



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 11:24 AM BST

PDB ID : 6VAX  
Title : Crystal structure of human SDHA-ADHAF2 assembly intermediate  
Authors : Sharma, P.; Maklashina, E.; Cecchini, G.; Iverson, T.M.  
Deposited on : 2019-12-18  
Resolution : 2.59 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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 : 2.14.4.dev1  
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) : 2.14.4.dev1

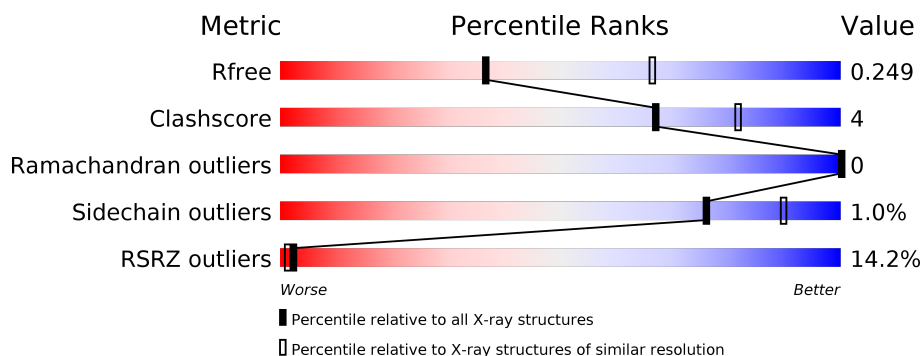
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	632	<div> <div>11%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	C	632	<div> <div>14%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	B	166	<div> <div>13%</div> <div>63%</div> <div>5%</div> <div>.</div> <div>32%</div> </div>
2	D	166	<div> <div>17%</div> <div>56%</div> <div>11%</div> <div>.</div> <div>32%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLI	A	703	-	-	-	X
6	GOL	A	704	-	-	-	X
8	EDO	A	707	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11494 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 Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4662	2918	825	887	32			
1	C	611	Total	C	N	O	S	0	0	0
			4668	2921	833	882	32			

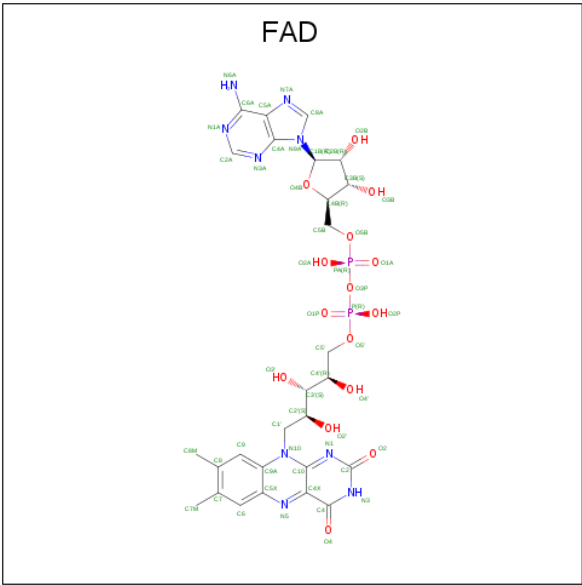
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	expression tag	UNP P31040
A	34	ARG	-	expression tag	UNP P31040
A	35	GLY	-	expression tag	UNP P31040
A	36	SER	-	expression tag	UNP P31040
A	37	HIS	-	expression tag	UNP P31040
A	38	HIS	-	expression tag	UNP P31040
A	39	HIS	-	expression tag	UNP P31040
A	40	HIS	-	expression tag	UNP P31040
A	41	HIS	-	expression tag	UNP P31040
A	42	HIS	-	expression tag	UNP P31040
A	43	GLY	-	expression tag	UNP P31040
C	33	MET	-	expression tag	UNP P31040
C	34	ARG	-	expression tag	UNP P31040
C	35	GLY	-	expression tag	UNP P31040
C	36	SER	-	expression tag	UNP P31040
C	37	HIS	-	expression tag	UNP P31040
C	38	HIS	-	expression tag	UNP P31040
C	39	HIS	-	expression tag	UNP P31040
C	40	HIS	-	expression tag	UNP P31040
C	41	HIS	-	expression tag	UNP P31040
C	42	HIS	-	expression tag	UNP P31040
C	43	GLY	-	expression tag	UNP P31040

- Molecule 2 is a protein called Succinate dehydrogenase assembly factor 2, mitochondrial.

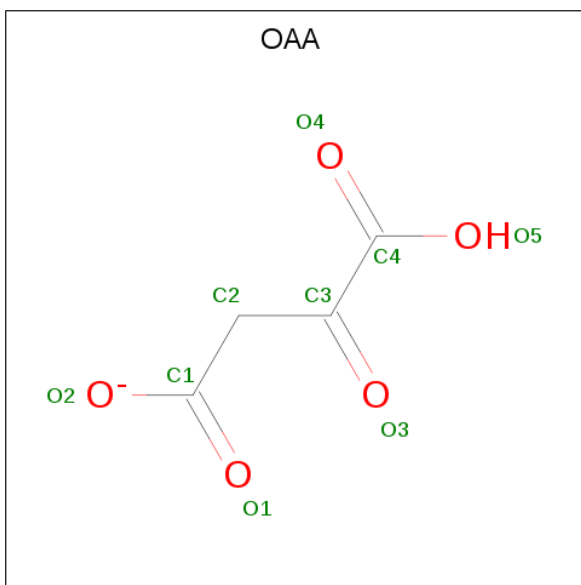
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	0
			954	610	164	176	4			
2	D	113	Total	C	N	O	S	0	0	0
			930	595	162	169	4			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by author).



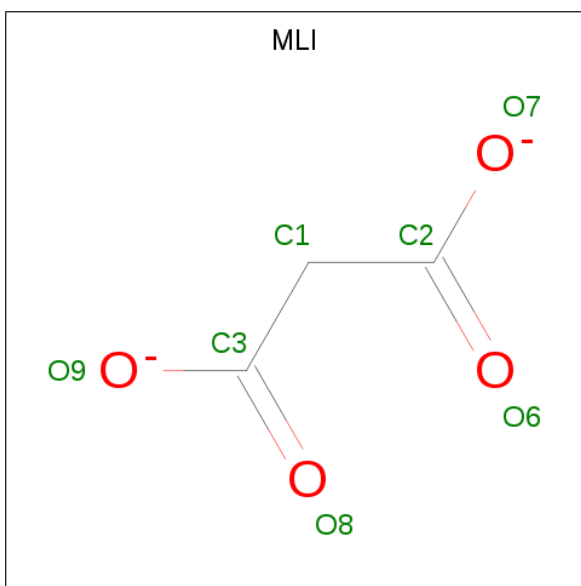
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is OXALOACETATE ION (three-letter code: OAA) (formula: C<sub>4</sub>H<sub>3</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		
4	C	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		
7	C	1	Total	K	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	48	Total O 48 48	0	0
9	B	3	Total O 3 3	0	0
9	C	45	Total O 45 45	0	0

*Continued on next page...*



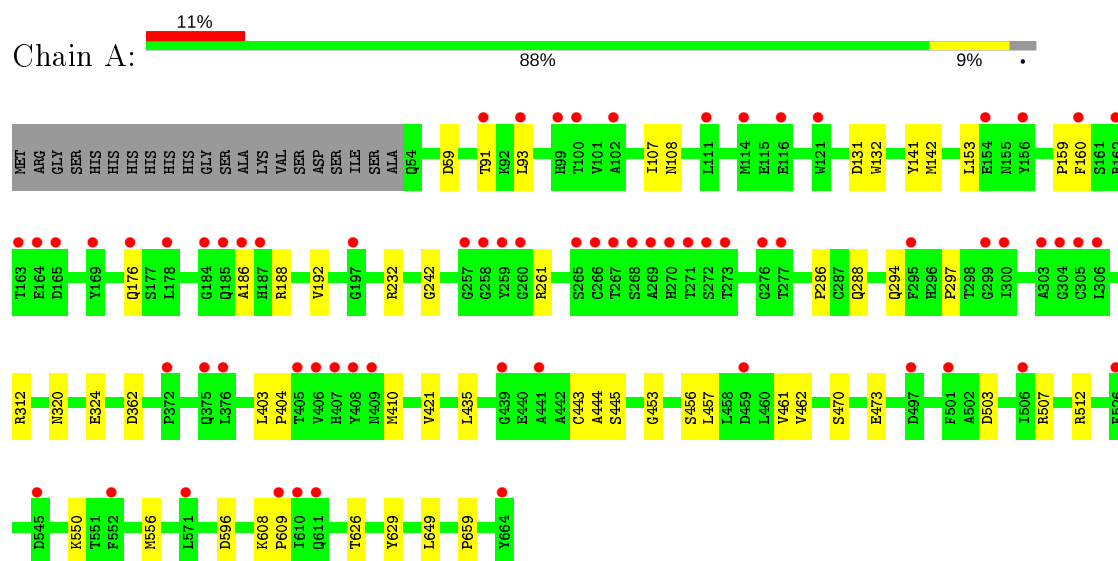
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	3	Total	O	0	0
			3	3		

### 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.

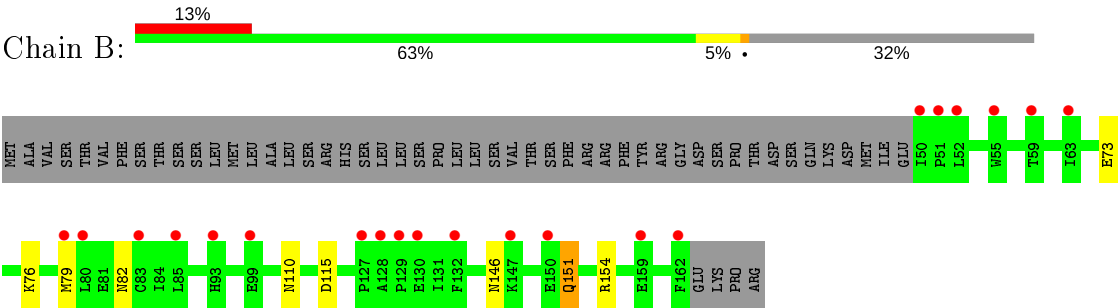
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



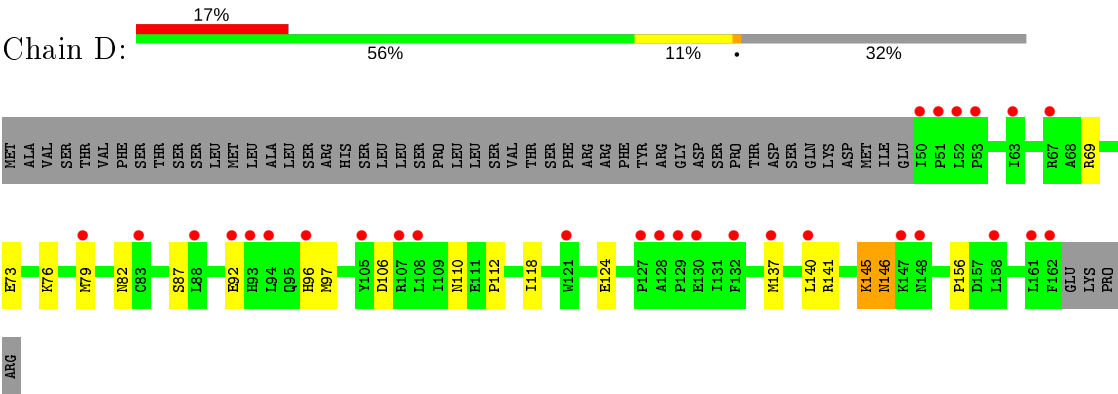
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



● Molecule 2: Succinate dehydrogenase assembly factor 2, mitochondrial



● Molecule 2: Succinate dehydrogenase assembly factor 2, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.56 Å 68.78 Å 126.58 Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	45.05 – 2.59 45.05 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.05-2.59) 99.3 (45.05-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.05 (at 2.58 Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.199 , 0.249 0.200 , 0.249	Depositor DCC
$R_{free}$ test set	2839 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.3	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4715e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, OAA, K, MLI, EDO, 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	0.24	0/4762	0.42	0/6452
1	C	0.24	0/4768	0.43	0/6457
2	B	0.24	0/977	0.38	0/1322
2	D	0.23	0/953	0.38	0/1293
All	All	0.24	0/11460	0.42	0/15524

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	4662	0	4506	31	0
1	C	4668	0	4526	42	0
2	B	954	0	935	5	0
2	D	930	0	895	13	0
3	A	53	0	29	1	0
3	C	53	0	29	1	0
4	A	9	0	2	0	0
4	C	9	0	2	0	0
5	A	7	0	2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	6	0	8	0	0
6	C	6	0	8	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	16	0	24	0	0
8	C	20	0	30	2	0
9	A	48	0	0	0	0
9	B	3	0	0	1	0
9	C	45	0	0	0	0
9	D	3	0	0	0	0
All	All	11494	0	10996	87	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 (87) 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:91:THR:HG22	1:A:93:LEU:H	1.52	0.73
1:C:600:ARG:HB2	8:C:708:EDO:H11	1.79	0.64
1:C:444:ALA:N	1:C:445:SER:HA	2.17	0.60
1:A:242:GLY:HA3	1:A:556:MET:HB3	1.83	0.59
2:B:73:GLU:OE1	2:B:110:ASN:ND2	2.36	0.58
1:A:444:ALA:N	1:A:445:SER:HA	2.19	0.58
2:D:92:GLU:O	2:D:96:HIS:NE2	2.34	0.57
1:A:456:SER:HB3	3:A:701:FAD:H2'	1.88	0.55
1:A:176:GLN:OE1	1:A:188:ARG:NH1	2.37	0.55
1:A:141:TYR:HB2	1:A:649:LEU:HD11	1.88	0.55
1:C:525:VAL:HG13	8:C:709:EDO:H22	1.89	0.54
1:C:451:ARG:HD2	1:C:456:SER:OG	2.10	0.52
2:D:146:ASN:HD22	2:D:146:ASN:H	1.57	0.52
1:A:93:LEU:HD21	2:B:76:LYS:HB3	1.90	0.52
1:A:108:ASN:ND2	1:A:453:GLY:O	2.42	0.52
2:D:79:MET:HG3	2:D:82:ASN:H	1.75	0.52
1:C:142:MET:HA	1:C:462:VAL:HG11	1.91	0.52
1:A:160:PHE:HA	1:A:192:VAL:HG22	1.91	0.51
1:A:512:ARG:HE	2:B:154:ARG:HH22	1.56	0.51
1:A:142:MET:HA	1:A:462:VAL:HG11	1.92	0.50
1:C:320:ASN:HD21	1:C:324:GLU:HB2	1.76	0.50
1:A:153:LEU:HD21	1:A:461:VAL:HG11	1.93	0.50
1:C:290:LEU:HD12	1:C:577:GLN:HB2	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:GLU:HG2	2:D:141:ARG:NH1	2.27	0.50
1:C:141:TYR:HB2	1:C:649:LEU:HD11	1.94	0.49
1:C:532:LEU:HD13	1:C:583:GLU:HA	1.94	0.49
1:A:320:ASN:HD21	1:A:324:GLU:HB2	1.76	0.49
1:C:93:LEU:HD22	2:D:76:LYS:HB3	1.95	0.49
1:C:153:LEU:HD11	1:C:461:VAL:HG21	1.94	0.49
1:C:600:ARG:NH2	1:C:660:ALA:O	2.42	0.49
2:B:79:MET:HG3	2:B:82:ASN:H	1.79	0.48
1:C:218:GLU:HG2	1:C:558:TRP:CZ3	2.49	0.48
1:C:320:ASN:HB2	1:C:355:ARG:HB3	1.96	0.47
1:C:460:LEU:HD11	3:C:702:FAD:H4'	1.95	0.47
1:A:132:TRP:CE2	1:A:659:PRO:HA	2.50	0.47
1:A:421:VAL:HG21	1:A:435:LEU:HG	1.96	0.47
1:C:408:TYR:CD2	1:C:451:ARG:HD3	2.50	0.46
1:C:172:ALA:HB2	1:C:187:HIS:CD2	2.50	0.46
1:C:242:GLY:HA3	1:C:556:MET:HB3	1.96	0.46
1:C:273:THR:HG21	1:C:567:GLU:HB3	1.97	0.46
2:B:151:GLN:O	9:B:201:HOH:O	2.21	0.46
1:C:280:ILE:HG13	1:C:413:ILE:HG12	1.97	0.46
1:C:294:GLN:HB2	1:C:410:MET:SD	2.56	0.46
1:C:95:PRO:HG2	1:C:205:TYR:CE1	2.51	0.45
1:A:176:GLN:HB3	1:A:186:ALA:HB3	1.96	0.45
1:C:117:ASP:OD1	1:C:118:ASN:N	2.47	0.45
1:C:610:ILE:HA	1:C:613:GLN:HE21	1.82	0.45
1:C:288:GLN:HA	1:C:626:THR:O	2.17	0.45
1:C:413:ILE:O	1:C:443:CYS:N	2.46	0.45
1:A:294:GLN:HB2	1:A:410:MET:SD	2.57	0.45
1:A:288:GLN:HA	1:A:626:THR:O	2.16	0.45
1:A:297:PRO:HG2	1:A:312:ARG:HH12	1.82	0.44
1:A:403:LEU:HD12	1:A:404:PRO:HD2	1.98	0.44
1:C:362:ASP:N	1:C:362:ASP:OD1	2.50	0.44
1:A:159:PRO:O	1:A:192:VAL:HG13	2.16	0.44
1:C:472:GLU:HG3	1:C:476:ARG:HH22	1.82	0.44
1:C:298:THR:HG21	1:C:312:ARG:HE	1.83	0.44
2:D:145:LYS:HD2	2:D:145:LYS:HA	1.61	0.44
1:C:125:ASP:OD1	1:C:177:SER:OG	2.35	0.43
1:A:261:ARG:HD3	1:A:261:ARG:HA	1.77	0.43
1:C:596:ASP:N	1:C:596:ASP:OD1	2.48	0.43
1:A:507:ARG:HE	1:A:550:LYS:HD3	1.84	0.43
1:A:596:ASP:N	1:A:596:ASP:OD1	2.41	0.42
1:A:286:PRO:HB3	1:A:629:TYR:CZ	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:TRP:CE2	1:C:659:PRO:HA	2.54	0.42
1:C:393:VAL:HG13	1:C:398:GLU:HB2	2.01	0.42
2:D:112:PRO:HG3	2:D:118:ILE:HD11	2.00	0.42
1:C:137:ASP:OD1	1:C:138:ALA:N	2.52	0.42
2:D:118:ILE:HD13	2:D:118:ILE:HA	1.87	0.42
1:A:362:ASP:OD1	1:A:362:ASP:N	2.53	0.41
2:D:69:ARG:NH2	2:D:106:ASP:OD2	2.46	0.41
1:A:107:ILE:HG12	1:A:457:LEU:HB2	2.02	0.41
1:C:218:GLU:HG2	1:C:558:TRP:HZ3	1.85	0.41
1:C:59:ASP:OD2	1:C:246:ARG:NH2	2.48	0.41
1:C:291:GLU:HA	1:C:578:THR:HG23	2.02	0.41
1:A:503:ASP:HA	1:A:550:LYS:HG3	2.02	0.41
1:C:482:PRO:HA	1:C:483:PRO:HD3	1.96	0.41
1:A:443:CYS:SG	1:A:445:SER:HB2	2.61	0.41
1:A:608:LYS:HB3	1:A:609:PRO:HD2	2.02	0.41
2:D:73:GLU:OE1	2:D:110:ASN:ND2	2.54	0.41
1:A:470:SER:HA	1:A:473:GLU:HG2	2.03	0.41
1:C:99:HIS:CE1	1:C:268:SER:HA	2.56	0.41
2:D:137:MET:HE1	2:D:140:LEU:HD23	2.02	0.41
1:C:273:THR:HA	1:C:571:LEU:HD21	2.02	0.40
1:C:388:MET:HG3	2:D:145:LYS:HD3	2.03	0.40
2:D:87:SER:OG	2:D:156:PRO:HD2	2.21	0.40
1:C:253:VAL:HG22	1:C:436:TYR:HB2	2.04	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	609/632 (96%)	585 (96%)	24 (4%)	0	100	100
1	C	609/632 (96%)	586 (96%)	23 (4%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	111/166 (67%)	104 (94%)	7 (6%)	0	100	100
2	D	111/166 (67%)	104 (94%)	7 (6%)	0	100	100
All	All	1440/1596 (90%)	1379 (96%)	61 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	485/512 (95%)	482 (99%)	3 (1%)	86	95
1	C	485/512 (95%)	482 (99%)	3 (1%)	86	95
2	B	102/154 (66%)	99 (97%)	3 (3%)	42	68
2	D	96/154 (62%)	93 (97%)	3 (3%)	40	66
All	All	1168/1332 (88%)	1156 (99%)	12 (1%)	76	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	131	ASP
1	A	232	ARG
2	B	115	ASP
2	B	146	ASN
2	B	151	GLN
1	C	131	ASP
1	C	218	GLU
1	C	232	ARG
2	D	97	MET
2	D	145	LYS
2	D	146	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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$
8	EDO	C	706	-	3,3,3	0.45	0	2,2,2	0.36	0
6	GOL	C	701	-	5,5,5	0.92	0	5,5,5	0.99	0
8	EDO	C	707	-	3,3,3	0.46	0	2,2,2	0.35	0
4	OAA	A	702	-	2,8,8	3.91	1 (50%)	2,10,10	1.92	1 (50%)
8	EDO	A	708	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EDO	A	707	-	3,3,3	0.48	0	2,2,2	0.29	0
3	FAD	C	702	1	51,58,58	1.22	5 (9%)	60,89,89	2.23	8 (13%)
8	EDO	C	709	-	3,3,3	0.46	0	2,2,2	0.35	0
3	FAD	A	701	1	51,58,58	1.21	5 (9%)	60,89,89	2.23	8 (13%)
5	MLI	A	703	-	0,6,6	0.00	-	0,7,7	0.00	-
4	OAA	C	703	-	2,8,8	3.96	1 (50%)	2,10,10	1.82	1 (50%)
8	EDO	C	705	-	3,3,3	0.45	0	2,2,2	0.34	0
8	EDO	C	708	-	3,3,3	0.46	0	2,2,2	0.31	0
6	GOL	A	704	-	5,5,5	0.90	0	5,5,5	0.97	0
8	EDO	A	706	-	3,3,3	0.45	0	2,2,2	0.40	0
8	EDO	A	709	-	3,3,3	0.46	0	2,2,2	0.39	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
8	EDO	C	706	-	-	1/1/1/1	-
6	GOL	C	701	-	-	2/4/4/4	-
8	EDO	C	707	-	-	0/1/1/1	-
4	OAA	A	702	-	-	0/2/8/8	-
8	EDO	A	708	-	-	1/1/1/1	-
8	EDO	A	707	-	-	0/1/1/1	-
3	FAD	C	702	1	-	5/30/50/50	0/6/6/6
8	EDO	C	709	-	-	0/1/1/1	-
3	FAD	A	701	1	-	6/30/50/50	0/6/6/6
5	MLI	A	703	-	-	0/0/4/4	-
4	OAA	C	703	-	-	1/2/8/8	-
8	EDO	C	705	-	-	0/1/1/1	-
8	EDO	C	708	-	-	0/1/1/1	-
6	GOL	A	704	-	-	2/4/4/4	-
8	EDO	A	706	-	-	1/1/1/1	-
8	EDO	A	709	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	703	OAA	O3-C3	5.58	1.31	1.22
3	C	702	FAD	C4X-C10	5.58	1.44	1.38
3	A	701	FAD	C4X-C10	5.55	1.44	1.38
4	A	702	OAA	O3-C3	5.50	1.31	1.22
3	A	701	FAD	C4-N3	3.19	1.38	1.33
3	C	702	FAD	C4-N3	3.14	1.38	1.33
3	A	701	FAD	C4-C4X	2.38	1.45	1.41
3	C	702	FAD	C4-C4X	2.38	1.45	1.41
3	A	701	FAD	C5X-N5	2.32	1.39	1.35
3	C	702	FAD	C5X-N5	2.28	1.39	1.35
3	C	702	FAD	C9A-N10	2.13	1.41	1.38
3	A	701	FAD	C9A-N10	2.11	1.41	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	FAD	C4-N3-C2	12.96	126.08	115.14
3	A	701	FAD	C4-N3-C2	12.96	126.08	115.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	FAD	C4X-C4-N3	-6.99	113.88	123.43
3	A	701	FAD	C4X-C4-N3	-6.98	113.88	123.43
3	C	702	FAD	C10-C4X-N5	4.68	124.50	121.26
3	A	701	FAD	C10-C4X-N5	4.67	124.48	121.26
3	A	701	FAD	C4-C4X-C10	-3.78	117.45	119.95
3	C	702	FAD	C4-C4X-C10	-3.76	117.46	119.95
3	A	701	FAD	C4X-C10-N10	-3.51	116.70	120.30
3	C	702	FAD	C4X-C10-N10	-3.50	116.71	120.30
3	C	702	FAD	C1'-N10-C9A	2.89	120.57	118.29
3	A	701	FAD	C1'-N10-C9A	2.81	120.51	118.29
4	A	702	OAA	C1-C2-C3	-2.60	110.88	115.51
3	C	702	FAD	P-O3P-PA	-2.57	124.02	132.83
4	C	703	OAA	C1-C2-C3	-2.50	111.06	115.51
3	A	701	FAD	P-O3P-PA	-2.49	124.27	132.83
3	A	701	FAD	C5A-C6A-N6A	2.38	123.96	120.35
3	C	702	FAD	C5A-C6A-N6A	2.36	123.94	120.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

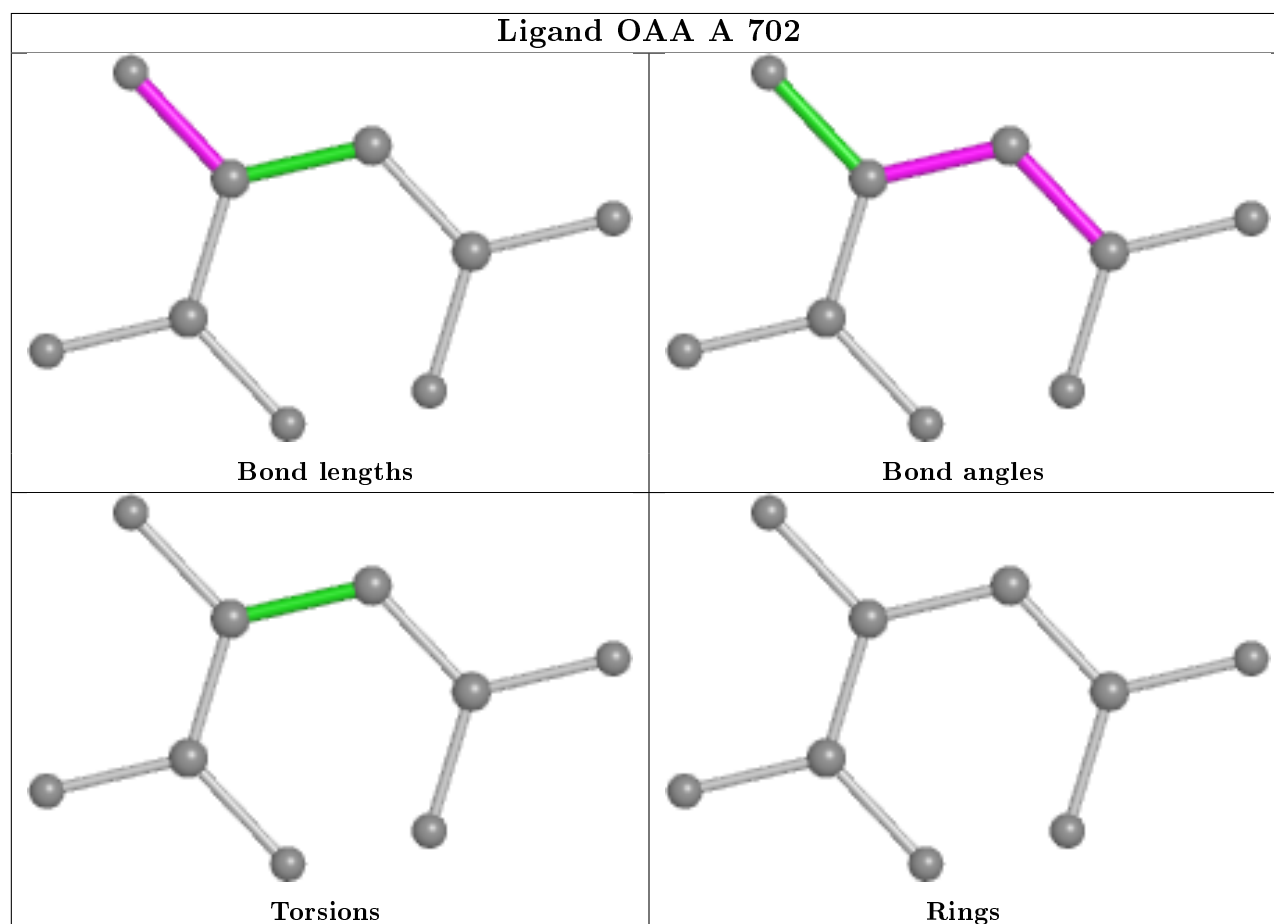
Mol	Chain	Res	Type	Atoms
3	C	702	FAD	N10-C1'-C2'-O2'
3	C	702	FAD	N10-C1'-C2'-C3'
3	C	702	FAD	C5'-O5'-P-O3P
3	A	701	FAD	N10-C1'-C2'-O2'
3	A	701	FAD	N10-C1'-C2'-C3'
3	A	701	FAD	C5'-O5'-P-O3P
6	C	701	GOL	C1-C2-C3-O3
8	C	706	EDO	O1-C1-C2-O2
6	C	701	GOL	O2-C2-C3-O3
6	A	704	GOL	O2-C2-C3-O3
4	C	703	OAA	C1-C2-C3-C4
3	A	701	FAD	C5'-O5'-P-O2P
3	A	701	FAD	O4B-C4B-C5B-O5B
3	C	702	FAD	O4B-C4B-C5B-O5B
8	A	708	EDO	O1-C1-C2-O2
8	A	709	EDO	O1-C1-C2-O2
6	A	704	GOL	C1-C2-C3-O3
8	A	706	EDO	O1-C1-C2-O2
3	C	702	FAD	C5'-O5'-P-O1P
3	A	701	FAD	C5'-O5'-P-O1P

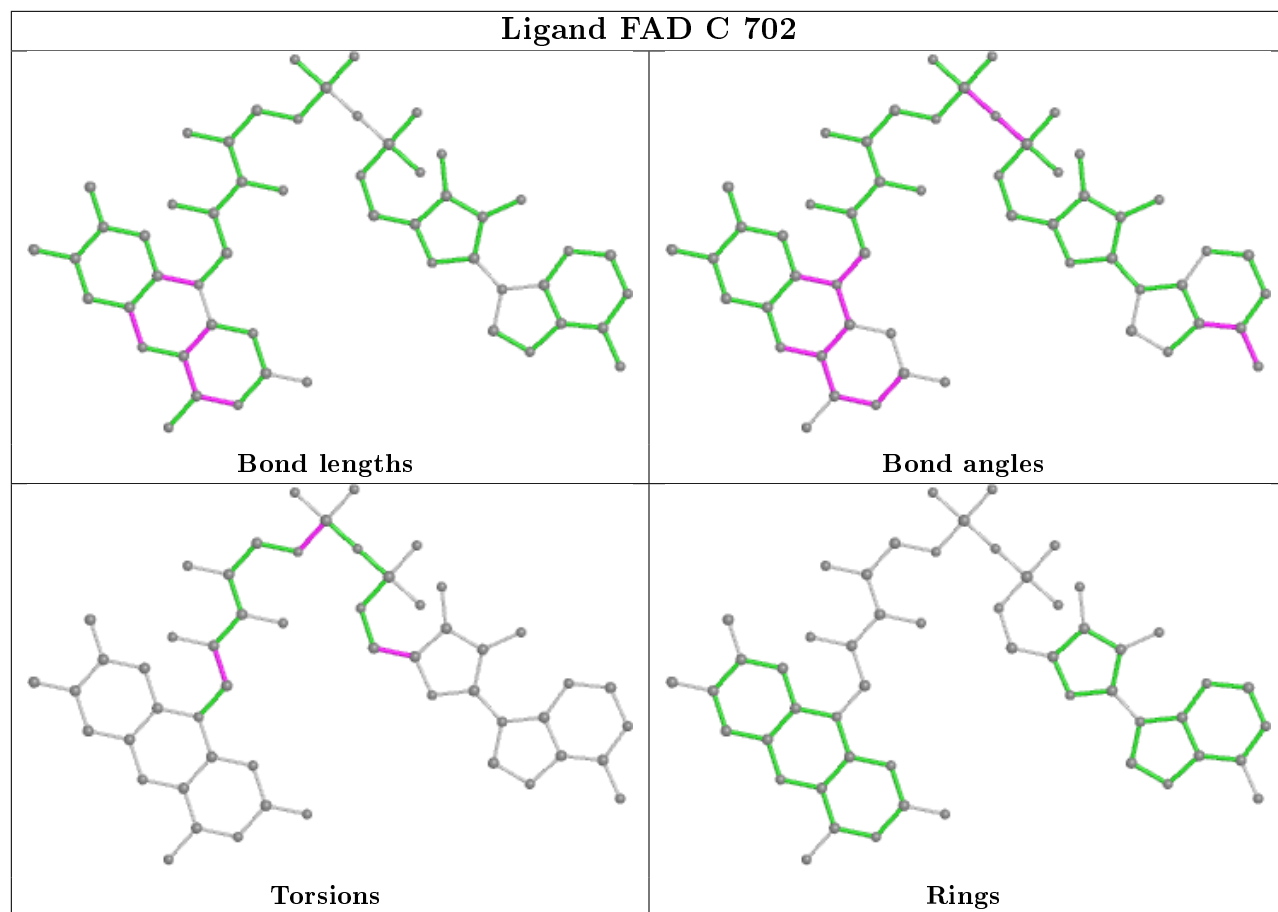
There are no ring outliers.

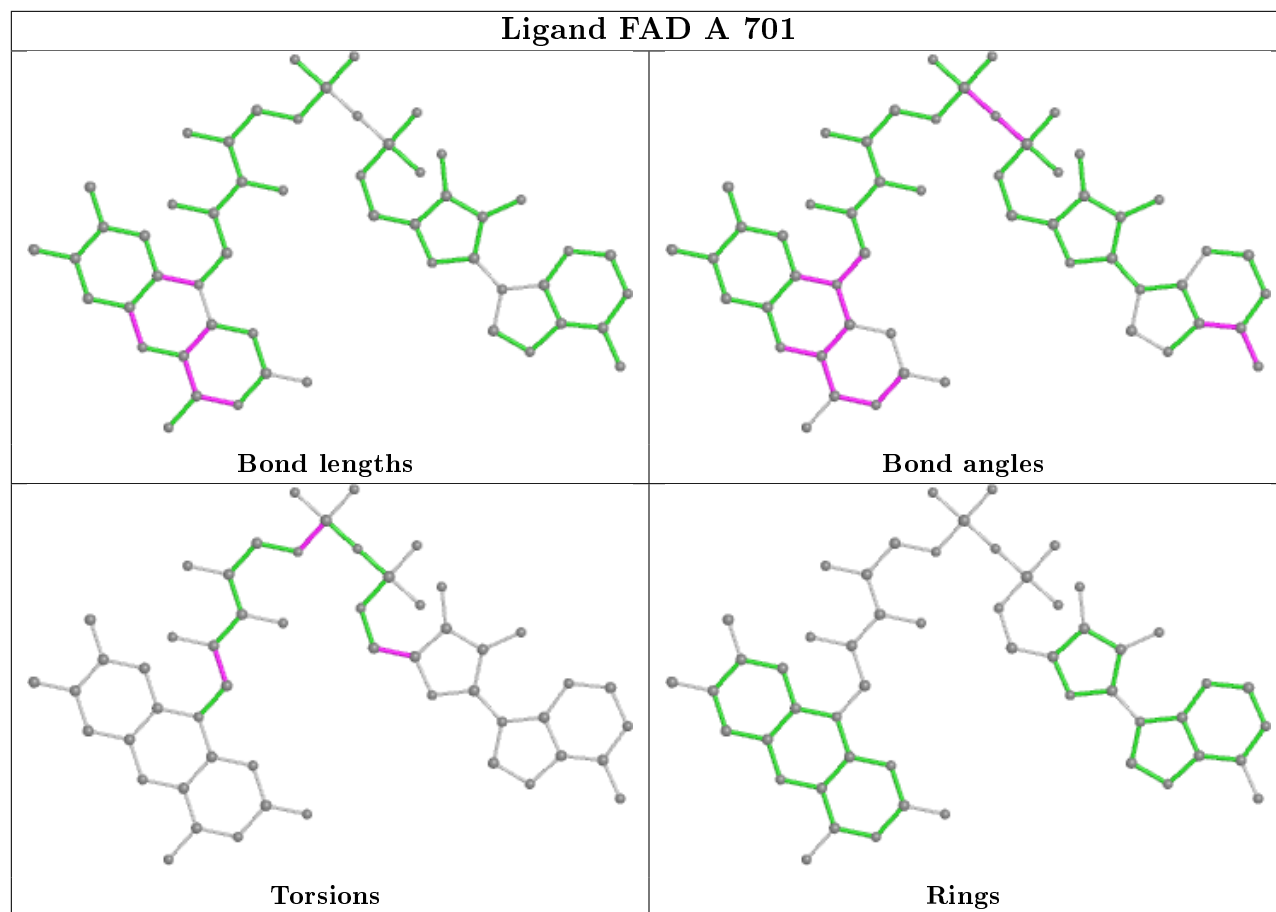
4 monomers are involved in 4 short contacts:

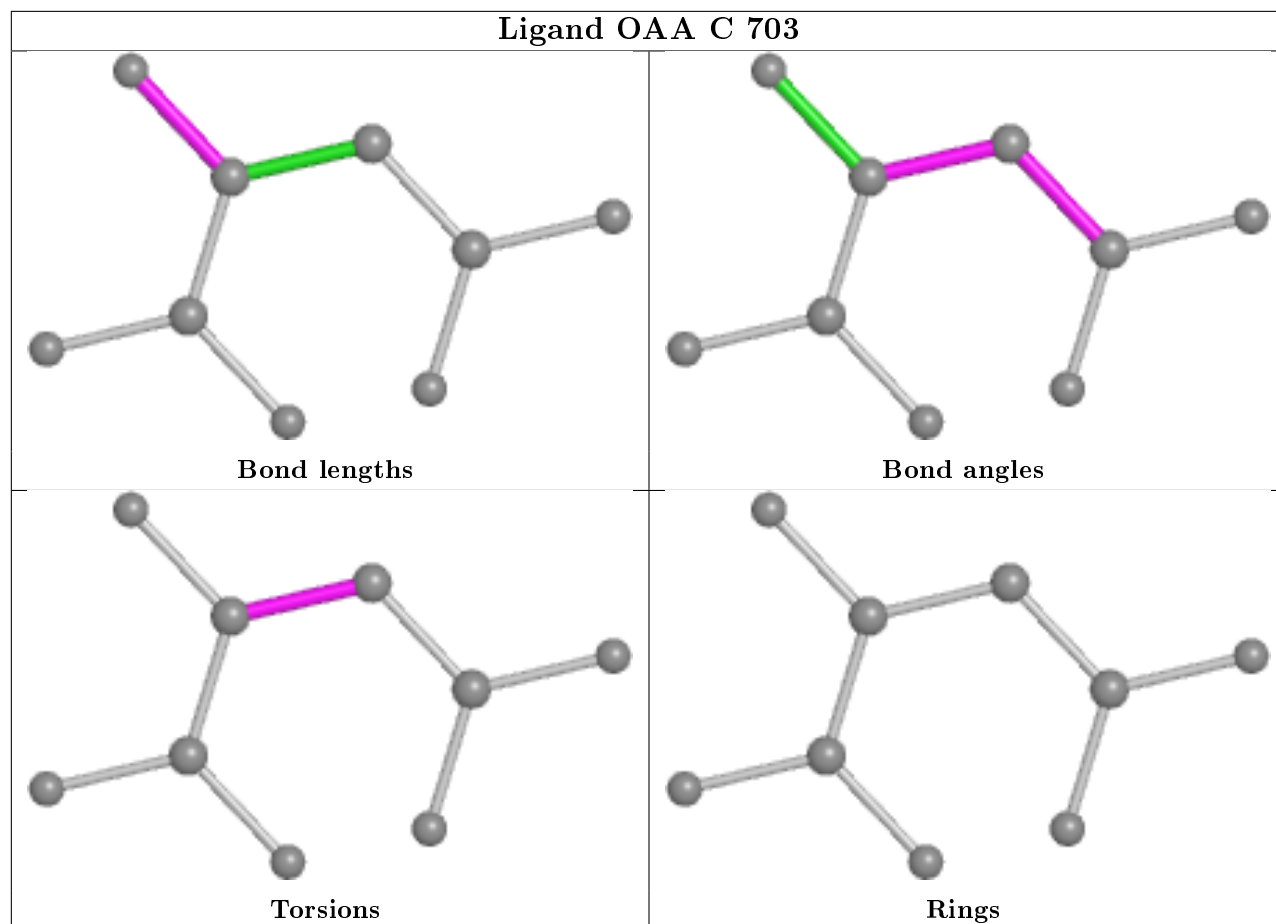
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	FAD	1	0
8	C	709	EDO	1	0
3	A	701	FAD	1	0
8	C	708	EDO	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	611/632 (96%)	0.71	68 (11%) 5 3	51, 82, 127, 175	0
1	C	611/632 (96%)	0.73	87 (14%) 2 1	48, 89, 136, 184	0
2	B	113/166 (68%)	0.95	21 (18%) 1 0	62, 100, 141, 164	0
2	D	113/166 (68%)	1.36	29 (25%) 0 0	83, 123, 161, 185	0
All	All	1448/1596 (90%)	0.79	205 (14%) 2 1	48, 89, 140, 185	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	ILE	7.0
2	D	158	LEU	6.6
1	C	268	SER	5.9
1	C	267	THR	5.6
1	C	270	HIS	5.5
1	C	266	CYS	5.4
1	C	260	GLY	5.3
1	A	266	CYS	5.2
2	D	94	LEU	5.1
1	C	408	TYR	5.0
1	C	258	GLY	5.0
1	A	163	THR	4.9
1	A	268	SER	4.8
2	D	121	TRP	4.7
2	D	50	ILE	4.6
1	A	408	TYR	4.6
1	C	406	VAL	4.5
1	C	272	SER	4.5
1	A	552	PHE	4.5
1	A	506	ILE	4.4
1	C	269	ALA	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	552	PHE	4.2
1	C	506	ILE	4.2
1	A	611	GLN	4.2
1	A	178	LEU	4.2
1	C	376	LEU	4.1
1	C	505	SER	4.1
1	A	114	MET	4.0
2	D	128	ALA	4.0
1	C	526	PHE	4.0
1	A	409	ASN	4.0
1	A	406	VAL	3.9
1	A	272	SER	3.9
1	C	169	TYR	3.9
2	D	51	PRO	3.9
1	C	259	TYR	3.9
1	A	259	TYR	3.9
1	A	376	LEU	3.9
1	C	407	HIS	3.8
2	B	99	GLU	3.8
1	A	407	HIS	3.8
1	A	267	THR	3.8
1	A	164	GLU	3.8
2	D	67	ARG	3.8
1	C	501	PHE	3.7
2	D	63	ILE	3.7
1	C	160	PHE	3.7
2	B	52	LEU	3.7
1	C	164	GLU	3.7
2	D	129	PRO	3.7
1	A	271	THR	3.6
1	C	265	SER	3.6
1	A	501	PHE	3.6
1	C	256	THR	3.6
1	C	271	THR	3.6
2	D	108	LEU	3.5
1	C	610	ILE	3.5
1	A	258	GLY	3.5
2	D	105	TYR	3.4
1	A	304	GLY	3.4
1	A	270	HIS	3.4
1	A	265	SER	3.4
1	A	260	GLY	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	497	ASP	3.4
1	A	305	CYS	3.3
1	C	664	TYR	3.3
1	C	100	THR	3.3
1	C	55	TYR	3.3
1	A	375	GLN	3.3
1	C	173	PHE	3.2
2	D	132	PHE	3.2
2	D	92	GLU	3.2
2	B	50	ILE	3.2
2	D	96	HIS	3.2
1	A	160	PHE	3.1
1	A	609	PRO	3.1
2	D	53	PRO	3.1
1	C	379	ARG	3.1
1	C	409	ASN	3.1
1	A	176	GLN	3.1
1	A	303	ALA	3.0
2	B	79	MET	3.0
1	A	169	TYR	3.0
2	D	147	LYS	3.0
1	C	568	LEU	3.0
1	C	499	LEU	3.0
1	A	257	GLY	3.0
1	C	176	GLN	3.0
2	D	83	CYS	3.0
2	B	162	PHE	3.0
1	C	306	LEU	3.0
1	A	102	ALA	2.9
1	C	257	GLY	2.9
1	A	111	LEU	2.9
2	B	130	GLU	2.9
1	C	296	HIS	2.9
1	A	184	GLY	2.9
1	C	168	ILE	2.9
1	C	404	PRO	2.9
1	A	441	ALA	2.8
2	B	150	GLU	2.8
1	C	103	ALA	2.8
1	C	54	GLN	2.8
1	A	91	THR	2.8
2	D	148	ASN	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	493	VAL	2.8
1	C	503	ASP	2.8
1	A	93	LEU	2.8
1	A	116	GLU	2.8
1	C	614	GLN	2.8
1	C	166	GLY	2.8
2	D	52	LEU	2.8
1	A	273	THR	2.7
1	A	295	PHE	2.7
2	B	127	PRO	2.7
1	C	156	TYR	2.7
1	C	159	PRO	2.7
2	D	140	LEU	2.7
1	A	439	GLY	2.7
1	C	305	CYS	2.7
1	A	526	PHE	2.6
1	C	295	PHE	2.6
1	C	302	GLY	2.6
1	C	405	THR	2.6
2	D	93	HIS	2.6
2	B	51	PRO	2.6
1	C	375	GLN	2.6
1	C	615	LYS	2.6
1	A	405	THR	2.6
1	C	599	VAL	2.5
1	C	280	ILE	2.5
2	B	63	ILE	2.5
2	B	80	LEU	2.5
1	A	99	HIS	2.5
1	C	439	GLY	2.5
1	A	276	GLY	2.5
2	B	132	PHE	2.5
2	D	162	PHE	2.5
1	A	156	TYR	2.4
1	C	304	GLY	2.4
1	A	306	LEU	2.4
1	C	93	LEU	2.4
1	A	187	HIS	2.4
1	A	165	ASP	2.4
1	C	300	ILE	2.4
2	B	55	TRP	2.4
1	A	300	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	264	PHE	2.4
2	B	83	CYS	2.4
2	D	130	GLU	2.4
1	A	269	ALA	2.4
1	C	273	THR	2.4
2	D	127	PRO	2.4
1	A	497	ASP	2.4
2	B	159	GLU	2.4
1	A	571	LEU	2.3
1	C	95	PRO	2.3
1	A	664	TYR	2.3
2	D	79	MET	2.3
1	C	504	GLY	2.3
1	C	307	ILE	2.3
1	A	277	THR	2.3
1	C	287	CYS	2.3
1	A	162	ARG	2.2
1	A	197	GLY	2.2
1	C	440	GLU	2.2
2	D	137	MET	2.2
1	A	154	GLU	2.2
1	C	372	PRO	2.2
2	B	129	PRO	2.2
1	C	456	SER	2.2
2	B	93	HIS	2.2
2	B	147	LYS	2.2
1	A	186	ALA	2.2
1	C	162	ARG	2.2
1	C	114	MET	2.1
1	C	165	ASP	2.1
2	D	107	ARG	2.1
1	A	121	TRP	2.1
1	C	102	ALA	2.1
2	B	85	LEU	2.1
2	D	88	LEU	2.1
2	B	128	ALA	2.1
1	A	372	PRO	2.1
1	C	546	LEU	2.1
1	C	70	GLY	2.1
1	C	276	GLY	2.1
1	C	299	GLY	2.1
1	C	197	GLY	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	442	ALA	2.1
1	C	101	VAL	2.1
1	A	299	GLY	2.1
1	A	545	ASP	2.0
1	C	167	LYS	2.0
1	A	100	THR	2.0
1	C	277	THR	2.0
1	C	263	TYR	2.0
2	D	161	LEU	2.0
1	C	94	PHE	2.0
1	C	618	PHE	2.0
1	A	459	ASP	2.0
2	B	59	THR	2.0
1	C	451	ARG	2.0
1	C	458	LEU	2.0
1	A	185	GLN	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 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

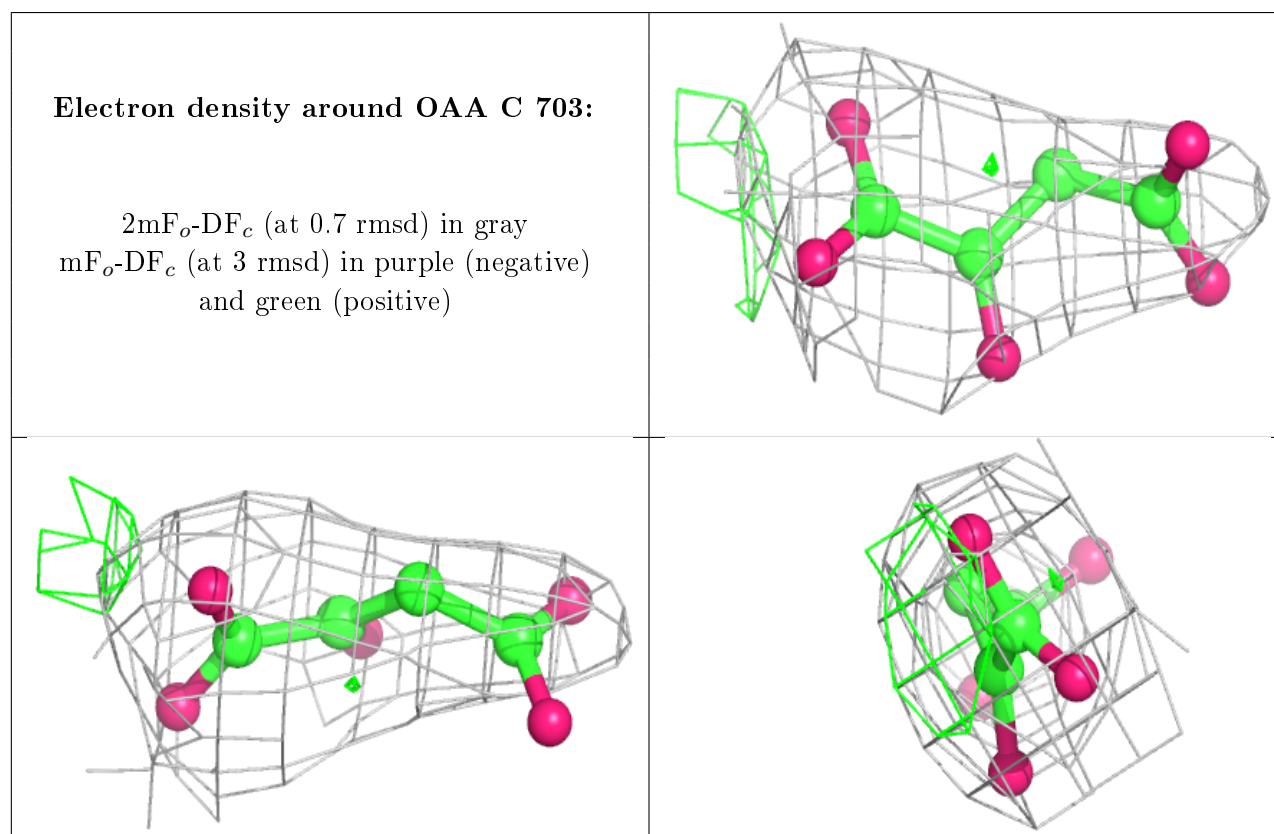
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	EDO	C	708	4/4	0.49	0.30	77,84,85,94	0
8	EDO	A	707	4/4	0.67	0.55	82,86,99,102	0
8	EDO	C	709	4/4	0.79	0.39	113,113,121,130	0
5	MLI	A	703	7/7	0.80	0.66	98,107,114,116	0
6	GOL	A	704	6/6	0.80	0.46	89,103,105,108	0
8	EDO	C	707	4/4	0.82	0.47	96,104,105,117	0
4	OAA	C	703	9/9	0.84	0.59	104,113,127,134	0

*Continued on next page...*

Continued from previous page...

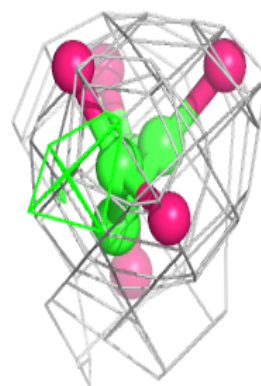
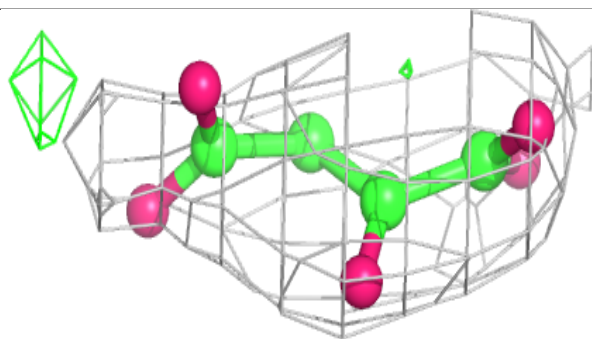
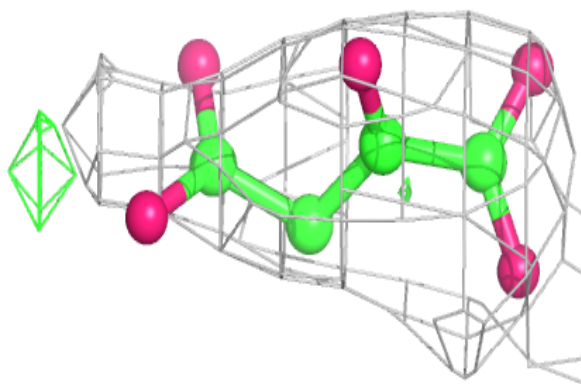
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EDO	A	706	4/4	0.84	0.32	102,103,104,104	0
8	EDO	C	706	4/4	0.85	0.33	117,120,121,132	0
4	OAA	A	702	9/9	0.89	0.44	93,102,123,134	0
6	GOL	C	701	6/6	0.89	0.42	76,95,107,113	0
8	EDO	A	708	4/4	0.91	0.23	93,102,108,111	0
8	EDO	C	705	4/4	0.92	0.17	78,87,96,105	0
7	K	C	704	1/1	0.93	0.18	74,74,74,74	0
8	EDO	A	709	4/4	0.93	0.17	93,96,97,111	0
7	K	A	705	1/1	0.96	0.21	77,77,77,77	0
3	FAD	C	702	53/53	0.96	0.31	54,72,87,95	0
3	FAD	A	701	53/53	0.97	0.29	45,65,84,88	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.

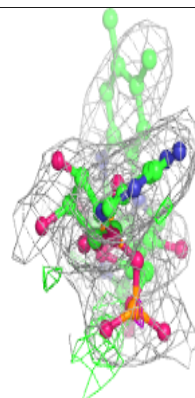
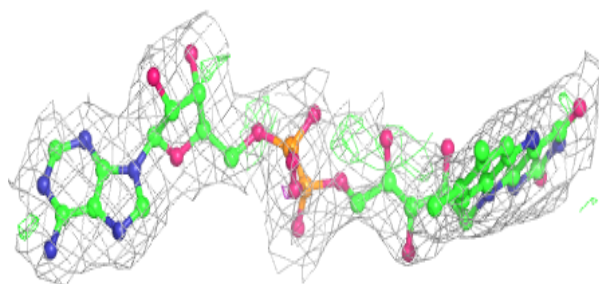
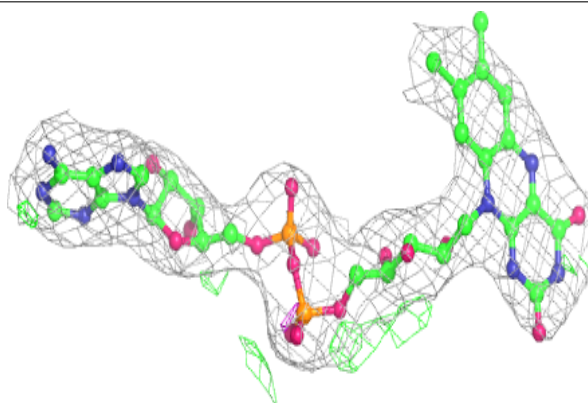


**Electron density around OAA A 702:**

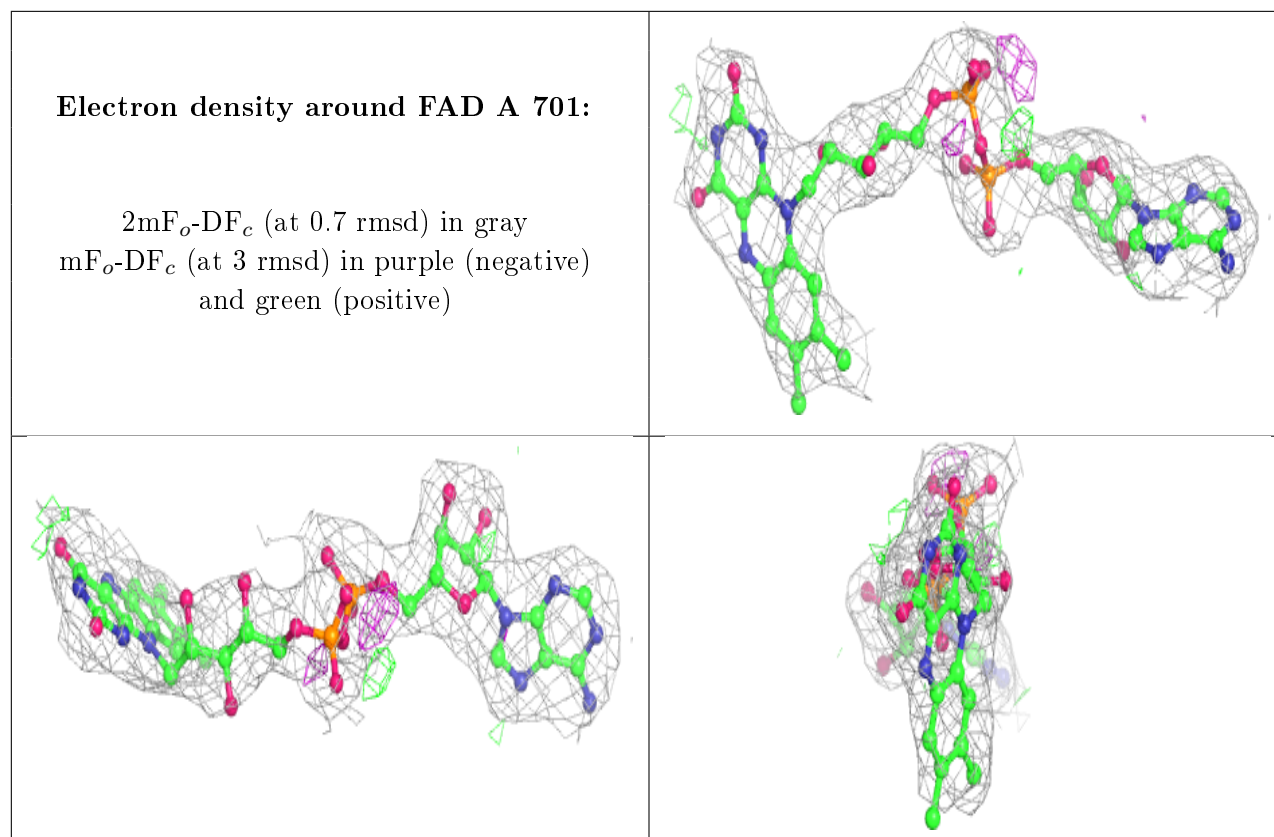
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FAD C 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.