4-C3-O2-C2
6	A	707	PEG	O2-C3-C4-O4
4	A	703	ASP	O-C-CA-CB
4	B	703	ASP	O-C-CA-CB
6	A	708	PEG	C1-C2-O2-C3
6	B	704	PEG	O2-C3-C4-O4
3	A	702	NAP	C4N-C3N-C7N-O7N
4	A	703	ASP	N-CA-CB-CG
6	B	705	PEG	C4-C3-O2-C2
2	A	701	FAD	O4B-C4B-C5B-O5B
3	A	702	NAP	C2N-C3N-C7N-N7N
3	B	702	NAP	C2B-O2B-P2B-O2X
3	B	702	NAP	C4N-C3N-C7N-N7N
2	B	701	FAD	O4B-C4B-C5B-O5B
3	A	702	NAP	O4B-C4B-C5B-O5B
3	B	702	NAP	C4N-C3N-C7N-O7N
2	A	701	FAD	N10-C1'-C2'-O2'
2	B	701	FAD	C2'-C1'-N10-C10

There are no ring outliers.

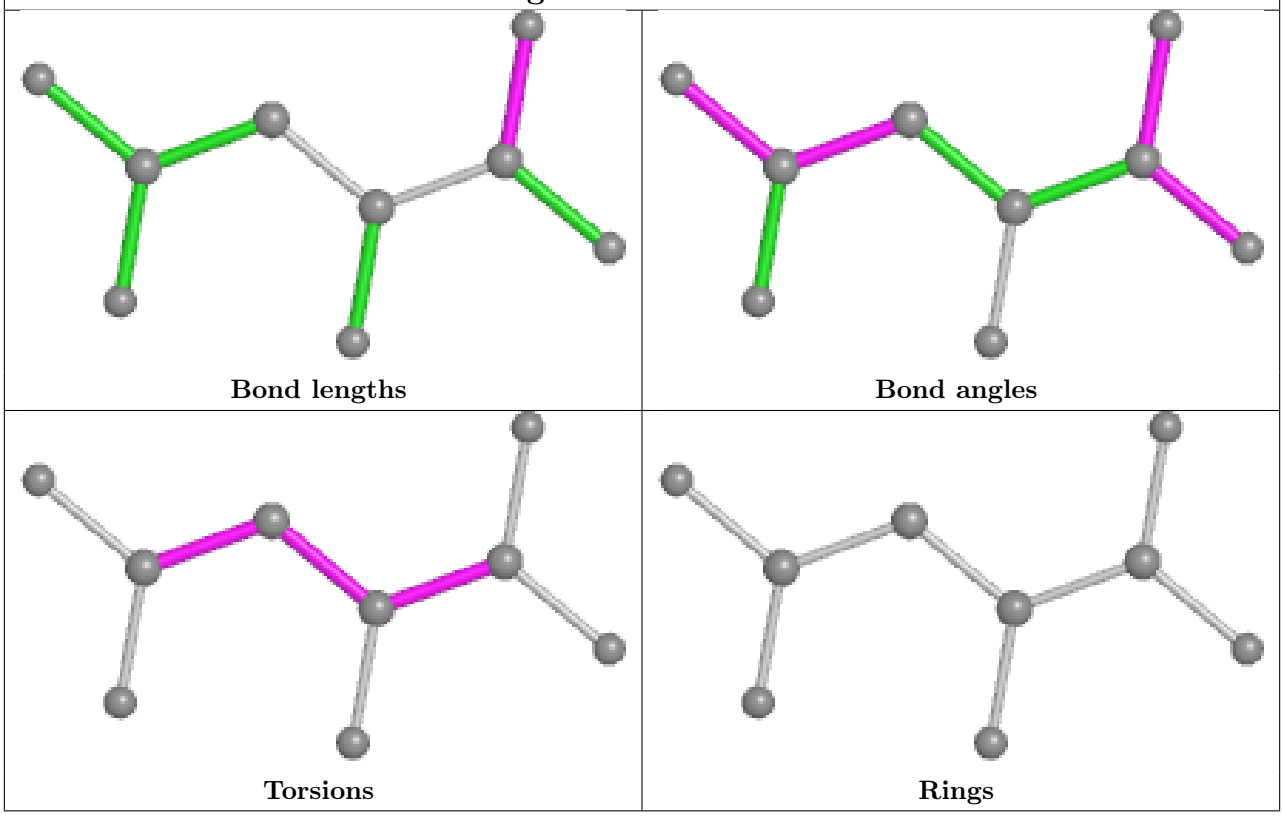
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	ASP	1	0
4	A	703	ASP	1	0
2	A	701	FAD	1	0
3	A	702	NAP	1	0
4	A	704	ASP	3	0
6	A	707	PEG	5	0
6	A	706	PEG	6	0

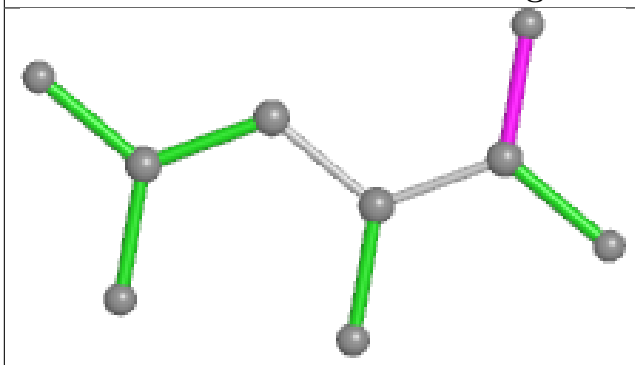
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

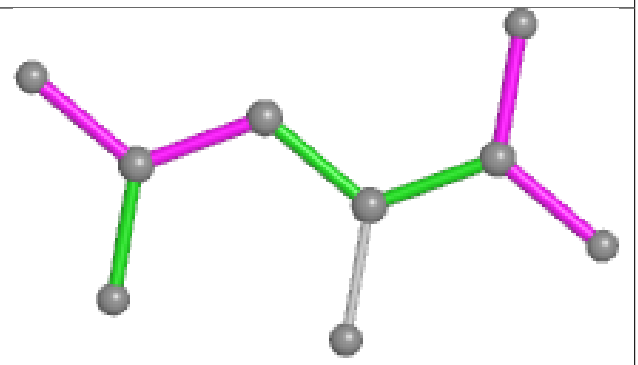
Ligand ASP B 703



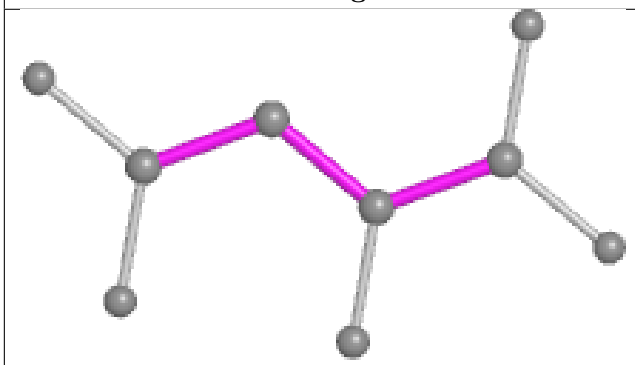
Ligand ASP A 703



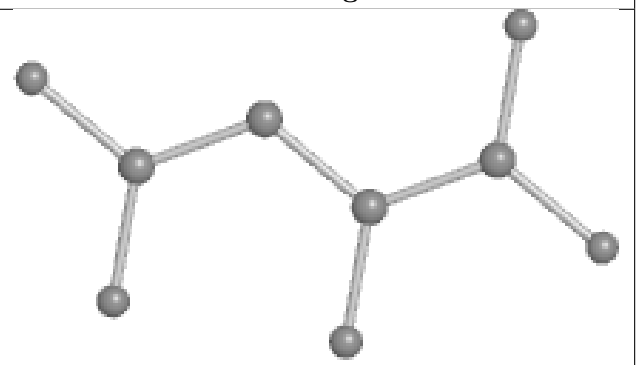
Bond lengths



Bond angles

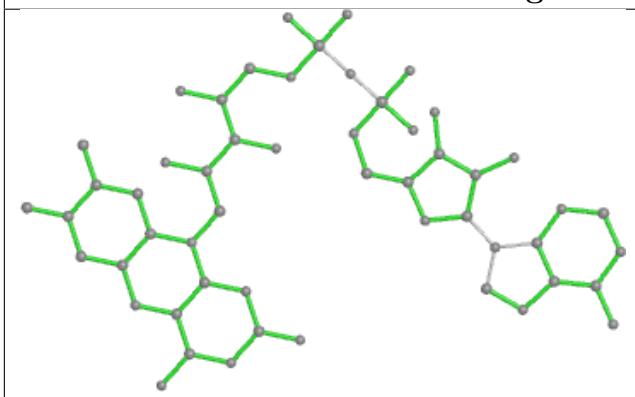


Torsions



Rings

Ligand FAD B 701



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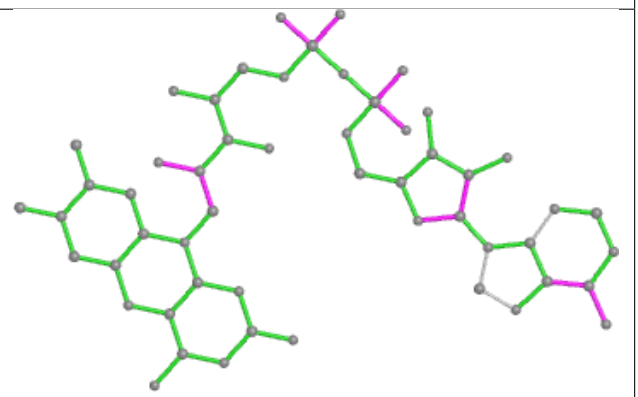
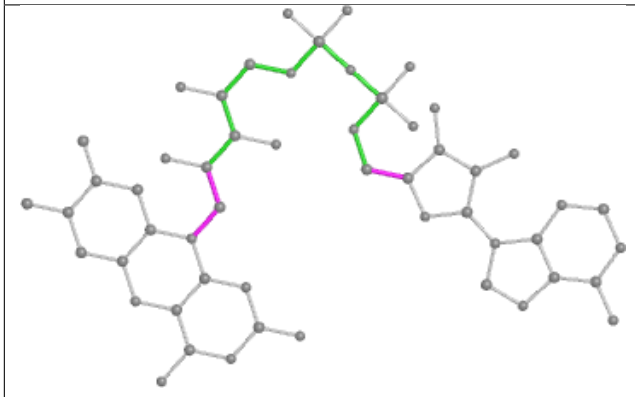


Bond angles



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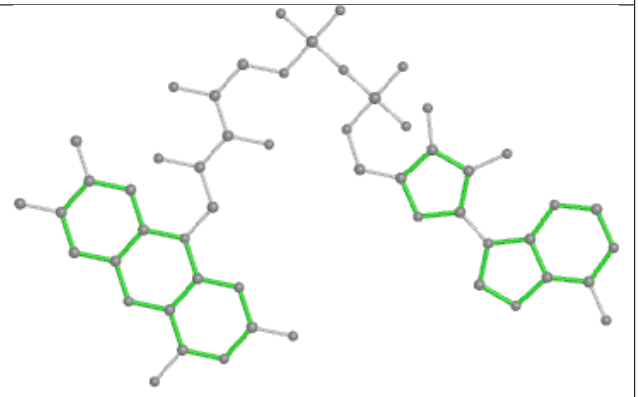

Rings

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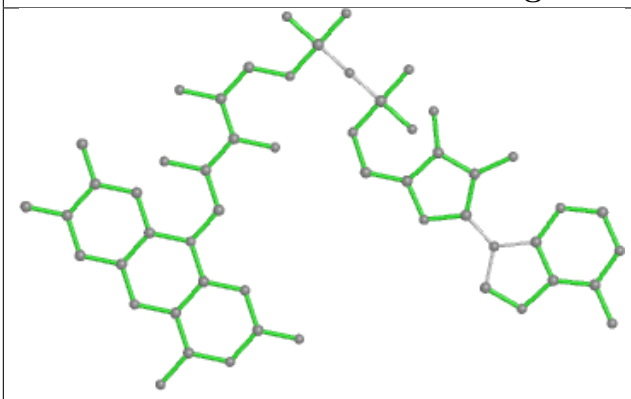

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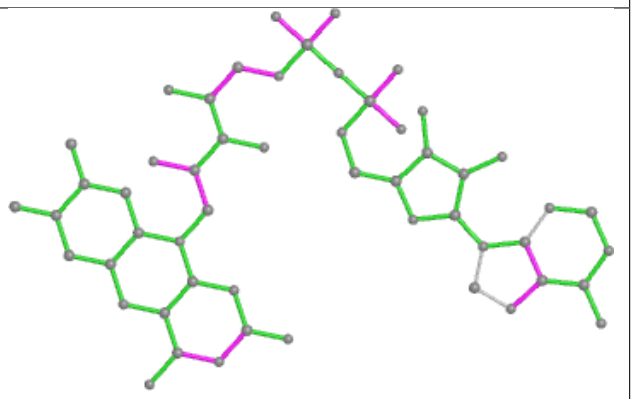
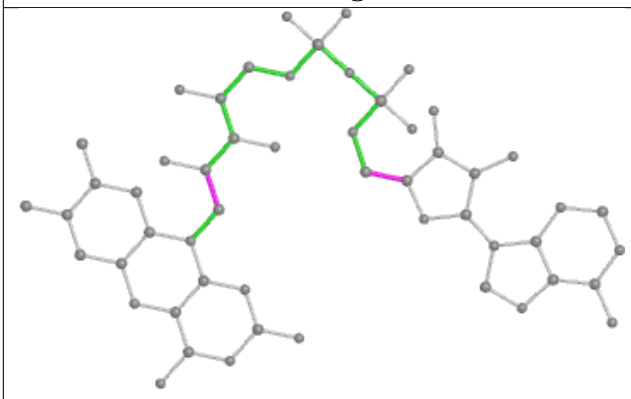


Bond angles



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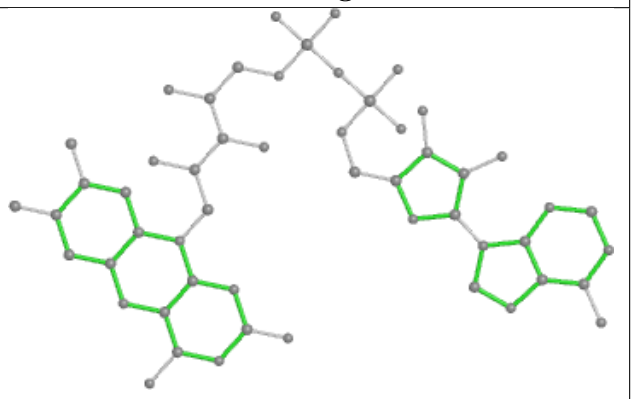
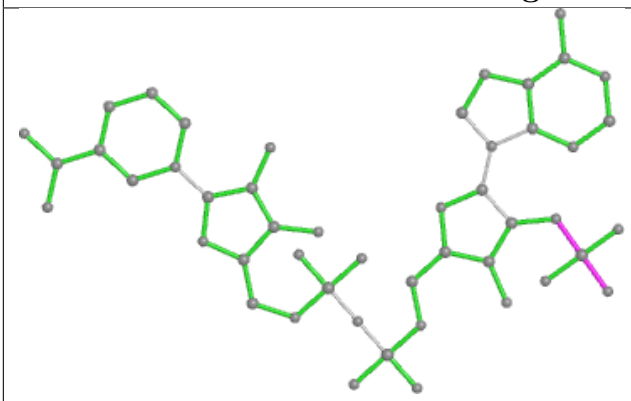


Rings

Ligand NAP B 702



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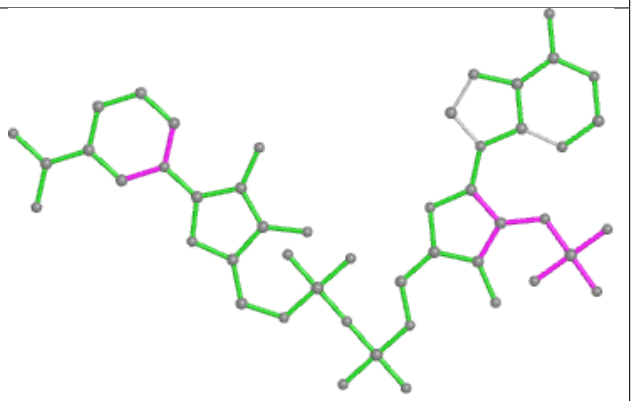
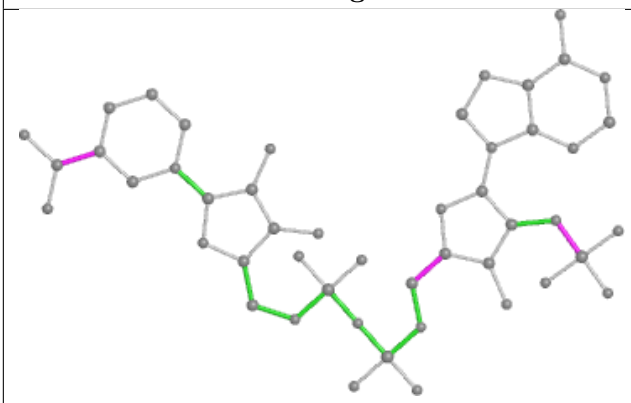


Bond angles



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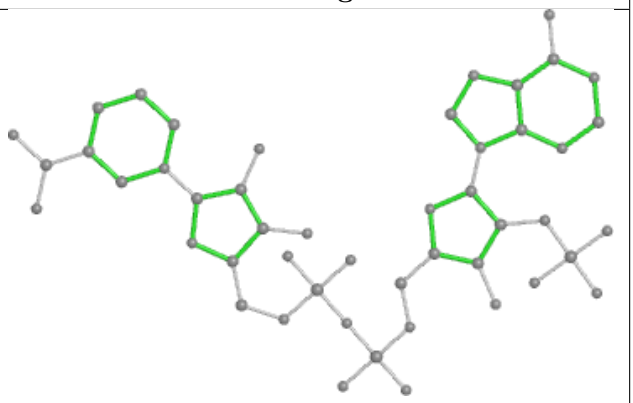
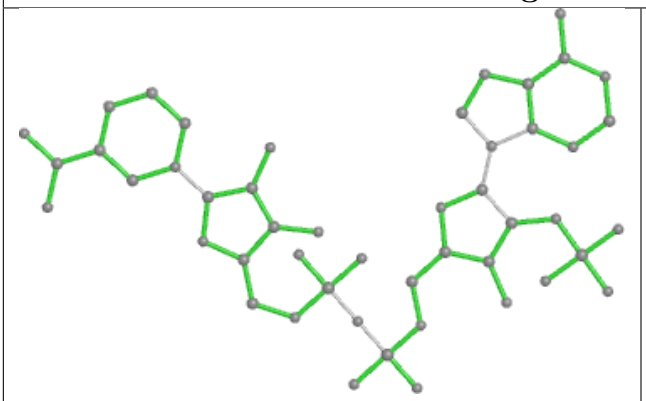
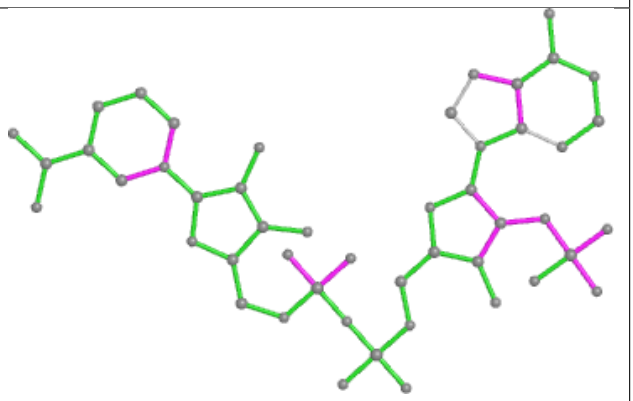


Rings

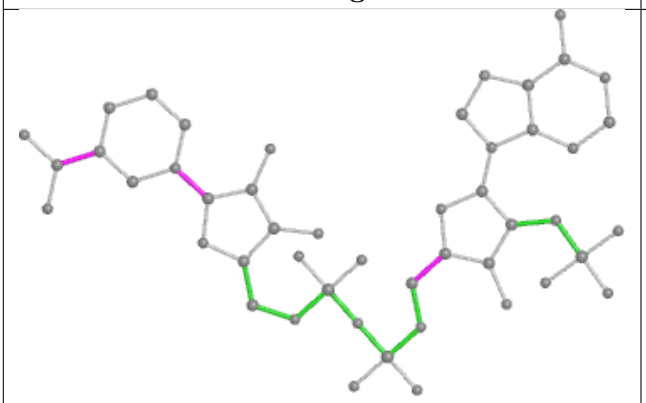
Ligand NAP A 702



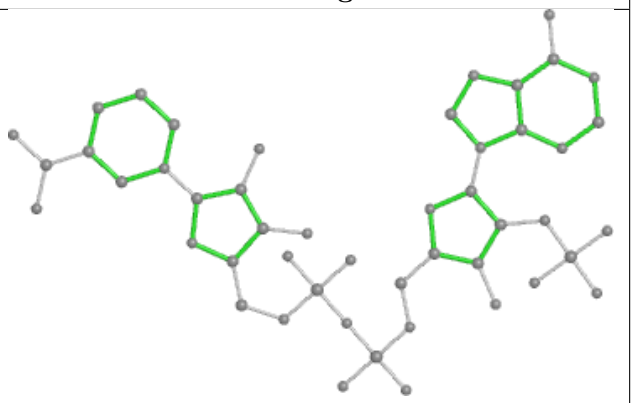
Bond lengths



Bond angles

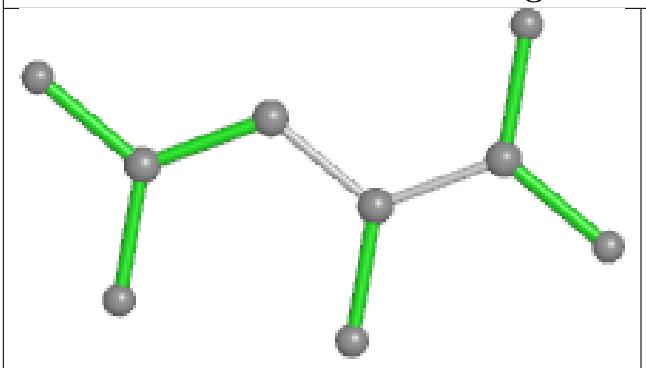


Torsions

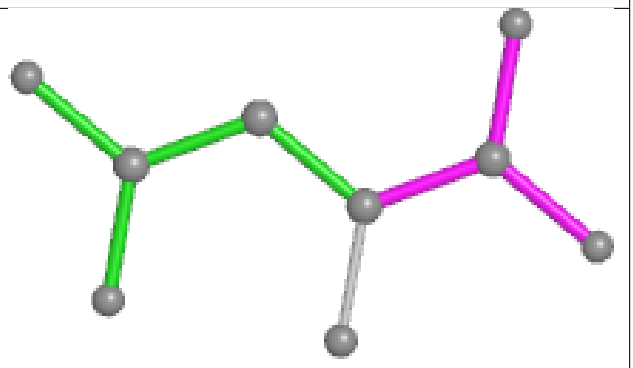


Rings

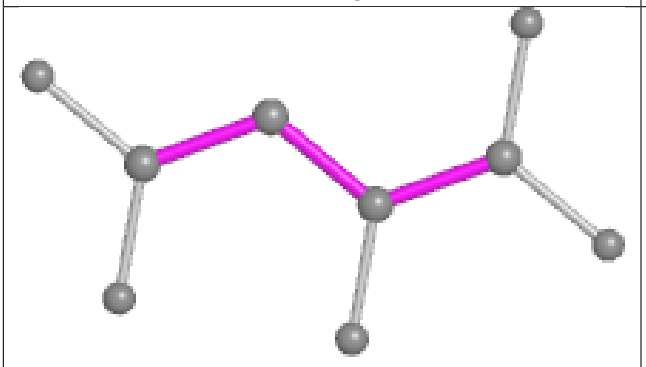
Ligand ASP A 704



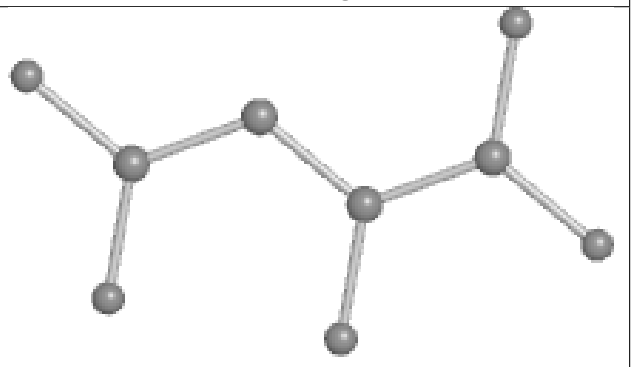
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	600/601 (99%)	-0.20	1 (0%)	95	95	18, 28, 52, 93	0
1	B	600/601 (99%)	-0.19	7 (1%)	79	82	22, 37, 66, 103	0
All	All	1200/1202 (99%)	-0.20	8 (0%)	87	89	18, 32, 61, 103	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.3
1	B	354	ASP	2.8
1	B	350	GLY	2.7
1	B	142	ALA	2.4
1	A	239	ASP	2.4
1	B	352	ASP	2.2
1	B	58	ASP	2.1
1	B	93	ASP	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

There are no monosaccharides in this entry.

6.4 Ligands

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

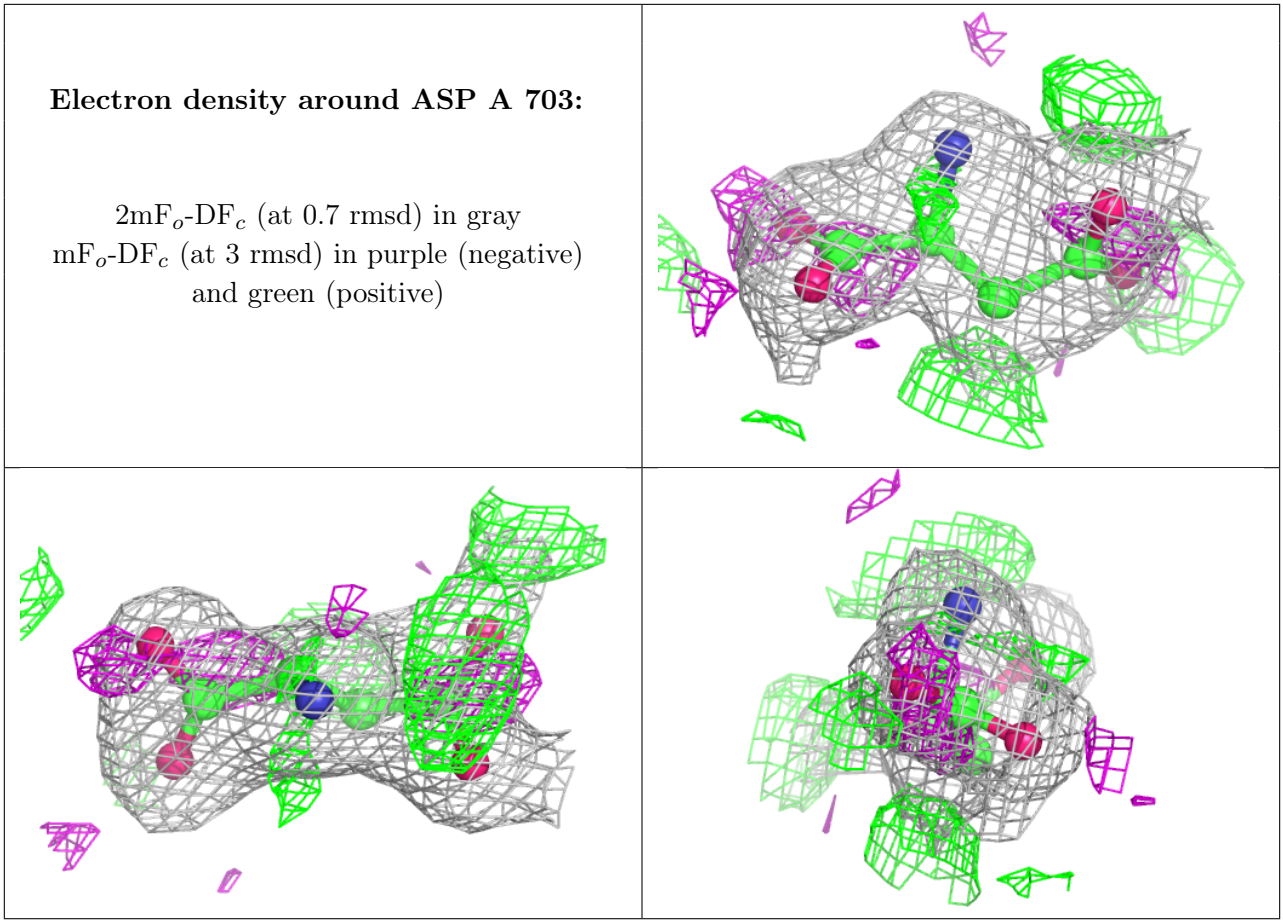
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	A	708	7/7	0.59	0.15	65,76,81,88	0
6	PEG	B	704	7/7	0.68	0.14	70,74,77,83	0
4	ASP	A	703	9/9	0.85	0.14	32,44,57,61	0
5	3NP	A	705	8/8	0.87	0.21	50,53,75,76	0
6	PEG	A	706	7/7	0.88	0.14	57,61,70,71	0
6	PEG	A	707	7/7	0.88	0.13	61,67,72,73	0
6	PEG	B	705	7/7	0.89	0.14	56,61,69,70	0
4	ASP	B	703	9/9	0.91	0.17	35,47,57,60	0
4	ASP	A	704	9/9	0.92	0.11	26,40,48,50	0
6	PEG	B	706	7/7	0.92	0.15	61,64,67,71	0
7	GOL	A	709	6/6	0.97	0.14	27,30,30,33	0
3	NAP	B	702	48/48	0.98	0.12	28,38,48,54	0
2	FAD	B	701	53/53	0.98	0.11	22,28,40,46	0
2	FAD	A	701	53/53	0.99	0.11	15,23,26,28	0
3	NAP	A	702	48/48	0.99	0.12	19,26,42,62	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.

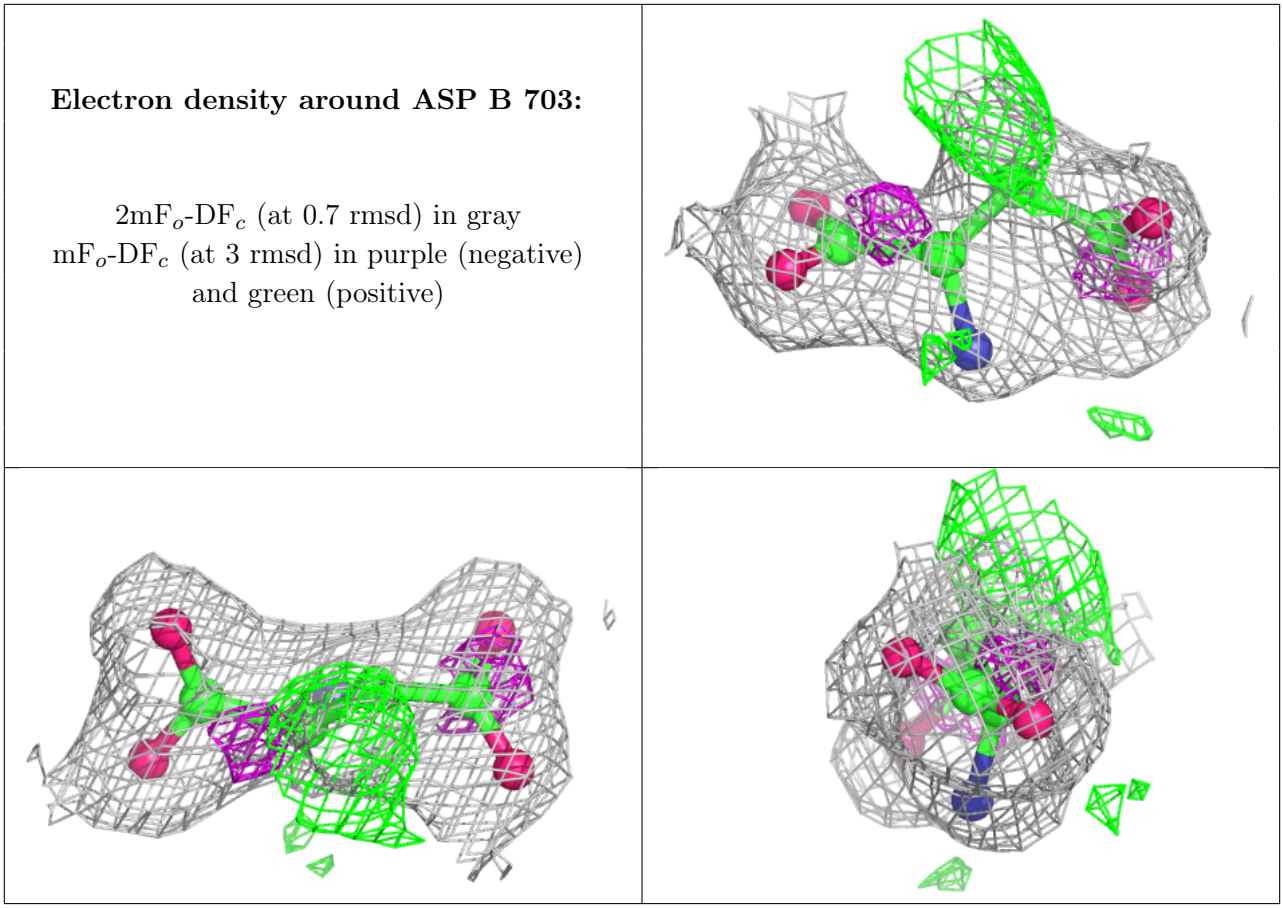
Electron density around ASP A 703:

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



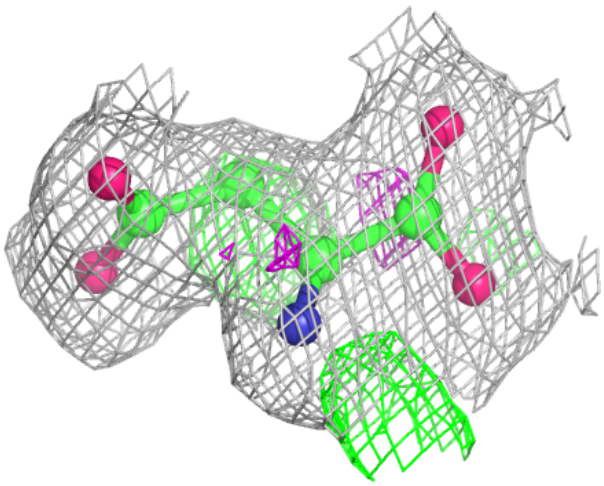
Electron density around ASP B 703:

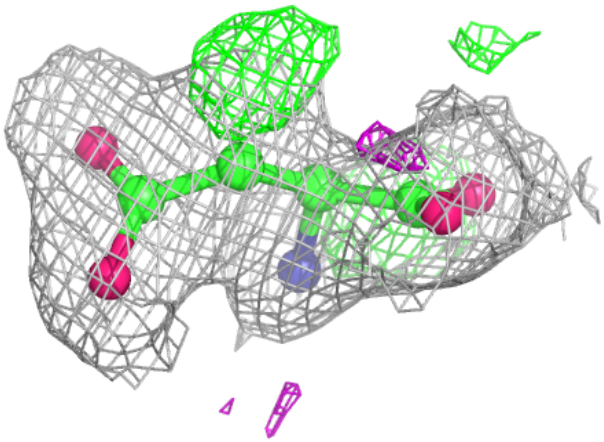
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

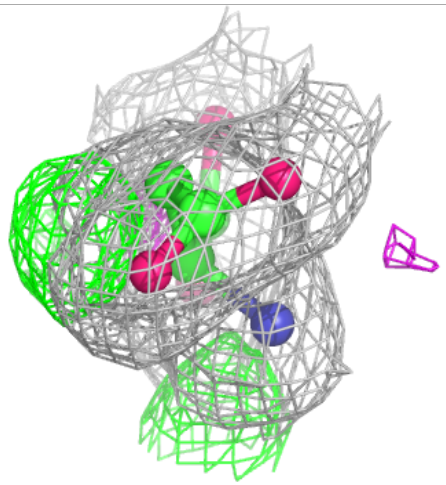


Electron density around ASP A 704:

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

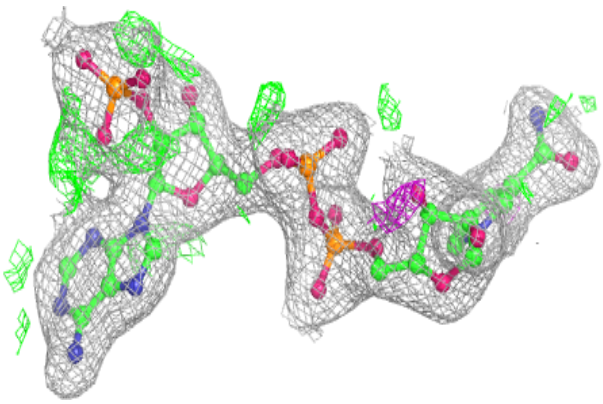


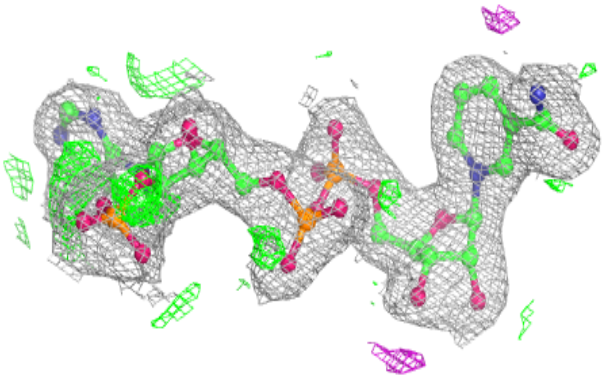


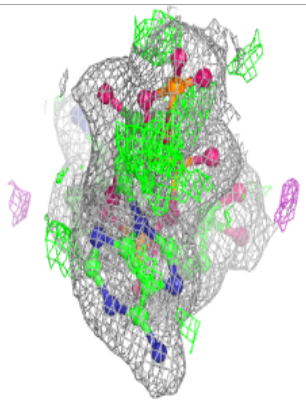


Electron density around NAP B 702:

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

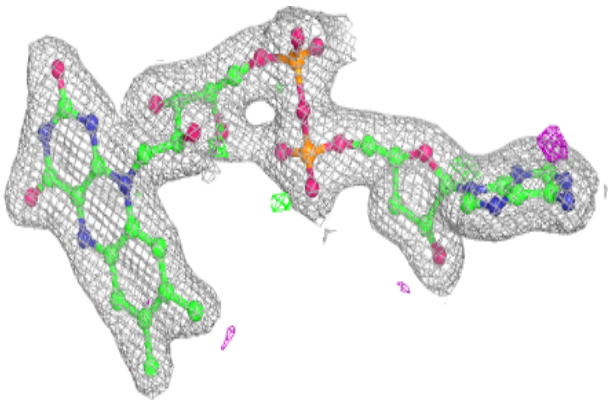


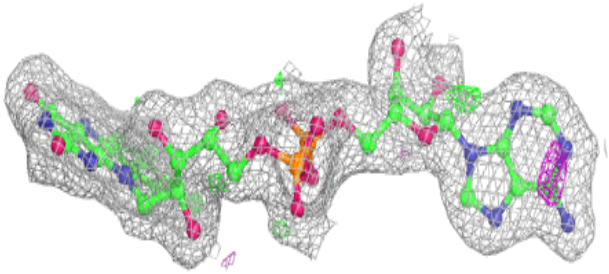


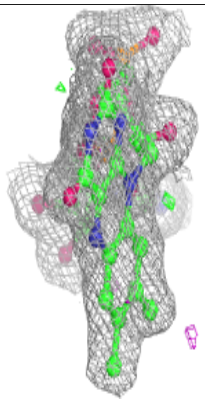


Electron density around FAD B 701:

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

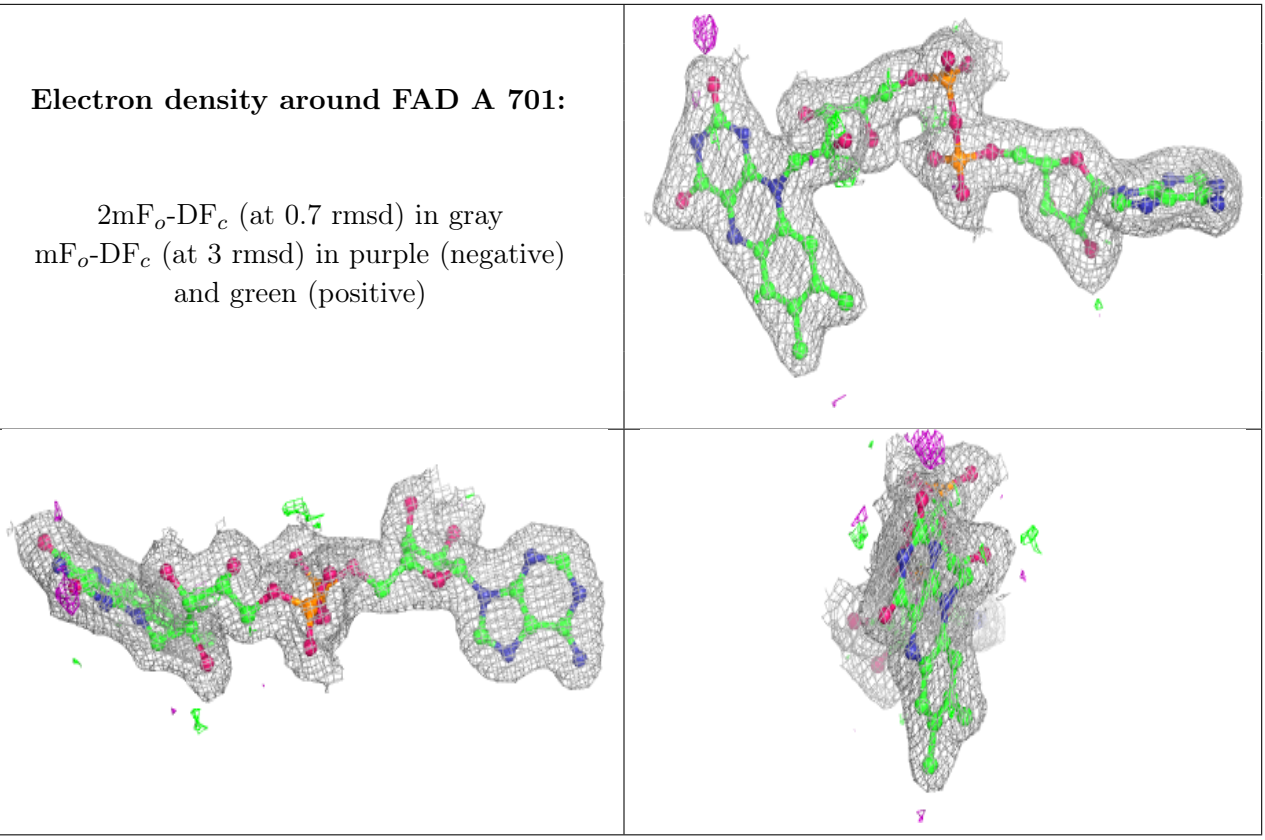






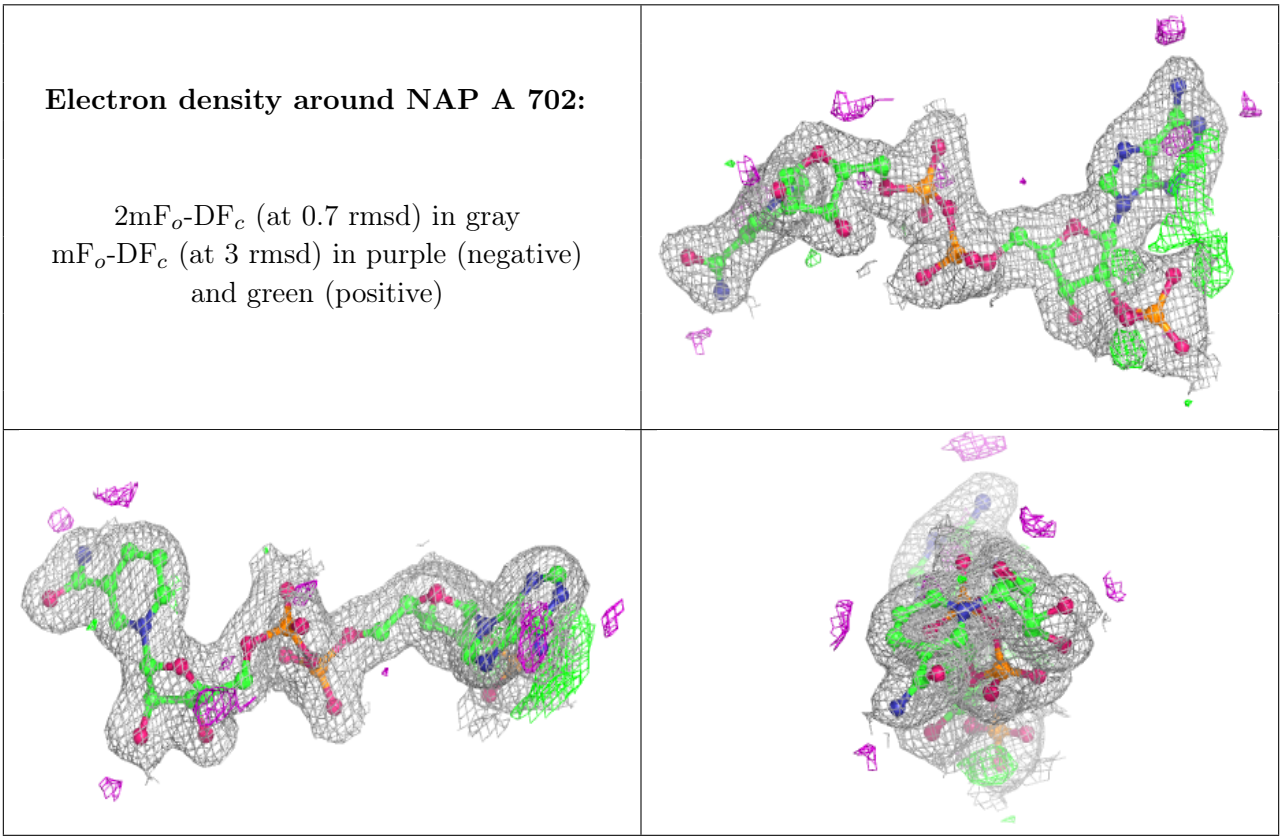
Electron density around FAD A 701:

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



Electron density around NAP A 702:

$2mF_o$-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.