



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:40 PM UTC

PDB ID : 3MPI / pdb_00003mpi
Title : Structure of the glutaryl-coenzyme A dehydrogenase glutaryl-CoA complex
Authors : Wischgoll, S.; Warkentin, E.; Boll, M.; Ermler, U.
Deposited on : 2010-04-27
Resolution : 2.05 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

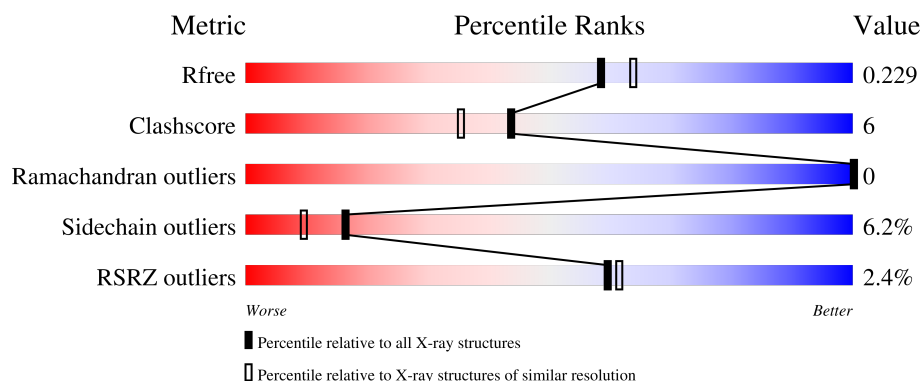
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	397	% 84% 13% ..
1	B	397	5% 85% 11% ..
1	C	397	% 85% 12% ..
1	D	397	3% 85% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12936 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 Glutaryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	4	0
			3023	1913	515	575	20			
1	B	390	Total	C	N	O	S	0	0	0
			2984	1888	510	566	20			
1	C	395	Total	C	N	O	S	0	0	0
			3028	1914	523	571	20			
1	D	390	Total	C	N	O	S	0	1	0
			2989	1892	510	566	21			

There are 32 discrepancies between the modelled and reference sequences:

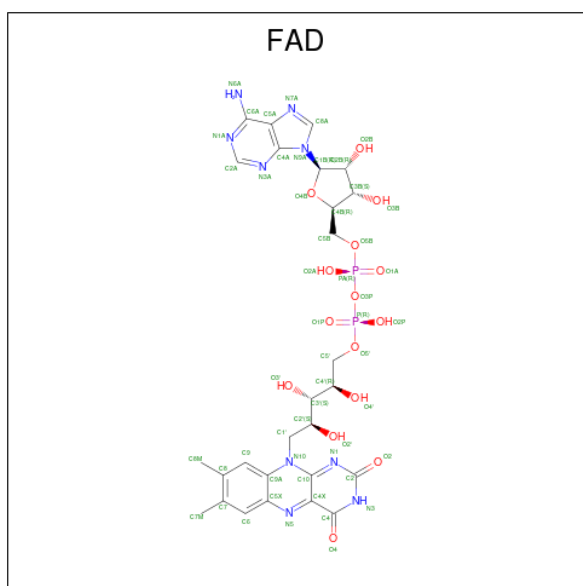
Chain	Residue	Modelled	Actual	Comment	Reference
A	390	LYS	-	expression tag	UNP C3UVB0
A	391	GLY	-	expression tag	UNP C3UVB0
A	392	HIS	-	expression tag	UNP C3UVB0
A	393	HIS	-	expression tag	UNP C3UVB0
A	394	HIS	-	expression tag	UNP C3UVB0
A	395	HIS	-	expression tag	UNP C3UVB0
A	396	HIS	-	expression tag	UNP C3UVB0
A	397	HIS	-	expression tag	UNP C3UVB0
B	390	LYS	-	expression tag	UNP C3UVB0
B	391	GLY	-	expression tag	UNP C3UVB0
B	392	HIS	-	expression tag	UNP C3UVB0
B	393	HIS	-	expression tag	UNP C3UVB0
B	394	HIS	-	expression tag	UNP C3UVB0
B	395	HIS	-	expression tag	UNP C3UVB0
B	396	HIS	-	expression tag	UNP C3UVB0
B	397	HIS	-	expression tag	UNP C3UVB0
C	390	LYS	-	expression tag	UNP C3UVB0
C	391	GLY	-	expression tag	UNP C3UVB0
C	392	HIS	-	expression tag	UNP C3UVB0
C	393	HIS	-	expression tag	UNP C3UVB0
C	394	HIS	-	expression tag	UNP C3UVB0

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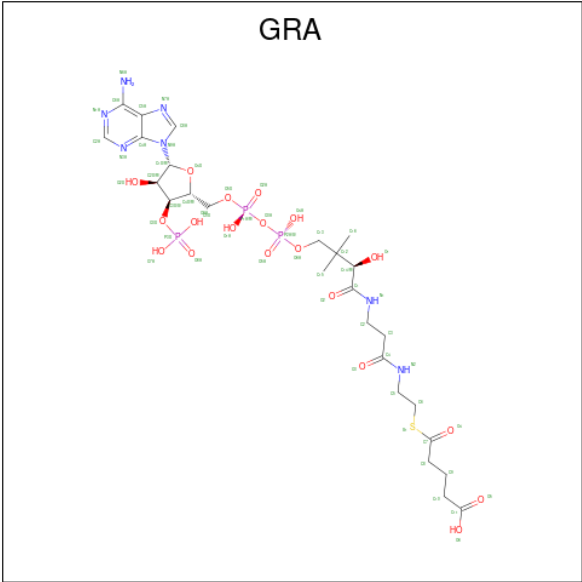
Chain	Residue	Modelled	Actual	Comment	Reference
C	395	HIS	-	expression tag	UNP C3UVB0
C	396	HIS	-	expression tag	UNP C3UVB0
C	397	HIS	-	expression tag	UNP C3UVB0
D	390	LYS	-	expression tag	UNP C3UVB0
D	391	GLY	-	expression tag	UNP C3UVB0
D	392	HIS	-	expression tag	UNP C3UVB0
D	393	HIS	-	expression tag	UNP C3UVB0
D	394	HIS	-	expression tag	UNP C3UVB0
D	395	HIS	-	expression tag	UNP C3UVB0
D	396	HIS	-	expression tag	UNP C3UVB0
D	397	HIS	-	expression tag	UNP C3UVB0

- 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

- Molecule 3 is glutaryl-coenzyme A (CCD ID: GRA) (formula: $C_{26}H_{42}N_7O_{19}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		

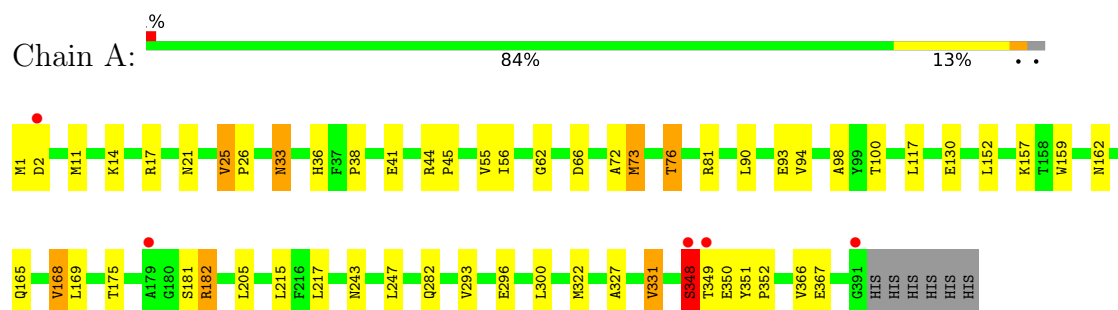
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	158	Total	O	0	0
			158	158		
4	B	58	Total	O	0	0
			58	58		
4	C	155	Total	O	0	0
			155	155		
4	D	105	Total	O	0	0
			105	105		

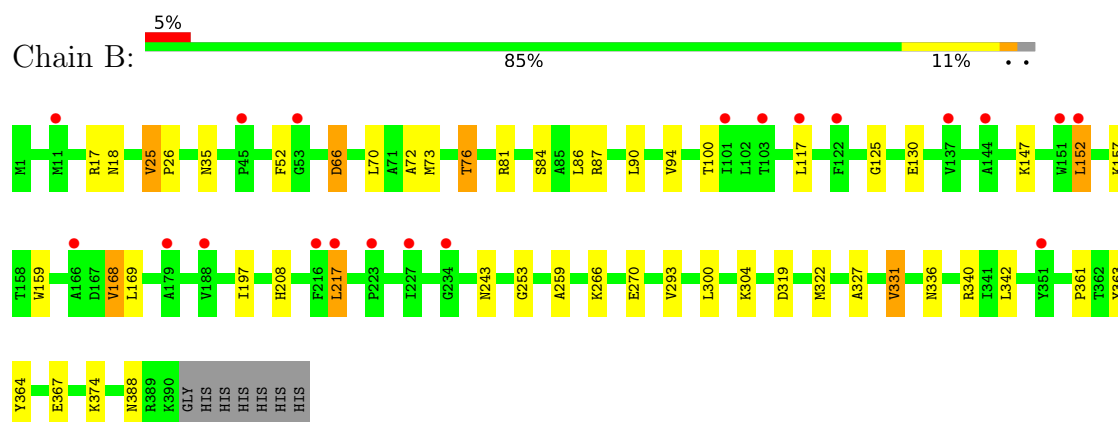
3 Residue-property plots

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.

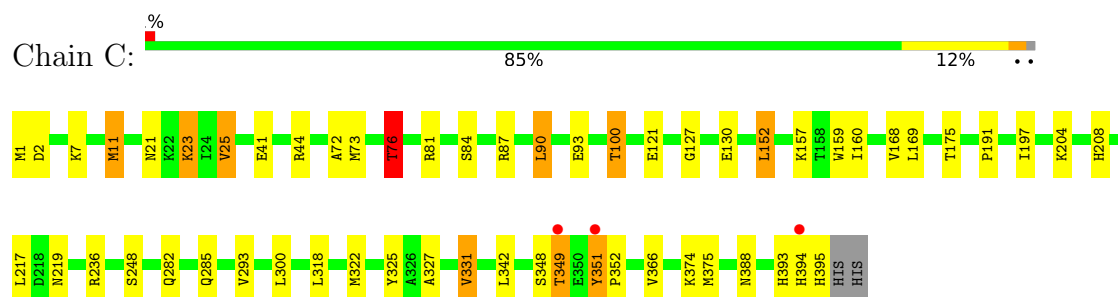
• Molecule 1: Glutaryl-CoA dehydrogenase



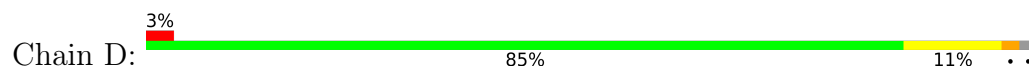
• Molecule 1: Glutaryl-CoA dehydrogenase

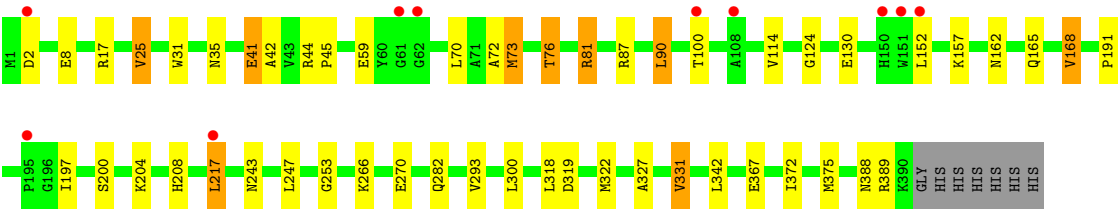


• Molecule 1: Glutaryl-CoA dehydrogenase



• Molecule 1: Glutaryl-CoA dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.99Å 114.79Å 122.24Å 90.00° 133.95° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 30.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-2.05) 97.0 (30.00-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.176 , 0.219 0.193 , 0.229	Depositor DCC
R_{free} test set	5434 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h+2*k,-h-l 0.014 for h,-k,-h-l 0.017 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12936	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: GRA, 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	0.80	1/3083 (0.0%)	0.91	2/4162 (0.0%)
1	B	0.67	1/3042 (0.0%)	0.87	1/4105 (0.0%)
1	C	0.81	2/3090 (0.1%)	0.92	7/4170 (0.2%)
1	D	0.71	2/3050 (0.1%)	0.87	5/4115 (0.1%)
All	All	0.75	6/12265 (0.0%)	0.89	15/16552 (0.1%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	VAL	CA-CB	10.47	1.59	1.54
1	A	25	VAL	CA-CB	9.44	1.58	1.54
1	D	25	VAL	CA-CB	7.70	1.59	1.53
1	C	25	VAL	CA-CB	7.38	1.58	1.53
1	C	76	THR	CA-CB	5.83	1.62	1.53
1	D	114	VAL	CA-CB	5.26	1.57	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	VAL	N-CA-CB	8.62	116.30	110.52
1	C	25	VAL	N-CA-CB	8.62	115.93	110.50
1	D	25	VAL	N-CA-CB	8.09	115.60	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	VAL	N-CA-CB	7.80	115.74	110.52
1	C	351	TYR	CA-C-N	-7.29	112.20	119.56
1	C	351	TYR	C-N-CA	-7.29	112.20	119.56
1	C	349	THR	CB-CA-C	-6.23	100.09	110.68
1	C	349	THR	N-CA-C	6.21	118.85	111.33
1	D	25	VAL	CA-C-N	-6.18	113.32	119.56
1	D	25	VAL	C-N-CA	-6.18	113.32	119.56
1	D	44	ARG	CA-C-N	-5.65	112.78	119.05
1	D	44	ARG	C-N-CA	-5.65	112.78	119.05
1	A	33	ASN	N-CA-C	5.49	117.26	111.28
1	C	100	THR	CB-CA-C	5.14	119.59	110.85
1	C	76	THR	N-CA-CB	5.09	117.69	110.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	SER	Peptide

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	3023	0	2981	43	0
1	B	2984	0	2950	37	0
1	C	3028	0	2981	35	0
1	D	2989	0	2959	32	0
2	A	53	0	31	4	0
2	B	53	0	31	6	0
2	C	53	0	31	7	0
2	D	53	0	31	5	0
3	A	56	0	37	3	0
3	B	56	0	37	4	0
3	C	56	0	37	1	0
3	D	56	0	37	3	0
4	A	158	0	0	6	0
4	B	58	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	155	0	0	2	0
4	D	105	0	0	3	0
All	All	12936	0	12143	151	0

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

All (151) 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:17:ARG:NH1	1:B:81:ARG:HH22	1.60	0.98
1:A:350[B]:GLU:OE2	1:A:351[B]:TYR:CE2	2.15	0.98
1:C:393:HIS:HE1	1:C:395:HIS:HD2	1.21	0.87
1:B:18:ASN:HB3	4:B:473:HOH:O	1.76	0.84
1:B:81:ARG:HD2	4:B:404:HOH:O	1.77	0.83
1:C:21:ASN:HD21	1:C:81:ARG:HH22	1.25	0.81
1:A:17:ARG:NH2	4:A:533:HOH:O	2.15	0.79
1:C:393:HIS:CE1	1:C:395:HIS:HD2	2.02	0.78
1:C:351:TYR:CD1	1:C:352:PRO:HD2	2.18	0.76
1:C:393:HIS:HE1	1:C:395:HIS:CD2	2.04	0.76
1:C:21:ASN:ND2	1:C:81:ARG:HH22	1.83	0.75
1:A:17:ARG:CZ	4:A:533:HOH:O	2.35	0.74
1:B:117:LEU:HD21	1:B:168:VAL:HG13	1.69	0.72
2:B:400:FAD:N5	3:B:402:GRA:H9A	2.04	0.71
1:B:17:ARG:HH12	1:B:81:ARG:HH22	1.39	0.67
1:A:17:ARG:NE	4:A:533:HOH:O	2.28	0.67
1:A:350[B]:GLU:OE2	1:A:351[B]:TYR:HE2	1.78	0.66
1:A:81:ARG:HD2	4:A:435:HOH:O	1.95	0.66
2:C:400:FAD:C9	2:C:400:FAD:H2'	2.26	0.65
2:B:400:FAD:C9	2:B:400:FAD:H2'	2.26	0.65
1:B:17:ARG:NH1	1:B:81:ARG:NH2	2.40	0.64
2:B:400:FAD:H2'	2:B:400:FAD:H9	1.80	0.64
1:A:350[B]:GLU:CD	1:A:351[B]:TYR:CD2	2.77	0.63
1:B:35:ASN:HD22	1:B:208:HIS:HB3	1.64	0.62
2:C:400:FAD:H2'	2:C:400:FAD:H9	1.81	0.62
2:A:400:FAD:C9	2:A:400:FAD:H2'	2.29	0.62
2:A:400:FAD:N5	3:A:402:GRA:H9A	2.15	0.61
2:D:400:FAD:N5	3:D:402:GRA:H9A	2.15	0.61
1:A:350[B]:GLU:OE2	1:A:351[B]:TYR:CD2	2.54	0.61
1:A:327:ALA:O	1:A:331:VAL:HG13	2.01	0.60
1:D:35:ASN:HD22	1:D:208:HIS:HB3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:HH11	1:B:81:ARG:HH22	1.45	0.60
1:A:130:GLU:HG2	1:A:157:LYS:HD3	1.84	0.58
1:A:25:VAL:CG2	1:A:26:PRO:HD3	2.33	0.58
1:B:331:VAL:HG21	1:B:363:TYR:HB2	1.84	0.58
1:D:17:ARG:NH1	1:D:81:ARG:NH2	2.52	0.58
1:A:25:VAL:HG22	1:A:26:PRO:HD3	1.86	0.57
1:C:318:LEU:H	1:C:388:ASN:ND2	2.02	0.57
2:A:400:FAD:H2'	2:A:400:FAD:H9	1.87	0.57
1:D:327:ALA:O	1:D:331:VAL:HG13	2.06	0.56
1:B:81:ARG:HG2	1:B:259:ALA:HB2	1.87	0.56
1:B:147:LYS:HE3	1:B:152:LEU:HD12	1.88	0.56
1:D:162:ASN:HA	1:D:165:GLN:HE21	1.71	0.56
1:D:72:ALA:O	1:D:76:THR:CG2	2.54	0.55
1:B:72:ALA:O	1:B:76:THR:HG22	2.07	0.55
1:B:327:ALA:O	1:B:331:VAL:HG13	2.07	0.55
1:A:348:SER:HB3	1:A:350[B]:GLU:H	1.73	0.54
1:B:25:VAL:CG2	1:B:26:PRO:HD3	2.37	0.54
1:C:1:MET:HG2	1:D:70:LEU:HD21	1.88	0.54
1:C:72:ALA:O	1:C:76:THR:HG22	2.07	0.54
2:C:400:FAD:N5	3:C:402:GRA:H9A	2.23	0.54
2:D:400:FAD:H2'	2:D:400:FAD:C9	2.37	0.54
1:A:21:ASN:O	1:A:25:VAL:HG22	2.07	0.54
1:A:17:ARG:HH12	1:A:81:ARG:NH2	2.06	0.54
1:A:350[B]:GLU:O	1:A:350[B]:GLU:HG2	2.07	0.54
1:D:72:ALA:O	1:D:76:THR:HG22	2.08	0.54
1:A:117:LEU:HD21	1:A:168:VAL:HG13	1.90	0.53
1:C:204:LYS:O	1:C:208:HIS:HE1	1.90	0.53
1:C:375:MET:HE1	2:C:400:FAD:N1A	2.24	0.53
1:D:76:THR:HG22	1:D:90:LEU:HD23	1.90	0.53
1:A:76:THR:HG22	1:A:90:LEU:HD23	1.91	0.53
1:D:197:ILE:HG12	1:D:217:LEU:HD22	1.91	0.53
2:D:400:FAD:H2'	2:D:400:FAD:H9	1.90	0.53
1:D:73:MET:HE3	1:D:247:LEU:HD23	1.90	0.53
1:B:76:THR:HG22	1:B:90:LEU:HD23	1.91	0.52
1:A:162:ASN:HA	1:A:165:GLN:HE21	1.74	0.51
1:C:44:ARG:HH21	1:C:121:GLU:HG3	1.76	0.51
1:A:293:VAL:HA	1:B:322:MET:CE	2.41	0.51
1:B:197:ILE:HG12	1:B:217:LEU:HD22	1.93	0.50
2:C:400:FAD:H2A	1:D:282:GLN:HE22	1.76	0.50
1:B:66:ASP:N	1:B:66:ASP:OD1	2.43	0.50
1:C:393:HIS:CE1	1:C:395:HIS:CD2	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:VAL:HA	1:D:322:MET:HE3	1.93	0.49
1:C:159:TRP:O	2:C:400:FAD:C4X	2.61	0.49
1:D:124:GLY:HA2	1:D:168:VAL:O	2.13	0.49
2:D:400:FAD:C4	3:D:402:GRA:H8	2.43	0.49
1:C:351:TYR:HA	4:C:480:HOH:O	2.13	0.48
1:D:8:GLU:HB2	4:D:467:HOH:O	2.14	0.48
1:A:72:ALA:O	1:A:76:THR:HG22	2.14	0.48
1:C:76:THR:HG21	1:C:248:SER:OG	2.14	0.48
1:C:285:GLN:OE1	1:D:375[B]:MET:SD	2.71	0.48
1:C:152:LEU:HD11	1:C:219:ASN:OD1	2.14	0.48
1:A:56:ILE:HB	1:A:62:GLY:HA3	1.95	0.48
1:C:130:GLU:HG2	1:C:157:LYS:HD3	1.96	0.47
1:D:81:ARG:NH1	4:D:401:HOH:O	2.47	0.47
1:A:296:GLU:OE1	1:B:304:LYS:NZ	2.42	0.47
1:C:76:THR:HG22	1:C:90:LEU:HD23	1.95	0.47
1:C:327:ALA:O	1:C:331:VAL:HG13	2.15	0.47
1:C:282:GLN:HE22	2:D:400:FAD:H2A	1.79	0.47
1:A:55:VAL:HG22	4:A:482:HOH:O	2.14	0.47
1:B:25:VAL:HG22	1:B:26:PRO:HD3	1.97	0.46
1:C:191:PRO:HA	1:C:197:ILE:HD12	1.97	0.46
1:C:394:HIS:HD2	4:C:436:HOH:O	1.98	0.46
1:B:253:GLY:O	1:B:331:VAL:HG12	2.16	0.46
1:B:361:PRO:HA	1:B:364:TYR:CZ	2.49	0.46
1:C:159:TRP:O	2:C:400:FAD:C10	2.64	0.45
1:A:94:VAL:HA	1:A:98:ALA:HB3	1.97	0.45
1:A:351[B]:TYR:HB3	1:A:352[B]:PRO:HD2	1.99	0.45
2:B:400:FAD:C4X	3:B:402:GRA:H9A	2.47	0.45
1:D:130:GLU:HG2	1:D:157:LYS:HD3	1.97	0.45
1:B:336:ASN:OD1	1:B:340:ARG:NE	2.49	0.45
1:A:1:MET:HG2	1:B:70:LEU:CD2	2.46	0.45
1:A:11:MET:O	1:A:11:MET:HE3	2.17	0.44
1:A:350[B]:GLU:OE1	1:A:351[B]:TYR:HD2	2.01	0.44
1:B:72:ALA:O	1:B:76:THR:CG2	2.65	0.44
1:A:367:GLU:OE2	3:A:402:GRA:H8B	2.16	0.44
1:D:87:ARG:HD2	1:D:87:ARG:C	2.43	0.44
1:A:44:ARG:HB3	1:A:45:PRO:HD3	2.00	0.44
1:A:182:ARG:HG3	1:A:182:ARG:NH1	2.33	0.44
1:C:127:GLY:HA2	1:C:160:ILE:HD12	2.00	0.44
1:C:322:MET:HE3	1:D:293:VAL:HA	2.00	0.44
1:D:266:LYS:HE3	1:D:270:GLU:OE1	2.18	0.44
1:C:72:ALA:O	1:C:76:THR:CG2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:TRP:CZ2	1:D:41:GLU:HG3	2.53	0.43
1:C:351:TYR:HD1	1:C:352:PRO:HD2	1.77	0.43
1:A:322:MET:HE3	1:B:293:VAL:HA	2.01	0.43
1:D:191:PRO:HA	1:D:197:ILE:HD13	2.00	0.43
2:B:400:FAD:C4	3:B:402:GRA:H8	2.49	0.43
1:D:42:ALA:C	1:D:45:PRO:HD2	2.43	0.43
1:B:159:TRP:O	2:B:400:FAD:C4X	2.67	0.43
1:B:84:SER:O	1:B:87:ARG:HG3	2.19	0.43
1:B:266:LYS:HE2	1:B:270:GLU:OE1	2.19	0.43
1:A:293:VAL:HA	1:B:322:MET:HE3	2.01	0.43
1:B:130:GLU:HG2	1:B:157:LYS:HD3	2.01	0.43
1:A:25:VAL:HG21	4:A:423:HOH:O	2.18	0.42
1:D:72:ALA:O	1:D:76:THR:HG23	2.19	0.42
1:A:11:MET:HE1	1:A:14:LYS:HD2	2.01	0.42
1:B:319:ASP:H	1:B:388:ASN:HD21	1.65	0.42
1:D:367:GLU:OE2	3:D:402:GRA:H8B	2.18	0.42
1:D:81:ARG:NH2	4:D:488:HOH:O	2.52	0.42
1:A:17:ARG:HH11	1:A:17:ARG:HG3	1.83	0.42
1:C:84:SER:O	1:C:87:ARG:HG3	2.20	0.42
1:A:73:MET:HE3	1:A:247:LEU:HD23	2.01	0.42
1:D:319:ASP:H	1:D:388:ASN:HD21	1.67	0.42
1:A:1:MET:HG2	1:B:70:LEU:HD21	2.02	0.42
1:C:325:TYR:CE1	1:C:374:LYS:HE3	2.53	0.42
1:B:367:GLU:OE2	3:B:402:GRA:H8B	2.20	0.42
1:C:11:MET:HA	1:C:11:MET:HE3	2.02	0.42
1:D:204:LYS:O	1:D:208:HIS:HE1	2.02	0.42
1:D:243:ASN:HD22	1:D:243:ASN:HA	1.63	0.42
1:A:159:TRP:O	2:A:400:FAD:C4X	2.68	0.41
1:D:253:GLY:O	1:D:331:VAL:HG12	2.20	0.41
1:D:318:LEU:H	1:D:388:ASN:ND2	2.18	0.41
1:B:243:ASN:HD22	1:B:243:ASN:HA	1.70	0.41
1:C:1:MET:HG2	1:D:70:LEU:CD2	2.51	0.41
1:A:181:SER:HB2	3:A:402:GRA:H4X	2.03	0.41
1:B:52:PHE:O	1:B:94:VAL:HG21	2.21	0.40
1:A:243:ASN:HD22	1:A:243:ASN:HA	1.69	0.40
1:A:36:HIS:O	1:A:38:PRO:HD3	2.22	0.40
1:C:23:LYS:HB3	1:C:23:LYS:HE2	1.69	0.40
1:B:125:GLY:HA3	1:B:169:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	393/397 (99%)	381 (97%)	12 (3%)	0	100	100
1	B	388/397 (98%)	378 (97%)	10 (3%)	0	100	100
1	C	393/397 (99%)	385 (98%)	8 (2%)	0	100	100
1	D	389/397 (98%)	382 (98%)	7 (2%)	0	100	100
All	All	1563/1588 (98%)	1526 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/309 (99%)	284 (92%)	23 (8%)	12	6
1	B	303/309 (98%)	291 (96%)	12 (4%)	28	22
1	C	307/309 (99%)	284 (92%)	23 (8%)	12	6
1	D	304/309 (98%)	286 (94%)	18 (6%)	18	10
All	All	1221/1236 (99%)	1145 (94%)	76 (6%)	16	9

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	33	ASN

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Mol	Chain	Res	Type
1	A	41	GLU
1	A	66	ASP
1	A	73	MET
1	A	76	THR
1	A	93	GLU
1	A	100	THR
1	A	152	LEU
1	A	168	VAL
1	A	169	LEU
1	A	175	THR
1	A	182	ARG
1	A	205	LEU
1	A	215	LEU
1	A	217	LEU
1	A	282	GLN
1	A	300	LEU
1	A	331	VAL
1	A	348	SER
1	A	349[A]	THR
1	A	349[B]	THR
1	A	366	VAL
1	B	66	ASP
1	B	73	MET
1	B	76	THR
1	B	86	LEU
1	B	100	THR
1	B	152	LEU
1	B	168	VAL
1	B	217	LEU
1	B	300	LEU
1	B	331	VAL
1	B	342	LEU
1	B	374	LYS
1	C	2	ASP
1	C	7	LYS
1	C	11	MET
1	C	23	LYS
1	C	25	VAL
1	C	41	GLU
1	C	73	MET
1	C	76	THR
1	C	90	LEU

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Mol	Chain	Res	Type
1	C	93	GLU
1	C	100	THR
1	C	152	LEU
1	C	168	VAL
1	C	169	LEU
1	C	175	THR
1	C	217	LEU
1	C	236	ARG
1	C	300	LEU
1	C	331	VAL
1	C	342	LEU
1	C	348	SER
1	C	349	THR
1	C	366	VAL
1	D	2	ASP
1	D	25	VAL
1	D	41	GLU
1	D	59	GLU
1	D	73	MET
1	D	76	THR
1	D	81	ARG
1	D	90	LEU
1	D	100	THR
1	D	152	LEU
1	D	168	VAL
1	D	200	SER
1	D	217	LEU
1	D	300	LEU
1	D	331	VAL
1	D	342	LEU
1	D	372	ILE
1	D	389	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	30	GLN
1	A	35	ASN
1	A	165	GLN
1	A	208	HIS
1	A	226	ASN

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Mol	Chain	Res	Type
1	A	243	ASN
1	A	269	ASN
1	A	282	GLN
1	A	388	ASN
1	B	21	ASN
1	B	30	GLN
1	B	33	ASN
1	B	35	ASN
1	B	165	GLN
1	B	208	HIS
1	B	243	ASN
1	B	282	GLN
1	B	388	ASN
1	C	21	ASN
1	C	30	GLN
1	C	35	ASN
1	C	165	GLN
1	C	208	HIS
1	C	226	ASN
1	C	243	ASN
1	C	269	ASN
1	C	282	GLN
1	C	388	ASN
1	C	393	HIS
1	C	395	HIS
1	D	21	ASN
1	D	30	GLN
1	D	33	ASN
1	D	35	ASN
1	D	165	GLN
1	D	208	HIS
1	D	243	ASN
1	D	269	ASN
1	D	282	GLN
1	D	388	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GRA	D	402	-	56,58,58	1.58	8 (14%)	79,85,85	1.87	19 (24%)
2	FAD	D	400	-	58,58,58	1.28	7 (12%)	85,89,89	1.61	18 (21%)
3	GRA	B	402	-	56,58,58	1.43	10 (17%)	79,85,85	1.87	19 (24%)
2	FAD	C	400	-	58,58,58	1.15	7 (12%)	85,89,89	1.65	21 (24%)
2	FAD	A	400	-	58,58,58	1.25	6 (10%)	85,89,89	1.58	16 (18%)
2	FAD	B	400	-	58,58,58	1.26	6 (10%)	85,89,89	1.57	17 (20%)
3	GRA	C	402	-	56,58,58	1.53	9 (16%)	79,85,85	1.81	19 (24%)
3	GRA	A	402	-	56,58,58	1.60	9 (16%)	79,85,85	1.87	21 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GRA	D	402	-	-	6/57/73/73	0/3/3/3
2	FAD	D	400	-	-	7/34/50/50	0/6/6/6
3	GRA	B	402	-	-	7/57/73/73	0/3/3/3
2	FAD	C	400	-	-	5/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	400	-	-	4/34/50/50	0/6/6/6
2	FAD	B	400	-	-	3/34/50/50	0/6/6/6
3	GRA	C	402	-	-	6/57/73/73	0/3/3/3
3	GRA	A	402	-	-	6/57/73/73	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	GRA	O4-C7	6.30	1.30	1.21
3	D	402	GRA	O4-C7	5.93	1.30	1.21
3	B	402	GRA	O4-C7	5.52	1.29	1.21
3	C	402	GRA	O4-C7	5.35	1.29	1.21
3	D	402	GRA	C9-C8	-4.71	1.35	1.52
3	C	402	GRA	C8-C7	-4.45	1.46	1.50
3	A	402	GRA	C9-C8	-4.44	1.36	1.52
3	D	402	GRA	C8-C7	-4.37	1.46	1.50
2	D	400	FAD	PA-O3P	4.34	1.64	1.59
2	A	400	FAD	C4X-N5	4.33	1.40	1.30
3	C	402	GRA	C9-C8	-4.32	1.36	1.52
2	C	400	FAD	C4X-N5	3.80	1.39	1.30
2	D	400	FAD	C4X-N5	3.75	1.38	1.30
2	B	400	FAD	C4X-N5	3.65	1.38	1.30
2	B	400	FAD	PA-O3P	3.51	1.63	1.59
2	B	400	FAD	C1'-C2'	3.34	1.57	1.52
3	B	402	GRA	C9-C8	-3.33	1.40	1.52
2	A	400	FAD	C10-N1	3.27	1.39	1.33
2	D	400	FAD	P-O3P	3.10	1.62	1.59
2	C	400	FAD	C2A-N1A	3.09	1.39	1.33
3	B	402	GRA	C2A-N3A	-3.06	1.28	1.33
3	A	402	GRA	C2A-N3A	-3.05	1.28	1.33
3	A	402	GRA	C8-C7	-3.04	1.47	1.50
3	D	402	GRA	C2A-N3A	-2.95	1.28	1.33
2	B	400	FAD	C10-N1	2.90	1.39	1.33
2	D	400	FAD	C1'-C2'	2.85	1.56	1.52
2	C	400	FAD	C1'-C2'	2.83	1.56	1.52
3	C	402	GRA	C2A-N3A	-2.80	1.29	1.33
2	A	400	FAD	C1'-C2'	2.74	1.56	1.52
2	B	400	FAD	P-O3P	2.70	1.62	1.59
3	D	402	GRA	C8A-N7A	2.70	1.36	1.31
3	A	402	GRA	C5A-C6A	2.66	1.48	1.41
2	A	400	FAD	C8A-N7A	2.65	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	FAD	C2A-N1A	2.65	1.38	1.33
3	B	402	GRA	C2A-N1A	-2.61	1.29	1.33
2	C	400	FAD	C5'-C4'	2.57	1.55	1.51
2	B	400	FAD	C2A-N1A	2.53	1.38	1.33
3	C	402	GRA	C4A-N3A	2.52	1.39	1.34
3	C	402	GRA	C8A-N7A	2.51	1.36	1.31
3	D	402	GRA	C4A-N9A	-2.49	1.32	1.37
3	C	402	GRA	C5A-C6A	2.48	1.47	1.41
3	B	402	GRA	C8A-N7A	2.47	1.36	1.31
2	C	400	FAD	C10-N1	2.44	1.38	1.33
2	A	400	FAD	C2A-N3A	2.43	1.38	1.33
3	A	402	GRA	P2A-O3A	2.42	1.62	1.59
3	A	402	GRA	C8A-N7A	2.40	1.36	1.31
2	A	400	FAD	PA-O3P	2.39	1.62	1.59
3	B	402	GRA	C5A-C6A	2.37	1.47	1.41
2	D	400	FAD	C10-N1	2.34	1.38	1.33
3	C	402	GRA	C4A-N9A	-2.33	1.32	1.37
3	A	402	GRA	C2A-N1A	-2.33	1.29	1.33
2	D	400	FAD	C2A-N3A	2.32	1.38	1.33
3	B	402	GRA	C4A-N9A	-2.32	1.32	1.37
2	C	400	FAD	C1'-N10	2.29	1.53	1.47
3	D	402	GRA	C5A-C6A	2.28	1.47	1.41
3	D	402	GRA	C2A-N1A	-2.25	1.29	1.33
3	C	402	GRA	C2A-N1A	-2.23	1.30	1.33
3	B	402	GRA	C5A-N7A	-2.14	1.35	1.39
3	B	402	GRA	C4A-N3A	2.12	1.38	1.34
2	C	400	FAD	C2A-N3A	2.09	1.37	1.33
3	A	402	GRA	C4A-N9A	-2.04	1.33	1.37
3	B	402	GRA	C8-C7	-2.02	1.48	1.50

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	GRA	C6-S1-C7	7.23	123.21	101.84
2	C	400	FAD	N3A-C2A-N1A	-6.75	118.36	128.58
2	A	400	FAD	N3A-C2A-N1A	-6.41	118.88	128.58
3	D	402	GRA	C6-S1-C7	6.39	120.73	101.84
2	B	400	FAD	N3A-C2A-N1A	-5.85	119.73	128.58
3	C	402	GRA	C6-S1-C7	5.76	118.86	101.84
2	D	400	FAD	N3A-C2A-N1A	-5.57	120.15	128.58
3	A	402	GRA	C6-S1-C7	5.46	117.99	101.84
3	A	402	GRA	C5A-C4A-N3A	-4.73	120.20	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	GRA	O4-C7-S1	-4.62	116.81	122.68
3	A	402	GRA	C5A-C4A-N9A	4.55	110.77	105.81
3	D	402	GRA	C5A-C4A-N9A	4.48	110.69	105.81
3	D	402	GRA	O4-C7-S1	-4.45	117.02	122.68
3	A	402	GRA	O4-C7-S1	-4.45	117.02	122.68
3	B	402	GRA	C5A-C4A-N3A	-4.43	120.62	126.72
3	B	402	GRA	C5A-C4A-N9A	4.39	110.59	105.81
3	D	402	GRA	C5A-C4A-N3A	-4.33	120.76	126.72
3	A	402	GRA	C8-C7-S1	4.14	118.34	113.40
3	D	402	GRA	C8-C7-S1	4.12	118.31	113.40
3	C	402	GRA	C5A-C4A-N3A	-4.10	121.07	126.72
3	B	402	GRA	O4-C7-S1	-4.07	117.51	122.68
2	D	400	FAD	N9A-C8A-N7A	-4.05	108.18	113.94
3	B	402	GRA	C8-C7-S1	4.01	118.18	113.40
3	C	402	GRA	C8-C7-S1	3.99	118.16	113.40
2	A	400	FAD	N9A-C8A-N7A	-3.92	108.37	113.94
2	B	400	FAD	C5A-C4A-N3A	-3.89	121.35	126.72
3	C	402	GRA	C5A-C4A-N9A	3.81	109.96	105.81
2	C	400	FAD	C5A-C4A-N3A	-3.79	121.49	126.72
2	C	400	FAD	N9A-C8A-N7A	-3.72	108.66	113.94
3	C	402	GRA	N1A-C2A-N3A	-3.58	123.16	128.58
2	D	400	FAD	C4-N3-C2	-3.57	119.30	125.64
2	C	400	FAD	C2A-N3A-C4A	3.55	120.50	111.83
3	A	402	GRA	C2A-N3A-C4A	3.47	120.31	111.83
3	A	402	GRA	N1A-C2A-N3A	-3.38	123.47	128.58
2	D	400	FAD	C5A-C4A-N3A	-3.37	122.08	126.72
2	A	400	FAD	C5A-C4A-N3A	-3.35	122.10	126.72
2	B	400	FAD	C4-N3-C2	-3.35	119.70	125.64
2	B	400	FAD	C2A-N3A-C4A	3.34	119.99	111.83
2	B	400	FAD	N9A-C8A-N7A	-3.30	109.26	113.94
3	A	402	GRA	C4A-C5A-N7A	-3.29	106.83	110.58
3	A	402	GRA	C2X-C1X-N9A	-3.26	105.20	113.30
3	D	402	GRA	N6A-C6A-N1A	3.25	125.62	118.38
3	C	402	GRA	C2A-N3A-C4A	3.20	119.65	111.83
2	D	400	FAD	C9A-C5X-N5	-3.20	119.06	122.45
2	D	400	FAD	C5A-N7A-C8A	3.19	108.46	103.45
2	A	400	FAD	C2A-N3A-C4A	3.19	119.61	111.83
2	C	400	FAD	C5A-N7A-C8A	3.12	108.36	103.45
3	C	402	GRA	O4A-P2A-O3A	3.12	115.71	107.27
3	D	402	GRA	C2X-C1X-N9A	-3.11	105.56	113.30
3	B	402	GRA	N1A-C2A-N3A	-3.08	123.92	128.58
2	C	400	FAD	C4X-C10-N10	3.08	120.89	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	FAD	C4-N3-C2	-3.07	120.19	125.64
3	C	402	GRA	C2X-C1X-N9A	-3.07	105.69	113.30
3	D	402	GRA	C3-C2-N1	-3.01	105.60	112.00
3	B	402	GRA	C2A-N3A-C4A	3.00	119.15	111.83
3	D	402	GRA	C6-C5-N2	-2.99	106.17	112.41
2	C	400	FAD	C5X-C9A-N10	2.95	120.64	117.97
2	A	400	FAD	C4-N3-C2	-2.94	120.41	125.64
3	B	402	GRA	C6-C5-N2	-2.94	106.28	112.41
2	B	400	FAD	C10-C4X-N5	-2.92	118.85	124.81
3	D	402	GRA	C2A-N3A-C4A	2.91	118.94	111.83
2	D	400	FAD	C2A-N3A-C4A	2.91	118.93	111.83
2	B	400	FAD	C5A-N7A-C8A	2.89	108.00	103.45
2	B	400	FAD	C4X-C10-N1	-2.89	117.50	124.59
3	A	402	GRA	O4A-P2A-O3A	2.88	115.06	107.27
3	D	402	GRA	N1A-C2A-N3A	-2.85	124.26	128.58
3	B	402	GRA	C2X-C1X-N9A	-2.85	106.23	113.30
2	A	400	FAD	C5A-N7A-C8A	2.84	107.92	103.45
3	A	402	GRA	O7A-P3X-O9A	2.82	118.38	107.80
2	D	400	FAD	C5X-C9A-N10	2.80	120.50	117.97
3	C	402	GRA	C6-C5-N2	-2.79	106.59	112.41
3	B	402	GRA	N6A-C6A-N1A	2.78	124.57	118.38
2	A	400	FAD	O4-C4-C4X	-2.78	119.19	126.53
3	B	402	GRA	C4A-C5A-N7A	-2.75	107.44	110.58
3	A	402	GRA	O3A-P2A-O5A	-2.75	102.45	110.70
3	C	402	GRA	C15-C12-C14	2.74	113.44	108.77
3	A	402	GRA	N9A-C8A-N7A	-2.72	110.07	113.94
3	C	402	GRA	C2A-N1A-C6A	2.71	123.19	118.73
2	B	400	FAD	C4-C4X-C10	2.71	121.58	116.93
2	B	400	FAD	C9A-C5X-N5	-2.68	119.61	122.45
3	A	402	GRA	C6-C5-N2	-2.62	106.95	112.41
2	C	400	FAD	C1'-C2'-C3'	2.62	116.75	109.66
3	B	402	GRA	C10-C9-C8	-2.60	106.77	112.20
3	C	402	GRA	O3A-P2A-O5A	-2.59	102.92	110.70
2	D	400	FAD	C4A-N9A-C8A	2.59	108.45	105.74
3	C	402	GRA	C3-C2-N1	-2.57	106.54	112.00
3	D	402	GRA	O4A-P2A-O3A	2.55	114.16	107.27
3	D	402	GRA	O3A-P2A-O5A	-2.54	103.06	110.70
3	B	402	GRA	C3-C2-N1	-2.53	106.62	112.00
2	D	400	FAD	O4-C4-C4X	-2.51	119.91	126.53
3	D	402	GRA	C4A-C5A-N7A	-2.50	107.72	110.58
3	D	402	GRA	C2-N1-C1	2.48	127.00	122.55
3	B	402	GRA	N9A-C8A-N7A	-2.47	110.43	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	FAD	C5X-N5-C4X	2.47	122.08	118.09
2	D	400	FAD	C10-C4X-N5	-2.46	119.78	124.81
2	D	400	FAD	C4X-C4-N3	2.44	119.46	113.25
2	A	400	FAD	C4X-C4-N3	2.41	119.39	113.25
3	D	402	GRA	O1A-P1A-O2A	2.41	123.66	112.44
2	C	400	FAD	N3A-C4A-N9A	2.41	131.26	127.17
2	B	400	FAD	N3A-C4A-N9A	2.41	131.26	127.17
3	D	402	GRA	C2A-N1A-C6A	2.40	122.67	118.73
3	D	402	GRA	N9A-C8A-N7A	-2.39	110.54	113.94
2	C	400	FAD	C4A-C5A-N7A	-2.39	107.86	110.58
2	D	400	FAD	C4X-C10-N10	2.38	119.89	116.48
3	C	402	GRA	C2-N1-C1	2.36	126.78	122.55
3	A	402	GRA	C3-C2-N1	-2.35	106.99	112.00
3	B	402	GRA	C2A-N1A-C6A	2.35	122.59	118.73
2	B	400	FAD	C4X-C4-N3	2.35	119.24	113.25
2	C	400	FAD	C4-C4X-C10	2.35	120.97	116.93
2	D	400	FAD	N3A-C4A-N9A	2.33	131.13	127.17
2	A	400	FAD	O2P-P-O3P	2.33	113.57	107.27
2	D	400	FAD	C4-C4X-C10	2.33	120.92	116.93
3	C	402	GRA	O7A-P3X-O9A	2.32	116.50	107.80
2	B	400	FAD	C4X-C10-N10	2.32	119.80	116.48
2	A	400	FAD	C2A-N1A-C6A	2.32	122.53	118.73
3	A	402	GRA	C16-C12-C14	2.31	112.71	108.77
2	A	400	FAD	C4X-C10-N10	2.30	119.78	116.48
3	C	402	GRA	N6A-C6A-N1A	2.30	123.50	118.38
2	A	400	FAD	C9A-C5X-N5	-2.29	120.02	122.45
2	A	400	FAD	O3P-P-O1P	-2.27	103.87	110.70
3	A	402	GRA	N6A-C6A-N1A	2.27	123.42	118.38
2	D	400	FAD	C4X-C10-N1	-2.26	119.05	124.59
2	C	400	FAD	O4-C4-C4X	-2.25	120.59	126.53
2	B	400	FAD	C4A-C5A-N7A	-2.24	108.02	110.58
2	A	400	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
3	C	402	GRA	N9A-C8A-N7A	-2.22	110.78	113.94
3	C	402	GRA	C4A-C5A-N7A	-2.21	108.06	110.58
3	B	402	GRA	O7A-P3X-O9A	2.20	116.07	107.80
2	C	400	FAD	O2-C2-N1	-2.20	118.14	121.80
3	A	402	GRA	C2A-N1A-C6A	2.19	122.33	118.73
2	B	400	FAD	C1'-C2'-C3'	2.19	115.60	109.66
2	D	400	FAD	C4A-C5A-N7A	-2.16	108.11	110.58
2	A	400	FAD	C10-C4X-N5	-2.16	120.39	124.81
2	C	400	FAD	O2A-PA-O3P	2.16	113.11	107.27
3	B	402	GRA	C15-C12-C14	2.16	112.44	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	GRA	O3A-P2A-O5A	-2.16	104.22	110.70
3	D	402	GRA	O7A-P3X-O9A	2.15	115.88	107.80
2	C	400	FAD	O3P-P-O1P	-2.13	104.28	110.70
3	A	402	GRA	C6A-C5A-N7A	2.12	136.18	132.09
2	C	400	FAD	C2B-C1B-N9A	-2.11	108.07	113.30
2	A	400	FAD	C4X-C10-N1	-2.10	119.44	124.59
2	D	400	FAD	C5B-C4B-C3B	-2.09	107.68	115.21
3	A	402	GRA	O4A-P2A-O5A	2.07	122.05	112.44
2	C	400	FAD	C10-C4X-N5	-2.06	120.60	124.81
2	C	400	FAD	C4X-C4-N3	2.05	118.47	113.25
2	C	400	FAD	C4A-N9A-C8A	2.04	107.89	105.74
3	B	402	GRA	O4A-P2A-O3A	2.04	112.79	107.27
3	A	402	GRA	C5A-N7A-C8A	2.03	106.64	103.45
2	C	400	FAD	C4X-C10-N1	-2.01	119.67	124.59
2	B	400	FAD	C10-N1-C2	2.01	121.19	116.85

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	FAD	C1'-C2'-C3'-O3'
2	A	400	FAD	C1'-C2'-C3'-C4'
2	A	400	FAD	PA-O3P-P-O5'
2	C	400	FAD	C1'-C2'-C3'-O3'
2	C	400	FAD	C1'-C2'-C3'-C4'
2	C	400	FAD	PA-O3P-P-O5'
2	D	400	FAD	C1'-C2'-C3'-O3'
2	D	400	FAD	C1'-C2'-C3'-C4'
3	C	402	GRA	N1-C2-C3-C4
3	C	402	GRA	C11-C10-C9-C8
3	D	402	GRA	C11-C10-C9-C8
3	A	402	GRA	C11-C10-C9-C8
3	B	402	GRA	C11-C10-C9-C8
2	D	400	FAD	PA-O3P-P-O5'
3	A	402	GRA	N1-C2-C3-C4
3	B	402	GRA	N1-C2-C3-C4
3	D	402	GRA	N1-C2-C3-C4
3	B	402	GRA	P1A-O3A-P2A-O4A
3	B	402	GRA	C5-C6-S1-C7
2	C	400	FAD	C2'-C1'-N10-C10
2	D	400	FAD	C5B-O5B-PA-O1A
3	A	402	GRA	P1A-O3A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
3	C	402	GRA	P1A-O3A-P2A-O4A
3	D	402	GRA	P1A-O3A-P2A-O4A
2	A	400	FAD	C4'-C5'-O5'-P
2	D	400	FAD	O3'-C3'-C4'-C5'
2	C	400	FAD	C4'-C5'-O5'-P
3	A	402	GRA	C9-C10-C11-O5
3	B	402	GRA	C9-C10-C11-O5
3	D	402	GRA	C9-C10-C11-O5
3	C	402	GRA	C9-C10-C11-O5
2	B	400	FAD	PA-O3P-P-O5'
2	D	400	FAD	C4'-C5'-O5'-P
3	B	402	GRA	C9-C10-C11-O6
3	D	402	GRA	C9-C10-C11-O6
3	C	402	GRA	C9-C10-C11-O6
3	A	402	GRA	C9-C10-C11-O6
2	B	400	FAD	C1'-C2'-C3'-O3'
2	B	400	FAD	C4'-C5'-O5'-P
2	D	400	FAD	O2'-C2'-C3'-O3'
3	A	402	GRA	P1A-O3A-P2A-O5A
3	B	402	GRA	P1A-O3A-P2A-O5A
3	C	402	GRA	P1A-O3A-P2A-O5A
3	D	402	GRA	P1A-O3A-P2A-O5A

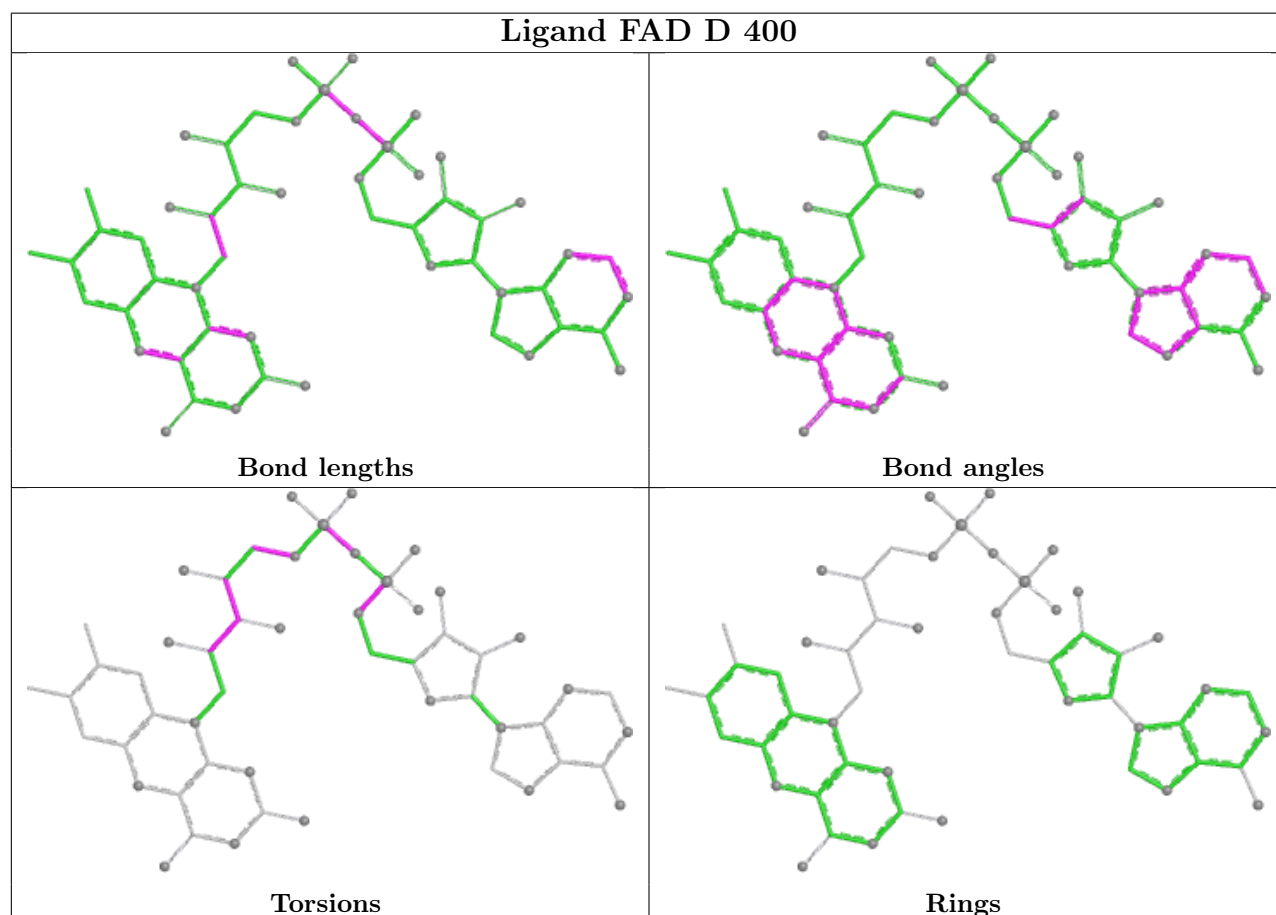
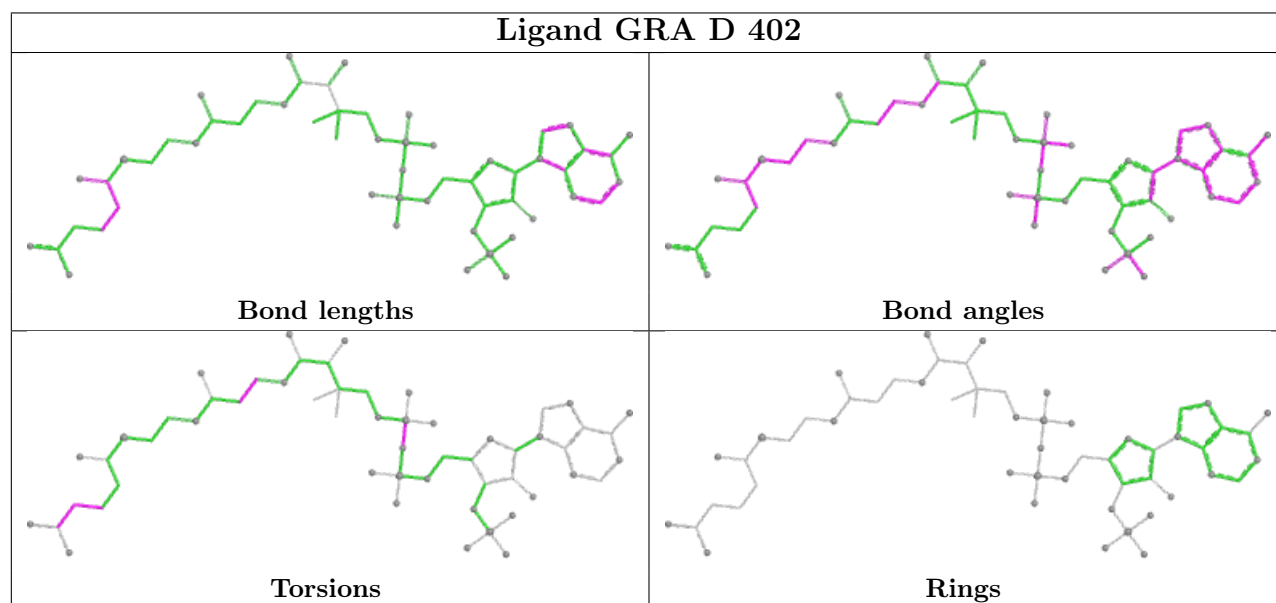
There are no ring outliers.

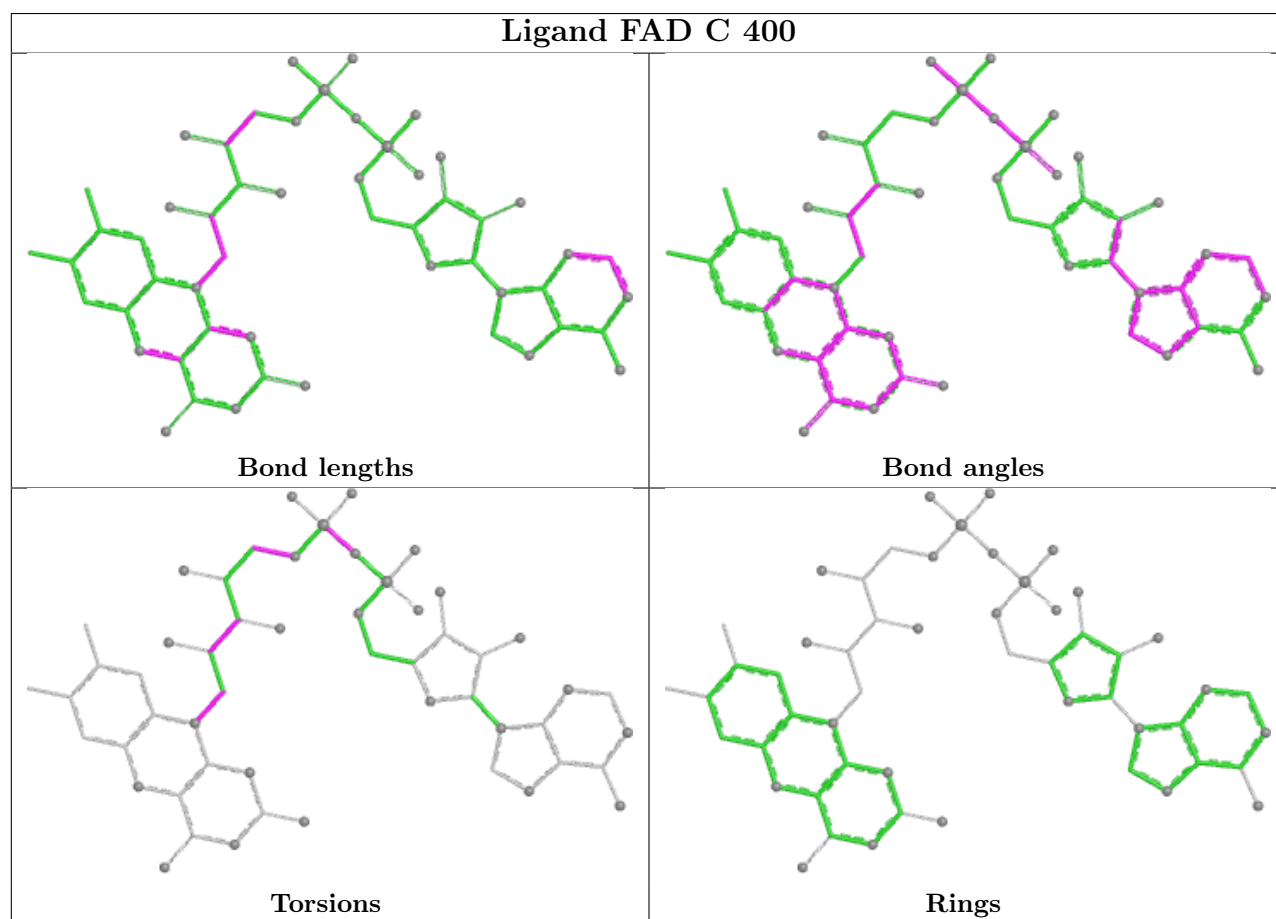
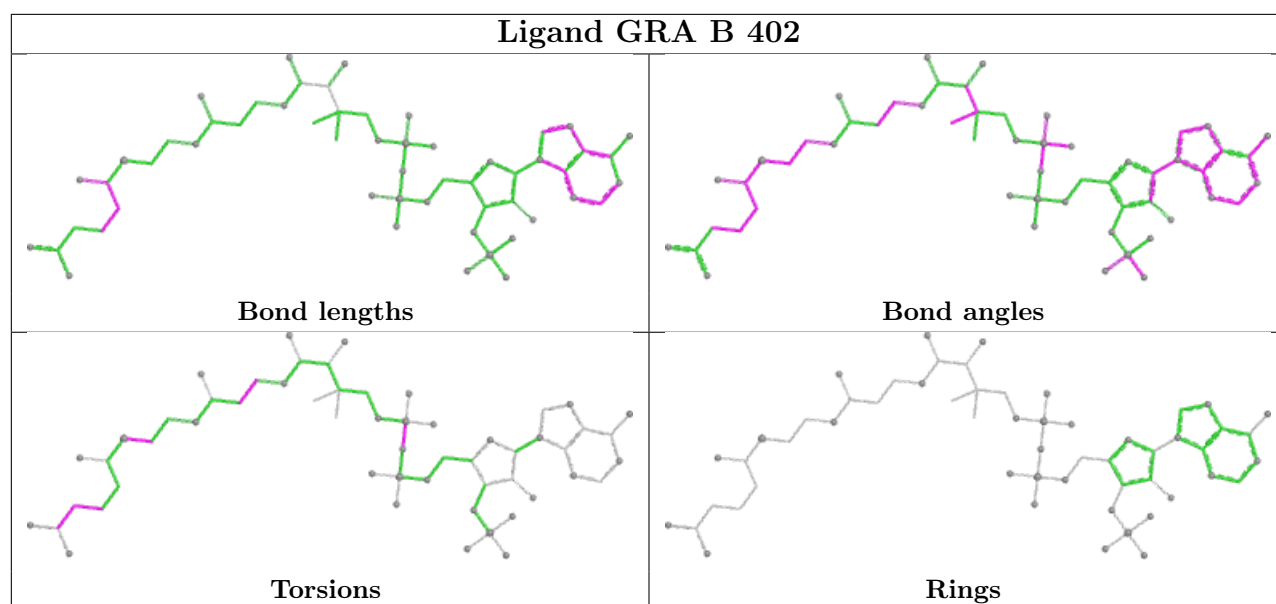
8 monomers are involved in 26 short contacts:

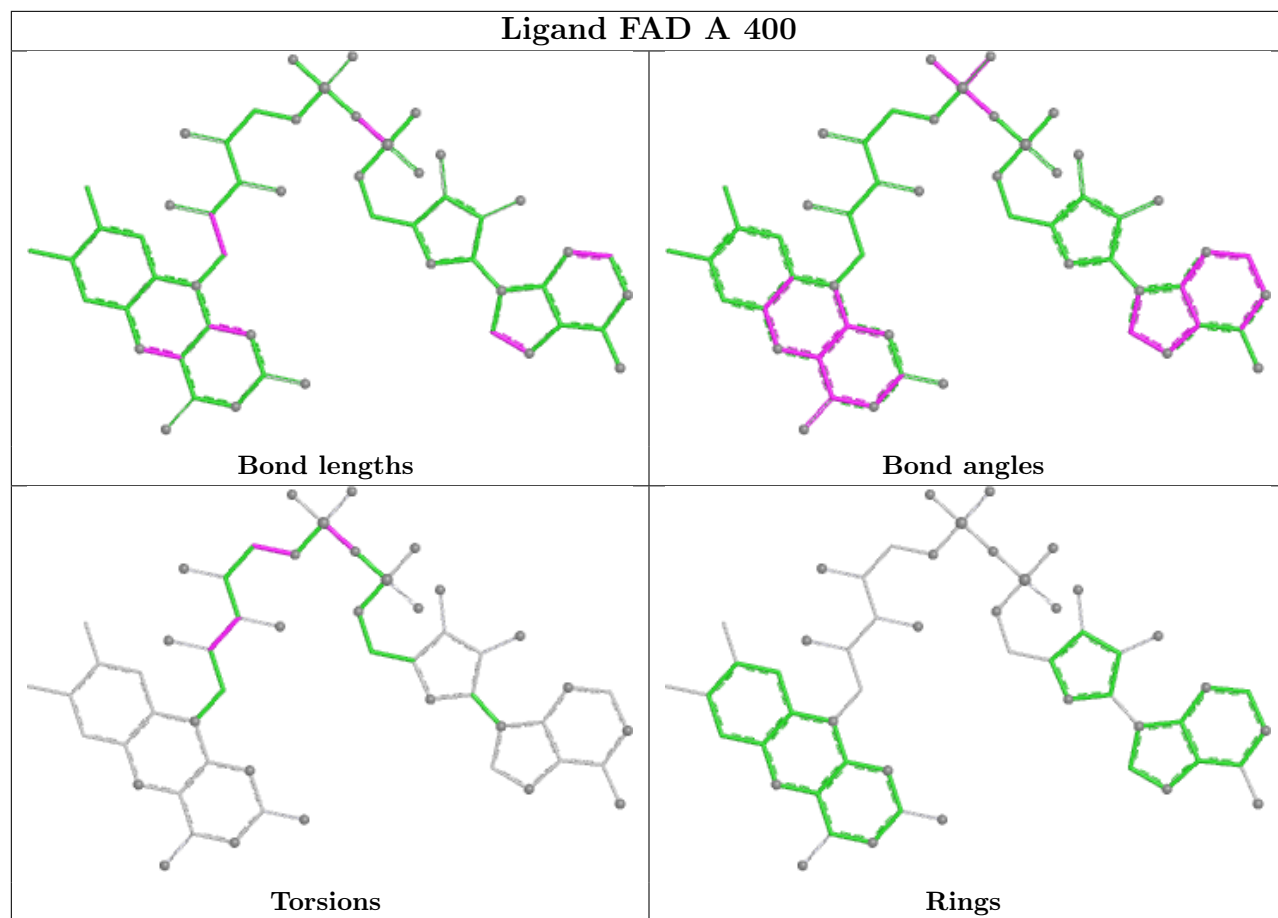
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	GRA	3	0
2	D	400	FAD	5	0
3	B	402	GRA	4	0
2	C	400	FAD	7	0
2	A	400	FAD	4	0
2	B	400	FAD	6	0
3	C	402	GRA	1	0
3	A	402	GRA	3	0

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

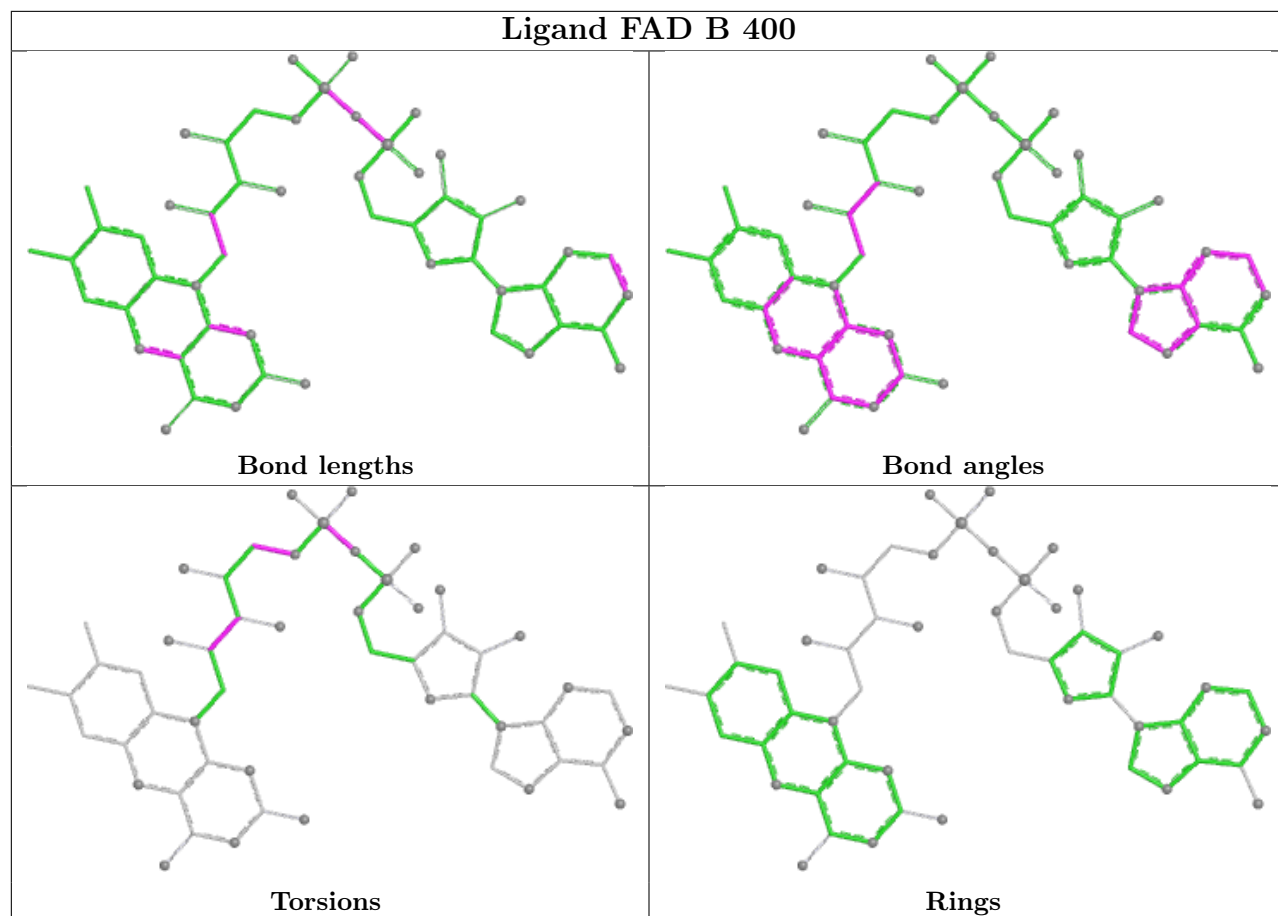
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



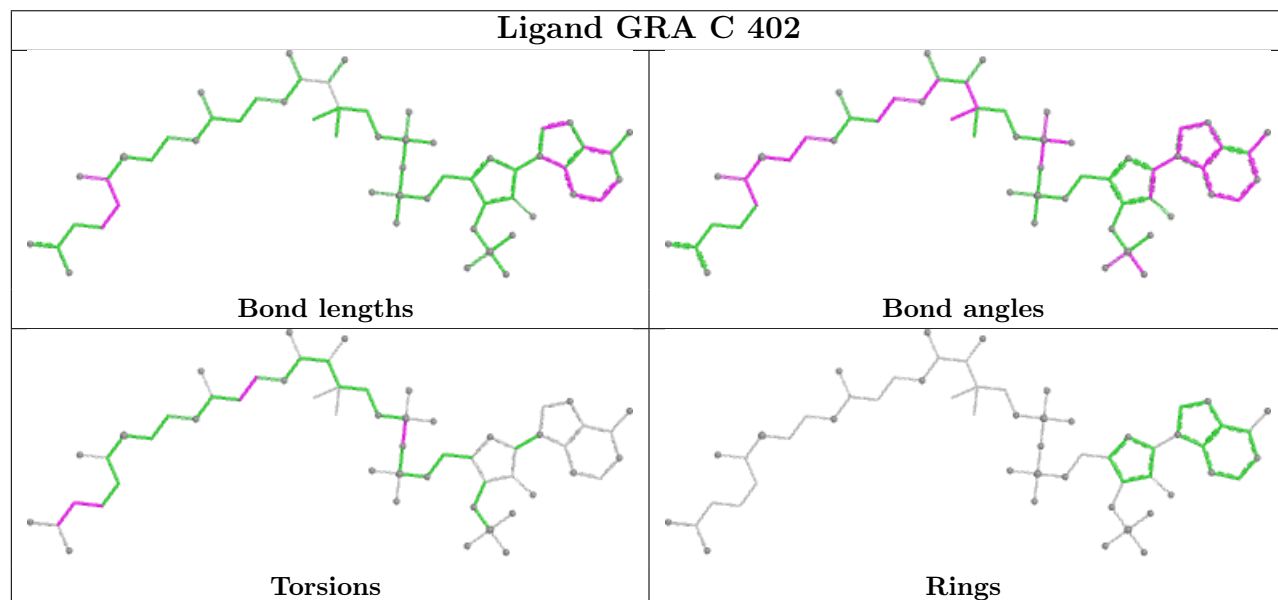


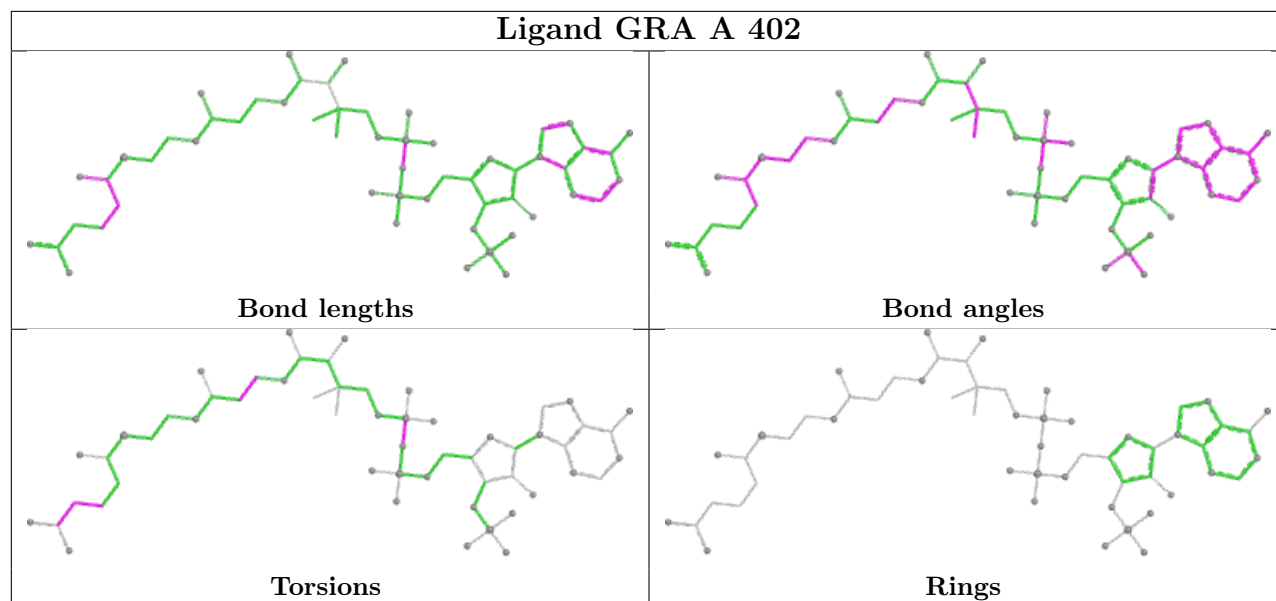


Ligand FAD B 400



Ligand GRA C 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	391/397 (98%)	-0.11	5 (1%) 75 76	20, 43, 63, 76	4 (1%)
1	B	390/397 (98%)	0.54	20 (5%) 33 33	39, 59, 83, 97	0
1	C	395/397 (99%)	-0.06	3 (0%) 82 84	31, 43, 66, 90	0
1	D	390/397 (98%)	0.34	10 (2%) 57 59	28, 53, 76, 89	1 (0%)
All	All	1566/1588 (98%)	0.18	38 (2%) 59 61	20, 49, 75, 97	5 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	THR	3.6
1	D	152	LEU	3.4
1	D	2	ASP	3.1
1	B	152	LEU	3.1
1	B	103	THR	3.0
1	B	45	PRO	3.0
1	B	151	TRP	2.8
1	B	166	ALA	2.7
1	B	217	LEU	2.7
1	C	351	TYR	2.7
1	A	179	ALA	2.6
1	D	151	TRP	2.6
1	B	179	ALA	2.6
1	A	348	SER	2.6
1	B	122	PHE	2.6
1	B	227	ILE	2.5
1	D	195	PRO	2.5
1	B	101	ILE	2.5
1	C	394	HIS	2.4
1	A	2	ASP	2.4
1	B	223	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	2.4
1	A	349[A]	THR	2.4
1	B	53	GLY	2.3
1	B	117	LEU	2.3
1	D	150	HIS	2.3
1	D	100	THR	2.3
1	B	144	ALA	2.2
1	B	216	PHE	2.1
1	B	188	VAL	2.1
1	D	61	GLY	2.1
1	D	108	ALA	2.1
1	B	11	MET	2.1
1	B	137	VAL	2.1
1	D	217	LEU	2.1
1	A	391	GLY	2.1
1	D	62	GLY	2.1
1	B	351	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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.

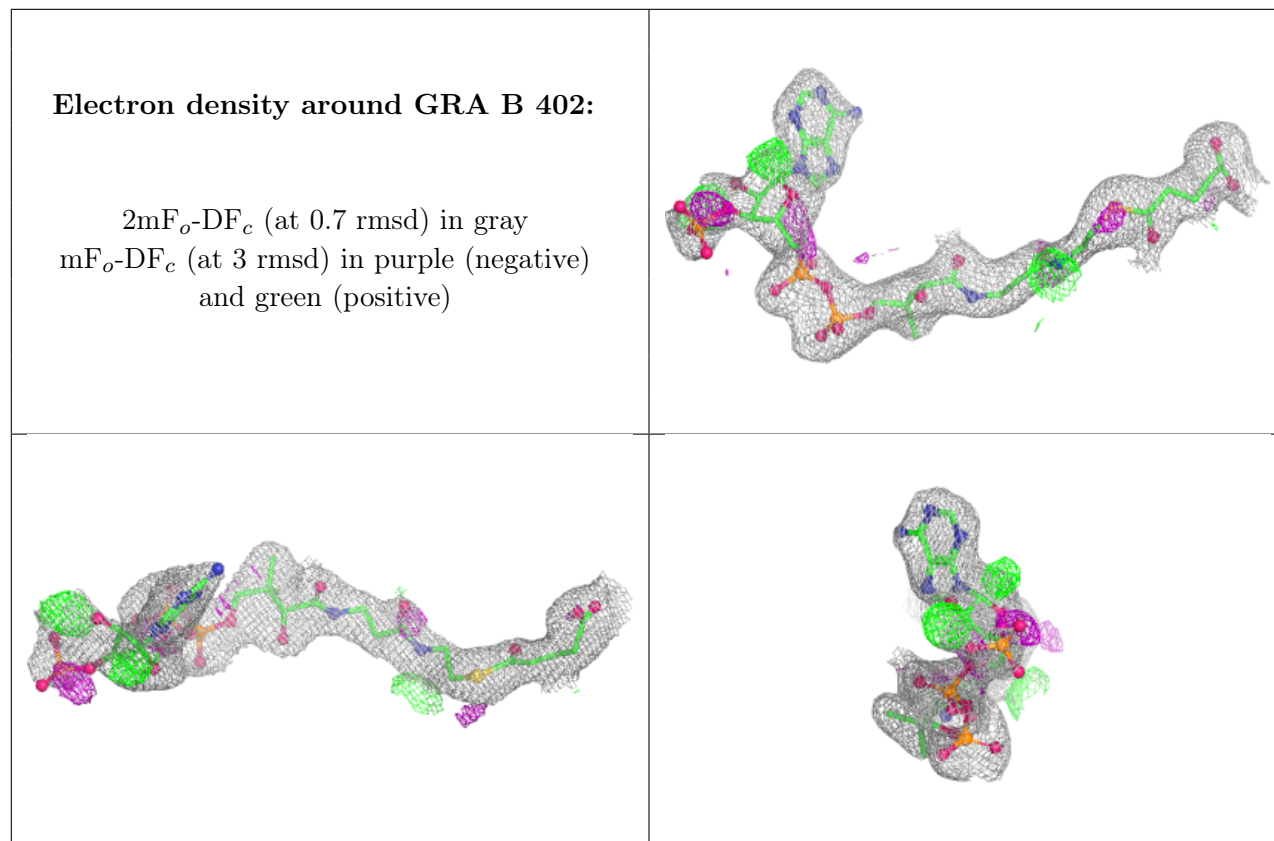
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GRA	B	402	56/56	0.90	0.10	49,62,107,117	0
2	FAD	B	400	53/53	0.94	0.11	52,59,67,69	0
3	GRA	D	402	56/56	0.94	0.08	43,57,83,91	0
2	FAD	D	400	53/53	0.95	0.09	45,52,59,62	0
3	GRA	C	402	56/56	0.95	0.07	34,45,56,61	0
3	GRA	A	402	56/56	0.95	0.07	35,46,69,78	0

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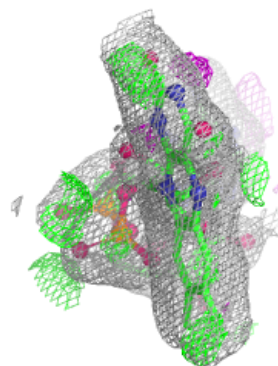
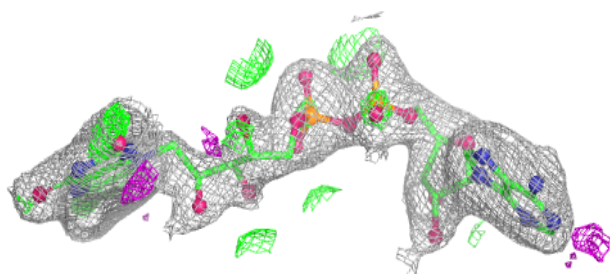
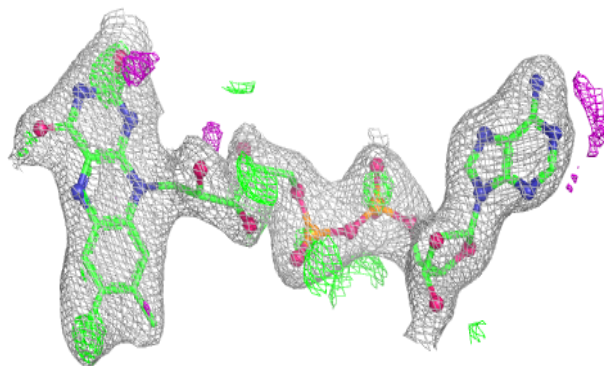
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	C	400	53/53	0.96	0.07	35,40,43,45	0
2	FAD	A	400	53/53	0.97	0.06	34,40,46,48	0

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.

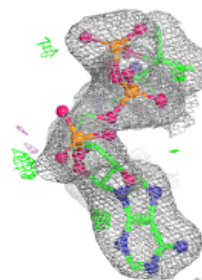
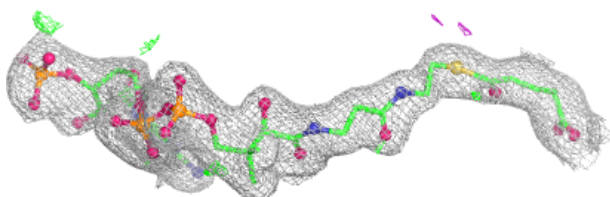
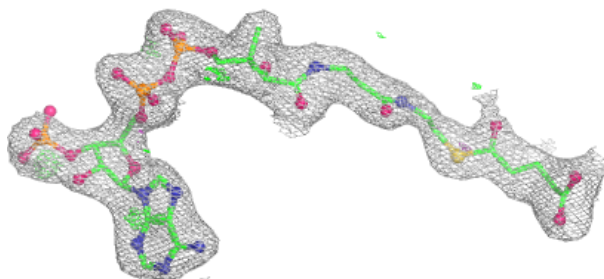


Electron density around FAD B 400:

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

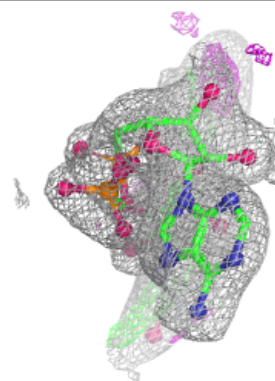
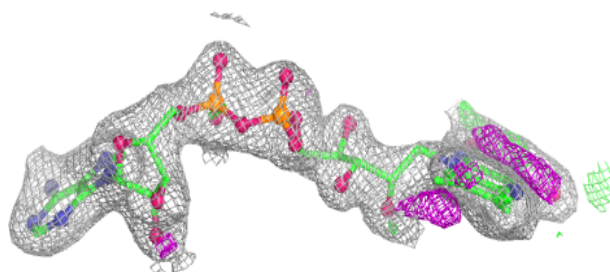
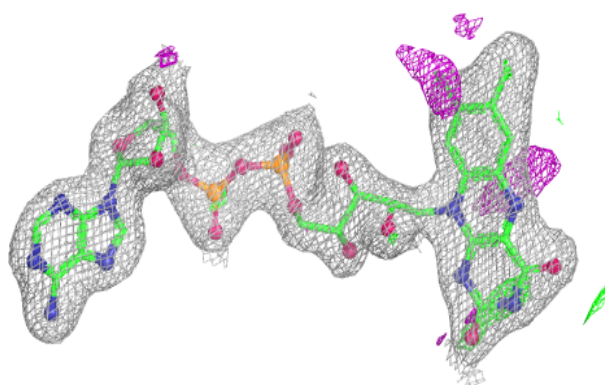
**Electron density around GRA D 402:**

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

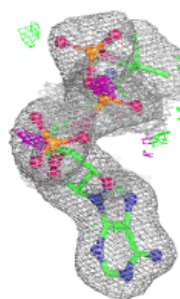
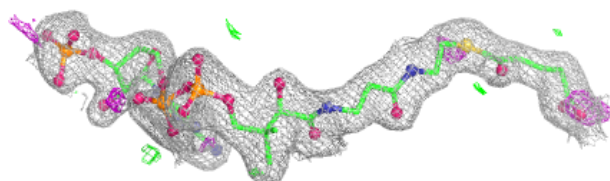
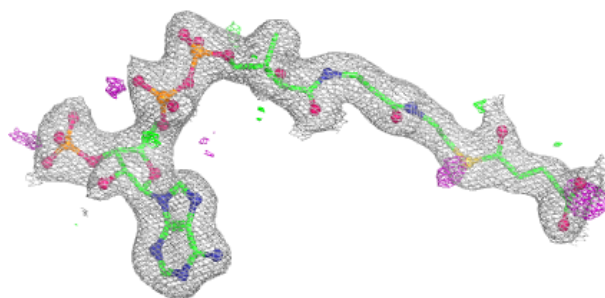


Electron density around FAD D 400:

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

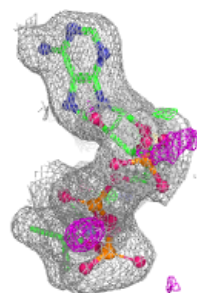
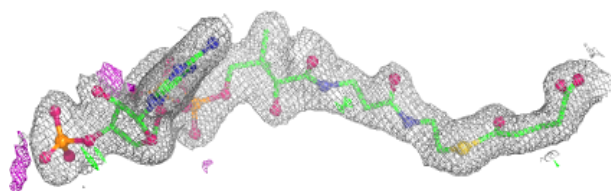
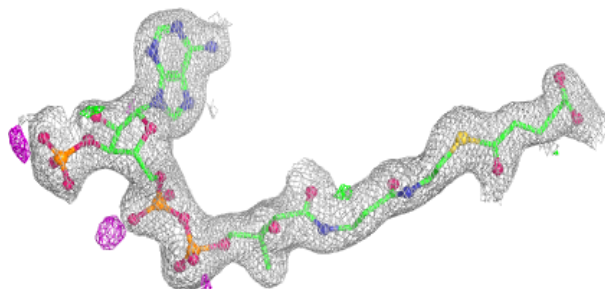
**Electron density around GRA C 402:**

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

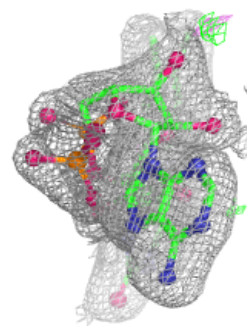
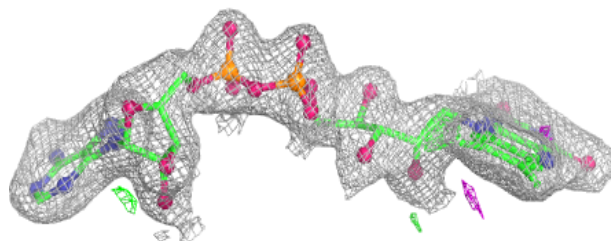
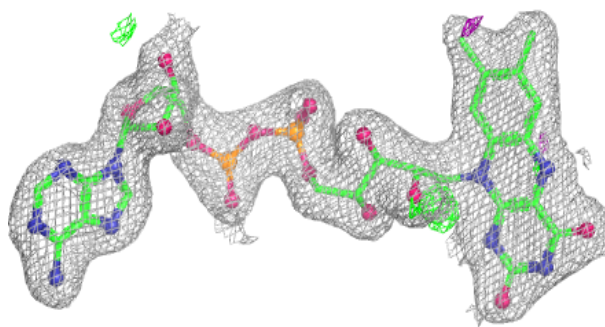


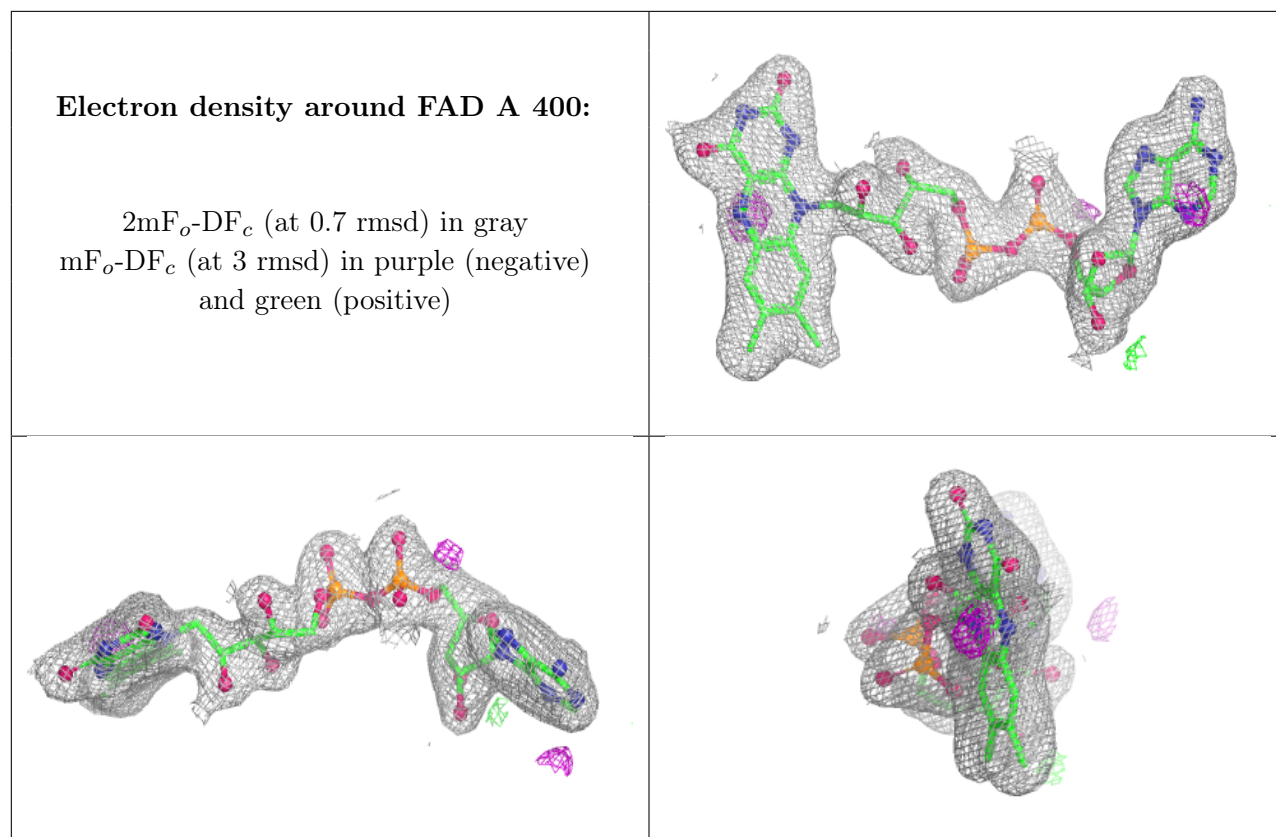
Electron density around GRA A 402:

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

**Electron density around FAD C 400:**

$2mF_o-DF_c$ (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.