Full wwPDB EM Validation Report (i)

Aug 4, 2026 – 10:47 PM EDT

PDB ID	:	7KOE / pdb_00007koe
EMDB ID	:	EMD-22973
Title	:	Electron bifurcating flavoprotein Fix/EtfABCX
Authors	:	Feng, X.; Li, H.
Deposited on	:	2020-11-08
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

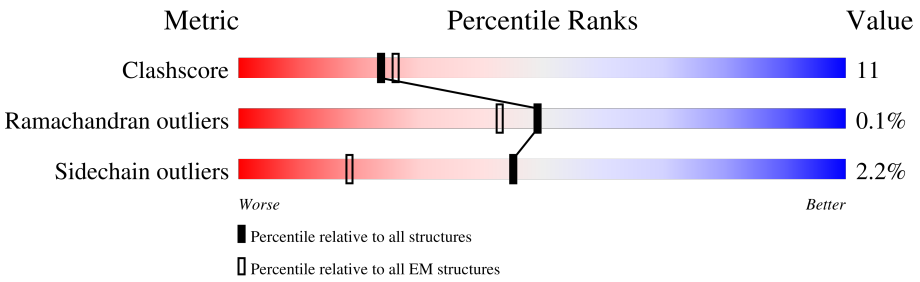
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

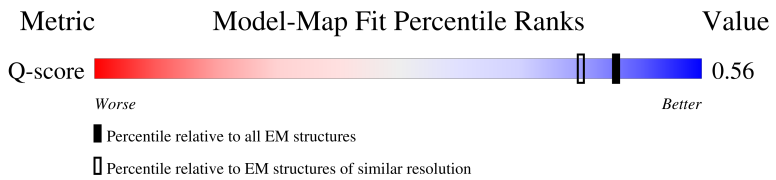
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	296	69% 22% • 5%
1	E	296	70% 22% • 5%
2	B	338	80% 19% •
2	F	338	80% 19% •

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Mol	Chain	Length	Quality of chain
3	C	438	79% 20%
3	G	438	79% 21%
4	D	92	78% 21%
4	H	92	77% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MQ7	C	502	-	X	-	-
6	MQ7	G	502	-	X	-	-
7	SF4	D	601	-	-	X	-
7	SF4	D	602	-	-	X	-
7	SF4	H	601	-	-	X	-
7	SF4	H	602	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18348 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Electron transfer flavoprotein, beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	282	2195	1401	380	410	4	0	0
1	E	282	2195	1401	380	410	4	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q9X1L6
A	-9	ALA	-	expression tag	UNP Q9X1L6
A	-8	HIS	-	expression tag	UNP Q9X1L6
A	-7	HIS	-	expression tag	UNP Q9X1L6
A	-6	HIS	-	expression tag	UNP Q9X1L6
A	-5	HIS	-	expression tag	UNP Q9X1L6
A	-4	HIS	-	expression tag	UNP Q9X1L6
A	-3	HIS	-	expression tag	UNP Q9X1L6
A	-2	HIS	-	expression tag	UNP Q9X1L6
A	-1	HIS	-	expression tag	UNP Q9X1L6
A	0	HIS	-	expression tag	UNP Q9X1L6
A	1	ALA	-	expression tag	UNP Q9X1L6
E	-10	MET	-	expression tag	UNP Q9X1L6
E	-9	ALA	-	expression tag	UNP Q9X1L6
E	-8	HIS	-	expression tag	UNP Q9X1L6
E	-7	HIS	-	expression tag	UNP Q9X1L6
E	-6	HIS	-	expression tag	UNP Q9X1L6
E	-5	HIS	-	expression tag	UNP Q9X1L6
E	-4	HIS	-	expression tag	UNP Q9X1L6
E	-3	HIS	-	expression tag	UNP Q9X1L6
E	-2	HIS	-	expression tag	UNP Q9X1L6
E	-1	HIS	-	expression tag	UNP Q9X1L6
E	0	HIS	-	expression tag	UNP Q9X1L6
E	1	ALA	-	expression tag	UNP Q9X1L6

- Molecule 2 is a protein called Electron transfer flavoprotein, alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	336	2565	1643	433	478	11	0	0
2	F	336	2565	1643	433	478	11	0	0

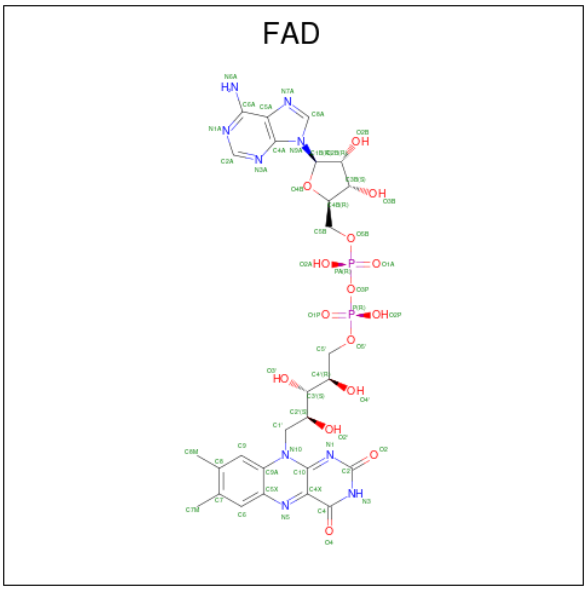
- Molecule 3 is a protein called Electron transfer flavoprotein-quinone oxidoreductase FixC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	438	3445	2207	593	628	17	0	0
3	G	438	3445	2207	593	628	17	0	0

- Molecule 4 is a protein called Ferredoxin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	92	746	467	125	143	11	0	0
4	H	92	746	467	125	143	11	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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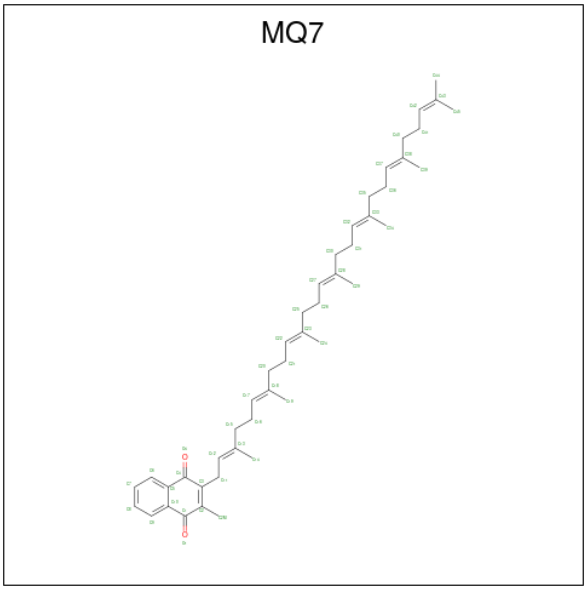
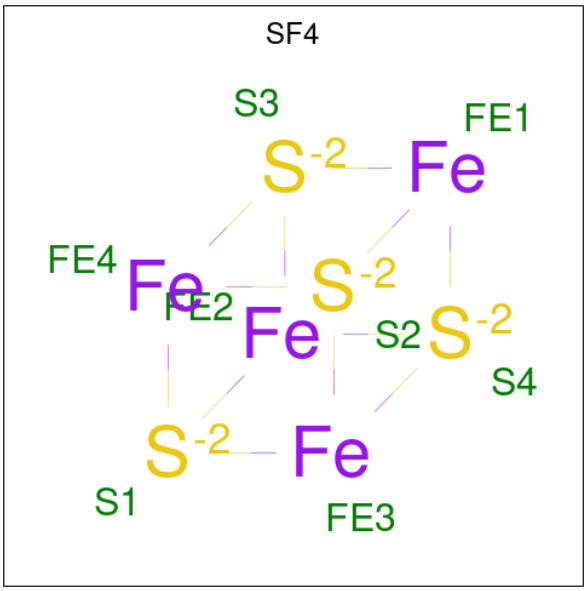
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	B	1	53	27	9	15	2	0
5	C	1	53	27	9	15	2	0
5	E	1	53	27	9	15	2	0
5	F	1	53	27	9	15	2	0
5	G	1	53	27	9	15	2	0

- Molecule 6 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	C	1	48	46	2	0
6	G	1	48	46	2	0

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



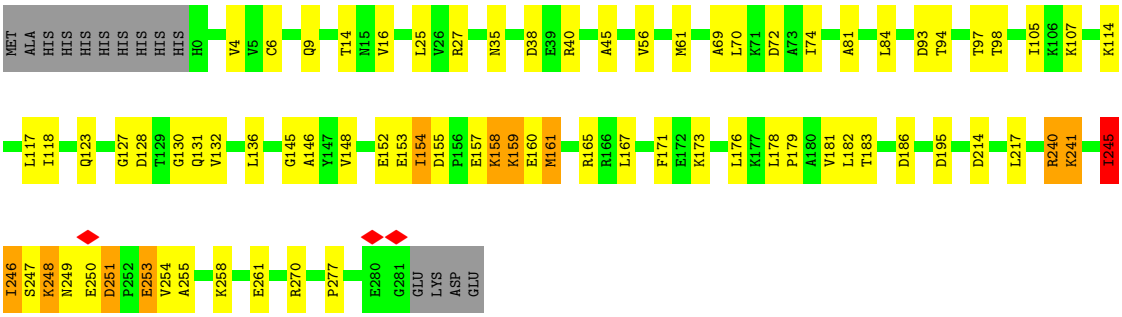
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
7	D	1	8	4	4	0
			Total	Fe	S	
7	D	1	8	4	4	0
			Total	Fe	S	
7	H	1	8	4	4	0
			Total	Fe	S	
7	H	1	8	4	4	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

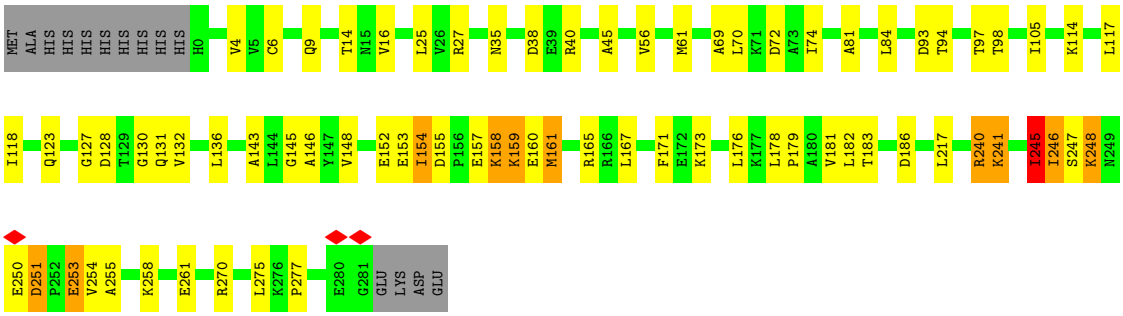
• Molecule 1: Electron transfer flavoprotein, beta subunit

Chain A:



• Molecule 1: Electron transfer flavoprotein, beta subunit

Chain E:

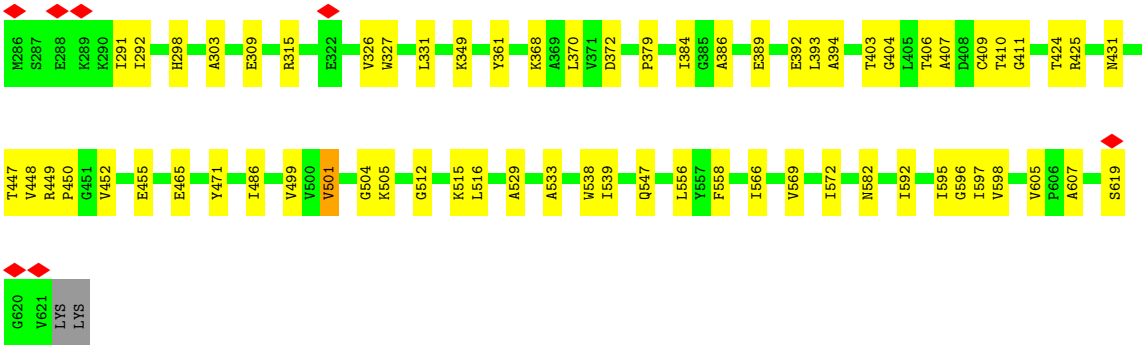


• Molecule 2: Electron transfer flavoprotein, alpha subunit

Chain B:

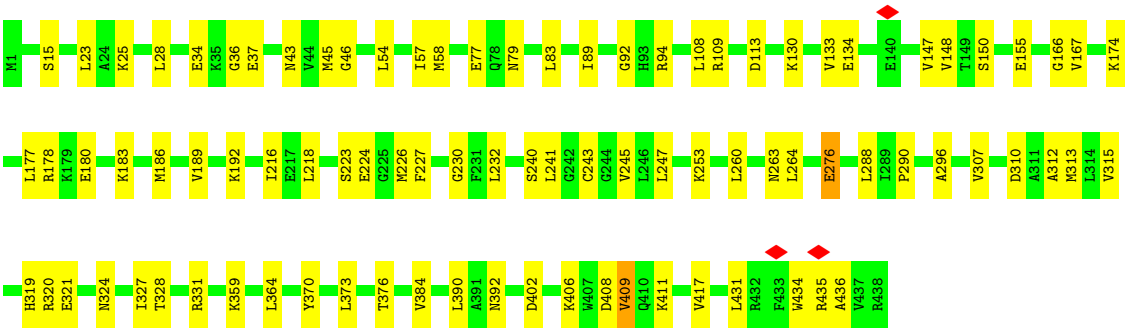
• Molecule 2: Electron transfer flavoprotein, alpha subunit

Chain F:



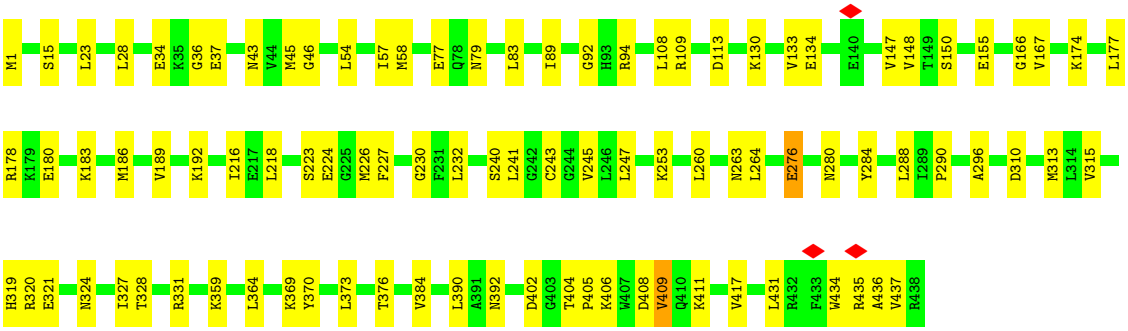
• Molecule 3: Electron transfer flavoprotein-quinone oxidoreductase FixC

Chain C:



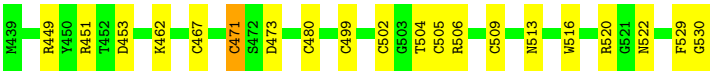
• Molecule 3: Electron transfer flavoprotein-quinone oxidoreductase FixC

Chain G:



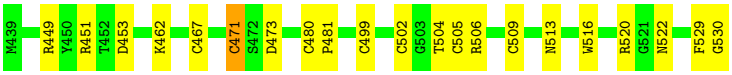
• Molecule 4: Ferredoxin-like protein

Chain D:



- Molecule 4: Ferredoxin-like protein

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	285377	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	329.28003, 329.28003, 329.28003	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.029, 1.029, 1.029	Depositor

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: MQ7, SF4, 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	0.40	0/2233	0.56	0/3026
1	E	0.40	0/2233	0.56	0/3026
2	B	0.23	0/2610	0.50	0/3531
2	F	0.23	0/2610	0.50	0/3531
3	C	0.36	0/3511	0.55	2/4737 (0.0%)
3	G	0.36	0/3511	0.55	2/4737 (0.0%)
4	D	0.45	0/764	0.65	0/1029
4	H	0.45	0/764	0.65	0/1029
All	All	0.35	0/18236	0.55	4/24646 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	276	GLU	CA-CB-CG	5.73	125.55	114.10
3	G	276	GLU	CA-CB-CG	5.73	125.55	114.10
3	C	276	GLU	CB-CG-CD	5.57	122.06	112.60
3	G	276	GLU	CB-CG-CD	5.57	122.06	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2195	0	2278	91	0
1	E	2195	0	2278	88	0
2	B	2565	0	2651	53	0
2	F	2565	0	2651	54	0
3	C	3445	0	3524	58	0
3	G	3445	0	3524	62	0
4	D	746	0	703	27	0
4	H	746	0	703	28	0
5	A	53	0	31	15	0
5	B	53	0	31	2	0
5	C	53	0	31	2	0
5	E	53	0	31	14	0
5	F	53	0	31	1	0
5	G	53	0	31	2	0
6	C	48	0	64	2	0
6	G	48	0	64	1	0
7	D	16	0	0	16	0
7	H	16	0	0	16	0
All	All	18348	0	18626	408	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 11.

All (408) 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:E:251:ASP:HB3	1:E:254:VAL:CG2	1.59	1.31
1:A:251:ASP:HB3	1:A:254:VAL:CG2	1.59	1.31
1:E:247:SER:OG	2:F:597:ILE:HG23	1.51	1.10
1:A:247:SER:OG	2:B:597:ILE:HG23	1.51	1.09
1:A:251:ASP:HB3	1:A:254:VAL:HG23	1.31	1.08
1:E:251:ASP:HB3	1:E:254:VAL:HG23	1.31	1.07
4:D:509:CYS:SG	7:D:602:SF4:S1	2.52	1.07
4:H:509:CYS:SG	7:H:602:SF4:S1	2.52	1.06
4:H:505:CYS:HG	7:H:601:SF4:FE3	0.69	0.99
1:E:251:ASP:HB3	1:E:254:VAL:HG22	1.46	0.98
4:D:467:CYS:HG	7:D:602:SF4:FE1	0.68	0.95
1:E:247:SER:HG	2:F:597:ILE:HG23	1.28	0.95
1:A:251:ASP:HB3	1:A:254:VAL:HG22	1.46	0.94
4:H:467:CYS:HG	7:H:602:SF4:FE1	0.65	0.94
4:D:505:CYS:HG	7:D:601:SF4:FE3	0.67	0.91
4:H:509:CYS:SG	7:H:602:SF4:FE4	1.63	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:509:CYS:SG	7:D:602:SF4:FE4	1.63	0.90
4:D:499:CYS:HG	7:D:601:SF4:FE1	0.57	0.88
1:A:158:LYS:HE2	1:A:160:GLU:OE2	1.74	0.86
1:E:240:ARG:HD2	2:F:592:ILE:HG12	1.57	0.86
1:A:247:SER:HG	2:B:597:ILE:HG23	1.39	0.86
1:A:240:ARG:HD2	2:B:592:ILE:HG12	1.57	0.86
1:E:158:LYS:HE2	1:E:160:GLU:OE2	1.74	0.86
1:A:154:ILE:HA	1:A:161:MET:HB2	1.58	0.85
4:H:499:CYS:HG	7:H:601:SF4:FE1	0.57	0.84
1:E:154:ILE:HA	1:E:161:MET:HB2	1.58	0.83
1:E:6:CYS:O	5:E:301:FAD:O2B	1.98	0.81
1:E:241:LYS:HB2	1:E:241:LYS:NZ	1.96	0.81
1:A:6:CYS:O	5:A:301:FAD:O2B	1.98	0.81
1:A:241:LYS:HB2	1:A:241:LYS:NZ	1.96	0.80
1:A:97:THR:OG1	5:A:301:FAD:O4'	2.00	0.80
1:E:97:THR:OG1	5:E:301:FAD:O4'	2.00	0.80
1:E:245:ILE:HA	2:F:596:GLY:O	1.83	0.78
1:A:245:ILE:HA	2:B:596:GLY:O	1.83	0.78
4:D:480:CYS:SG	7:D:601:SF4:FE4	1.75	0.78
4:D:467:CYS:SG	7:D:602:SF4:FE1	1.75	0.77
4:H:480:CYS:SG	7:H:601:SF4:FE4	1.75	0.77
4:H:467:CYS:SG	7:H:602:SF4:FE1	1.75	0.77
1:E:251:ASP:OD1	1:E:251:ASP:N	2.17	0.77
4:H:502:CYS:SG	7:H:601:SF4:FE2	1.77	0.76
4:H:502:CYS:HG	7:H:601:SF4:FE2	1.02	0.75
4:D:505:CYS:SG	7:D:601:SF4:FE3	1.79	0.75
1:A:127:GLY:O	5:A:301:FAD:O1P	2.05	0.74
1:E:127:GLY:O	5:E:301:FAD:O1P	2.05	0.74
4:D:502:CYS:SG	7:D:601:SF4:FE2	1.77	0.74
4:H:471:CYS:SG	7:H:602:SF4:FE2	1.80	0.74
4:D:471:CYS:SG	7:D:602:SF4:FE2	1.80	0.74
4:D:502:CYS:HG	7:D:601:SF4:FE2	1.03	0.74
1:E:247:SER:CB	1:E:255:ALA:HB1	2.18	0.74
1:A:247:SER:CB	1:A:255:ALA:HB1	2.18	0.73
4:H:480:CYS:HG	7:H:601:SF4:FE4	1.06	0.73
1:A:154:ILE:HD12	1:A:154:ILE:C	2.14	0.73
1:E:155:ASP:HB3	1:E:158:LYS:HG3	1.71	0.73
1:A:93:ASP:HA	5:A:301:FAD:O3'	1.89	0.72
1:E:247:SER:HB2	1:E:255:ALA:HB2	1.71	0.72
1:A:93:ASP:C	5:A:301:FAD:O3'	2.33	0.72
1:E:93:ASP:HA	5:E:301:FAD:O3'	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:CB	1:A:254:VAL:HG23	2.16	0.71
1:E:253:GLU:HG3	2:F:607:ALA:HB1	1.72	0.71
1:A:155:ASP:HB3	1:A:158:LYS:HG3	1.71	0.71
1:A:251:ASP:OD1	1:A:251:ASP:N	2.17	0.71
4:H:505:CYS:SG	7:H:601:SF4:FE3	1.79	0.71
1:E:93:ASP:C	5:E:301:FAD:O3'	2.33	0.71
1:A:247:SER:HB2	1:A:255:ALA:HB2	1.71	0.71
1:E:154:ILE:C	1:E:154:ILE:HD12	2.14	0.71
1:A:253:GLU:HG3	2:B:607:ALA:HB1	1.72	0.70
1:A:248:LYS:C	2:B:598:VAL:O	2.34	0.70
1:E:248:LYS:C	2:F:598:VAL:O	2.34	0.70
2:B:349:LYS:HD2	2:B:465:GLU:HG2	1.72	0.70
1:E:247:SER:OG	2:F:597:ILE:CG2	2.37	0.70
1:E:247:SER:CB	1:E:255:ALA:CB	2.70	0.70
1:E:251:ASP:CB	1:E:254:VAL:HG23	2.16	0.69
1:A:247:SER:CB	1:A:255:ALA:CB	2.70	0.69
4:D:480:CYS:HG	7:D:601:SF4:FE4	1.07	0.69
2:F:349:LYS:HD2	2:F:465:GLU:HG2	1.72	0.69
1:E:251:ASP:CB	1:E:254:VAL:CG2	2.55	0.69
1:A:94:THR:HG21	1:A:131:GLN:HB2	1.76	0.68
1:A:251:ASP:CB	1:A:254:VAL:CG2	2.55	0.68
1:E:94:THR:HG21	1:E:131:GLN:HB2	1.76	0.68
4:H:471:CYS:HG	7:H:602:SF4:FE2	1.10	0.68
1:E:93:ASP:CA	5:E:301:FAD:O3'	2.43	0.67
1:A:93:ASP:CA	5:A:301:FAD:O3'	2.43	0.67
1:A:241:LYS:HB2	1:A:241:LYS:HZ3	1.60	0.67
1:A:247:SER:OG	2:B:597:ILE:CG2	2.37	0.67
1:A:248:LYS:O	2:B:598:VAL:O	2.13	0.66
1:E:248:LYS:O	2:F:598:VAL:O	2.13	0.66
1:A:251:ASP:CB	1:A:254:VAL:HG22	2.26	0.64
2:B:291:ILE:HG23	2:B:379:PRO:HA	1.80	0.64
1:E:247:SER:HB2	1:E:255:ALA:CB	2.28	0.64
2:F:291:ILE:HG23	2:F:379:PRO:HA	1.80	0.63
1:A:247:SER:HB2	1:A:255:ALA:CB	2.28	0.63
2:B:529:ALA:HB2	2:B:539:ILE:HD12	1.81	0.62
1:A:146:ALA:HA	1:A:183:THR:HB	1.82	0.62
3:C:178:ARG:NH2	3:C:296:ALA:O	2.33	0.62
3:G:178:ARG:NH2	3:G:296:ALA:O	2.33	0.62
1:E:251:ASP:CB	1:E:254:VAL:HG22	2.26	0.61
1:E:154:ILE:HD12	1:E:154:ILE:O	2.00	0.61
2:F:529:ALA:HB2	2:F:539:ILE:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:148:VAL:HG12	3:G:155:GLU:HG2	1.82	0.61
1:A:247:SER:HB3	1:A:255:ALA:HB1	1.83	0.61
3:C:148:VAL:HG12	3:C:155:GLU:HG2	1.82	0.61
1:A:154:ILE:HD12	1:A:154:ILE:O	2.00	0.60
1:E:247:SER:HB3	1:E:255:ALA:HB1	1.83	0.60
1:E:146:ALA:HA	1:E:183:THR:HB	1.82	0.60
2:F:298:HIS:HA	2:F:303:ALA:HA	1.84	0.59
2:B:298:HIS:HA	2:B:303:ALA:HA	1.84	0.59
1:E:25:LEU:HD21	2:F:431:ASN:HB3	1.86	0.58
3:C:319:HIS:HE2	3:C:370:TYR:HH	1.52	0.58
1:E:246:ILE:HG12	2:F:595:ILE:HG23	1.86	0.57
1:A:25:LEU:HD21	2:B:431:ASN:HB3	1.86	0.57
4:H:499:CYS:SG	7:H:601:SF4:S4	3.02	0.57
2:B:309:GLU:HG2	2:B:455:GLU:HG3	1.85	0.57
1:A:246:ILE:HG12	2:B:595:ILE:HG23	1.86	0.57
4:D:499:CYS:SG	7:D:601:SF4:S4	3.02	0.57
1:E:130:GLY:N	5:E:301:FAD:O1A	2.38	0.56
2:F:309:GLU:HG2	2:F:455:GLU:HG3	1.85	0.56
3:C:37:GLU:OE1	4:D:449:ARG:NH1	2.37	0.56
3:G:390:LEU:HD11	3:G:417:VAL:HA	1.87	0.56
4:H:451:ARG:NH1	4:H:522:ASN:OD1	2.38	0.56
4:D:451:ARG:NH1	4:D:522:ASN:OD1	2.38	0.56
3:G:408:ASP:HA	3:G:411:LYS:HG2	1.88	0.56
1:A:130:GLY:N	5:A:301:FAD:O1A	2.38	0.56
1:E:158:LYS:CE	1:E:160:GLU:OE2	2.52	0.56
4:D:471:CYS:HG	7:D:602:SF4:FE2	1.21	0.55
5:E:301:FAD:N1	5:E:301:FAD:H2'	2.22	0.55
3:C:390:LEU:HD11	3:C:417:VAL:HA	1.87	0.55
3:C:408:ASP:HA	3:C:411:LYS:HG2	1.88	0.54
5:A:301:FAD:H2'	5:A:301:FAD:N1	2.22	0.54
1:A:38:ASP:OD2	5:A:301:FAD:O3B	2.15	0.54
2:F:298:HIS:NE2	2:F:331:LEU:O	2.36	0.54
1:A:131:GLN:HE21	2:B:407:ALA:HB2	1.73	0.54
3:G:37:GLU:OE1	4:H:449:ARG:NH1	2.37	0.54
2:B:298:HIS:NE2	2:B:331:LEU:O	2.36	0.53
1:E:241:LYS:HB2	1:E:241:LYS:HZ3	1.71	0.53
1:E:158:LYS:HB2	1:E:160:GLU:HG2	1.90	0.53
3:C:34:GLU:HG3	3:C:36:GLY:H	1.73	0.53
1:E:131:GLN:HE21	2:F:407:ALA:HB2	1.73	0.53
3:C:223:SER:HA	3:C:260:LEU:HD22	1.90	0.53
4:H:471:CYS:SG	7:H:602:SF4:S3	2.99	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:O	2:B:547:GLN:NE2	2.42	0.53
3:C:192:LYS:NZ	4:D:530:GLY:OXT	2.38	0.52
3:G:223:SER:HA	3:G:260:LEU:HD22	1.90	0.52
1:A:61:MET:HB2	1:A:84:LEU:HD12	1.92	0.52
1:A:270:ARG:NH2	2:B:309:GLU:OE2	2.42	0.52
1:E:14:THR:O	2:F:547:GLN:NE2	2.42	0.52
2:F:386:ALA:HB3	2:F:450:PRO:HD3	1.91	0.52
4:H:467:CYS:SG	7:H:602:SF4:S2	3.08	0.52
1:A:158:LYS:CE	1:A:160:GLU:OE2	2.52	0.52
4:D:467:CYS:SG	7:D:602:SF4:S2	3.08	0.52
1:E:165:ARG:NH2	2:F:392:GLU:OE2	2.43	0.52
1:E:270:ARG:NH2	2:F:309:GLU:OE2	2.42	0.52
3:G:226:MET:HE3	3:G:245:VAL:HG21	1.92	0.52
1:A:158:LYS:HB2	1:A:160:GLU:HG2	1.90	0.52
3:C:320:ARG:HH21	6:C:502:MQ7:H141	1.75	0.52
4:D:471:CYS:SG	7:D:602:SF4:S3	2.99	0.52
3:G:34:GLU:HG3	3:G:36:GLY:H	1.73	0.52
3:G:320:ARG:HH21	6:G:502:MQ7:H141	1.75	0.52
2:B:386:ALA:HB3	2:B:450:PRO:HD3	1.91	0.52
3:C:226:MET:HE3	3:C:245:VAL:HG21	1.92	0.52
3:C:230:GLY:HA2	3:C:243:CYS:HA	1.92	0.52
1:E:61:MET:HB2	1:E:84:LEU:HD12	1.92	0.52
2:F:407:ALA:HA	2:F:447:THR:HB	1.92	0.52
3:C:224:GLU:OE2	3:C:263:ASN:ND2	2.43	0.52
3:G:192:LYS:NZ	4:H:530:GLY:OXT	2.38	0.51
3:C:431:LEU:HA	3:C:434:TRP:HB2	1.92	0.51
1:E:240:ARG:HH11	1:E:240:ARG:CG	2.23	0.51
3:G:431:LEU:HA	3:G:434:TRP:HB2	1.92	0.51
1:A:240:ARG:CG	1:A:240:ARG:HH11	2.23	0.51
2:B:410:THR:HA	2:B:452:VAL:HG11	1.92	0.51
3:G:23:LEU:HD22	3:G:28:LEU:HD12	1.92	0.51
3:G:224:GLU:OE2	3:G:263:ASN:ND2	2.43	0.51
3:G:230:GLY:HA2	3:G:243:CYS:HA	1.92	0.51
1:A:148:VAL:HG21	1:A:182:LEU:HD22	1.93	0.51
1:E:130:GLY:HA2	5:E:301:FAD:O1A	2.11	0.51
1:E:277:PRO:HB3	2:F:619:SER:HB3	1.93	0.51
3:C:45:MET:HB3	3:C:109:ARG:HG3	1.93	0.51
2:F:361:TYR:HE1	2:F:393:LEU:HD12	1.76	0.51
3:C:216:ILE:HB	3:C:232:LEU:HB3	1.93	0.51
1:E:38:ASP:OD2	5:E:301:FAD:O3B	2.15	0.51
1:A:277:PRO:HB3	2:B:619:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ASP:OD1	3:G:130:LYS:NZ	2.44	0.51
2:F:410:THR:HA	2:F:452:VAL:HG11	1.92	0.51
1:A:72:ASP:OD1	3:C:130:LYS:NZ	2.44	0.50
1:A:130:GLY:HA2	5:A:301:FAD:O1A	2.11	0.50
1:A:165:ARG:NH2	2:B:392:GLU:OE2	2.43	0.50
1:E:148:VAL:HG21	1:E:182:LEU:HD22	1.93	0.50
3:G:45:MET:HB3	3:G:109:ARG:HG3	1.93	0.50
2:B:361:TYR:HE1	2:B:393:LEU:HD12	1.76	0.50
2:B:407:ALA:HA	2:B:447:THR:HB	1.92	0.50
2:B:569:VAL:HA	2:B:572:ILE:HG12	1.93	0.50
2:F:569:VAL:HA	2:F:572:ILE:HG12	1.93	0.50
3:G:186:MET:HB3	3:G:313:MET:HE1	1.93	0.50
3:C:23:LEU:HD22	3:C:28:LEU:HD12	1.92	0.50
1:A:167:LEU:HD22	2:B:389:GLU:HG3	1.93	0.50
3:G:232:LEU:HD12	3:G:241:LEU:HB2	1.94	0.50
3:C:186:MET:HB3	3:C:313:MET:HE1	1.93	0.49
3:G:216:ILE:HB	3:G:232:LEU:HB3	1.93	0.49
1:A:154:ILE:C	1:A:154:ILE:CD1	2.86	0.49
3:C:108:LEU:HD13	4:D:529:PHE:HB2	1.95	0.49
1:E:167:LEU:HD22	2:F:389:GLU:HG3	1.93	0.49
3:G:79:ASN:HA	3:G:92:GLY:HA2	1.94	0.49
3:G:77:GLU:OE1	3:G:94:ARG:NH1	2.46	0.49
3:C:77:GLU:OE1	3:C:94:ARG:NH1	2.46	0.49
1:E:4:VAL:HG11	1:E:105:ILE:HG12	1.95	0.49
3:G:319:HIS:HE2	3:G:370:TYR:HH	1.59	0.49
3:C:109:ARG:N	4:D:530:GLY:O	2.39	0.49
3:C:79:ASN:HA	3:C:92:GLY:HA2	1.94	0.49
3:C:83:LEU:HD11	3:C:218:LEU:HD22	1.95	0.49
3:C:227:PHE:HA	3:C:384:VAL:HG21	1.95	0.49
3:G:227:PHE:HA	3:G:384:VAL:HG21	1.95	0.49
3:G:108:LEU:HD13	4:H:529:PHE:HB2	1.95	0.49
3:G:83:LEU:HD11	3:G:218:LEU:HD22	1.95	0.48
3:C:232:LEU:HD12	3:C:241:LEU:HB2	1.94	0.48
3:G:406:LYS:HA	3:G:409:VAL:HG22	1.95	0.48
3:C:57:ILE:HG22	3:C:58:MET:HG3	1.95	0.48
3:G:134:GLU:OE2	3:G:150:SER:OG	2.31	0.48
1:A:117:LEU:HD11	1:A:182:LEU:HG	1.95	0.48
2:F:411:GLY:HA3	2:F:424:THR:HB	1.94	0.48
3:G:189:VAL:HG23	3:G:247:LEU:HG	1.96	0.48
1:A:4:VAL:HG11	1:A:105:ILE:HG12	1.95	0.48
2:B:411:GLY:HA3	2:B:424:THR:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:ASP:CB	1:E:158:LYS:HG3	2.43	0.48
3:C:15:SER:OG	5:C:501:FAD:O1P	2.31	0.48
3:G:57:ILE:HG22	3:G:58:MET:HG3	1.95	0.48
3:G:130:LYS:HB3	4:H:522:ASN:HB2	1.96	0.48
3:C:130:LYS:HB3	4:D:522:ASN:HB2	1.96	0.48
1:E:159:LYS:HD3	1:E:159:LYS:HA	1.60	0.48
3:G:376:THR:HG21	3:G:436:ALA:HB2	1.96	0.48
3:C:406:LYS:HA	3:C:409:VAL:HG22	1.95	0.47
1:A:45:ALA:HB1	1:A:56:VAL:HG11	1.96	0.47
1:E:117:LEU:HD11	1:E:182:LEU:HG	1.95	0.47
1:A:145:GLY:HA3	1:A:176:LEU:HD11	1.96	0.47
3:C:189:VAL:HG23	3:C:247:LEU:HG	1.96	0.47
3:C:376:THR:HG21	3:C:436:ALA:HB2	1.96	0.47
1:E:93:ASP:CA	5:E:301:FAD:HO3'	2.27	0.47
3:C:134:GLU:OE2	3:C:150:SER:OG	2.31	0.47
3:C:290:PRO:HD2	3:C:315:VAL:HG21	1.97	0.47
2:F:406:THR:OG1	2:F:409:CYS:SG	2.63	0.47
1:A:240:ARG:HB3	1:A:241:LYS:H	1.55	0.47
3:G:109:ARG:N	4:H:530:GLY:O	2.39	0.47
1:A:40:ARG:HG3	1:A:186:ASP:HA	1.96	0.46
1:A:240:ARG:HD2	2:B:592:ILE:CG1	2.39	0.46
2:B:406:THR:OG1	2:B:409:CYS:SG	2.63	0.46
3:C:192:LYS:HE3	3:C:240:SER:HB2	1.97	0.46
1:E:70:LEU:HD22	1:E:81:ALA:HB1	1.97	0.46
1:E:45:ALA:HB1	1:E:56:VAL:HG11	1.96	0.46
1:E:145:GLY:HA3	1:E:176:LEU:HD11	1.96	0.46
1:E:40:ARG:HG3	1:E:186:ASP:HA	1.96	0.46
1:A:155:ASP:CB	1:A:158:LYS:HG3	2.43	0.46
3:G:43:ASN:ND2	3:G:113:ASP:OD2	2.44	0.46
1:A:70:LEU:HD22	1:A:81:ALA:HB1	1.97	0.46
3:C:133:VAL:HG13	3:C:147:VAL:HG13	1.97	0.46
1:E:240:ARG:HD2	2:F:592:ILE:CG1	2.39	0.46
2:F:505:LYS:H	2:F:538:TRP:HZ3	1.62	0.46
3:G:328:THR:HG23	3:G:331:ARG:HH21	1.80	0.46
1:E:16:VAL:HG13	1:E:27:ARG:HB3	1.98	0.46
2:F:370:LEU:HD13	2:F:393:LEU:HD21	1.97	0.46
3:G:290:PRO:HD2	3:G:315:VAL:HG21	1.97	0.46
2:B:384:ILE:HD12	2:B:394:ALA:HB2	1.97	0.46
3:G:313:MET:HE2	3:G:313:MET:HB3	1.89	0.46
3:C:328:THR:HG23	3:C:331:ARG:HH21	1.80	0.46
1:A:132:VAL:HG23	5:A:301:FAD:O2A	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:LYS:H	2:B:538:TRP:HZ3	1.62	0.45
1:E:245:ILE:CA	2:F:596:GLY:O	2.59	0.45
3:C:134:GLU:O	3:C:174:LYS:NZ	2.48	0.45
2:B:370:LEU:HD13	2:B:393:LEU:HD21	1.97	0.45
2:B:582:ASN:HB2	5:B:701:FAD:H1B	1.98	0.45
3:C:43:ASN:ND2	3:C:113:ASP:OD2	2.44	0.45
1:E:253:GLU:C	1:E:255:ALA:N	2.74	0.45
3:C:25:LYS:HD2	3:C:25:LYS:HA	1.77	0.45
1:E:9:GLN:HG3	1:E:69:ALA:HB2	1.98	0.45
3:G:192:LYS:HE3	3:G:240:SER:HB2	1.97	0.45
2:B:315:ARG:HA	2:B:315:ARG:HD2	1.81	0.45
3:C:46:GLY:H	5:C:501:FAD:C6	2.30	0.45
2:F:384:ILE:HD12	2:F:394:ALA:HB2	1.97	0.45
3:G:133:VAL:HG13	3:G:147:VAL:HG13	1.97	0.45
1:A:248:LYS:HD2	1:A:248:LYS:HA	1.38	0.45
1:E:159:LYS:HD3	1:E:178:LEU:HD12	1.98	0.45
1:A:246:ILE:N	2:B:596:GLY:O	2.50	0.45
1:E:247:SER:HB3	1:E:255:ALA:CB	2.44	0.45
2:F:315:ARG:HD2	2:F:315:ARG:HA	1.81	0.45
2:F:372:ASP:OD2	2:F:471:TYR:OH	2.30	0.45
1:A:16:VAL:HG13	1:A:27:ARG:HB3	1.98	0.45
1:E:35:ASN:ND2	1:E:123:GLN:O	2.42	0.45
1:E:171:PHE:HB2	2:F:486:ILE:HB	1.99	0.45
2:F:386:ALA:HB3	2:F:449:ARG:HA	1.99	0.45
3:G:134:GLU:O	3:G:174:LYS:NZ	2.48	0.45
3:G:247:LEU:HD21	4:H:504:THR:HG23	1.99	0.45
3:C:177:LEU:H	3:C:177:LEU:HG	1.62	0.45
1:E:114:LYS:HE3	1:E:179:PRO:HG2	1.99	0.45
1:E:132:VAL:HG23	5:E:301:FAD:O2A	2.16	0.45
3:G:166:GLY:HA2	3:G:310:ASP:HB2	1.99	0.45
3:C:166:GLY:HA2	3:C:310:ASP:HB2	1.99	0.44
2:F:501:VAL:HA	2:F:558:PHE:HB2	1.99	0.44
3:G:46:GLY:H	5:G:501:FAD:C6	2.30	0.44
1:A:118:ILE:HB	1:A:181:VAL:HG22	1.99	0.44
1:A:253:GLU:C	1:A:255:ALA:N	2.74	0.44
1:E:248:LYS:HD2	1:E:248:LYS:HA	1.38	0.44
1:A:9:GLN:HG3	1:A:69:ALA:HB2	1.98	0.44
2:B:386:ALA:HB3	2:B:449:ARG:HA	1.99	0.44
2:F:582:ASN:HB2	5:F:701:FAD:H1B	1.98	0.44
2:B:386:ALA:N	2:B:448:VAL:O	2.50	0.44
1:E:118:ILE:HB	1:E:181:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:ILE:N	2:F:596:GLY:O	2.50	0.44
1:A:171:PHE:HB2	2:B:486:ILE:HB	1.99	0.44
2:F:386:ALA:N	2:F:448:VAL:O	2.50	0.44
1:A:159:LYS:HD3	1:A:178:LEU:HD12	1.98	0.44
1:E:130:GLY:CA	5:E:301:FAD:O1A	2.66	0.44
3:C:247:LEU:HD21	4:D:504:THR:HG23	1.99	0.44
3:G:369:LYS:NZ	3:G:437:VAL:O	2.50	0.44
1:A:93:ASP:CA	5:A:301:FAD:HO3'	2.31	0.43
1:A:114:LYS:HE3	1:A:179:PRO:HG2	1.99	0.43
1:A:154:ILE:HD13	1:A:161:MET:HB2	2.00	0.43
3:G:1:MET:HE3	3:G:1:MET:HB3	1.84	0.43
2:B:566:ILE:HA	2:B:569:VAL:HG22	2.00	0.43
3:C:216:ILE:HG13	3:C:232:LEU:HD23	2.00	0.43
3:C:313:MET:HE2	3:C:313:MET:HB3	1.89	0.43
1:A:240:ARG:CG	1:A:240:ARG:NH1	2.80	0.43
2:B:403:THR:OG1	2:B:404:GLY:N	2.52	0.43
4:D:473:ASP:OD1	4:D:473:ASP:N	2.44	0.43
1:E:240:ARG:CG	1:E:240:ARG:NH1	2.80	0.43
2:B:501:VAL:HA	2:B:558:PHE:HB2	1.99	0.43
6:C:502:MQ7:H452	6:C:502:MQ7:H411	1.83	0.43
2:F:566:ILE:HA	2:F:569:VAL:HG22	2.00	0.43
2:B:504:GLY:HA2	2:B:533:ALA:HB2	2.00	0.43
4:D:462:LYS:HD2	4:D:513:ASN:HA	2.00	0.43
2:F:516:LEU:HD23	2:F:605:VAL:HG11	2.01	0.43
1:A:128:ASP:OD1	1:A:128:ASP:N	2.52	0.43
4:D:453:ASP:OD2	4:D:520:ARG:NE	2.48	0.43
1:E:128:ASP:OD1	1:E:128:ASP:N	2.52	0.43
2:F:504:GLY:HA2	2:F:533:ALA:HB2	2.00	0.43
4:H:473:ASP:OD1	4:H:473:ASP:N	2.44	0.43
1:A:249:ASN:OD1	1:A:249:ASN:N	2.45	0.43
3:G:284:TYR:OH	4:H:481:PRO:O	2.36	0.43
4:H:462:LYS:HD2	4:H:513:ASN:HA	2.00	0.43
2:B:516:LEU:HD23	2:B:605:VAL:HG11	2.01	0.43
3:G:180:GLU:OE2	3:G:183:LYS:NZ	2.52	0.43
3:G:216:ILE:HG13	3:G:232:LEU:HD23	2.00	0.43
4:H:453:ASP:OD2	4:H:520:ARG:NE	2.48	0.43
1:A:173:LYS:HG3	2:B:486:ILE:HD11	2.00	0.42
1:E:154:ILE:HD13	1:E:161:MET:HB2	2.00	0.42
1:A:245:ILE:CA	2:B:596:GLY:O	2.59	0.42
1:A:130:GLY:CA	5:A:301:FAD:O1A	2.66	0.42
3:G:167:VAL:HG11	3:G:288:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HA	1:A:261:GLU:HB2	2.02	0.42
3:C:180:GLU:OE2	3:C:183:LYS:NZ	2.52	0.42
1:A:195:ASP:OD1	1:A:195:ASP:N	2.53	0.42
1:E:173:LYS:HG3	2:F:486:ILE:HD11	2.00	0.42
2:F:368:LYS:HE3	2:F:368:LYS:HB2	1.88	0.42
3:G:15:SER:OG	5:G:501:FAD:O1P	2.31	0.42
3:C:224:GLU:O	3:C:253:LYS:NZ	2.53	0.42
3:G:370:TYR:HB3	3:G:373:LEU:HD22	2.02	0.42
1:A:159:LYS:HD3	1:A:159:LYS:HA	1.60	0.42
2:F:291:ILE:HD11	2:F:327:TRP:CE2	2.55	0.42
3:G:431:LEU:HA	3:G:434:TRP:CB	2.49	0.42
1:A:35:ASN:ND2	1:A:123:GLN:O	2.42	0.41
2:B:406:THR:HB	2:B:425:ARG:HD2	2.02	0.41
3:C:218:LEU:HD13	3:C:264:LEU:HD11	2.02	0.41
3:G:224:GLU:O	3:G:253:LYS:NZ	2.53	0.41
3:C:167:VAL:HG11	3:C:288:LEU:HB2	2.01	0.41
3:C:370:TYR:HB3	3:C:373:LEU:HD22	2.02	0.41
3:C:402:ASP:N	3:C:402:ASP:OD1	2.53	0.41
4:D:506:ARG:HD3	4:D:516:TRP:HB3	2.02	0.41
1:E:98:THR:HG23	1:E:136:LEU:HG	2.02	0.41
2:F:292:ILE:HD11	2:F:326:VAL:HG22	2.01	0.41
2:F:403:THR:OG1	2:F:404:GLY:N	2.52	0.41
3:G:177:LEU:H	3:G:177:LEU:HG	1.62	0.41
2:B:291:ILE:HD11	2:B:327:TRP:CE2	2.55	0.41
3:C:431:LEU:HA	3:C:434:TRP:CB	2.49	0.41
3:G:54:LEU:HG	3:G:327:ILE:HD13	2.03	0.41
1:A:74:ILE:HD11	1:A:81:ALA:HB2	2.02	0.41
3:C:307:VAL:HG12	3:C:312:ALA:HB2	2.02	0.41
1:A:247:SER:HB3	1:A:255:ALA:CB	2.44	0.41
3:C:54:LEU:HG	3:C:327:ILE:HD13	2.03	0.41
3:G:404:THR:HA	3:G:405:PRO:HD3	1.87	0.41
1:A:98:THR:HG23	1:A:136:LEU:HG	2.02	0.41
2:B:292:ILE:HD11	2:B:326:VAL:HG22	2.01	0.41
1:E:245:ILE:N	1:E:245:ILE:HD13	2.36	0.41
3:G:89:ILE:HD11	3:G:392:ASN:HA	2.02	0.41
1:A:245:ILE:HD13	1:A:245:ILE:N	2.36	0.41
1:E:258:LYS:HA	1:E:261:GLU:HB2	2.02	0.41
1:E:275:LEU:HD23	1:E:275:LEU:HA	1.91	0.41
3:G:280:ASN:OD1	3:G:280:ASN:N	2.53	0.41
2:B:512:GLY:HA2	2:B:515:LYS:HD2	2.03	0.41
3:C:89:ILE:HD11	3:C:392:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ILE:HD11	1:E:81:ALA:HB2	2.02	0.41
3:G:364:LEU:HD23	3:G:364:LEU:HA	1.89	0.41
3:G:402:ASP:N	3:G:402:ASP:OD1	2.53	0.41
5:A:301:FAD:H9	5:A:301:FAD:H1'1	1.79	0.41
1:A:93:ASP:C	5:A:301:FAD:HO3'	2.27	0.40
3:C:321:GLU:HB3	3:C:324:ASN:HB3	2.03	0.40
1:E:245:ILE:CG2	2:F:598:VAL:HG23	2.51	0.40
2:B:445:MET:HE2	2:B:445:MET:HB3	1.81	0.40
3:G:321:GLU:HB3	3:G:324:ASN:HB3	2.03	0.40
1:E:240:ARG:HB3	1:E:241:LYS:H	1.55	0.40
3:G:218:LEU:HD13	3:G:264:LEU:HD11	2.02	0.40
1:A:107:LYS:NZ	1:A:214:ASP:O	2.44	0.40
1:A:245:ILE:CG2	2:B:598:VAL:HG23	2.51	0.40
5:B:701:FAD:H4'	5:B:701:FAD:H1'2	1.85	0.40
3:C:359:LYS:HA	3:C:364:LEU:HB2	2.04	0.40
5:E:301:FAD:H1'1	5:E:301:FAD:H9	1.79	0.40
3:G:359:LYS:HA	3:G:364:LEU:HB2	2.04	0.40
4:H:506:ARG:HD3	4:H:516:TRP:HB3	2.02	0.40
2:B:606:PRO:HA	2:B:609:THR:HG22	2.03	0.40
1:E:143:ALA:HB1	1:E:176:LEU:HD22	2.03	0.40
2:F:406:THR:HB	2:F:425:ARG:HD2	2.02	0.40
2:F:499:VAL:HG22	2:F:556:LEU:HB3	2.04	0.40
2:F:512:GLY:HA2	2:F:515:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	280/296 (95%)	262 (94%)	17 (6%)	1 (0%)	30	59
1	E	280/296 (95%)	263 (94%)	16 (6%)	1 (0%)	30	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	334/338 (99%)	315 (94%)	19 (6%)	0	100	100
2	F	334/338 (99%)	315 (94%)	19 (6%)	0	100	100
3	C	436/438 (100%)	399 (92%)	37 (8%)	0	100	100
3	G	436/438 (100%)	399 (92%)	37 (8%)	0	100	100
4	D	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
4	H	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	2280/2328 (98%)	2125 (93%)	153 (7%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ILE
1	E	245	ILE

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 PDB entries followed by that with respect to all EM entries.

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	236/249 (95%)	220 (93%)	16 (7%)	14	42
1	E	236/249 (95%)	220 (93%)	16 (7%)	14	42
2	B	273/275 (99%)	272 (100%)	1 (0%)	84	94
2	F	273/275 (99%)	272 (100%)	1 (0%)	84	94
3	C	370/370 (100%)	367 (99%)	3 (1%)	73	90
3	G	370/370 (100%)	367 (99%)	3 (1%)	73	90
4	D	83/83 (100%)	82 (99%)	1 (1%)	63	86
4	H	83/83 (100%)	82 (99%)	1 (1%)	63	86
All	All	1924/1954 (98%)	1882 (98%)	42 (2%)	45	77

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	GLU
1	A	153	GLU
1	A	154	ILE
1	A	157	GLU
1	A	158	LYS
1	A	159	LYS
1	A	161	MET
1	A	217	LEU
1	A	240	ARG
1	A	241	LYS
1	A	245	ILE
1	A	246	ILE
1	A	248	LYS
1	A	250	GLU
1	A	251	ASP
1	A	253	GLU
2	B	501	VAL
3	C	276	GLU
3	C	409	VAL
3	C	435	ARG
4	D	471	CYS
1	E	152	GLU
1	E	153	GLU
1	E	154	ILE
1	E	157	GLU
1	E	158	LYS
1	E	159	LYS
1	E	161	MET
1	E	217	LEU
1	E	240	ARG
1	E	241	LYS
1	E	245	ILE
1	E	246	ILE
1	E	248	LYS
1	E	250	GLU
1	E	251	ASP
1	E	253	GLU
2	F	501	VAL
3	G	276	GLU
3	G	409	VAL
3	G	435	ARG
4	H	471	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	131	GLN
2	B	359	ASN
2	B	441	HIS
2	B	547	GLN
3	C	67	ASN
3	C	168	ASN
3	C	203	ASN
3	C	235	ASN
3	C	287	HIS
3	C	382	GLN
4	D	448	ASN
1	E	15	ASN
1	E	131	GLN
2	F	359	ASN
2	F	441	HIS
2	F	547	GLN
3	G	67	ASN
3	G	168	ASN
3	G	203	ASN
3	G	235	ASN
3	G	287	HIS
3	G	382	GLN
4	H	448	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
5	FAD	F	701	-	58,58,58	0.58	1 (1%)	85,89,89	0.34	0
5	FAD	G	501	-	58,58,58	0.56	1 (1%)	85,89,89	0.39	0
5	FAD	C	501	-	58,58,58	0.56	1 (1%)	85,89,89	0.39	0
7	SF4	H	602	4	0,12,12	-	-	-		
7	SF4	H	601	-	0,12,12	-	-	-		
6	MQ7	C	502	-	49,49,49	4.17	18 (36%)	61,63,63	3.14	37 (60%)
5	FAD	B	701	-	58,58,58	0.58	1 (1%)	85,89,89	0.34	0
5	FAD	E	301	-	58,58,58	0.56	0	85,89,89	0.58	1 (1%)
5	FAD	A	301	-	58,58,58	0.56	0	85,89,89	0.58	1 (1%)
6	MQ7	G	502	-	49,49,49	4.17	18 (36%)	61,63,63	3.14	37 (60%)
7	SF4	D	602	4	0,12,12	-	-	-		
7	SF4	D	601	-	0,12,12	-	-	-		

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	FAD	F	701	-	-	9/34/50/50	0/6/6/6
5	FAD	G	501	-	-	14/34/50/50	0/6/6/6
5	FAD	C	501	-	-	14/34/50/50	0/6/6/6
7	SF4	H	602	4	-	-	0/6/5/5
7	SF4	H	601	-	-	-	0/6/5/5
6	MQ7	C	502	-	-	20/41/61/61	0/2/2/2
5	FAD	B	701	-	-	9/34/50/50	0/6/6/6
5	FAD	E	301	-	-	14/34/50/50	0/6/6/6
5	FAD	A	301	-	-	14/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MQ7	G	502	-	-	20/41/61/61	0/2/2/2
7	SF4	D	602	4	-	-	0/6/5/5
7	SF4	D	601	-	-	-	0/6/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	502	MQ7	C17-C18	10.04	1.56	1.33
6	G	502	MQ7	C17-C18	10.04	1.56	1.33
6	C	502	MQ7	C32-C33	9.86	1.55	1.33
6	G	502	MQ7	C32-C33	9.86	1.55	1.33
6	C	502	MQ7	C12-C13	9.83	1.55	1.33
6	G	502	MQ7	C12-C13	9.83	1.55	1.33
6	C	502	MQ7	C27-C28	9.76	1.55	1.33
6	G	502	MQ7	C27-C28	9.76	1.55	1.33
6	C	502	MQ7	C37-C38	9.38	1.54	1.33
6	G	502	MQ7	C37-C38	9.38	1.54	1.33
6	C	502	MQ7	C22-C23	9.35	1.54	1.33
6	G	502	MQ7	C22-C23	9.35	1.54	1.33
6	C	502	MQ7	C42-C43	7.51	1.54	1.32
6	G	502	MQ7	C42-C43	7.51	1.54	1.32
6	C	502	MQ7	O1-C1	7.17	1.38	1.23
6	G	502	MQ7	O1-C1	7.17	1.38	1.23
6	C	502	MQ7	O4-C4	6.84	1.37	1.23
6	G	502	MQ7	O4-C4	6.84	1.37	1.23
6	C	502	MQ7	C3-C2	4.24	1.42	1.35
6	G	502	MQ7	C3-C2	4.24	1.42	1.35
6	C	502	MQ7	C2-C1	-4.07	1.38	1.47
6	G	502	MQ7	C2-C1	-4.07	1.38	1.47
6	C	502	MQ7	C11-C12	3.59	1.56	1.50
6	G	502	MQ7	C11-C12	3.59	1.56	1.50
6	C	502	MQ7	C3-C4	-3.21	1.39	1.47
6	G	502	MQ7	C3-C4	-3.21	1.39	1.47
6	C	502	MQ7	C10-C1	-3.10	1.42	1.48
6	G	502	MQ7	C10-C1	-3.10	1.42	1.48
6	C	502	MQ7	C15-C13	2.78	1.57	1.51
6	G	502	MQ7	C15-C13	2.78	1.57	1.51
6	C	502	MQ7	C5-C4	-2.70	1.42	1.48
6	G	502	MQ7	C5-C4	-2.70	1.42	1.48
5	C	501	FAD	P-O2P	-2.49	1.43	1.55
5	G	501	FAD	P-O2P	-2.49	1.43	1.55
6	C	502	MQ7	C20-C18	2.31	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	502	MQ7	C20-C18	2.31	1.56	1.51
6	C	502	MQ7	C40-C38	2.23	1.55	1.51
6	G	502	MQ7	C40-C38	2.23	1.55	1.51
5	B	701	FAD	P-O2P	-2.09	1.45	1.55
5	F	701	FAD	P-O2P	-2.09	1.45	1.55

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	502	MQ7	C14-C13-C12	-5.80	108.74	123.63
6	G	502	MQ7	C14-C13-C12	-5.80	108.74	123.63
6	C	502	MQ7	C31-C32-C33	-5.69	114.61	127.62
6	G	502	MQ7	C31-C32-C33	-5.69	114.61	127.62
6	C	502	MQ7	C34-C33-C32	-5.51	109.47	123.63
6	G	502	MQ7	C34-C33-C32	-5.51	109.47	123.63
6	C	502	MQ7	C11-C12-C13	-5.29	117.72	126.83
6	G	502	MQ7	C11-C12-C13	-5.29	117.72	126.83
6	C	502	MQ7	C39-C38-C37	-5.20	110.27	123.63
6	G	502	MQ7	C39-C38-C37	-5.20	110.27	123.63
6	C	502	MQ7	C19-C18-C17	-5.08	110.58	123.63
6	G	502	MQ7	C19-C18-C17	-5.08	110.58	123.63
6	C	502	MQ7	C36-C37-C38	-5.04	116.08	127.62
6	G	502	MQ7	C36-C37-C38	-5.04	116.08	127.62
6	C	502	MQ7	C21-C22-C23	-5.04	116.10	127.62
6	G	502	MQ7	C21-C22-C23	-5.04	116.10	127.62
6	C	502	MQ7	C24-C23-C22	-4.84	111.20	123.63
6	G	502	MQ7	C24-C23-C22	-4.84	111.20	123.63
6	C	502	MQ7	C29-C28-C27	-4.56	111.90	123.63
6	G	502	MQ7	C29-C28-C27	-4.56	111.90	123.63
6	C	502	MQ7	C11-C3-C4	4.21	123.01	118.58
6	G	502	MQ7	C11-C3-C4	4.21	123.01	118.58
6	C	502	MQ7	C16-C17-C18	-4.09	118.27	127.62
6	G	502	MQ7	C16-C17-C18	-4.09	118.27	127.62
6	C	502	MQ7	C26-C27-C28	-3.90	118.69	127.62
6	G	502	MQ7	C26-C27-C28	-3.90	118.69	127.62
6	C	502	MQ7	C35-C33-C32	-3.87	112.47	121.17
6	G	502	MQ7	C35-C33-C32	-3.87	112.47	121.17
6	C	502	MQ7	C5-C10-C1	-3.83	116.60	120.71
6	G	502	MQ7	C5-C10-C1	-3.83	116.60	120.71
6	C	502	MQ7	C24-C23-C25	-3.78	108.67	115.23
6	G	502	MQ7	C24-C23-C25	-3.78	108.67	115.23
6	C	502	MQ7	C20-C18-C17	-3.77	112.71	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	502	MQ7	C20-C18-C17	-3.77	112.71	121.17
6	C	502	MQ7	C41-C42-C43	-3.71	115.27	127.64
6	G	502	MQ7	C41-C42-C43	-3.71	115.27	127.64
6	C	502	MQ7	C45-C43-C42	-3.70	111.55	122.66
6	G	502	MQ7	C45-C43-C42	-3.70	111.55	122.66
6	C	502	MQ7	C5-C4-C3	3.67	125.00	118.27
6	G	502	MQ7	C5-C4-C3	3.67	125.00	118.27
6	C	502	MQ7	C10-C1-C2	3.57	123.94	118.97
6	G	502	MQ7	C10-C1-C2	3.57	123.94	118.97
6	C	502	MQ7	C44-C43-C42	-3.54	112.02	122.66
6	G	502	MQ7	C44-C43-C42	-3.54	112.02	122.66
6	C	502	MQ7	C25-C23-C22	-3.42	113.48	121.17
6	G	502	MQ7	C25-C23-C22	-3.42	113.48	121.17
6	C	502	MQ7	C15-C13-C12	-3.42	113.48	121.17
6	G	502	MQ7	C15-C13-C12	-3.42	113.48	121.17
6	C	502	MQ7	C14-C13-C15	-3.40	109.33	115.23
6	G	502	MQ7	C14-C13-C15	-3.40	109.33	115.23
6	C	502	MQ7	C34-C33-C35	-3.30	109.49	115.23
6	G	502	MQ7	C34-C33-C35	-3.30	109.49	115.23
6	C	502	MQ7	C40-C38-C37	-3.22	113.94	121.17
6	G	502	MQ7	C40-C38-C37	-3.22	113.94	121.17
6	C	502	MQ7	C30-C28-C27	-2.97	114.50	121.17
6	G	502	MQ7	C30-C28-C27	-2.97	114.50	121.17
6	C	502	MQ7	C12-C11-C3	2.95	119.34	112.08
6	G	502	MQ7	C12-C11-C3	2.95	119.34	112.08
6	C	502	MQ7	O1-C1-C10	-2.91	116.91	121.57
6	G	502	MQ7	O1-C1-C10	-2.91	116.91	121.57
6	C	502	MQ7	C9-C10-C1	2.82	124.21	120.10
6	G	502	MQ7	C9-C10-C1	2.82	124.21	120.10
6	C	502	MQ7	C19-C18-C20	-2.80	110.37	115.23
6	G	502	MQ7	C19-C18-C20	-2.80	110.37	115.23
6	C	502	MQ7	O4-C4-C5	-2.77	117.14	121.57
6	G	502	MQ7	O4-C4-C5	-2.77	117.14	121.57
6	C	502	MQ7	C39-C38-C40	-2.71	110.52	115.23
6	G	502	MQ7	C39-C38-C40	-2.71	110.52	115.23
6	C	502	MQ7	C45-C43-C44	-2.28	109.34	114.59
6	G	502	MQ7	C45-C43-C44	-2.28	109.34	114.59
5	A	301	FAD	C4-N3-C2	-2.10	121.91	125.64
5	E	301	FAD	C4-N3-C2	-2.10	121.91	125.64
6	C	502	MQ7	C2M-C2-C3	-2.06	121.07	124.45
6	G	502	MQ7	C2M-C2-C3	-2.06	121.07	124.45
6	C	502	MQ7	C10-C5-C4	-2.04	118.52	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	502	MQ7	C10-C5-C4	-2.04	118.52	120.71

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	FAD	C3'-C4'-C5'-O5'
5	A	301	FAD	O4'-C4'-C5'-O5'
5	A	301	FAD	C5'-O5'-P-O1P
5	A	301	FAD	C5'-O5'-P-O2P
5	A	301	FAD	C5'-O5'-P-O3P
5	B	701	FAD	C5B-O5B-PA-O1A
5	B	701	FAD	C5B-O5B-PA-O3P
5	C	501	FAD	C5B-O5B-PA-O2A
5	C	501	FAD	C1'-C2'-C3'-O3'
5	C	501	FAD	C1'-C2'-C3'-C4'
5	C	501	FAD	C2'-C3'-C4'-O4'
5	C	501	FAD	C2'-C3'-C4'-C5'
5	C	501	FAD	O3'-C3'-C4'-O4'
5	C	501	FAD	O3'-C3'-C4'-C5'
5	E	301	FAD	C3'-C4'-C5'-O5'
5	E	301	FAD	O4'-C4'-C5'-O5'
5	E	301	FAD	C5'-O5'-P-O1P
5	E	301	FAD	C5'-O5'-P-O2P
5	E	301	FAD	C5'-O5'-P-O3P
5	F	701	FAD	C5B-O5B-PA-O1A
5	F	701	FAD	C5B-O5B-PA-O3P
5	G	501	FAD	C5B-O5B-PA-O2A
5	G	501	FAD	C1'-C2'-C3'-O3'
5	G	501	FAD	C1'-C2'-C3'-C4'
5	G	501	FAD	C2'-C3'-C4'-O4'
5	G	501	FAD	C2'-C3'-C4'-C5'
5	G	501	FAD	O3'-C3'-C4'-O4'
5	G	501	FAD	O3'-C3'-C4'-C5'
6	C	502	MQ7	C11-C12-C13-C14
6	C	502	MQ7	C21-C22-C23-C24
6	C	502	MQ7	C35-C36-C37-C38
6	C	502	MQ7	C36-C37-C38-C40
6	G	502	MQ7	C11-C12-C13-C14
6	G	502	MQ7	C21-C22-C23-C24
6	G	502	MQ7	C35-C36-C37-C38
6	G	502	MQ7	C36-C37-C38-C40

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Mol	Chain	Res	Type	Atoms
6	C	502	MQ7	C16-C17-C18-C19
6	C	502	MQ7	C26-C27-C28-C29
6	C	502	MQ7	C31-C32-C33-C34
6	G	502	MQ7	C16-C17-C18-C19
6	G	502	MQ7	C26-C27-C28-C29
6	G	502	MQ7	C31-C32-C33-C34
6	C	502	MQ7	C11-C12-C13-C15
6	G	502	MQ7	C11-C12-C13-C15
6	C	502	MQ7	C23-C25-C26-C27
6	C	502	MQ7	C33-C35-C36-C37
6	G	502	MQ7	C23-C25-C26-C27
6	G	502	MQ7	C33-C35-C36-C37
5	A	301	FAD	C2'-C3'-C4'-C5'
5	E	301	FAD	C2'-C3'-C4'-C5'
6	C	502	MQ7	C41-C42-C43-C45
6	G	502	MQ7	C41-C42-C43-C45
5	B	701	FAD	O4B-C4B-C5B-O5B
5	F	701	FAD	O4B-C4B-C5B-O5B
5	A	301	FAD	O3'-C3'-C4'-C5'
5	E	301	FAD	O3'-C3'-C4'-C5'
6	C	502	MQ7	C13-C15-C16-C17
6	G	502	MQ7	C13-C15-C16-C17
5	C	501	FAD	O2'-C2'-C3'-O3'
5	G	501	FAD	O2'-C2'-C3'-O3'
5	B	701	FAD	C3B-C4B-C5B-O5B
5	F	701	FAD	C3B-C4B-C5B-O5B
6	C	502	MQ7	C41-C42-C43-C44
6	G	502	MQ7	C41-C42-C43-C44
5	C	501	FAD	O4B-C4B-C5B-O5B
5	G	501	FAD	O4B-C4B-C5B-O5B
6	C	502	MQ7	C22-C23-C25-C26
6	G	502	MQ7	C22-C23-C25-C26
5	C	501	FAD	O2'-C2'-C3'-C4'
5	G	501	FAD	O2'-C2'-C3'-C4'
5	A	301	FAD	O3'-C3'-C4'-O4'
5	E	301	FAD	O3'-C3'-C4'-O4'
5	C	501	FAD	C3B-C4B-C5B-O5B
5	G	501	FAD	C3B-C4B-C5B-O5B
6	C	502	MQ7	C34-C33-C35-C36
6	G	502	MQ7	C34-C33-C35-C36
5	A	301	FAD	C2'-C3'-C4'-O4'
5	E	301	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
6	C	502	MQ7	C27-C28-C30-C31
6	G	502	MQ7	C27-C28-C30-C31
5	B	701	FAD	C2B-C1B-N9A-C8A
5	F	701	FAD	C2B-C1B-N9A-C8A
5	A	301	FAD	PA-O3P-P-O2P
5	B	701	FAD	PA-O3P-P-O2P
5	E	301	FAD	PA-O3P-P-O2P
5	F	701	FAD	PA-O3P-P-O2P
5	A	301	FAD	C5B-O5B-PA-O1A
5	A	301	FAD	C2'-C1'-N10-C10
5	B	701	FAD	C5B-O5B-PA-O2A
5	C	501	FAD	C5B-O5B-PA-O1A
5	C	501	FAD	C5B-O5B-PA-O3P
5	E	301	FAD	C5B-O5B-PA-O1A
5	E	301	FAD	C2'-C1'-N10-C10
5	F	701	FAD	C5B-O5B-PA-O2A
5	G	501	FAD	C5B-O5B-PA-O1A
5	G	501	FAD	C5B-O5B-PA-O3P
6	C	502	MQ7	C19-C18-C20-C21
6	G	502	MQ7	C19-C18-C20-C21
6	C	502	MQ7	C39-C38-C40-C41
6	G	502	MQ7	C39-C38-C40-C41
6	C	502	MQ7	C12-C13-C15-C16
6	G	502	MQ7	C12-C13-C15-C16
6	C	502	MQ7	C38-C40-C41-C42
6	G	502	MQ7	C38-C40-C41-C42
5	B	701	FAD	PA-O3P-P-O1P
5	C	501	FAD	P-O3P-PA-O2A
5	F	701	FAD	PA-O3P-P-O1P
5	G	501	FAD	P-O3P-PA-O2A
5	A	301	FAD	O2'-C2'-C3'-C4'
5	E	301	FAD	O2'-C2'-C3'-C4'
5	B	701	FAD	O4B-C1B-N9A-C8A
5	F	701	FAD	O4B-C1B-N9A-C8A
5	A	301	FAD	PA-O3P-P-O1P
5	E	301	FAD	PA-O3P-P-O1P

There are no ring outliers.

12 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	701	FAD	1	0

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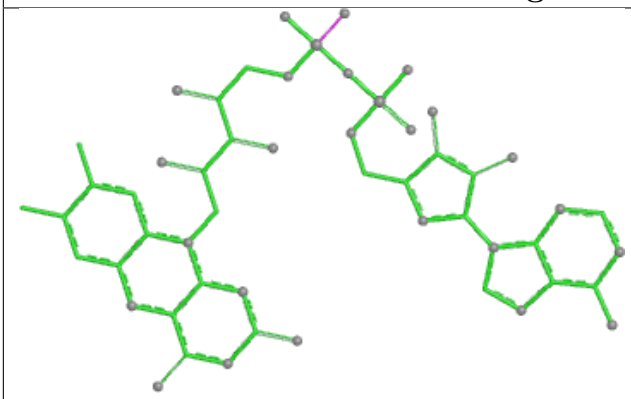
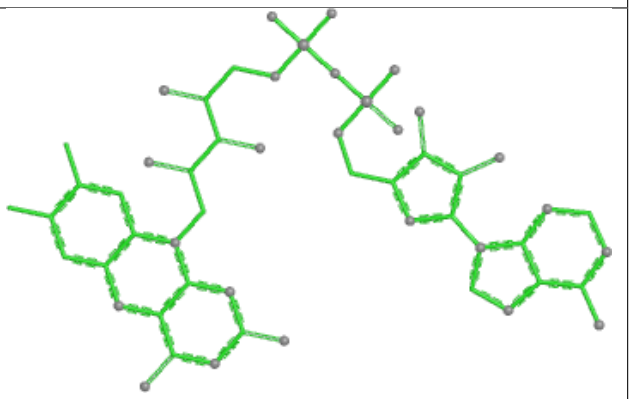
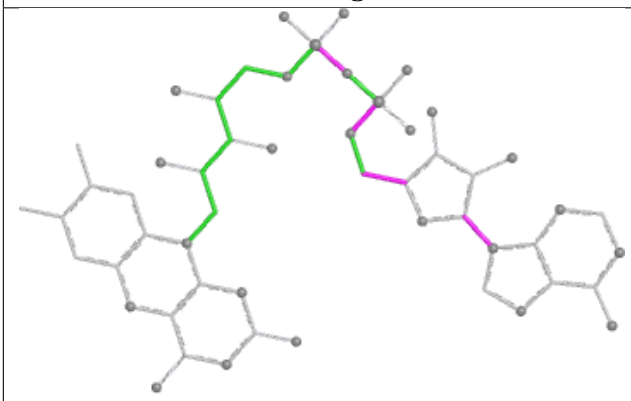
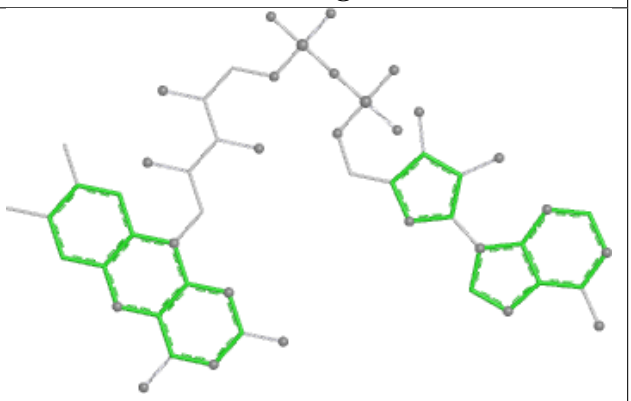
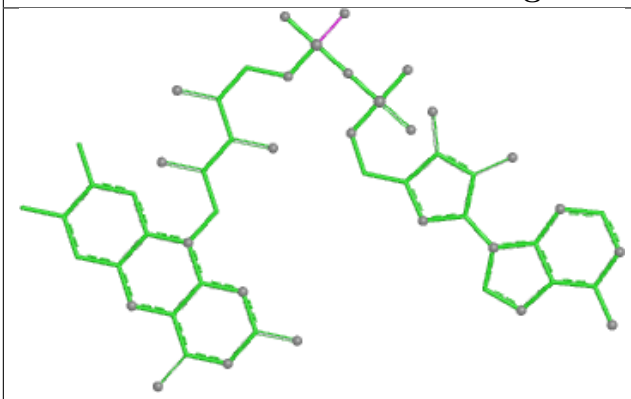
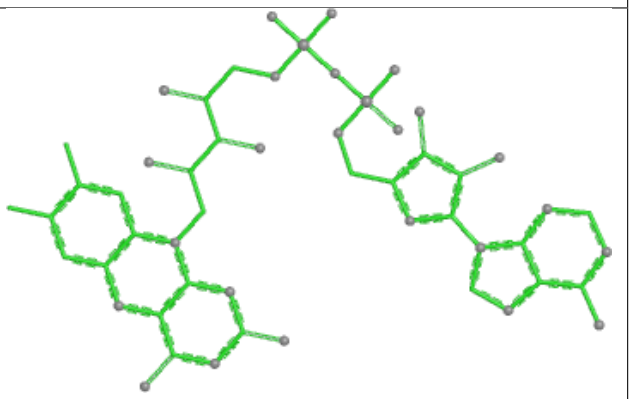
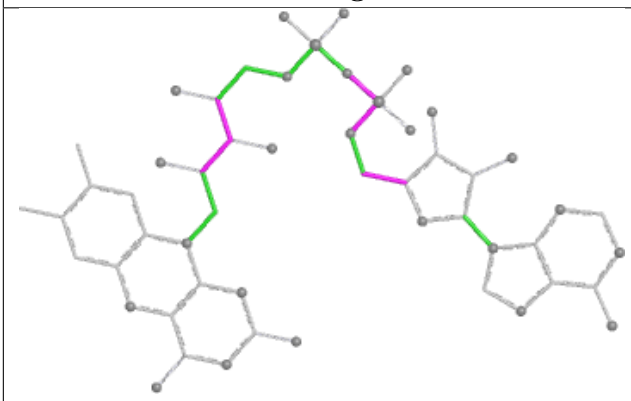
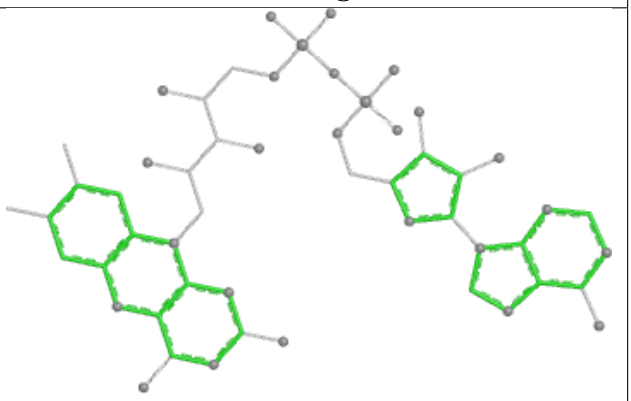
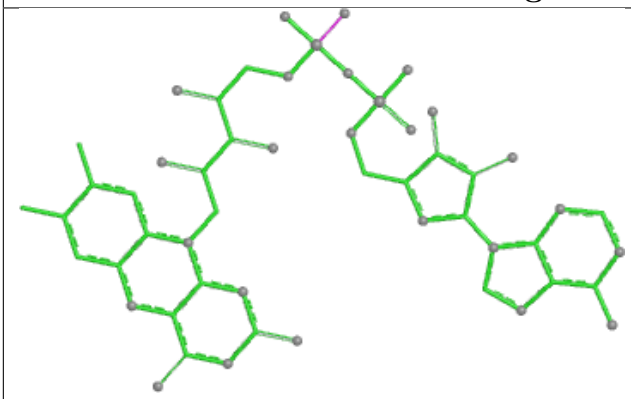
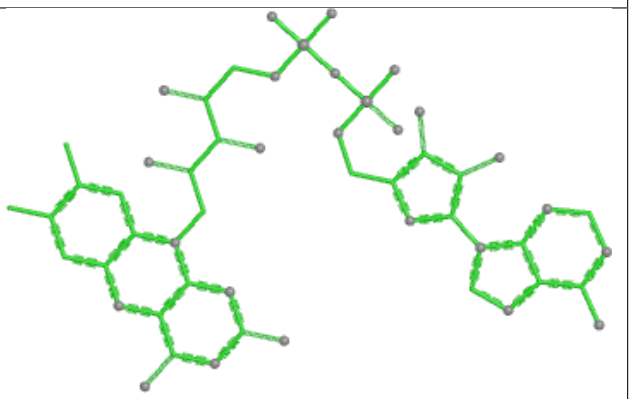
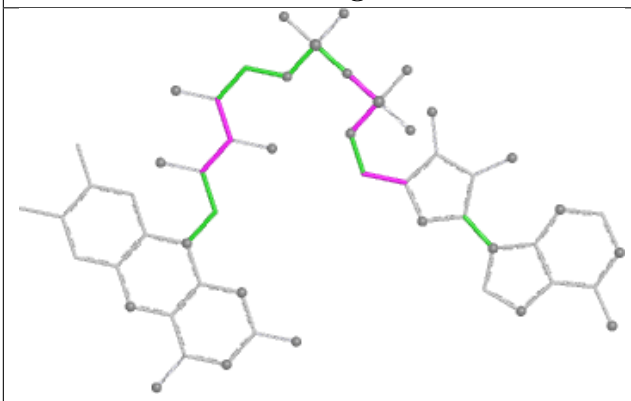
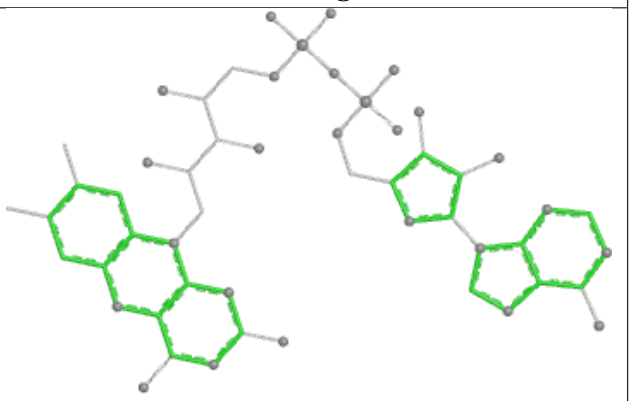
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	501	FAD	2	0
5	C	501	FAD	2	0
7	H	602	SF4	8	0
7	H	601	SF4	8	0
6	C	502	MQ7	2	0
5	B	701	FAD	2	0
5	E	301	FAD	14	0
5	A	301	FAD	15	0
6	G	502	MQ7	1	0
7	D	602	SF4	8	0
7	D	601	SF4	8	0

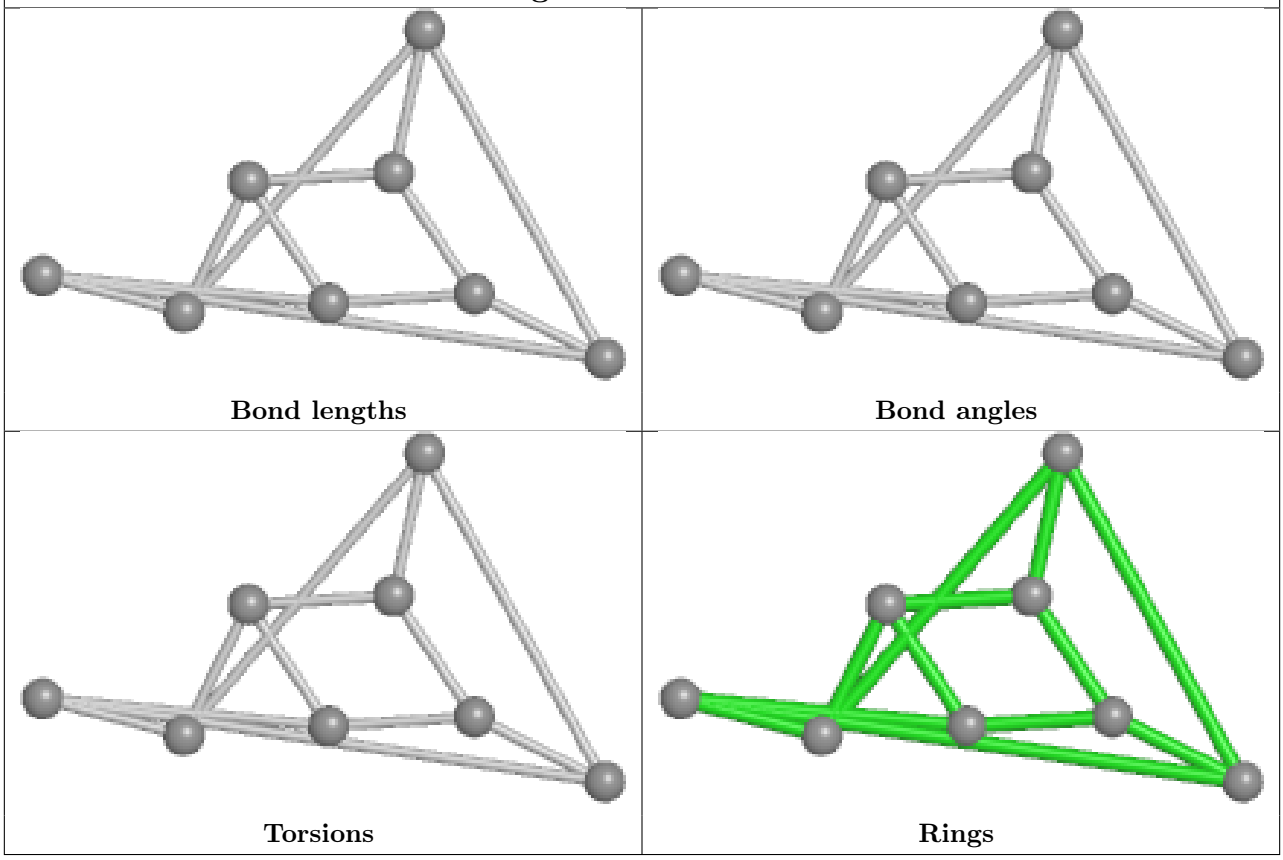
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 F 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

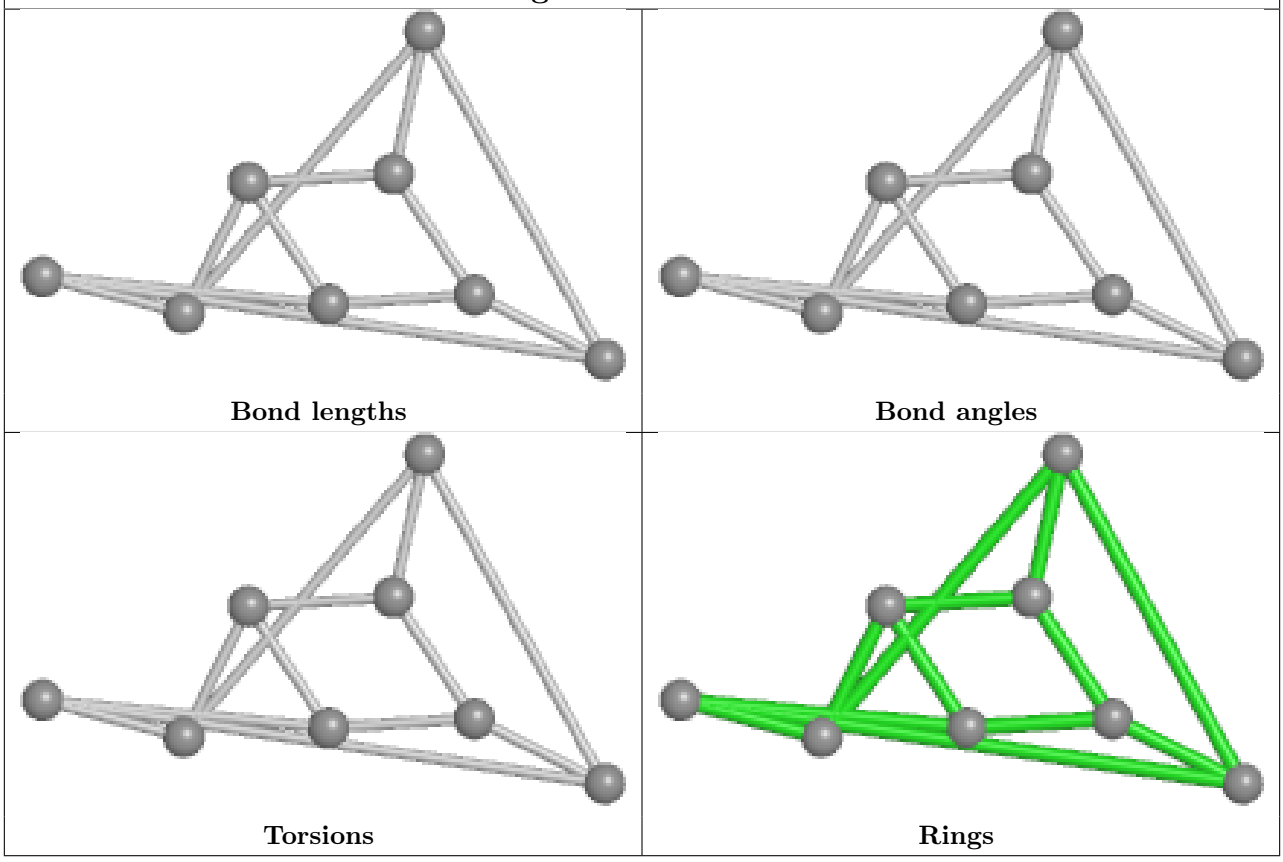
Ligand FAD G 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 H 602



Ligand SF4 H 601



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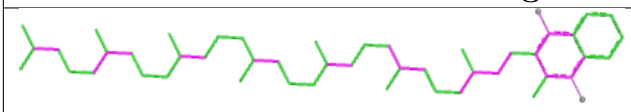
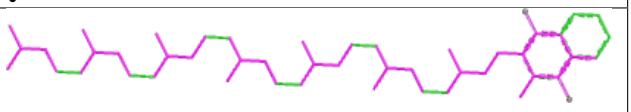
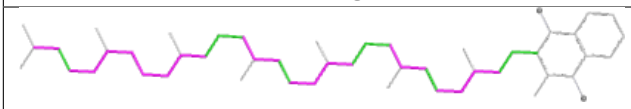
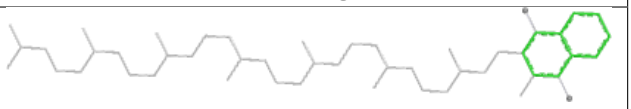
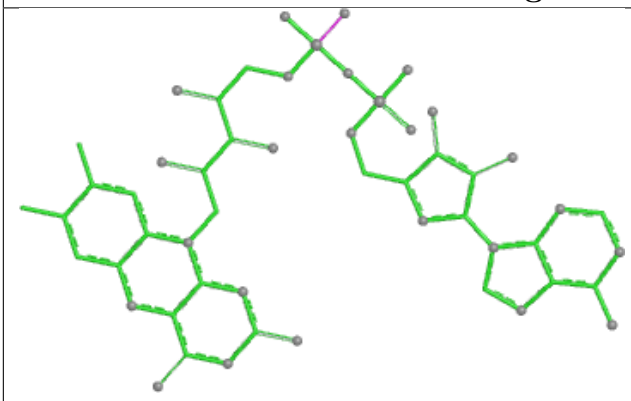
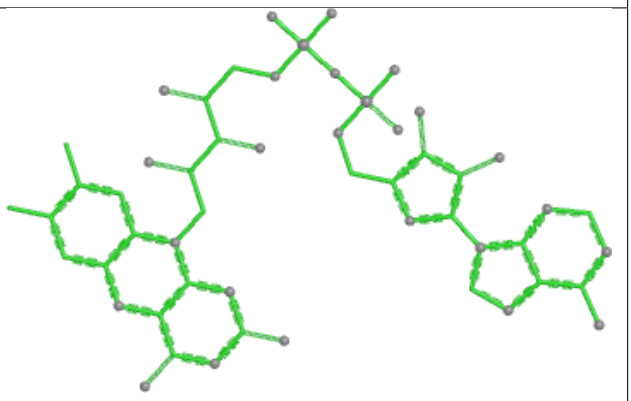
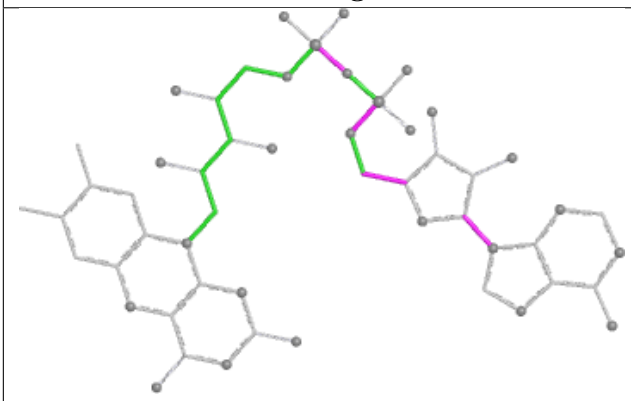
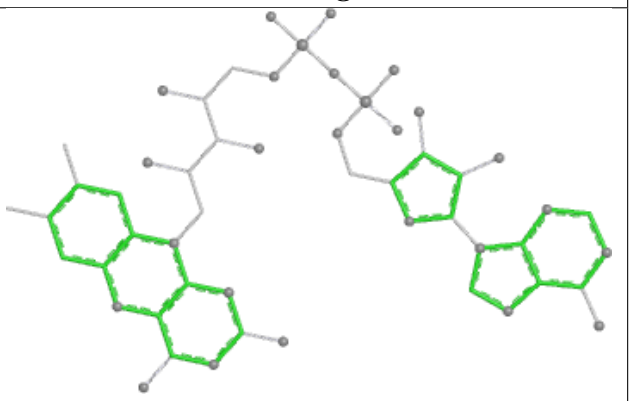
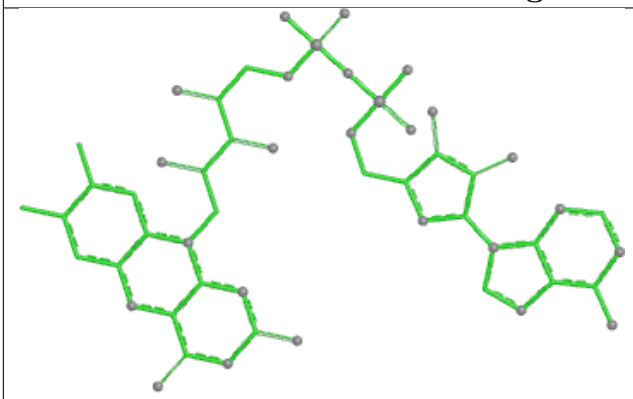
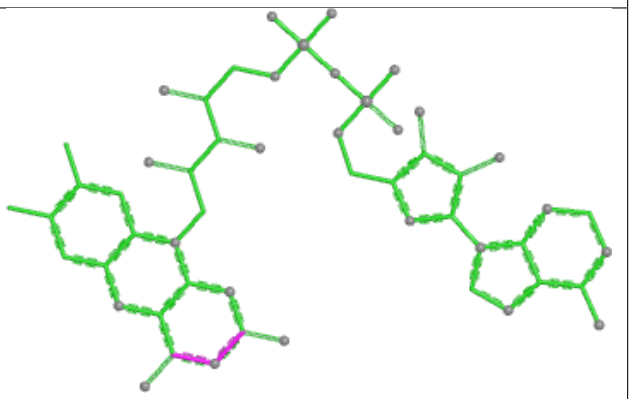
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD B 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

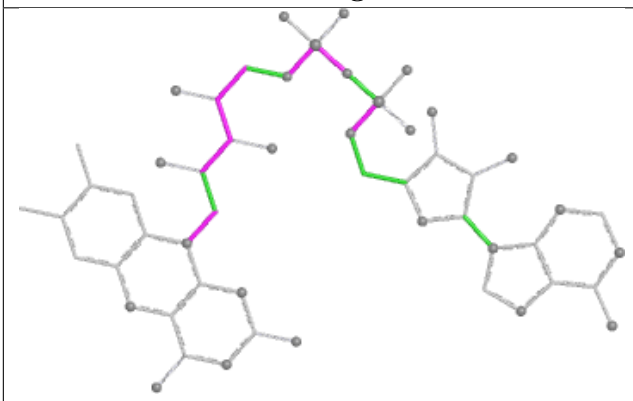
Ligand FAD E 301



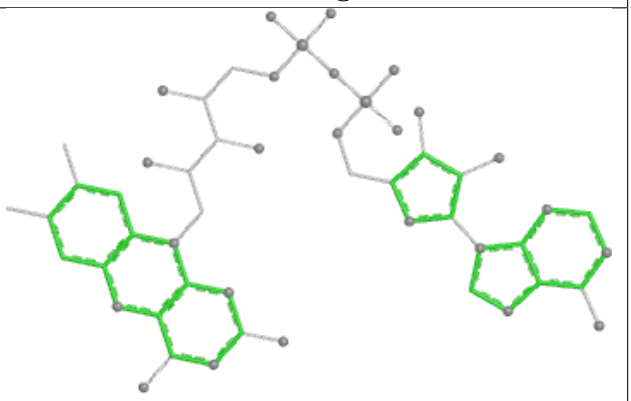
Bond lengths



Bond angles

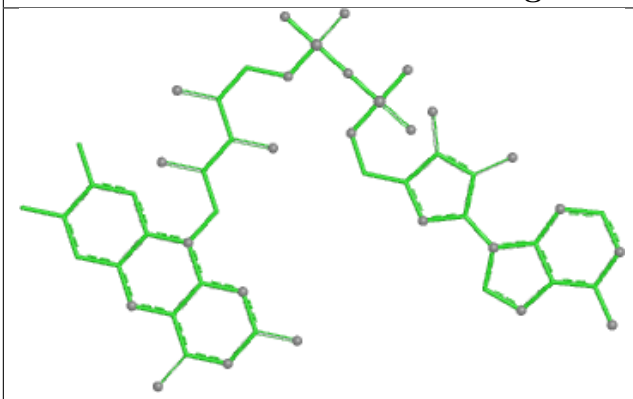


Torsions

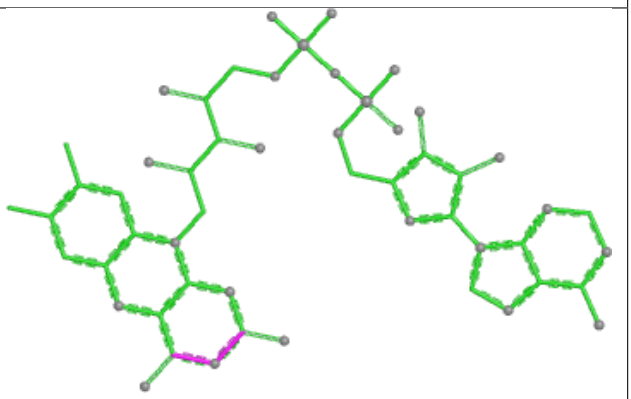


Rings

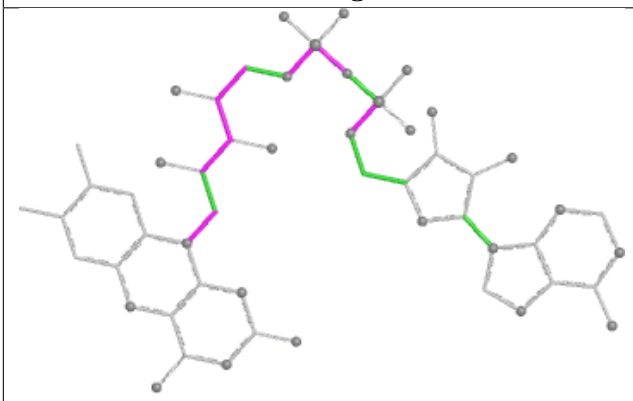
Ligand FAD A 301



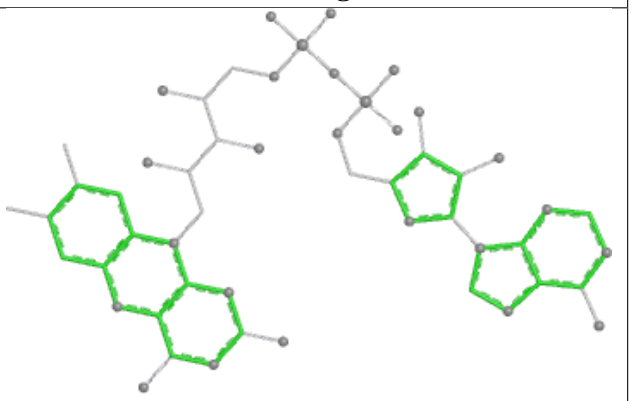
Bond lengths



Bond angles

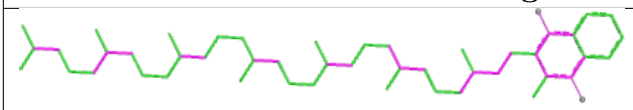


Torsions



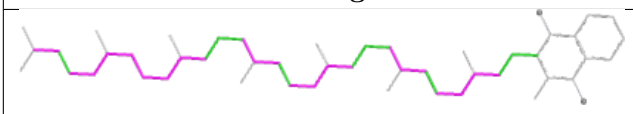
Rings

Ligand MQ7 G 502

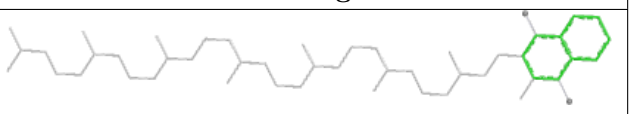


Bond lengths

Bond angles

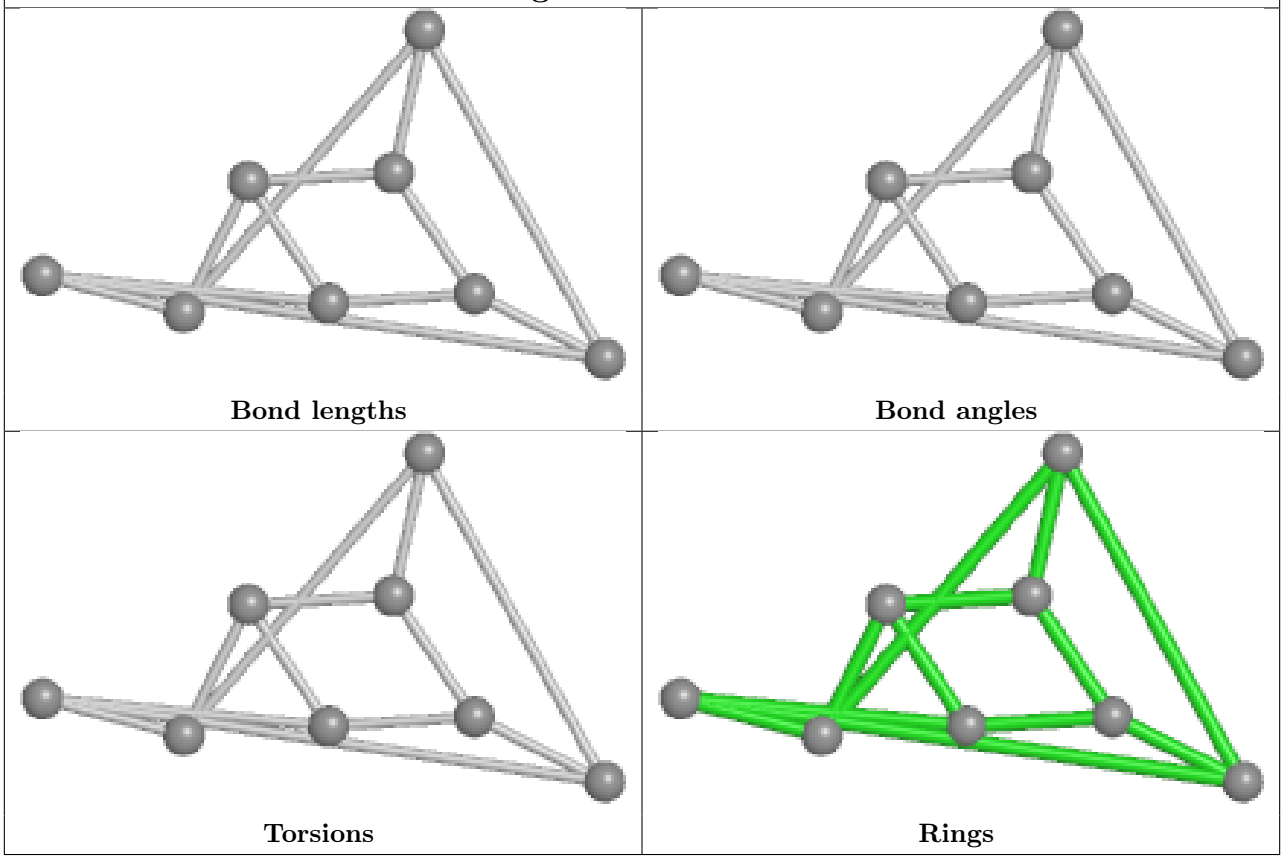


Torsions

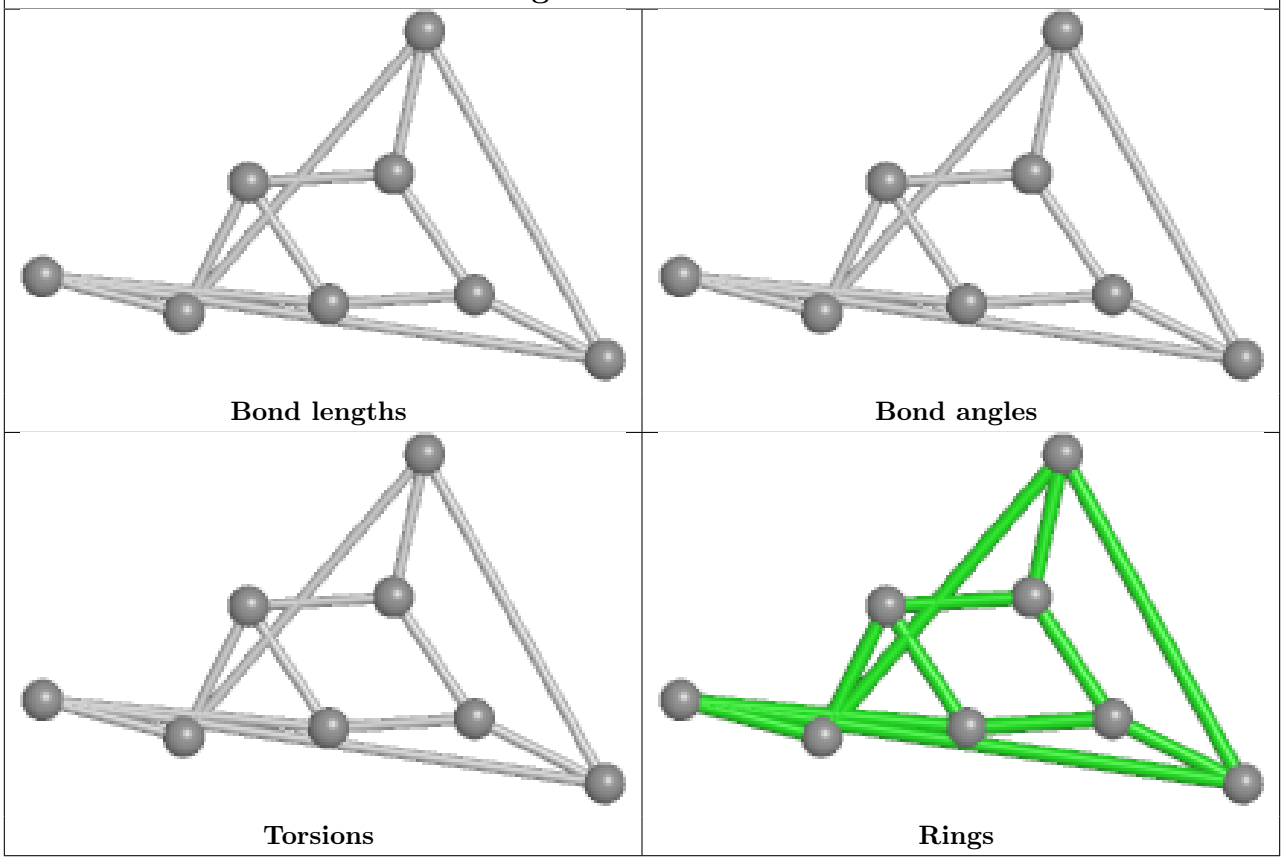


Rings

Ligand SF4 D 602



Ligand SF4 D 601



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.

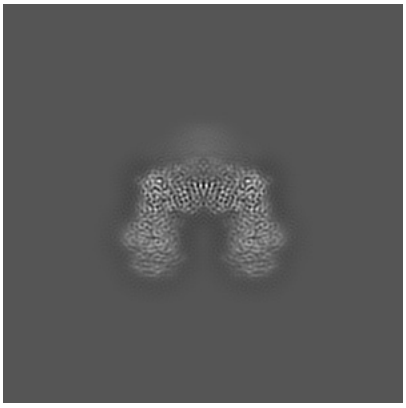
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22973. These allow visual inspection of the internal detail of the map and identification of artifacts.

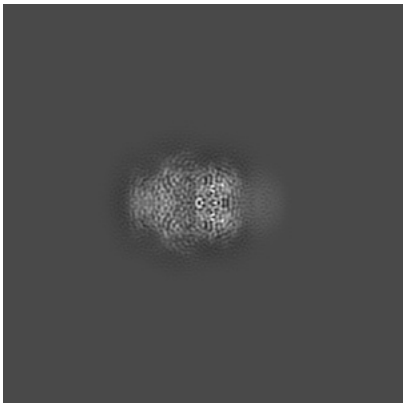
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

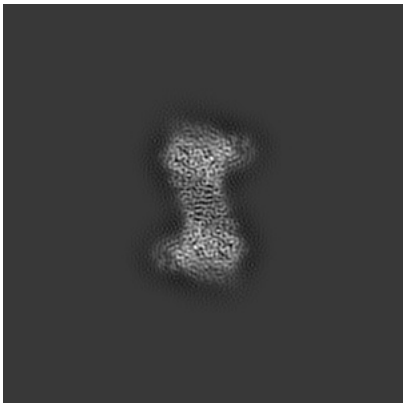
6.1.1 Primary map



X



Y



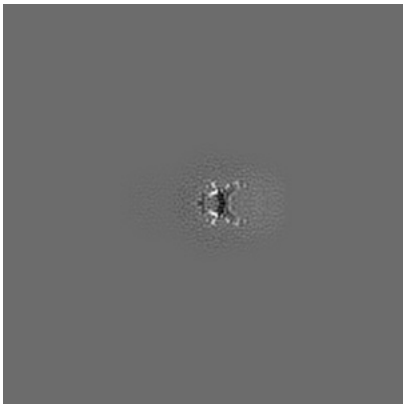
Z

The images above show the map projected in three orthogonal directions.

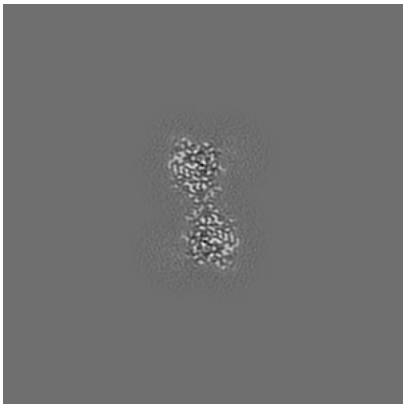
6.2 Central slices (i)

6.2.1 Primary map

X Index: 160



Y Index: 160



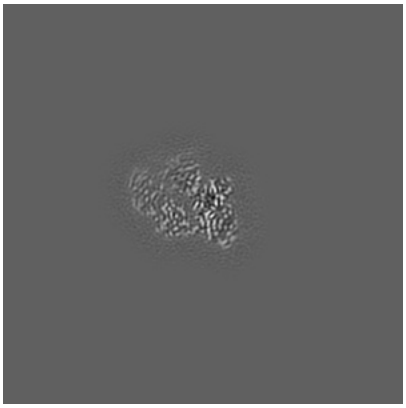
Z Index: 160

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 160



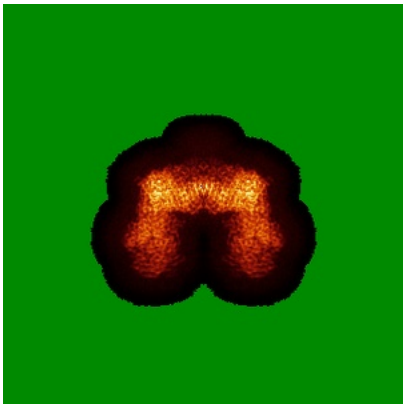
Y Index: 198

Z Index: 168

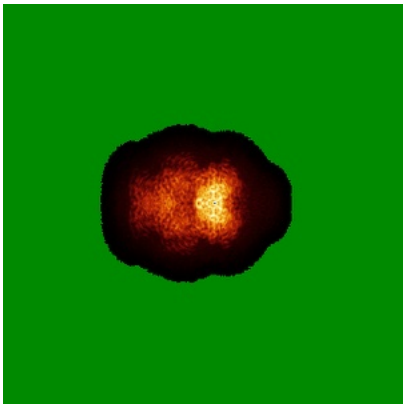
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

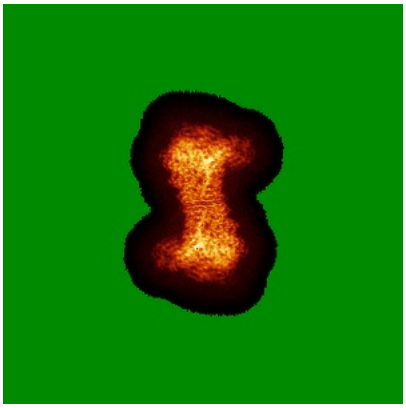
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

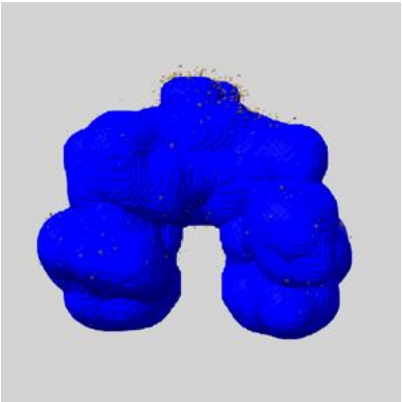
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

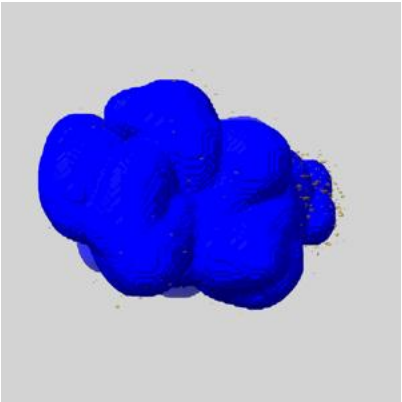
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

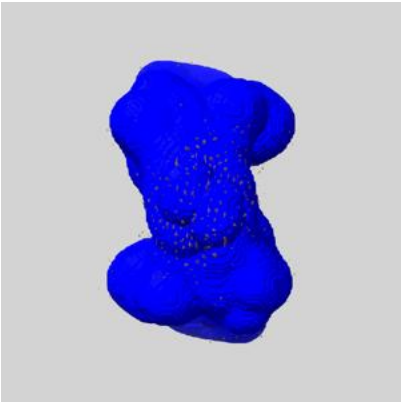
6.6.1 emd_22973_msk_1.map (i)



X



Y

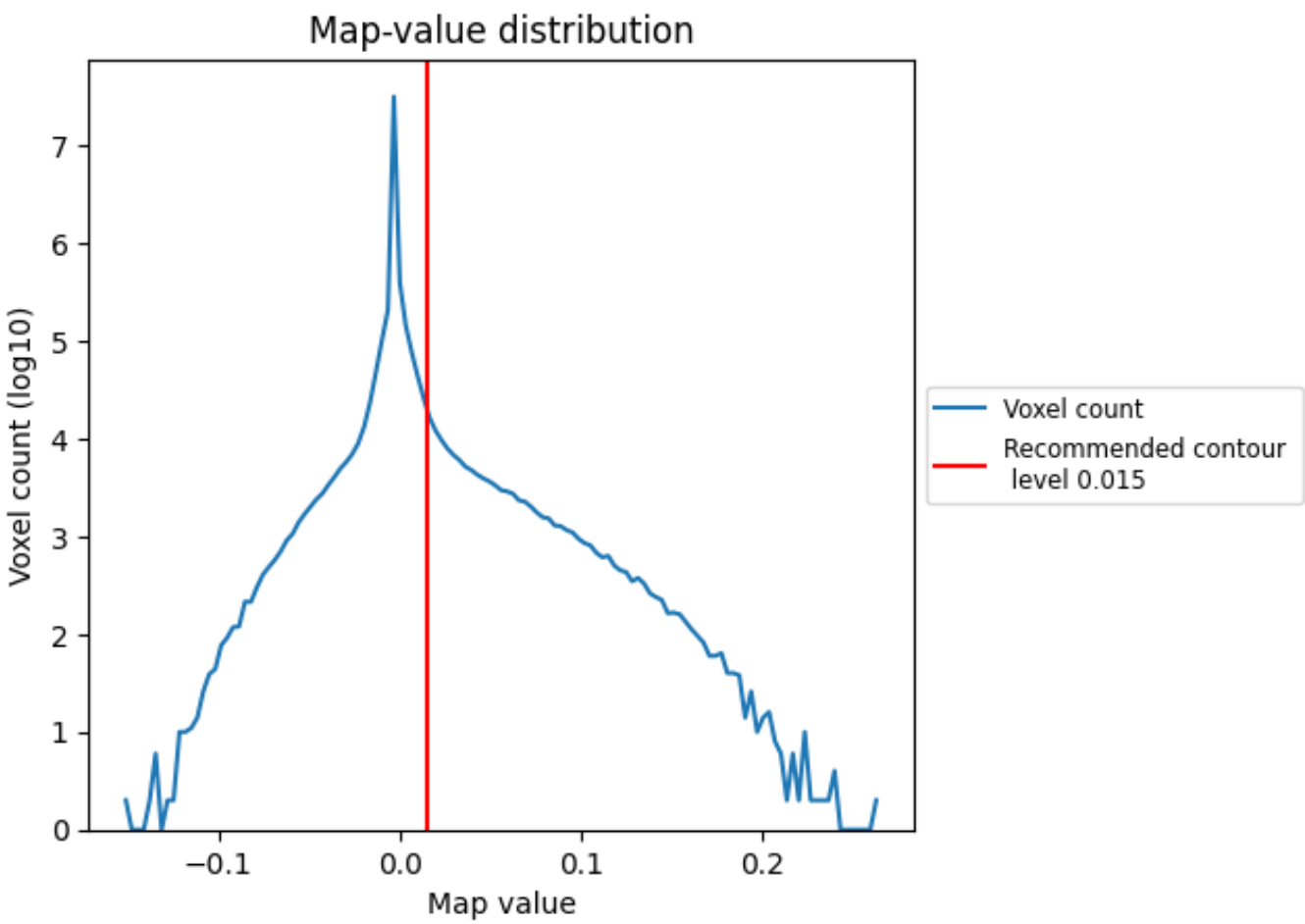


Z

7 Map analysis (i)

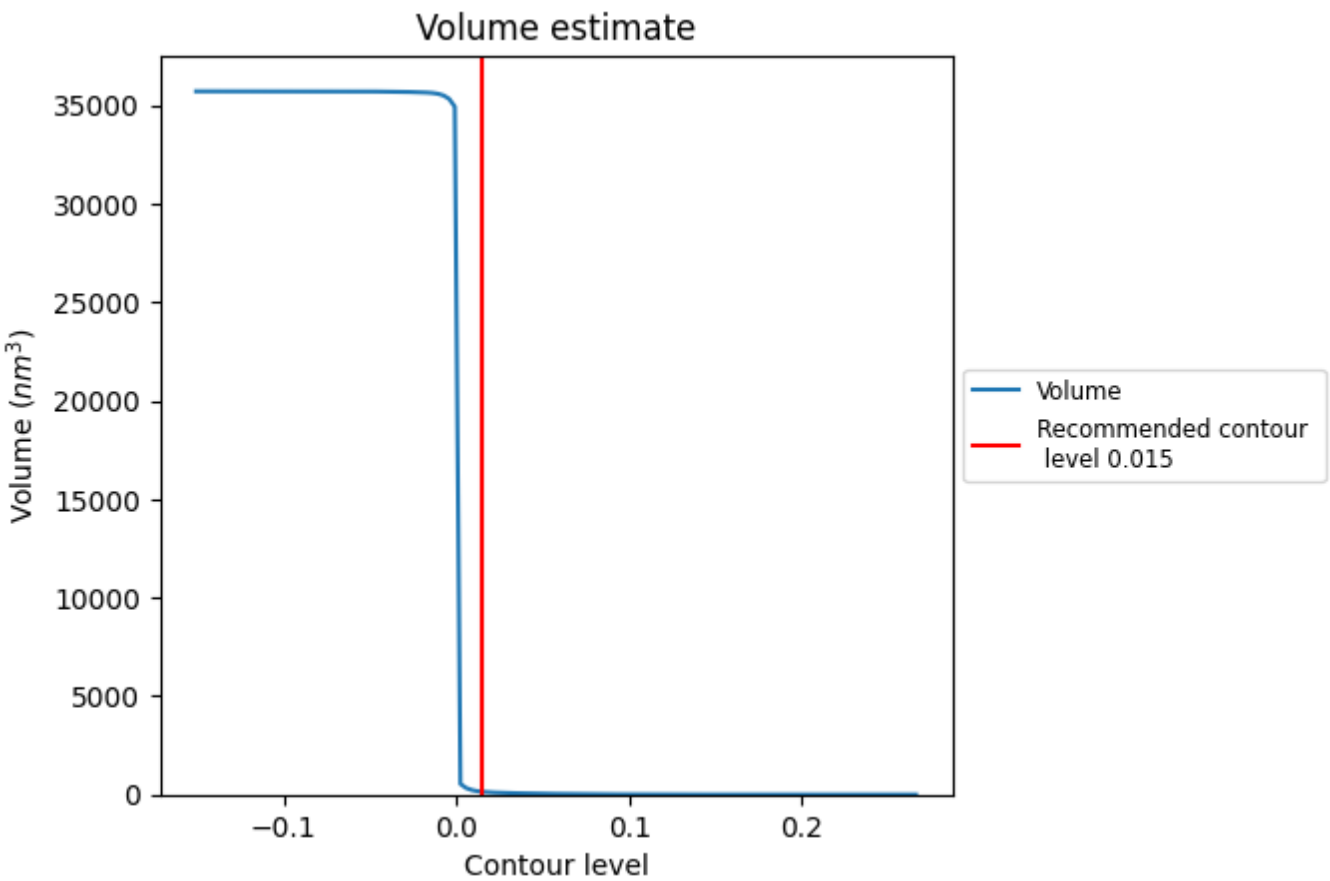
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

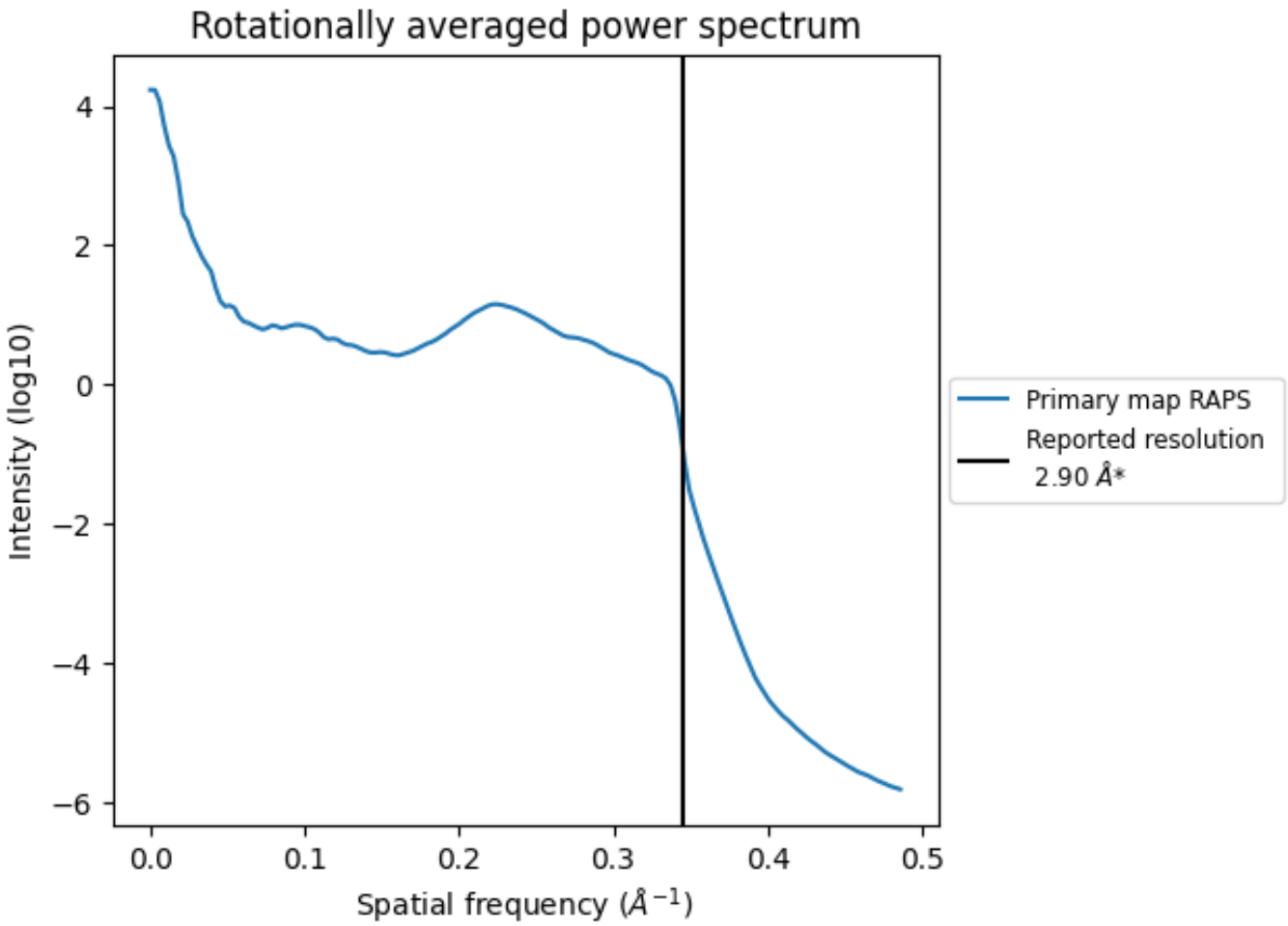
7.2 Volume estimate (i)



The volume at the recommended contour level is 143 nm^3; this corresponds to an approximate mass of 129 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

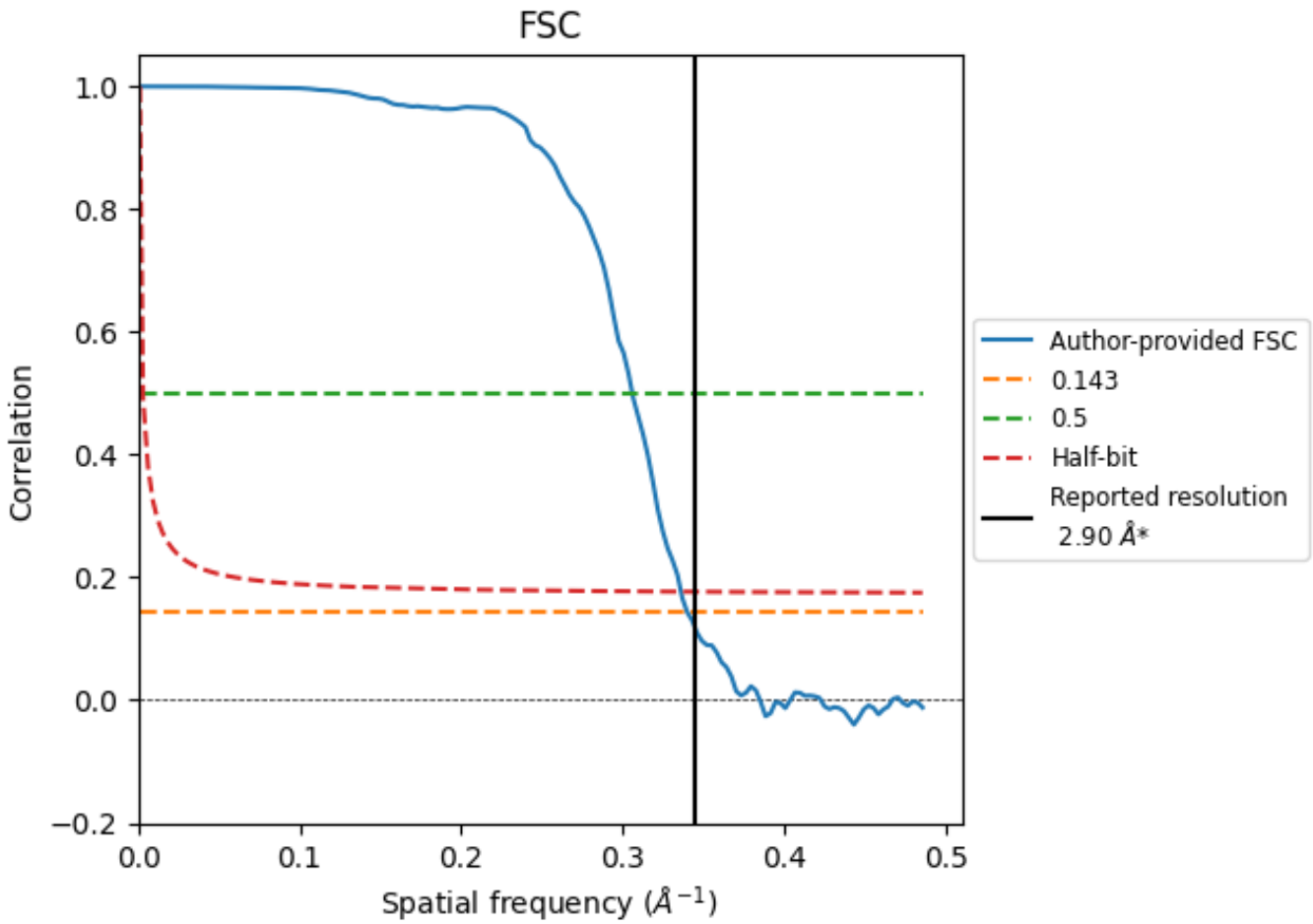


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

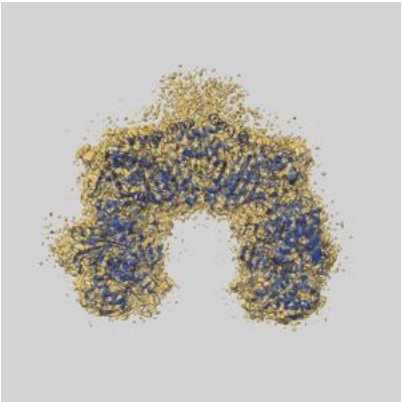
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.27	2.97
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

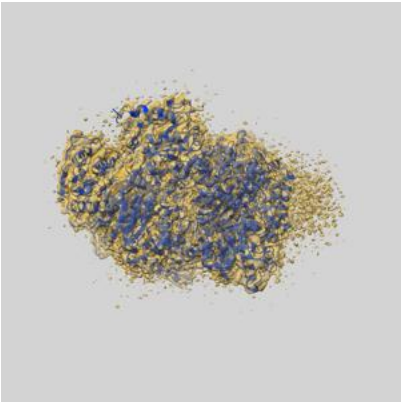
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22973 and PDB model 7KOE. Per-residue inclusion information can be found in section 3 on page 8.

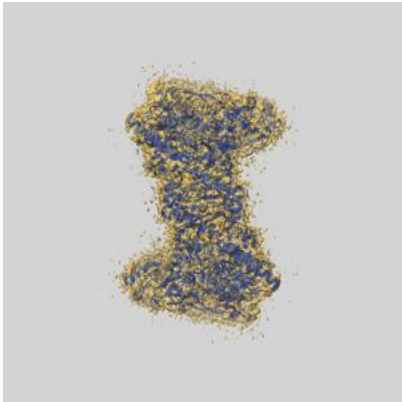
9.1 Map-model overlay (i)



X



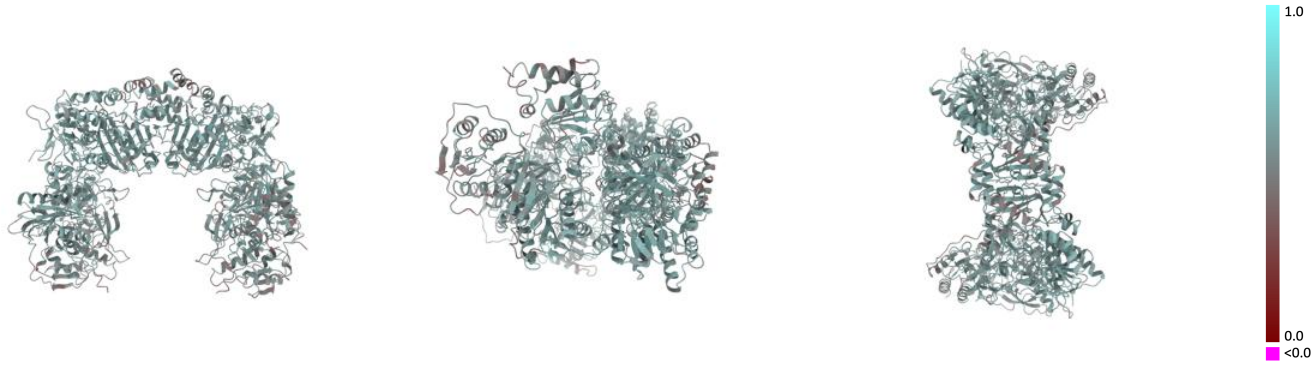
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

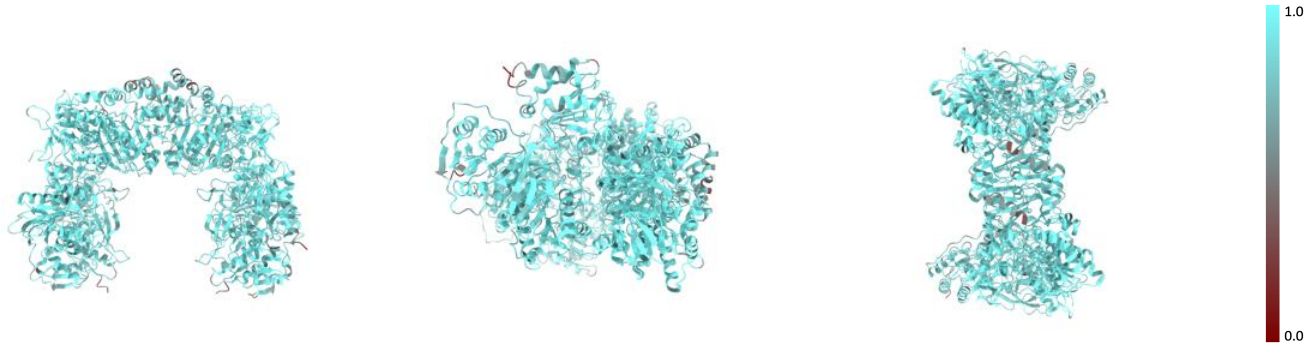
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

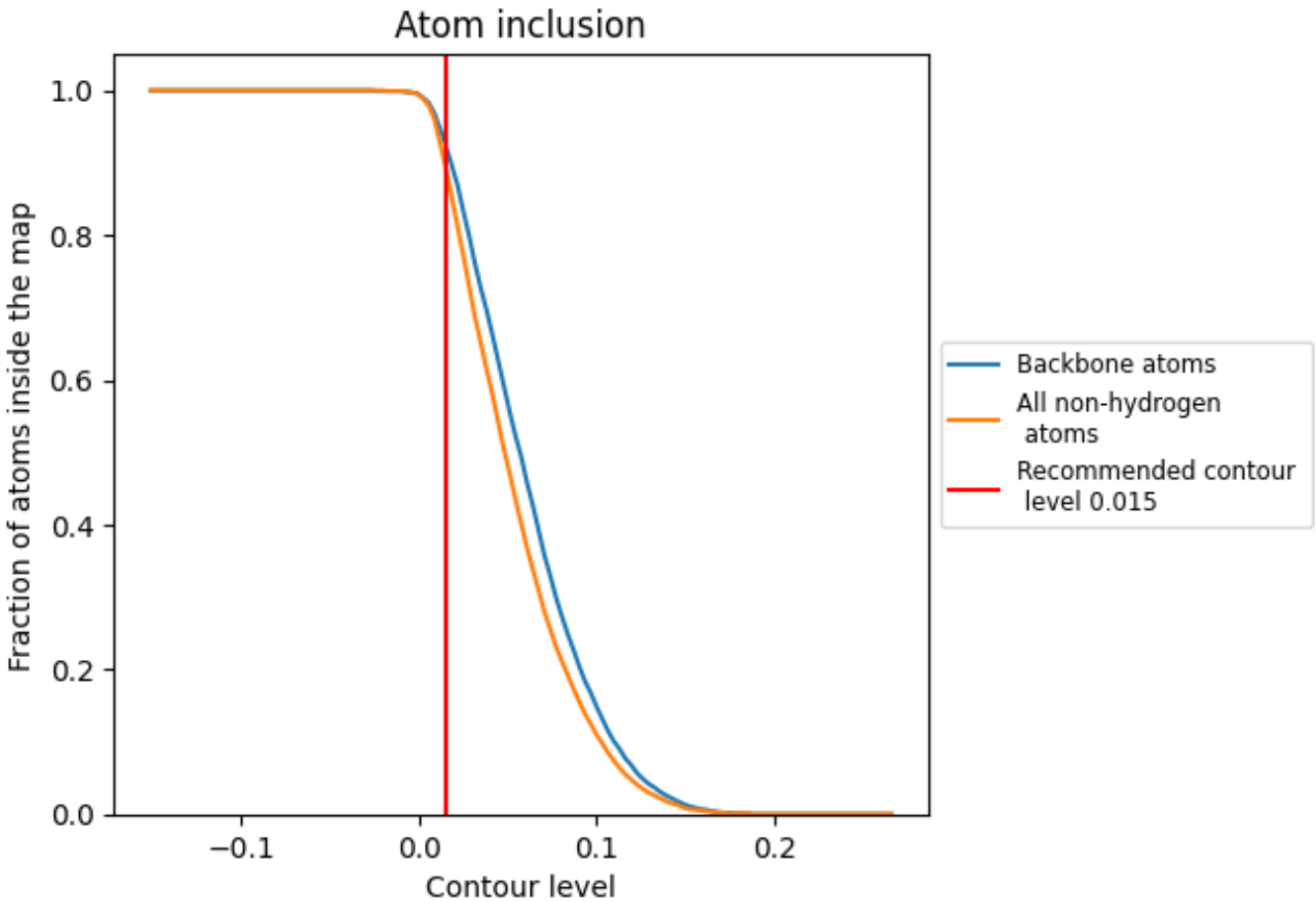
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.5600
A	0.8850	0.5480
B	0.8650	0.5390
C	0.9190	0.5790
D	0.9390	0.5860
E	0.8850	0.5460
F	0.8650	0.5360
G	0.9200	0.5790
H	0.9390	0.5820