



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 10:30 AM BST

PDB ID : 5WWV
Title : Crystal structure of porcine kidney D-amino acid oxidase mutant (I230A/R283G)
Authors : Motojima, F.; Yasukawa, K.; Ohno, A.; Asano, Y.
Deposited on : 2017-01-05
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

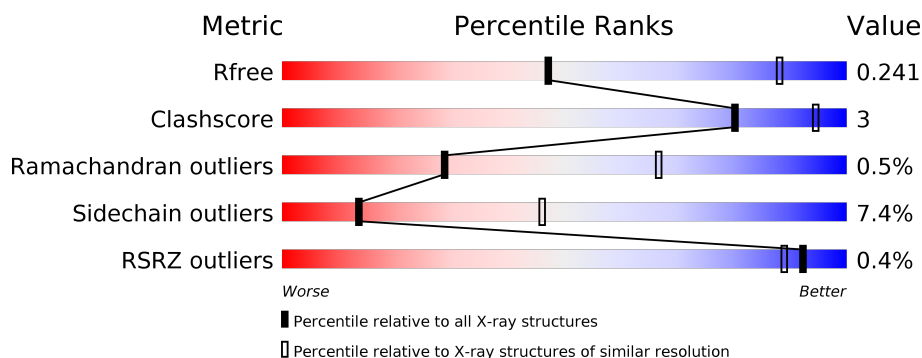
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	347	<div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	B	347	<div> <div>83%</div> <div>12%</div> <div>..</div> </div>
1	C	347	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	D	347	<div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	E	347	<div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	F	347	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	347	<div><div>%</div><div><div></div><div>86%</div><div>9%</div><div></div></div><div></div></div>
1	H	347	<div><div>%</div><div><div></div><div>81%</div><div>15%</div><div></div></div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22427 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 D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	1	0
			2720	1748	473	490	9			
1	B	339	Total	C	N	O	S	0	0	0
			2710	1742	470	489	9			
1	C	339	Total	C	N	O	S	0	0	0
			2710	1742	470	489	9			
1	D	339	Total	C	N	O	S	0	1	0
			2719	1750	470	490	9			
1	E	338	Total	C	N	O	S	0	2	0
			2718	1749	471	489	9			
1	F	338	Total	C	N	O	S	0	0	0
			2702	1736	469	488	9			
1	G	338	Total	C	N	O	S	0	0	0
			2702	1736	469	488	9			
1	H	337	Total	C	N	O	S	0	1	0
			2704	1738	470	487	9			

There are 16 discrepancies between the modelled and reference sequences:

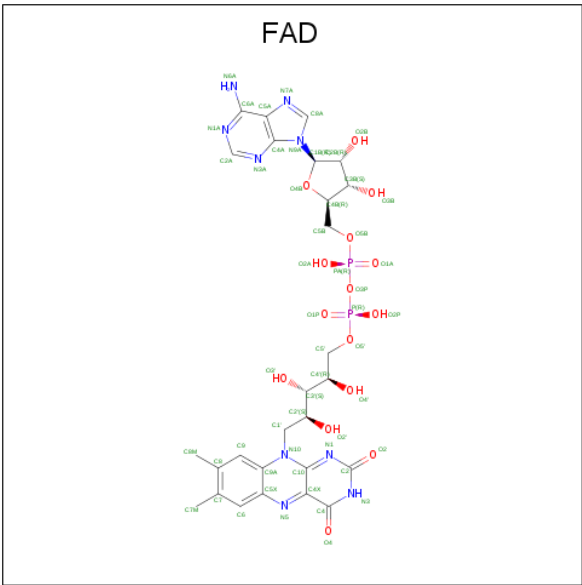
Chain	Residue	Modelled	Actual	Comment	Reference
A	230	ALA	ILE	engineered mutation	UNP P00371
A	283	GLY	ARG	engineered mutation	UNP P00371
B	230	ALA	ILE	engineered mutation	UNP P00371
B	283	GLY	ARG	engineered mutation	UNP P00371
C	230	ALA	ILE	engineered mutation	UNP P00371
C	283	GLY	ARG	engineered mutation	UNP P00371
D	230	ALA	ILE	engineered mutation	UNP P00371
D	283	GLY	ARG	engineered mutation	UNP P00371
E	230	ALA	ILE	engineered mutation	UNP P00371
E	283	GLY	ARG	engineered mutation	UNP P00371
F	230	ALA	ILE	engineered mutation	UNP P00371
F	283	GLY	ARG	engineered mutation	UNP P00371
G	230	ALA	ILE	engineered mutation	UNP P00371

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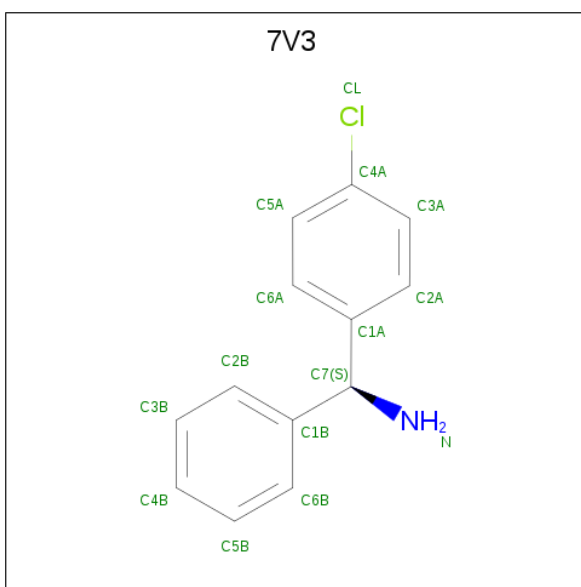
Chain	Residue	Modelled	Actual	Comment	Reference
G	283	GLY	ARG	engineered mutation	UNP P00371
H	230	ALA	ILE	engineered mutation	UNP P00371
H	283	GLY	ARG	engineered mutation	UNP P00371

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is (S)-(4-chlorophenyl)-phenyl-methanamine (three-letter code: 7V3) (formula: C₁₃H₁₂ClN).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			15	13	1	1		
3	C	1	Total	C	Cl	N	0	0
			15	13	1	1		
3	D	1	Total	C	Cl	N	0	0
			15	13	1	1		
3	F	1	Total	C	Cl	N	0	0
			15	13	1	1		
3	G	1	Total	C	Cl	N	0	0
			15	13	1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



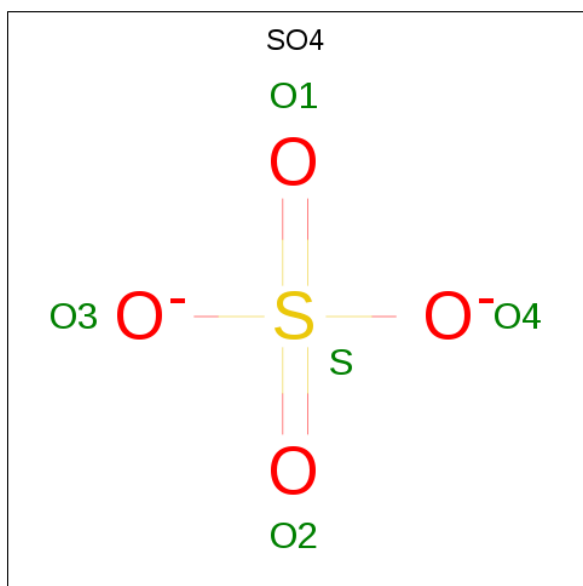
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		


- Molecule 6 is water.

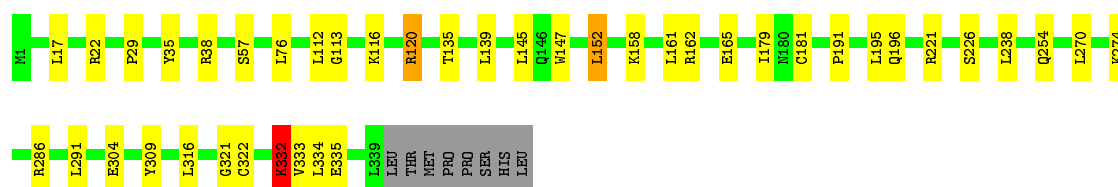
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	8	Total	O	0	0
			8	8		
6	C	9	Total	O	0	0
			9	9		
6	D	9	Total	O	0	0
			9	9		
6	E	5	Total	O	0	0
			5	5		
6	F	2	Total	O	0	0
			2	2		
6	H	5	Total	O	0	0
			5	5		

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.

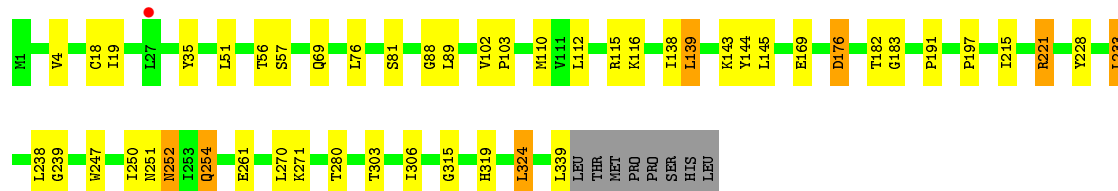
• Molecule 1: D-amino-acid oxidase

Chain A: 




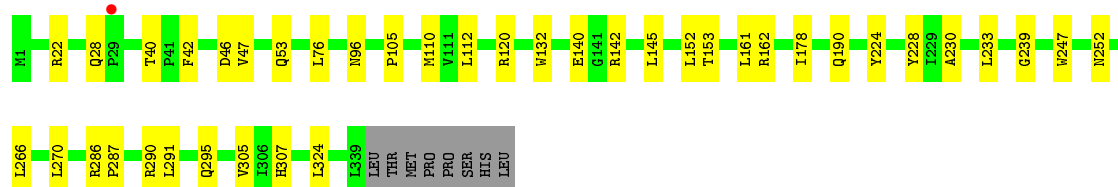
• Molecule 1: D-amino-acid oxidase

Chain B: 




• Molecule 1: D-amino-acid oxidase

Chain C: 



• Molecule 1: D-amino-acid oxidase

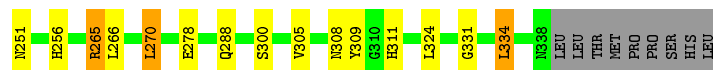
Chain D: 





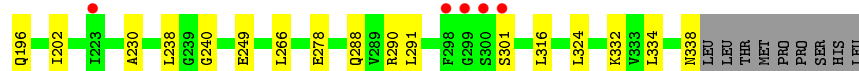
- Molecule 1: D-amino-acid oxidase

Chain E: 83% 13% . .



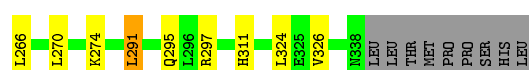
- Molecule 1: D-amino-acid oxidase

Chain F: 2% 84% 14% .



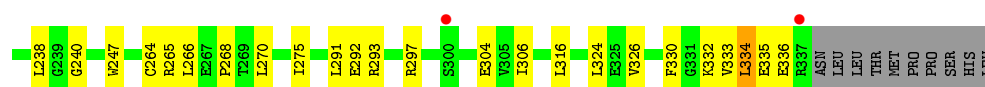
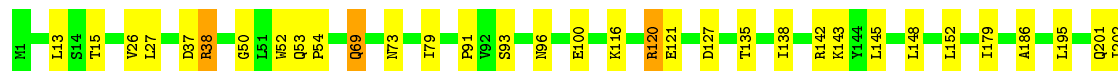
- Molecule 1: D-amino-acid oxidase

Chain G: 0% 86% 9% . .



- Molecule 1: D-amino-acid oxidase

Chain H: 0% 81% 15% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	170.06Å 273.95Å 136.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 – 3.20 48.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.73-3.20) 100.0 (48.73-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.145 , 0.242 0.152 , 0.241	Depositor DCC
R_{free} test set	2657 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22427	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: 7V3, MPD, SO4, 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	0.70	1/2797 (0.0%)	0.87	3/3810 (0.1%)
1	B	0.67	0/2786	0.84	1/3795 (0.0%)
1	C	0.64	1/2786 (0.0%)	0.83	2/3795 (0.1%)
1	D	0.65	0/2799	0.84	3/3813 (0.1%)
1	E	0.60	0/2802	0.82	4/3817 (0.1%)
1	F	0.64	0/2778	0.81	0/3784
1	G	0.59	0/2778	0.79	0/3784
1	H	0.61	1/2781 (0.0%)	0.77	2/3788 (0.1%)
All	All	0.64	3/22307 (0.0%)	0.82	15/30386 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	247	TRP	CB-CG	6.38	1.61	1.50
1	C	247	TRP	CB-CG	5.80	1.60	1.50
1	A	147	TRP	CB-CG	5.24	1.59	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	H	120	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	120	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	E	151	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	221	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	120	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	22	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	E	2	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	H	293	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	99	ARG	NE-CZ-NH2	5.29	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	ARG	CG-CD-NE	5.24	122.80	111.80
1	D	139	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	120	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	286	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	D	286	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2720	0	2665	10	0
1	B	2710	0	2659	19	0
1	C	2710	0	2659	14	0
1	D	2719	0	2668	11	0
1	E	2718	0	2664	16	0
1	F	2702	0	2648	17	0
1	G	2702	0	2648	16	0
1	H	2704	0	2648	23	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
2	E	53	0	31	1	0
2	F	53	0	31	1	0
2	G	53	0	31	1	0
2	H	53	0	31	0	0
3	A	15	0	0	0	0
3	C	15	0	0	2	0
3	D	15	0	0	1	0
3	F	15	0	0	1	0
3	G	15	0	0	0	0
4	A	32	0	56	0	0
4	B	16	0	28	0	0
4	C	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	16	0	28	0	0
4	E	32	0	56	2	0
4	F	24	0	42	0	0
4	G	16	0	28	0	0
4	H	24	0	42	3	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	1	0
5	H	5	0	0	0	0
6	A	7	0	0	0	0
6	B	8	0	0	0	0
6	C	9	0	0	1	0
6	D	9	0	0	0	0
6	E	5	0	0	0	0
6	F	2	0	0	0	0
6	H	5	0	0	0	0
All	All	22427	0	21801	121	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 3.

All (121) 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)
4:E:404:MPD:H52	4:E:404:MPD:H12	1.71	0.73
1:H:334:LEU:HA	1:H:335:GLU:C	2.13	0.69
1:D:96:ASN:ND2	1:D:217:HIS:NE2	2.38	0.69
1:A:120:ARG:NH2	1:B:110:MET:O	2.28	0.66
1:H:330:PHE:O	1:H:333:VAL:HG22	2.00	0.62
1:G:291:LEU:HD11	1:G:326:VAL:HG22	1.81	0.62
1:C:40:THR:HG22	1:C:142:ARG:HH11	1.65	0.61
1:E:127:ASP:OD2	1:E:265:ARG:NH1	2.34	0.61
1:D:215:ILE:HG12	3:D:402:7V3:CL	2.37	0.60
1:H:306:ILE:HG21	1:H:326:VAL:HG13	1.82	0.60
1:F:120:ARG:CZ	5:F:406:SO4:S	2.90	0.59
1:E:178:ILE:HB	1:E:305:VAL:HG22	1.86	0.58
1:D:178:ILE:HB	1:D:305:VAL:HG22	1.87	0.57
1:D:291:LEU:HD13	1:D:326:VAL:HG22	1.86	0.57
1:C:53:GLN:NE2	1:C:96:ASN:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:TYR:CZ	1:B:239:GLY:HA3	2.41	0.56
1:G:112:LEU:HD23	1:H:121:GLU:HG2	1.88	0.56
1:E:113:GLY:HA3	1:F:115:ARG:NH2	2.22	0.54
1:D:291:LEU:HA	1:D:307:HIS:O	2.08	0.54
1:B:88:GLY:HA2	1:B:233:LEU:HD21	1.90	0.54
1:H:127:ASP:OD2	1:H:265:ARG:NH1	2.42	0.53
1:G:11:ILE:HD12	1:G:311:HIS:CE1	2.43	0.52
1:G:127:ASP:N	1:G:127:ASP:OD1	2.42	0.52
1:G:1:MET:N	1:G:29:PRO:O	2.42	0.52
1:B:4:VAL:HG13	1:B:35:TYR:CD1	2.45	0.51
1:B:69:GLN:HB2	1:B:110:MET:HE3	1.94	0.50
1:C:190:GLN:HE22	1:C:290:ARG:HH22	1.60	0.50
1:A:179:ILE:HG22	1:A:181:CYS:SG	2.52	0.50
1:F:168:GLU:OE2	1:F:172:ARG:NH1	2.44	0.50
1:G:17:LEU:HA	1:G:152:LEU:HD11	1.94	0.49
1:B:250:ILE:N	1:B:250:ILE:HD13	2.26	0.49
4:H:403:MPD:H52	4:H:403:MPD:H12	1.93	0.49
1:H:13:LEU:CB	1:H:148:LEU:HD13	2.41	0.49
1:D:22:ARG:HB2	1:D:23:TYR:CE2	2.48	0.49
1:E:144:TYR:CE2	1:E:148:LEU:HD11	2.48	0.49
1:F:101:ALA:HA	1:F:130:TYR:CD2	2.47	0.49
1:F:230:ALA:HB2	3:F:402:7V3:CL	2.51	0.47
1:E:26:VAL:HG23	1:E:27:LEU:HD12	1.95	0.47
1:A:195:LEU:HD22	1:A:309:TYR:CE2	2.50	0.47
1:B:51:LEU:CD2	1:B:215:ILE:HD11	2.45	0.47
1:A:332:LYS:O	1:A:334:LEU:N	2.49	0.46
1:C:228:TYR:CZ	1:C:239:GLY:HA3	2.50	0.46
1:H:142:ARG:CD	4:H:403:MPD:HM2	2.45	0.46
1:G:112:LEU:HD23	1:H:121:GLU:CG	2.46	0.46
1:E:250:ILE:HG22	1:E:251:ASN:O	2.16	0.46
1:F:27:LEU:HD11	1:F:334:LEU:HD21	1.97	0.46
1:G:216:THR:HG21	1:G:266:LEU:HD21	1.96	0.46
1:C:178:ILE:HB	1:C:305:VAL:HG22	1.98	0.46
1:H:50:GLY:O	1:H:138:ILE:HA	2.15	0.46
1:E:331:GLY:HA2	1:E:334:LEU:HD22	1.98	0.46
1:G:51:LEU:HA	1:G:138:ILE:HD13	1.98	0.46
1:H:69:GLN:O	1:H:73:ASN:ND2	2.49	0.46
1:A:17:LEU:HD13	1:A:152:LEU:HD13	1.98	0.46
1:H:13:LEU:HB2	1:H:148:LEU:HD13	1.98	0.45
1:E:78:HIS:O	1:E:81:SER:HB3	2.15	0.45
1:A:321:GLY:O	1:A:322:CYS:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:ASP:OD1	1:H:38:ARG:HD2	2.17	0.45
1:C:291:LEU:HA	1:C:307:HIS:O	2.17	0.45
1:C:40:THR:HG23	1:C:46:ASP:OD1	2.17	0.45
1:F:20:HIS:CD2	1:F:155:ARG:HB3	2.52	0.45
1:B:182:THR:O	1:B:183:GLY:C	2.55	0.45
1:B:18:CYS:SG	1:B:324:LEU:HD12	2.56	0.45
1:E:11:ILE:HG23	1:E:308:ASN:ND2	2.32	0.44
1:F:139:LEU:HD21	1:F:144:TYR:CG	2.52	0.44
1:G:15:THR:HG21	1:G:179:ILE:HG21	1.98	0.44
1:B:4:VAL:HG13	1:B:35:TYR:HD1	1.81	0.44
1:F:45:THR:O	1:F:48:ALA:HB3	2.18	0.44
1:H:50:GLY:HA2	1:H:316:LEU:CD1	2.47	0.44
1:D:89:LEU:HA	1:D:138:ILE:O	2.17	0.44
1:C:224:TYR:CZ	3:C:402:7V3:N	2.85	0.44
1:H:53:GLN:NE2	1:H:96:ASN:OD1	2.50	0.44
1:H:79:ILE:HD12	1:H:91:PRO:HD3	1.99	0.44
1:C:42:PHE:HA	4:C:403:MPD:HM2	2.00	0.44
1:B:139:LEU:HD11	1:B:144:TYR:CD2	2.52	0.43
1:G:110:MET:O	1:H:120:ARG:NH2	2.41	0.43
1:E:228:TYR:CE2	1:E:239:GLY:HA3	2.53	0.43
1:F:182:THR:O	1:F:183:GLY:C	2.57	0.43
1:B:315:GLY:O	1:B:319:HIS:HB3	2.18	0.43
1:H:142:ARG:HD3	4:H:403:MPD:HM2	2.01	0.43
1:C:105:PRO:HD3	1:C:132:TRP:CZ2	2.54	0.43
1:B:89:LEU:HA	1:B:138:ILE:O	2.18	0.43
1:B:252:ASN:OD1	1:B:254:GLN:HG2	2.18	0.43
1:F:37:ASP:OD1	2:F:401:FAD:O2B	2.31	0.43
1:C:142:ARG:NH2	6:C:501:HOH:O	2.50	0.43
1:C:230:ALA:HB2	3:C:402:7V3:CL	2.55	0.43
1:F:20:HIS:O	1:F:20:HIS:CD2	2.72	0.43
1:B:197:PRO:HG3	1:B:247:TRP:CE2	2.54	0.42
1:D:45:THR:OG1	2:D:401:FAD:O1A	2.29	0.42
1:E:210:LEU:HD11	1:E:270:LEU:CD1	2.50	0.42
1:G:291:LEU:CD1	1:G:326:VAL:HG22	2.49	0.42
1:A:332:LYS:O	1:A:335:GLU:N	2.53	0.42
1:A:112:LEU:HB2	1:A:135:THR:HB	2.02	0.42
1:D:52:TRP:CE2	1:D:317:THR:HG23	2.55	0.42
1:G:197:PRO:HG3	1:G:247:TRP:CD2	2.54	0.42
1:H:264:CYS:O	1:H:268:PRO:HA	2.19	0.42
1:B:251:ASN:ND2	1:B:280:THR:OG1	2.53	0.41
1:E:121:GLU:HG2	1:F:112:LEU:HD23	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:ALA:HB3	1:H:195:LEU:HD22	2.02	0.41
1:E:11:ILE:HG13	1:E:311:HIS:CE1	2.56	0.41
1:A:113:GLY:HA3	1:B:115:ARG:NH2	2.35	0.41
1:C:110:MET:O	1:D:120:ARG:NH2	2.53	0.41
1:G:72:PHE:O	1:G:76:LEU:HB2	2.21	0.41
1:H:15:THR:HG21	1:H:179:ILE:HG21	2.03	0.41
1:C:286:ARG:O	1:C:287:PRO:C	2.59	0.41
1:E:309:TYR:HA	1:E:311:HIS:CE1	2.56	0.41
1:H:13:LEU:HB3	1:H:148:LEU:HD13	2.02	0.41
1:F:45:THR:HG23	1:F:316:LEU:HD21	2.03	0.41
1:H:93:SER:HA	1:H:135:THR:HA	2.02	0.41
1:H:52:TRP:CZ3	1:H:54:PRO:HD3	2.56	0.41
1:A:35:TYR:CD2	1:A:162:ARG:HD2	2.56	0.40
1:G:20:HIS:CE1	1:G:155:ARG:HB3	2.55	0.40
1:F:45:THR:CG2	1:F:145:LEU:HD11	2.51	0.40
1:G:11:ILE:HD13	2:G:401:FAD:O1P	2.21	0.40
1:D:66:ASN:HB3	1:D:70:GLN:HE21	1.85	0.40
2:E:401:FAD:C4	4:E:402:MPD:HM3	2.52	0.40
1:F:202:ILE:O	1:F:278:GLU:HG3	2.22	0.40
1:F:190:GLN:NE2	1:F:290:ARG:HH22	2.19	0.40
1:E:20:HIS:ND1	1:E:155:ARG:HD3	2.37	0.40
1:B:102:VAL:HB	1:B:103:PRO:HD2	2.03	0.40
1:B:176:ASP:OD1	1:B:176:ASP:N	2.55	0.40
1:E:256:HIS:HD1	1:E:278:GLU:CD	2.24	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	338/347 (97%)	310 (92%)	24 (7%)	4 (1%)	13 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	337/347 (97%)	308 (91%)	27 (8%)	2 (1%)	25	64
1	C	337/347 (97%)	314 (93%)	23 (7%)	0	100	100
1	D	338/347 (97%)	317 (94%)	20 (6%)	1 (0%)	41	74
1	E	338/347 (97%)	308 (91%)	29 (9%)	1 (0%)	41	74
1	F	336/347 (97%)	299 (89%)	34 (10%)	3 (1%)	17	56
1	G	336/347 (97%)	304 (90%)	31 (9%)	1 (0%)	41	74
1	H	336/347 (97%)	309 (92%)	25 (7%)	2 (1%)	25	64
All	All	2696/2776 (97%)	2469 (92%)	213 (8%)	14 (0%)	29	67

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	VAL
1	D	338	ASN
1	B	56	THR
1	F	29	PRO
1	G	29	PRO
1	A	332	LYS
1	A	57	SER
1	A	29	PRO
1	H	26	VAL
1	F	126	PRO
1	F	240	GLY
1	H	240	GLY
1	B	19	ILE
1	E	126	PRO

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	289/296 (98%)	268 (93%)	21 (7%)	14	46
1	B	288/296 (97%)	265 (92%)	23 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	288/296 (97%)	271 (94%)	17 (6%)	19	54
1	D	289/296 (98%)	267 (92%)	22 (8%)	13	45
1	E	289/296 (98%)	267 (92%)	22 (8%)	13	45
1	F	287/296 (97%)	266 (93%)	21 (7%)	14	46
1	G	287/296 (97%)	266 (93%)	21 (7%)	14	46
1	H	287/296 (97%)	265 (92%)	22 (8%)	13	44
All	All	2304/2368 (97%)	2135 (93%)	169 (7%)	13	46

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	76	LEU
1	A	116	LYS
1	A	139	LEU
1	A	145	LEU
1	A	152	LEU
1	A	158	LYS
1	A	161	LEU
1	A	165	GLU
1	A	191	PRO
1	A	196	GLN
1	A	221	ARG
1	A	226	SER
1	A	238	LEU
1	A	254	GLN
1	A	270	LEU
1	A	274	LYS
1	A	291	LEU
1	A	304	GLU
1	A	316	LEU
1	A	332	LYS
1	B	57	SER
1	B	76	LEU
1	B	81	SER
1	B	112	LEU
1	B	116	LYS
1	B	139	LEU
1	B	143	LYS
1	B	145	LEU

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Mol	Chain	Res	Type
1	B	169	GLU
1	B	176	ASP
1	B	191	PRO
1	B	221	ARG
1	B	233	LEU
1	B	238	LEU
1	B	252	ASN
1	B	254	GLN
1	B	261	GLU
1	B	270	LEU
1	B	271	LYS
1	B	303	THR
1	B	306	ILE
1	B	324	LEU
1	B	339	LEU
1	C	22	ARG
1	C	28	GLN
1	C	47	VAL
1	C	76	LEU
1	C	112	LEU
1	C	140	GLU
1	C	145	LEU
1	C	152	LEU
1	C	153	THR
1	C	161	LEU
1	C	162	ARG
1	C	233	LEU
1	C	252	ASN
1	C	266	LEU
1	C	270	LEU
1	C	295	GLN
1	C	324	LEU
1	D	21	GLU
1	D	22	ARG
1	D	27	LEU
1	D	28	GLN
1	D	40	THR
1	D	56	THR
1	D	81	SER
1	D	83	ASN
1	D	116	LYS
1	D	139	LEU

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Mol	Chain	Res	Type
1	D	140	GLU
1	D	145	LEU
1	D	152	LEU
1	D	153	THR
1	D	206	ASP
1	D	218	ASP
1	D	238	LEU
1	D	291	LEU
1	D	293	ARG
1	D	324	LEU
1	D	334	LEU
1	D	339	LEU
1	E	1	MET
1	E	76	LEU
1	E	81	SER
1	E	112	LEU
1	E	116	LYS
1	E	120	ARG
1	E	139	LEU
1	E	152	LEU
1	E	188	VAL
1	E	190	GLN
1	E	216	THR
1	E	221	ARG
1	E	226	SER
1	E	233	LEU
1	E	249	GLU
1	E	265	ARG
1	E	266	LEU
1	E	270	LEU
1	E	288	GLN
1	E	300	SER
1	E	324	LEU
1	E	334	LEU
1	F	18	CYS
1	F	31	ASP
1	F	40	THR
1	F	116	LYS
1	F	129	ARG
1	F	139	LEU
1	F	143	LYS
1	F	149	THR

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Mol	Chain	Res	Type
1	F	152	LEU
1	F	161	LEU
1	F	169	GLU
1	F	196	GLN
1	F	238	LEU
1	F	249	GLU
1	F	266	LEU
1	F	288	GLN
1	F	291	LEU
1	F	301	SER
1	F	324	LEU
1	F	332	LYS
1	F	338	ASN
1	G	1	MET
1	G	11	ILE
1	G	38	ARG
1	G	57	SER
1	G	76	LEU
1	G	77	SER
1	G	127	ASP
1	G	134	ASN
1	G	139	LEU
1	G	145	LEU
1	G	152	LEU
1	G	158	LYS
1	G	172	ARG
1	G	176	ASP
1	G	233	LEU
1	G	270	LEU
1	G	274	LYS
1	G	291	LEU
1	G	295	GLN
1	G	297	ARG
1	G	324	LEU
1	H	27	LEU
1	H	38	ARG
1	H	69	GLN
1	H	100	GLU
1	H	116	LYS
1	H	143	LYS
1	H	145	LEU
1	H	152	LEU

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Mol	Chain	Res	Type
1	H	201	GLN
1	H	202	ILE
1	H	238	LEU
1	H	266	LEU
1	H	270	LEU
1	H	275	ILE
1	H	291	LEU
1	H	292	GLU
1	H	297	ARG
1	H	304	GLU
1	H	324	LEU
1	H	332	LYS
1	H	334	LEU
1	H	336	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	78	HIS
1	A	196	GLN
1	B	20	HIS
1	B	96	ASN
1	B	251	ASN
1	C	53	GLN
1	C	70	GLN
1	C	86	ASN
1	C	96	ASN
1	C	146	GLN
1	C	295	GLN
1	D	66	ASN
1	D	68	ASN
1	D	96	ASN
1	E	86	ASN
1	E	134	ASN
1	E	190	GLN
1	F	20	HIS
1	F	68	ASN
1	F	190	GLN
1	F	338	ASN
1	G	53	GLN
1	G	68	ASN

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Mol	Chain	Res	Type
1	G	96	ASN
1	G	190	GLN
1	H	53	GLN
1	H	61	ASN
1	H	73	ASN
1	H	96	ASN
1	H	146	GLN
1	H	288	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

40 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MPD	G	403	-	7,7,7	0.58	0	9,10,10	0.65	0
4	MPD	H	402	-	7,7,7	0.63	0	9,10,10	0.66	0
4	MPD	C	403	-	7,7,7	0.51	0	9,10,10	0.86	0
4	MPD	A	404	-	7,7,7	0.45	0	9,10,10	1.36	1 (11%)
3	7V3	C	402	-	15,16,16	2.72	4 (26%)	15,21,21	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	D	403	-	7,7,7	0.52	0	9,10,10	1.26	1 (11%)
4	MPD	F	403	-	7,7,7	0.29	0	9,10,10	0.29	0
2	FAD	C	401	-	51,58,58	1.76	9 (17%)	60,89,89	1.63	8 (13%)
5	SO4	A	407	-	4,4,4	0.30	0	6,6,6	0.52	0
4	MPD	B	402	-	7,7,7	0.50	0	9,10,10	1.10	0
3	7V3	A	402	-	15,16,16	1.82	2 (13%)	15,21,21	0.95	1 (6%)
5	SO4	F	406	-	4,4,4	0.39	0	6,6,6	0.38	0
5	SO4	E	405	-	4,4,4	0.31	0	6,6,6	0.36	0
3	7V3	F	402	-	15,16,16	2.08	5 (33%)	15,21,21	0.97	1 (6%)
4	MPD	F	405	-	7,7,7	0.59	0	9,10,10	1.48	1 (11%)
2	FAD	H	401	-	51,58,58	1.76	8 (15%)	60,89,89	1.86	10 (16%)
4	MPD	A	405	-	7,7,7	0.52	0	9,10,10	0.70	0
4	MPD	B	403	-	7,7,7	0.37	0	9,10,10	0.52	0
5	SO4	H	405	-	4,4,4	0.36	0	6,6,6	0.16	0
4	MPD	E	406	-	7,7,7	0.36	0	9,10,10	0.46	0
4	MPD	A	403	-	7,7,7	0.33	0	9,10,10	0.77	0
3	7V3	D	402	-	15,16,16	1.66	3 (20%)	15,21,21	1.22	1 (6%)
4	MPD	F	404	-	7,7,7	0.53	0	9,10,10	0.74	0
4	MPD	D	404	-	7,7,7	0.41	0	9,10,10	0.76	0
2	FAD	F	401	-	51,58,58	1.87	7 (13%)	60,89,89	2.18	10 (16%)
2	FAD	A	401	-	51,58,58	1.79	6 (11%)	60,89,89	1.88	12 (20%)
2	FAD	G	401	-	51,58,58	1.92	8 (15%)	60,89,89	2.28	13 (21%)
4	MPD	A	406	-	7,7,7	0.44	0	9,10,10	0.57	0
4	MPD	E	403	-	7,7,7	0.51	0	9,10,10	0.77	0
4	MPD	H	403	-	7,7,7	0.40	0	9,10,10	0.89	0
3	7V3	G	402	-	15,16,16	1.47	4 (26%)	15,21,21	0.91	0
4	MPD	E	404	-	7,7,7	0.51	0	9,10,10	0.77	0
5	SO4	C	404	-	4,4,4	0.36	0	6,6,6	0.63	0
4	MPD	G	404	-	7,7,7	0.48	0	9,10,10	1.03	0
4	MPD	H	404	-	7,7,7	0.46	0	9,10,10	1.55	2 (22%)
5	SO4	D	405	-	4,4,4	0.44	0	6,6,6	0.48	0
2	FAD	B	401	-	51,58,58	1.85	8 (15%)	60,89,89	1.86	10 (16%)
2	FAD	D	401	-	51,58,58	1.82	5 (9%)	60,89,89	1.90	13 (21%)
4	MPD	E	402	-	7,7,7	0.75	0	9,10,10	1.11	0
2	FAD	E	401	-	51,58,58	1.86	5 (9%)	60,89,89	2.10	14 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	G	403	-	-	2/5/5/5	-
4	MPD	H	402	-	-	2/5/5/5	-
4	MPD	C	403	-	-	3/5/5/5	-
4	MPD	A	404	-	-	0/5/5/5	-
3	7V3	C	402	-	-	2/8/8/8	0/2/2/2
4	MPD	D	403	-	-	1/5/5/5	-
4	MPD	F	403	-	-	2/5/5/5	-
2	FAD	C	401	-	-	1/30/50/50	0/6/6/6
4	MPD	B	402	-	-	0/5/5/5	-
3	7V3	A	402	-	-	1/8/8/8	0/2/2/2
3	7V3	F	402	-	-	2/8/8/8	0/2/2/2
4	MPD	F	405	-	-	2/5/5/5	-
2	FAD	H	401	-	-	1/30/50/50	0/6/6/6
4	MPD	A	405	-	-	2/5/5/5	-
4	MPD	B	403	-	-	2/5/5/5	-
4	MPD	E	406	-	-	2/5/5/5	-
4	MPD	A	403	-	-	2/5/5/5	-
3	7V3	D	402	-	-	0/8/8/8	0/2/2/2
4	MPD	F	404	-	-	2/5/5/5	-
4	MPD	D	404	-	-	2/5/5/5	-
2	FAD	F	401	-	-	1/30/50/50	0/6/6/6
2	FAD	A	401	-	-	2/30/50/50	0/6/6/6
2	FAD	G	401	-	-	2/30/50/50	0/6/6/6
4	MPD	A	406	-	-	0/5/5/5	-
4	MPD	E	403	-	-	1/5/5/5	-
4	MPD	H	403	-	-	1/5/5/5	-
3	7V3	G	402	-	-	0/8/8/8	0/2/2/2
4	MPD	E	404	-	-	2/5/5/5	-
4	MPD	G	404	-	-	2/5/5/5	-
4	MPD	H	404	-	-	0/5/5/5	-
2	FAD	B	401	-	-	3/30/50/50	0/6/6/6
2	FAD	D	401	-	-	4/30/50/50	0/6/6/6
4	MPD	E	402	-	-	3/5/5/5	-
2	FAD	E	401	-	-	1/30/50/50	0/6/6/6

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FAD	C4X-C10	9.77	1.48	1.38
2	F	401	FAD	C4X-C10	9.22	1.48	1.38
2	G	401	FAD	C4X-C10	9.15	1.48	1.38
2	A	401	FAD	C4X-C10	9.15	1.48	1.38
2	E	401	FAD	C4X-C10	9.05	1.47	1.38
2	D	401	FAD	C4X-C10	9.03	1.47	1.38
2	H	401	FAD	C4X-C10	8.64	1.47	1.38
3	C	402	7V3	C1A-C7	-7.80	1.44	1.52
2	C	401	FAD	C4X-C10	7.43	1.46	1.38
3	F	402	7V3	C1B-C7	6.02	1.58	1.52
3	C	402	7V3	C1B-C7	5.44	1.58	1.52
2	D	401	FAD	C4-C4X	5.07	1.50	1.41
3	A	402	7V3	C1A-C7	-5.00	1.47	1.52
2	G	401	FAD	C4-C4X	4.84	1.49	1.41
2	E	401	FAD	C4-C4X	4.79	1.49	1.41
2	C	401	FAD	C9A-C5X	4.35	1.51	1.42
2	E	401	FAD	C9A-C5X	4.34	1.51	1.42
2	F	401	FAD	C9A-N10	4.12	1.44	1.38
3	D	402	7V3	C1B-C7	4.06	1.56	1.52
2	B	401	FAD	C9A-C5X	4.04	1.50	1.42
2	F	401	FAD	C4-C4X	3.93	1.48	1.41
2	F	401	FAD	C9A-C5X	3.84	1.50	1.42
2	D	401	FAD	C9A-C5X	3.78	1.50	1.42
2	G	401	FAD	C9A-C5X	3.71	1.50	1.42
2	C	401	FAD	C8-C7	3.70	1.50	1.40
2	A	401	FAD	C4-C4X	3.69	1.47	1.41
2	H	401	FAD	C4-C4X	3.55	1.47	1.41
2	H	401	FAD	C9A-N10	3.46	1.43	1.38
3	A	402	7V3	C1B-C7	3.45	1.56	1.52
2	E	401	FAD	C8-C7	3.31	1.49	1.40
2	B	401	FAD	C4-C4X	3.29	1.47	1.41
2	G	401	FAD	C8-C7	3.28	1.49	1.40
3	D	402	7V3	C4A-CL	3.23	1.81	1.74
2	D	401	FAD	C8-C7	3.16	1.48	1.40
2	B	401	FAD	C8-C7	3.11	1.48	1.40
2	H	401	FAD	C6-C5X	-3.11	1.37	1.41
2	A	401	FAD	C9A-C5X	3.08	1.48	1.42
2	C	401	FAD	C9A-N10	3.08	1.42	1.38
3	F	402	7V3	C2B-C1B	3.05	1.44	1.39
2	A	401	FAD	C9A-N10	2.98	1.42	1.38
2	C	401	FAD	C1'-N10	-2.92	1.45	1.48
3	C	402	7V3	C6B-C1B	2.89	1.43	1.39
2	A	401	FAD	C8-C7	2.88	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	C4-C4X	2.85	1.46	1.41
2	G	401	FAD	C5A-C4A	2.82	1.48	1.40
3	G	402	7V3	C1B-C7	2.68	1.55	1.52
2	H	401	FAD	C9A-C5X	2.66	1.47	1.42
2	B	401	FAD	C9A-N10	2.63	1.42	1.38
3	G	402	7V3	C4A-CL	2.57	1.80	1.74
2	G	401	FAD	C9A-N10	2.55	1.42	1.38
2	E	401	FAD	C9A-N10	2.53	1.41	1.38
2	G	401	FAD	C2A-N3A	2.51	1.36	1.32
2	H	401	FAD	C8-C7	2.46	1.47	1.40
2	H	401	FAD	C2A-N3A	2.43	1.36	1.32
2	F	401	FAD	C8-C7	2.42	1.46	1.40
2	B	401	FAD	C10-N1	2.41	1.36	1.33
3	G	402	7V3	C1A-C7	2.39	1.55	1.52
2	A	401	FAD	C5A-C4A	2.38	1.47	1.40
2	F	401	FAD	C5A-C4A	2.36	1.47	1.40
3	G	402	7V3	C2B-C1B	2.34	1.42	1.39
2	C	401	FAD	C2-N3	-2.30	1.33	1.38
2	H	401	FAD	C5A-C4A	2.29	1.47	1.40
2	C	401	FAD	C5A-N7A	-2.27	1.31	1.39
2	D	401	FAD	C5A-C4A	2.26	1.46	1.40
2	B	401	FAD	C5A-C4A	2.22	1.46	1.40
2	B	401	FAD	O4B-C1B	2.21	1.44	1.41
2	C	401	FAD	O4B-C1B	2.19	1.44	1.41
3	C	402	7V3	C2B-C1B	2.18	1.42	1.39
2	F	401	FAD	C2A-N3A	2.13	1.35	1.32
3	F	402	7V3	C6B-C1B	2.13	1.42	1.39
3	D	402	7V3	C1A-C7	-2.06	1.50	1.52
3	F	402	7V3	C4A-CL	2.04	1.78	1.74
3	F	402	7V3	C1A-C7	-2.02	1.50	1.52
2	G	401	FAD	C10-N1	2.01	1.35	1.33

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	C4-N3-C2	8.06	121.95	115.14
2	F	401	FAD	C4-N3-C2	8.00	121.90	115.14
2	F	401	FAD	C1'-N10-C9A	7.92	124.52	118.29
2	G	401	FAD	C1'-N10-C9A	7.84	124.46	118.29
2	G	401	FAD	C4-N3-C2	7.78	121.71	115.14
2	H	401	FAD	C4-N3-C2	7.74	121.68	115.14
2	D	401	FAD	C4-N3-C2	7.70	121.64	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	FAD	C4-N3-C2	7.32	121.33	115.14
2	B	401	FAD	C4-N3-C2	7.14	121.17	115.14
2	B	401	FAD	C1'-N10-C9A	6.68	123.55	118.29
2	C	401	FAD	C4-N3-C2	6.40	120.55	115.14
2	F	401	FAD	C4-C4X-C10	-6.26	115.81	119.95
2	G	401	FAD	C4-C4X-C10	-6.12	115.90	119.95
2	H	401	FAD	C4X-N5-C5X	5.87	122.63	116.77
2	G	401	FAD	C4-C4X-N5	5.77	125.20	118.60
2	E	401	FAD	C1'-N10-C9A	5.29	122.45	118.29
2	A	401	FAD	C1'-N10-C9A	4.97	122.20	118.29
2	E	401	FAD	C4-C4X-C10	-4.96	116.67	119.95
2	C	401	FAD	C4X-N5-C5X	4.95	121.72	116.77
2	E	401	FAD	N3A-C2A-N1A	-4.73	121.28	128.68
2	E	401	FAD	C4-C4X-N5	4.64	123.90	118.60
2	E	401	FAD	C4X-N5-C5X	4.60	121.37	116.77
2	D	401	FAD	C4X-N5-C5X	4.59	121.36	116.77
2	G	401	FAD	C4X-N5-C5X	4.40	121.17	116.77
2	A	401	FAD	C4X-N5-C5X	4.40	121.16	116.77
2	C	401	FAD	C4-C4X-C10	-4.19	117.17	119.95
2	F	401	FAD	C4X-N5-C5X	4.08	120.85	116.77
2	B	401	FAD	N3A-C2A-N1A	-4.00	122.42	128.68
2	E	401	FAD	O4B-C1B-C2B	-3.93	101.18	106.93
2	G	401	FAD	N3A-C2A-N1A	-3.85	122.67	128.68
2	D	401	FAD	C4X-C4-N3	-3.82	118.21	123.43
2	F	401	FAD	C4-C4X-N5	3.80	122.94	118.60
2	H	401	FAD	N3A-C2A-N1A	-3.80	122.74	128.68
2	D	401	FAD	N3A-C2A-N1A	-3.79	122.75	128.68
2	H	401	FAD	C1'-N10-C9A	3.79	121.28	118.29
2	H	401	FAD	C4X-C4-N3	-3.75	118.30	123.43
4	F	405	MPD	CM-C2-C1	3.69	118.26	110.57
2	F	401	FAD	N3A-C2A-N1A	-3.68	122.93	128.68
2	D	401	FAD	C4-C4X-N5	3.54	122.64	118.60
2	G	401	FAD	C10-C4X-N5	-3.42	118.89	121.26
2	B	401	FAD	C4-C4X-C10	-3.41	117.69	119.95
2	F	401	FAD	O4B-C1B-C2B	-3.38	101.98	106.93
2	A	401	FAD	C4X-C4-N3	-3.37	118.82	123.43
2	A	401	FAD	N3A-C2A-N1A	-3.36	123.43	128.68
2	C	401	FAD	N3A-C2A-N1A	-3.35	123.45	128.68
2	D	401	FAD	O4B-C1B-C2B	-3.34	102.04	106.93
2	B	401	FAD	C4X-N5-C5X	3.23	120.00	116.77
2	A	401	FAD	C4-C4X-C10	-3.19	117.84	119.95
2	B	401	FAD	C9A-N10-C10	-3.10	117.84	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FAD	C1'-N10-C9A	3.03	120.68	118.29
2	D	401	FAD	C10-C4X-N5	-3.03	119.16	121.26
2	F	401	FAD	C9A-N10-C10	-2.94	118.06	121.91
2	B	401	FAD	C4X-C4-N3	-2.91	119.46	123.43
2	G	401	FAD	C9A-N10-C10	-2.85	118.18	121.91
2	E	401	FAD	N6A-C6A-N1A	2.85	124.48	118.57
2	E	401	FAD	C4X-C4-N3	-2.80	119.60	123.43
4	H	404	MPD	O2-C2-C3	-2.74	99.49	109.80
2	A	401	FAD	C4-C4X-N5	2.74	121.73	118.60
2	G	401	FAD	C4X-C4-N3	-2.74	119.69	123.43
4	D	403	MPD	CM-C2-C1	2.71	116.23	110.57
2	G	401	FAD	N6A-C6A-N1A	2.70	124.18	118.57
2	D	401	FAD	C4-C4X-C10	-2.68	118.18	119.95
2	E	401	FAD	C10-C4X-N5	-2.65	119.42	121.26
2	A	401	FAD	N6A-C6A-N1A	2.64	124.05	118.57
2	A	401	FAD	C2A-N1A-C6A	2.63	123.25	118.75
2	F	401	FAD	C4A-C5A-N7A	-2.61	106.68	109.40
2	F	401	FAD	C4X-C4-N3	-2.58	119.91	123.43
2	D	401	FAD	O2A-PA-O1A	2.53	124.77	112.24
4	A	404	MPD	CM-C2-C1	-2.52	105.32	110.57
2	C	401	FAD	C4X-C10-N10	-2.51	117.72	120.30
4	H	404	MPD	O2-C2-CM	2.50	116.12	108.08
2	D	401	FAD	O2'-C2'-C1'	2.49	115.59	109.59
2	E	401	FAD	C1B-N9A-C4A	-2.48	122.28	126.64
2	D	401	FAD	C9A-N10-C10	-2.45	118.70	121.91
2	D	401	FAD	C1'-N10-C10	2.45	120.60	118.41
2	C	401	FAD	C4X-C4-N3	-2.44	120.10	123.43
2	C	401	FAD	N6A-C6A-N1A	2.42	123.60	118.57
2	H	401	FAD	C1B-N9A-C4A	-2.41	122.40	126.64
2	G	401	FAD	C2A-N1A-C6A	2.41	122.87	118.75
3	D	402	7V3	C2B-C1B-C6B	-2.35	115.37	118.29
2	E	401	FAD	C5A-C6A-N6A	-2.26	116.91	120.35
2	B	401	FAD	N6A-C6A-N1A	2.24	123.22	118.57
3	C	402	7V3	C2B-C1B-C6B	-2.22	115.52	118.29
2	E	401	FAD	C2A-N1A-C6A	2.20	122.52	118.75
2	H	401	FAD	C9A-N10-C10	-2.18	119.05	121.91
2	A	401	FAD	O5'-P-O1P	-2.18	100.55	109.07
2	B	401	FAD	C6-C5X-N5	-2.17	116.66	119.05
2	H	401	FAD	C4-C4X-N5	2.12	121.02	118.60
3	F	402	7V3	C3A-C2A-C1A	2.12	123.33	121.20
3	A	402	7V3	C2B-C1B-C6B	-2.11	115.65	118.29
2	C	401	FAD	C1'-N10-C9A	2.11	119.95	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	FAD	O2A-PA-O1A	2.07	122.48	112.24
2	H	401	FAD	C4-C4X-C10	-2.05	118.59	119.95
2	E	401	FAD	C9A-N10-C10	-2.05	119.22	121.91
2	A	401	FAD	P-O3P-PA	-2.04	125.81	132.83
2	H	401	FAD	N6A-C6A-N1A	2.03	122.79	118.57
2	B	401	FAD	C2A-N1A-C6A	2.01	122.20	118.75
2	A	401	FAD	C5A-C6A-N1A	-2.01	115.79	120.35
2	G	401	FAD	O2P-P-O1P	2.00	122.13	112.24

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	402	MPD	C2-C3-C4-O4
4	C	403	MPD	C1-C2-C3-C4
4	C	403	MPD	O2-C2-C3-C4
4	A	403	MPD	C2-C3-C4-O4
4	E	403	MPD	C2-C3-C4-O4
4	H	403	MPD	C2-C3-C4-O4
4	G	404	MPD	C2-C3-C4-O4
4	G	404	MPD	C2-C3-C4-C5
3	C	402	7V3	C6B-C1B-C7-C1A
3	C	402	7V3	C2B-C1B-C7-C1A
3	A	402	7V3	C2B-C1B-C7-C1A
3	F	402	7V3	C6B-C1B-C7-C1A
3	F	402	7V3	C2B-C1B-C7-C1A
2	A	401	FAD	P-O3P-PA-O5B
2	G	401	FAD	PA-O3P-P-O5'
4	E	402	MPD	O2-C2-C3-C4
4	F	405	MPD	C2-C3-C4-C5
4	A	405	MPD	C2-C3-C4-C5
4	B	403	MPD	C2-C3-C4-C5
4	E	406	MPD	C2-C3-C4-C5
4	A	403	MPD	C2-C3-C4-C5
4	F	404	MPD	C2-C3-C4-C5
4	E	404	MPD	C2-C3-C4-O4
4	G	403	MPD	C1-C2-C3-C4
4	C	403	MPD	CM-C2-C3-C4
4	D	404	MPD	C1-C2-C3-C4
4	E	402	MPD	C1-C2-C3-C4
4	E	402	MPD	CM-C2-C3-C4
2	D	401	FAD	C2'-C3'-C4'-O4'

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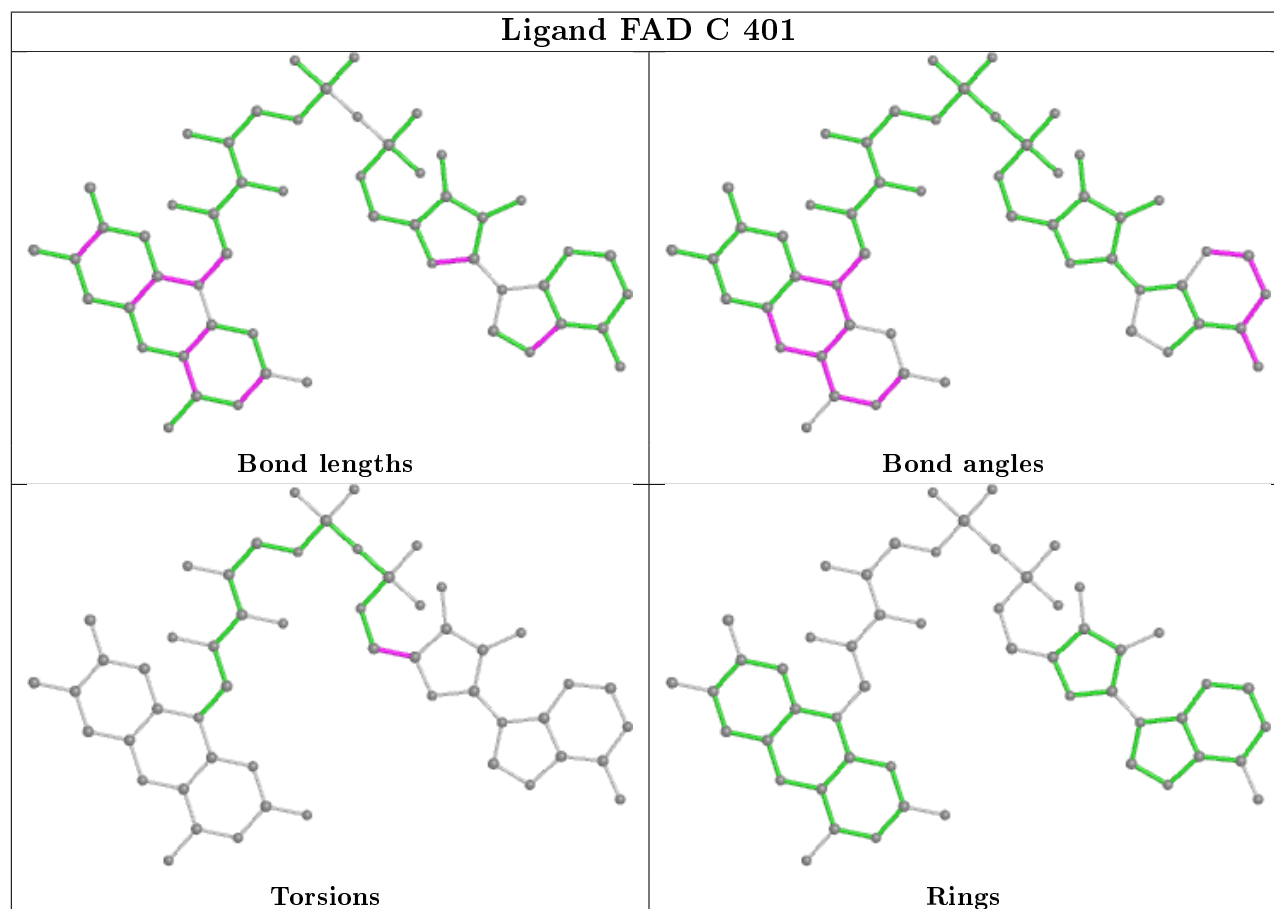
Mol	Chain	Res	Type	Atoms
2	B	401	FAD	O4B-C4B-C5B-O5B
2	F	401	FAD	O4B-C4B-C5B-O5B
4	G	403	MPD	O2-C2-C3-C4
4	D	404	MPD	O2-C2-C3-C4
2	C	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	O4B-C4B-C5B-O5B
2	G	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	O4B-C4B-C5B-O5B
2	E	401	FAD	O4B-C4B-C5B-O5B
4	H	402	MPD	C2-C3-C4-C5
4	D	403	MPD	C2-C3-C4-C5
4	F	403	MPD	C2-C3-C4-C5
4	E	404	MPD	C2-C3-C4-C5
2	D	401	FAD	O3'-C3'-C4'-O4'
2	H	401	FAD	O4B-C4B-C5B-O5B
2	B	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	C1'-C2'-C3'-O3'
2	B	401	FAD	O2'-C2'-C3'-C4'
4	F	403	MPD	C2-C3-C4-O4
4	F	405	MPD	C2-C3-C4-O4
4	A	405	MPD	C2-C3-C4-O4
4	B	403	MPD	C2-C3-C4-O4
4	E	406	MPD	C2-C3-C4-O4
4	F	404	MPD	C2-C3-C4-O4

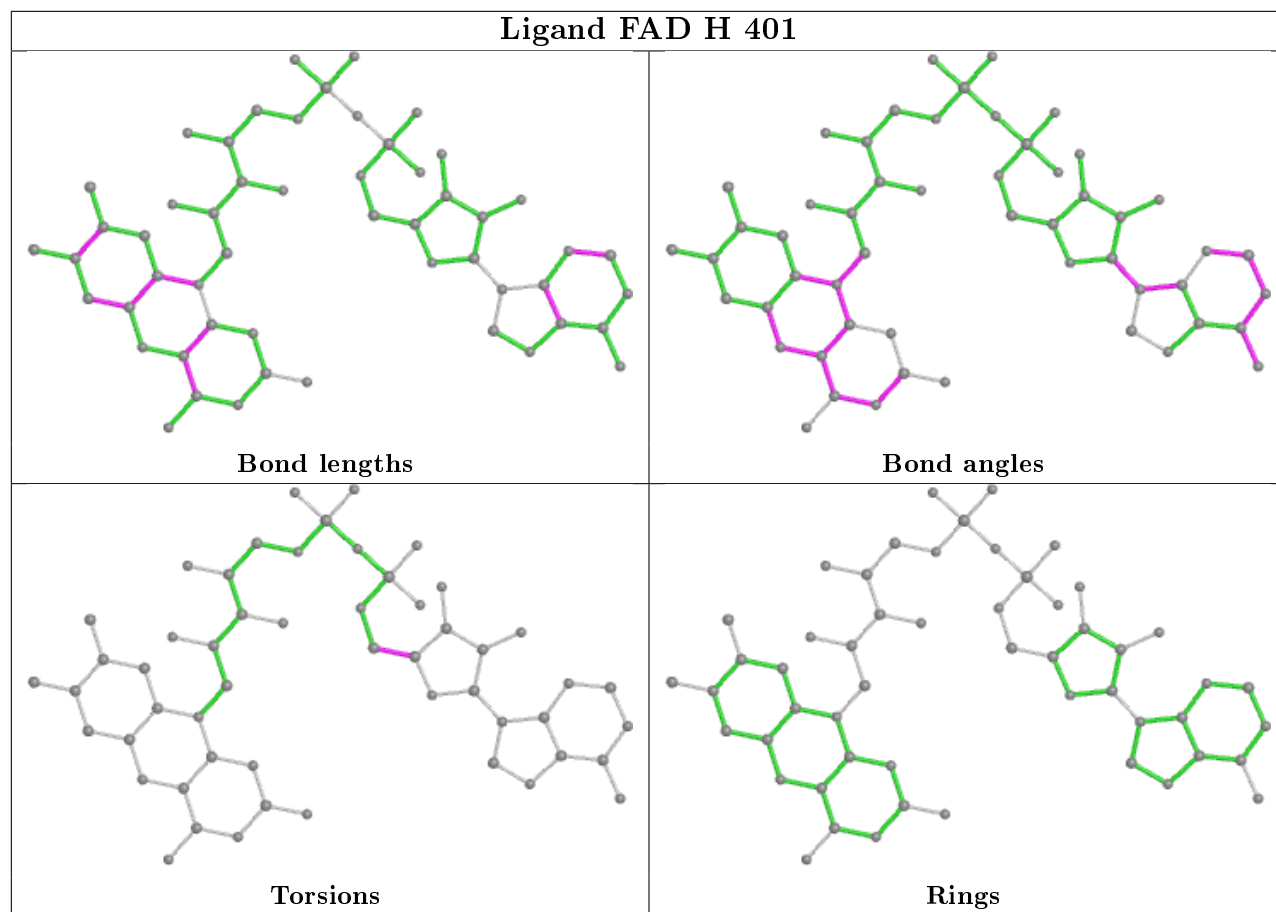
There are no ring outliers.

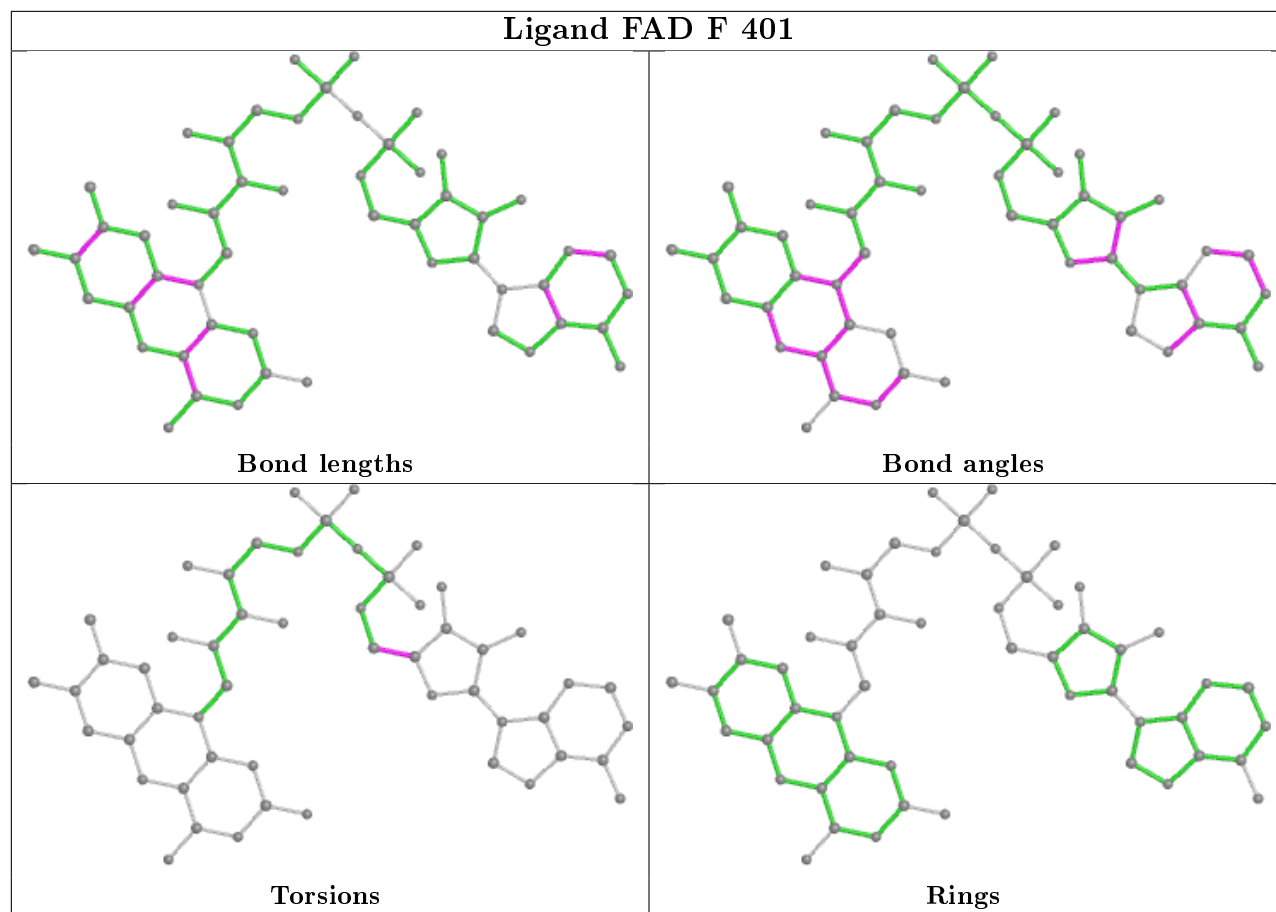
12 monomers are involved in 14 short contacts:

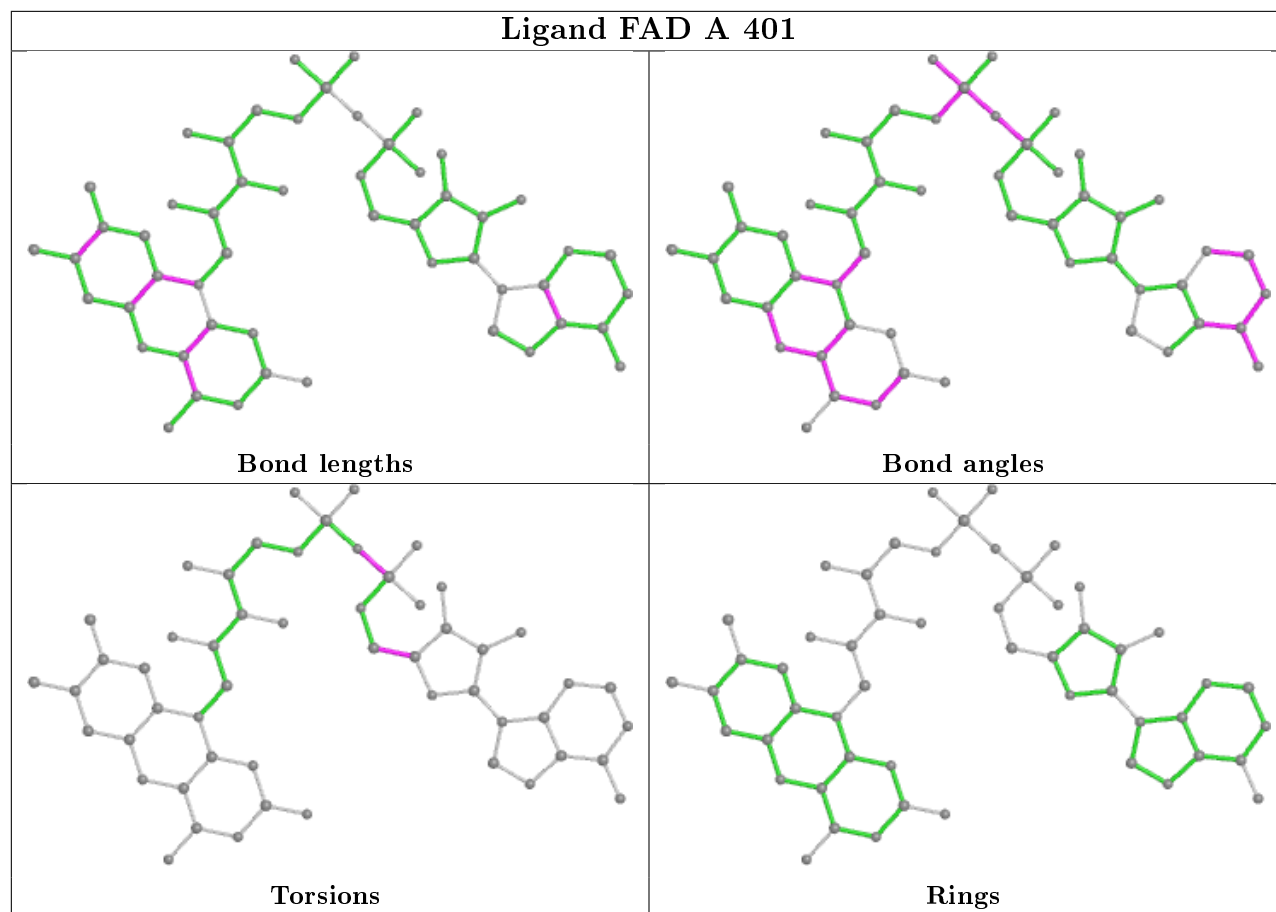
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	MPD	1	0
3	C	402	7V3	2	0
5	F	406	SO4	1	0
3	F	402	7V3	1	0
3	D	402	7V3	1	0
2	F	401	FAD	1	0
2	G	401	FAD	1	0
4	H	403	MPD	3	0
4	E	404	MPD	1	0
2	D	401	FAD	1	0
4	E	402	MPD	1	0
2	E	401	FAD	1	0

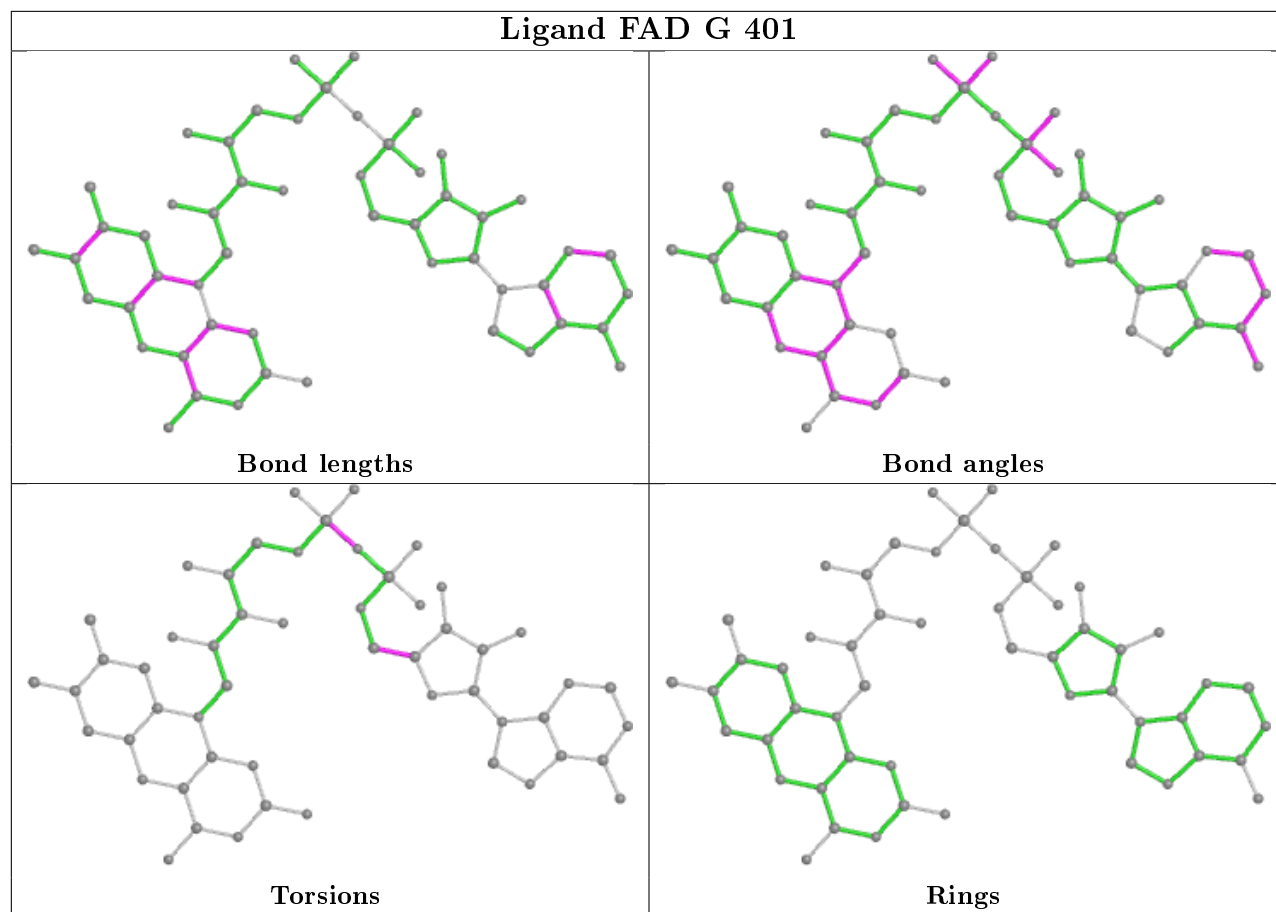
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



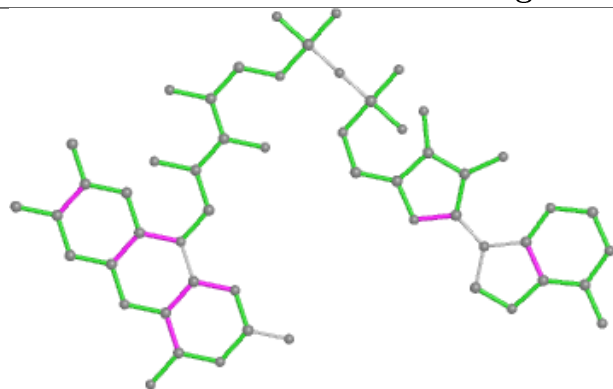




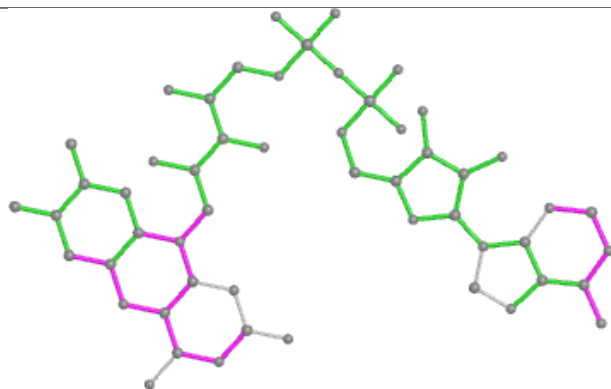




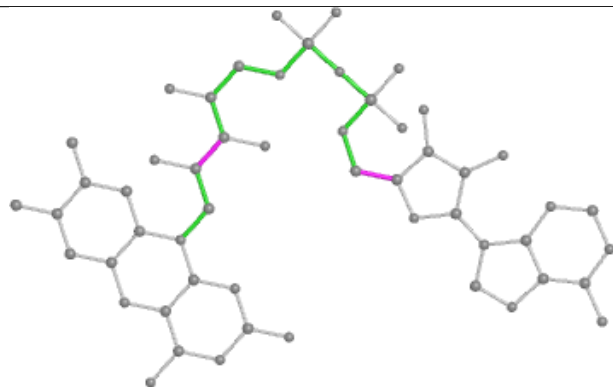
Ligand FAD B 401



Bond lengths



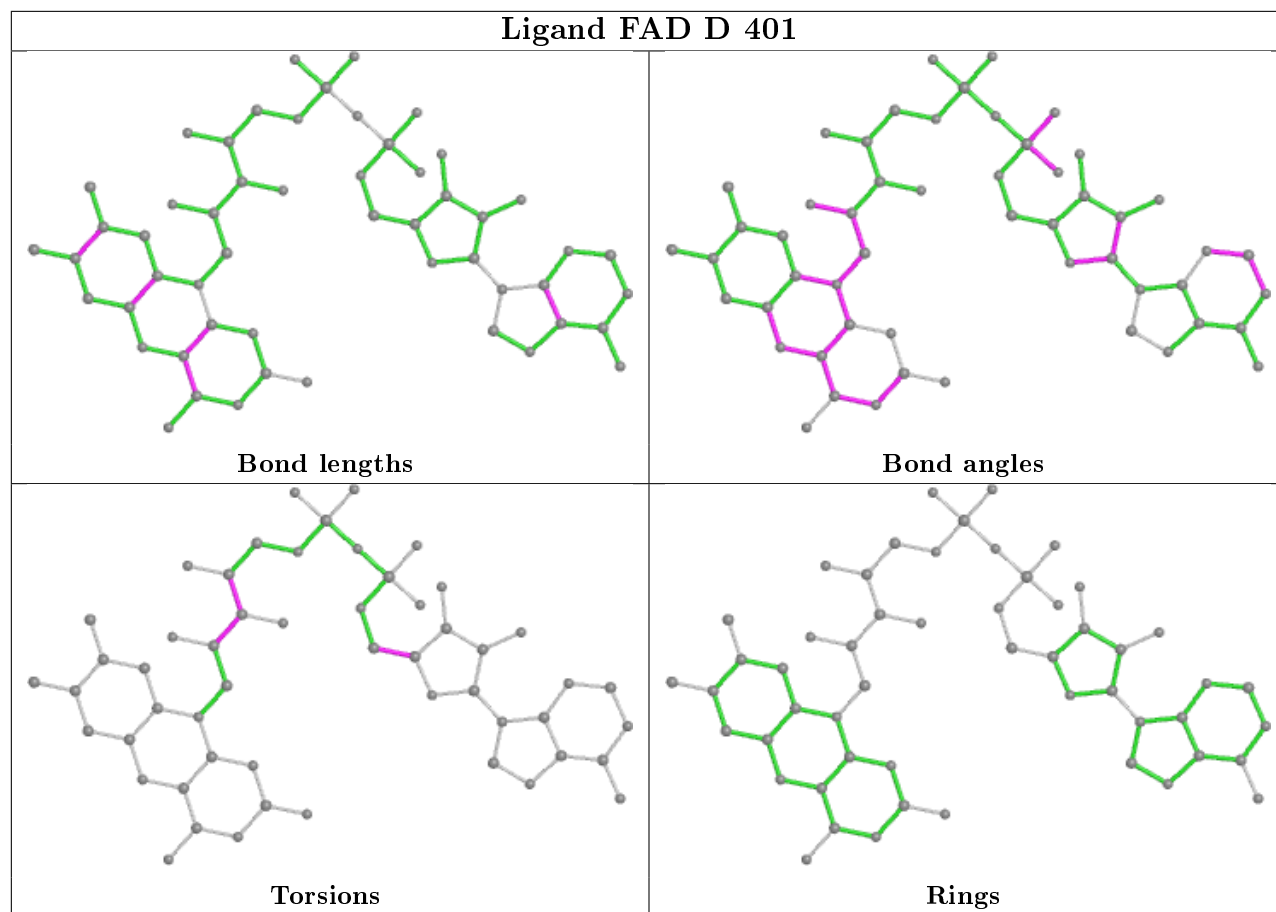
Bond angles

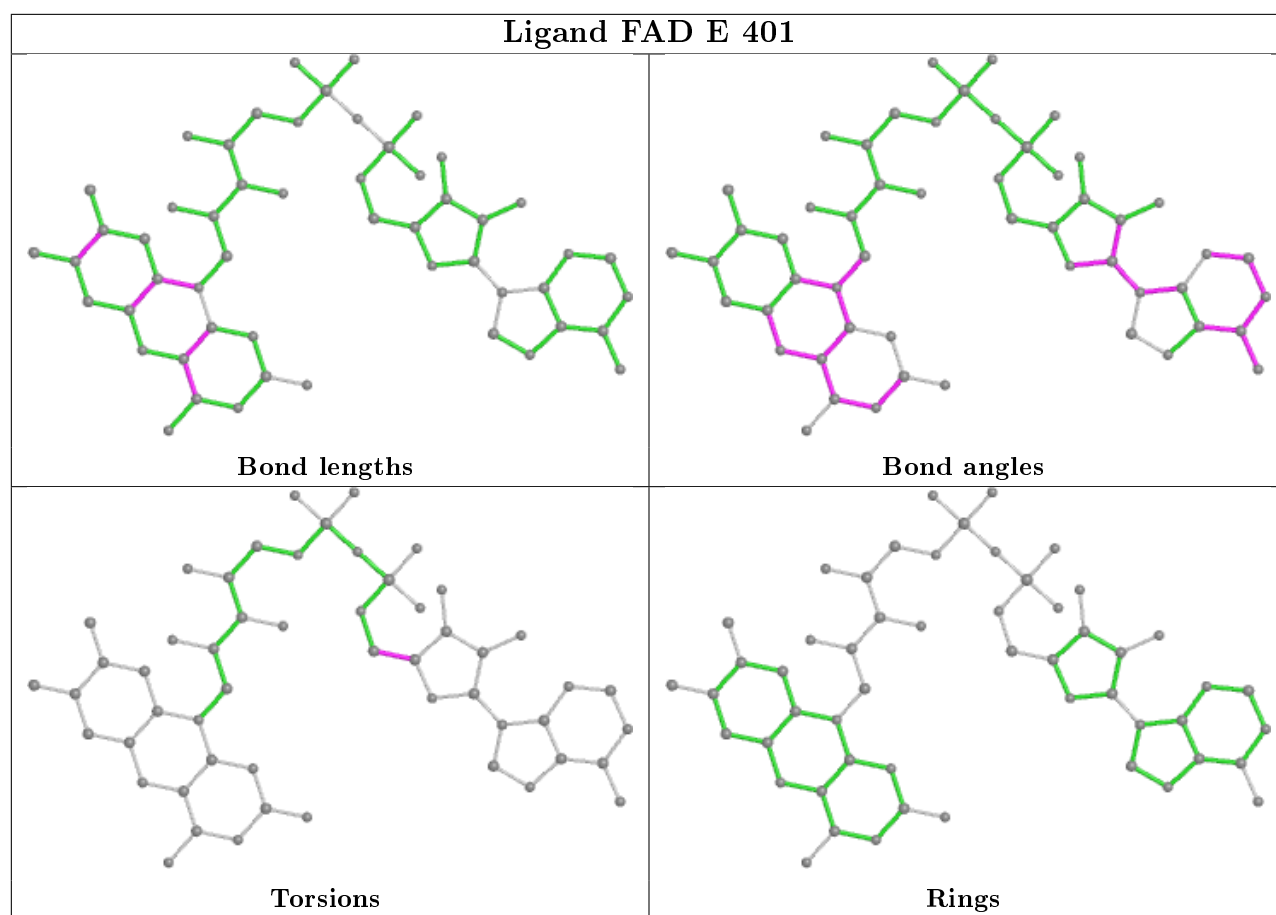


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	339/347 (97%)	-0.61	0 100 100	38, 59, 111, 146	0
1	B	339/347 (97%)	-0.54	1 (0%) 94 92	39, 64, 125, 180	0
1	C	339/347 (97%)	-0.51	1 (0%) 94 92	42, 63, 111, 161	0
1	D	339/347 (97%)	-0.50	0 100 100	43, 67, 120, 172	1 (0%)
1	E	338/347 (97%)	-0.42	0 100 100	44, 78, 124, 157	0
1	F	338/347 (97%)	-0.34	6 (1%) 68 55	51, 81, 120, 152	0
1	G	338/347 (97%)	-0.29	2 (0%) 89 83	60, 86, 131, 149	0
1	H	337/347 (97%)	-0.30	2 (0%) 89 83	57, 87, 132, 194	0
All	All	2707/2776 (97%)	-0.44	12 (0%) 92 89	38, 75, 125, 194	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	300	SER	4.5
1	H	300	SER	3.2
1	F	301	SER	2.8
1	F	223	ILE	2.8
1	F	60	SER	2.7
1	F	298	PHE	2.7
1	H	337	ARG	2.6
1	B	27	LEU	2.4
1	C	29	PRO	2.2
1	F	299	GLY	2.1
1	G	249	GLU	2.0
1	G	65	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
5	SO4	H	405	5/5	0.82	0.22	144,146,156,157	0
5	SO4	D	405	5/5	0.86	0.21	115,120,122,132	0
5	SO4	F	406	5/5	0.87	0.28	177,191,197,221	0
4	MPD	E	406	8/8	0.88	0.40	87,106,113,118	0
4	MPD	A	406	8/8	0.89	0.26	94,98,102,104	0
4	MPD	E	404	8/8	0.89	0.65	101,112,121,122	0
5	SO4	A	407	5/5	0.89	0.25	121,123,131,136	0
4	MPD	G	403	8/8	0.90	0.24	85,95,101,107	0
3	7V3	G	402	15/15	0.90	0.53	114,122,140,160	0
4	MPD	B	402	8/8	0.91	0.30	85,87,88,97	0
4	MPD	G	404	8/8	0.91	0.43	88,98,104,106	0
4	MPD	B	403	8/8	0.91	0.33	112,120,123,125	0
4	MPD	F	403	8/8	0.92	0.25	102,109,111,114	0
4	MPD	H	403	8/8	0.93	0.25	68,74,83,83	0
5	SO4	E	405	5/5	0.93	0.15	122,126,131,141	0
3	7V3	F	402	15/15	0.93	0.54	87,94,104,111	0
4	MPD	D	404	8/8	0.93	0.23	84,93,99,104	0
4	MPD	H	404	8/8	0.93	0.26	71,75,78,79	0
4	MPD	D	403	8/8	0.93	0.24	74,93,108,123	0
4	MPD	E	403	8/8	0.94	0.21	82,84,89,95	0
3	7V3	C	402	15/15	0.94	0.53	95,102,117,125	0
4	MPD	F	405	8/8	0.94	0.20	67,73,79,80	0
3	7V3	D	402	15/15	0.94	0.44	87,98,106,120	0
4	MPD	F	404	8/8	0.94	0.25	65,77,92,94	0
4	MPD	A	405	8/8	0.94	0.25	84,89,97,103	0
3	7V3	A	402	15/15	0.94	0.24	82,89,101,106	0
4	MPD	E	402	8/8	0.94	0.19	82,97,105,107	0

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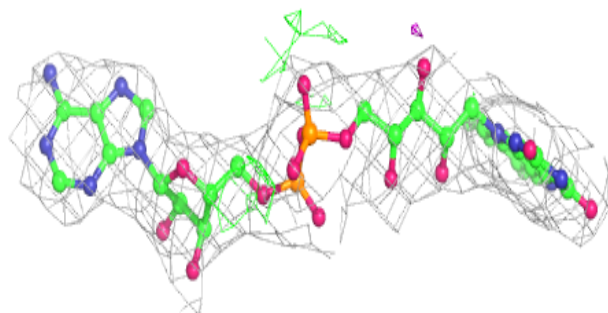
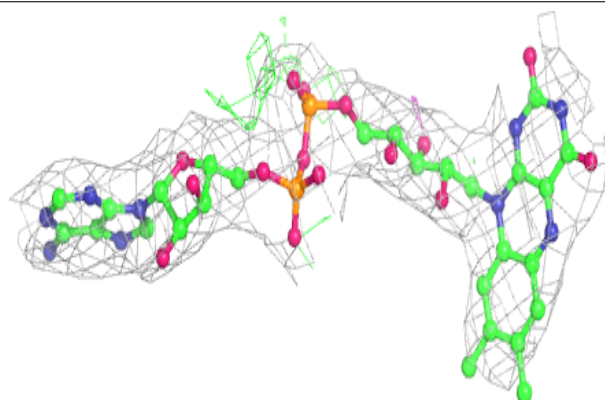
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MPD	A	403	8/8	0.95	0.27	70,81,88,92	0
5	SO4	C	404	5/5	0.95	0.13	91,97,108,110	0
4	MPD	H	402	8/8	0.95	0.24	92,99,101,105	0
4	MPD	A	404	8/8	0.96	0.19	47,49,58,69	0
2	FAD	F	401	53/53	0.97	0.15	51,60,67,74	0
2	FAD	G	401	53/53	0.97	0.14	65,75,88,91	0
4	MPD	C	403	8/8	0.97	0.16	56,61,63,64	0
2	FAD	A	401	53/53	0.98	0.14	36,42,58,71	0
2	FAD	H	401	53/53	0.98	0.16	63,69,79,80	0
2	FAD	B	401	53/53	0.98	0.15	44,56,84,95	0
2	FAD	D	401	53/53	0.98	0.15	43,55,61,65	0
2	FAD	C	401	53/53	0.98	0.15	40,48,56,64	0
2	FAD	E	401	53/53	0.98	0.14	45,58,69,78	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.

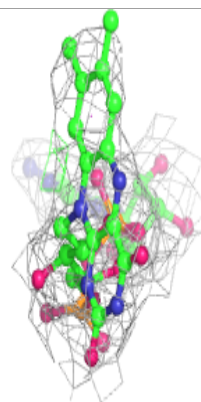
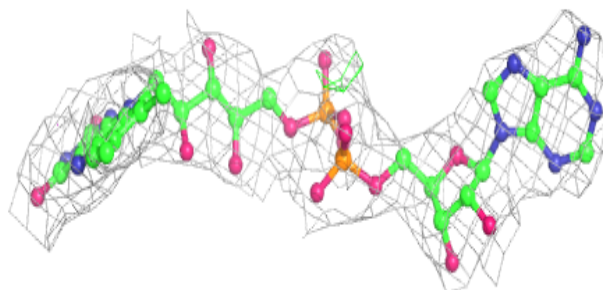
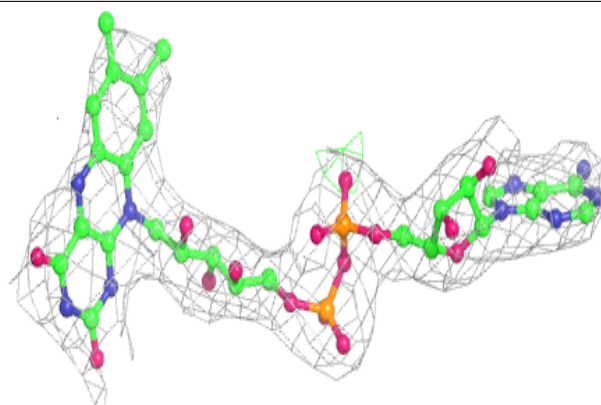
Electron density around FAD F 401:

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

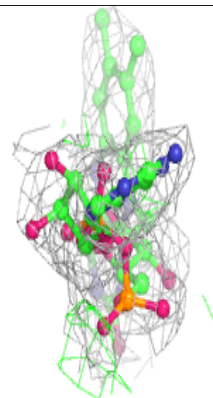
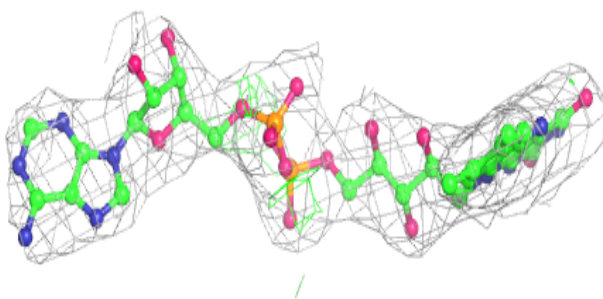
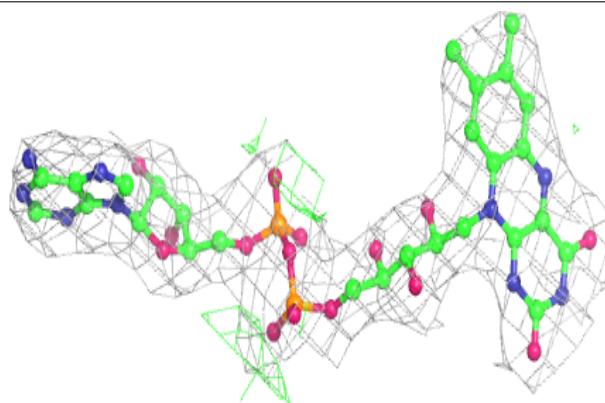


Electron density around FAD G 401:

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

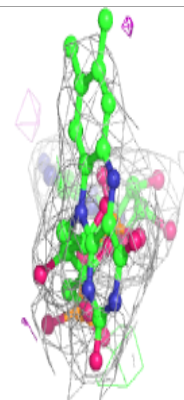
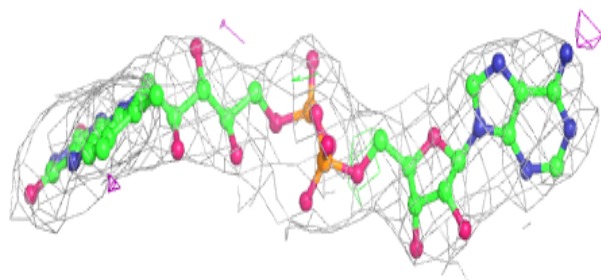
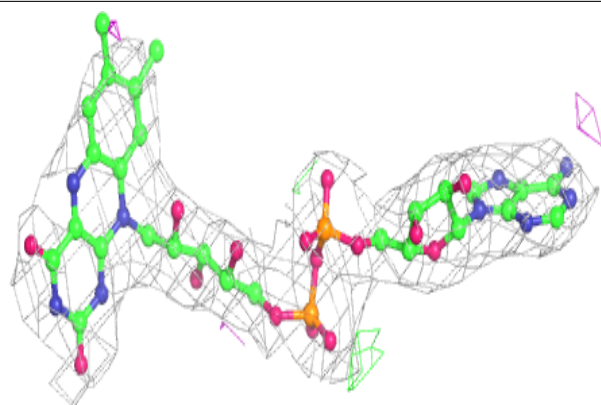
**Electron density around FAD A 401:**

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

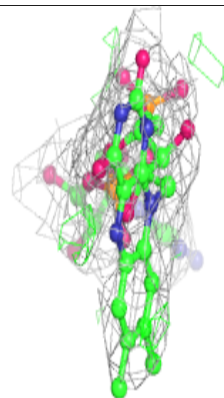
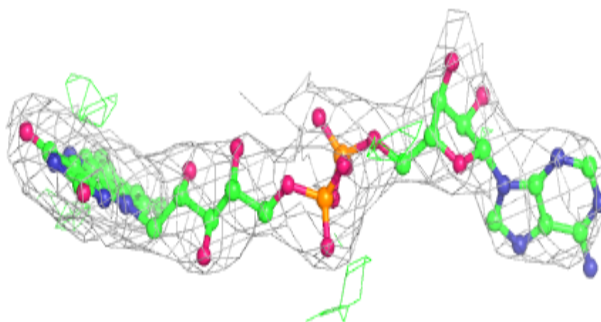
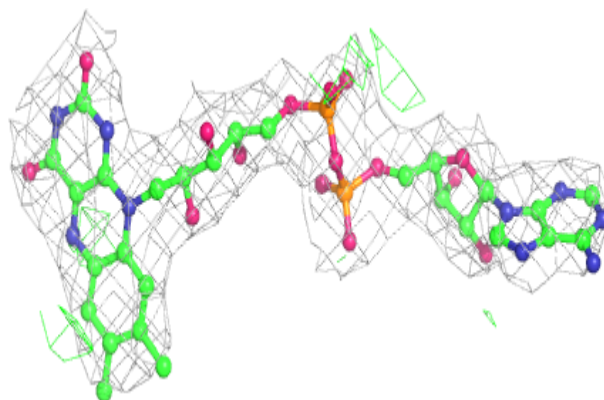


Electron density around FAD H 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

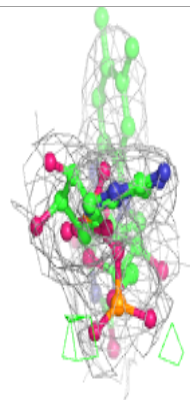
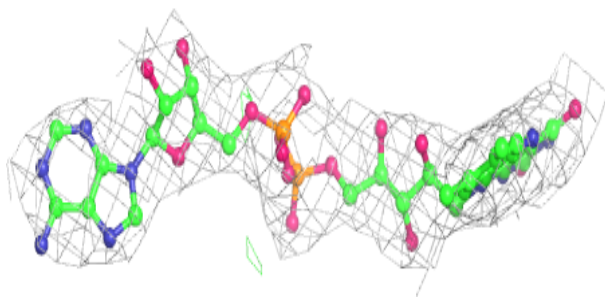
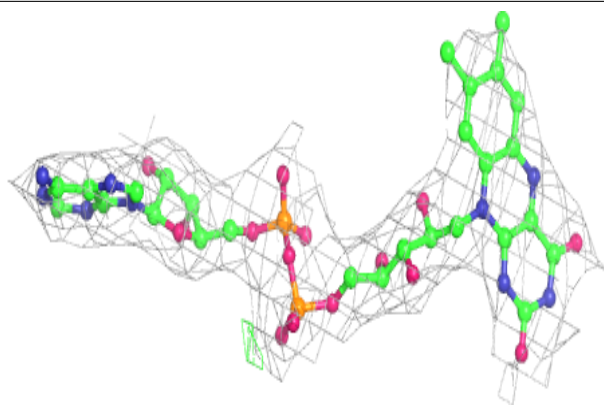
**Electron density around FAD B 401:**

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

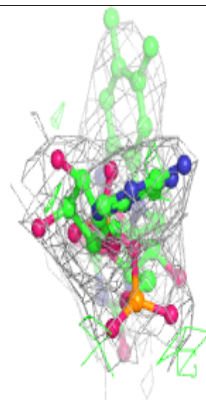
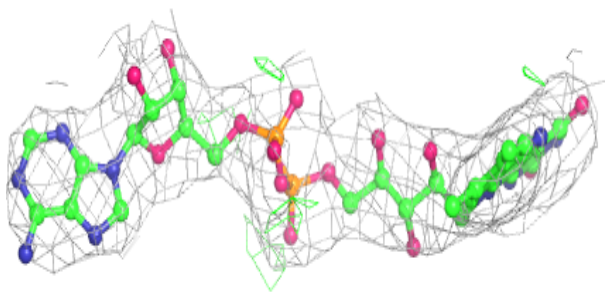
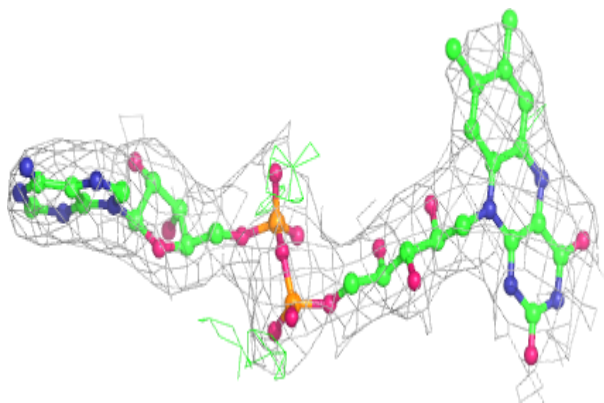


Electron density around FAD D 401:

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

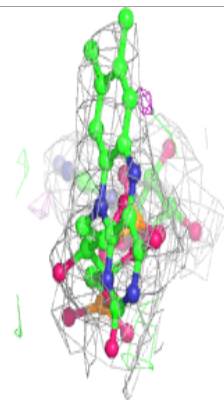
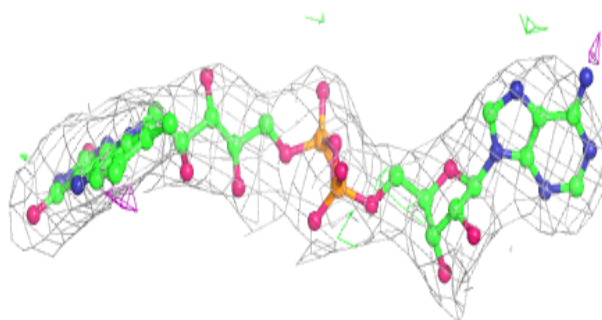
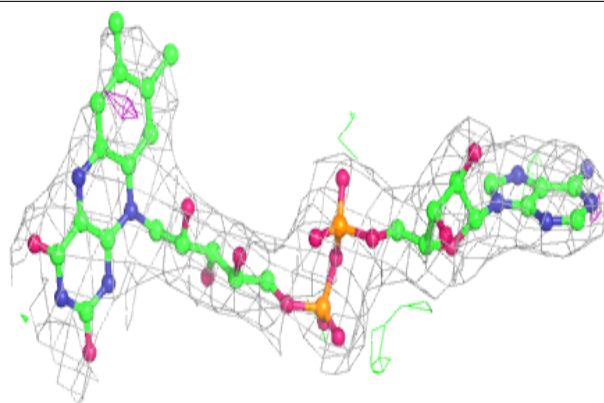
**Electron density around FAD C 401:**

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



Electron density around FAD E 401:

$2mF_o - DF_c$ (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.