



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2022 – 02:31 pm BST

PDB ID : 7R35
Title : Difference-refined structure of fatty acid photodecarboxylase 300 ns following 400-nm laser irradiation of the dark-state determined by SFX
Authors : Hadjidemetriou, K.; Coquelle, N.; Barends, T.R.M.; De Zitter, E.; Schlichting, I.; Colletier, J.P.; Weik, W.
Deposited on : 2022-02-06
Resolution : 2.00 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 : 2.30
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.30

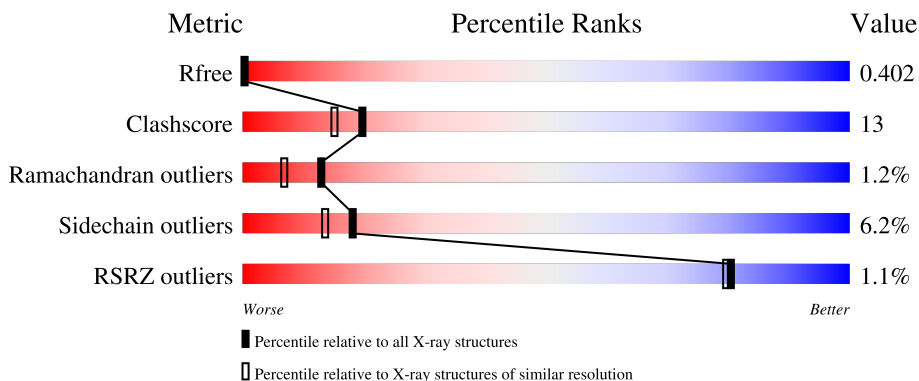
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	578	
1	B	578	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9184 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 Fatty acid photodecarboxylase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	563	Total	C	N	O	S	0	15	0
			4328	2702	778	833	15			
1	B	562	Total	C	N	O	S	0	13	0
			4302	2690	772	825	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP A0A248QE08
B	?	-	GLY	deletion	UNP A0A248QE08

- 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).



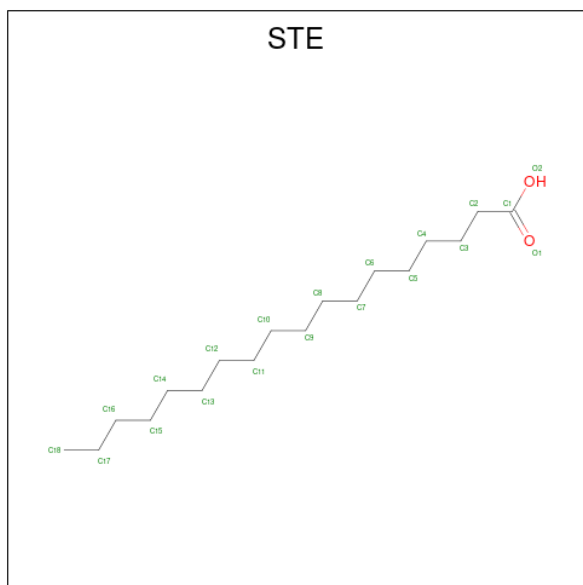
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			17	17		
3	A	1	Total	C	0	0
			10	10		
3	B	1	Total	C	0	0
			17	17		
3	B	1	Total	C	0	0
			10	10		

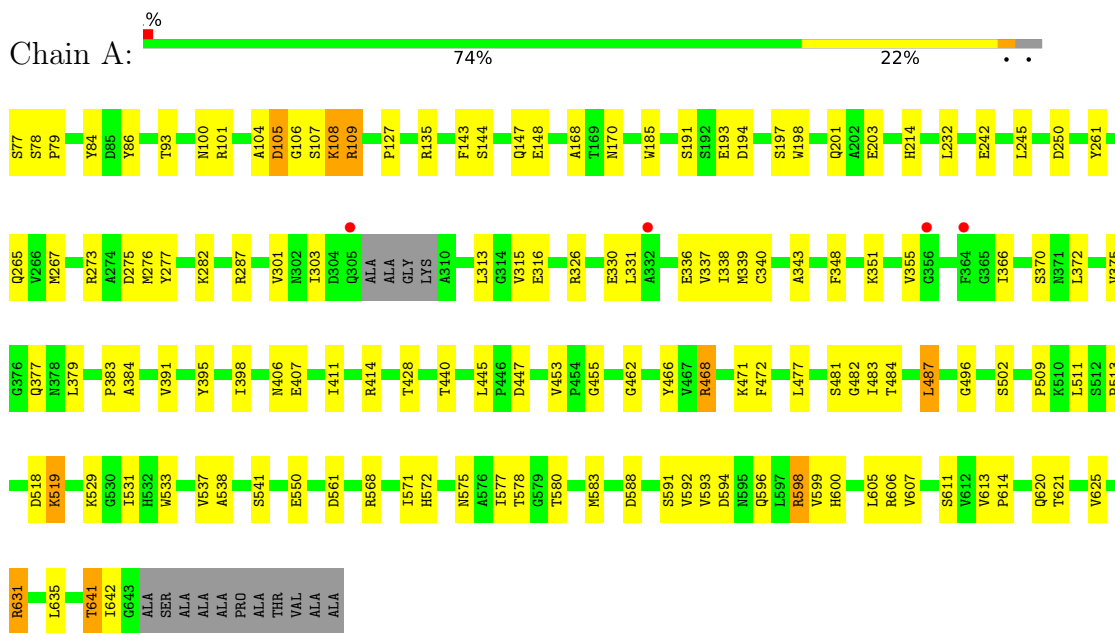
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total	O	0	0
			209	209		
4	B	185	Total	O	0	0
			185	185		

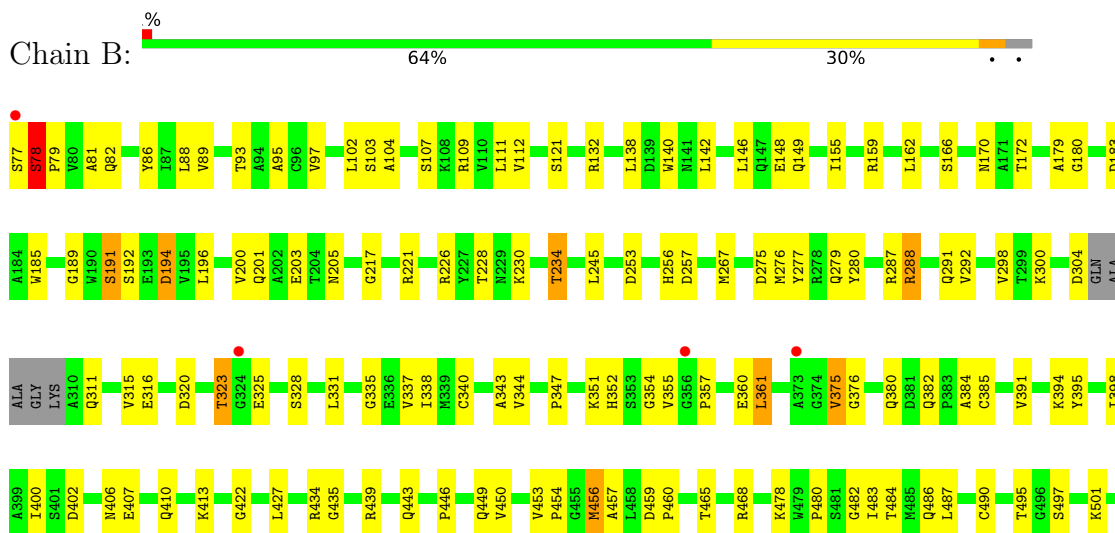
3 Residue-property plots

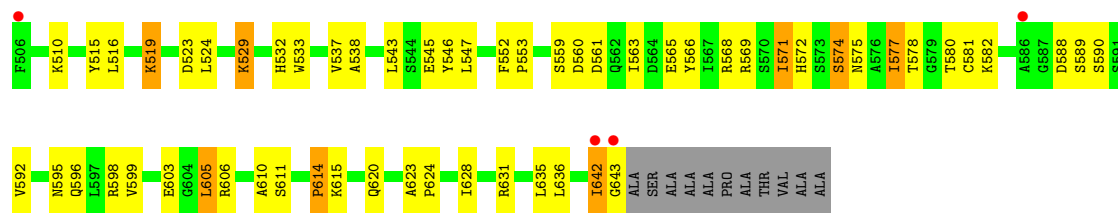
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fatty acid photodecarboxylase, chloroplastic



- Molecule 1: Fatty acid photodecarboxylase, chloroplastic





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.39Å 60.01Å 182.90Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.00) 97.0 (10.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.330 , 0.402 0.330 , 0.402	Depositor DCC
R_{free} test set	4477 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.177 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9184	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: FAD, STE

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	0.44	0/4428	0.63	1/6001 (0.0%)
1	B	0.43	0/4403	0.61	0/5969
All	All	0.43	0/8831	0.62	1/11970 (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	487	LEU	CA-CB-CG	-5.08	103.61	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	4328	0	4264	96	0
1	B	4302	0	4252	123	0
2	A	53	0	31	5	0
2	B	53	0	31	4	0
3	A	27	0	49	5	0
3	B	27	0	49	7	0
4	A	209	0	0	14	0
4	B	185	0	0	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9184	0	8676	222	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 13.

All (222) 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:B:354:GLY:HA2	1:B:361:LEU:HD11	1.47	0.95
1:B:221:ARG:NH1	4:B:802:HOH:O	2.03	0.84
1:B:89:VAL:HG13	1:B:298:VAL:HG21	1.63	0.80
1:B:149:GLN:O	1:B:568[B]:ARG:NH1	2.15	0.80
1:A:568[A]:ARG:NH1	4:A:802:HOH:O	2.14	0.79
1:B:560:ASP:OD1	4:B:801:HOH:O	2.01	0.77
1:B:180:GLY:HA2	1:B:183:ASP:HB2	1.68	0.75
1:B:449:GLN:OE1	4:B:803:HOH:O	2.06	0.72
1:A:351:LYS:HE3	1:A:375:VAL:HG12	1.72	0.70
1:B:538:ALA:HA	1:B:543:LEU:HD12	1.75	0.69
1:B:382:GLN:O	1:B:574:SER:OG	2.10	0.69
1:B:457:ALA:HB1	1:B:465:THR:HG21	1.76	0.68
1:B:395:TYR:OH	1:B:545:GLU:OE2	2.07	0.68
1:A:411:ILE:HD13	3:A:703:STE:H141	1.74	0.67
1:B:328:SER:OG	4:B:804:HOH:O	2.10	0.67
1:B:347:PRO:HG2	1:B:580:THR:HB	1.77	0.67
1:B:459:ASP:OD2	1:B:468[C]:ARG:NH2	2.23	0.66
1:A:93:THR:HG23	1:A:276:MET:HG3	1.79	0.65
1:B:453:VAL:HG11	3:B:702:STE:H82	1.77	0.65
1:B:380:GLN:OE1	4:B:805:HOH:O	2.15	0.65
1:A:275:ASP:OD2	4:A:801:HOH:O	2.14	0.65
1:A:445:LEU:O	4:A:803:HOH:O	2.15	0.64
1:B:132:ARG:O	4:B:807:HOH:O	2.15	0.64
1:B:468[B]:ARG:NH1	4:B:810:HOH:O	2.29	0.64
1:B:82:GLN:OE1	1:B:109:ARG:NH2	2.29	0.64
1:B:355:VAL:O	1:B:375:VAL:HG21	1.98	0.63
1:B:575:ASN:O	4:B:806:HOH:O	2.15	0.63
1:B:578:THR:HG22	1:B:610:ALA:HB1	1.79	0.63
1:B:501:LYS:HG3	1:B:510:LYS:HB2	1.81	0.63
1:B:620:GLN:HB3	2:B:701:FAD:C2	2.27	0.62
1:B:331:LEU:HD11	1:B:337:VAL:HG23	1.82	0.62
1:B:395:TYR:O	1:B:398:ILE:HG12	2.00	0.61
1:B:81:ALA:O	1:B:82:GLN:NE2	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:O	1:B:323:THR:OG1	2.19	0.60
1:A:592:VAL:HG12	1:A:593:VAL:HG13	1.82	0.60
1:B:588:ASP:OD1	1:B:590:SER:OG	2.17	0.60
1:B:599:VAL:HB	1:B:605:LEU:HB3	1.83	0.60
1:B:533:TRP:CZ3	1:B:537:VAL:HG21	2.37	0.60
1:A:277:TYR:OH	1:A:282:LYS:NZ	2.28	0.59
1:B:533:TRP:CH2	1:B:537:VAL:HG21	2.38	0.58
1:B:185:TRP:CG	1:B:614:PRO:HG2	2.38	0.58
1:B:93:THR:HG23	1:B:276:MET:HG3	1.85	0.58
1:B:357:PRO:HG2	1:B:360:GLU:HB3	1.85	0.58
1:A:193:GLU:O	4:A:804:HOH:O	2.18	0.57
1:B:138:LEU:HD22	1:B:162:LEU:HD13	1.87	0.57
1:B:460:PRO:HG3	1:B:552:PHE:CD1	2.39	0.57
1:A:466:TYR:HE1	3:A:702:STE:H91	1.69	0.57
1:B:88:LEU:HD12	1:B:112:VAL:HG22	1.88	0.56
1:B:203:GLU:OE2	1:B:205:ASN:ND2	2.34	0.56
1:A:383:PRO:HB2	1:A:571:ILE:HD11	1.86	0.55
1:A:621:THR:O	1:A:625:VAL:HG23	2.06	0.55
1:B:427:LEU:HD22	3:B:703:STE:H172	1.88	0.55
1:B:351:LYS:HE3	1:B:375:VAL:HG12	1.88	0.55
1:A:86:TYR:HD1	1:A:338:ILE:HD11	1.72	0.55
1:A:203:GLU:OE1	1:A:214:HIS:HA	2.07	0.54
1:B:484:THR:HG21	3:B:702:STE:H62	1.89	0.54
1:B:351:LYS:HE2	1:B:357:PRO:HD2	1.89	0.54
1:A:466:TYR:CE1	3:A:702:STE:H71	2.43	0.54
1:A:170:ASN:ND2	4:A:820:HOH:O	2.36	0.54
1:A:487:LEU:HD13	1:A:531:ILE:HD13	1.89	0.54
1:A:104:ALA:HA	1:A:287:ARG:NH1	2.22	0.53
1:B:391:VAL:HG13	1:B:482:GLY:HA2	1.89	0.53
1:A:275:ASP:OD1	1:A:277:TYR:HB3	2.08	0.53
1:B:170:ASN:HB2	2:B:701:FAD:C5X	2.39	0.52
1:A:406:ASN:ND2	4:A:822:HOH:O	2.40	0.52
1:A:170:ASN:HB2	2:A:701:FAD:C5X	2.40	0.52
1:B:226:ARG:NH2	1:B:422:GLY:O	2.43	0.52
1:B:191:SER:N	1:B:194:ASP:OD2	2.43	0.52
1:A:105:ASP:OD2	1:A:107:SER:OG	2.28	0.51
1:B:407[A]:GLU:H	1:B:407[A]:GLU:CD	2.13	0.51
1:B:406:ASN:HD21	1:B:410[A]:GLN:HB2	1.75	0.51
1:A:277:TYR:CE2	1:A:282:LYS:HD2	2.45	0.51
1:A:620:GLN:HB3	2:A:701:FAD:C2	2.40	0.51
1:B:575:ASN:HA	4:B:889:HOH:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:ASP:N	4:B:813:HOH:O	2.44	0.51
1:A:84:TYR:CD1	1:A:109[B]:ARG:HG2	2.46	0.51
1:A:185:TRP:CG	1:A:614:PRO:HG2	2.45	0.51
1:B:257:ASP:OD1	1:B:439:ARG:NH2	2.43	0.51
1:B:382:GLN:HG2	1:B:490:CYS:HA	1.93	0.51
1:B:439:ARG:HG2	1:B:446:PRO:HA	1.93	0.50
1:B:624:PRO:O	1:B:628:ILE:HG13	2.12	0.50
1:A:635:LEU:HD22	1:A:642:ILE:HD13	1.92	0.50
1:B:155:ILE:HG21	1:B:515:TYR:HE2	1.77	0.50
1:A:198:TRP:NE1	4:A:805:HOH:O	2.19	0.50
1:A:379:LEU:O	1:A:496:GLY:N	2.43	0.50
1:A:472:PHE:CZ	1:A:477:LEU:HB2	2.46	0.50
1:A:599:VAL:HG11	1:A:605:LEU:HD23	1.94	0.50
1:A:265:GLN:OE1	4:A:806:HOH:O	2.19	0.49
1:A:355:VAL:HG13	1:A:370:SER:HB3	1.93	0.49
1:B:189:GLY:O	1:B:642:ILE:HD12	2.12	0.49
1:B:191:SER:OG	1:B:192:SER:N	2.44	0.49
1:A:372:LEU:HD11	1:A:600:HIS:O	2.12	0.49
1:A:331:LEU:HD11	1:A:337:VAL:HG23	1.95	0.49
1:A:343:ALA:HA	1:A:611[A]:SER:OG	2.11	0.49
1:A:214:HIS:NE2	1:A:250:ASP:OD2	2.37	0.49
1:A:519:LYS:NZ	1:A:519:LYS:HB3	2.26	0.49
1:A:533:TRP:CH2	1:A:537:VAL:HG21	2.48	0.49
1:B:107:SER:N	4:B:817:HOH:O	2.46	0.49
1:A:594:ASP:OD1	1:A:598:ARG:HG3	2.12	0.49
1:A:583:MET:HA	1:A:593:VAL:O	2.12	0.49
1:A:538:ALA:O	4:A:807:HOH:O	2.20	0.48
1:A:301:VAL:HG22	1:A:315:VAL:HG12	1.95	0.48
1:B:257:ASP:CG	1:B:439:ARG:HH22	2.16	0.48
1:B:140:TRP:HB3	1:B:142:LEU:HG	1.96	0.48
1:B:331:LEU:HD13	1:B:335:GLY:O	2.13	0.48
1:B:354:GLY:HA2	1:B:361:LEU:CD1	2.32	0.48
1:A:592:VAL:O	1:A:600:HIS:ND1	2.44	0.47
1:B:529:LYS:HD3	1:B:532:HIS:HB2	1.96	0.47
1:A:395:TYR:O	1:A:398:ILE:HG12	2.14	0.47
1:A:588:ASP:O	1:A:591:SER:OG	2.30	0.47
1:B:483:ILE:HG12	1:B:547:LEU:HD21	1.97	0.47
1:A:440:THR:OG1	1:A:447:ASP:OD2	2.29	0.47
1:A:185:TRP:CE2	1:A:614:PRO:HD2	2.50	0.47
1:B:149:GLN:OE1	1:B:149:GLN:N	2.45	0.47
1:B:343:ALA:HA	1:B:611[A]:SER:OG	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HB3	1:A:261:TYR:HD2	1.80	0.47
1:B:300[B]:LYS:NZ	1:B:316:GLU:OE2	2.48	0.47
1:A:108:LYS:N	1:A:108:LYS:HD3	2.30	0.47
1:B:104:ALA:HA	1:B:287:ARG:NH1	2.30	0.47
1:B:97:VAL:HA	1:B:280:TYR:CD2	2.50	0.47
1:B:598:ARG:HG2	1:B:606:ARG:HG2	1.97	0.47
3:B:702:STE:H121	3:B:702:STE:H91	1.45	0.47
1:A:191:SER:OG	1:A:194:ASP:OD2	2.20	0.46
1:A:348:PHE:CD1	1:A:509:PRO:HB3	2.50	0.46
1:B:111:LEU:HA	1:B:291:GLN:O	2.15	0.46
1:B:221:ARG:HG2	1:B:279:GLN:NE2	2.31	0.46
1:B:459:ASP:HB3	1:B:465:THR:HG23	1.97	0.46
1:B:196:LEU:O	1:B:200:VAL:HG23	2.15	0.46
1:A:198:TRP:CG	1:A:631:ARG:HG3	2.50	0.46
1:B:456:MET:HB2	1:B:482:GLY:HA3	1.97	0.46
1:A:316:GLU:OE2	1:A:326:ARG:HD2	2.15	0.46
1:A:326:ARG:HD3	1:A:326:ARG:HA	1.52	0.46
1:B:581:CYS:HB2	1:B:611[B]:SER:OG	2.16	0.45
1:B:230:LYS:O	1:B:234[B]:THR:HB	2.16	0.45
1:B:486:GLN:NE2	3:B:702:STE:H31	2.31	0.45
1:A:383:PRO:CB	1:A:571:ILE:HD11	2.47	0.45
1:B:228:THR:HA	1:B:434:ARG:NH2	2.30	0.45
1:B:642:ILE:HG13	1:B:643:GLY:N	2.30	0.45
1:B:595:ASN:ND2	1:B:642:ILE:HD11	2.32	0.45
1:A:242:GLU:OE2	1:A:541:SER:OG	2.35	0.45
1:A:326:ARG:HG3	1:B:589:SER:HB2	1.99	0.45
1:A:462:GLY:H	1:A:572:HIS:CE1	2.34	0.45
1:B:338:ILE:HA	1:B:606:ARG:O	2.16	0.45
1:A:336:GLU:OE1	1:A:606:ARG:HG3	2.16	0.44
1:A:578:THR:HB	1:A:613:VAL:HB	1.99	0.44
1:A:384:ALA:HA	1:A:487:LEU:O	2.18	0.44
1:B:179:ALA:O	1:B:192:SER:HB3	2.16	0.44
1:B:343:ALA:HB3	1:B:577:ILE:HG22	1.99	0.44
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.80	0.44
3:B:702:STE:H71	3:B:702:STE:H102	1.77	0.44
1:A:144:SER:HB2	1:A:513:PRO:HD3	2.00	0.44
1:A:519:LYS:N	4:A:841:HOH:O	2.51	0.44
1:B:112:VAL:HB	1:B:292:VAL:HG22	2.00	0.44
1:A:641:THR:HG22	1:A:642:ILE:H	1.83	0.43
1:B:166:SER:O	1:B:170:ASN:HB3	2.18	0.43
1:A:84:TYR:HD1	1:A:109[B]:ARG:HG2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:SER:H	1:B:79:PRO:CD	2.30	0.43
1:B:159:ARG:HB3	4:B:898:HOH:O	2.18	0.43
1:B:288:ARG:CZ	1:B:288:ARG:HB2	2.49	0.43
1:A:127:PRO:HG2	1:A:428:THR:HA	2.00	0.43
1:A:267:MET:HE2	4:A:888:HOH:O	2.17	0.43
1:B:86:TYR:CD2	1:B:102:LEU:HD13	2.54	0.43
1:B:456:MET:O	3:B:702:STE:H101	2.19	0.43
1:A:377:GLN:O	1:A:580:THR:HA	2.19	0.43
1:B:478:LYS:O	4:B:808:HOH:O	2.21	0.43
1:B:385:CYS:HA	1:B:572:HIS:CE1	2.53	0.43
1:B:620:GLN:HB3	2:B:701:FAD:N3	2.34	0.43
1:B:185:TRP:CD1	1:B:614:PRO:HG2	2.53	0.43
1:B:456:MET:HE3	1:B:480:PRO:HG2	2.00	0.43
1:A:339:MET:HB2	1:A:607:VAL:HG22	2.01	0.43
1:B:623:ALA:HB3	1:B:624:PRO:HD3	2.01	0.43
1:A:107:SER:C	1:A:108:LYS:HD3	2.40	0.43
1:B:636:LEU:HD23	1:B:636:LEU:HA	1.65	0.43
1:B:582:LYS:HG3	1:B:614:PRO:HA	2.01	0.42
1:A:468:ARG:NH1	1:A:471:LYS:HD2	2.34	0.42
1:B:172:THR:O	1:B:267:MET:N	2.50	0.42
1:A:468:ARG:HA	1:A:468:ARG:HD3	1.75	0.42
1:B:275:ASP:OD2	1:B:277:TYR:HB3	2.19	0.42
1:A:232:LEU:HD13	1:A:483:ILE:HG22	2.01	0.42
1:A:340:CYS:O	2:A:701:FAD:H52A	2.20	0.42
1:B:516:LEU:HD11	1:B:571:ILE:HD12	2.01	0.42
1:B:230:LYS:O	1:B:234[A]:THR:HB	2.18	0.42
1:B:559:SER:O	1:B:563:ILE:HG13	2.19	0.42
1:A:198:TRP:CD1	1:A:631:ARG:HG3	2.53	0.42
1:B:606:ARG:HH12	1:B:635:LEU:HD21	1.85	0.42
1:B:581:CYS:HA	1:B:592:VAL:HG21	2.00	0.42
1:B:95:ALA:HB2	1:B:340:CYS:CB	2.50	0.42
1:B:376:GLY:O	1:B:497:SER:HA	2.20	0.42
1:B:384:ALA:HA	1:B:487:LEU:O	2.20	0.42
1:A:105:ASP:OD1	1:A:105:ASP:N	2.39	0.41
1:A:313:LEU:C	1:A:331:LEU:HD12	2.40	0.41
1:A:453:VAL:C	1:A:455:GLY:H	2.22	0.41
1:A:135:ARG:NH1	1:A:143:PHE:HE1	2.18	0.41
1:A:484:THR:HG21	3:A:702:STE:H61	2.02	0.41
1:B:569[A]:ARG:NH2	4:B:819:HOH:O	2.46	0.41
1:A:641:THR:C	1:A:642:ILE:HD12	2.41	0.41
1:B:245:LEU:HD12	1:B:245:LEU:HA	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ASN:HB3	2:A:701:FAD:C8	2.50	0.41
1:A:391:VAL:HG13	1:A:482:GLY:HA2	2.02	0.41
1:A:518:ASP:HB2	4:A:841:HOH:O	2.20	0.41
1:B:406:ASN:ND2	1:B:410[A]:GLN:HB2	2.36	0.41
1:B:435:GLY:HA3	1:B:450:VAL:O	2.20	0.41
1:B:140:TRP:HE1	2:B:701:FAD:H2B	1.85	0.41
1:B:543:LEU:O	1:B:546:TYR:N	2.42	0.41
1:A:100:ASN:OD1	1:A:101:ARG:HD3	2.21	0.41
1:A:147:GLN:OE1	1:A:513:PRO:HD2	2.20	0.41
1:A:414[B]:ARG:HB2	4:A:985:HOH:O	2.19	0.41
1:A:550:GLU:HG3	4:A:962:HOH:O	2.21	0.41
1:A:588:ASP:HB3	1:A:591:SER:OG	2.20	0.41
1:A:596:GLN:O	1:A:606:ARG:NH1	2.52	0.41
1:B:553:PRO:HB3	1:B:566:TYR:CG	2.56	0.41
1:A:168:ALA:HA	1:A:273:ARG:HD3	2.02	0.41
1:A:511:LEU:HD12	1:A:511:LEU:HA	1.81	0.41
1:B:402:ASP:HA	4:B:862:HOH:O	2.20	0.41
1:B:519:LYS:H	1:B:519:LYS:HG2	1.57	0.40
1:B:606:ARG:CZ	1:B:636:LEU:HD21	2.50	0.40
2:A:701:FAD:H9	2:A:701:FAD:H1'1	1.86	0.40
3:A:702:STE:H91	3:A:702:STE:H122	1.69	0.40
1:B:400:ILE:HB	1:B:454:PRO:HG2	2.04	0.40
1:B:460:PRO:HD3	1:B:552:PHE:CZ	2.57	0.40
1:A:301:VAL:O	1:A:303:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	573/578 (99%)	530 (92%)	38 (7%)	5 (1%)	17 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	571/578 (99%)	522 (91%)	41 (7%)	8 (1%)	11	5
All	All	1144/1156 (99%)	1052 (92%)	79 (7%)	13 (1%)	13	8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253	ASP
1	A	577	ILE
1	B	78	SER
1	B	443	GLN
1	A	105	ASP
1	B	103	SER
1	B	577	ILE
1	A	78	SER
1	A	106	GLY
1	B	217	GLY
1	B	614	PRO
1	A	79	PRO
1	B	375	VAL

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	452/442 (102%)	432 (96%)	20 (4%)	28	25
1	B	449/442 (102%)	410 (91%)	39 (9%)	10	6
All	All	901/884 (102%)	842 (94%)	59 (6%)	18	12

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	108	LYS
1	A	109[A]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109[B]	ARG
1	A	148[A]	GLU
1	A	148[B]	GLU
1	A	197	SER
1	A	201[A]	GLN
1	A	201[B]	GLN
1	A	330	GLU
1	A	366	ILE
1	A	468	ARG
1	A	481	SER
1	A	502	SER
1	A	519	LYS
1	A	529	LYS
1	A	561	ASP
1	A	598	ARG
1	A	631	ARG
1	A	641	THR
1	B	77	SER
1	B	78	SER
1	B	121	SER
1	B	146	LEU
1	B	148	GLU
1	B	191	SER
1	B	194	ASP
1	B	201	GLN
1	B	234[A]	THR
1	B	234[B]	THR
1	B	256	HIS
1	B	288	ARG
1	B	304	ASP
1	B	311	GLN
1	B	315	VAL
1	B	320	ASP
1	B	323	THR
1	B	325	GLU
1	B	344	VAL
1	B	352	HIS
1	B	361	LEU
1	B	394	LYS
1	B	413	LYS
1	B	456	MET
1	B	495	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	519	LYS
1	B	524	LEU
1	B	529	LYS
1	B	561	ASP
1	B	565[A]	GLU
1	B	565[B]	GLU
1	B	571	ILE
1	B	574	SER
1	B	596	GLN
1	B	603	GLU
1	B	605	LEU
1	B	615	LYS
1	B	631	ARG
1	B	642	ILE

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

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](#)

6 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
2	FAD	A	701	-	53,58,58	0.60	0	68,89,89	0.77	2 (2%)
3	STE	B	702	-	16,16,19	0.25	0	15,15,19	0.75	0
2	FAD	B	701	-	53,58,58	0.64	0	68,89,89	0.81	3 (4%)
3	STE	A	702	-	16,16,19	0.25	0	15,15,19	0.68	0
3	STE	B	703	-	9,9,19	0.27	0	8,8,19	0.62	0
3	STE	A	703	-	9,9,19	0.30	0	8,8,19	0.47	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
2	FAD	A	701	-	-	1/30/50/50	0/6/6/6
3	STE	B	702	-	-	10/14/14/17	-
2	FAD	B	701	-	-	2/30/50/50	0/6/6/6
3	STE	A	702	-	-	8/14/14/17	-
3	STE	B	703	-	-	3/7/7/17	-
3	STE	A	703	-	-	1/7/7/17	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FAD	O4B-C1B-C2B	-2.58	103.15	106.93
2	A	701	FAD	C5A-C6A-N6A	2.34	123.92	120.35
2	B	701	FAD	C5A-C6A-N6A	2.30	123.84	120.35
2	B	701	FAD	O4B-C1B-C2B	-2.08	103.89	106.93
2	B	701	FAD	C4-N3-C2	-2.04	121.88	125.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	STE	C9-C10-C11-C12
3	B	702	STE	C9-C10-C11-C12
3	B	702	STE	C6-C7-C8-C9
3	B	702	STE	C2-C3-C4-C5
3	B	702	STE	C4-C5-C6-C7
3	B	703	STE	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	702	STE	C11-C12-C13-C14
3	A	702	STE	C12-C13-C14-C15
3	A	702	STE	C10-C11-C12-C13
3	A	702	STE	C14-C15-C16-C17
3	B	703	STE	C15-C16-C17-C18
2	B	701	FAD	O4B-C4B-C5B-O5B
3	A	702	STE	C11-C10-C9-C8
3	B	702	STE	C13-C14-C15-C16
3	B	702	STE	C11-C10-C9-C8
3	B	703	STE	C11-C12-C13-C14
3	B	702	STE	C12-C13-C14-C15
3	A	702	STE	C4-C5-C6-C7
3	A	703	STE	C15-C16-C17-C18
3	B	702	STE	C5-C6-C7-C8
3	B	702	STE	C7-C8-C9-C10
2	A	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	C3B-C4B-C5B-O5B
3	A	702	STE	C2-C3-C4-C5
3	A	702	STE	C6-C7-C8-C9

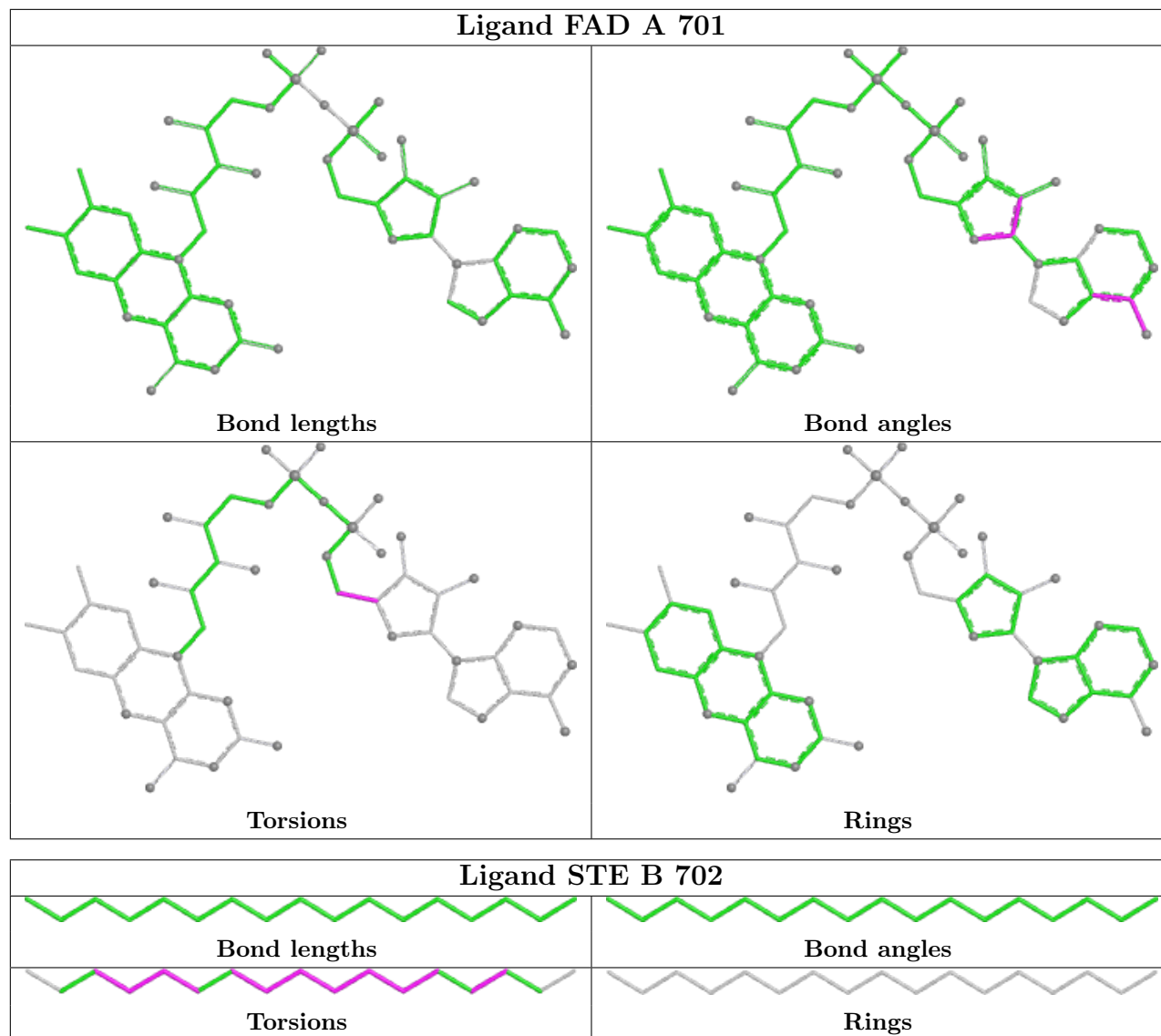
There are no ring outliers.

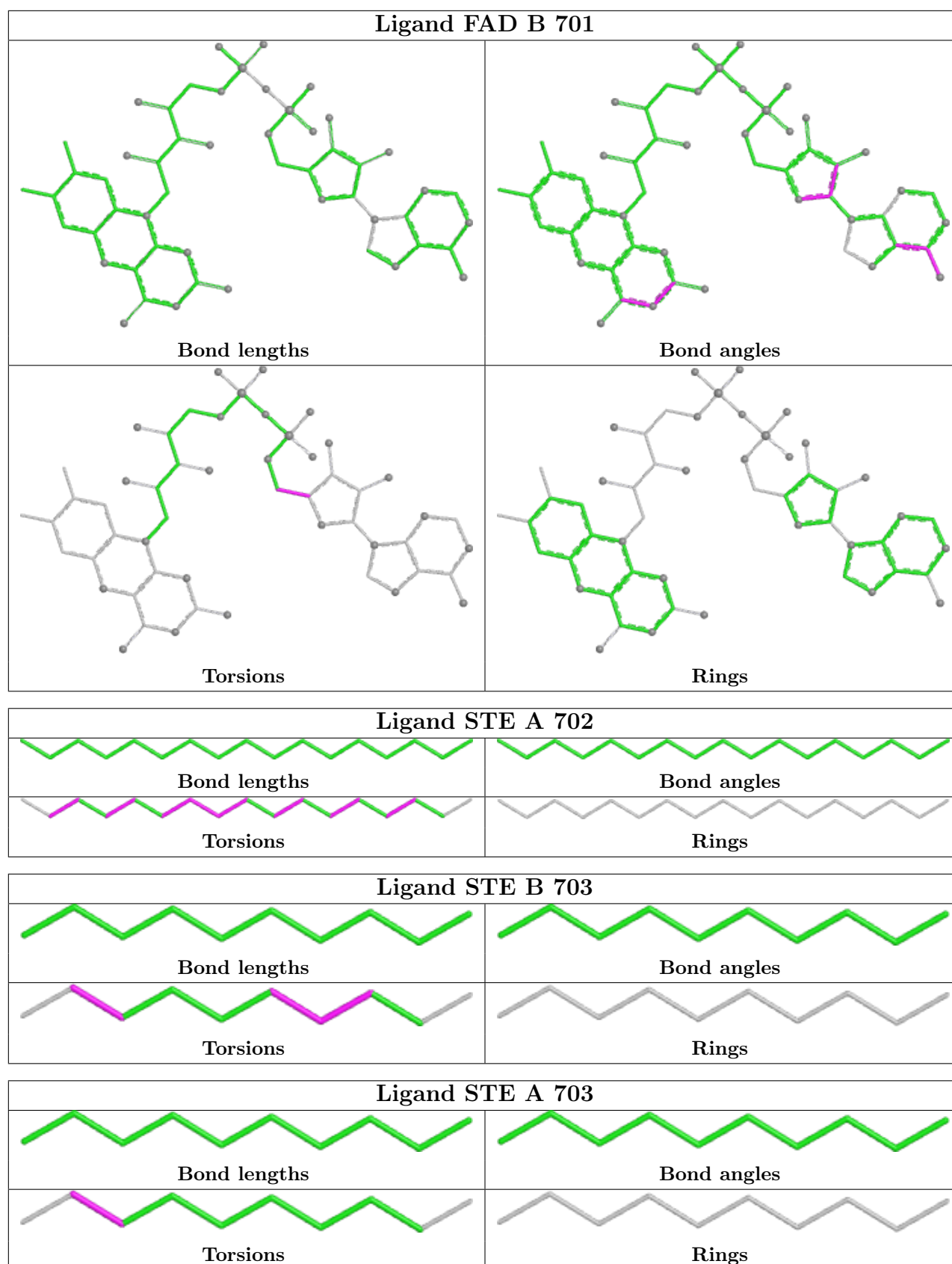
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	5	0
3	B	702	STE	6	0
2	B	701	FAD	4	0
3	A	702	STE	4	0
3	B	703	STE	1	0
3	A	703	STE	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	563/578 (97%)	-0.21	4 (0%) 87 87	13, 25, 57, 76	0
1	B	562/578 (97%)	-0.10	8 (1%) 75 74	11, 29, 59, 75	0
All	All	1125/1156 (97%)	-0.15	12 (1%) 80 79	11, 27, 58, 76	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	GLY	4.3
1	B	356	GLY	4.2
1	B	642	ILE	3.2
1	B	586	ALA	2.9
1	A	305[A]	GLN	2.8
1	A	332	ALA	2.6
1	B	77	SER	2.5
1	B	373	ALA	2.4
1	B	506	PHE	2.4
1	B	324	GLY	2.4
1	B	643	GLY	2.2
1	A	364	PHE	2.2

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](#)

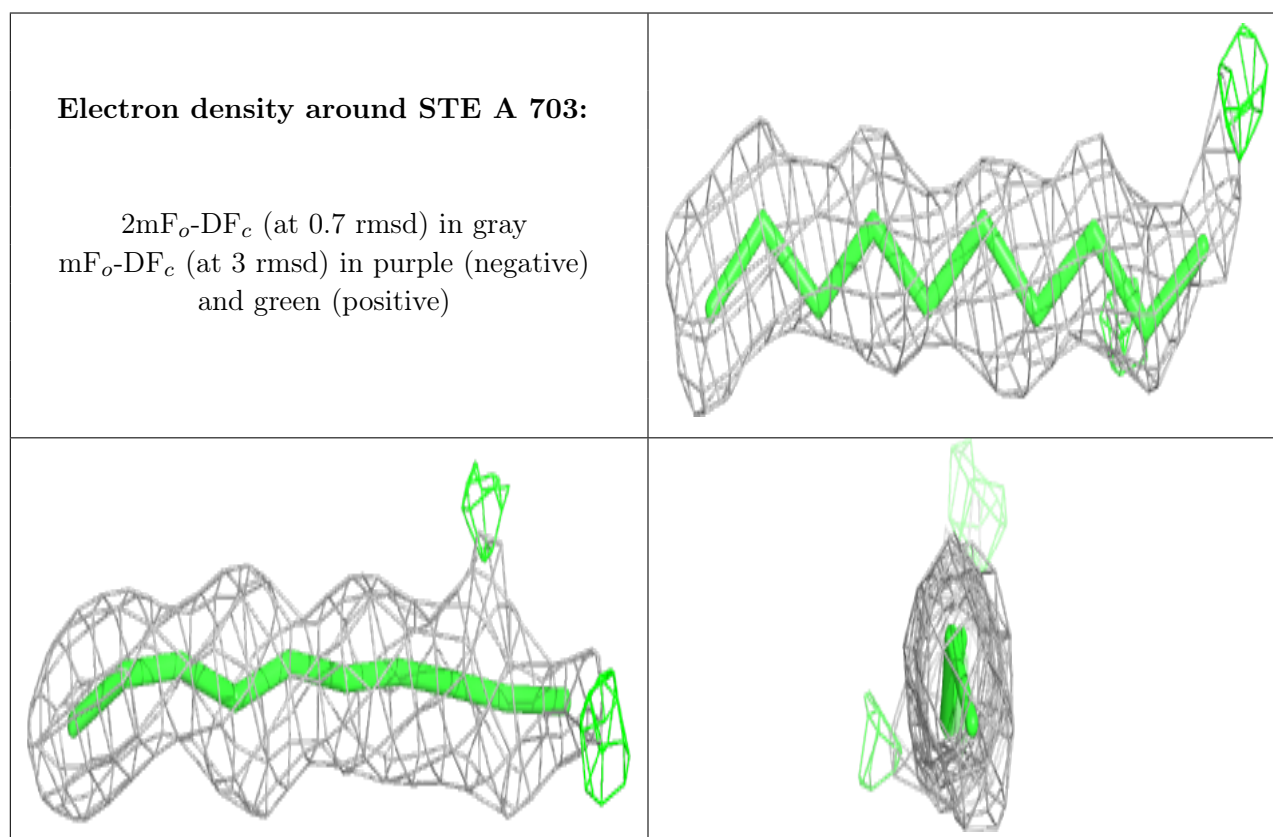
There are no monosaccharides in this entry.

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

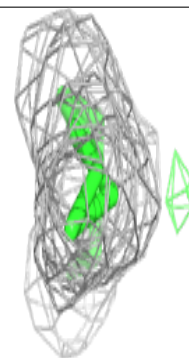
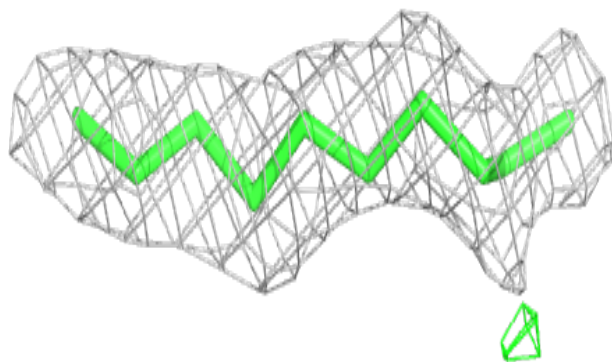
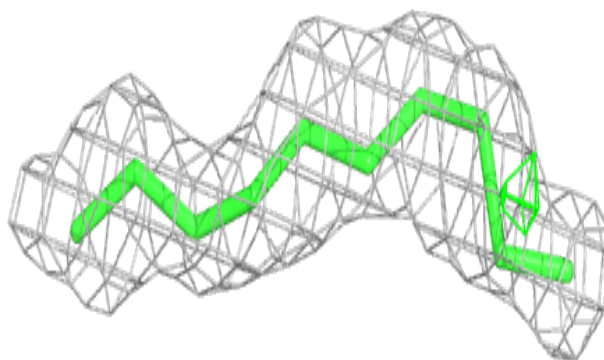
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	STE	A	703	10/20	0.90	0.15	13,29,41,42	0
3	STE	B	703	10/20	0.91	0.14	15,25,34,36	0
3	STE	B	702	17/20	0.92	0.14	11,18,27,63	0
3	STE	A	702	17/20	0.93	0.12	11,21,27,37	0
2	FAD	A	701	53/53	0.96	0.11	11,20,52,58	0
2	FAD	B	701	53/53	0.96	0.10	10,22,35,48	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.

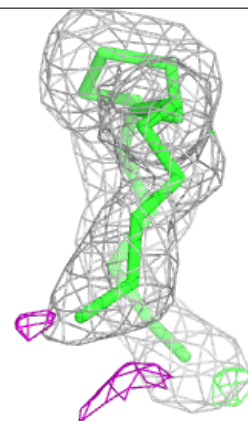
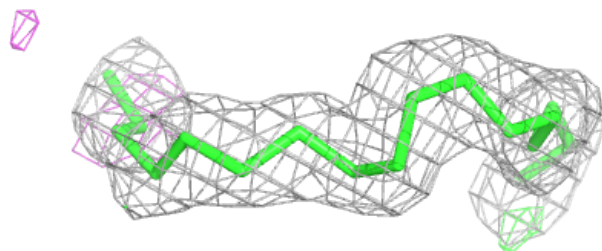
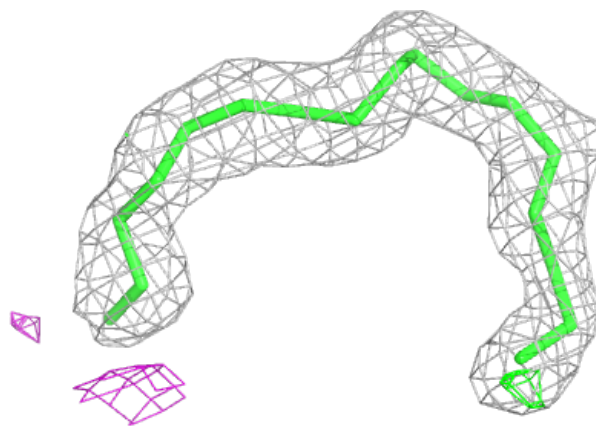


Electron density around STE B 703:

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

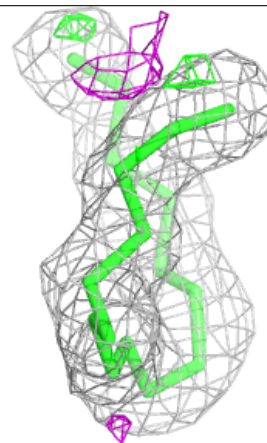
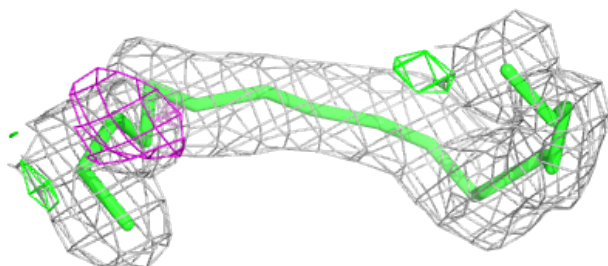
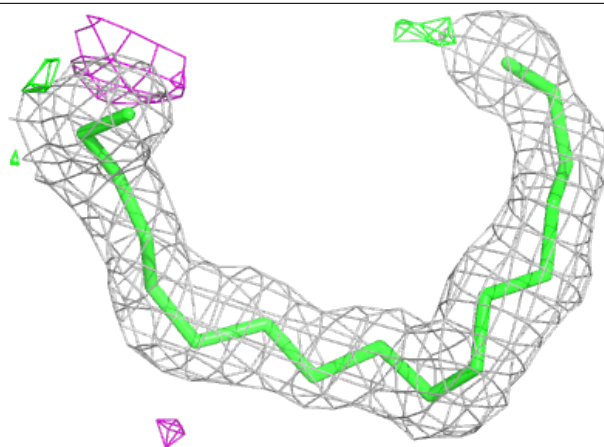
**Electron density around STE B 702:**

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

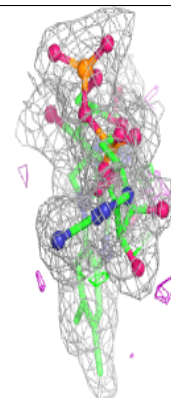
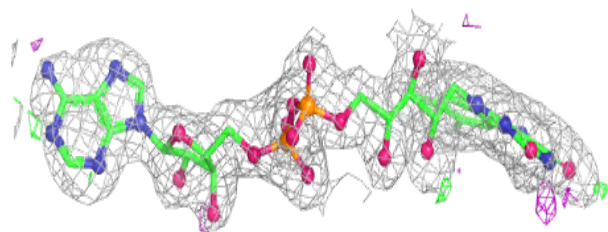
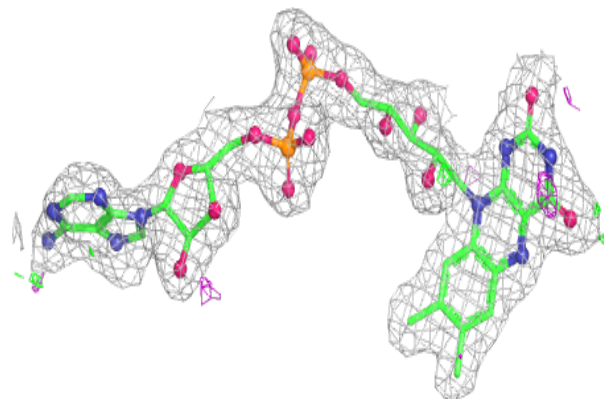


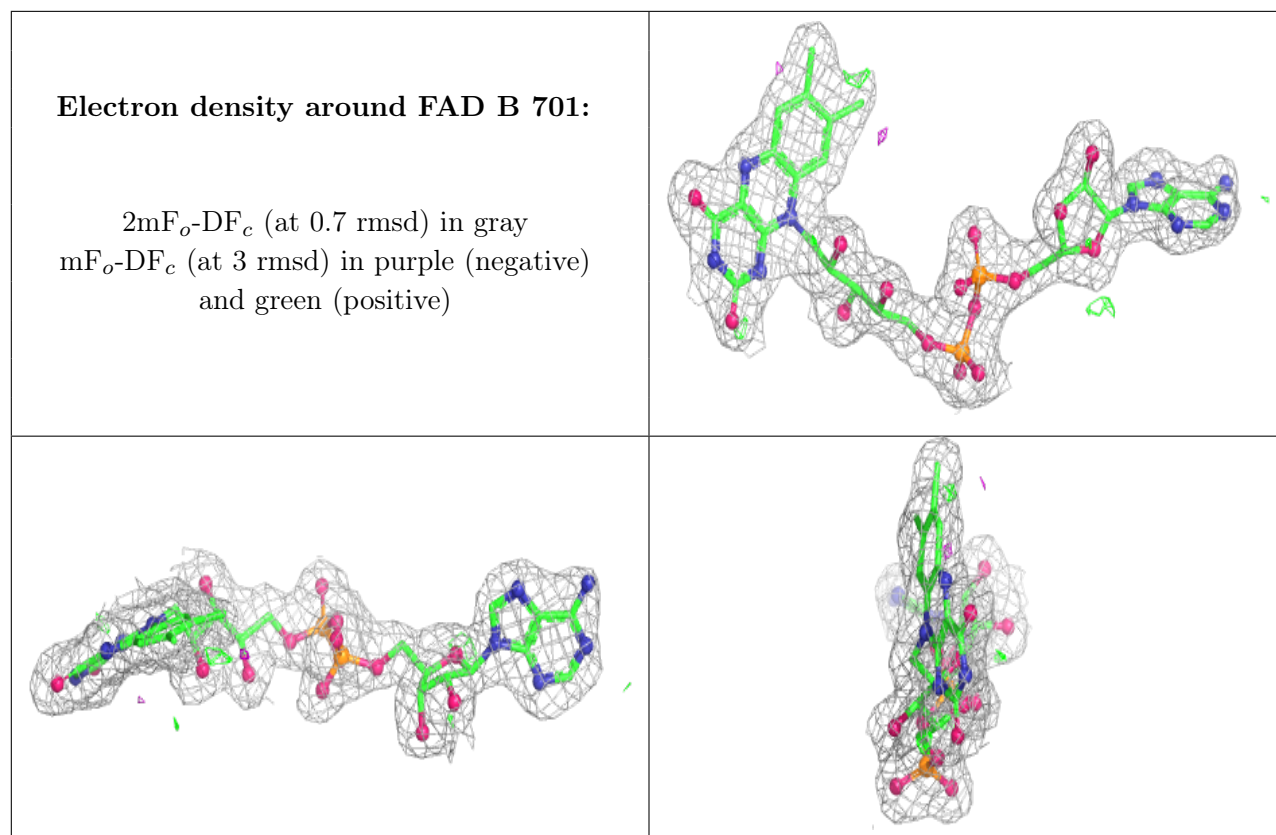
Electron density around STE A 702:

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

**Electron density around FAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.