Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 02:26 PM EST

PDB ID	:	1RX0
Title	:	Crystal structure of isobutyryl-CoA dehydrogenase complexed with substrate/ligand.
Authors	:	Battaile, K.P.; Nguyen, T.V.; Vockley, J.; Kim, J.J.
Deposited on	:	2003-12-18
Resolution	:	1.77 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 (i) 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 (i)) were used in the production of this report:

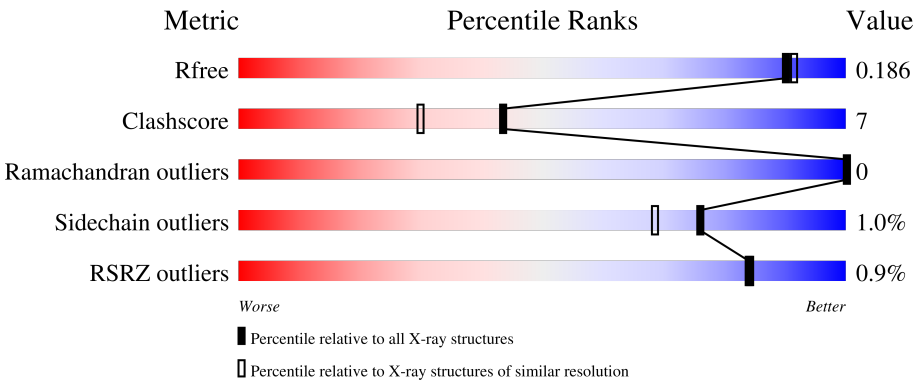
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 <=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	393	.% 86% 11% • •
1	B	393	.% 87% 11% •
1	C	393	.% 82% 15% •
1	D	393	2% 84% 13% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13784 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.

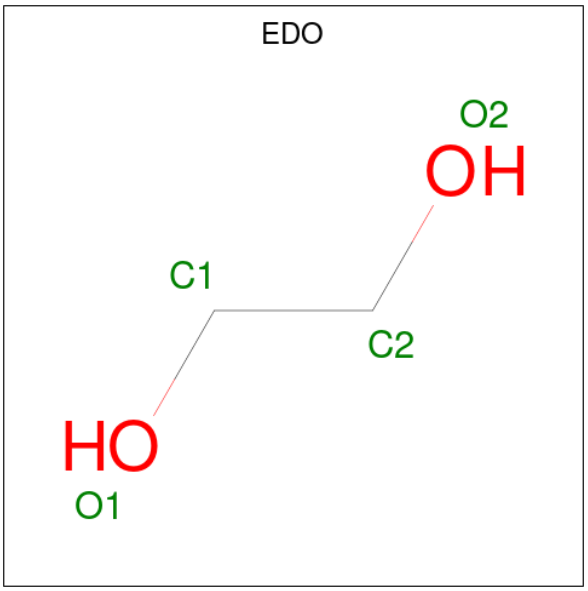
- Molecule 1 is a protein called Acyl-CoA dehydrogenase family member 8, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	2964	1855	518	564	27	0	7	0
1	B	384	2961	1852	517	565	27	0	7	0
1	C	383	2978	1861	521	569	27	0	10	0
1	D	384	3019	1887	529	575	28	0	14	0

There are 4 discrepancies between the modelled and reference sequences:

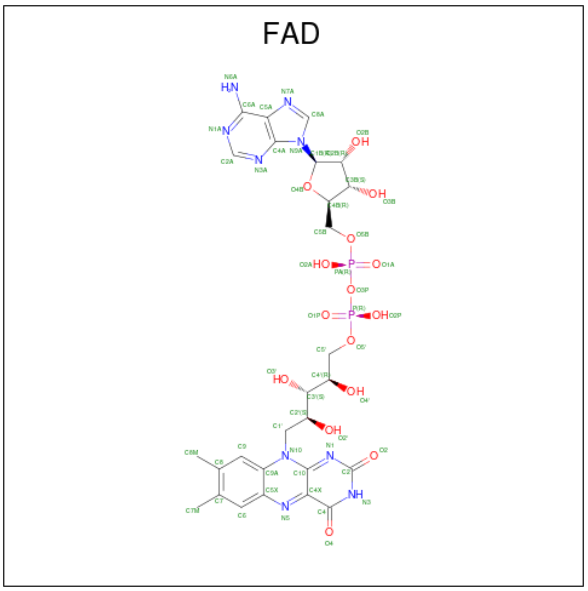
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q9UKU7
B	1	MET	-	cloning artifact	UNP Q9UKU7
C	1	MET	-	cloning artifact	UNP Q9UKU7
D	1	MET	-	cloning artifact	UNP Q9UKU7

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



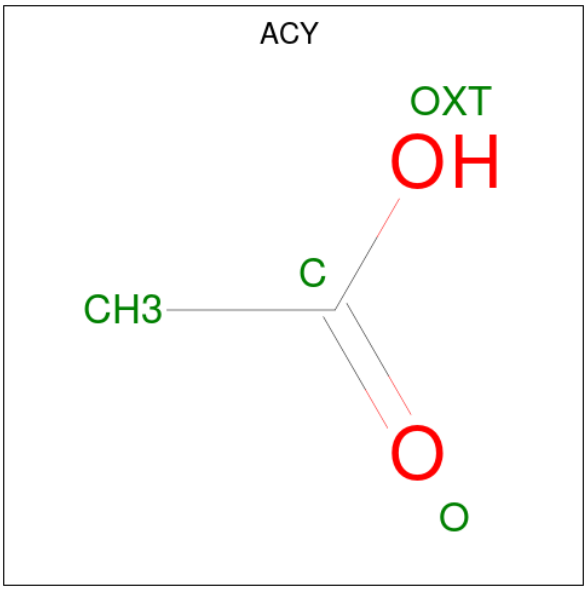
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	C	1	4	2	2	0	0
			Total	C	O		
2	C	1	4	2	2	0	0
			Total	C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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



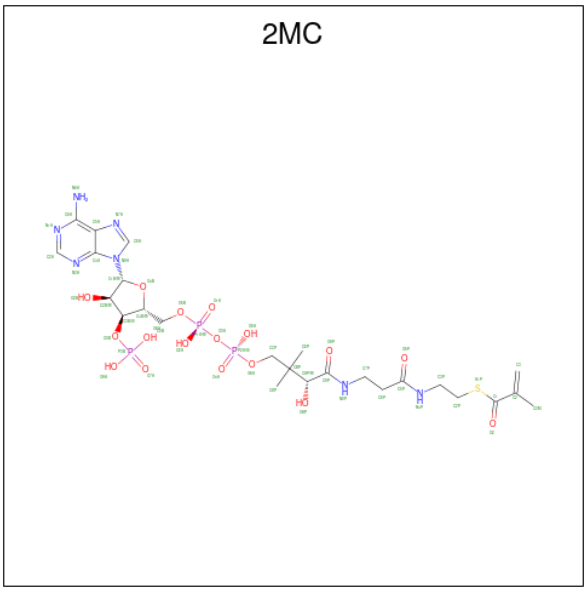
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is METHACRYLYL-COENZYME A (three-letter code: 2MC) (formula: $C_{25}H_{40}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	C	1	53	25	7	17	3	1	0	0
5	D	1	53	25	7	17	3	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	374	374	374	0	0

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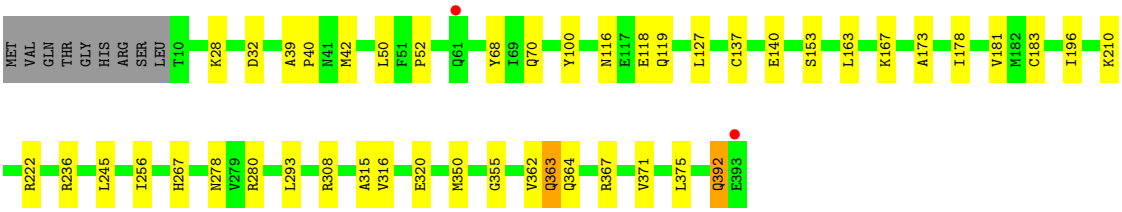
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	402	402	402	0	0
			Total	O		
6	C	352	352	352	0	0
			Total	O		
6	D	344	344	344	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

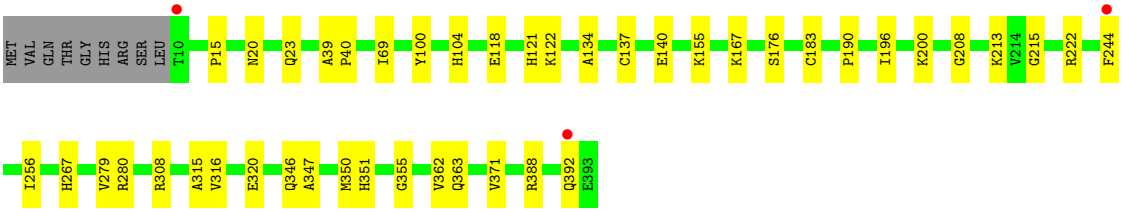
• Molecule 1: Acyl-CoA dehydrogenase family member 8, mitochondrial

Chain A:



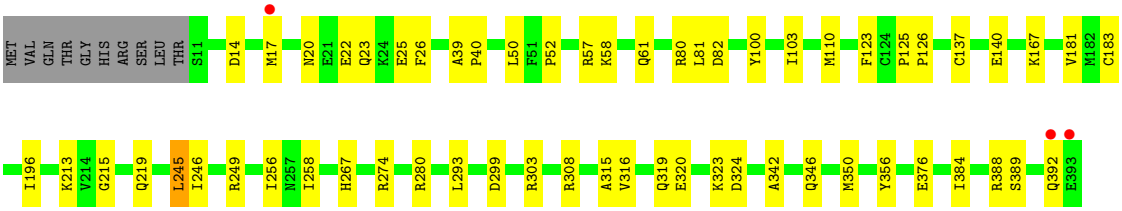
• Molecule 1: Acyl-CoA dehydrogenase family member 8, mitochondrial

Chain B:



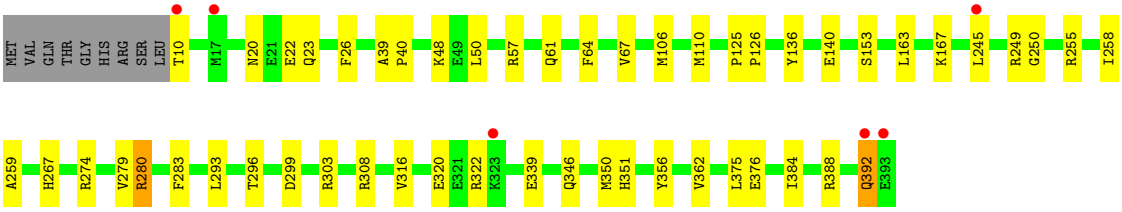
• Molecule 1: Acyl-CoA dehydrogenase family member 8, mitochondrial

Chain C:



• Molecule 1: Acyl-CoA dehydrogenase family member 8, mitochondrial

Chain D:


MET
VAL
GLN
THR
GLY
HIS
ARG
SER
LEU
T10
M17
N20
E21
E22
Q23
F26
A39
P40
K48
E49
L50
R57
Q61
F64
V67
M106
M110
P125
P126
Y136
E140
S153
L163
K167
L245
R249
G250
R255
I258
A259
H267
R274
V279
R280
F283
L293
T296
D299
R303
R308
V316
E320
E321
R322
K323
E339
Q346
M350
H351
Y356
V362
L375
E376
I384
R388
Q392
E393

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.20Å 134.34Å 189.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.77 94.82 – 1.77	Depositor EDS
% Data completeness (in resolution range)	92.7 (50.00-1.77) 92.8 (94.82-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 1.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.179 , 0.192 0.174 , 0.186	Depositor DCC
R_{free} test set	22775 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13784	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0214e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, FAD, ACY, 2MC

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	0.29	0/3015	0.55	0/4064
1	B	0.29	0/3012	0.55	0/4061
1	C	0.28	0/3029	0.54	0/4083
1	D	0.28	0/3070	0.55	0/4138
All	All	0.29	0/12126	0.55	0/16346

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TYR	Sidechain
1	B	100	TYR	Sidechain
1	C	100	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2964	0	2935	38	0
1	B	2961	0	2927	33	0
1	C	2978	0	2938	46	0
1	D	3019	0	2983	57	0
2	A	8	0	12	2	0
2	B	16	0	24	2	0
2	C	12	0	18	0	0
2	D	8	0	12	1	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	4	0	3	1	0
4	B	8	0	6	0	0
4	C	4	0	3	0	0
4	D	12	0	9	0	0
5	C	53	0	36	2	0
5	D	53	0	36	0	0
6	A	374	0	0	4	1
6	B	402	0	0	13	0
6	C	352	0	0	1	0
6	D	344	0	0	3	1
All	All	13784	0	12066	164	1

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 7.

All (164) 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:D:110[B]:MET:HE1	1:D:136:TYR:HE1	1.29	0.98
1:D:296:THR:HG21	1:D:346[A]:GLN:NE2	1.82	0.92
1:D:110[B]:MET:CE	1:D:136:TYR:HE1	1.82	0.92
1:D:258[A]:ILE:HG13	1:D:376:GLU:HG3	1.52	0.89
1:C:303:ARG:NH2	1:D:303:ARG:HH12	1.70	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:HH22	2:A:2011:EDO:H22	1.39	0.88
1:C:258:ILE:HG13	1:C:376:GLU:HG3	1.55	0.86
1:A:350:MET:HE3	6:A:9193:HOH:O	1.75	0.86
1:A:363:GLN:HE22	1:A:367:ARG:HH21	1.25	0.81
1:D:296:THR:HG21	1:D:346[A]:GLN:HE21	1.45	0.78
1:A:293:LEU:HD22	1:A:350:MET:CE	2.16	0.76
1:D:267:HIS:CD2	1:D:308:ARG:HH22	2.04	0.76
1:D:258[B]:ILE:HD12	1:D:376:GLU:HG3	1.68	0.75
1:C:303:ARG:NH2	1:D:303:ARG:NH1	2.34	0.75
1:C:267:HIS:CD2	1:C:308:ARG:HH22	2.06	0.73
1:D:267:HIS:HD2	1:D:308:ARG:HH22	1.37	0.72
1:A:267:HIS:CD2	1:A:308:ARG:HH22	2.08	0.72
1:C:303:ARG:HH21	1:D:303:ARG:HH12	1.35	0.72
1:D:110[B]:MET:HE1	1:D:136:TYR:CE1	2.19	0.72
1:C:323:LYS:HB2	1:D:10:THR:HG22	1.72	0.71
1:C:299:ASP:O	1:C:303:ARG:HG2	1.91	0.70
1:C:384:ILE:O	1:C:388:ARG:HG3	1.91	0.70
1:C:267:HIS:HD2	1:C:308:ARG:HH22	1.40	0.69
1:D:110[B]:MET:HE2	1:D:250:GLY:HA3	1.72	0.69
1:A:173:ALA:HB3	1:A:222:ARG:HG2	1.75	0.69
1:A:267:HIS:HD2	1:A:308:ARG:HH22	1.39	0.69
1:B:267:HIS:CD2	1:B:308:ARG:HH22	2.11	0.68
1:D:57:ARG:O	1:D:61:GLN:HG3	1.93	0.68
1:A:293:LEU:HD22	1:A:350:MET:HE2	1.75	0.67
1:B:190:PRO:HB3	1:B:244:PHE:CD2	2.29	0.67
1:A:28:LYS:HE2	1:A:32:ASP:OD1	1.96	0.66
1:C:342:ALA:O	1:C:346[B]:GLN:HG3	1.95	0.66
1:D:258[B]:ILE:CD1	1:D:375:LEU:CD1	2.73	0.66
1:D:258[B]:ILE:HD11	1:D:375:LEU:CD1	2.26	0.66
1:D:258[B]:ILE:HD11	1:D:375:LEU:HD11	1.78	0.66
1:D:299:ASP:OD1	6:D:9246:HOH:O	2.13	0.65
1:A:68:TYR:HB2	4:A:9005:ACY:H2	1.77	0.65
1:D:125:PRO:HB2	1:D:126:PRO:HD3	1.79	0.64
1:D:110[B]:MET:CE	1:D:136:TYR:CE1	2.74	0.62
1:B:267:HIS:HD2	1:B:308:ARG:HH22	1.47	0.61
1:B:69:ILE:HG12	6:B:9338:HOH:O	2.01	0.61
1:D:388:ARG:O	1:D:392:GLN:NE2	2.33	0.61
1:D:258[B]:ILE:CD1	1:D:375:LEU:HD12	2.31	0.60
1:C:183[A]:CYS:SG	1:C:196[A]:ILE:HD12	2.41	0.60
1:C:258:ILE:HG13	1:C:376:GLU:CG	2.32	0.59
1:B:104:HIS:HD2	1:B:134:ALA:H	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ARG:HH22	1:D:303:ARG:NH1	2.00	0.58
1:C:125:PRO:HB2	1:C:126:PRO:HD3	1.87	0.57
1:D:346[A]:GLN:NE2	1:D:350:MET:CE	2.68	0.57
1:B:362[A]:VAL:HG13	6:B:9204:HOH:O	2.04	0.56
1:B:388:ARG:O	1:B:392:GLN:HG3	2.05	0.56
1:A:236:ARG:NH2	2:A:2011:EDO:H22	2.17	0.56
1:B:316:VAL:O	1:B:320:GLU:HG3	2.05	0.56
1:B:392:GLN:HG3	6:B:9375:HOH:O	2.06	0.55
1:B:122:LYS:HD3	6:B:9287:HOH:O	2.07	0.55
1:B:256:ILE:HD13	1:B:315:ALA:HA	1.88	0.55
1:A:392:GLN:HE21	1:A:392:GLN:N	2.04	0.55
1:C:316:VAL:O	1:C:320:GLU:HG3	2.06	0.55
1:D:316:VAL:O	1:D:320:GLU:HG3	2.07	0.55
1:B:183[A]:CYS:SG	1:B:196[A]:ILE:HD12	2.46	0.54
1:A:70:GLN:HB3	6:A:9106:HOH:O	2.06	0.54
1:B:137:CYS:HB3	1:B:167:LYS:HG3	1.90	0.54
1:C:324:ASP:HB3	1:D:10:THR:HG23	1.90	0.54
1:A:293:LEU:HD22	1:A:350:MET:HE1	1.88	0.53
1:C:22:GLU:HG2	1:C:26:PHE:CZ	2.44	0.53
1:A:39:ALA:HB3	1:A:40:PRO:HD3	1.90	0.53
1:D:39:ALA:HB3	1:D:40:PRO:HD3	1.89	0.53
1:D:258[A]:ILE:HG13	1:D:376:GLU:CG	2.32	0.53
1:D:255:ARG:O	1:D:258[B]:ILE:HG22	2.10	0.52
1:D:303:ARG:HD2	1:D:339:GLU:OE1	2.09	0.52
1:D:303:ARG:CD	1:D:339:GLU:OE1	2.58	0.52
1:D:293:LEU:HD22	1:D:350:MET:SD	2.50	0.51
1:A:140:GLU:HG2	1:A:167:LYS:HD3	1.92	0.51
1:B:355:GLY:O	1:B:363:GLN:HB3	2.11	0.51
1:C:39:ALA:HB3	1:C:40:PRO:HD3	1.93	0.51
1:D:346[A]:GLN:NE2	1:D:350:MET:HE3	2.26	0.51
1:B:347:ALA:O	1:B:351:HIS:HD2	1.93	0.50
1:A:137:CYS:HB3	1:A:167:LYS:HG3	1.92	0.50
1:D:140:GLU:HG2	1:D:167:LYS:HD3	1.93	0.50
1:C:57:ARG:O	1:C:61:GLN:HG3	2.12	0.50
1:D:245:LEU:O	1:D:249:ARG:HG2	2.12	0.49
1:B:140:GLU:HG2	1:B:167:LYS:HD3	1.95	0.49
1:B:15:PRO:HG3	2:B:2006:EDO:H12	1.94	0.49
1:C:323:LYS:CB	1:D:10:THR:HG22	2.42	0.49
1:D:20:ASN:OD1	1:D:23:GLN:HG3	2.13	0.48
1:D:274:ARG:HH11	1:D:274:ARG:HG3	1.78	0.48
1:B:155:LYS:NZ	6:B:9310:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ASP:HB3	1:C:17:MET:HG2	1.94	0.48
1:C:103:ILE:HG12	5:C:400:2MC:H2M1	1.95	0.48
1:B:39:ALA:HB3	1:B:40:PRO:HD3	1.96	0.47
1:C:293:LEU:HD22	1:C:350:MET:SD	2.55	0.47
1:A:127:LEU:HD21	1:A:178[B]:ILE:HD12	1.95	0.47
1:A:116:ASN:H	1:A:119:GLN:NE2	2.12	0.47
1:C:58:LYS:HA	1:C:61:GLN:NE2	2.30	0.47
1:D:283:PHE:HA	2:D:2010:EDO:H21	1.97	0.47
1:A:316:VAL:O	1:A:320:GLU:HG3	2.16	0.46
1:C:140:GLU:HG2	1:C:167:LYS:HD3	1.96	0.46
1:D:64:PHE:HA	1:D:67:VAL:HG22	1.98	0.46
1:D:258[B]:ILE:HD12	1:D:375:LEU:CD1	2.46	0.46
1:D:362[B]:VAL:HG13	6:D:9195:HOH:O	2.14	0.46
1:B:20:ASN:OD1	1:B:23:GLN:HG3	2.16	0.46
1:C:245:LEU:N	1:C:245:LEU:CD1	2.79	0.45
1:A:116:ASN:H	1:A:119:GLN:HE21	1.63	0.45
1:A:183[A]:CYS:SG	1:A:196:ILE:HD12	2.55	0.45
1:C:103:ILE:HD11	5:C:400:2MC:H12	1.97	0.45
1:C:181:VAL:HG12	1:C:183[B]:CYS:SG	2.57	0.45
1:D:384:ILE:O	1:D:388:ARG:HG3	2.17	0.45
1:A:362[B]:VAL:HG13	6:A:9369:HOH:O	2.15	0.45
1:C:123:PHE:O	1:C:126:PRO:HD2	2.17	0.45
1:B:351:HIS:HE1	6:B:9019:HOH:O	1.99	0.44
1:B:121:HIS:HD2	6:B:9098:HOH:O	1.99	0.44
1:B:392:GLN:HB2	6:B:9378:HOH:O	2.17	0.44
1:D:22:GLU:HG2	1:D:26:PHE:CZ	2.53	0.44
1:A:181:VAL:HG12	1:A:183[B]:CYS:SG	2.58	0.44
1:C:137:CYS:HB3	1:C:167:LYS:HG3	2.00	0.44
1:C:213:LYS:HE2	1:C:215:GLY:O	2.17	0.44
1:C:20:ASN:OD1	1:C:23:GLN:HG3	2.17	0.44
1:A:256:ILE:HD13	1:A:315:ALA:HA	2.00	0.44
1:B:346:GLN:O	1:B:350:MET:HG2	2.17	0.44
1:B:392:GLN:CG	6:B:9375:HOH:O	2.65	0.44
1:C:346[B]:GLN:O	1:C:350:MET:HG2	2.17	0.44
1:D:48:LYS:HB2	1:D:50:LEU:HG	1.99	0.43
1:A:245:LEU:C	1:A:245:LEU:HD13	2.39	0.43
1:A:363:GLN:HE22	1:A:367:ARG:NH2	2.05	0.43
1:C:389:SER:O	1:C:392:GLN:HG2	2.18	0.43
1:C:17:MET:HE2	1:D:322:ARG:NE	2.33	0.43
1:D:351:HIS:CE1	1:D:362[B]:VAL:HG11	2.54	0.43
2:B:2003:EDO:H21	6:D:9255:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258[B]:ILE:HG23	1:D:259:ALA:N	2.34	0.43
1:D:388:ARG:O	1:D:392:GLN:HB2	2.18	0.43
1:D:106:MET:O	1:D:110[B]:MET:HG3	2.19	0.43
1:A:173:ALA:HB3	1:A:222:ARG:CG	2.46	0.42
1:A:392:GLN:HE21	1:A:392:GLN:CA	2.31	0.42
1:B:213:LYS:HE2	1:B:215:GLY:O	2.19	0.42
1:C:50:LEU:O	1:C:52:PRO:HD3	2.19	0.42
1:B:155:LYS:HE2	6:B:9310:HOH:O	2.17	0.42
1:A:173:ALA:O	1:A:222:ARG:HD3	2.20	0.42
1:A:50:LEU:O	1:A:52:PRO:HD3	2.19	0.42
1:B:279:VAL:HG23	6:B:9015:HOH:O	2.19	0.42
1:A:355:GLY:O	1:A:363:GLN:HB3	2.20	0.42
1:A:210:LYS:HD2	6:A:9213:HOH:O	2.20	0.42
1:C:80:ARG:HG2	1:C:319[A]:GLN:OE1	2.19	0.42
1:D:346[A]:GLN:HE22	1:D:350:MET:CE	2.31	0.42
1:B:118:GLU:HG3	6:B:9104:HOH:O	2.20	0.42
1:B:176:SER:O	1:B:200:LYS:HE3	2.19	0.42
1:B:208:GLY:O	1:B:222:ARG:NH1	2.50	0.41
1:C:23:GLN:HG2	1:C:82:ASP:OD1	2.20	0.41
1:C:256:ILE:HD13	1:C:315:ALA:HA	2.01	0.41
1:C:274:ARG:HH11	1:C:274:ARG:HG3	1.85	0.41
1:B:371:VAL:HB	1:D:356:TYR:CZ	2.55	0.41
1:D:153:SER:O	1:D:163:LEU:HA	2.21	0.41
1:D:279[A]:VAL:HG13	1:D:280:ARG:N	2.36	0.41
1:D:392:GLN:HE21	1:D:392:GLN:N	2.19	0.41
1:A:153:SER:O	1:A:163:LEU:HA	2.20	0.41
1:C:249:ARG:HD2	6:C:9149:HOH:O	2.21	0.41
1:C:110:MET:CE	1:C:246:ILE:HG22	2.50	0.41
1:A:371:VAL:HB	1:C:356:TYR:CE1	2.56	0.41
1:C:346[A]:GLN:O	1:C:350:MET:HG2	2.20	0.41
1:A:371:VAL:HB	1:C:356:TYR:CZ	2.56	0.40
1:C:23:GLN:HE22	1:C:81:LEU:HD23	1.86	0.40
1:D:346[B]:GLN:O	1:D:350:MET:HG2	2.20	0.40
1:A:42:MET:HG2	1:A:364:GLN:NE2	2.36	0.40
1:A:278:ASN:HD22	1:A:278:ASN:HA	1.71	0.40
1:B:155:LYS:CE	6:B:9310:HOH:O	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9015:HOH:O	6:D:9087:HOH:O[3_545]	2.14	0.06

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	389/393 (99%)	384 (99%)	5 (1%)	0	100	100
1	B	389/393 (99%)	383 (98%)	6 (2%)	0	100	100
1	C	391/393 (100%)	386 (99%)	5 (1%)	0	100	100
1	D	396/393 (101%)	391 (99%)	5 (1%)	0	100	100
All	All	1565/1572 (100%)	1544 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/317 (100%)	311 (98%)	5 (2%)	62	51
1	B	316/317 (100%)	315 (100%)	1 (0%)	92	90
1	C	318/317 (100%)	314 (99%)	4 (1%)	69	59
1	D	323/317 (102%)	321 (99%)	2 (1%)	86	82
All	All	1273/1268 (100%)	1261 (99%)	12 (1%)	76	72

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

Mol	Chain	Res	Type
1	A	118	GLU
1	A	280	ARG
1	A	363	GLN
1	A	375	LEU
1	A	392	GLN
1	B	280	ARG
1	C	25	GLU
1	C	219	GLN
1	C	245	LEU
1	C	280	ARG
1	D	280	ARG
1	D	392	GLN

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

Mol	Chain	Res	Type
1	A	27	GLN
1	A	61	GLN
1	A	119	GLN
1	A	267	HIS
1	A	276	HIS
1	A	278	ASN
1	A	294	GLN
1	A	363	GLN
1	A	364	GLN
1	A	392	GLN
1	B	27	GLN
1	B	104	HIS
1	B	267	HIS
1	B	278	ASN
1	B	294	GLN
1	B	313	ASN
1	B	351	HIS
1	B	364	GLN
1	C	27	GLN
1	C	61	GLN
1	C	219	GLN
1	C	267	HIS
1	C	278	ASN
1	C	294	GLN
1	C	364	GLN
1	D	27	GLN
1	D	61	GLN

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Mol	Chain	Res	Type
1	D	267	HIS
1	D	278	ASN
1	D	294	GLN
1	D	364	GLN
1	D	392	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)

24 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	ACY	D	9003	-	3,3,3	1.45	0	3,3,3	1.39	0
3	FAD	D	399	-	53,58,58	1.47	7 (13%)	68,89,89	1.13	7 (10%)
2	EDO	C	2008	-	3,3,3	0.54	0	2,2,2	0.43	0
2	EDO	B	2006	-	3,3,3	0.52	0	2,2,2	0.42	0
2	EDO	D	2010	-	3,3,3	0.52	0	2,2,2	0.43	0
2	EDO	A	2011	-	3,3,3	0.52	0	2,2,2	0.42	0
2	EDO	A	2001	-	3,3,3	0.55	0	2,2,2	0.41	0
4	ACY	D	9002	-	3,3,3	1.46	0	3,3,3	1.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	C	399	-	53,58,58	1.51	8 (15%)	68,89,89	1.14	7 (10%)
3	FAD	A	399	-	53,58,58	1.48	7 (13%)	68,89,89	1.14	5 (7%)
2	EDO	C	2002	-	3,3,3	0.55	0	2,2,2	0.42	0
4	ACY	D	9007	-	3,3,3	1.46	0	3,3,3	1.36	0
2	EDO	D	2009	-	3,3,3	0.53	0	2,2,2	0.42	0
4	ACY	C	9004	-	3,3,3	1.45	0	3,3,3	1.37	0
4	ACY	B	9006	-	3,3,3	1.46	0	3,3,3	1.38	0
5	2MC	C	400	-	47,55,55	1.93	10 (21%)	55,82,82	1.70	8 (14%)
2	EDO	B	2007	-	3,3,3	0.52	0	2,2,2	0.41	0
4	ACY	A	9005	-	3,3,3	1.45	0	3,3,3	1.37	0
2	EDO	B	2003	-	3,3,3	0.52	0	2,2,2	0.42	0
5	2MC	D	400	-	47,55,55	1.91	10 (21%)	55,82,82	1.68	7 (12%)
2	EDO	B	2004	-	3,3,3	0.53	0	2,2,2	0.42	0
3	FAD	B	399	-	53,58,58	1.50	7 (13%)	68,89,89	1.14	5 (7%)
2	EDO	C	2005	-	3,3,3	0.54	0	2,2,2	0.43	0
4	ACY	B	9001	-	3,3,3	1.43	0	3,3,3	1.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2MC	C	400	-	-	5/48/71/71	0/3/3/3
3	FAD	A	399	-	-	1/30/50/50	0/6/6/6
2	EDO	C	2002	-	-	1/1/1/1	-
2	EDO	B	2006	-	-	1/1/1/1	-
2	EDO	D	2010	-	-	0/1/1/1	-
3	FAD	C	399	-	-	0/30/50/50	0/6/6/6
2	EDO	D	2009	-	-	0/1/1/1	-
2	EDO	B	2007	-	-	0/1/1/1	-
3	FAD	D	399	-	-	0/30/50/50	0/6/6/6
2	EDO	B	2003	-	-	1/1/1/1	-
5	2MC	D	400	-	-	4/48/71/71	0/3/3/3
2	EDO	A	2011	-	-	1/1/1/1	-
2	EDO	A	2001	-	-	1/1/1/1	-
2	EDO	B	2004	-	-	0/1/1/1	-
3	FAD	B	399	-	-	1/30/50/50	0/6/6/6
2	EDO	C	2005	-	-	1/1/1/1	-
2	EDO	C	2008	-	-	1/1/1/1	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	400	2MC	C4A-N3A	6.48	1.44	1.35
5	C	400	2MC	C4A-N3A	6.41	1.44	1.35
3	A	399	FAD	C4X-N5	6.04	1.42	1.30
3	B	399	FAD	C4X-N5	6.01	1.42	1.30
3	C	399	FAD	C4X-N5	5.84	1.42	1.30
3	D	399	FAD	C4X-N5	5.71	1.41	1.30
5	C	400	2MC	O4B-C1B	4.81	1.47	1.41
5	D	400	2MC	O4B-C1B	4.68	1.47	1.41
5	C	400	2MC	C2A-N3A	4.02	1.38	1.32
5	D	400	2MC	C2A-N3A	3.94	1.38	1.32
3	C	399	FAD	C9A-C5X	3.67	1.47	1.41
3	D	399	FAD	C9A-C5X	3.66	1.47	1.41
3	B	399	FAD	C9A-C5X	3.57	1.47	1.41
5	C	400	2MC	C9P-N8P	3.51	1.41	1.33
5	D	400	2MC	OAP-CAP	3.48	1.48	1.42
3	A	399	FAD	C9A-C5X	3.46	1.47	1.41
5	C	400	2MC	OAP-CAP	3.40	1.48	1.42
5	D	400	2MC	C9P-N8P	3.32	1.40	1.33
5	D	400	2MC	C1-C2	3.04	1.55	1.46
5	C	400	2MC	C1-C2	2.97	1.54	1.46
3	C	399	FAD	C9A-N10	2.97	1.46	1.41
3	A	399	FAD	C9A-N10	2.81	1.46	1.41
3	B	399	FAD	C9A-N10	2.77	1.46	1.41
3	C	399	FAD	C10-N1	2.62	1.38	1.33
3	D	399	FAD	C9A-N10	2.59	1.45	1.41
3	B	399	FAD	C6-C7	2.57	1.43	1.39
3	C	399	FAD	C6-C7	2.57	1.43	1.39
5	C	400	2MC	C5P-N4P	2.55	1.39	1.33
5	C	400	2MC	C2A-N1A	2.55	1.38	1.33
5	D	400	2MC	C5P-N4P	2.50	1.39	1.33
5	D	400	2MC	C2A-N1A	2.50	1.38	1.33
3	D	399	FAD	C10-N1	2.47	1.38	1.33
3	B	399	FAD	C10-N1	2.46	1.38	1.33
3	D	399	FAD	C6-C7	2.44	1.43	1.39
3	A	399	FAD	C10-N1	2.40	1.38	1.33
5	C	400	2MC	P3B-O3B	2.34	1.63	1.59
3	A	399	FAD	C6-C7	2.34	1.43	1.39
3	D	399	FAD	C2A-N3A	2.26	1.35	1.32
3	C	399	FAD	C9-C9A	2.24	1.43	1.39
5	C	400	2MC	C8A-N7A	-2.23	1.30	1.34
3	C	399	FAD	C2A-N3A	2.22	1.35	1.32
3	C	399	FAD	C10-N10	2.22	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	400	2MC	C8A-N7A	-2.19	1.30	1.34
5	D	400	2MC	P3B-O3B	2.13	1.63	1.59
3	B	399	FAD	C2A-N3A	2.12	1.35	1.32
3	B	399	FAD	C8A-N7A	-2.10	1.30	1.34
3	A	399	FAD	C9-C9A	2.06	1.43	1.39
3	A	399	FAD	C2A-N3A	2.02	1.35	1.32
3	D	399	FAD	C8A-N7A	-2.01	1.31	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	400	2MC	C2P-S1P-C1	8.59	110.59	99.80
5	D	400	2MC	C2P-S1P-C1	8.15	110.04	99.80
5	D	400	2MC	CEP-CBP-CAP	3.17	114.31	108.82
5	C	400	2MC	CEP-CBP-CAP	3.16	114.31	108.82
3	B	399	FAD	O5'-C5'-C4'	3.13	117.73	109.36
3	A	399	FAD	O5'-C5'-C4'	3.05	117.51	109.36
3	D	399	FAD	O5'-C5'-C4'	2.89	117.09	109.36
3	B	399	FAD	C1'-N10-C9A	-2.78	115.88	120.51
3	C	399	FAD	O5'-C5'-C4'	2.77	116.76	109.36
3	C	399	FAD	C1'-N10-C9A	-2.67	116.06	120.51
5	D	400	2MC	C6P-C7P-N8P	-2.62	106.60	111.90
3	A	399	FAD	C1'-N10-C9A	-2.61	116.15	120.51
5	C	400	2MC	C6P-C7P-N8P	-2.55	106.74	111.90
3	D	399	FAD	C1'-N10-C9A	-2.53	116.29	120.51
3	A	399	FAD	C10-N1-C2	2.51	121.93	116.90
3	B	399	FAD	C10-N1-C2	2.40	121.69	116.90
3	D	399	FAD	C10-N1-C2	2.38	121.66	116.90
3	D	399	FAD	P-O3P-PA	-2.34	124.79	132.83
3	C	399	FAD	C10-N1-C2	2.34	121.58	116.90
3	C	399	FAD	P-O3P-PA	-2.33	124.84	132.83
5	C	400	2MC	O3B-P3B-O7A	-2.26	100.66	109.39
5	C	400	2MC	O9A-P3B-O8A	2.26	116.26	107.64
5	D	400	2MC	O9A-P3B-O8A	2.23	116.15	107.64
5	D	400	2MC	O3B-P3B-O7A	-2.21	100.85	109.39
5	D	400	2MC	C3P-N4P-C5P	-2.16	118.82	122.84
3	C	399	FAD	C4X-C10-N1	-2.16	119.72	124.73
5	C	400	2MC	C3P-N4P-C5P	-2.15	118.84	122.84
3	A	399	FAD	P-O3P-PA	-2.13	125.50	132.83
3	C	399	FAD	C9-C9A-N10	2.11	124.69	121.84
3	D	399	FAD	C4X-C10-N1	-2.11	119.84	124.73
3	B	399	FAD	P-O3P-PA	-2.10	125.64	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	399	FAD	C4X-C10-N1	-2.09	119.89	124.73
5	C	400	2MC	C6P-C5P-N4P	-2.07	112.94	116.42
3	A	399	FAD	C4X-C10-N1	-2.06	119.94	124.73
5	D	400	2MC	C6P-C5P-N4P	-2.03	113.00	116.42
3	C	399	FAD	C5X-C9A-N10	-2.03	115.86	117.95
5	C	400	2MC	O6A-CCP-CBP	2.02	113.80	110.55
3	D	399	FAD	C5X-C9A-N10	-2.02	115.87	117.95
3	D	399	FAD	C9-C9A-N10	2.00	124.55	121.84

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2011	EDO	O1-C1-C2-O2
2	C	2002	EDO	O1-C1-C2-O2
2	C	2005	EDO	O1-C1-C2-O2
2	C	2008	EDO	O1-C1-C2-O2
2	B	2003	EDO	O1-C1-C2-O2
2	B	2006	EDO	O1-C1-C2-O2
5	C	400	2MC	P1A-O3A-P2A-O4A
5	D	400	2MC	P1A-O3A-P2A-O4A
5	D	400	2MC	N8P-C9P-CAP-OAP
5	C	400	2MC	C5P-C6P-C7P-N8P
5	D	400	2MC	C5P-C6P-C7P-N8P
3	B	399	FAD	C3'-C4'-C5'-O5'
5	C	400	2MC	O9P-C9P-CAP-OAP
5	D	400	2MC	O9P-C9P-CAP-OAP
5	C	400	2MC	N8P-C9P-CAP-OAP
5	C	400	2MC	P1A-O3A-P2A-O5A
3	A	399	FAD	C3'-C4'-C5'-O5'
2	A	2001	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2006	EDO	1	0
2	D	2010	EDO	1	0
2	A	2011	EDO	2	0
5	C	400	2MC	2	0
4	A	9005	ACY	1	0

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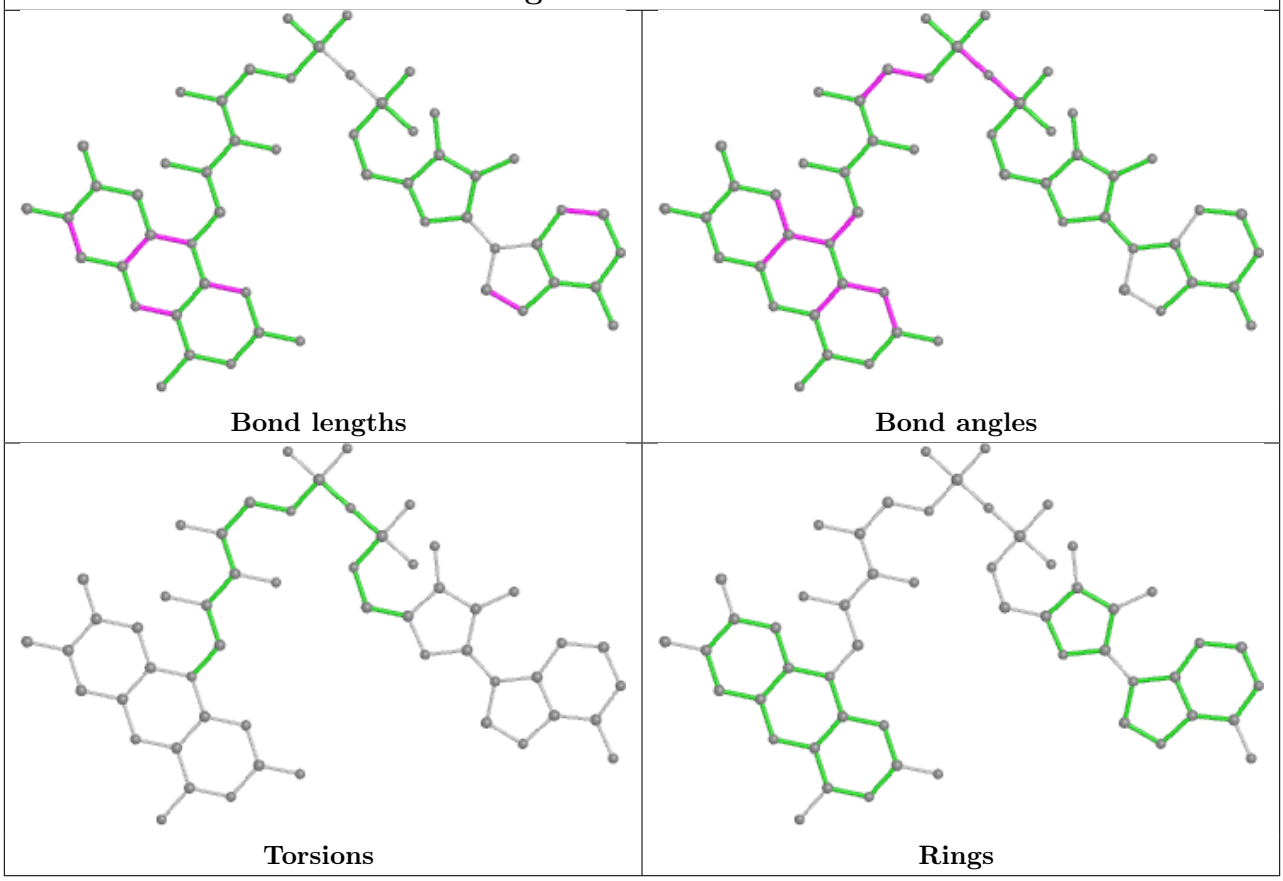
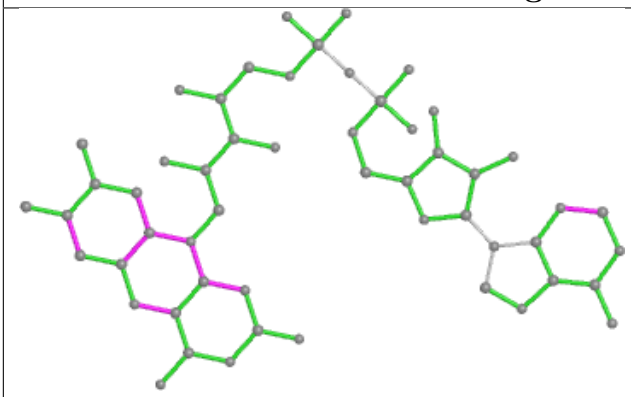
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2003	EDO	1	0

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

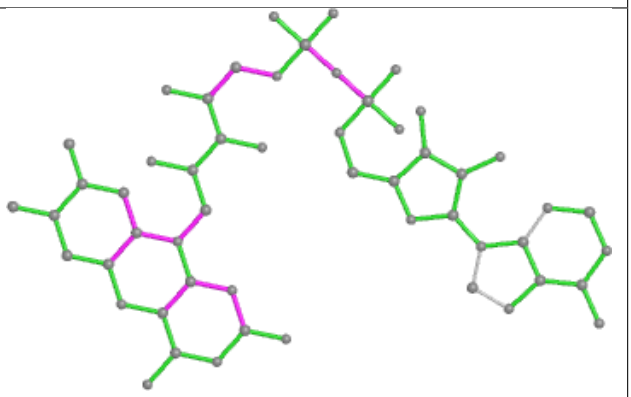
Ligand FAD D 399



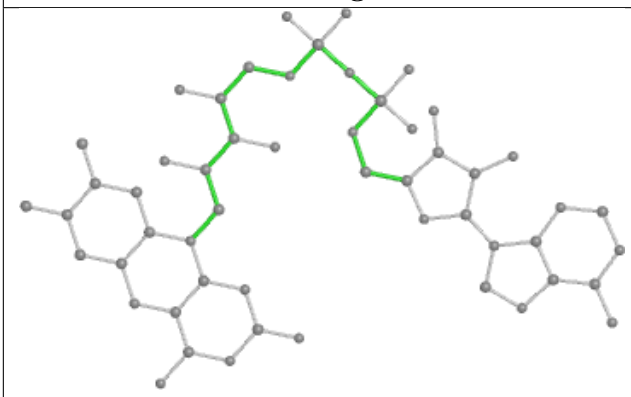
Ligand FAD C 399



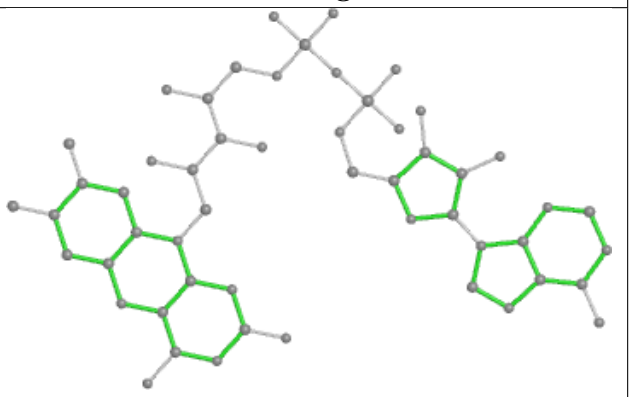
Bond lengths



Bond angles

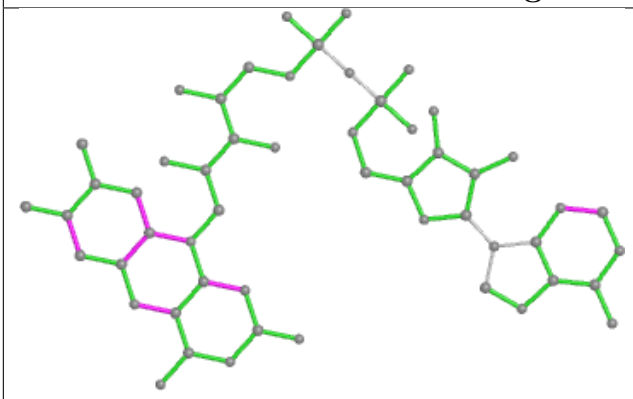


Torsions

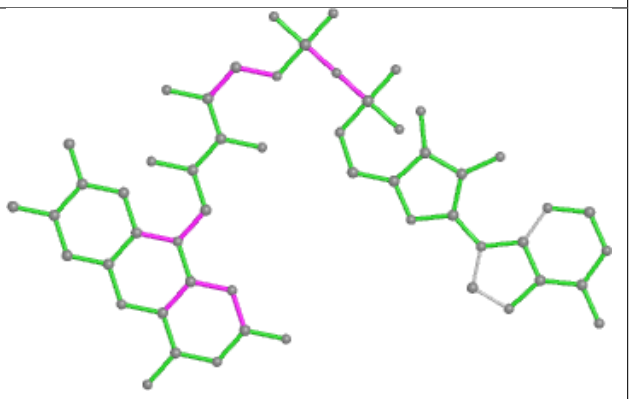


Rings

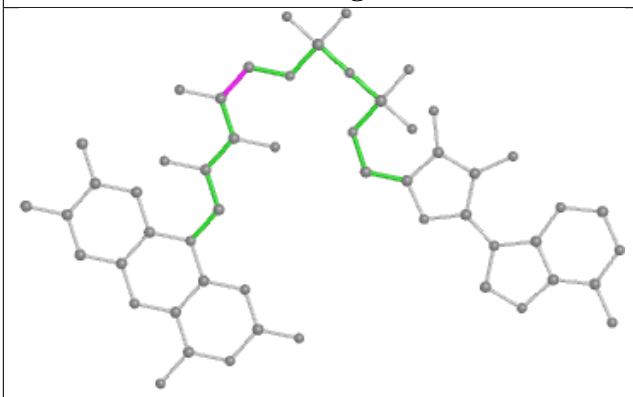
Ligand FAD A 399



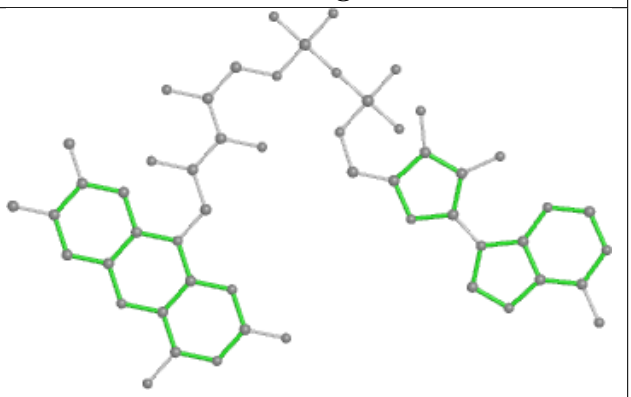
Bond lengths



Bond angles

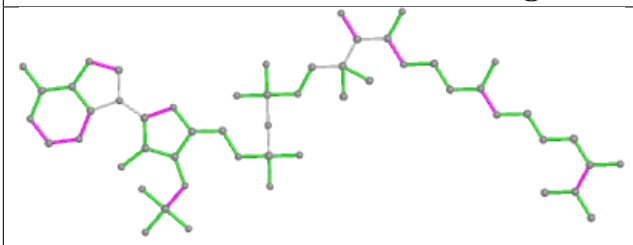


Torsions

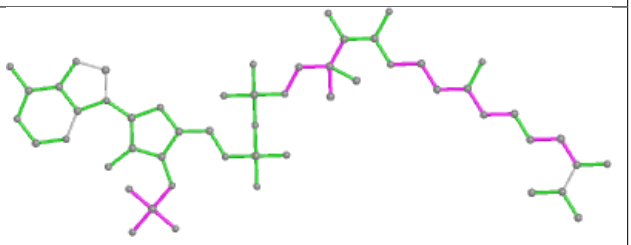


Rings

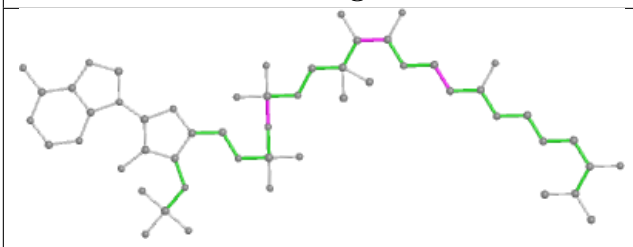
Ligand 2MC C 400



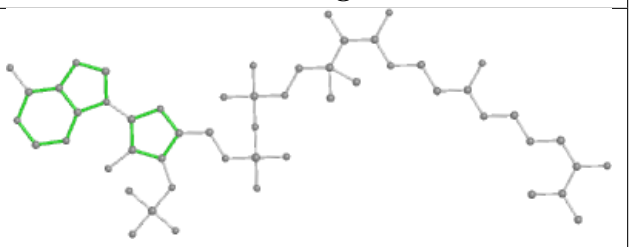
Bond lengths



Bond angles

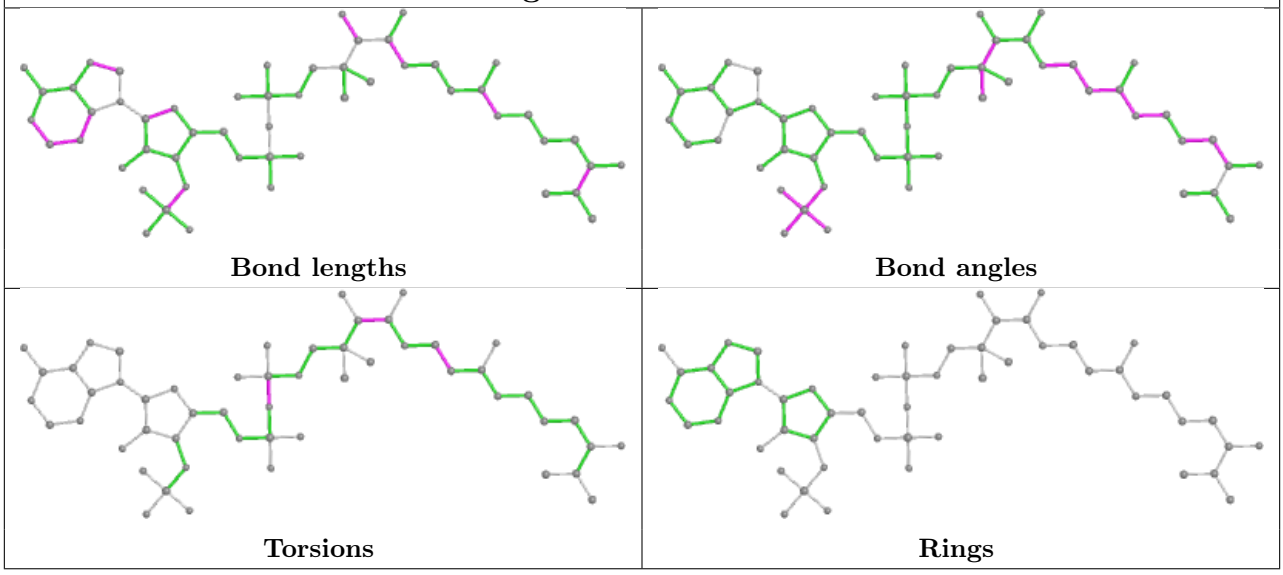


Torsions

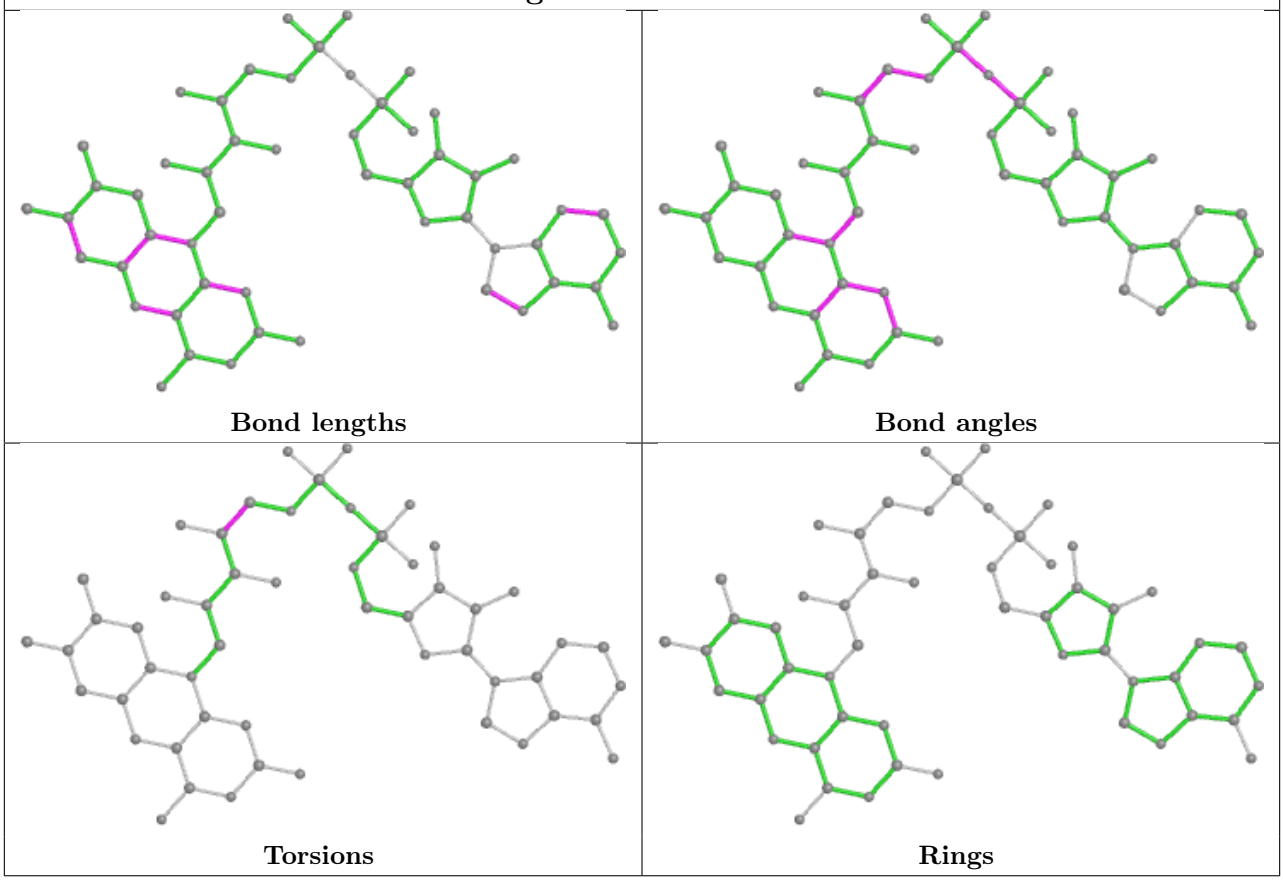


Rings

Ligand 2MC D 400



Ligand FAD B 399



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	384/393 (97%)	0.02	2 (0%)	91	91	9, 17, 28, 45	0
1	B	384/393 (97%)	-0.04	3 (0%)	86	86	9, 16, 26, 42	0
1	C	383/393 (97%)	0.01	3 (0%)	86	86	10, 18, 29, 56	0
1	D	384/393 (97%)	0.02	6 (1%)	72	72	10, 17, 29, 52	0
All	All	1535/1572 (97%)	0.00	14 (0%)	84	84	9, 17, 28, 56	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	THR	4.5
1	D	393	GLU	3.6
1	C	393	GLU	3.4
1	C	17	MET	3.0
1	C	392	GLN	2.8
1	D	392	GLN	2.7
1	B	10	THR	2.7
1	D	17	MET	2.5
1	D	323	LYS	2.4
1	B	244	PHE	2.3
1	A	393	GLU	2.2
1	A	61	GLN	2.2
1	D	245	LEU	2.2
1	B	392	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

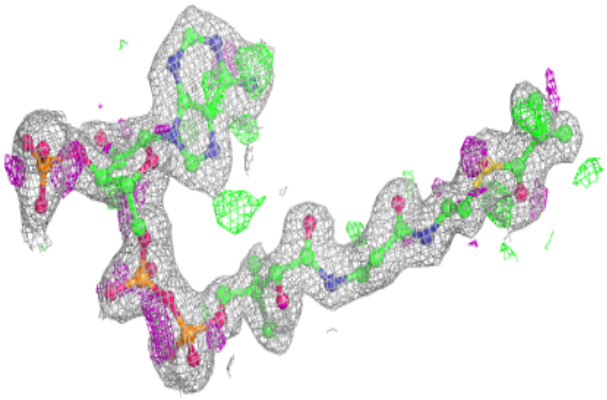
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

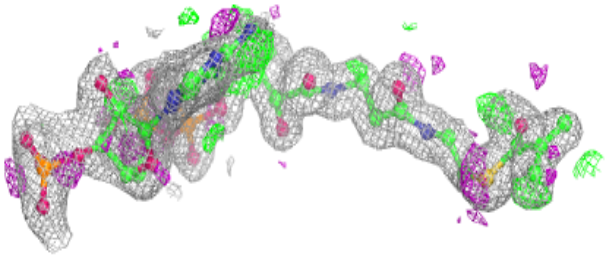
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACY	D	9007	4/4	0.41	0.32	50,51,51,51	0
4	ACY	A	9005	4/4	0.54	0.34	49,50,50,51	0
4	ACY	C	9004	4/4	0.56	0.33	52,52,53,53	0
2	EDO	D	2010	4/4	0.73	0.24	49,49,49,50	0
4	ACY	D	9002	4/4	0.74	0.16	52,53,53,53	0
2	EDO	C	2005	4/4	0.75	0.20	58,58,58,59	0
4	ACY	B	9006	4/4	0.78	0.22	61,62,62,62	0
4	ACY	B	9001	4/4	0.78	0.18	47,47,48,48	0
2	EDO	B	2007	4/4	0.79	0.20	46,47,47,47	0
4	ACY	D	9003	4/4	0.80	0.20	50,50,50,51	0
2	EDO	B	2003	4/4	0.82	0.20	40,41,41,42	0
2	EDO	A	2011	4/4	0.83	0.16	41,41,41,44	0
2	EDO	A	2001	4/4	0.84	0.15	36,37,38,40	0
2	EDO	B	2004	4/4	0.84	0.19	41,41,42,42	0
2	EDO	C	2002	4/4	0.85	0.11	45,45,45,46	0
2	EDO	D	2009	4/4	0.86	0.12	47,48,48,48	0
2	EDO	B	2006	4/4	0.88	0.13	38,38,38,40	0
5	2MC	C	400	53/53	0.90	0.15	21,37,50,51	0
2	EDO	C	2008	4/4	0.91	0.14	46,46,47,47	0
5	2MC	D	400	53/53	0.91	0.13	22,34,52,53	0
3	FAD	A	399	53/53	0.97	0.10	11,13,15,19	0
3	FAD	B	399	53/53	0.97	0.10	11,12,15,18	0
3	FAD	D	399	53/53	0.97	0.10	10,12,15,16	0
3	FAD	C	399	53/53	0.98	0.10	10,12,14,16	0

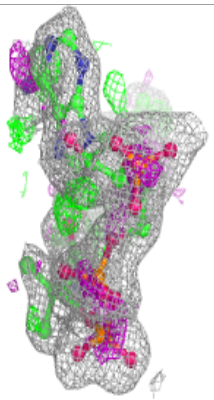
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2MC 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)

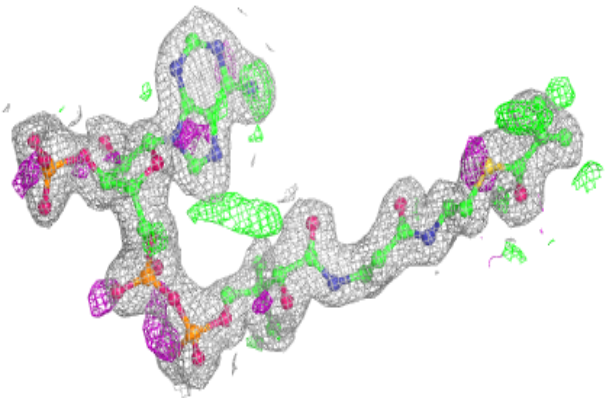


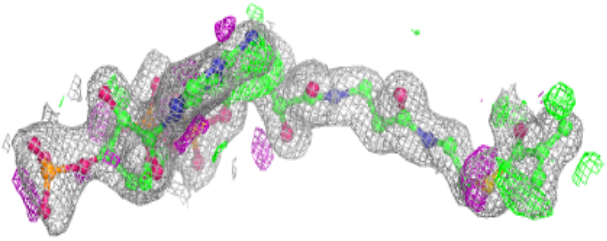


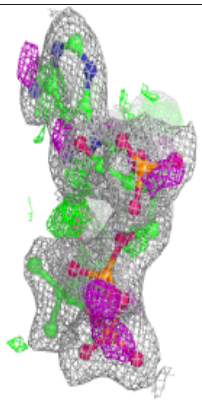


Electron density around 2MC D 400:

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

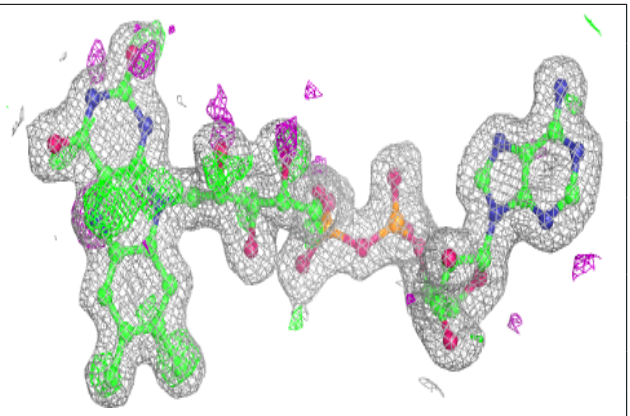


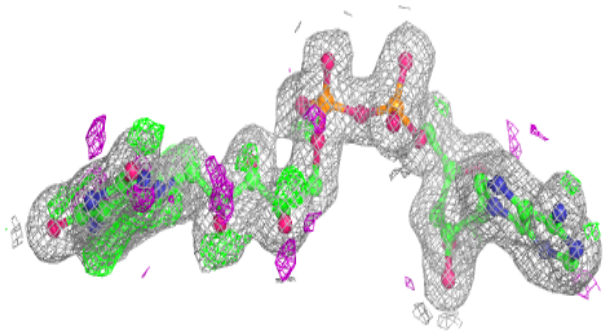


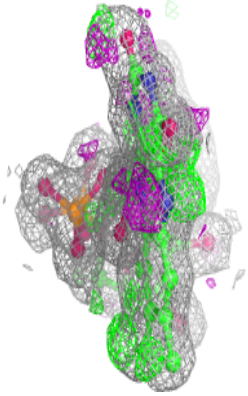


Electron density around FAD A 399:

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

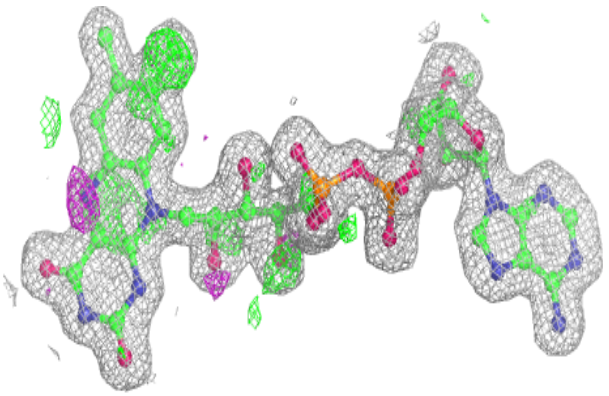


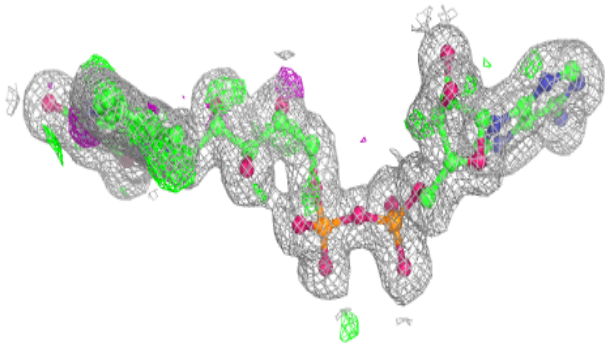


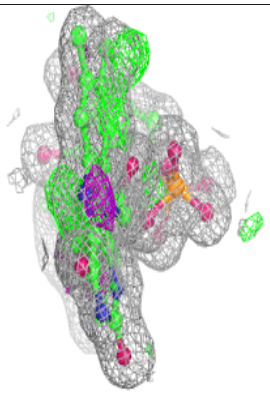


Electron density around FAD B 399:

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

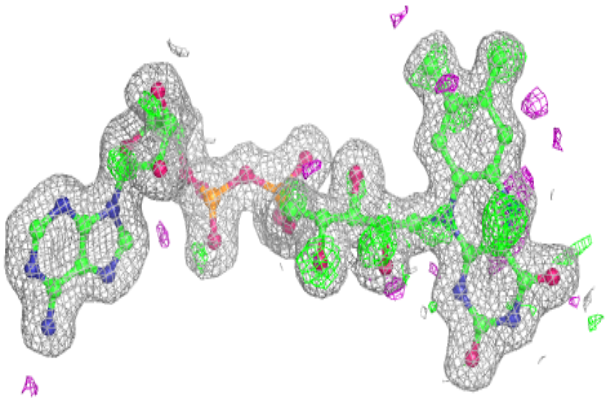


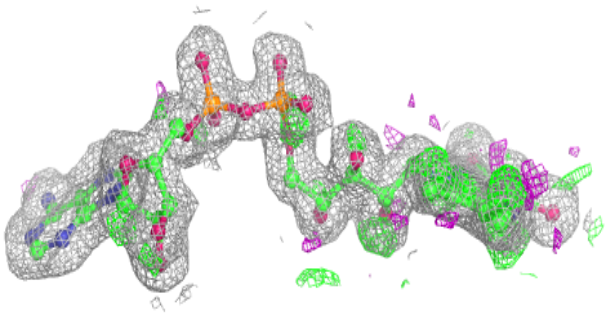


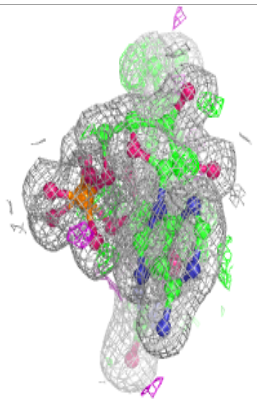


Electron density around FAD D 399:

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

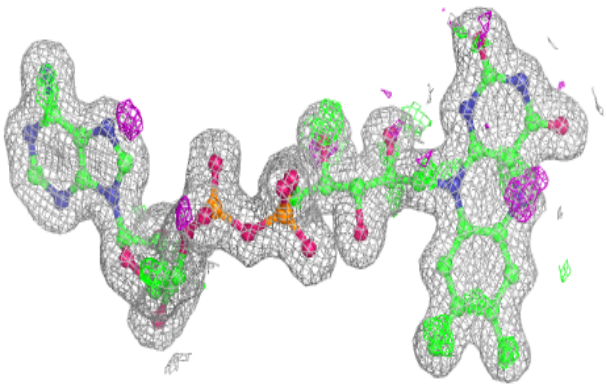


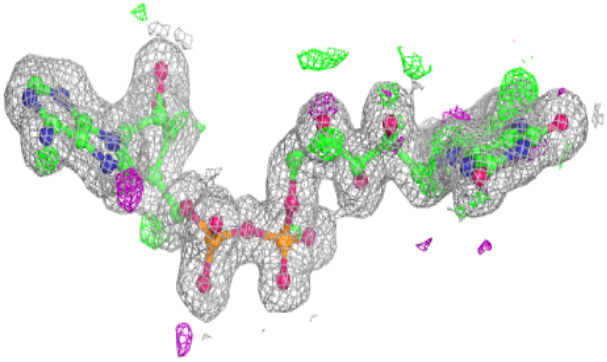


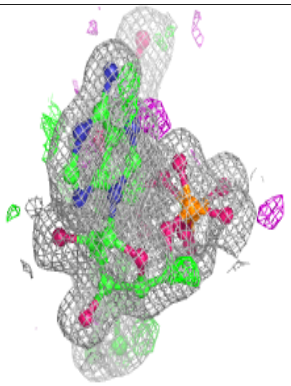


Electron density around FAD C 399:

$2mF_o$-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.