



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:50 AM UTC

PDB ID : 6H3G / pdb_00006h3g
Title : Alcohol oxidase from Phanerochaete chrysosporium
Authors : Nguyen, Q.-T.; Romero, E.; Dijkman, W.P.; de Vasconcellos, S.P.; Binda, C.;
Mattevi, A.; Fraaije, M.W.
Deposited on : 2018-07-18
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

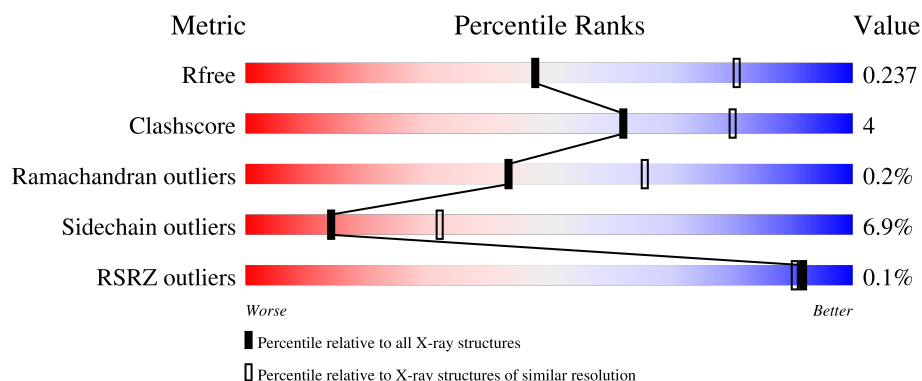
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	651	 84% 14% ..
1	B	651	 84% 13% ..
1	C	651	 83% 14% ..
1	D	651	 86% 11% ..
1	E	651	 86% 12% .

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Mol	Chain	Length	Quality of chain
1	F	651	 84%13%..
1	G	651	 84%12%..
1	H	651	 82%14%..

2 Entry composition

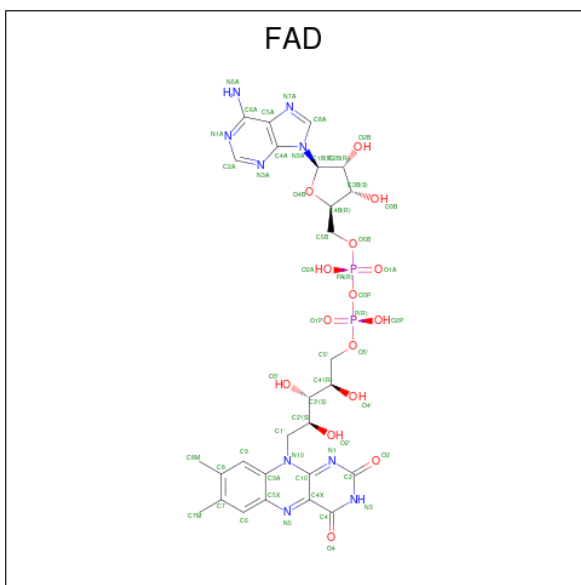
There are 4 unique types of molecules in this entry. The entry contains 41161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alcohol oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	1	0
			5052	3178	893	956	25			
1	B	642	Total	C	N	O	S	0	0	0
			5036	3169	889	953	25			
1	C	636	Total	C	N	O	S	0	1	0
			5003	3147	884	947	25			
1	D	636	Total	C	N	O	S	0	0	0
			4992	3141	880	946	25			
1	E	637	Total	C	N	O	S	0	0	0
			4999	3146	881	947	25			
1	F	646	Total	C	N	O	S	0	1	0
			5074	3190	900	959	25			
1	G	635	Total	C	N	O	S	0	0	0
			4985	3136	879	945	25			
1	H	636	Total	C	N	O	S	0	0	0
			4992	3141	880	946	25			

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



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	101	Total	O	0	0
			101	101		
4	C	72	Total	O	0	0
			72	72		
4	D	85	Total	O	0	0
			85	85		
4	E	45	Total	O	0	0
			45	45		
4	F	66	Total	O	0	0
			66	66		
4	G	73	Total	O	0	0
			73	73		

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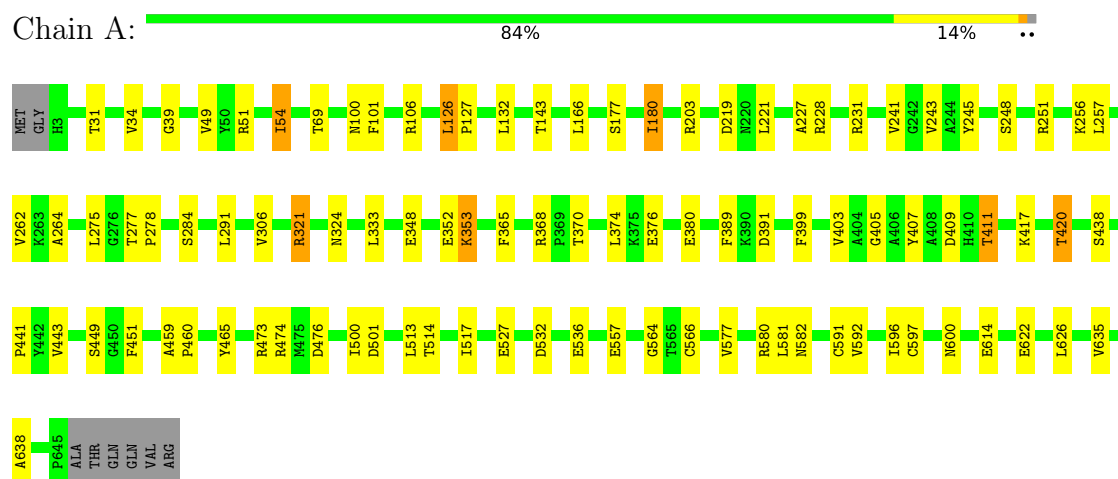
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	89	Total	O	0	0
			89	89		

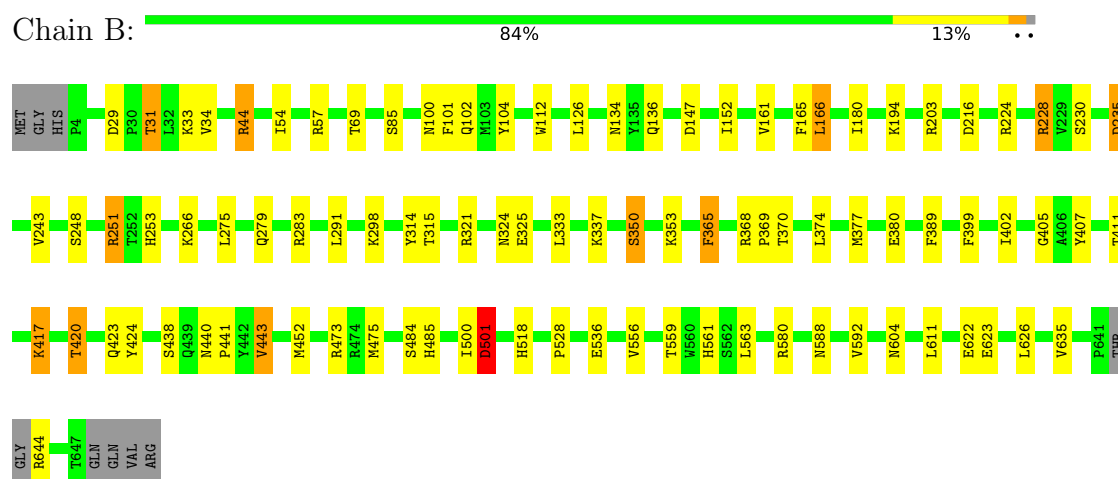
3 Residue-property plots

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.

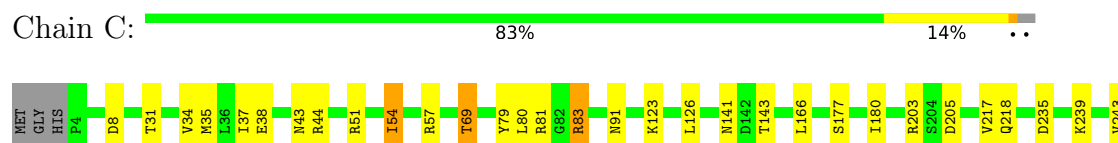
• Molecule 1: Alcohol oxidase

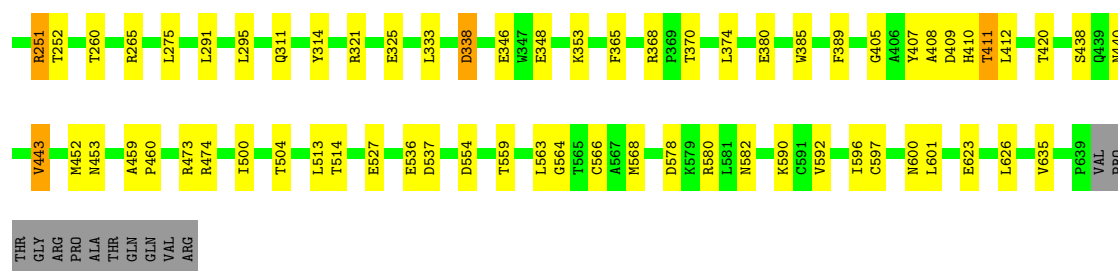


• Molecule 1: Alcohol oxidase



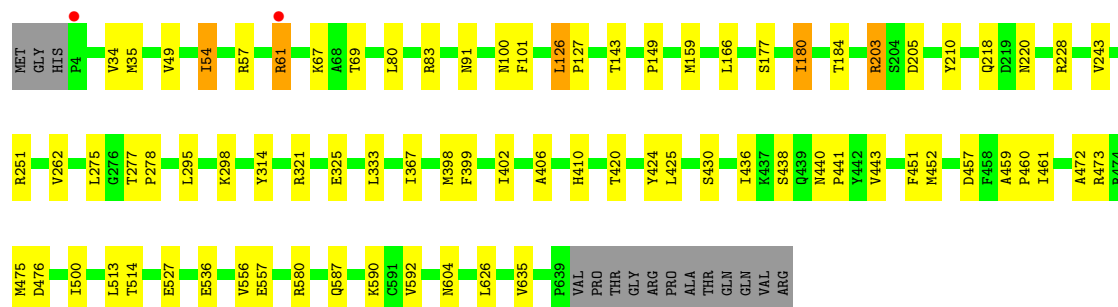
• Molecule 1: Alcohol oxidase





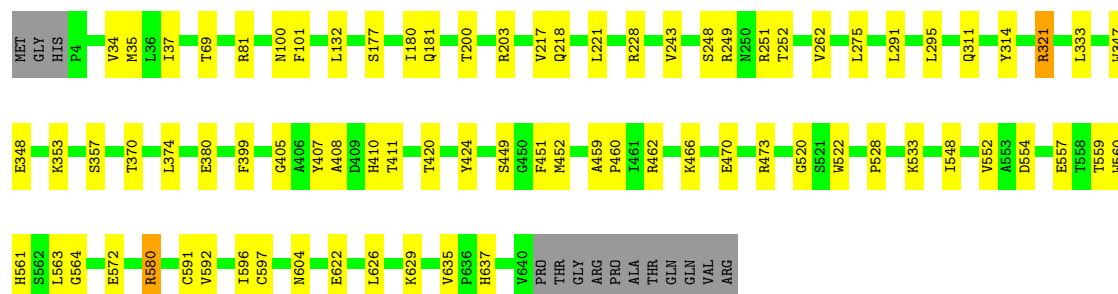
• Molecule 1: Alcohol oxidase

Chain D: 86% 11% ..



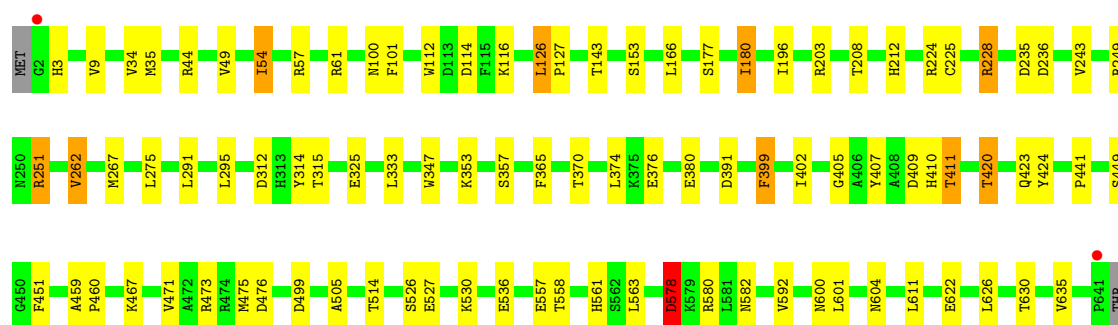
• Molecule 1: Alcohol oxidase

Chain E: 86% 12% .



• Molecule 1: Alcohol oxidase

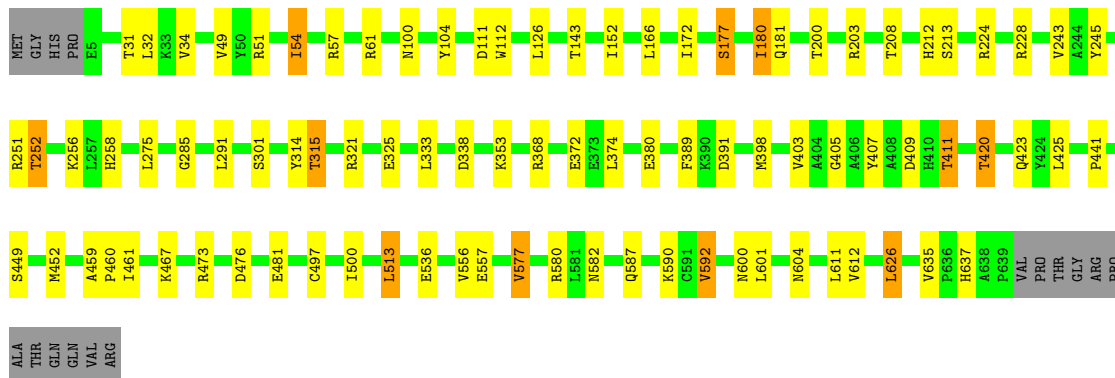
Chain F: 84% 13% ..





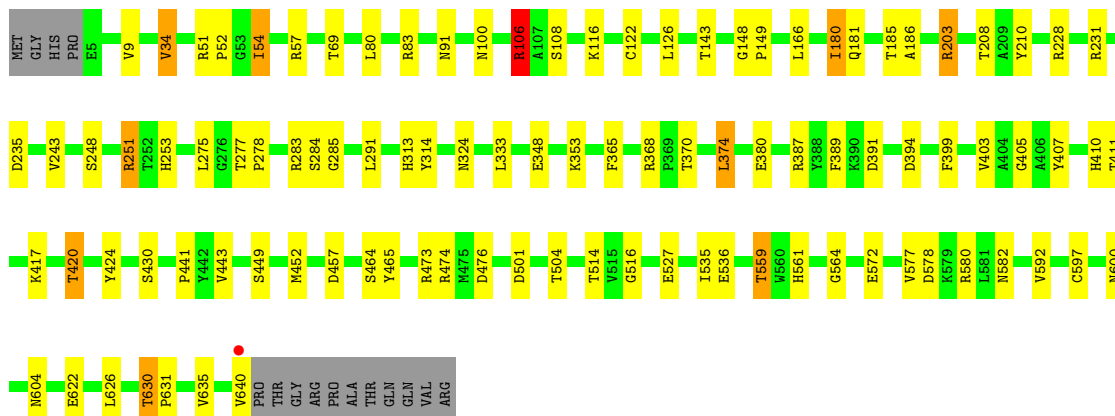
• Molecule 1: Alcohol oxidase

Chain G: 84% 12% ..



• Molecule 1: Alcohol oxidase

Chain H: 82% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.67Å 204.04Å 116.52Å 90.00° 105.02° 90.00°	Depositor
Resolution (Å)	49.32 – 2.60 49.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.32-2.60) 97.6 (49.32-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.193 , 0.264 (Not available) , 0.237	Depositor DCC
R_{free} test set	7538 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	41161	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.66	0/5178	0.97	0/7031
1	B	0.68	0/5160	0.97	1/7004 (0.0%)
1	C	0.67	0/5126	0.98	0/6956
1	D	0.68	1/5115 (0.0%)	0.98	2/6942 (0.0%)
1	E	0.68	0/5122	0.98	0/6952
1	F	0.69	0/5199	0.98	0/7056
1	G	0.68	0/5107	0.98	2/6931 (0.0%)
1	H	0.69	0/5114	0.99	3/6941 (0.0%)
All	All	0.68	1/41121 (0.0%)	0.98	8/55813 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	E	0	2
1	H	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	367	ILE	N-CA	5.28	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	527	GLU	CB-CA-C	5.50	117.36	109.11
1	D	205	ASP	CA-CB-CG	5.32	117.92	112.60
1	H	122	CYS	CA-C-N	5.28	127.67	120.54
1	H	122	CYS	C-N-CA	5.28	127.67	120.54
1	G	577	VAL	CA-C-N	5.23	129.71	120.87
1	G	577	VAL	C-N-CA	5.23	129.71	120.87
1	D	527	GLU	CB-CA-C	5.22	116.22	108.87
1	B	365	PHE	CA-CB-CG	5.15	118.95	113.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	ARG	Sidechain
1	B	321	ARG	Sidechain
1	B	500	ILE	Peptide
1	C	203	ARG	Sidechain
1	E	321	ARG	Sidechain
1	E	462	ARG	Sidechain
1	H	106	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5052	0	4923	42	0
1	B	5036	0	4912	42	0
1	C	5003	0	4877	39	0
1	D	4992	0	4865	43	0
1	E	4999	0	4874	36	0
1	F	5074	0	4944	51	0
1	G	4985	0	4857	40	0
1	H	4992	0	4866	54	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
2	C	53	0	31	1	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	53	0	31	3	0
2	G	53	0	31	2	0
2	H	53	0	31	1	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	H	12	0	16	2	0
4	A	43	0	0	0	0
4	B	101	0	0	3	0
4	C	72	0	0	2	0
4	D	85	0	0	1	0
4	E	45	0	0	3	0
4	F	66	0	0	1	0
4	G	73	0	0	2	0
4	H	89	0	0	3	0
All	All	41161	0	39406	327	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 (327) 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:228:ARG:NH1	1:A:441:PRO:O	1.92	1.02
1:D:580:ARG:O	1:D:590:LYS:NZ	2.00	0.94
1:D:410:HIS:ND1	1:H:514:THR:HG21	1.86	0.89
1:F:61[B]:ARG:HH11	1:F:61[B]:ARG:CG	1.95	0.79
1:H:580:ARG:NH2	1:H:622:GLU:OE1	2.14	0.79
1:E:81:ARG:NH1	1:E:554:ASP:OD2	2.20	0.74
1:H:368:ARG:NH2	1:H:389:PHE:O	2.24	0.71
1:A:405:GLY:O	1:A:420:THR:HG22	1.91	0.70
1:D:228:ARG:NH1	1:D:441:PRO:O	2.24	0.70
1:E:100:ASN:O	1:E:203:ARG:NH2	2.25	0.69
1:B:473:ARG:NH2	1:B:536:GLU:O	2.26	0.69
1:C:568:MET:O	4:C:801:HOH:O	2.12	0.68
1:H:283:ARG:NH2	4:H:801:HOH:O	2.25	0.67
1:C:368:ARG:NH2	1:C:389:PHE:O	2.28	0.67
1:C:514:THR:HG21	1:F:410:HIS:ND1	2.09	0.67
1:F:473:ARG:NH2	1:F:536:GLU:O	2.27	0.66
1:B:407:TYR:H	1:B:420:THR:HG21	1.59	0.66
1:F:100:ASN:O	1:F:203:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:228:ARG:NH1	1:H:441:PRO:O	2.29	0.65
1:E:101:PHE:HB2	2:E:701:FAD:O4	1.98	0.64
1:G:473:ARG:NH2	1:G:536:GLU:O	2.32	0.63
1:H:100:ASN:O	1:H:203:ARG:NH2	2.33	0.62
1:F:61[B]:ARG:HH11	1:F:61[B]:ARG:HG2	1.66	0.61
1:G:228:ARG:NH1	1:G:441:PRO:O	2.34	0.61
1:D:399:PHE:CD1	1:D:424:TYR:CD2	2.89	0.60
1:F:101:PHE:HB2	2:F:701:FAD:O4	2.02	0.60
1:A:473:ARG:NH2	1:A:536:GLU:O	2.33	0.60
1:H:108:SER:OG	1:H:394:ASP:O	2.15	0.59
1:F:580:ARG:HH22	1:F:622:GLU:CD	2.10	0.59
1:C:8:ASP:OD1	1:C:265:ARG:NH1	2.34	0.59
1:C:38:GLU:OE1	2:C:701:FAD:O2B	2.10	0.59
1:E:399:PHE:CG	1:E:424:TYR:CE2	2.90	0.59
1:F:604:ASN:HB3	2:F:701:FAD:C2	2.32	0.59
1:A:514[B]:THR:HG23	1:A:517:ILE:HD12	1.85	0.59
1:F:347:TRP:CD1	1:F:357:SER:HG	2.20	0.59
1:A:409:ASP:OD1	1:A:411:THR:HB	2.02	0.59
1:E:203:ARG:NH1	4:E:801:HOH:O	2.36	0.58
1:E:217:VAL:HG23	1:E:218:GLN:HG3	1.84	0.58
1:F:312:ASP:OD2	1:F:558:THR:OG1	2.19	0.58
1:F:407:TYR:H	1:F:420:THR:HG21	1.67	0.58
1:D:101:PHE:HB2	2:D:701:FAD:O4	2.04	0.58
1:E:314:TYR:O	1:E:424:TYR:HA	2.04	0.58
1:C:409:ASP:OD1	1:C:411:THR:HB	2.04	0.58
1:A:438:SER:HB3	1:A:443:VAL:HG21	1.86	0.58
1:D:399:PHE:CD1	1:D:424:TYR:CE2	2.91	0.57
1:E:347:TRP:CD1	1:E:357:SER:HG	2.21	0.57
1:A:514[A]:THR:HG21	1:E:410:HIS:HB2	1.85	0.57
1:D:430:SER:HB2	1:D:457:ASP:OD2	2.05	0.57
1:A:39:GLY:O	1:A:248:SER:OG	2.22	0.57
1:C:338:ASP:OD1	1:C:338:ASP:N	2.38	0.57
1:B:57:ARG:HD2	4:B:821:HOH:O	2.06	0.56
1:F:61[B]:ARG:HH11	1:F:61[B]:ARG:HG3	1.71	0.56
1:C:141:ASN:OD1	1:C:143:THR:OG1	2.19	0.56
1:A:407:TYR:H	1:A:420:THR:HG21	1.70	0.56
1:C:438:SER:HB3	1:C:443:VAL:HG21	1.86	0.56
1:B:230:SER:O	1:B:283:ARG:HD2	2.05	0.56
1:H:69:THR:HG23	1:H:91:ASN:HB2	1.88	0.55
1:A:403:VAL:HB	1:A:420:THR:HG23	1.89	0.55
2:B:701:FAD:O2A	2:B:701:FAD:O4'	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:THR:HA	1:G:423:GLN:O	2.07	0.55
1:H:407:TYR:H	1:H:420:THR:HG21	1.72	0.55
1:F:100:ASN:HB2	2:F:701:FAD:C5X	2.37	0.55
1:G:411:THR:HG21	4:G:806:HOH:O	2.07	0.55
1:E:466:LYS:O	1:E:470:GLU:HG2	2.07	0.55
1:B:161:VAL:HG13	4:B:840:HOH:O	2.06	0.54
1:B:561:HIS:CE1	1:B:604:ASN:HA	2.42	0.54
1:G:100:ASN:O	1:G:203:ARG:NH2	2.40	0.54
1:H:405:GLY:O	1:H:420:THR:HG22	2.06	0.54
1:C:43:ASN:ND2	1:C:205:ASP:OD2	2.40	0.54
1:G:405:GLY:O	1:G:420:THR:HG22	2.06	0.54
1:G:580:ARG:O	1:G:590:LYS:NZ	2.40	0.54
1:H:313:HIS:HB2	1:H:559:THR:HG23	1.88	0.54
1:G:403:VAL:HB	1:G:420:THR:HG23	1.90	0.54
1:F:499:ASP:O	1:F:526:SER:OG	2.21	0.53
1:B:402:ILE:HD12	1:B:475:MET:HE1	1.89	0.53
1:F:35:MET:CE	1:F:262:VAL:HG21	2.37	0.53
1:B:101:PHE:HB2	2:B:701:FAD:O4	2.07	0.53
1:D:452:MET:HE1	1:D:461:ILE:CD1	2.38	0.53
1:C:440:ASN:HB3	1:C:443:VAL:HG13	1.90	0.53
1:C:459:ALA:N	1:C:460:PRO:HD2	2.23	0.53
1:F:402:ILE:HD12	1:F:475:MET:HE1	1.91	0.53
1:G:208:THR:HA	1:G:212:HIS:HB2	1.91	0.53
1:C:473:ARG:NH2	1:C:536:GLU:O	2.41	0.53
1:A:51:ARG:HB2	1:A:54:ILE:HD13	1.91	0.53
1:D:80:LEU:O	1:D:83:ARG:HG2	2.09	0.53
1:C:346:GLU:HB3	4:C:810:HOH:O	2.09	0.52
1:D:149:PRO:HG2	1:D:210:TYR:CE1	2.44	0.52
1:E:311:GLN:HB2	1:E:563:LEU:HD12	1.91	0.52
1:A:580:ARG:HH22	1:A:622:GLU:CD	2.18	0.52
1:B:251:ARG:NH1	1:D:476:ASP:OD1	2.42	0.51
1:A:368:ARG:NH2	1:A:389:PHE:O	2.43	0.51
1:B:100:ASN:O	1:B:203:ARG:NH2	2.42	0.51
1:F:35:MET:HE2	1:F:262:VAL:HG21	1.91	0.51
1:F:399:PHE:CD1	1:F:424:TYR:CD2	2.98	0.51
1:H:51:ARG:HB2	1:H:54:ILE:HD13	1.91	0.51
1:A:449:SER:OG	1:A:451:PHE:CD1	2.63	0.51
1:E:459:ALA:N	1:E:460:PRO:HD2	2.25	0.51
1:G:368:ARG:NH2	1:G:389:PHE:O	2.44	0.51
1:G:452:MET:HE3	1:G:556:VAL:HG21	1.92	0.51
1:A:352:GLU:HG2	1:A:353:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:O	1:A:203:ARG:HD2	2.10	0.50
1:C:578:ASP:OD2	1:C:582:ASN:HB2	2.12	0.50
1:G:557:GLU:HG3	4:G:808:HOH:O	2.11	0.50
1:D:473:ARG:NH2	1:D:536:GLU:O	2.44	0.50
1:A:101:PHE:HB2	2:A:701:FAD:O4	2.11	0.50
1:C:405:GLY:O	1:C:420:THR:HG22	2.11	0.50
1:G:49:VAL:O	1:G:203:ARG:HD2	2.11	0.50
1:E:180:ILE:HG22	1:E:181:GLN:NE2	2.27	0.50
1:F:228:ARG:NH1	1:F:441:PRO:O	2.45	0.50
1:H:578:ASP:OD2	1:H:582:ASN:HB2	2.11	0.50
1:F:112:TRP:CZ2	1:F:611:LEU:HD23	2.47	0.50
1:G:321:ARG:HD3	1:G:500:ILE:HB	1.94	0.50
1:A:635:VAL:HG13	1:A:638:ALA:CB	2.42	0.50
1:B:104:TYR:CE1	1:B:152:ILE:HD13	2.47	0.50
1:H:106:ARG:HH22	1:H:143:THR:HG22	1.76	0.49
1:F:314:TYR:O	1:F:424:TYR:HA	2.12	0.49
1:H:57:ARG:HD2	4:H:825:HOH:O	2.12	0.49
1:D:514:THR:HG21	1:H:410:HIS:ND1	2.28	0.49
1:F:578:ASP:HB3	1:F:580:ARG:H	1.77	0.49
1:H:604:ASN:HB3	2:H:701:FAD:C2	2.42	0.49
1:C:69:THR:HG23	1:C:91:ASN:HB2	1.95	0.49
1:E:580:ARG:HH22	1:E:622:GLU:CD	2.21	0.49
1:D:410:HIS:H	1:H:514:THR:HG23	1.77	0.49
1:G:314:TYR:CD2	1:G:452:MET:HE2	2.47	0.49
1:H:561:HIS:CE1	1:H:604:ASN:HA	2.47	0.49
1:A:277:THR:HB	1:A:278:PRO:HD3	1.95	0.49
1:D:126:LEU:HB3	1:D:127:PRO:HD3	1.95	0.49
1:D:406:ALA:HA	1:D:420:THR:HG22	1.95	0.49
1:G:476:ASP:OD1	1:H:251:ARG:NH1	2.46	0.49
1:H:180:ILE:CD1	1:H:185:THR:HG21	2.42	0.49
1:H:148:GLY:C	3:H:703:GOL:H32	2.38	0.48
1:A:476:ASP:OD1	1:C:251:ARG:NH1	2.46	0.48
1:G:604:ASN:HB3	2:G:701:FAD:C2	2.43	0.48
1:B:266:LYS:O	1:B:588:ASN:ND2	2.46	0.48
1:C:385:TRP:CE3	1:C:389:PHE:HB2	2.49	0.48
1:B:368:ARG:NH2	1:B:389:PHE:O	2.47	0.48
1:B:438:SER:HB3	1:B:443:VAL:CG2	2.44	0.48
1:C:81:ARG:NH1	1:C:554:ASP:OD2	2.46	0.47
1:H:564:GLY:HA2	1:H:597:CYS:O	2.14	0.47
1:B:518:HIS:HB3	1:G:61:ARG:NH1	2.30	0.47
1:A:227:ALA:HB1	1:A:245:TYR:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:THR:HG23	1:D:91:ASN:HB2	1.94	0.47
1:D:438:SER:HB3	1:D:443:VAL:HG21	1.97	0.47
1:G:407:TYR:H	1:G:420:THR:HG21	1.79	0.47
1:A:321:ARG:HD3	1:A:500:ILE:HB	1.97	0.47
1:C:321:ARG:NH1	1:C:500:ILE:HD12	2.29	0.47
1:C:566:CYS:O	1:C:596:ILE:HA	2.14	0.47
1:D:440:ASN:ND2	1:D:441:PRO:HD2	2.30	0.47
1:A:566:CYS:O	1:A:596:ILE:HA	2.14	0.47
1:B:134:ASN:O	1:B:136:GLN:HG3	2.14	0.47
1:C:474:ARG:NH2	1:C:537:ASP:OD1	2.48	0.47
1:D:402:ILE:HD12	1:D:475:MET:HE1	1.95	0.47
1:E:449:SER:HB3	1:E:451:PHE:CD1	2.50	0.47
1:B:580:ARG:NH1	1:B:623:GLU:OE2	2.48	0.47
1:C:79:TYR:CD2	1:C:453:ASN:HA	2.50	0.47
1:F:177:SER:HB3	1:F:180:ILE:CD1	2.45	0.47
1:H:399:PHE:CG	1:H:424:TYR:CE2	3.03	0.47
1:G:104:TYR:CE1	1:G:152:ILE:HD13	2.50	0.47
1:D:321:ARG:NH1	1:D:500:ILE:HD12	2.30	0.46
1:D:67:LYS:NZ	4:D:805:HOH:O	2.49	0.46
1:F:409:ASP:OD1	1:F:411:THR:HB	2.15	0.46
1:F:578:ASP:OD2	1:F:582:ASN:HB2	2.16	0.46
1:D:459:ALA:N	1:D:460:PRO:HD2	2.30	0.46
1:F:251:ARG:HG2	1:H:535:ILE:HD12	1.97	0.46
1:E:405:GLY:O	1:E:420:THR:HG22	2.15	0.46
1:F:644:ARG:HB2	1:F:645:PRO:HD2	1.98	0.46
1:H:577:VAL:HA	1:H:582:ASN:O	2.15	0.46
1:A:577:VAL:HA	1:A:582:ASN:O	2.16	0.46
1:D:277:THR:HB	1:D:278:PRO:HD3	1.98	0.46
1:E:629:LYS:HE2	4:E:839:HOH:O	2.16	0.46
1:A:219:ASP:OD1	1:A:219:ASP:C	2.59	0.45
1:B:100:ASN:HB2	2:B:701:FAD:C5X	2.46	0.45
1:B:165:PHE:CD1	1:B:165:PHE:C	2.94	0.45
1:F:54:ILE:O	1:F:57:ARG:HG2	2.16	0.45
1:F:153:SER:OG	1:F:196:ILE:O	2.29	0.45
1:G:32:LEU:HD22	1:G:626:LEU:HD21	1.96	0.45
1:B:452:MET:HE3	1:B:556:VAL:HG21	1.99	0.45
1:C:51:ARG:HB2	1:C:54:ILE:HD13	1.98	0.45
1:H:186:ALA:HB2	1:H:394:ASP:C	2.42	0.45
1:H:580:ARG:HH22	1:H:622:GLU:CD	2.23	0.45
1:D:49:VAL:O	1:D:203:ARG:HD2	2.17	0.45
1:F:235:ASP:OD1	1:F:236:ASP:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ARG:NH2	1:B:622:GLU:OE1	2.50	0.45
1:D:452:MET:HE1	1:D:461:ILE:HD12	1.99	0.45
1:E:399:PHE:CD1	1:E:424:TYR:CE2	3.05	0.45
1:G:513:LEU:N	1:G:513:LEU:HD23	2.32	0.45
1:A:132:LEU:HD23	1:A:614:GLU:HG3	1.99	0.45
1:B:399:PHE:CG	1:B:424:TYR:CE2	3.05	0.45
1:D:314:TYR:CD2	1:D:452:MET:HE2	2.52	0.45
1:G:180:ILE:HG22	1:G:181:GLN:NE2	2.32	0.45
1:H:106:ARG:NH1	1:H:181:GLN:O	2.50	0.45
1:G:112:TRP:CZ2	1:G:611:LEU:HD23	2.52	0.44
1:A:100:ASN:HB2	2:A:701:FAD:C5X	2.46	0.44
1:H:374:LEU:HD13	1:H:374:LEU:HA	1.89	0.44
1:B:44:ARG:NH2	1:B:216:ASP:OD1	2.45	0.44
1:G:111:ASP:HB3	1:G:601:LEU:HD23	1.99	0.44
1:G:200:THR:HG21	1:G:637:HIS:O	2.17	0.44
1:C:580:ARG:NH1	1:C:623:GLU:OE2	2.46	0.44
1:D:100:ASN:O	1:D:203:ARG:NH2	2.50	0.44
1:C:311:GLN:HB2	1:C:563:LEU:HD12	1.98	0.44
1:B:484:SER:OG	1:B:485:HIS:ND1	2.45	0.44
1:D:218:GLN:NE2	1:D:220:ASN:OD1	2.48	0.44
1:A:324:ASN:O	1:A:417:LYS:NZ	2.50	0.44
1:B:314:TYR:CD2	1:B:452:MET:HE2	2.53	0.44
1:C:217:VAL:HG23	1:C:218:GLN:HG3	2.00	0.44
1:D:61:ARG:NH1	1:H:516:GLY:O	2.48	0.44
1:F:314:TYR:CE1	1:F:451:PHE:CD1	3.06	0.44
1:F:563:LEU:C	1:F:563:LEU:HD12	2.43	0.44
1:C:235:ASP:HB2	1:C:239:LYS:O	2.18	0.44
1:D:513:LEU:O	1:H:57:ARG:HA	2.18	0.44
1:C:408:ALA:O	1:F:514:THR:OG1	2.34	0.44
1:F:61[B]:ARG:HG2	1:F:61[B]:ARG:NH1	2.33	0.44
1:H:314:TYR:CD2	1:H:452:MET:HE2	2.53	0.43
1:C:411:THR:HG21	1:F:505:ALA:HB1	1.99	0.43
1:G:100:ASN:HB2	2:G:701:FAD:C5X	2.49	0.43
1:H:313:HIS:HB2	1:H:559:THR:CG2	2.48	0.43
1:A:411:THR:O	1:E:321:ARG:NH2	2.51	0.43
1:E:35:MET:HE3	1:E:37:ILE:HG12	2.00	0.43
1:E:399:PHE:CD1	1:E:424:TYR:CD2	3.06	0.43
1:F:399:PHE:CD1	1:F:424:TYR:CE2	3.06	0.43
1:B:501:ASP:CG	1:B:528:PRO:HA	2.44	0.43
1:F:405:GLY:O	1:F:420:THR:HG22	2.18	0.43
1:G:459:ALA:N	1:G:460:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:HB3	1:A:180:ILE:CD1	2.48	0.43
1:A:514[B]:THR:HG21	1:E:408:ALA:O	2.18	0.43
1:B:57:ARG:CD	4:B:821:HOH:O	2.65	0.43
1:G:577:VAL:HA	1:G:582:ASN:O	2.18	0.43
1:B:29:ASP:OD1	1:B:31:THR:OG1	2.37	0.43
1:D:177:SER:HB3	1:D:180:ILE:CD1	2.48	0.43
1:D:399:PHE:CG	1:D:424:TYR:CE2	3.06	0.43
1:G:252:THR:HG21	1:G:258:HIS:HB2	2.00	0.43
1:A:100:ASN:N	1:A:203:ARG:NH2	2.67	0.43
1:B:405:GLY:O	1:B:420:THR:HG22	2.19	0.43
1:E:69:THR:HG22	4:E:835:HOH:O	2.18	0.43
1:G:452:MET:HE1	1:G:461:ILE:HD12	2.01	0.43
1:A:126:LEU:N	1:A:127:PRO:HD2	2.34	0.43
1:A:459:ALA:N	1:A:460:PRO:HD2	2.33	0.43
1:C:564:GLY:HA2	1:C:597:CYS:O	2.19	0.43
1:D:100:ASN:HB2	2:D:701:FAD:C5X	2.48	0.43
1:B:102:GLN:O	1:B:194:LYS:HA	2.19	0.43
1:E:314:TYR:CD2	1:E:452:MET:HE2	2.54	0.43
1:H:501:ASP:OD2	1:H:504:THR:OG1	2.31	0.43
1:A:564:GLY:HA2	1:A:597:CYS:O	2.19	0.43
1:A:241:VAL:O	1:A:264:ALA:N	2.47	0.42
1:C:80:LEU:HB3	1:C:83:ARG:HG3	2.01	0.42
1:E:560:TRP:CE3	2:E:701:FAD:C6	3.02	0.42
1:B:501:ASP:OD2	1:B:528:PRO:HA	2.19	0.42
1:D:452:MET:HE3	1:D:556:VAL:HG21	2.01	0.42
1:E:34:VAL:HG22	1:E:221:LEU:HD13	2.01	0.42
1:F:126:LEU:N	1:F:127:PRO:CD	2.82	0.42
1:D:35:MET:CE	1:D:262:VAL:HG21	2.50	0.42
1:D:604:ASN:HB3	2:D:701:FAD:C2	2.48	0.42
1:F:9:VAL:HA	1:F:267:MET:O	2.19	0.42
1:F:203:ARG:NH1	4:F:802:HOH:O	2.51	0.42
1:G:398:MET:SD	1:G:425:LEU:HA	2.58	0.42
1:H:149:PRO:N	3:H:703:GOL:H32	2.34	0.42
1:H:231:ARG:HB2	1:H:284:SER:HA	2.00	0.42
1:F:459:ALA:N	1:F:460:PRO:HD2	2.35	0.42
1:H:324:ASN:O	1:H:417:LYS:NZ	2.52	0.42
1:B:440:ASN:OD1	1:B:441:PRO:HD2	2.19	0.42
1:H:277:THR:HB	1:H:278:PRO:HD3	2.00	0.42
1:D:436:ILE:HD12	1:D:438:SER:O	2.19	0.42
1:G:172:ILE:HD12	1:G:467:LYS:HD2	2.02	0.42
1:G:177:SER:HB3	1:G:180:ILE:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:481:GLU:OE1	1:G:497:CYS:HA	2.19	0.42
1:H:640:VAL:HG22	4:H:855:HOH:O	2.18	0.42
1:A:348:GLU:HG3	1:B:350:SER:OG	2.19	0.42
1:B:279:GLN:HB3	1:B:283:ARG:NH2	2.34	0.42
1:C:314:TYR:CD2	1:C:452:MET:HE2	2.55	0.42
1:C:407:TYR:H	1:C:420:THR:HG21	1.85	0.42
1:E:249:ARG:NH1	1:F:476:ASP:OD2	2.52	0.42
1:H:180:ILE:HG22	1:H:181:GLN:NE2	2.35	0.42
1:H:403:VAL:HB	1:H:420:THR:HG23	2.02	0.42
1:D:398:MET:SD	1:D:425:LEU:HA	2.60	0.42
1:B:112:TRP:CZ2	1:B:611:LEU:HD23	2.54	0.42
1:F:315:THR:HA	1:F:423:GLN:O	2.20	0.42
1:E:200:THR:HG21	1:E:637:HIS:O	2.20	0.41
1:E:591:CYS:O	1:E:596:ILE:HG21	2.20	0.41
1:F:224:ARG:NH1	1:F:225:CYS:O	2.53	0.41
1:H:149:PRO:HG2	1:H:210:TYR:CZ	2.55	0.41
1:B:315:THR:HA	1:B:423:GLN:O	2.20	0.41
1:H:464:SER:O	1:H:465:TYR:C	2.63	0.41
1:G:245:TYR:CD1	1:G:245:TYR:C	2.98	0.41
1:H:106:ARG:HH12	1:H:143:THR:HG22	1.85	0.41
1:B:166:LEU:HD12	1:B:166:LEU:HA	1.97	0.41
1:H:399:PHE:CD1	1:H:424:TYR:CD2	3.08	0.41
1:B:324:ASN:O	1:B:417:LYS:NZ	2.52	0.41
1:C:410:HIS:HB2	1:F:514:THR:HG21	2.02	0.41
1:C:500:ILE:HD11	1:C:504:THR:HG22	2.02	0.41
1:B:438:SER:HB3	1:B:443:VAL:HG21	2.02	0.41
1:C:35:MET:HE2	1:C:37:ILE:HD11	2.02	0.41
1:D:314:TYR:CE1	1:D:451:PHE:CD1	3.09	0.41
1:D:472:ALA:HA	1:D:475:MET:HE3	2.03	0.41
1:F:249:ARG:NH1	1:H:476:ASP:OD2	2.53	0.41
1:F:208:THR:HA	1:F:212:HIS:HB2	2.03	0.41
1:G:51:ARG:HB2	1:G:54:ILE:HD13	2.03	0.41
1:H:630:THR:HA	1:H:631:PRO:HA	1.95	0.41
1:D:159:MET:HE2	1:D:159:MET:HA	2.02	0.41
1:E:561:HIS:CE1	1:E:604:ASN:HA	2.56	0.41
1:E:132:LEU:HD12	1:E:132:LEU:C	2.46	0.41
1:E:177:SER:HB3	1:E:180:ILE:CD1	2.51	0.41
1:F:561:HIS:CE1	1:F:604:ASN:HA	2.56	0.41
1:G:409:ASP:OD1	1:G:411:THR:HB	2.21	0.41
1:H:9:VAL:O	1:H:34:VAL:HA	2.19	0.41
1:H:51:ARG:HA	1:H:52:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:ARG:O	1:C:590:LYS:NZ	2.48	0.41
1:D:54:ILE:O	1:D:57:ARG:CG	2.69	0.41
1:E:564:GLY:HA2	1:E:597:CYS:O	2.21	0.41
1:H:80:LEU:O	1:H:83:ARG:HG2	2.20	0.41
1:A:581:LEU:HB3	1:A:591:CYS:O	2.21	0.40
1:B:369:PRO:HB3	1:B:377:MET:HE1	2.02	0.40
1:E:407:TYR:H	1:E:420:THR:HG21	1.86	0.40
1:E:520:GLY:HA3	1:E:522:TRP:NE1	2.36	0.40
1:F:251:ARG:CG	1:H:535:ILE:HD12	2.51	0.40
1:E:548:ILE:O	1:E:552:VAL:HG23	2.21	0.40
1:A:277:THR:O	1:A:278:PRO:C	2.64	0.40
1:B:399:PHE:CD1	1:B:424:TYR:CD2	3.09	0.40
1:F:49:VAL:O	1:F:203:ARG:HD2	2.21	0.40
1:F:467:LYS:O	1:F:471:VAL:HG23	2.22	0.40
1:H:473:ARG:NH2	1:H:536:GLU:O	2.55	0.40
1:A:449:SER:OG	1:A:451:PHE:CG	2.74	0.40
1:G:403:VAL:HB	1:G:420:THR:CG2	2.50	0.40
1:H:430:SER:OG	1:H:457:ASP:OD2	2.36	0.40
1:A:231:ARG:HB2	1:A:284:SER:HA	2.01	0.40
1:A:465:TYR:CD1	1:A:465:TYR:C	3.00	0.40
1:B:228:ARG:NH1	1:B:441:PRO:O	2.54	0.40
1:G:592:VAL:HG23	1:G:612:VAL:HG12	2.03	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	642/651 (99%)	606 (94%)	35 (6%)	1 (0%)	43 66
1	B	638/651 (98%)	603 (94%)	32 (5%)	3 (0%)	24 46
1	C	635/651 (98%)	593 (93%)	41 (6%)	1 (0%)	43 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	634/651 (97%)	598 (94%)	36 (6%)	0	100	100
1	E	635/651 (98%)	598 (94%)	36 (6%)	1 (0%)	43	66
1	F	643/651 (99%)	605 (94%)	37 (6%)	1 (0%)	43	66
1	G	633/651 (97%)	588 (93%)	44 (7%)	1 (0%)	43	66
1	H	634/651 (97%)	597 (94%)	34 (5%)	3 (0%)	24	46
All	All	5094/5208 (98%)	4788 (94%)	295 (6%)	11 (0%)	43	66

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	501	ASP
1	B	235	ASP
1	F	578	ASP
1	H	449	SER
1	B	253	HIS
1	E	528	PRO
1	A	306	VAL
1	C	123	LYS
1	H	253	HIS
1	H	285	GLY
1	G	285	GLY

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	543/548 (99%)	506 (93%)	37 (7%)	14	32
1	B	541/548 (99%)	501 (93%)	40 (7%)	13	29
1	C	537/548 (98%)	499 (93%)	38 (7%)	13	31
1	D	347/548 (63%)	326 (94%)	21 (6%)	17	37
1	E	390/548 (71%)	365 (94%)	25 (6%)	16	35
1	F	544/548 (99%)	502 (92%)	42 (8%)	12	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	535/548 (98%)	499 (93%)	36 (7%)	15	33
1	H	536/548 (98%)	501 (94%)	35 (6%)	15	35
All	All	3973/4384 (91%)	3699 (93%)	274 (7%)	14	32

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	34	VAL
1	A	54	ILE
1	A	69	THR
1	A	106	ARG
1	A	126	LEU
1	A	143	THR
1	A	166	LEU
1	A	180	ILE
1	A	221	LEU
1	A	243	VAL
1	A	251	ARG
1	A	256	LYS
1	A	257	LEU
1	A	262	VAL
1	A	275	LEU
1	A	291	LEU
1	A	333	LEU
1	A	353	LYS
1	A	365	PHE
1	A	370	THR
1	A	374	LEU
1	A	376	GLU
1	A	380	GLU
1	A	391	ASP
1	A	399	PHE
1	A	411	THR
1	A	420	THR
1	A	474	ARG
1	A	501	ASP
1	A	513	LEU
1	A	527	GLU
1	A	532	ASP
1	A	557	GLU

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Mol	Chain	Res	Type
1	A	592	VAL
1	A	600	ASN
1	A	626	LEU
1	B	31	THR
1	B	33	LYS
1	B	34	VAL
1	B	44	ARG
1	B	54	ILE
1	B	69	THR
1	B	85	SER
1	B	126	LEU
1	B	147	ASP
1	B	166	LEU
1	B	180	ILE
1	B	224	ARG
1	B	228	ARG
1	B	235	ASP
1	B	243	VAL
1	B	248	SER
1	B	251	ARG
1	B	275	LEU
1	B	291	LEU
1	B	298	LYS
1	B	325	GLU
1	B	333	LEU
1	B	337	LYS
1	B	350	SER
1	B	353	LYS
1	B	365	PHE
1	B	370	THR
1	B	374	LEU
1	B	380	GLU
1	B	411	THR
1	B	417	LYS
1	B	420	THR
1	B	443	VAL
1	B	501	ASP
1	B	559	THR
1	B	563	LEU
1	B	592	VAL
1	B	626	LEU
1	B	635	VAL

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Mol	Chain	Res	Type
1	B	644	ARG
1	C	31	THR
1	C	34	VAL
1	C	44	ARG
1	C	54	ILE
1	C	57	ARG
1	C	69	THR
1	C	83	ARG
1	C	126	LEU
1	C	166	LEU
1	C	177	SER
1	C	180	ILE
1	C	243	VAL
1	C	251	ARG
1	C	252	THR
1	C	260	THR
1	C	275	LEU
1	C	291	LEU
1	C	295	LEU
1	C	325	GLU
1	C	333	LEU
1	C	338	ASP
1	C	348	GLU
1	C	353	LYS
1	C	365	PHE
1	C	370	THR
1	C	374	LEU
1	C	380	GLU
1	C	411	THR
1	C	412	LEU
1	C	443	VAL
1	C	513	LEU
1	C	527	GLU
1	C	559	THR
1	C	592	VAL
1	C	600	ASN
1	C	601	LEU
1	C	626	LEU
1	C	635	VAL
1	D	34	VAL
1	D	54	ILE
1	D	61	ARG

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Mol	Chain	Res	Type
1	D	126	LEU
1	D	143	THR
1	D	166	LEU
1	D	180	ILE
1	D	184	THR
1	D	203	ARG
1	D	243	VAL
1	D	251	ARG
1	D	275	LEU
1	D	295	LEU
1	D	298	LYS
1	D	325	GLU
1	D	333	LEU
1	D	557	GLU
1	D	587	GLN
1	D	592	VAL
1	D	626	LEU
1	D	635	VAL
1	E	228	ARG
1	E	243	VAL
1	E	248	SER
1	E	251	ARG
1	E	252	THR
1	E	262	VAL
1	E	275	LEU
1	E	291	LEU
1	E	295	LEU
1	E	333	LEU
1	E	348	GLU
1	E	353	LYS
1	E	370	THR
1	E	374	LEU
1	E	380	GLU
1	E	411	THR
1	E	473	ARG
1	E	533	LYS
1	E	557	GLU
1	E	559	THR
1	E	572	GLU
1	E	580	ARG
1	E	592	VAL
1	E	626	LEU

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Mol	Chain	Res	Type
1	E	635	VAL
1	F	3	HIS
1	F	34	VAL
1	F	44	ARG
1	F	54	ILE
1	F	114	ASP
1	F	116	LYS
1	F	126	LEU
1	F	143	THR
1	F	166	LEU
1	F	180	ILE
1	F	228	ARG
1	F	243	VAL
1	F	251	ARG
1	F	262	VAL
1	F	275	LEU
1	F	291	LEU
1	F	295	LEU
1	F	325	GLU
1	F	333	LEU
1	F	353	LYS
1	F	365	PHE
1	F	370	THR
1	F	374	LEU
1	F	376	GLU
1	F	380	GLU
1	F	391	ASP
1	F	399	PHE
1	F	411	THR
1	F	420	THR
1	F	449	SER
1	F	527	GLU
1	F	530	LYS
1	F	557	GLU
1	F	578	ASP
1	F	592	VAL
1	F	600	ASN
1	F	601	LEU
1	F	626	LEU
1	F	630	THR
1	F	635	VAL
1	F	644	ARG

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Mol	Chain	Res	Type
1	F	647	THR
1	G	31	THR
1	G	34	VAL
1	G	54	ILE
1	G	57	ARG
1	G	126	LEU
1	G	143	THR
1	G	166	LEU
1	G	177	SER
1	G	180	ILE
1	G	213	SER
1	G	224	ARG
1	G	243	VAL
1	G	251	ARG
1	G	252	THR
1	G	256	LYS
1	G	275	LEU
1	G	291	LEU
1	G	301	SER
1	G	315	THR
1	G	325	GLU
1	G	333	LEU
1	G	338	ASP
1	G	353	LYS
1	G	372	GLU
1	G	374	LEU
1	G	380	GLU
1	G	391	ASP
1	G	411	THR
1	G	420	THR
1	G	449	SER
1	G	513	LEU
1	G	587	GLN
1	G	592	VAL
1	G	600	ASN
1	G	626	LEU
1	G	635	VAL
1	H	34	VAL
1	H	54	ILE
1	H	106	ARG
1	H	116	LYS
1	H	126	LEU

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Mol	Chain	Res	Type
1	H	166	LEU
1	H	180	ILE
1	H	203	ARG
1	H	208	THR
1	H	235	ASP
1	H	243	VAL
1	H	248	SER
1	H	251	ARG
1	H	275	LEU
1	H	291	LEU
1	H	333	LEU
1	H	348	GLU
1	H	353	LYS
1	H	365	PHE
1	H	370	THR
1	H	374	LEU
1	H	380	GLU
1	H	387	ARG
1	H	391	ASP
1	H	411	THR
1	H	420	THR
1	H	443	VAL
1	H	474	ARG
1	H	559	THR
1	H	572	GLU
1	H	592	VAL
1	H	600	ASN
1	H	626	LEU
1	H	630	THR
1	H	635	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	237	ASN
1	A	382	ASN
1	B	134	ASN
1	B	238	ASN
1	B	250	ASN
1	B	279	GLN
1	B	309	GLN

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Mol	Chain	Res	Type
1	B	439	GLN
1	C	309	GLN
1	C	311	GLN
1	C	440	ASN
1	C	518	HIS
1	C	531	HIS
1	C	582	ASN
1	C	600	ASN
1	D	157	GLN
1	D	199	HIS
1	D	218	GLN
1	D	637	HIS
1	E	218	GLN
1	E	309	GLN
1	E	311	GLN
1	E	423	GLN
1	E	587	GLN
1	F	157	GLN
1	F	218	GLN
1	F	253	HIS
1	F	309	GLN
1	F	523	HIS
1	F	524	GLN
1	F	531	HIS
1	F	573	GLN
1	F	587	GLN
1	G	65	ASN
1	G	136	GLN
1	G	170	HIS
1	G	311	GLN
1	G	524	GLN
1	G	600	ASN
1	H	311	GLN
1	H	531	HIS
1	H	600	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	C	701	-	58,58,58	1.57	10 (17%)	85,89,89	1.61	17 (20%)
2	FAD	A	701	-	58,58,58	1.55	8 (13%)	85,89,89	1.73	16 (18%)
2	FAD	G	701	-	58,58,58	1.55	7 (12%)	85,89,89	1.68	18 (21%)
3	GOL	B	702	-	5,5,5	0.77	0	5,5,5	0.62	0
3	GOL	D	702	-	5,5,5	0.45	0	5,5,5	0.36	0
2	FAD	D	701	-	58,58,58	1.63	9 (15%)	85,89,89	1.56	14 (16%)
2	FAD	F	701	-	58,58,58	1.52	10 (17%)	85,89,89	1.57	19 (22%)
2	FAD	H	701	-	58,58,58	1.66	10 (17%)	85,89,89	1.67	15 (17%)
2	FAD	E	701	-	58,58,58	1.61	9 (15%)	85,89,89	1.63	20 (23%)
3	GOL	H	703	-	5,5,5	0.72	0	5,5,5	1.20	1 (20%)
2	FAD	B	701	-	58,58,58	1.71	11 (18%)	85,89,89	1.54	15 (17%)
3	GOL	C	702	-	5,5,5	0.32	0	5,5,5	0.35	0
3	GOL	H	702	-	5,5,5	0.42	0	5,5,5	0.51	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	C	701	-	-	6/34/50/50	0/6/6/6
2	FAD	A	701	-	-	8/34/50/50	0/6/6/6
2	FAD	G	701	-	-	8/34/50/50	0/6/6/6
3	GOL	B	702	-	-	2/4/4/4	-
3	GOL	D	702	-	-	2/4/4/4	-
2	FAD	D	701	-	-	5/34/50/50	0/6/6/6
2	FAD	F	701	-	-	4/34/50/50	0/6/6/6
2	FAD	H	701	-	-	8/34/50/50	0/6/6/6
2	FAD	E	701	-	-	6/34/50/50	0/6/6/6
3	GOL	H	703	-	-	2/4/4/4	-
2	FAD	B	701	-	-	5/34/50/50	0/6/6/6
3	GOL	C	702	-	-	0/4/4/4	-
3	GOL	H	702	-	-	2/4/4/4	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	FAD	C9A-C5X	6.41	1.51	1.41
2	B	701	FAD	C9A-C5X	6.32	1.51	1.41
2	H	701	FAD	C9A-C5X	6.24	1.51	1.41
2	G	701	FAD	C9A-C5X	6.19	1.51	1.41
2	D	701	FAD	C9A-C5X	6.10	1.51	1.41
2	E	701	FAD	C9A-C5X	6.01	1.50	1.41
2	F	701	FAD	C9A-C5X	5.42	1.49	1.41
2	A	701	FAD	C9A-C5X	5.23	1.49	1.41
2	E	701	FAD	C5A-C4A	4.96	1.47	1.39
2	B	701	FAD	P-O3P	4.87	1.64	1.59
2	B	701	FAD	C5A-C4A	4.62	1.47	1.39
2	A	701	FAD	C5A-C4A	4.57	1.47	1.39
2	D	701	FAD	P-O3P	4.54	1.64	1.59
2	C	701	FAD	C5A-C4A	4.30	1.46	1.39
2	G	701	FAD	C5A-C4A	4.27	1.46	1.39
2	H	701	FAD	C5A-C4A	4.26	1.46	1.39
2	G	701	FAD	C8-C7	4.21	1.51	1.40
2	D	701	FAD	C5A-C4A	4.02	1.46	1.39
2	H	701	FAD	P-O3P	3.98	1.63	1.59
2	A	701	FAD	P-O3P	3.97	1.63	1.59
2	H	701	FAD	C8-C7	3.82	1.50	1.40
2	C	701	FAD	C8-C7	3.81	1.50	1.40
2	E	701	FAD	C8-C7	3.77	1.50	1.40
2	D	701	FAD	C8-C7	3.71	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAD	C8-C7	3.68	1.49	1.40
2	F	701	FAD	C5A-C4A	3.67	1.45	1.39
2	B	701	FAD	PA-O3P	3.61	1.63	1.59
2	F	701	FAD	C8-C7	3.55	1.49	1.40
2	E	701	FAD	P-O3P	3.49	1.63	1.59
2	B	701	FAD	C8-C7	3.48	1.49	1.40
2	D	701	FAD	PA-O3P	3.21	1.63	1.59
2	F	701	FAD	PA-O3P	3.14	1.62	1.59
2	H	701	FAD	PA-O3P	3.07	1.62	1.59
2	F	701	FAD	P-O3P	3.06	1.62	1.59
2	B	701	FAD	C5A-C6A	3.01	1.49	1.41
2	A	701	FAD	PA-O3P	2.95	1.62	1.59
2	A	701	FAD	C8A-N7A	2.89	1.37	1.31
2	E	701	FAD	C5A-C6A	2.87	1.49	1.41
2	C	701	FAD	C4A-N9A	-2.85	1.31	1.37
2	H	701	FAD	C5A-C6A	2.80	1.48	1.41
2	A	701	FAD	C5A-C6A	2.75	1.48	1.41
2	G	701	FAD	C5A-C6A	2.73	1.48	1.41
2	E	701	FAD	C8A-N7A	2.72	1.36	1.31
2	F	701	FAD	C4A-N9A	-2.68	1.32	1.37
2	F	701	FAD	C5A-C6A	2.65	1.48	1.41
2	E	701	FAD	PA-O3P	2.60	1.62	1.59
2	G	701	FAD	C8A-N7A	2.56	1.36	1.31
2	D	701	FAD	C5A-C6A	2.56	1.48	1.41
2	D	701	FAD	C4A-N9A	-2.48	1.32	1.37
2	H	701	FAD	C5A-N7A	-2.46	1.34	1.39
2	D	701	FAD	C8A-N7A	2.37	1.36	1.31
2	B	701	FAD	C8A-N7A	2.37	1.36	1.31
2	B	701	FAD	C4A-N9A	-2.35	1.32	1.37
2	H	701	FAD	C4X-N5	2.33	1.35	1.30
2	H	701	FAD	C8A-N7A	2.33	1.36	1.31
2	C	701	FAD	C4X-N5	2.31	1.35	1.30
2	F	701	FAD	C8A-N9A	-2.28	1.33	1.37
2	B	701	FAD	C4X-N5	2.27	1.35	1.30
2	C	701	FAD	C8A-N7A	2.26	1.36	1.31
2	D	701	FAD	C5A-N7A	-2.25	1.35	1.39
2	E	701	FAD	C4A-N9A	-2.25	1.33	1.37
2	F	701	FAD	C8A-N7A	2.22	1.35	1.31
2	G	701	FAD	C4X-N5	2.19	1.35	1.30
2	C	701	FAD	C5A-C6A	2.18	1.47	1.41
2	C	701	FAD	C5A-N7A	-2.18	1.35	1.39
2	G	701	FAD	C4A-N9A	-2.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	FAD	C5A-N7A	-2.16	1.35	1.39
2	E	701	FAD	C10-N10	2.12	1.41	1.37
2	C	701	FAD	C10-N10	2.11	1.41	1.37
2	B	701	FAD	C4-N3	-2.11	1.34	1.38
2	B	701	FAD	C5A-N7A	-2.09	1.35	1.39
2	C	701	FAD	P-O3P	2.04	1.61	1.59
2	H	701	FAD	C4A-N9A	-2.03	1.33	1.37
2	A	701	FAD	C4-N3	-2.02	1.35	1.38

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FAD	C5A-C4A-N3A	-6.21	118.17	126.72
2	H	701	FAD	C5A-C4A-N3A	-5.79	118.75	126.72
2	B	701	FAD	C5A-C4A-N3A	-5.26	119.47	126.72
2	H	701	FAD	N3A-C4A-N9A	4.88	135.47	127.17
2	F	701	FAD	C5A-C4A-N3A	-4.81	120.09	126.72
2	D	701	FAD	C5A-C4A-N3A	-4.68	120.28	126.72
2	G	701	FAD	C5A-C4A-N3A	-4.64	120.33	126.72
2	E	701	FAD	C5A-C4A-N3A	-4.61	120.36	126.72
2	A	701	FAD	N3A-C4A-N9A	4.50	134.82	127.17
2	A	701	FAD	C4'-C3'-C2'	-4.37	106.29	113.57
2	A	701	FAD	C2A-N3A-C4A	4.36	122.48	111.83
2	C	701	FAD	C4A-N9A-C8A	4.36	110.31	105.74
2	G	701	FAD	N3A-C2A-N1A	-4.30	122.07	128.58
2	C	701	FAD	N3A-C2A-N1A	-4.29	122.08	128.58
2	D	701	FAD	N3A-C2A-N1A	-4.27	122.12	128.58
2	A	701	FAD	N3A-C2A-N1A	-4.19	122.24	128.58
2	C	701	FAD	C5A-C4A-N3A	-4.16	120.99	126.72
2	E	701	FAD	N3A-C2A-N1A	-4.16	122.29	128.58
2	G	701	FAD	C4A-N9A-C8A	4.10	110.05	105.74
2	B	701	FAD	C4A-C5A-N7A	-4.02	105.99	110.58
2	C	701	FAD	N3A-C4A-N9A	3.98	133.93	127.17
2	F	701	FAD	C4A-N9A-C8A	3.86	109.79	105.74
2	F	701	FAD	N3A-C2A-N1A	-3.86	122.74	128.58
2	B	701	FAD	N3A-C4A-N9A	3.86	133.73	127.17
2	C	701	FAD	C4-C4X-N5	3.85	123.53	118.21
2	G	701	FAD	N3A-C4A-N9A	3.83	133.67	127.17
2	H	701	FAD	C2A-N3A-C4A	3.79	121.09	111.83
2	F	701	FAD	C4A-C5A-N7A	-3.79	106.25	110.58
2	G	701	FAD	C2A-N3A-C4A	3.78	121.06	111.83
2	H	701	FAD	C4A-N9A-C8A	3.76	109.68	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	N3A-C2A-N1A	-3.75	122.90	128.58
2	F	701	FAD	N3A-C4A-N9A	3.75	133.54	127.17
2	B	701	FAD	C2A-N3A-C4A	3.75	120.98	111.83
2	A	701	FAD	C4A-C5A-N7A	-3.71	106.34	110.58
2	D	701	FAD	C2A-N3A-C4A	3.69	120.84	111.83
2	G	701	FAD	C4A-C5A-N7A	-3.67	106.39	110.58
2	D	701	FAD	N3A-C4A-N9A	3.67	133.41	127.17
2	F	701	FAD	C2A-N3A-C4A	3.66	120.78	111.83
2	H	701	FAD	C4'-C3'-C2'	-3.66	107.47	113.57
2	E	701	FAD	N3A-C4A-N9A	3.65	133.38	127.17
2	D	701	FAD	C4A-N9A-C8A	3.64	109.56	105.74
2	D	701	FAD	C4A-C5A-N7A	-3.64	106.42	110.58
2	G	701	FAD	C4-C4X-N5	3.59	123.17	118.21
2	E	701	FAD	C2A-N3A-C4A	3.54	120.49	111.83
2	E	701	FAD	C4A-C5A-N7A	-3.53	106.55	110.58
2	B	701	FAD	C4-C4X-N5	3.53	123.08	118.21
2	H	701	FAD	C4A-C5A-N7A	-3.44	106.65	110.58
2	E	701	FAD	C4'-C3'-C2'	-3.41	107.89	113.57
2	E	701	FAD	C4A-N9A-C8A	3.39	109.30	105.74
2	C	701	FAD	C2A-N3A-C4A	3.38	120.08	111.83
2	H	701	FAD	N3A-C2A-N1A	-3.33	123.54	128.58
2	A	701	FAD	C4-C4X-N5	3.24	122.69	118.21
2	G	701	FAD	N9A-C8A-N7A	-3.21	109.38	113.94
2	G	701	FAD	C6A-C5A-N7A	3.18	138.23	132.09
2	F	701	FAD	C4-C4X-N5	3.12	122.52	118.21
2	E	701	FAD	C4-C4X-N5	3.08	122.46	118.21
2	C	701	FAD	C9A-C5X-N5	-3.06	119.21	122.45
2	G	701	FAD	C5A-N7A-C8A	3.00	108.17	103.45
2	D	701	FAD	O4-C4-C4X	-2.98	118.66	126.53
2	H	701	FAD	C5A-N7A-C8A	2.96	108.10	103.45
2	B	701	FAD	C4A-N9A-C8A	2.95	108.83	105.74
2	H	701	FAD	C4-C4X-N5	2.94	122.27	118.21
2	H	701	FAD	N9A-C8A-N7A	-2.92	109.79	113.94
2	E	701	FAD	C6A-C5A-N7A	2.90	137.69	132.09
2	D	701	FAD	C4'-C3'-C2'	-2.89	108.77	113.57
2	G	701	FAD	C4'-C3'-C2'	-2.88	108.77	113.57
2	F	701	FAD	N9A-C8A-N7A	-2.84	109.90	113.94
2	C	701	FAD	C2A-N1A-C6A	2.84	123.40	118.73
2	D	701	FAD	C6A-C5A-N7A	2.84	137.56	132.09
2	D	701	FAD	N9A-C8A-N7A	-2.83	109.92	113.94
2	B	701	FAD	C5A-N7A-C8A	2.79	107.84	103.45
2	E	701	FAD	C2A-N1A-C6A	2.76	123.27	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	FAD	C5A-N7A-C8A	2.75	107.78	103.45
2	F	701	FAD	C6A-C5A-N7A	2.75	137.39	132.09
2	D	701	FAD	O2A-PA-O3P	2.74	114.69	107.27
2	G	701	FAD	C2A-N1A-C6A	2.73	123.21	118.73
2	C	701	FAD	O2A-PA-O3P	2.71	114.59	107.27
2	F	701	FAD	C5A-N7A-C8A	2.69	107.68	103.45
2	A	701	FAD	C6A-C5A-N7A	2.68	137.26	132.09
2	A	701	FAD	C5A-N7A-C8A	2.67	107.65	103.45
2	C	701	FAD	N9A-C8A-N7A	-2.62	110.22	113.94
2	D	701	FAD	C2A-N1A-C6A	2.61	123.02	118.73
2	E	701	FAD	C5A-N7A-C8A	2.59	107.52	103.45
2	A	701	FAD	O2A-PA-O3P	2.58	114.24	107.27
2	C	701	FAD	C4X-C10-N10	2.57	120.17	116.48
2	E	701	FAD	O4B-C1B-N9A	2.57	113.03	108.09
2	G	701	FAD	C4A-N9A-C1B	-2.56	120.64	126.63
2	E	701	FAD	N9A-C8A-N7A	-2.50	110.38	113.94
2	B	701	FAD	C2A-N1A-C6A	2.45	122.76	118.73
2	C	701	FAD	C9-C9A-N10	-2.45	118.56	121.85
2	C	701	FAD	C4A-C5A-N7A	-2.45	107.79	110.58
2	B	701	FAD	C6A-C5A-N7A	2.43	136.78	132.09
2	F	701	FAD	C4X-C10-N1	-2.43	118.64	124.59
2	D	701	FAD	C4A-N9A-C1B	-2.42	120.97	126.63
2	H	701	FAD	O4-C4-C4X	-2.41	120.16	126.53
2	E	701	FAD	C4X-C10-N1	-2.41	118.68	124.59
2	B	701	FAD	N9A-C8A-N7A	-2.40	110.53	113.94
3	H	703	GOL	O3-C3-C2	2.38	121.11	110.38
2	E	701	FAD	C9A-C5X-N5	-2.38	119.93	122.45
2	E	701	FAD	C4A-N9A-C1B	-2.37	121.10	126.63
2	G	701	FAD	C9A-C5X-N5	-2.35	119.96	122.45
2	E	701	FAD	C10-N1-C2	2.35	121.93	116.85
2	H	701	FAD	C4X-C4-N3	2.34	119.22	113.25
2	A	701	FAD	C4A-N9A-C8A	2.34	108.20	105.74
2	E	701	FAD	O4-C4-C4X	-2.34	120.36	126.53
2	A	701	FAD	O4-C4-C4X	-2.33	120.38	126.53
2	C	701	FAD	C9A-N10-C10	-2.32	117.22	120.75
2	G	701	FAD	C10-C4X-N5	-2.29	120.14	124.81
2	A	701	FAD	C4X-C4-N3	2.28	119.06	113.25
2	F	701	FAD	O4-C4-C4X	-2.28	120.53	126.53
2	A	701	FAD	N9A-C8A-N7A	-2.22	110.79	113.94
2	F	701	FAD	C4X-C4-N3	2.22	118.89	113.25
2	F	701	FAD	C10-N1-C2	2.21	121.64	116.85
2	H	701	FAD	C10-N1-C2	2.21	121.63	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	FAD	C10-C4X-N5	-2.19	120.33	124.81
2	E	701	FAD	C4X-C4-N3	2.18	118.80	113.25
2	G	701	FAD	C4X-C10-N1	-2.17	119.27	124.59
2	A	701	FAD	C4X-C10-N1	-2.17	119.28	124.59
2	E	701	FAD	C9A-N10-C10	-2.15	117.47	120.75
2	B	701	FAD	C9A-C5X-N5	-2.15	120.17	122.45
2	F	701	FAD	C2A-N1A-C6A	2.15	122.26	118.73
2	B	701	FAD	C4'-C3'-C2'	-2.14	110.00	113.57
2	F	701	FAD	O2A-PA-O3P	2.14	113.07	107.27
2	C	701	FAD	C4X-C10-N1	-2.12	119.38	124.59
2	B	701	FAD	C4X-C10-N10	2.12	119.52	116.48
2	A	701	FAD	C4-N3-C2	-2.11	121.89	125.64
2	G	701	FAD	O4-C4-C4X	-2.09	121.01	126.53
2	G	701	FAD	C4X-C10-N10	2.08	119.46	116.48
2	H	701	FAD	C4X-C10-N1	-2.07	119.52	124.59
2	C	701	FAD	C6A-C5A-N7A	2.06	136.06	132.09
2	H	701	FAD	O3'-C3'-C2'	2.06	113.60	108.93
2	F	701	FAD	C10-C4X-N5	-2.05	120.61	124.81
2	B	701	FAD	C4X-C4-N3	2.05	118.48	113.25
2	F	701	FAD	C4-N3-C2	-2.04	122.02	125.64
2	F	701	FAD	C4A-N9A-C1B	-2.01	121.93	126.63

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	N10-C1'-C2'-O2'
2	A	701	FAD	N10-C1'-C2'-C3'
2	B	701	FAD	N10-C1'-C2'-O2'
2	C	701	FAD	N10-C1'-C2'-O2'
2	D	701	FAD	N10-C1'-C2'-O2'
2	E	701	FAD	N10-C1'-C2'-O2'
2	E	701	FAD	N10-C1'-C2'-C3'
2	F	701	FAD	N10-C1'-C2'-O2'
2	G	701	FAD	N10-C1'-C2'-O2'
2	G	701	FAD	N10-C1'-C2'-C3'
2	H	701	FAD	N10-C1'-C2'-O2'
3	D	702	GOL	O1-C1-C2-C3
3	H	703	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-O2
3	B	702	GOL	O1-C1-C2-C3
3	H	702	GOL	O1-C1-C2-C3

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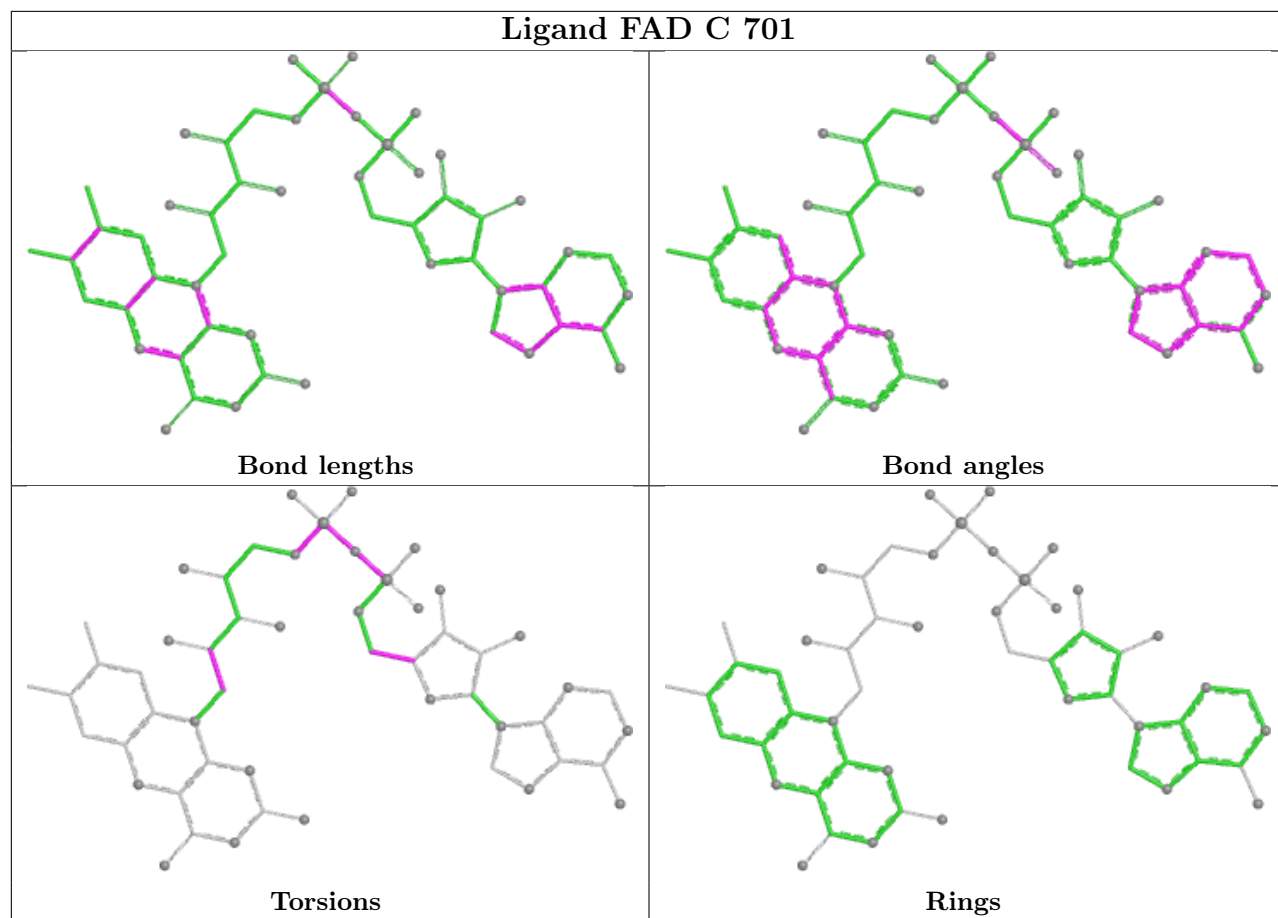
Mol	Chain	Res	Type	Atoms
3	D	702	GOL	O1-C1-C2-O2
3	H	703	GOL	O2-C2-C3-O3
2	H	701	FAD	O4'-C4'-C5'-O5'
2	E	701	FAD	O4B-C4B-C5B-O5B
2	H	701	FAD	P-O3P-PA-O1A
2	H	701	FAD	PA-O3P-P-O1P
3	H	702	GOL	O1-C1-C2-O2
2	A	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	PA-O3P-P-O5'
2	D	701	FAD	PA-O3P-P-O5'
2	E	701	FAD	PA-O3P-P-O5'
2	F	701	FAD	PA-O3P-P-O5'
2	G	701	FAD	PA-O3P-P-O5'
2	H	701	FAD	PA-O3P-P-O5'
2	A	701	FAD	P-O3P-PA-O2A
2	E	701	FAD	O4'-C4'-C5'-O5'
2	G	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	N10-C1'-C2'-C3'
2	H	701	FAD	N10-C1'-C2'-C3'
2	A	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5'-O5'-P-O1P
2	C	701	FAD	C5'-O5'-P-O1P
2	H	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	P-O3P-PA-O1A
2	D	701	FAD	P-O3P-PA-O2A
2	D	701	FAD	PA-O3P-P-O1P
2	G	701	FAD	P-O3P-PA-O2A
2	E	701	FAD	C3B-C4B-C5B-O5B
2	A	701	FAD	O4'-C4'-C5'-O5'
2	F	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	P-O3P-PA-O1A
2	G	701	FAD	P-O3P-PA-O1A
2	G	701	FAD	PA-O3P-P-O1P
2	B	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	P-O3P-PA-O1A
2	A	701	FAD	PA-O3P-P-O1P
2	C	701	FAD	P-O3P-PA-O2A
2	D	701	FAD	P-O3P-PA-O1A
2	H	701	FAD	P-O3P-PA-O2A
2	G	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	O3'-C3'-C4'-C5'

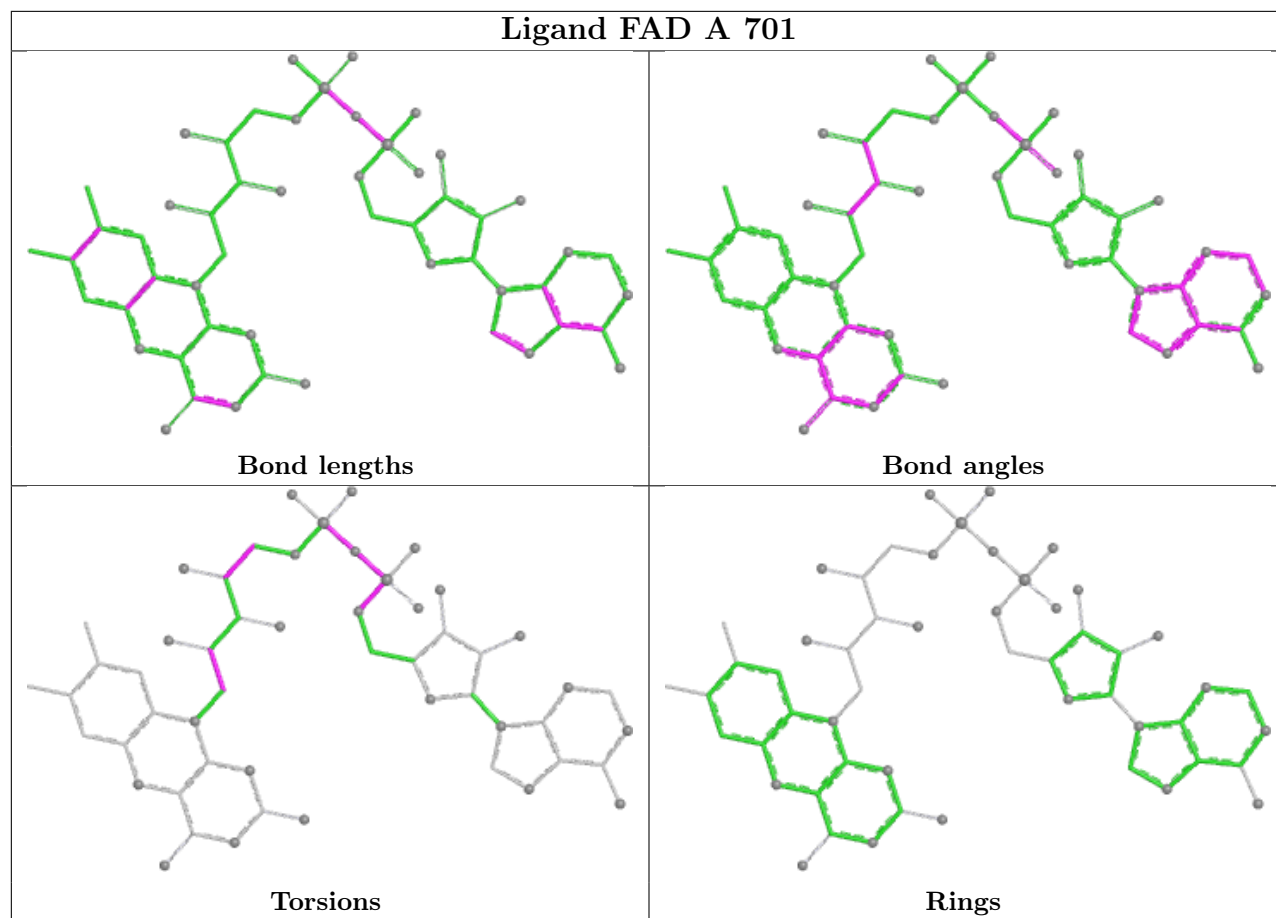
There are no ring outliers.

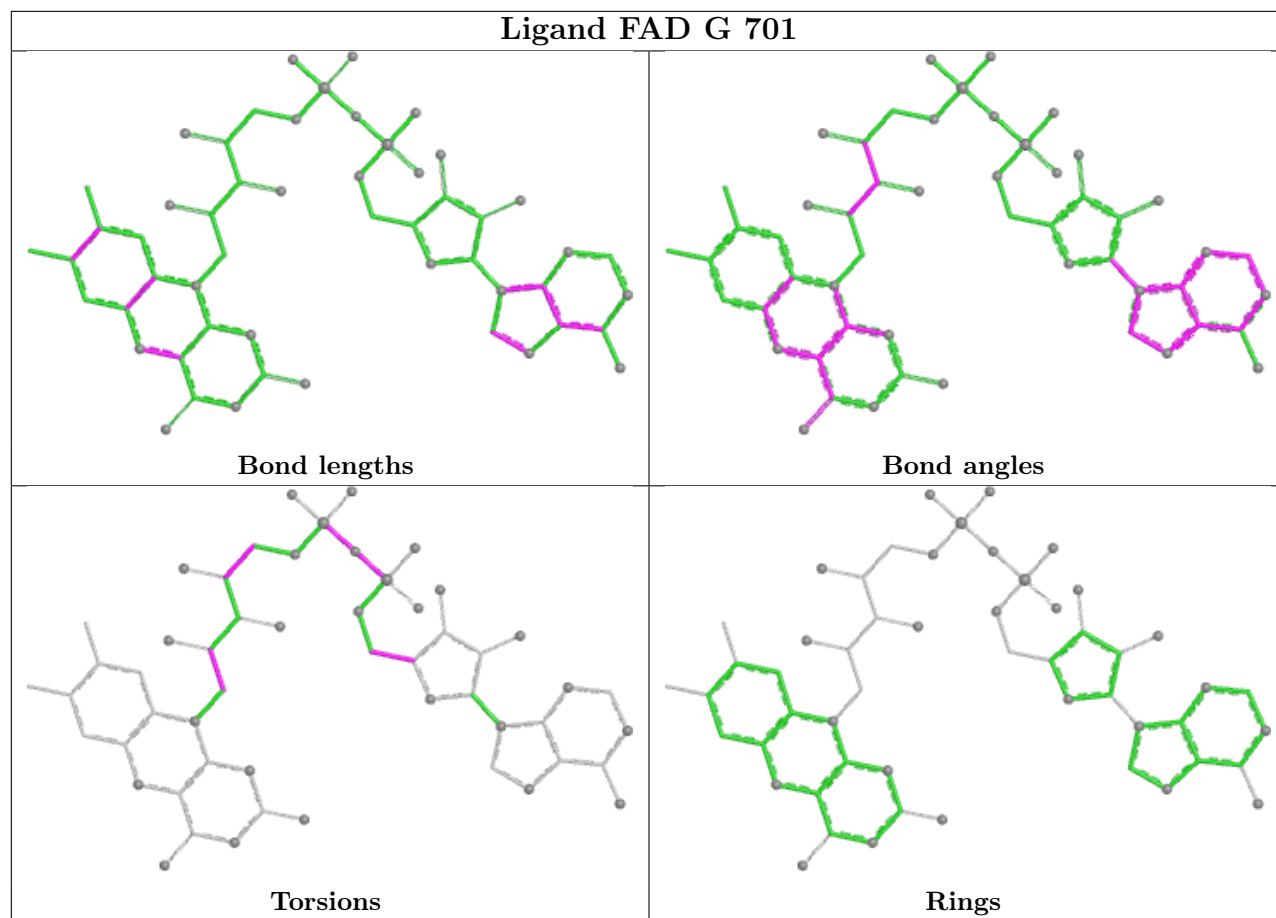
9 monomers are involved in 19 short contacts:

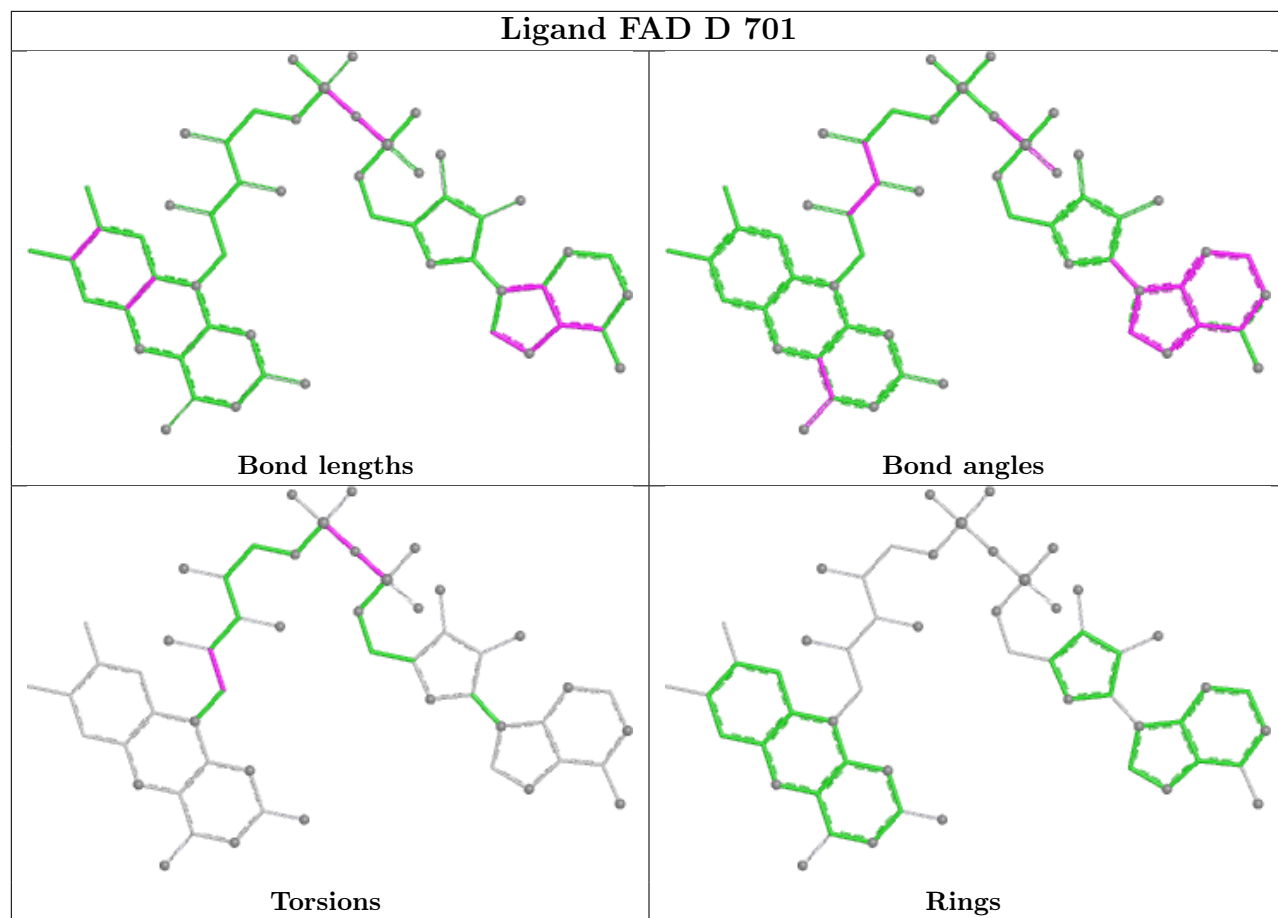
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	FAD	1	0
2	A	701	FAD	2	0
2	G	701	FAD	2	0
2	D	701	FAD	3	0
2	F	701	FAD	3	0
2	H	701	FAD	1	0
2	E	701	FAD	2	0
3	H	703	GOL	2	0
2	B	701	FAD	3	0

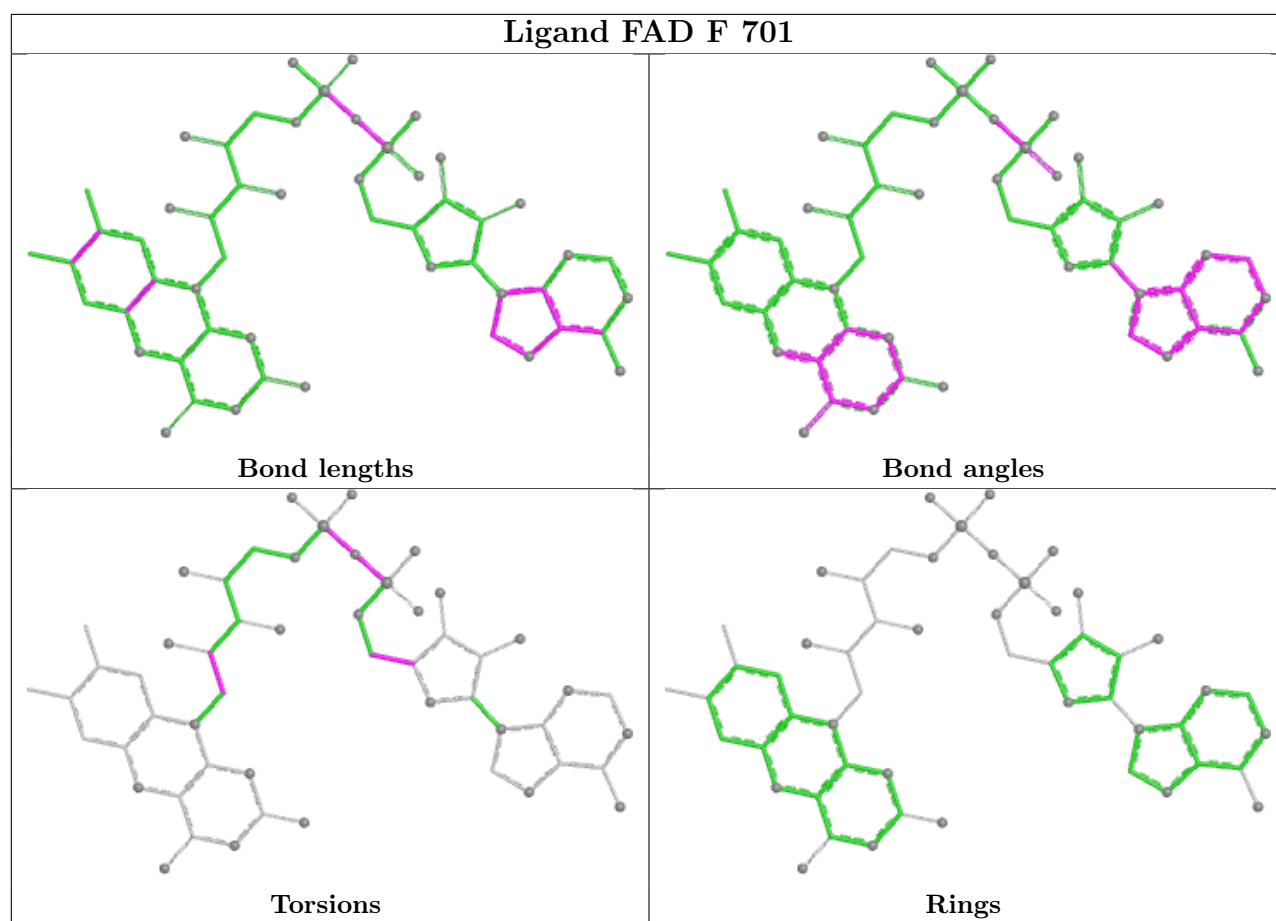
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

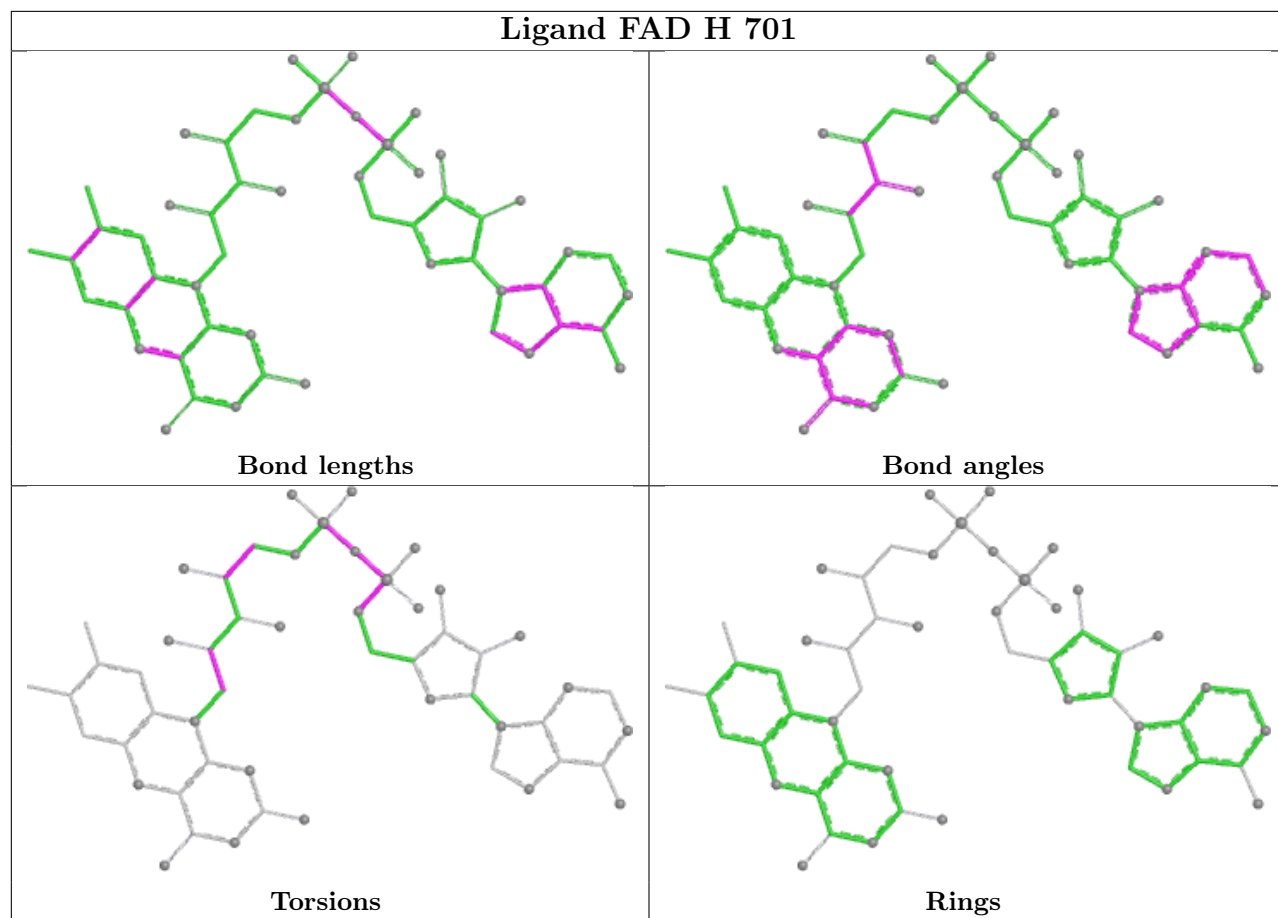


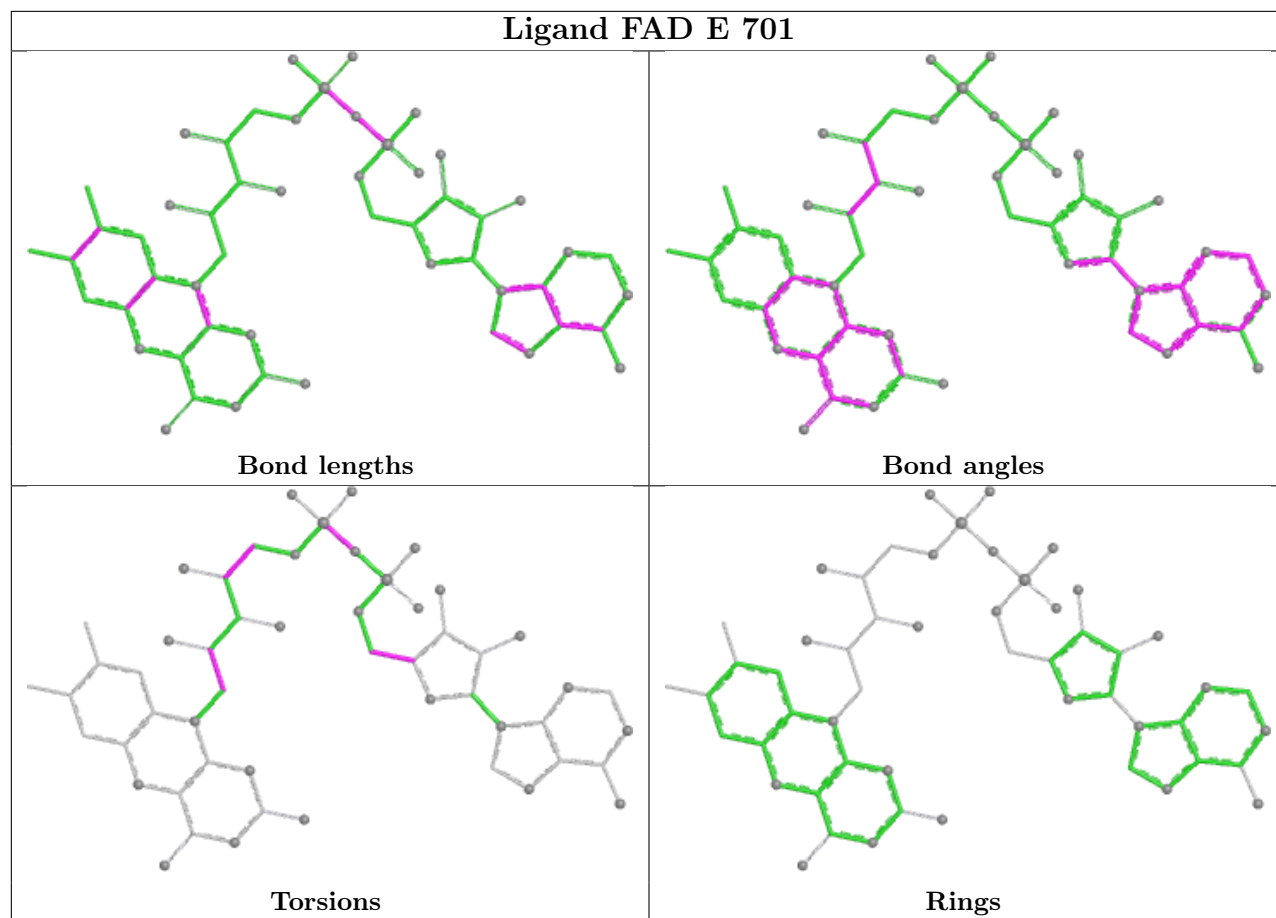


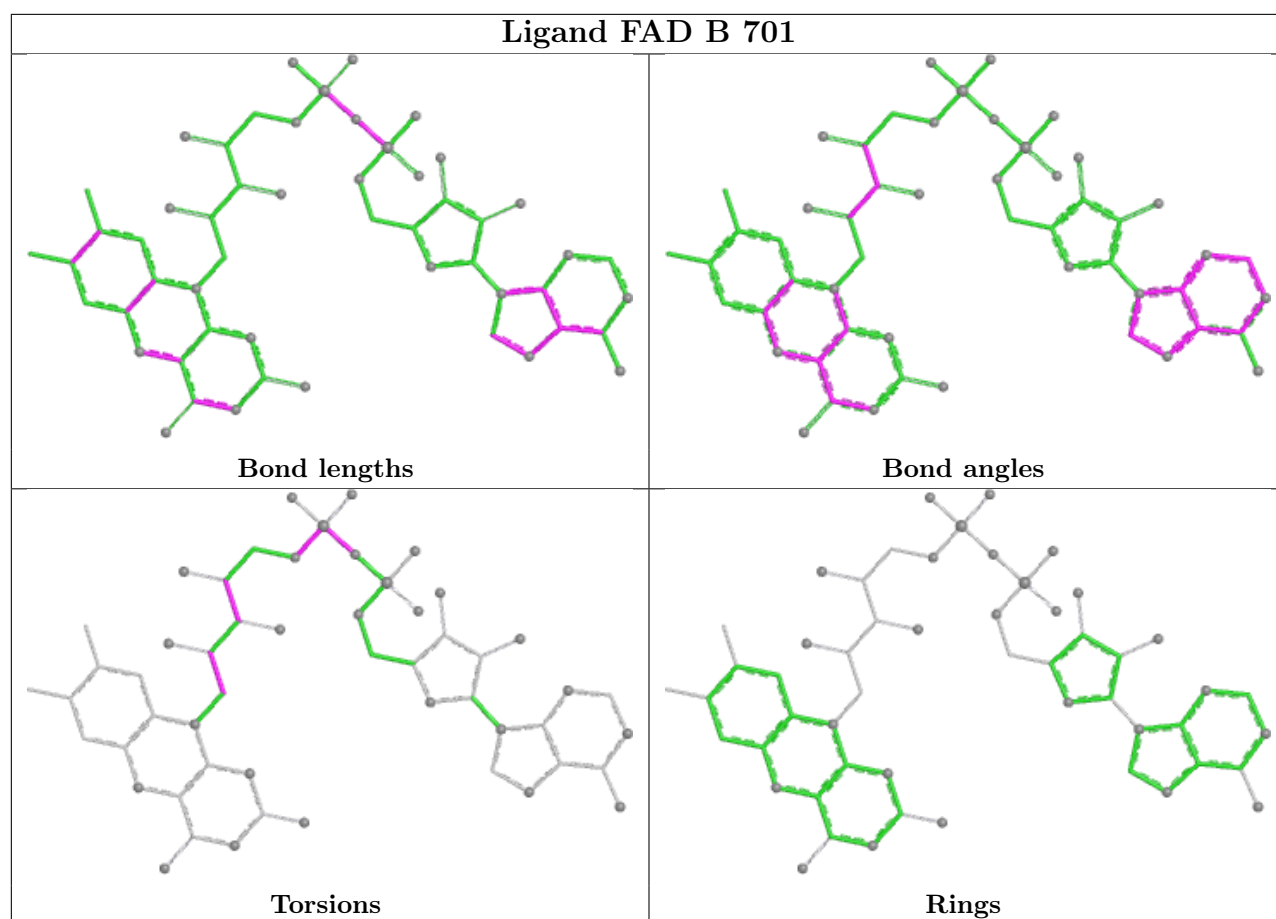












5.7 Other polymers [i](#)

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	643/651 (98%)	-0.32	0	100	100	25, 60, 83, 124	1 (0%)
1	B	642/651 (98%)	-0.52	0	100	100	35, 50, 74, 107	0
1	C	636/651 (97%)	-0.34	0	100	100	23, 57, 79, 95	1 (0%)
1	D	636/651 (97%)	-0.48	2 (0%)	90	88	15, 51, 77, 99	1 (0%)
1	E	637/651 (97%)	-0.26	0	100	100	45, 69, 92, 112	0
1	F	646/651 (99%)	-0.41	2 (0%)	90	88	19, 54, 78, 120	1 (0%)
1	G	635/651 (97%)	-0.33	0	100	100	37, 58, 90, 114	0
1	H	636/651 (97%)	-0.44	1 (0%)	91	90	36, 52, 79, 108	0
All	All	5111/5208 (98%)	-0.39	5 (0%)	92	90	15, 56, 84, 124	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	ARG	4.0
1	F	2	GLY	2.9
1	D	4	PRO	2.6
1	H	640	VAL	2.0
1	F	641	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

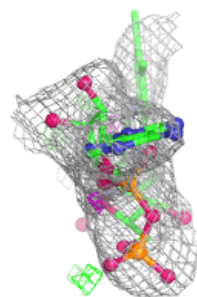
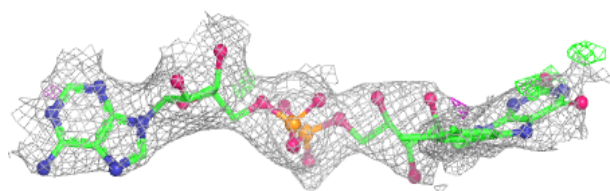
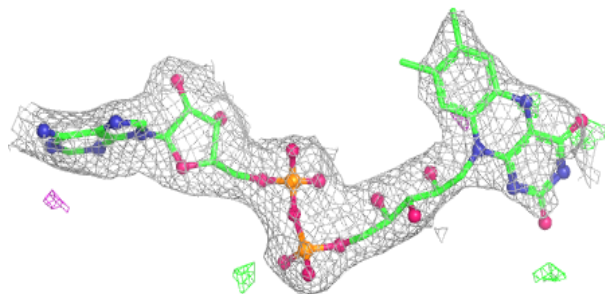
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	H	703	6/6	0.82	0.14	56,57,60,63	0
3	GOL	B	702	6/6	0.85	0.12	59,63,65,66	0
3	GOL	H	702	6/6	0.89	0.11	61,65,68,68	0
3	GOL	D	702	6/6	0.90	0.08	55,63,64,67	0
2	FAD	E	701	53/53	0.92	0.10	68,76,102,108	0
3	GOL	C	702	6/6	0.93	0.08	65,66,67,68	0
2	FAD	G	701	53/53	0.93	0.09	51,78,86,87	0
2	FAD	C	701	53/53	0.94	0.08	51,70,82,86	0
2	FAD	H	701	53/53	0.95	0.09	41,66,96,102	0
2	FAD	A	701	53/53	0.95	0.07	44,70,81,85	0
2	FAD	D	701	53/53	0.95	0.08	49,68,88,90	0
2	FAD	F	701	53/53	0.96	0.07	38,64,87,91	0
2	FAD	B	701	53/53	0.96	0.07	44,53,81,87	0

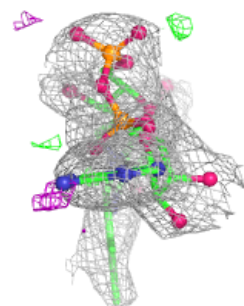
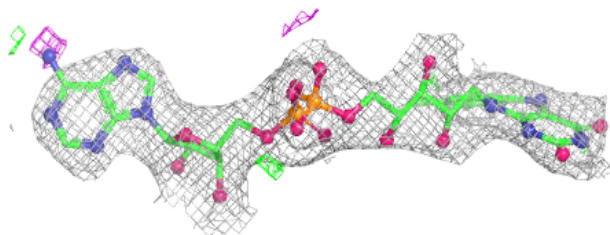
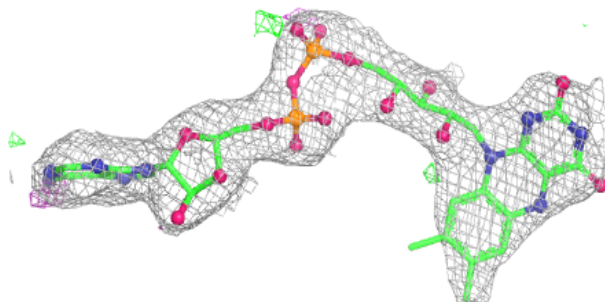
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD E 701:

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

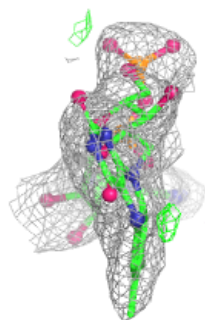
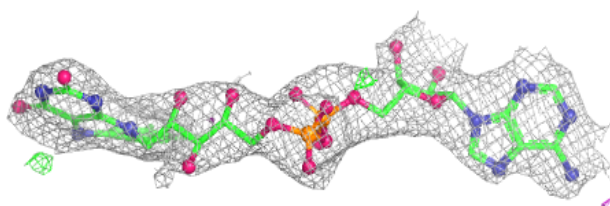
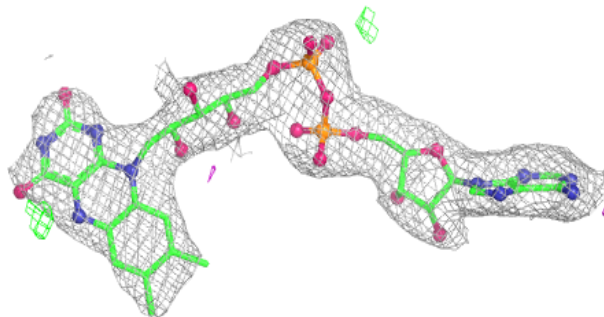
**Electron density around FAD G 701:**

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

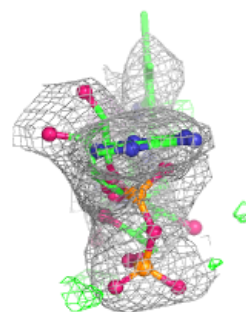
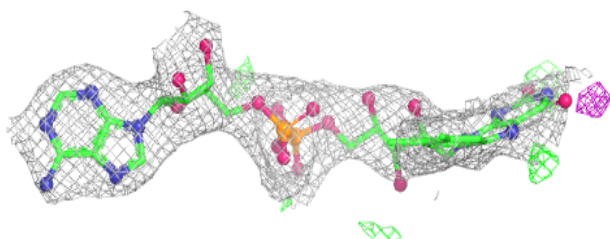
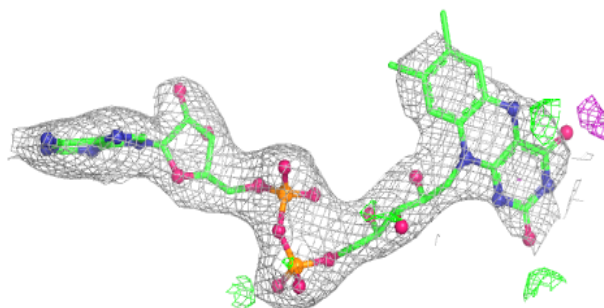


Electron density around FAD C 701:

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

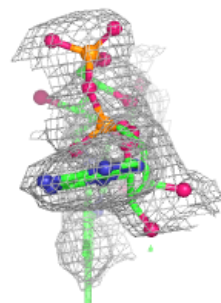
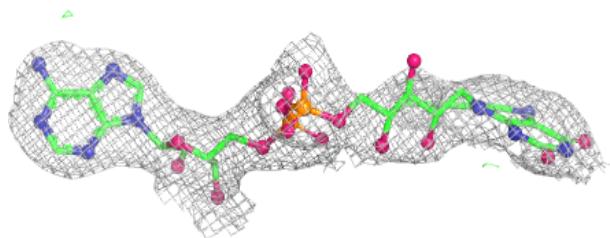
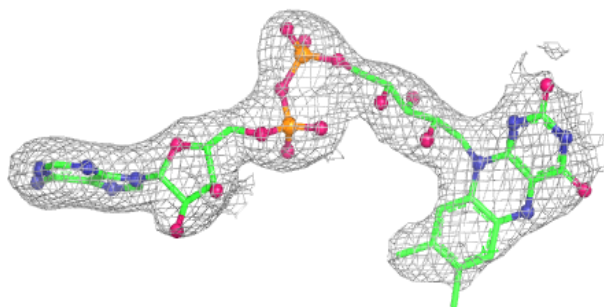
**Electron density around FAD H 701:**

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

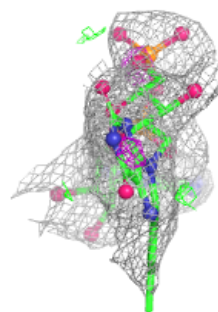
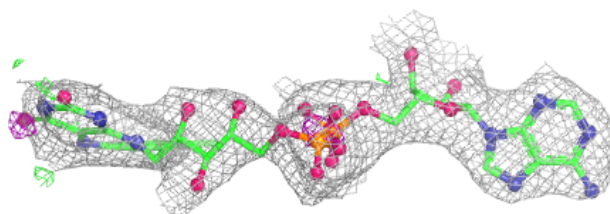
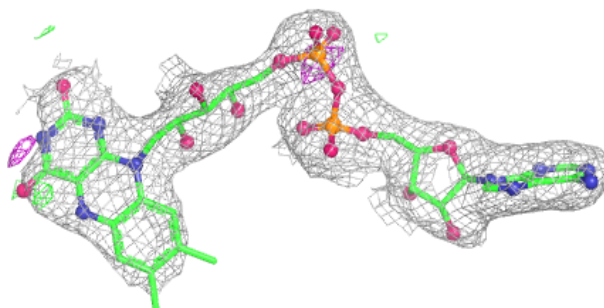


Electron density around FAD A 701:

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

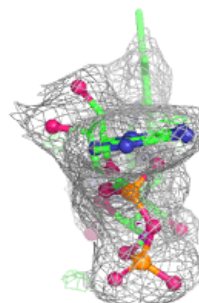
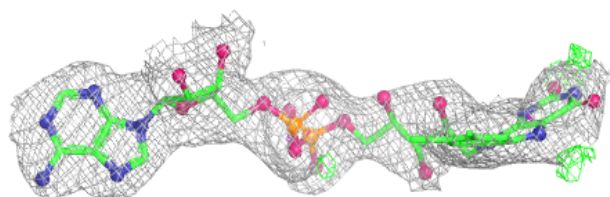
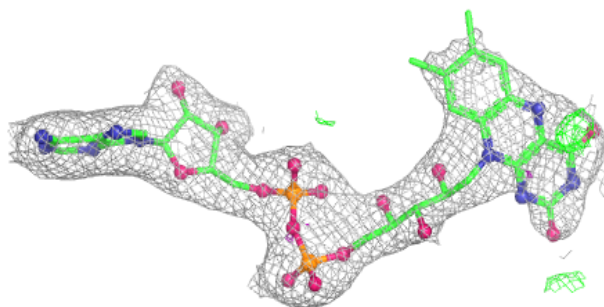
**Electron density around FAD D 701:**

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

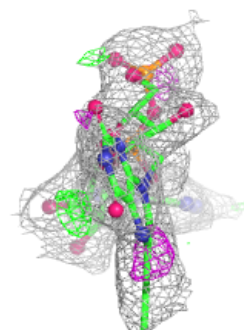
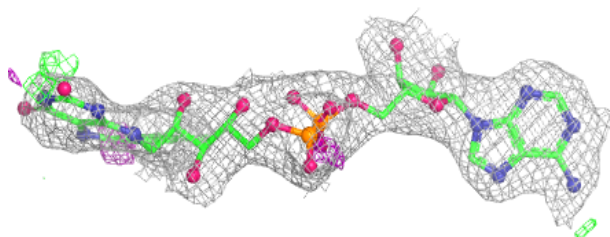
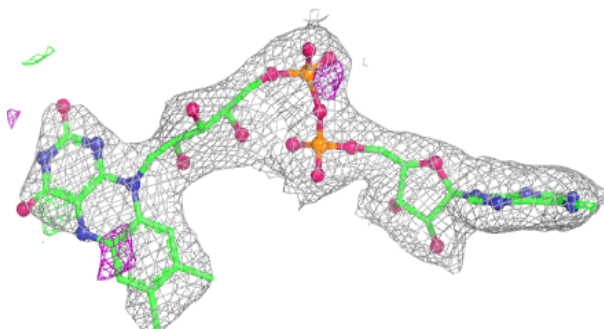


Electron density around FAD F 701:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.