



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:01 PM UTC

PDB ID : 1QLB / pdb_00001qlb
Title : respiratory complex II-like fumarate reductase from Wolinella succinogenes
Authors : Lancaster, C.R.D.; Kroeger, A.; Auer, M.; Michel, H.
Deposited on : 1999-08-25
Resolution : 2.33 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

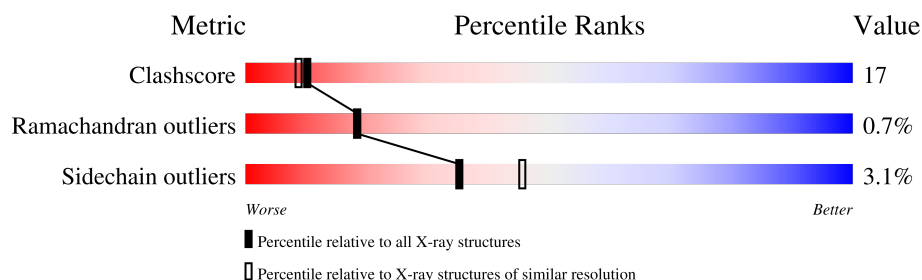
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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))
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	656	
1	D	656	
2	B	239	
2	E	239	
3	C	256	
3	F	256	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19056 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 FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	88	0	0
			5101	3194	913	962	32			
1	D	655	Total	C	N	O	S	88	0	0
			5101	3194	913	962	32			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	ASP	ARG	conflict	UNP P17412
A	282	VAL	CYS	conflict	UNP P17412
A	283	ASP	GLY	conflict	UNP P17412
A	284	GLY	TRP	conflict	UNP P17412
A	285	HIS	THR	conflict	UNP P17412
A	286	ARG	PRO	conflict	UNP P17412
A	287	PHE	ILE	conflict	UNP P17412
A	288	MET	HIS	conflict	UNP P17412
A	289	PRO	ALA	conflict	UNP P17412
D	281	ASP	ARG	conflict	UNP P17412
D	282	VAL	CYS	conflict	UNP P17412
D	283	ASP	GLY	conflict	UNP P17412
D	284	GLY	TRP	conflict	UNP P17412
D	285	HIS	THR	conflict	UNP P17412
D	286	ARG	PRO	conflict	UNP P17412
D	287	PHE	ILE	conflict	UNP P17412
D	288	MET	HIS	conflict	UNP P17412
D	289	PRO	ALA	conflict	UNP P17412

- Molecule 2 is a protein called FUMARATE REDUCTASE IRON-SULFUR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1893	1194	322	354	23			

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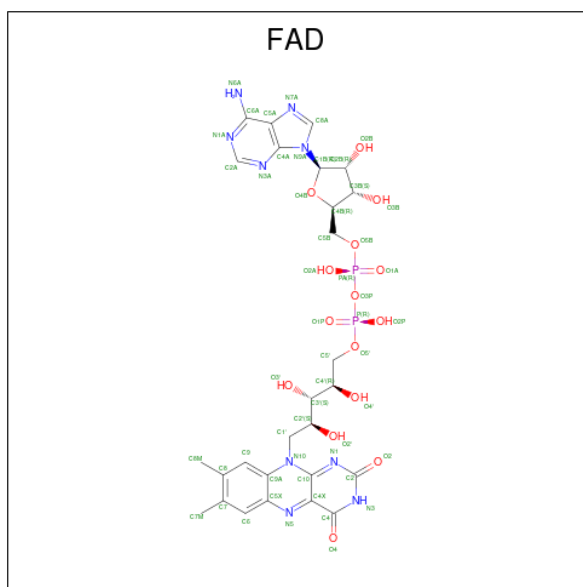
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	239	Total	C	N	O	S	0	0	0
			1893	1194	322	354	23			

- Molecule 3 is a protein called FUMARATE REDUCTASE CYTOCHROME B SUBUNIT.

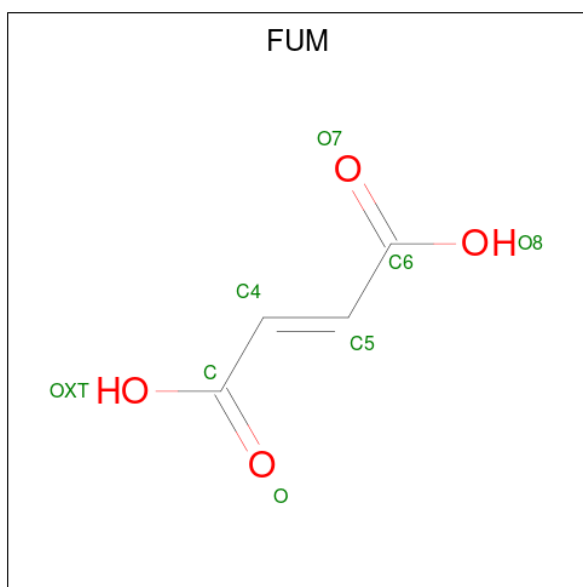
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	254	Total	C	N	O	S	111	0	0
			2080	1388	333	345	14			
3	F	254	Total	C	N	O	S	111	0	0
			2080	1388	333	345	14			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).

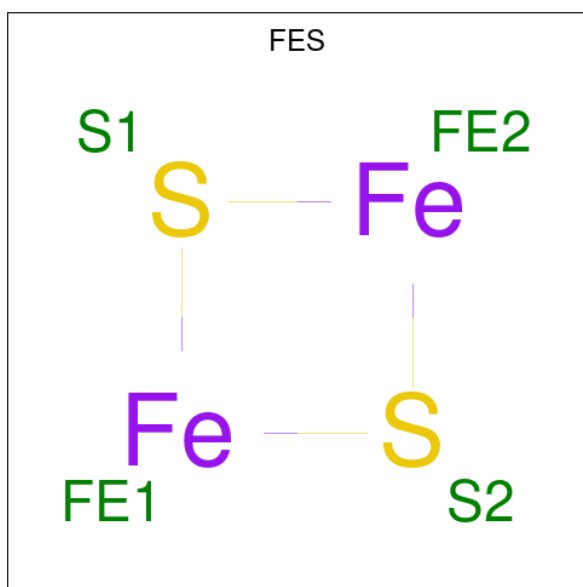


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

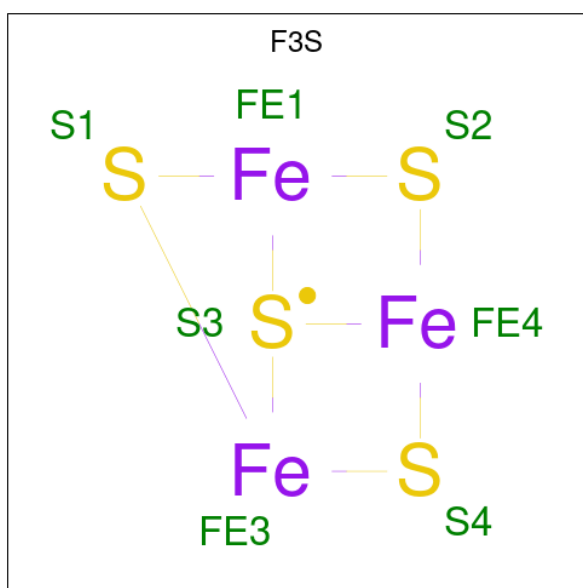
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		

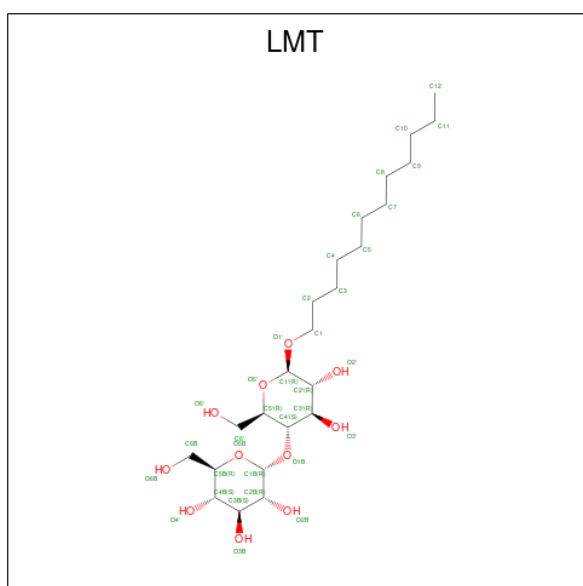
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 8	Fe 4	S 4	0	0
9	E	1	Total 8	Fe 4	S 4	0	0

- # HEM

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 11 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O		
			35	24	11	16	0
11	F	1	Total	C	O		
			35	24	11	16	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	149	Total	O		
			149	149	0	0
12	B	79	Total	O		
			79	79	0	0
12	C	23	Total	O		
			23	23	0	0
12	D	148	Total	O		
			148	148	0	0

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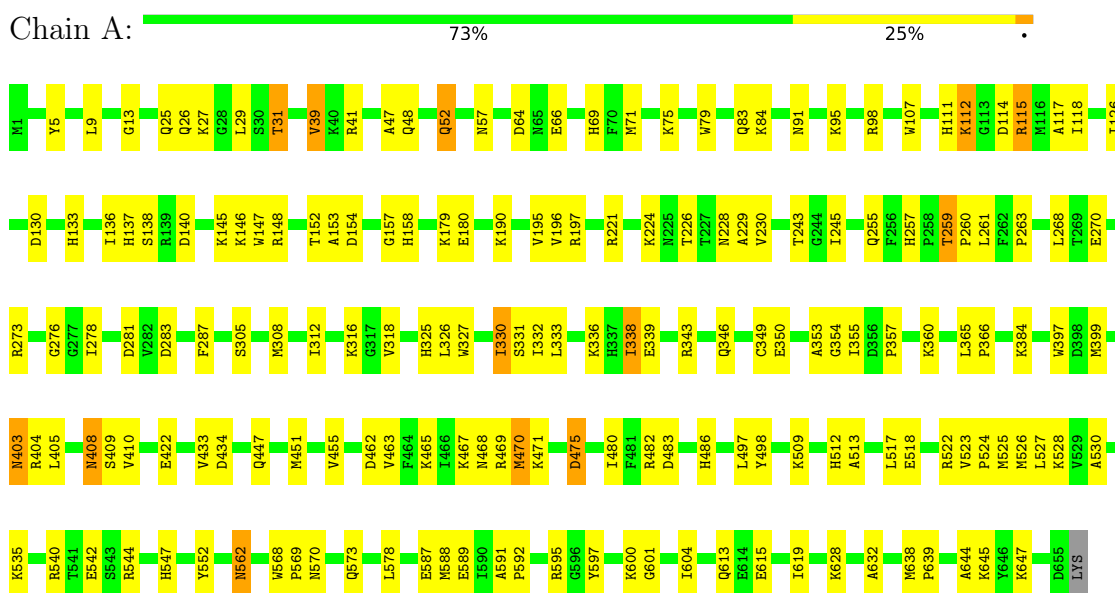
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	83	Total	O	0	0
			83	83		
12	F	22	Total	O	0	0
			22	22		

3 Residue-property plots

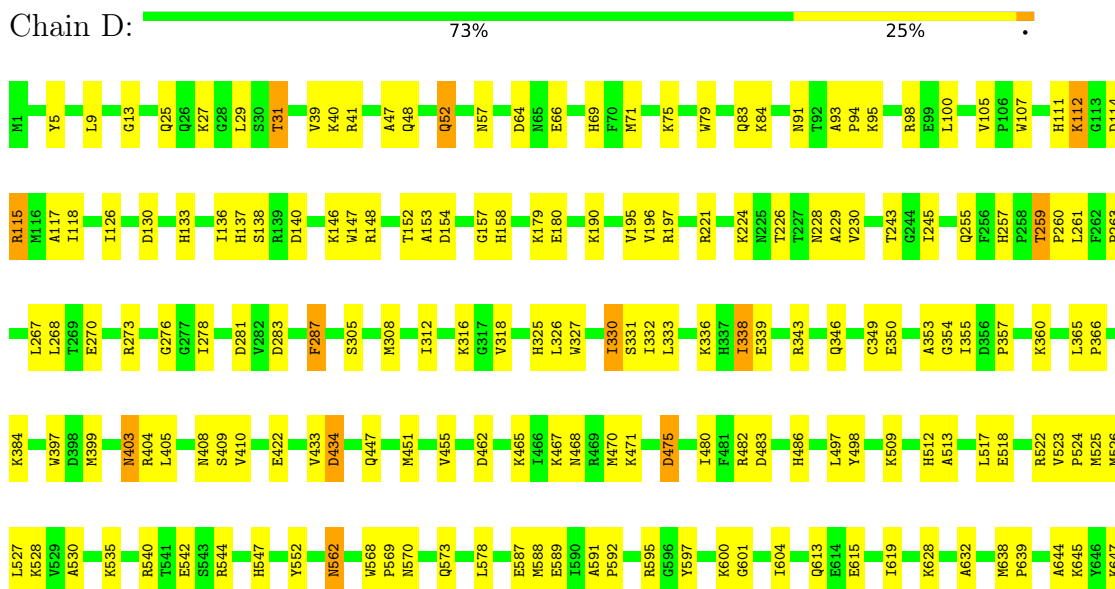
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT



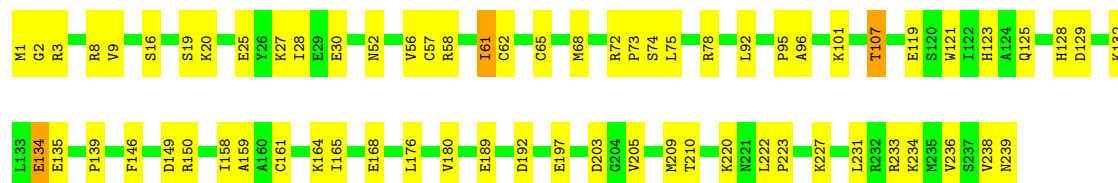
• Molecule 1: FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT





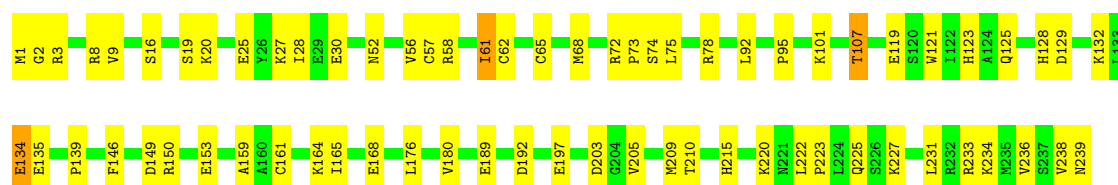
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain B: 72% 27%



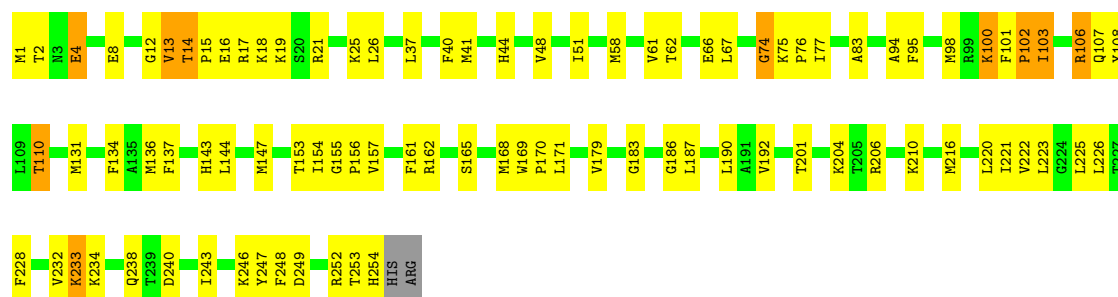
• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN

Chain E: 71% 28%



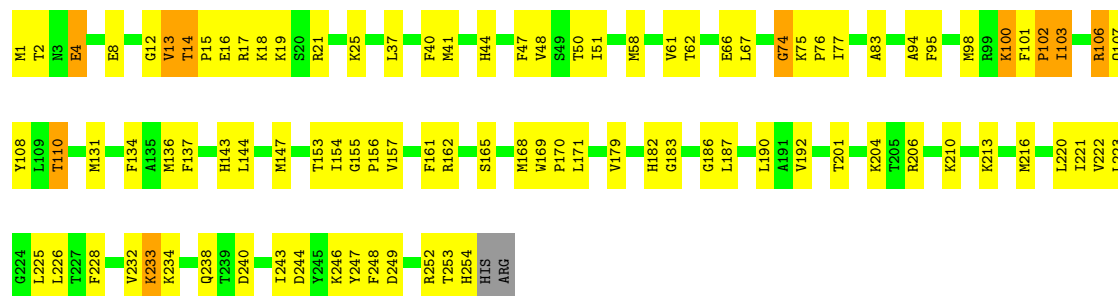
• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

Chain C: 63% 32%



• Molecule 3: FUMARATE REDUCTASE CYTOCHROME B SUBUNIT

Chain F: 62% 34%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.40Å 85.05Å 188.85Å 90.00° 96.46° 90.00°	Depositor
Resolution (Å)	38.87 – 2.33	Depositor
% Data completeness (in resolution range)	95.8 (38.87-2.33)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.213 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19056	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S, HEM, FAD, FUM, LMT, CA, FES

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	0.41	1/5197 (0.0%)	0.91	13/7006 (0.2%)
1	D	0.39	0/5197	0.91	12/7006 (0.2%)
2	B	0.41	0/1930	0.90	7/2604 (0.3%)
2	E	0.40	0/1930	0.90	6/2604 (0.2%)
3	C	0.34	0/2146	0.83	3/2904 (0.1%)
3	F	0.34	0/2146	0.83	3/2904 (0.1%)
All	All	0.39	1/18546 (0.0%)	0.89	44/25028 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	MET	SD-CE	-5.13	1.66	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	397	TRP	N-CA-C	-10.52	99.89	111.36
1	A	397	TRP	N-CA-C	-10.47	99.95	111.36
3	C	102	PRO	N-CA-C	-9.15	96.82	111.19
3	F	102	PRO	N-CA-C	-9.13	96.85	111.19
1	A	399	MET	N-CA-C	-7.78	102.87	113.30
1	D	399	MET	N-CA-C	-7.76	102.89	113.30
1	D	568	TRP	CA-C-N	7.19	126.71	119.24
1	D	568	TRP	C-N-CA	7.19	126.71	119.24
2	E	65	CYS	N-CA-C	6.96	120.35	112.97
2	B	65	CYS	N-CA-C	6.95	120.33	112.97
1	A	568	TRP	CA-C-N	6.69	126.20	119.24
1	A	568	TRP	C-N-CA	6.69	126.20	119.24
3	C	103	ILE	N-CA-C	6.40	119.05	112.90
1	A	259	THR	N-CA-C	6.31	123.75	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	GLU	N-CA-C	6.30	118.96	111.33
1	D	259	THR	N-CA-C	6.30	123.74	109.81
2	E	168	GLU	N-CA-C	6.23	118.87	111.33
3	F	103	ILE	N-CA-C	6.20	118.85	112.90
1	D	195	VAL	N-CA-C	-5.84	100.17	108.58
1	A	195	VAL	N-CA-C	-5.84	100.18	108.58
1	D	552	TYR	CA-C-N	5.83	125.53	119.82
1	D	552	TYR	C-N-CA	5.83	125.53	119.82
1	A	552	TYR	CA-C-N	5.80	125.50	119.82
1	A	552	TYR	C-N-CA	5.80	125.50	119.82
2	E	9	VAL	N-CA-C	5.66	116.03	108.11
2	B	9	VAL	N-CA-C	5.64	116.00	108.11
2	E	2	GLY	N-CA-C	-5.60	108.31	115.42
2	B	2	GLY	N-CA-C	-5.52	108.41	115.42
2	E	161	CYS	N-CA-C	5.44	117.10	108.67
2	B	161	CYS	N-CA-C	5.43	117.09	108.67
1	D	287	PHE	N-CA-C	5.39	119.97	112.90
1	D	410	VAL	N-CA-C	-5.33	104.29	111.44
1	A	39	VAL	N-CA-C	5.33	117.71	111.05
1	A	287	PHE	N-CA-C	5.32	119.88	112.90
1	A	243	THR	N-CA-C	-5.32	106.30	112.89
2	E	203	ASP	N-CA-C	-5.31	106.85	113.38
1	A	410	VAL	N-CA-C	-5.29	104.36	111.44
1	D	243	THR	N-CA-C	-5.21	106.44	112.89
3	C	249	ASP	N-CA-C	5.14	116.78	108.41
3	F	249	ASP	N-CA-C	5.12	116.75	108.41
1	D	153	ALA	CB-CA-C	-5.10	110.67	116.54
1	A	153	ALA	CB-CA-C	-5.08	110.70	116.54
2	B	158	ILE	N-CA-C	-5.05	106.76	111.45
2	B	203	ASP	N-CA-C	-5.03	107.20	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5101	0	5079	165	0
1	D	5101	0	5079	163	0
2	B	1893	0	1861	63	0
2	E	1893	0	1861	65	0
3	C	2080	0	2101	103	0
3	F	2080	0	2101	105	0
4	A	53	0	29	1	0
4	D	53	0	29	1	0
5	A	8	0	1	2	0
5	D	8	0	1	1	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
8	B	7	0	0	0	0
8	E	7	0	0	0	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
10	C	86	0	60	7	0
10	F	86	0	60	8	0
11	C	35	0	46	7	0
11	F	35	0	46	8	0
12	A	149	0	0	9	0
12	B	79	0	0	2	0
12	C	23	0	0	0	0
12	D	148	0	0	7	0
12	E	83	0	0	3	0
12	F	22	0	0	0	0
All	All	19056	0	18354	618	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 17.

All (618) 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)
3:F:253:THR:HG22	3:F:254:HIS:H	1.25	0.99
3:C:253:THR:HG22	3:C:254:HIS:H	1.25	0.98
2:B:239:ASN:ND2	3:C:21:ARG:HH21	1.64	0.96
2:E:239:ASN:ND2	3:F:21:ARG:HH21	1.64	0.95
2:E:239:ASN:HD22	3:F:21:ARG:HH21	1.15	0.91
2:B:239:ASN:HD22	3:C:21:ARG:HH21	1.14	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:ARG:HG2	2:B:25:GLU:HG2	1.52	0.91
2:E:8:ARG:HG2	2:E:25:GLU:HG2	1.52	0.90
3:F:14:THR:HG22	3:F:16:GLU:H	1.36	0.90
1:A:41:ARG:HH21	2:B:107:THR:CG2	1.86	0.89
3:C:248:PHE:HB3	3:C:254:HIS:HD2	1.38	0.87
1:A:535:LYS:HG3	1:A:578:LEU:HD11	1.57	0.87
1:D:41:ARG:HH21	2:E:107:THR:CG2	1.87	0.87
3:C:14:THR:HG22	3:C:16:GLU:H	1.37	0.86
3:F:248:PHE:HB3	3:F:254:HIS:HD2	1.38	0.86
1:D:535:LYS:HG3	1:D:578:LEU:HD11	1.57	0.85
3:C:103:ILE:H	3:C:107:GLN:NE2	1.75	0.84
3:F:103:ILE:H	3:F:107:GLN:NE2	1.75	0.84
1:D:112:LYS:HG3	1:D:130:ASP:HA	1.60	0.84
1:A:112:LYS:HG3	1:A:130:ASP:HA	1.59	0.84
1:A:346:GLN:HA	1:A:357:PRO:HG2	1.61	0.83
3:C:106:ARG:O	3:C:110:THR:HB	1.79	0.82
1:A:570:ASN:H	1:A:573:GLN:HE21	1.26	0.82
1:D:346:GLN:HA	1:D:357:PRO:HG2	1.61	0.82
3:F:106:ARG:O	3:F:110:THR:HB	1.79	0.82
1:D:570:ASN:H	1:D:573:GLN:HE21	1.26	0.82
1:D:338:ILE:HG12	1:D:339:GLU:H	1.45	0.82
1:A:338:ILE:HG12	1:A:339:GLU:H	1.45	0.81
3:C:94:ALA:HB2	10:C:1255:HEM:HBB2	1.64	0.80
1:D:83:GLN:HB2	1:D:638:MET:HE1	1.65	0.79
1:D:115:ARG:HG2	1:D:115:ARG:HH11	1.47	0.79
3:F:94:ALA:HB2	10:F:1255:HEM:HBB2	1.65	0.79
1:A:83:GLN:HB2	1:A:638:MET:HE1	1.64	0.79
3:C:248:PHE:O	3:C:254:HIS:HB3	1.83	0.79
3:F:248:PHE:O	3:F:254:HIS:HB3	1.83	0.78
1:A:115:ARG:HG2	1:A:115:ARG:HH11	1.48	0.78
1:A:587:GLU:O	1:A:638:MET:HE2	1.86	0.76
2:B:209:MET:SD	3:C:100:LYS:HG3	2.26	0.76
1:D:587:GLU:O	1:D:638:MET:HE2	1.86	0.76
1:A:482:ARG:HH11	1:A:547:HIS:HD2	1.33	0.76
1:D:570:ASN:O	1:D:573:GLN:HG2	1.87	0.75
3:C:248:PHE:HB3	3:C:254:HIS:CD2	2.21	0.75
1:A:112:LYS:H	1:A:133:HIS:HD2	1.34	0.75
3:F:248:PHE:HB3	3:F:254:HIS:CD2	2.21	0.75
1:A:570:ASN:O	1:A:573:GLN:HG2	1.87	0.75
1:D:112:LYS:H	1:D:133:HIS:HD2	1.35	0.75
1:D:482:ARG:HH11	1:D:547:HIS:HD2	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:MET:SD	3:F:100:LYS:HG3	2.27	0.75
1:A:470:MET:HE3	1:A:527:LEU:HD23	1.67	0.74
1:D:52:GLN:HG2	1:D:69:HIS:NE2	2.02	0.74
1:A:52:GLN:HG2	1:A:69:HIS:NE2	2.02	0.74
1:D:570:ASN:H	1:D:573:GLN:NE2	1.84	0.74
1:A:330:ILE:HD13	1:A:330:ILE:H	1.52	0.74
1:A:273:ARG:HE	1:A:273:ARG:HA	1.53	0.73
1:A:41:ARG:HH21	2:B:107:THR:HG23	1.52	0.73
1:A:570:ASN:H	1:A:573:GLN:NE2	1.84	0.73
1:D:470:MET:HE3	1:D:527:LEU:HD23	1.69	0.73
1:D:589:GLU:N	1:D:638:MET:HE3	2.04	0.73
1:D:261:LEU:HG	1:D:268:LEU:HG	1.71	0.72
1:A:470:MET:CE	1:A:527:LEU:HA	2.19	0.72
1:A:589:GLU:N	1:A:638:MET:HE3	2.04	0.72
1:D:470:MET:CE	1:D:527:LEU:HA	2.19	0.72
1:D:273:ARG:HE	1:D:273:ARG:HA	1.53	0.72
1:D:41:ARG:HH21	2:E:107:THR:HG23	1.52	0.72
1:A:261:LEU:HG	1:A:268:LEU:HG	1.71	0.72
1:D:330:ILE:HD13	1:D:330:ILE:H	1.52	0.72
1:A:83:GLN:CB	1:A:638:MET:HE1	2.20	0.71
1:D:136:ILE:HD12	2:E:134:GLU:HG2	1.72	0.71
1:A:179:LYS:HG3	1:A:196:VAL:CG1	2.21	0.71
1:D:83:GLN:CB	1:D:638:MET:HE1	2.20	0.71
1:D:179:LYS:HG3	1:D:196:VAL:CG1	2.21	0.71
2:E:165:ILE:HG22	3:F:110:THR:HG23	1.73	0.71
3:F:14:THR:HG23	3:F:15:PRO:HD2	1.74	0.70
3:F:108:TYR:HD2	11:F:1257:LMT:H52	1.56	0.70
2:B:239:ASN:HD22	3:C:21:ARG:NH2	1.89	0.70
3:C:108:TYR:HD2	11:C:1257:LMT:H52	1.56	0.70
2:E:239:ASN:HD22	3:F:21:ARG:NH2	1.89	0.70
1:A:136:ILE:HD12	2:B:134:GLU:HG2	1.73	0.69
2:B:165:ILE:HG22	3:C:110:THR:HG23	1.73	0.69
1:D:98:ARG:HG2	2:E:134:GLU:HG3	1.74	0.69
1:D:158:HIS:HD2	12:E:2021:HOH:O	1.74	0.69
1:D:255:GLN:HE21	1:D:403:ASN:ND2	1.91	0.69
2:E:128:HIS:CD2	2:E:135:GLU:HG3	2.28	0.69
1:A:98:ARG:HG2	2:B:134:GLU:HG3	1.75	0.69
2:B:128:HIS:CD2	2:B:135:GLU:HG3	2.28	0.69
1:D:278:ILE:HD12	1:D:332:ILE:HG13	1.75	0.69
1:A:255:GLN:HE21	1:A:403:ASN:ND2	1.91	0.69
1:A:278:ILE:HD12	1:A:332:ILE:HG13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:ARG:HE	3:C:252:ARG:HA	1.58	0.69
2:B:68:MET:HB2	2:B:92:LEU:HB2	1.73	0.69
1:A:355:ILE:HG12	1:A:360:LYS:HB2	1.74	0.68
1:A:330:ILE:HD13	12:A:2095:HOH:O	1.94	0.68
1:A:470:MET:HE1	1:A:526:MET:C	2.18	0.68
2:B:20:LYS:HE3	3:F:16:GLU:HA	1.76	0.68
1:D:64:ASP:HB2	1:D:146:LYS:HG2	1.76	0.67
1:D:338:ILE:HG23	1:D:339:GLU:N	2.09	0.67
1:D:355:ILE:HG12	1:D:360:LYS:HB2	1.74	0.67
1:D:470:MET:HE1	1:D:526:MET:C	2.18	0.67
2:E:68:MET:HB2	2:E:92:LEU:HB2	1.74	0.67
1:D:523:VAL:HA	1:D:526:MET:HE3	1.77	0.67
1:D:524:PRO:O	1:D:528:LYS:HG3	1.95	0.67
1:A:158:HIS:HD2	12:B:2019:HOH:O	1.76	0.67
3:C:157:VAL:HG22	3:C:254:HIS:NE2	2.10	0.67
1:D:338:ILE:HG12	1:D:339:GLU:N	2.10	0.67
1:A:111:HIS:HB3	2:B:139:PRO:HG3	1.77	0.67
1:A:338:ILE:HG12	1:A:339:GLU:N	2.10	0.67
1:D:467:LYS:O	1:D:471:LYS:HG3	1.95	0.67
3:F:252:ARG:HE	3:F:252:ARG:HA	1.57	0.67
3:C:14:THR:HG23	3:C:15:PRO:HD2	1.75	0.67
3:F:157:VAL:HG22	3:F:254:HIS:NE2	2.10	0.67
3:F:253:THR:HG22	3:F:254:HIS:N	2.06	0.67
1:A:338:ILE:HG23	1:A:339:GLU:N	2.10	0.66
3:C:253:THR:HG22	3:C:254:HIS:N	2.06	0.66
3:F:233:LYS:HZ3	3:F:233:LYS:HB2	1.60	0.66
1:D:179:LYS:HG3	1:D:196:VAL:HG11	1.76	0.66
1:A:524:PRO:O	1:A:528:LYS:HG3	1.96	0.66
1:A:179:LYS:HG3	1:A:196:VAL:HG11	1.76	0.66
1:D:111:HIS:HB3	2:E:139:PRO:HG3	1.76	0.66
1:A:467:LYS:O	1:A:471:LYS:HG3	1.96	0.66
1:A:523:VAL:HA	1:A:526:MET:HE3	1.77	0.66
1:A:64:ASP:HB2	1:A:146:LYS:HG2	1.77	0.65
3:C:16:GLU:HA	2:E:20:LYS:HE3	1.76	0.65
1:D:562:ASN:C	1:D:562:ASN:HD22	2.05	0.65
1:D:330:ILE:HD13	12:D:2092:HOH:O	1.97	0.65
3:C:233:LYS:HB2	3:C:233:LYS:HZ3	1.62	0.64
3:C:108:TYR:CD2	11:C:1257:LMT:H52	2.32	0.64
1:A:562:ASN:C	1:A:562:ASN:HD22	2.06	0.64
3:F:108:TYR:CD2	11:F:1257:LMT:H52	2.32	0.64
2:B:27:LYS:C	2:B:28:ILE:HD12	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:GLU:CD	1:D:645:LYS:HD3	2.23	0.63
1:A:136:ILE:CD1	2:B:134:GLU:HG2	2.28	0.63
1:A:422:GLU:CD	1:A:645:LYS:HD3	2.22	0.63
3:C:102:PRO:O	11:C:1257:LMT:H62	1.99	0.63
2:E:27:LYS:C	2:E:28:ILE:HD12	2.23	0.63
2:B:165:ILE:CG2	3:C:110:THR:HG23	2.29	0.63
3:F:156:PRO:HD2	3:F:254:HIS:HE1	1.63	0.63
3:C:156:PRO:HD2	3:C:254:HIS:HE1	1.63	0.62
2:B:239:ASN:HB2	3:C:21:ARG:HE	1.65	0.62
1:D:628:LYS:HG3	1:D:632:ALA:HB3	1.81	0.62
1:A:180:GLU:OE2	1:A:522:ARG:HD3	2.00	0.62
2:E:128:HIS:HD2	2:E:135:GLU:HG3	1.64	0.62
2:E:239:ASN:HB2	3:F:21:ARG:HE	1.65	0.62
1:D:136:ILE:CD1	2:E:134:GLU:HG2	2.28	0.62
3:F:102:PRO:O	11:F:1257:LMT:H62	1.99	0.62
3:C:4:GLU:CD	3:C:4:GLU:H	2.08	0.62
1:D:462:ASP:HB3	1:D:465:LYS:HG2	1.80	0.62
2:E:165:ILE:CG2	3:F:110:THR:HG23	2.30	0.62
1:A:462:ASP:HB3	1:A:465:LYS:HG2	1.81	0.62
1:A:628:LYS:HG3	1:A:632:ALA:HB3	1.81	0.61
1:D:535:LYS:O	1:D:535:LYS:HD3	2.01	0.61
3:F:155:GLY:HA3	3:F:254:HIS:CE1	2.35	0.61
2:E:238:VAL:HG12	2:E:239:ASN:ND2	2.16	0.61
1:D:180:GLU:OE2	1:D:522:ARG:HD3	2.00	0.61
2:B:165:ILE:HG22	3:C:110:THR:CG2	2.30	0.61
2:E:165:ILE:HG22	3:F:110:THR:CG2	2.30	0.61
1:D:137:HIS:CD2	1:D:138:SER:H	2.18	0.61
1:D:305:SER:HB3	1:D:480:ILE:HD13	1.82	0.61
1:D:639:PRO:HA	12:D:2140:HOH:O	2.00	0.61
1:D:41:ARG:NH2	2:E:107:THR:CG2	2.63	0.61
2:E:176:LEU:HD22	2:E:205:VAL:HG12	1.83	0.60
2:E:197:GLU:O	3:F:19:LYS:HD2	2.01	0.60
1:A:535:LYS:HD3	1:A:535:LYS:O	2.01	0.60
2:B:128:HIS:HD2	2:B:135:GLU:HG3	1.64	0.60
1:A:158:HIS:HE1	2:B:149:ASP:O	1.84	0.60
3:C:155:GLY:HA3	3:C:254:HIS:CE1	2.35	0.60
2:B:238:VAL:HG12	2:B:239:ASN:ND2	2.16	0.60
3:F:4:GLU:H	3:F:4:GLU:CD	2.09	0.60
1:D:66:GLU:HG2	1:D:91:ASN:HD22	1.67	0.60
2:B:197:GLU:O	3:C:19:LYS:HD2	2.02	0.60
3:C:12:GLY:HA2	3:F:106:ARG:NH2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:HIS:HE1	2:E:149:ASP:O	1.84	0.60
1:D:107:TRP:HA	1:D:152:THR:HG22	1.83	0.60
1:A:305:SER:HB3	1:A:480:ILE:HD13	1.84	0.59
3:C:221:ILE:O	3:C:225:LEU:HB2	2.02	0.59
3:C:247:TYR:O	3:C:248:PHE:C	2.44	0.59
2:E:205:VAL:HG11	2:E:231:LEU:HG	1.82	0.59
1:A:137:HIS:CD2	1:A:138:SER:H	2.19	0.59
2:B:176:LEU:HD22	2:B:205:VAL:HG12	1.83	0.59
2:E:146:PHE:O	2:E:150:ARG:HG3	2.02	0.59
1:A:41:ARG:NH2	2:B:107:THR:CG2	2.62	0.59
1:A:221:ARG:HD3	1:A:229:ALA:O	2.03	0.59
3:F:221:ILE:O	3:F:225:LEU:HB2	2.03	0.59
1:A:245:ILE:O	1:A:384:LYS:HE2	2.02	0.59
2:B:205:VAL:HG11	2:B:231:LEU:HG	1.82	0.59
3:C:14:THR:HG22	3:C:16:GLU:N	2.14	0.59
1:D:245:ILE:O	1:D:384:LYS:HE2	2.02	0.59
2:B:146:PHE:O	2:B:150:ARG:HG3	2.03	0.59
1:A:41:ARG:NH2	2:B:107:THR:HG23	2.17	0.58
1:A:470:MET:HE3	1:A:527:LEU:HA	1.85	0.58
1:D:570:ASN:N	1:D:573:GLN:HE21	2.00	0.58
3:C:8:GLU:HA	3:C:13:VAL:O	2.04	0.58
1:D:115:ARG:HG2	1:D:115:ARG:NH1	2.17	0.58
3:F:247:TYR:O	3:F:248:PHE:C	2.45	0.58
1:A:589:GLU:H	1:A:638:MET:HE3	1.68	0.58
3:F:13:VAL:CG1	3:F:17:ARG:HA	2.33	0.58
2:B:164:LYS:O	2:B:164:LYS:HD3	2.04	0.58
3:C:13:VAL:CG1	3:C:17:ARG:HA	2.33	0.58
2:E:164:LYS:O	2:E:164:LYS:HD3	2.03	0.58
3:F:14:THR:CG2	3:F:16:GLU:H	2.13	0.58
3:C:83:ALA:HA	10:C:1256:HEM:CBB	2.33	0.58
3:C:103:ILE:H	3:C:107:GLN:HE21	1.48	0.58
1:A:107:TRP:HA	1:A:152:THR:HG22	1.84	0.58
1:A:115:ARG:HG2	1:A:115:ARG:NH1	2.18	0.57
3:F:83:ALA:HA	10:F:1256:HEM:CBB	2.34	0.57
1:D:518:GLU:O	1:D:522:ARG:HG3	2.05	0.57
3:F:8:GLU:HA	3:F:13:VAL:O	2.05	0.57
1:A:66:GLU:HG2	1:A:91:ASN:HD22	1.69	0.57
3:C:40:PHE:HZ	10:C:1256:HEM:HAB	1.68	0.57
3:C:131:MET:HB2	11:C:1257:LMT:H123	1.85	0.57
3:C:106:ARG:NH2	3:F:12:GLY:HA2	2.20	0.57
1:A:518:GLU:O	1:A:522:ARG:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:THR:CG2	3:C:16:GLU:H	2.13	0.57
2:B:121:TRP:O	2:B:123:HIS:HD2	1.88	0.57
3:C:13:VAL:HG13	3:C:17:ARG:HA	1.87	0.57
1:D:111:HIS:HA	1:D:133:HIS:CD2	2.40	0.57
1:D:41:ARG:NH2	2:E:107:THR:HG23	2.18	0.57
3:F:40:PHE:HZ	10:F:1256:HEM:HAB	1.68	0.57
3:F:74:GLY:HA3	3:F:252:ARG:HG2	1.86	0.57
3:F:13:VAL:HG13	3:F:17:ARG:HA	1.87	0.57
3:F:103:ILE:H	3:F:107:GLN:HE21	1.48	0.57
1:D:470:MET:HE3	1:D:527:LEU:HA	1.86	0.56
3:F:131:MET:HB2	11:F:1257:LMT:H123	1.86	0.56
1:D:470:MET:HE2	1:D:530:ALA:HB2	1.87	0.56
3:F:14:THR:HG22	3:F:16:GLU:N	2.13	0.56
1:A:257:HIS:HE1	5:A:1657:FUM:O	1.88	0.56
1:D:221:ARG:HD3	1:D:229:ALA:O	2.04	0.56
2:E:57:CYS:O	2:E:58:ARG:HG3	2.05	0.56
3:F:169:TRP:CD1	3:F:170:PRO:HD3	2.40	0.56
1:A:470:MET:HE2	1:A:530:ALA:HB2	1.87	0.56
1:A:257:HIS:HD2	1:A:259:THR:H	1.54	0.56
1:D:257:HIS:HE1	5:D:1657:FUM:O	1.88	0.56
3:F:2:THR:HB	3:F:4:GLU:OE2	2.05	0.56
1:A:111:HIS:HA	1:A:133:HIS:CD2	2.40	0.56
3:F:37:LEU:HB3	10:F:1255:HEM:HAC	1.87	0.56
3:C:74:GLY:HA3	3:C:252:ARG:HG2	1.87	0.56
3:C:37:LEU:HB3	10:C:1255:HEM:HAC	1.87	0.56
1:D:455:VAL:O	1:D:509:LYS:HD2	2.06	0.56
1:D:115:ARG:HD2	12:D:2037:HOH:O	2.05	0.56
3:F:14:THR:HG23	3:F:15:PRO:CD	2.36	0.56
3:C:2:THR:HB	3:C:4:GLU:OE2	2.05	0.55
1:D:589:GLU:H	1:D:638:MET:HE3	1.69	0.55
2:B:1:MET:C	2:B:3:ARG:H	2.14	0.55
1:D:257:HIS:HD2	1:D:259:THR:H	1.54	0.55
2:E:1:MET:C	2:E:3:ARG:H	2.14	0.55
1:A:455:VAL:O	1:A:509:LYS:HD2	2.07	0.55
1:A:570:ASN:N	1:A:573:GLN:HE21	2.00	0.55
2:E:121:TRP:O	2:E:123:HIS:HD2	1.89	0.55
1:A:338:ILE:HG23	1:A:339:GLU:H	1.72	0.55
3:C:169:TRP:CD1	3:C:170:PRO:HD3	2.41	0.55
1:D:338:ILE:HG23	1:D:339:GLU:H	1.72	0.55
3:C:14:THR:HG23	3:C:15:PRO:CD	2.37	0.55
2:E:132:LYS:NZ	2:E:132:LYS:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:TYR:HA	1:A:527:LEU:HD13	1.88	0.55
1:D:331:SER:C	1:D:333:LEU:H	2.15	0.55
1:D:482:ARG:NH1	1:D:547:HIS:HD2	2.05	0.55
2:B:132:LYS:NZ	2:B:132:LYS:HB3	2.22	0.55
2:E:61:ILE:HG13	12:E:2020:HOH:O	2.07	0.55
2:B:134:GLU:CD	2:B:134:GLU:H	2.15	0.54
1:D:224:LYS:HB3	1:D:475:ASP:OD2	2.07	0.54
2:E:134:GLU:CD	2:E:134:GLU:H	2.15	0.54
1:A:639:PRO:HA	12:A:2143:HOH:O	2.06	0.54
1:A:569:PRO:HD2	1:A:573:GLN:HE22	1.72	0.54
1:A:615:GLU:O	1:A:619:ILE:HG13	2.08	0.54
3:C:41:MET:HE2	3:C:179:VAL:HG21	1.89	0.54
1:A:224:LYS:HB3	1:A:475:ASP:OD2	2.08	0.54
1:A:470:MET:HE3	1:A:527:LEU:CD2	2.37	0.54
1:A:57:ASN:HB2	12:A:2017:HOH:O	2.08	0.54
1:A:628:LYS:HG3	1:A:632:ALA:CB	2.38	0.54
1:D:330:ILE:HD11	1:D:357:PRO:HB3	1.90	0.54
2:E:180:VAL:HG11	2:E:227:LYS:HG3	1.90	0.54
1:D:498:TYR:HA	1:D:527:LEU:HD13	1.89	0.54
1:D:615:GLU:O	1:D:619:ILE:HG13	2.07	0.54
1:D:71:MET:O	1:D:75:LYS:HG3	2.08	0.53
1:D:628:LYS:HG3	1:D:632:ALA:CB	2.38	0.53
2:B:57:CYS:O	2:B:58:ARG:HG3	2.08	0.53
1:A:330:ILE:HD11	1:A:357:PRO:HB3	1.91	0.53
1:D:268:LEU:C	1:D:270:GLU:H	2.16	0.53
1:D:569:PRO:HD2	1:D:573:GLN:HE22	1.73	0.53
1:A:268:LEU:C	1:A:270:GLU:H	2.16	0.53
2:B:75:LEU:HB2	2:B:78:ARG:HG2	1.90	0.53
2:E:75:LEU:HB2	2:E:78:ARG:HG2	1.90	0.53
3:F:156:PRO:HD2	3:F:254:HIS:CE1	2.43	0.53
2:B:61:ILE:HG13	12:B:2020:HOH:O	2.08	0.53
2:B:180:VAL:HG11	2:B:227:LYS:HG3	1.89	0.53
3:F:144:LEU:HD21	10:F:1256:HEM:HMC3	1.91	0.53
1:D:283:ASP:OD2	1:D:316:LYS:HD2	2.09	0.53
2:E:95:PRO:HD2	2:E:159:ALA:HB1	1.91	0.53
1:A:261:LEU:HG	1:A:268:LEU:CG	2.37	0.52
1:A:331:SER:C	1:A:333:LEU:H	2.15	0.52
1:A:330:ILE:HD13	1:A:330:ILE:N	2.22	0.52
1:D:330:ILE:HD13	1:D:330:ILE:N	2.22	0.52
1:D:588:MET:HA	1:D:638:MET:CE	2.39	0.52
3:F:161:PHE:HD2	3:F:246:LYS:HE3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:MET:HE1	1:A:527:LEU:N	2.24	0.52
3:C:221:ILE:HG13	3:C:222:VAL:N	2.24	0.52
3:C:240:ASP:CG	3:C:243:ILE:HG12	2.34	0.52
1:D:470:MET:HE3	1:D:527:LEU:CD2	2.37	0.52
1:D:644:ALA:HA	1:D:647:LYS:HE3	1.90	0.52
3:F:41:MET:HE2	3:F:179:VAL:HG21	1.90	0.52
1:A:644:ALA:HA	1:A:647:LYS:HE3	1.91	0.52
3:C:222:VAL:O	3:C:226:LEU:HG	2.10	0.52
3:F:147:MET:HE1	3:F:154:ILE:CD1	2.40	0.52
1:A:71:MET:O	1:A:75:LYS:HG3	2.09	0.52
1:D:325:HIS:HD2	1:D:326:LEU:O	1.93	0.52
1:D:343:ARG:HD2	1:D:343:ARG:O	2.10	0.52
1:A:482:ARG:NH1	1:A:547:HIS:HD2	2.05	0.52
2:B:68:MET:SD	2:B:73:PRO:HG3	2.50	0.52
2:B:95:PRO:HD2	2:B:159:ALA:HB1	1.91	0.52
3:C:94:ALA:O	3:C:98:MET:HB2	2.10	0.52
3:F:240:ASP:CG	3:F:243:ILE:HG12	2.34	0.52
1:D:261:LEU:HG	1:D:268:LEU:CG	2.37	0.52
3:F:83:ALA:HA	10:F:1256:HEM:HBB1	1.92	0.52
1:A:343:ARG:HD2	1:A:343:ARG:O	2.10	0.52
3:C:156:PRO:HD2	3:C:254:HIS:CE1	2.44	0.52
3:C:147:MET:HE1	3:C:154:ILE:CD1	2.40	0.51
1:D:13:GLY:HA3	1:D:39:VAL:HG12	1.91	0.51
3:F:94:ALA:O	3:F:98:MET:HB2	2.10	0.51
3:F:222:VAL:O	3:F:226:LEU:HG	2.11	0.51
1:A:604:ILE:HD12	1:A:604:ILE:N	2.26	0.51
1:D:57:ASN:HB2	12:D:2041:HOH:O	2.10	0.51
1:D:604:ILE:HD12	1:D:604:ILE:N	2.26	0.51
1:A:325:HIS:HD2	1:A:326:LEU:O	1.93	0.51
2:E:68:MET:SD	2:E:73:PRO:HG3	2.50	0.51
3:F:221:ILE:HG13	3:F:222:VAL:N	2.24	0.51
1:A:588:MET:HA	1:A:638:MET:CE	2.40	0.51
1:A:13:GLY:HA3	1:A:39:VAL:HG12	1.92	0.51
2:B:192:ASP:OD2	2:B:234:LYS:HD2	2.10	0.51
3:C:131:MET:CB	11:C:1257:LMT:H123	2.40	0.51
2:E:192:ASP:OD2	2:E:234:LYS:HD2	2.10	0.51
3:F:44:HIS:CE1	3:F:48:VAL:HG21	2.46	0.51
3:F:131:MET:CB	11:F:1257:LMT:H123	2.41	0.51
3:F:147:MET:HE1	3:F:154:ILE:HD11	1.93	0.51
1:A:283:ASP:OD2	1:A:316:LYS:HD2	2.10	0.50
2:B:16:SER:O	3:F:17:ARG:NH1	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ASP:CB	1:D:146:LYS:HG2	2.40	0.50
1:D:447:GLN:O	1:D:451:MET:HG2	2.11	0.50
1:D:470:MET:HE1	1:D:527:LEU:N	2.25	0.50
2:B:210:THR:O	2:B:210:THR:HG22	2.11	0.50
1:D:257:HIS:O	1:D:366:PRO:HA	2.12	0.50
1:D:346:GLN:O	1:D:350:GLU:HG3	2.11	0.50
1:D:468:ASN:ND2	12:D:2117:HOH:O	2.43	0.50
3:C:44:HIS:CE1	3:C:48:VAL:HG21	2.46	0.50
3:C:144:LEU:HD21	10:C:1256:HEM:HMC3	1.92	0.50
1:D:197:ARG:NE	1:D:451:MET:HE2	2.27	0.50
1:A:64:ASP:CB	1:A:146:LYS:HG2	2.41	0.50
1:A:197:ARG:NE	1:A:451:MET:HE2	2.27	0.50
1:A:257:HIS:O	1:A:366:PRO:HA	2.12	0.50
1:A:331:SER:C	1:A:333:LEU:N	2.69	0.50
1:D:255:GLN:HE21	1:D:403:ASN:HD22	1.56	0.50
1:D:331:SER:C	1:D:333:LEU:N	2.69	0.50
2:B:223:PRO:O	2:B:227:LYS:HB2	2.12	0.50
2:E:210:THR:HG22	2:E:210:THR:O	2.11	0.50
1:A:228:ASN:N	1:A:228:ASN:HD22	2.08	0.50
1:A:467:LYS:HD3	1:A:526:MET:HE1	1.93	0.50
3:C:17:ARG:NH1	2:E:16:SER:O	2.35	0.50
3:C:161:PHE:HD2	3:C:246:LYS:HE3	1.76	0.50
1:A:346:GLN:O	1:A:350:GLU:HG3	2.11	0.50
2:B:52:ASN:OD1	2:B:101:LYS:HE3	2.12	0.50
3:C:75:LYS:N	3:C:76:PRO:HD3	2.27	0.50
3:C:83:ALA:HA	10:C:1256:HEM:HBB1	1.92	0.50
2:E:125:GLN:HG3	2:E:189:GLU:OE1	2.12	0.50
3:F:75:LYS:N	3:F:76:PRO:HD3	2.27	0.50
2:B:125:GLN:HG3	2:B:189:GLU:OE1	2.12	0.49
3:C:17:ARG:HD2	2:E:19:SER:O	2.11	0.49
1:A:255:GLN:HE21	1:A:403:ASN:HD22	1.56	0.49
1:A:257:HIS:CD2	1:A:259:THR:H	2.30	0.49
1:A:447:GLN:O	1:A:451:MET:HG2	2.12	0.49
1:D:228:ASN:N	1:D:228:ASN:HD22	2.09	0.49
2:E:215:HIS:HD1	2:E:225:GLN:H	1.61	0.49
2:E:223:PRO:O	2:E:227:LYS:HB2	2.12	0.49
3:F:186:GLY:O	3:F:190:LEU:HB2	2.12	0.49
2:E:164:LYS:HD3	12:E:2056:HOH:O	2.12	0.49
3:F:169:TRP:CG	3:F:170:PRO:HD3	2.48	0.49
3:C:147:MET:HE1	3:C:154:ILE:HD11	1.93	0.49
3:F:161:PHE:CD2	3:F:246:LYS:HE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:GLY:O	3:C:190:LEU:HB2	2.13	0.49
1:A:525:MET:HE1	12:A:2059:HOH:O	2.13	0.48
3:C:169:TRP:CG	3:C:170:PRO:HD3	2.48	0.48
1:A:535:LYS:HG3	1:A:578:LEU:CD1	2.39	0.48
1:D:5:TYR:CD1	1:D:5:TYR:C	2.91	0.48
1:A:591:ALA:HB3	1:A:613:GLN:HE21	1.79	0.48
1:A:52:GLN:HG3	1:A:148:ARG:HD2	1.96	0.48
2:E:52:ASN:OD1	2:E:101:LYS:HE3	2.13	0.48
3:C:143:HIS:O	3:C:147:MET:HG2	2.14	0.48
1:D:197:ARG:HD2	1:D:451:MET:HE2	1.95	0.48
1:A:115:ARG:HD2	12:A:2037:HOH:O	2.12	0.48
1:A:197:ARG:HD2	1:A:451:MET:HE2	1.96	0.47
2:B:119:GLU:OE1	2:B:123:HIS:HE1	1.97	0.47
2:E:119:GLU:OE1	2:E:123:HIS:HE1	1.97	0.47
3:C:161:PHE:CD2	3:C:246:LYS:HE3	2.49	0.47
1:D:522:ARG:HA	1:D:525:MET:HE3	1.96	0.47
1:D:591:ALA:HB3	1:D:613:GLN:HE21	1.79	0.47
3:F:228:PHE:O	3:F:232:VAL:HG23	2.14	0.47
1:D:25:GLN:OE1	1:D:31:THR:HG23	2.13	0.47
1:D:467:LYS:HD3	1:D:526:MET:HE1	1.95	0.47
3:F:162:ARG:CG	3:F:168:MET:HG3	2.44	0.47
1:A:112:LYS:HD2	1:A:130:ASP:HB3	1.96	0.47
2:E:197:GLU:OE1	3:F:19:LYS:HG3	2.14	0.47
3:F:13:VAL:HG13	3:F:14:THR:N	2.30	0.47
1:A:5:TYR:CD1	1:A:5:TYR:C	2.92	0.47
1:A:338:ILE:CG1	1:A:339:GLU:H	2.16	0.47
1:D:179:LYS:CG	1:D:196:VAL:HG11	2.44	0.47
1:A:197:ARG:CD	1:A:451:MET:HE2	2.45	0.47
1:D:52:GLN:HG3	1:D:148:ARG:HD2	1.97	0.47
1:D:114:ASP:HA	1:D:126:ILE:O	2.15	0.47
1:D:332:ILE:O	1:D:332:ILE:HG22	2.14	0.47
3:C:162:ARG:CG	3:C:168:MET:HG3	2.44	0.47
3:C:228:PHE:O	3:C:232:VAL:HG23	2.15	0.47
1:D:257:HIS:CD2	1:D:259:THR:H	2.31	0.47
3:F:17:ARG:O	3:F:17:ARG:HG2	2.15	0.47
1:A:332:ILE:O	1:A:332:ILE:HG22	2.14	0.47
3:F:246:LYS:HG3	3:F:247:TYR:CD1	2.50	0.47
3:F:248:PHE:CB	3:F:254:HIS:HD2	2.20	0.47
1:A:25:GLN:OE1	1:A:31:THR:HG23	2.15	0.46
1:A:114:ASP:HA	1:A:126:ILE:O	2.15	0.46
4:A:1656:FAD:H9	4:A:1656:FAD:H1'1	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:VAL:HG13	3:C:14:THR:N	2.29	0.46
1:D:197:ARG:CD	1:D:451:MET:HE2	2.44	0.46
3:F:143:HIS:O	3:F:147:MET:HG2	2.15	0.46
3:F:234:LYS:O	3:F:238:GLN:HG3	2.15	0.46
2:E:1:MET:N	2:E:30:GLU:OE1	2.49	0.46
1:A:483:ASP:CG	1:A:486:HIS:HD1	2.24	0.46
2:B:19:SER:O	3:F:17:ARG:HD2	2.16	0.46
3:C:234:LYS:O	3:C:238:GLN:HG3	2.15	0.46
3:C:246:LYS:HG3	3:C:247:TYR:CD1	2.50	0.46
3:F:252:ARG:HA	3:F:252:ARG:NE	2.28	0.46
1:A:542:GLU:OE2	1:A:544:ARG:HD2	2.16	0.46
2:B:1:MET:N	2:B:30:GLU:OE1	2.48	0.46
2:B:197:GLU:OE1	3:C:19:LYS:HG3	2.16	0.46
4:D:1656:FAD:H9	4:D:1656:FAD:H1'1	1.63	0.46
3:F:233:LYS:HZ3	3:F:233:LYS:CB	2.27	0.46
1:A:26:GLN:NE2	12:A:2003:HOH:O	2.46	0.46
2:B:8:ARG:HG2	2:B:25:GLU:CG	2.35	0.46
3:F:201:THR:HB	3:F:204:LYS:HG3	1.98	0.46
3:C:248:PHE:CB	3:C:254:HIS:HD2	2.20	0.46
3:F:136:MET:HB2	10:F:1255:HEM:HAB	1.98	0.46
1:A:455:VAL:HG13	1:A:509:LYS:HD3	1.98	0.46
3:C:157:VAL:HG21	3:C:248:PHE:CD2	2.51	0.46
1:D:470:MET:HE1	1:D:527:LEU:HA	1.97	0.46
3:F:61:VAL:HG23	3:F:62:THR:N	2.31	0.46
2:B:220:LYS:HB3	2:B:222:LEU:HD13	1.98	0.46
3:C:17:ARG:O	3:C:17:ARG:HG2	2.15	0.46
1:D:112:LYS:HD2	1:D:130:ASP:HB3	1.96	0.46
1:D:455:VAL:HG13	1:D:509:LYS:HD3	1.98	0.46
2:E:8:ARG:HG2	2:E:25:GLU:CG	2.36	0.45
11:C:1257:LMT:H42	3:F:95:PHE:CZ	2.51	0.45
1:D:48:GLN:HG2	1:D:154:ASP:O	2.17	0.45
1:A:52:GLN:HE21	1:A:52:GLN:HB2	1.50	0.45
1:D:349:CYS:O	1:D:354:GLY:N	2.50	0.45
3:F:157:VAL:HG21	3:F:248:PHE:CD2	2.51	0.45
1:A:137:HIS:HD2	1:A:138:SER:H	1.64	0.45
1:A:540:ARG:HH22	1:A:562:ASN:HD22	1.64	0.45
1:D:29:LEU:O	1:D:31:THR:HG22	2.16	0.45
1:D:79:TRP:CE2	1:D:592:PRO:HA	2.51	0.45
1:D:595:ARG:HD2	1:D:597:TYR:CZ	2.52	0.45
3:C:252:ARG:HA	3:C:252:ARG:NE	2.29	0.45
1:D:483:ASP:CG	1:D:486:HIS:HD1	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:HIS:O	1:D:513:ALA:C	2.59	0.45
1:A:179:LYS:CG	1:A:196:VAL:HG11	2.45	0.45
1:A:522:ARG:HA	1:A:525:MET:HE3	1.98	0.45
3:C:201:THR:HB	3:C:204:LYS:HG3	1.98	0.45
1:D:41:ARG:HG2	1:D:41:ARG:HH11	1.82	0.45
3:F:171:LEU:C	3:F:171:LEU:HD23	2.42	0.45
1:A:29:LEU:O	1:A:31:THR:HG22	2.17	0.45
1:D:221:ARG:HD2	1:D:226:THR:HG21	1.99	0.45
1:D:281:ASP:HB2	1:D:316:LYS:HG3	1.98	0.45
2:E:220:LYS:HB3	2:E:222:LEU:HD13	1.98	0.45
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.81	0.45
1:A:84:LYS:HE3	1:A:639:PRO:O	2.17	0.45
1:A:468:ASN:ND2	12:A:2120:HOH:O	2.46	0.45
3:C:61:VAL:HG23	3:C:62:THR:N	2.31	0.45
3:C:206:ARG:O	3:C:210:LYS:HG3	2.16	0.45
1:D:83:GLN:HB3	1:D:638:MET:HE1	1.98	0.45
1:D:540:ARG:HH22	1:D:562:ASN:HD22	1.65	0.45
2:E:233:ARG:O	2:E:236:VAL:HG12	2.17	0.45
1:A:349:CYS:O	1:A:354:GLY:N	2.50	0.45
1:A:512:HIS:O	1:A:513:ALA:C	2.60	0.44
1:A:595:ARG:HD2	1:A:597:TYR:CZ	2.52	0.44
3:C:136:MET:HB2	10:C:1255:HEM:HAB	1.99	0.44
1:A:83:GLN:HB3	1:A:638:MET:HE1	1.99	0.44
2:B:176:LEU:HD22	2:B:205:VAL:CG1	2.47	0.44
3:C:171:LEU:C	3:C:171:LEU:HD23	2.43	0.44
1:D:84:LYS:HE3	1:D:639:PRO:O	2.17	0.44
1:D:140:ASP:HB2	1:D:147:TRP:CE2	2.53	0.44
1:D:542:GLU:OE2	1:D:544:ARG:HD2	2.17	0.44
1:A:79:TRP:CE2	1:A:592:PRO:HA	2.51	0.44
1:A:145:LYS:HE3	12:A:2044:HOH:O	2.17	0.44
3:C:14:THR:HB	3:C:18:LYS:O	2.16	0.44
1:D:261:LEU:HG	1:D:268:LEU:CD1	2.48	0.44
3:F:161:PHE:O	3:F:165:SER:HB3	2.17	0.44
1:A:355:ILE:HD11	1:A:360:LYS:HG3	2.00	0.44
2:B:1:MET:H2	2:B:30:GLU:HB3	1.83	0.44
3:C:222:VAL:HG13	3:C:223:LEU:N	2.32	0.44
1:D:346:GLN:HA	1:D:357:PRO:CG	2.41	0.44
1:D:600:LYS:HG3	1:D:601:GLY:N	2.31	0.44
2:E:176:LEU:HD22	2:E:205:VAL:CG1	2.46	0.44
3:F:222:VAL:HG13	3:F:223:LEU:N	2.32	0.44
1:A:405:LEU:O	1:A:408:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:PHE:O	3:C:165:SER:HB3	2.18	0.44
1:D:52:GLN:HB3	1:D:408:ASN:HD22	1.82	0.44
1:D:112:LYS:CG	1:D:130:ASP:HA	2.41	0.44
1:D:338:ILE:CG1	1:D:339:GLU:N	2.77	0.44
1:D:467:LYS:HD3	1:D:523:VAL:HG22	1.99	0.44
1:A:140:ASP:HB2	1:A:147:TRP:CE2	2.53	0.44
1:A:281:ASP:HB2	1:A:316:LYS:HG3	1.99	0.44
1:A:600:LYS:HG3	1:A:601:GLY:N	2.32	0.44
1:D:47:ALA:HB3	1:D:157:GLY:HA3	2.00	0.44
2:B:233:ARG:O	2:B:236:VAL:HG12	2.17	0.44
1:A:52:GLN:HB3	1:A:408:ASN:HD22	1.82	0.44
1:D:318:VAL:HG21	1:D:327:TRP:NE1	2.32	0.43
3:F:206:ARG:O	3:F:210:LYS:HG3	2.17	0.43
1:A:462:ASP:HB3	1:A:465:LYS:CG	2.47	0.43
3:C:240:ASP:HB3	3:C:243:ILE:HG12	2.01	0.43
1:A:523:VAL:HB	1:A:524:PRO:HD3	2.00	0.43
3:F:14:THR:HB	3:F:18:LYS:O	2.18	0.43
5:A:1657:FUM:H5	12:A:2094:HOH:O	2.17	0.43
3:F:216:MET:O	3:F:220:LEU:HG	2.18	0.43
1:D:267:LEU:HD12	1:D:267:LEU:HA	1.86	0.43
1:D:260:PRO:HD2	1:D:365:LEU:O	2.18	0.43
1:D:308:MET:O	1:D:312:ILE:HG13	2.18	0.43
1:A:261:LEU:HG	1:A:268:LEU:CD1	2.48	0.43
1:D:349:CYS:O	1:D:353:ALA:HB3	2.19	0.43
1:D:355:ILE:HD11	1:D:360:LYS:HG3	2.00	0.43
2:E:210:THR:HG21	3:F:192:VAL:HG23	2.01	0.43
3:F:75:LYS:C	3:F:77:ILE:H	2.27	0.43
1:A:47:ALA:HB3	1:A:157:GLY:HA3	2.01	0.43
3:C:21:ARG:O	3:C:25:LYS:HG3	2.18	0.43
1:A:318:VAL:HG21	1:A:327:TRP:NE1	2.34	0.43
3:C:153:THR:HG21	3:C:246:LYS:HD2	2.00	0.43
1:A:112:LYS:CG	1:A:130:ASP:HA	2.41	0.42
2:B:128:HIS:ND1	2:B:129:ASP:N	2.67	0.42
3:C:75:LYS:C	3:C:77:ILE:H	2.27	0.42
3:C:216:MET:O	3:C:220:LEU:HG	2.18	0.42
1:D:509:LYS:HB2	12:D:2124:HOH:O	2.19	0.42
2:E:227:LYS:HD3	2:E:227:LYS:HA	1.90	0.42
3:F:21:ARG:O	3:F:25:LYS:HG3	2.18	0.42
1:A:349:CYS:O	1:A:353:ALA:HB3	2.20	0.42
1:D:137:HIS:HD2	1:D:138:SER:H	1.63	0.42
1:D:404:ARG:HD2	1:D:409:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LEU:O	1:D:408:ASN:HB2	2.19	0.42
1:D:523:VAL:HB	1:D:524:PRO:HD3	2.01	0.42
1:A:221:ARG:HD2	1:A:226:THR:HG21	2.01	0.42
1:A:260:PRO:HD2	1:A:365:LEU:O	2.19	0.42
1:D:100:LEU:HB3	1:D:105:VAL:HG21	2.02	0.42
2:E:128:HIS:ND1	2:E:129:ASP:N	2.67	0.42
3:F:240:ASP:HB3	3:F:243:ILE:HG12	2.01	0.42
2:B:234:LYS:HB2	2:B:234:LYS:HE3	1.87	0.42
3:C:95:PHE:CZ	11:F:1257:LMT:H42	2.53	0.42
2:E:72:ARG:HA	2:E:73:PRO:HD3	1.89	0.42
2:E:234:LYS:HE3	2:E:234:LYS:HB2	1.87	0.42
3:F:51:ILE:HD11	3:F:234:LYS:HD3	2.00	0.42
3:F:153:THR:HG21	3:F:246:LYS:HD2	2.01	0.42
3:C:51:ILE:HD11	3:C:234:LYS:HD3	2.00	0.42
2:E:57:CYS:C	2:E:58:ARG:HG3	2.45	0.42
1:A:308:MET:O	1:A:312:ILE:HG13	2.18	0.42
1:A:470:MET:HE1	1:A:527:LEU:HA	1.97	0.42
1:D:462:ASP:HB3	1:D:465:LYS:CG	2.47	0.42
1:A:628:LYS:HD3	1:A:628:LYS:HA	1.94	0.42
3:C:44:HIS:O	3:C:48:VAL:HG23	2.20	0.42
3:C:169:TRP:N	3:C:170:PRO:CD	2.83	0.42
3:C:233:LYS:HZ2	3:C:233:LYS:HA	1.84	0.42
1:D:471:LYS:HG3	1:D:471:LYS:H	1.70	0.42
1:A:259:THR:N	1:A:260:PRO:HD3	2.35	0.42
3:C:134:PHE:O	3:C:137:PHE:HB2	2.20	0.42
3:F:134:PHE:O	3:F:137:PHE:HB2	2.19	0.42
3:F:169:TRP:N	3:F:170:PRO:CD	2.83	0.42
1:A:540:ARG:HH22	1:A:562:ASN:ND2	2.18	0.41
1:D:338:ILE:CG1	1:D:339:GLU:H	2.15	0.41
3:F:44:HIS:O	3:F:48:VAL:HG23	2.20	0.41
1:A:48:GLN:HG2	1:A:154:ASP:O	2.19	0.41
1:A:455:VAL:CG1	1:A:509:LYS:HG3	2.51	0.41
1:A:467:LYS:HD3	1:A:523:VAL:HG22	2.00	0.41
2:B:72:ARG:HA	2:B:73:PRO:HD3	1.88	0.41
3:F:161:PHE:CD2	3:F:246:LYS:HB2	2.55	0.41
2:B:57:CYS:C	2:B:58:ARG:HG3	2.46	0.41
1:D:338:ILE:CG2	1:D:339:GLU:N	2.77	0.41
1:D:540:ARG:HH22	1:D:562:ASN:ND2	2.18	0.41
3:F:213:LYS:HE2	3:F:213:LYS:HB3	1.87	0.41
1:A:470:MET:HE1	1:A:527:LEU:CA	2.50	0.41
1:D:93:ALA:HB3	1:D:94:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ASN:HD22	1:D:403:ASN:HA	1.59	0.41
3:F:182:HIS:CD2	10:F:1255:HEM:NC	2.88	0.41
2:B:95:PRO:O	2:B:96:ALA:HB3	2.20	0.41
1:D:287:PHE:CZ	1:D:326:LEU:HD13	2.56	0.41
1:D:455:VAL:CG1	1:D:509:LYS:HG3	2.51	0.41
1:A:470:MET:HE2	1:A:530:ALA:CB	2.50	0.41
3:C:26:LEU:HD21	11:F:1257:LMT:H5'	2.02	0.41
3:F:244:ASP:OD2	3:F:247:TYR:HB2	2.20	0.41
1:A:281:ASP:HB2	1:A:316:LYS:O	2.21	0.41
1:A:465:LYS:HE2	1:A:465:LYS:HB3	1.85	0.41
1:A:467:LYS:CD	1:A:526:MET:HE1	2.50	0.41
3:C:161:PHE:CD2	3:C:246:LYS:HB2	2.56	0.41
3:C:225:LEU:HD12	3:C:225:LEU:HA	1.97	0.41
1:D:470:MET:HE1	1:D:527:LEU:CA	2.51	0.41
2:E:220:LYS:HD3	2:E:220:LYS:HA	1.90	0.41
3:F:13:VAL:HG13	3:F:14:THR:O	2.21	0.41
1:A:346:GLN:HA	1:A:357:PRO:CG	2.42	0.41
2:B:28:ILE:HD12	2:B:28:ILE:N	2.36	0.41
1:A:433:VAL:CG1	1:A:434:ASP:N	2.84	0.40
2:B:210:THR:HG21	3:C:192:VAL:HG23	2.02	0.40
2:E:121:TRP:O	2:E:123:HIS:CD2	2.72	0.40
1:A:64:ASP:HB2	1:A:146:LYS:CG	2.49	0.40
2:B:121:TRP:O	2:B:123:HIS:CD2	2.71	0.40
1:D:40:LYS:HE2	2:E:153:GLU:OE1	2.21	0.40
1:D:465:LYS:HE2	1:D:465:LYS:HB3	1.85	0.40
1:D:525:MET:HE1	12:D:2059:HOH:O	2.20	0.40
2:E:56:VAL:HB	2:E:62:CYS:SG	2.61	0.40
2:B:56:VAL:HB	2:B:62:CYS:SG	2.61	0.40
3:C:13:VAL:HG13	3:C:14:THR:O	2.21	0.40
1:D:433:VAL:CG1	1:D:434:ASP:N	2.82	0.40
3:F:47:PHE:HA	3:F:50:THR:HG23	2.04	0.40
1:A:463:VAL:HG22	1:A:523:VAL:HG21	2.03	0.40
3:C:101:PHE:HB3	11:C:1257:LMT:H71	2.03	0.40
3:C:183:GLY:O	3:C:187:LEU:HG	2.22	0.40
3:F:101:PHE:HB3	11:F:1257:LMT:H71	2.03	0.40
1:A:404:ARG:HD2	1:A:409:SER:OG	2.20	0.40
1:A:469:ARG:HA	1:A:469:ARG:HD2	1.90	0.40
3:F:183:GLY:O	3:F:187:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/656 (89%)	549 (94%)	32 (6%)	5 (1%)	14	13
1	D	653/656 (100%)	615 (94%)	33 (5%)	5 (1%)	16	16
2	B	237/239 (99%)	229 (97%)	8 (3%)	0	100	100
2	E	237/239 (99%)	229 (97%)	8 (3%)	0	100	100
3	C	252/256 (98%)	234 (93%)	15 (6%)	3 (1%)	10	8
3	F	252/256 (98%)	235 (93%)	14 (6%)	3 (1%)	10	8
All	All	2217/2302 (96%)	2091 (94%)	110 (5%)	16 (1%)	18	18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ALA
1	A	338	ILE
3	C	67	LEU
1	D	117	ALA
1	D	338	ILE
3	F	67	LEU
1	A	336	LYS
1	D	336	LYS
3	C	66	GLU
3	F	66	GLU
1	A	276	GLY
1	D	276	GLY
3	C	74	GLY
3	F	74	GLY
1	A	118	ILE
1	D	118	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	534/535 (100%)	517 (97%)	17 (3%)	34	44
1	D	534/535 (100%)	517 (97%)	17 (3%)	34	44
2	B	211/211 (100%)	207 (98%)	4 (2%)	50	63
2	E	211/211 (100%)	207 (98%)	4 (2%)	50	63
3	C	221/223 (99%)	212 (96%)	9 (4%)	27	35
3	F	221/223 (99%)	212 (96%)	9 (4%)	27	35
All	All	1932/1938 (100%)	1872 (97%)	60 (3%)	35	45

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	27	LYS
1	A	31	THR
1	A	52	GLN
1	A	95	LYS
1	A	112	LYS
1	A	115	ARG
1	A	190	LYS
1	A	230	VAL
1	A	263	PRO
1	A	330	ILE
1	A	403	ASN
1	A	408	ASN
1	A	475	ASP
1	A	497	LEU
1	A	517	LEU
1	A	562	ASN
2	B	61	ILE
2	B	74	SER
2	B	107	THR
2	B	134	GLU
3	C	1	MET

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Mol	Chain	Res	Type
3	C	4	GLU
3	C	13	VAL
3	C	14	THR
3	C	58	MET
3	C	100	LYS
3	C	106	ARG
3	C	110	THR
3	C	233	LYS
1	D	9	LEU
1	D	27	LYS
1	D	31	THR
1	D	52	GLN
1	D	95	LYS
1	D	112	LYS
1	D	115	ARG
1	D	190	LYS
1	D	230	VAL
1	D	263	PRO
1	D	330	ILE
1	D	403	ASN
1	D	434	ASP
1	D	475	ASP
1	D	497	LEU
1	D	517	LEU
1	D	562	ASN
2	E	61	ILE
2	E	74	SER
2	E	107	THR
2	E	134	GLU
3	F	1	MET
3	F	4	GLU
3	F	13	VAL
3	F	14	THR
3	F	58	MET
3	F	100	LYS
3	F	106	ARG
3	F	110	THR
3	F	233	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	57	ASN
1	A	91	ASN
1	A	133	HIS
1	A	137	HIS
1	A	158	HIS
1	A	225	ASN
1	A	228	ASN
1	A	247	GLN
1	A	257	HIS
1	A	319	GLN
1	A	324	GLN
1	A	325	HIS
1	A	368	GLN
1	A	403	ASN
1	A	408	ASN
1	A	430	ASN
1	A	468	ASN
1	A	547	HIS
1	A	562	ASN
1	A	573	GLN
1	A	613	GLN
2	B	24	GLN
2	B	123	HIS
2	B	177	ASN
2	B	239	ASN
3	C	107	GLN
3	C	208	ASN
3	C	238	GLN
3	C	254	HIS
1	D	48	GLN
1	D	57	ASN
1	D	91	ASN
1	D	133	HIS
1	D	137	HIS
1	D	158	HIS
1	D	225	ASN
1	D	228	ASN
1	D	247	GLN
1	D	257	HIS
1	D	319	GLN
1	D	324	GLN
1	D	325	HIS

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Mol	Chain	Res	Type
1	D	368	GLN
1	D	403	ASN
1	D	408	ASN
1	D	430	ASN
1	D	468	ASN
1	D	547	HIS
1	D	562	ASN
1	D	573	GLN
1	D	613	GLN
2	E	24	GLN
2	E	116	GLN
2	E	123	HIS
2	E	177	ASN
2	E	239	ASN
3	F	107	GLN
3	F	208	ASN
3	F	238	GLN
3	F	254	HIS

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](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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
11	LMT	F	1257	-	36,36,36	1.11	2 (5%)	47,47,47	1.27	4 (8%)
9	SF4	B	1242	2	0,12,12	-	-	-		
9	SF4	E	1242	2	0,12,12	-	-	-		
7	FES	E	1240	2	0,4,4	-	-	-		
11	LMT	C	1257	-	36,36,36	1.10	2 (5%)	47,47,47	1.27	4 (8%)
7	FES	B	1240	2	0,4,4	-	-	-		
8	F3S	B	1241	2	0,9,9	-	-	-		
10	HEM	C	1256	3	50,50,50	1.36	7 (14%)	67,82,82	1.00	4 (5%)
4	FAD	D	1656	1	58,58,58	1.96	13 (22%)	85,89,89	1.26	9 (10%)
5	FUM	D	1657	-	7,7,7	1.60	2 (28%)	8,8,8	0.79	0
5	FUM	A	1657	-	7,7,7	1.61	2 (28%)	8,8,8	0.79	0
4	FAD	A	1656	1	58,58,58	2.03	16 (27%)	85,89,89	1.26	9 (10%)
10	HEM	F	1256	3	50,50,50	1.34	7 (14%)	67,82,82	0.99	4 (5%)
10	HEM	F	1255	3	50,50,50	1.40	7 (14%)	67,82,82	0.80	0
8	F3S	E	1241	2	0,9,9	-	-	-		
10	HEM	C	1255	3	50,50,50	1.39	7 (14%)	67,82,82	0.79	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
11	LMT	F	1257	-	-	10/21/61/61	0/2/2/2
9	SF4	B	1242	2	-	-	0/6/5/5
9	SF4	E	1242	2	-	-	0/6/5/5
11	LMT	C	1257	-	-	10/21/61/61	0/2/2/2
7	FES	E	1240	2	-	-	0/1/1/1
7	FES	B	1240	2	-	-	0/1/1/1
10	HEM	C	1256	3	-	2/14/54/54	-
8	F3S	B	1241	2	-	-	0/3/3/3
4	FAD	D	1656	1	-	3/34/50/50	0/6/6/6
5	FUM	D	1657	-	-	2/5/5/5	-
5	FUM	A	1657	-	-	2/5/5/5	-
4	FAD	A	1656	1	-	4/34/50/50	0/6/6/6
10	HEM	F	1256	3	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	F	1255	3	-	4/14/54/54	-
8	F3S	E	1241	2	-	-	0/3/3/3
10	HEM	C	1255	3	-	4/14/54/54	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1656	FAD	P-O3P	-8.05	1.50	1.59
4	D	1656	FAD	P-O3P	-7.93	1.50	1.59
4	A	1656	FAD	C1'-C2'	4.19	1.58	1.52
4	A	1656	FAD	O5'-C5'	4.11	1.60	1.44
4	D	1656	FAD	C1'-C2'	4.10	1.58	1.52
4	A	1656	FAD	PA-O2A	-4.08	1.36	1.55
4	D	1656	FAD	O5'-C5'	4.01	1.59	1.44
4	D	1656	FAD	PA-O2A	-3.98	1.36	1.55
10	C	1255	HEM	FE-NC	3.62	2.07	1.95
10	C	1256	HEM	CBC-CAC	3.44	1.46	1.30
10	F	1256	HEM	FE-NC	3.43	2.06	1.95
10	F	1255	HEM	FE-NC	3.43	2.06	1.95
10	C	1256	HEM	FE-NC	3.42	2.06	1.95
10	F	1256	HEM	CBC-CAC	3.33	1.46	1.30
11	F	1257	LMT	O5B-C1B	3.29	1.50	1.41
11	C	1257	LMT	O5B-C1B	3.28	1.50	1.41
10	F	1256	HEM	CAB-C3B	-3.27	1.38	1.47
10	C	1256	HEM	CAB-C3B	-3.23	1.38	1.47
10	C	1256	HEM	FE-NB	3.23	2.04	1.94
10	F	1255	HEM	FE-NA	3.21	2.05	1.95
4	A	1656	FAD	P-O2P	-3.11	1.40	1.55
4	D	1656	FAD	P-O2P	-3.09	1.41	1.55
10	C	1255	HEM	CAC-C3C	-3.09	1.39	1.47
10	F	1255	HEM	CAC-C3C	-3.07	1.39	1.47
10	F	1255	HEM	CBC-CAC	3.03	1.45	1.30
10	C	1255	HEM	CBC-CAC	3.03	1.45	1.30
4	A	1656	FAD	C6-C5X	3.02	1.44	1.40
10	F	1255	HEM	CBB-CAB	2.96	1.44	1.30
10	F	1256	HEM	FE-ND	2.94	2.03	1.94
10	F	1255	HEM	CAB-C3B	-2.91	1.39	1.47
10	C	1256	HEM	FE-NA	2.90	2.04	1.95
10	C	1255	HEM	CBB-CAB	2.88	1.44	1.30
10	C	1255	HEM	CAB-C3B	-2.87	1.39	1.47
10	C	1255	HEM	FE-NB	2.86	2.03	1.94
11	C	1257	LMT	C3'-C4'	2.86	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	1257	LMT	C3'-C4'	2.85	1.60	1.52
10	C	1255	HEM	FE-NA	2.83	2.04	1.95
10	F	1256	HEM	FE-NA	2.83	2.04	1.95
10	F	1255	HEM	FE-NB	2.81	2.03	1.94
4	A	1656	FAD	O2-C2	-2.78	1.18	1.24
4	A	1656	FAD	PA-O3P	2.74	1.62	1.59
10	C	1256	HEM	CBB-CAB	2.74	1.43	1.30
4	D	1656	FAD	C6-C5X	2.73	1.44	1.40
4	A	1656	FAD	C5A-C6A	2.68	1.48	1.41
4	D	1656	FAD	C4X-N5	2.68	1.36	1.30
10	F	1256	HEM	CAC-C3C	-2.65	1.40	1.47
10	F	1256	HEM	CBB-CAB	2.62	1.43	1.30
4	D	1656	FAD	C5A-C6A	2.61	1.48	1.41
5	A	1657	FUM	C4-C	2.58	1.54	1.48
4	A	1656	FAD	C8-C7	2.57	1.47	1.40
5	D	1657	FUM	C4-C	2.56	1.54	1.48
10	C	1256	HEM	CAC-C3C	-2.53	1.40	1.47
4	D	1656	FAD	C9A-N10	2.46	1.45	1.41
5	D	1657	FUM	C5-C4	2.45	1.40	1.33
5	A	1657	FUM	C5-C4	2.43	1.40	1.33
4	D	1656	FAD	O2-C2	-2.38	1.19	1.24
4	D	1656	FAD	C8-C7	2.33	1.46	1.40
4	A	1656	FAD	C4X-N5	2.30	1.35	1.30
4	D	1656	FAD	C4A-N3A	2.20	1.38	1.34
4	A	1656	FAD	O4B-C1B	2.19	1.47	1.42
4	A	1656	FAD	C9A-N10	2.16	1.44	1.41
4	D	1656	FAD	O4B-C1B	2.15	1.47	1.42
4	A	1656	FAD	C2-N3	2.08	1.43	1.39
4	A	1656	FAD	C4A-N3A	2.08	1.38	1.34
4	A	1656	FAD	C5A-C4A	2.03	1.42	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1257	LMT	C1-O1'-C1'	4.93	122.11	113.68
11	F	1257	LMT	C1-O1'-C1'	4.89	122.03	113.68
4	A	1656	FAD	C1'-N10-C9A	-4.37	112.15	120.63
4	D	1656	FAD	C1'-N10-C9A	-4.33	112.22	120.63
4	D	1656	FAD	O4B-C1B-N9A	-3.50	101.36	108.09
4	A	1656	FAD	O4B-C1B-N9A	-3.47	101.43	108.09
11	F	1257	LMT	C3'-C4'-C5'	-3.43	103.34	110.93
11	C	1257	LMT	C3'-C4'-C5'	-3.41	103.38	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1256	HEM	CAD-C3D-C4D	3.33	130.51	124.70
10	F	1256	HEM	CAD-C3D-C4D	3.18	130.24	124.70
4	D	1656	FAD	C5'-C4'-C3'	-3.09	106.39	112.22
4	A	1656	FAD	C5'-C4'-C3'	-3.03	106.51	112.22
10	C	1256	HEM	CAD-C3D-C2D	-2.95	122.34	127.87
10	F	1256	HEM	CAD-C3D-C2D	-2.83	122.58	127.87
4	A	1656	FAD	C2A-N1A-C6A	2.60	123.01	118.73
4	D	1656	FAD	C2A-N1A-C6A	2.53	122.88	118.73
10	C	1256	HEM	CBA-CAA-C2A	2.45	119.31	112.53
4	A	1656	FAD	C4-N3-C2	-2.41	121.36	125.64
11	F	1257	LMT	O1'-C1'-C2'	-2.39	104.64	108.27
11	C	1257	LMT	O1'-C1'-C2'	-2.35	104.70	108.27
10	F	1256	HEM	CBA-CAA-C2A	2.35	119.03	112.53
10	F	1256	HEM	CAA-C2A-C1A	2.31	129.44	124.94
4	D	1656	FAD	O3'-C3'-C2'	2.30	114.17	108.93
4	A	1656	FAD	O4'-C4'-C3'	2.27	114.55	109.25
4	D	1656	FAD	C4-N3-C2	-2.26	121.62	125.64
4	A	1656	FAD	O3'-C3'-C2'	2.26	114.05	108.93
4	D	1656	FAD	C4'-C3'-C2'	-2.22	109.88	113.57
11	F	1257	LMT	O1B-C4'-C3'	2.19	112.79	107.23
4	A	1656	FAD	C4'-C3'-C2'	-2.17	109.95	113.57
4	D	1656	FAD	O4'-C4'-C3'	2.15	114.28	109.25
11	C	1257	LMT	O1B-C4'-C3'	2.14	112.68	107.23
4	D	1656	FAD	C2B-C1B-N9A	2.13	118.61	113.30
10	C	1256	HEM	CAA-C2A-C1A	2.13	129.11	124.94
4	A	1656	FAD	C2B-C1B-N9A	2.06	118.42	113.30

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1656	FAD	PA-O3P-P-O5'
4	D	1656	FAD	PA-O3P-P-O5'
10	C	1255	HEM	C2B-C3B-CAB-CBB
10	C	1255	HEM	C4B-C3B-CAB-CBB
10	C	1255	HEM	C2C-C3C-CAC-CBC
10	C	1255	HEM	C4C-C3C-CAC-CBC
10	C	1256	HEM	C2B-C3B-CAB-CBB
10	C	1256	HEM	C4B-C3B-CAB-CBB
10	F	1255	HEM	C2B-C3B-CAB-CBB
10	F	1255	HEM	C4B-C3B-CAB-CBB
10	F	1255	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
10	F	1255	HEM	C4C-C3C-CAC-CBC
10	F	1256	HEM	C2B-C3B-CAB-CBB
10	F	1256	HEM	C4B-C3B-CAB-CBB
11	C	1257	LMT	O5'-C5'-C6'-O6'
11	F	1257	LMT	O5'-C5'-C6'-O6'
11	C	1257	LMT	C4'-C5'-C6'-O6'
11	F	1257	LMT	C4'-C5'-C6'-O6'
5	A	1657	FUM	C4-C5-C6-O7
5	D	1657	FUM	C4-C5-C6-O7
11	C	1257	LMT	O1'-C1-C2-C3
11	F	1257	LMT	O1'-C1-C2-C3
5	A	1657	FUM	C4-C5-C6-O8
5	D	1657	FUM	C4-C5-C6-O8
11	C	1257	LMT	C7-C8-C9-C10
11	F	1257	LMT	C7-C8-C9-C10
11	F	1257	LMT	C11-C10-C9-C8
11	C	1257	LMT	C11-C10-C9-C8
4	A	1656	FAD	P-O3P-PA-O2A
4	D	1656	FAD	P-O3P-PA-O2A
11	F	1257	LMT	C5'-C4'-O1B-C1B
11	C	1257	LMT	C5'-C4'-O1B-C1B
11	C	1257	LMT	C2B-C1B-O1B-C4'
11	F	1257	LMT	C2B-C1B-O1B-C4'
11	C	1257	LMT	O5B-C1B-O1B-C4'
11	F	1257	LMT	O5B-C1B-O1B-C4'
11	F	1257	LMT	C9-C10-C11-C12
11	C	1257	LMT	C9-C10-C11-C12
4	A	1656	FAD	P-O3P-PA-O1A
4	D	1656	FAD	P-O3P-PA-O1A
11	F	1257	LMT	C3'-C4'-O1B-C1B
11	C	1257	LMT	C3'-C4'-O1B-C1B
4	A	1656	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

10 monomers are involved in 35 short contacts:

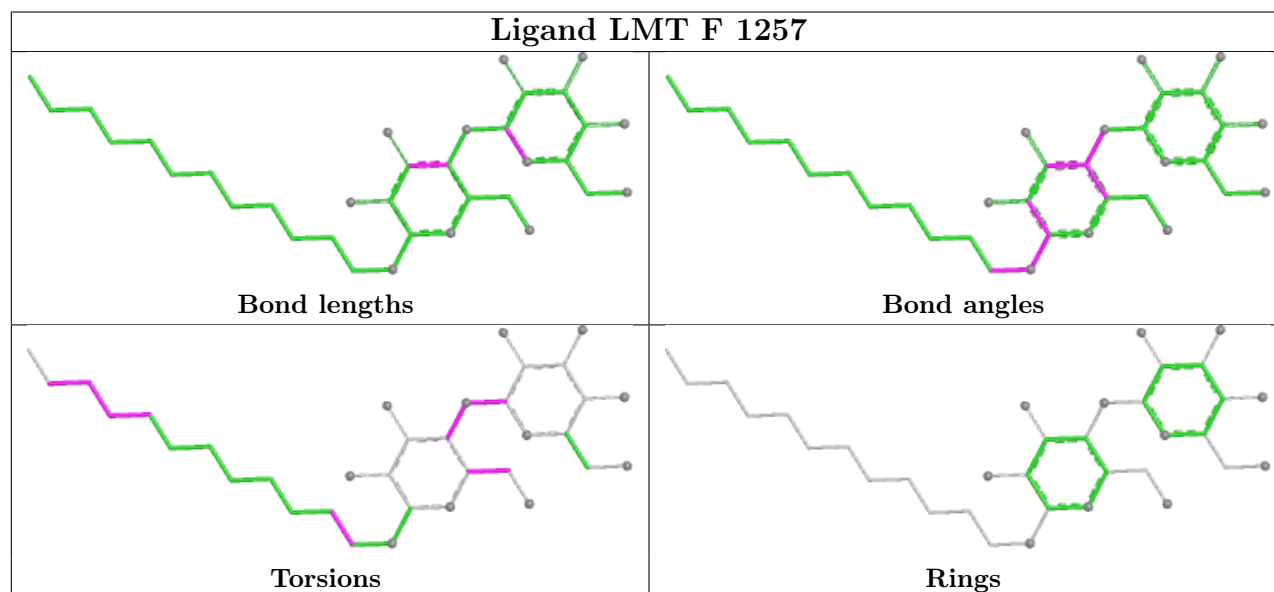
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	1257	LMT	8	0
11	C	1257	LMT	7	0
10	C	1256	HEM	4	0
4	D	1656	FAD	1	0
5	D	1657	FUM	1	0

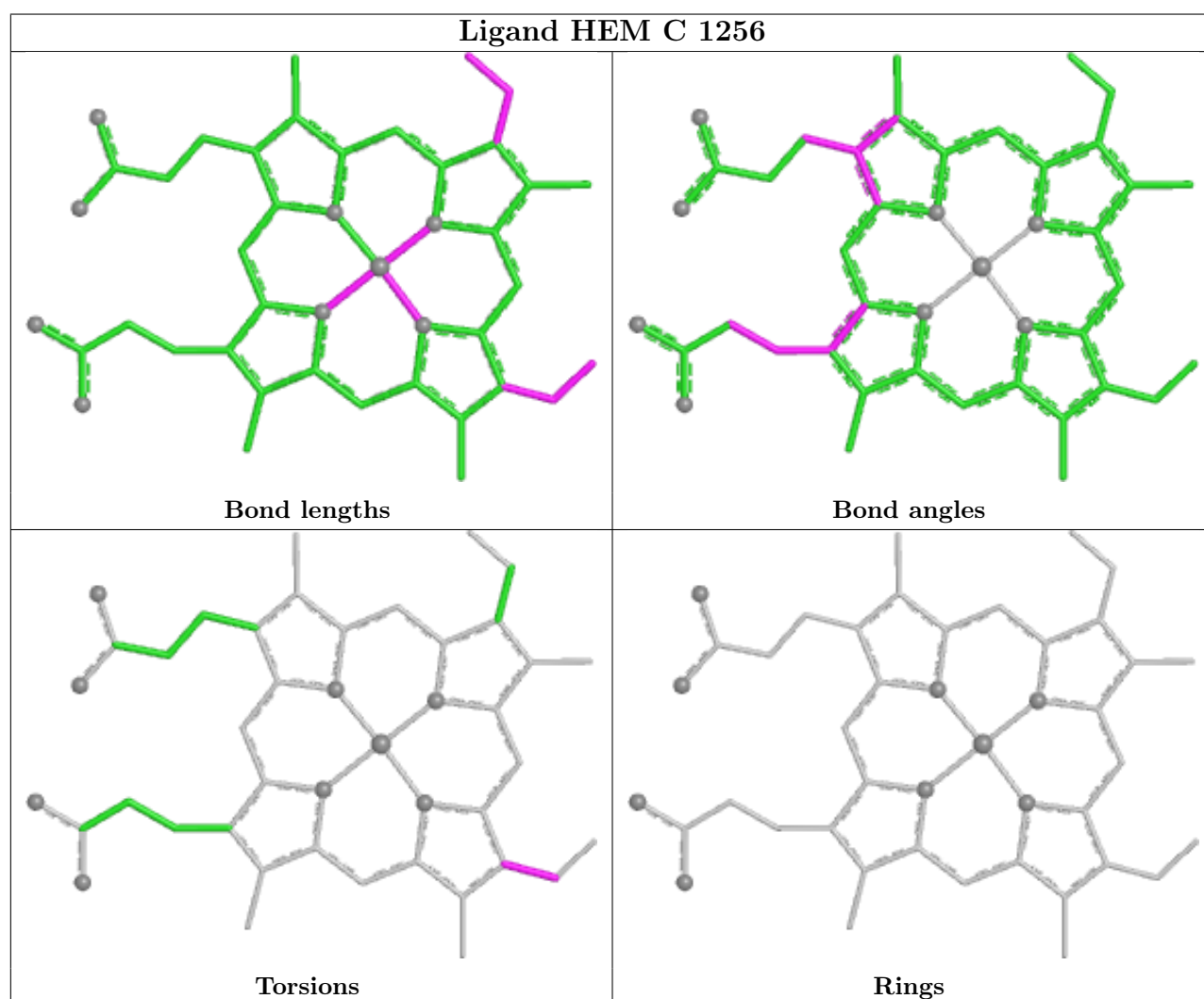
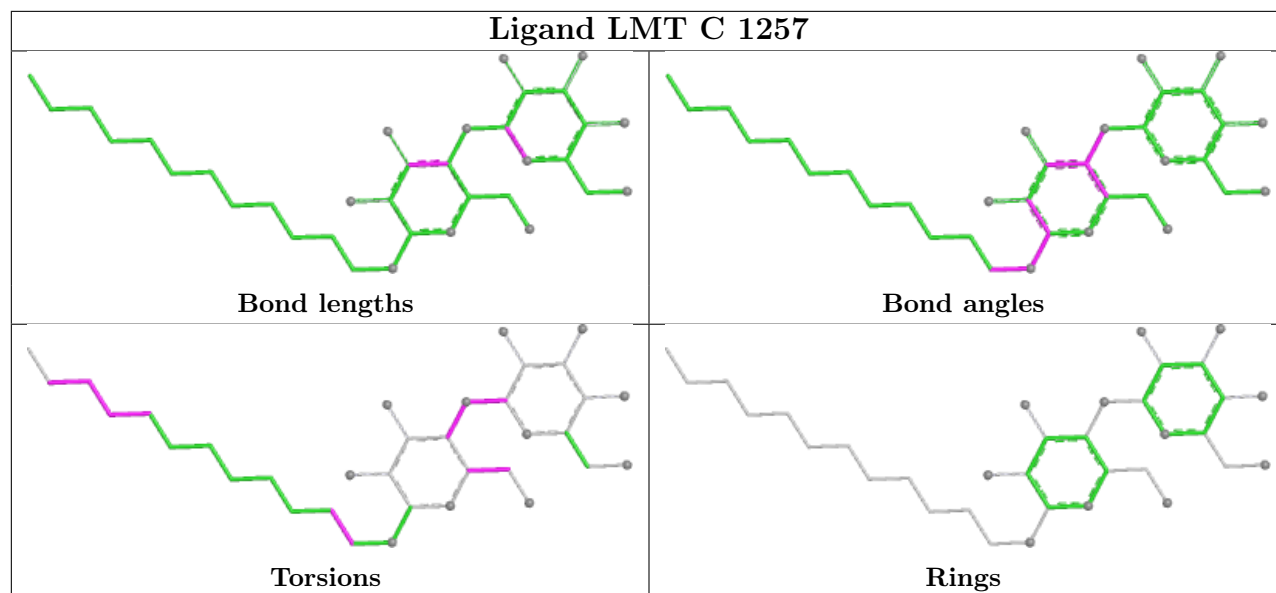
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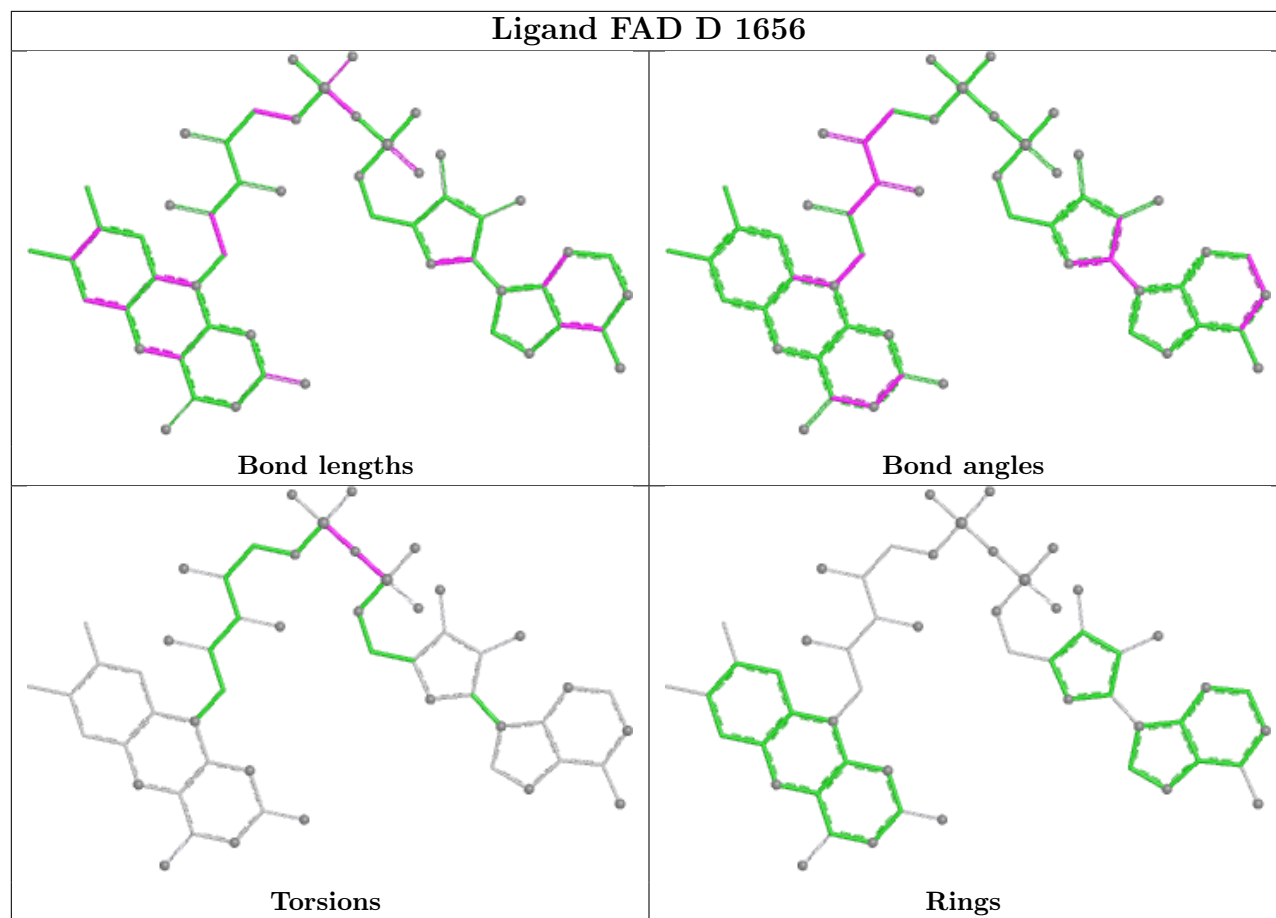
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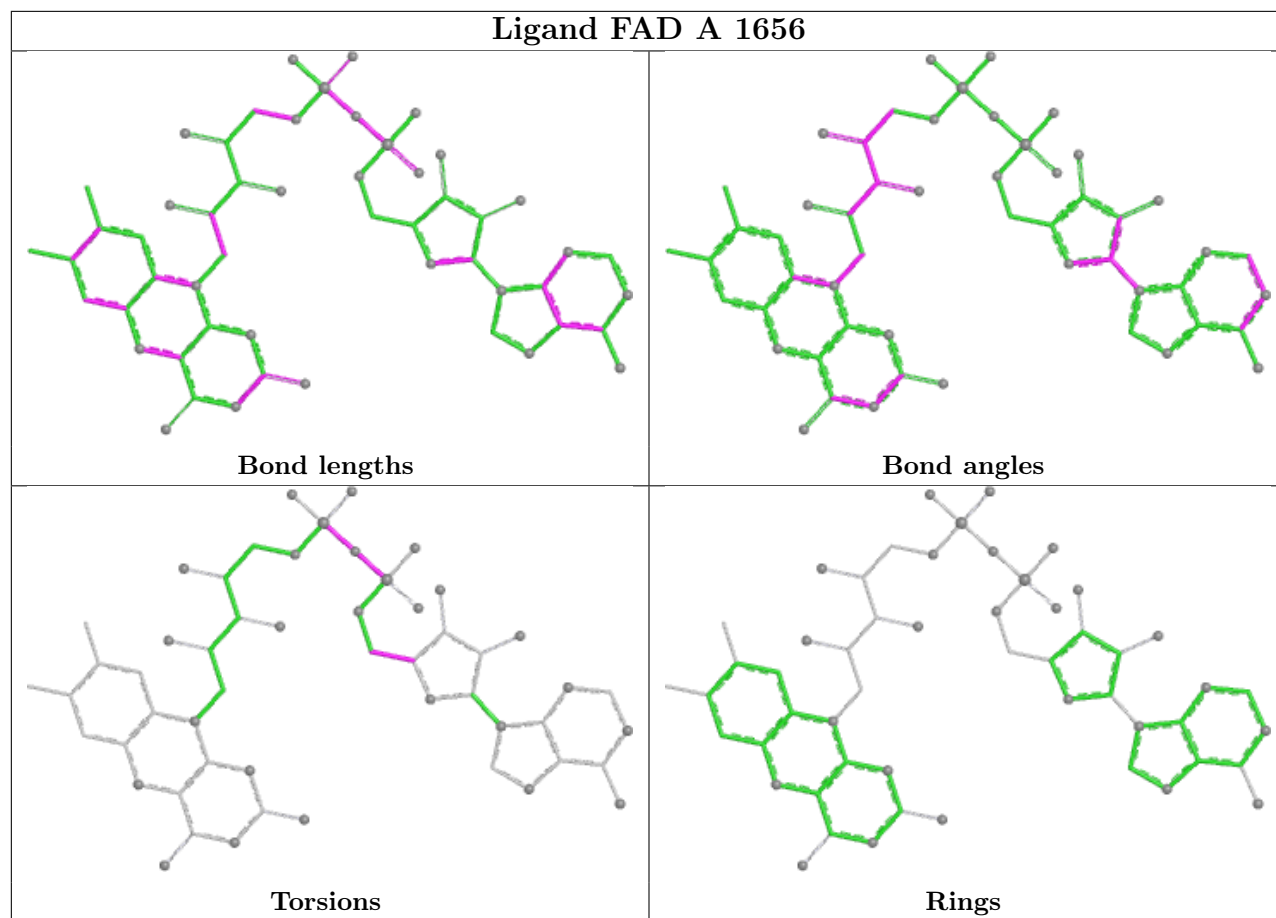
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1657	FUM	2	0
4	A	1656	FAD	1	0
10	F	1256	HEM	4	0
10	F	1255	HEM	4	0
10	C	1255	HEM	3	0

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

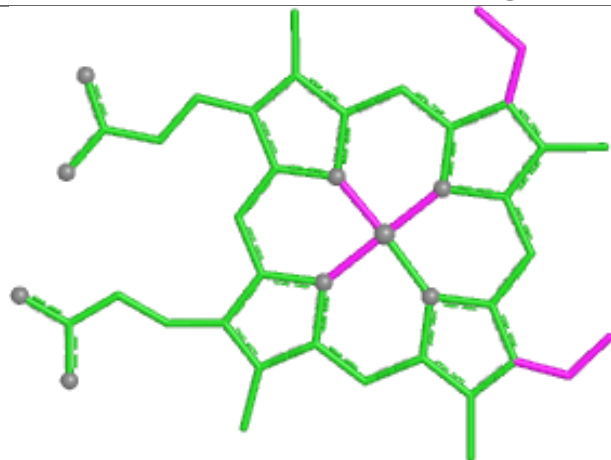




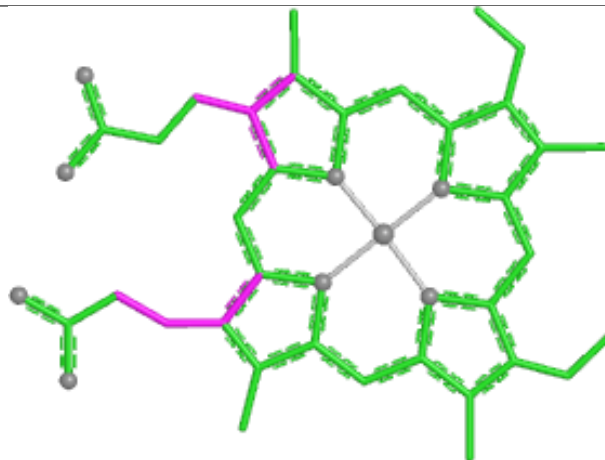




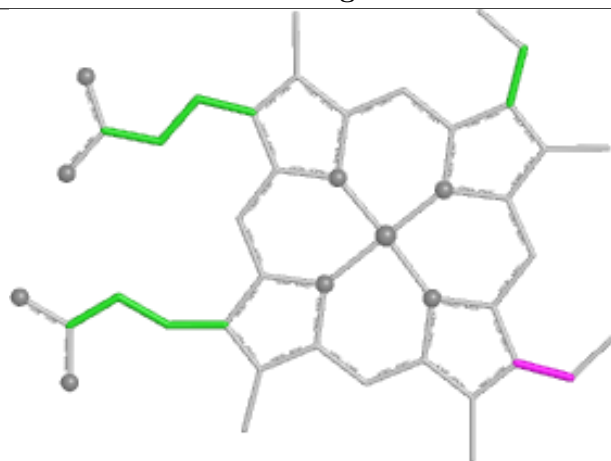
Ligand HEM F 1256



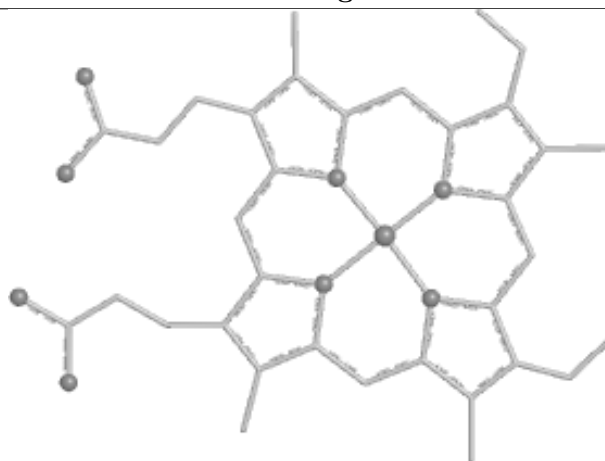
Bond lengths



Bond angles

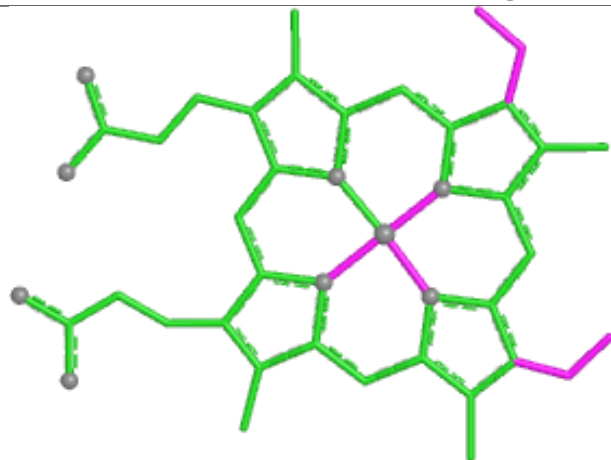


Torsions

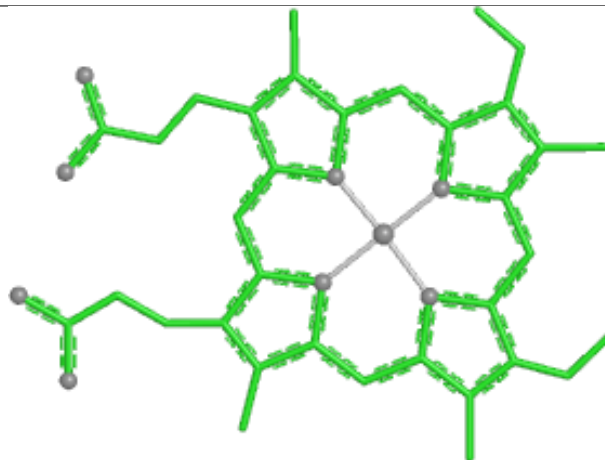


Rings

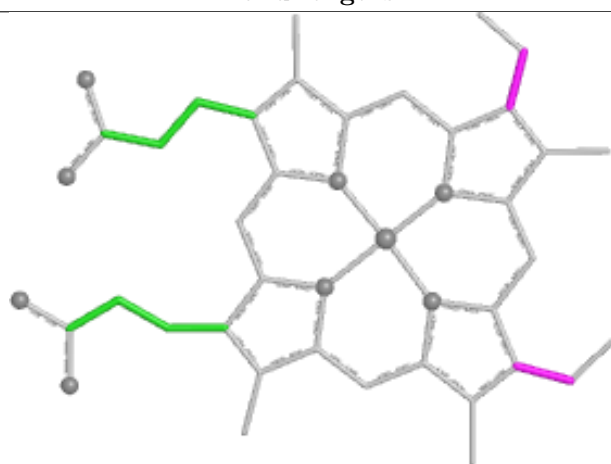
Ligand HEM F 1255



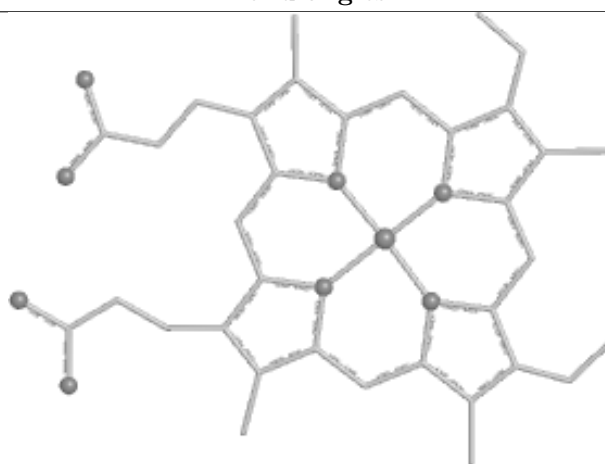
Bond lengths



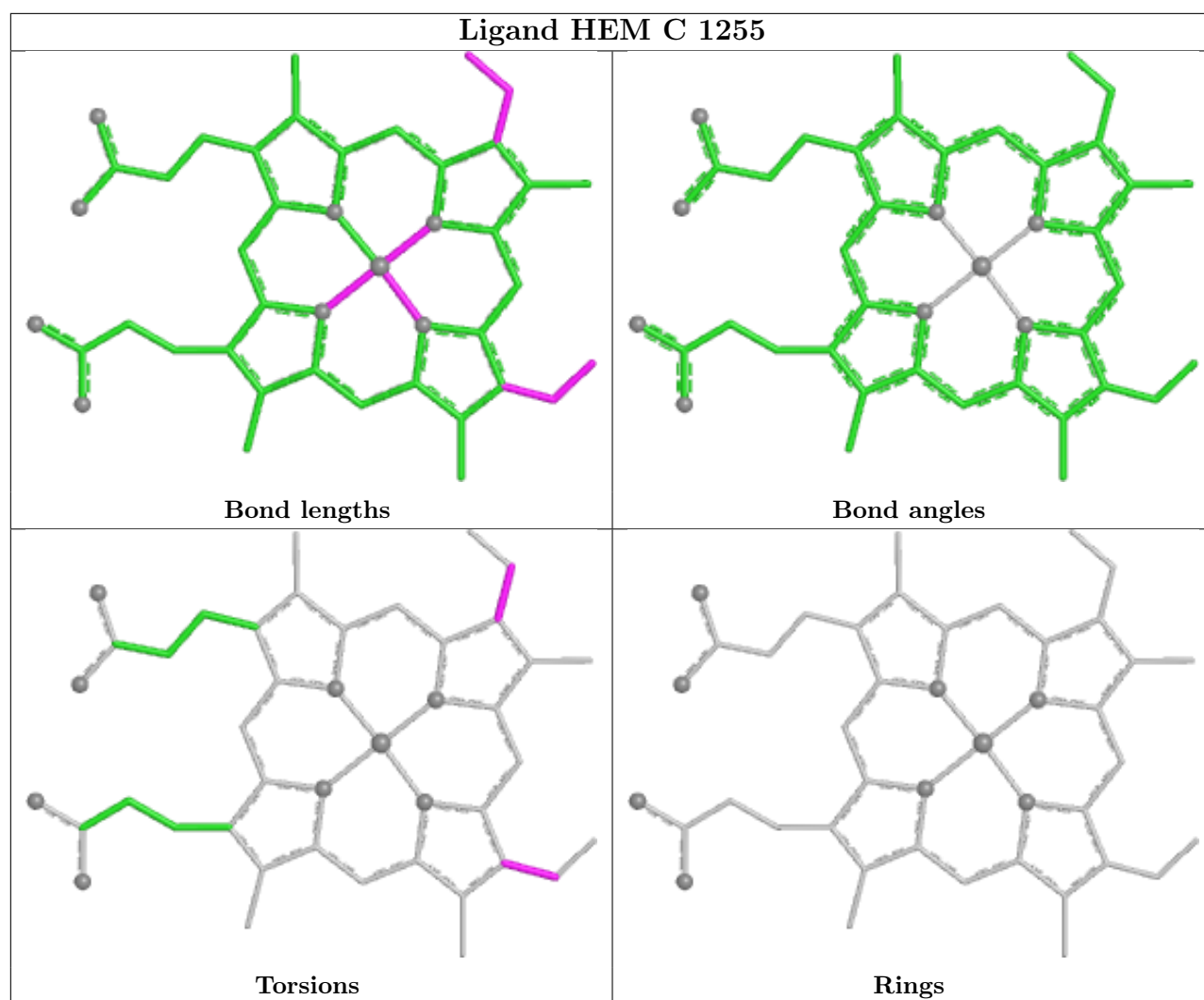
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.