Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:57 AM EDT

PDB ID	:	3WKT
Title	:	Complex structure of an open form of NADPH-cytochrome P450 reductase and heme oxygenase-1
Authors	:	Sugishima, M.; Sato, H.; Higashimoto, Y.; Harada, J.; Wada, K.; Fukuyama, K.; Noguchi, M.
Deposited on	:	2013-10-31
Resolution	:	4.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

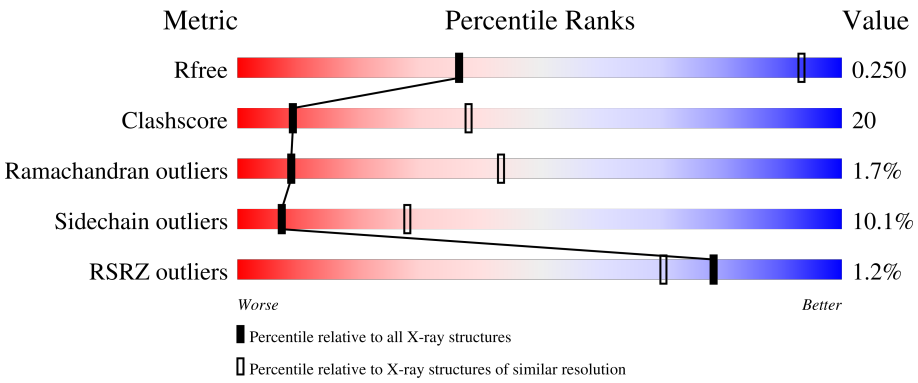
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	618	% 60% 33% • •
1	B	618	2% 54% 34% 7% 5%
2	C	267	51% 27% • 20%
2	D	267	47% 28% 5% 20%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13354 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 NADPH-cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	602	4834	3063	830	918	23	0	0	0
1	B	588	4720	2992	816	889	23	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

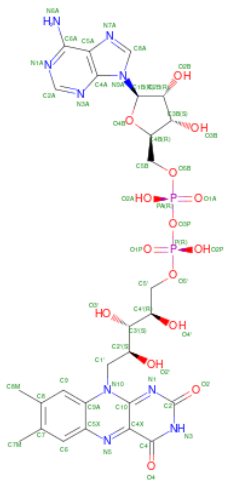
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MET	-	expression tag	UNP P00388
A	?	-	THR	deletion	UNP P00388
A	?	-	GLY	deletion	UNP P00388
A	?	-	GLU	deletion	UNP P00388
A	?	-	GLU	deletion	UNP P00388
B	57	MET	-	expression tag	UNP P00388
B	?	-	THR	deletion	UNP P00388
B	?	-	GLY	deletion	UNP P00388
B	?	-	GLU	deletion	UNP P00388
B	?	-	GLU	deletion	UNP P00388

- Molecule 2 is a protein called Heme oxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	214	1742	1116	298	322	6	0	0	0
2	D	214	1742	1116	298	322	6	0	0	0

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

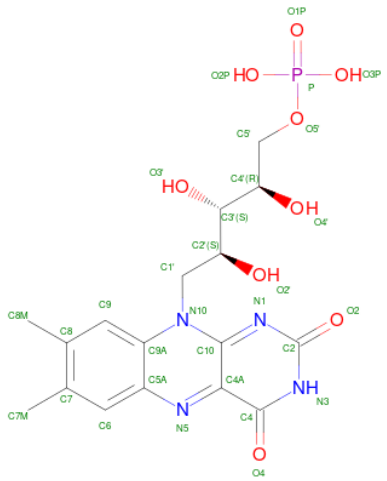
FAD



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

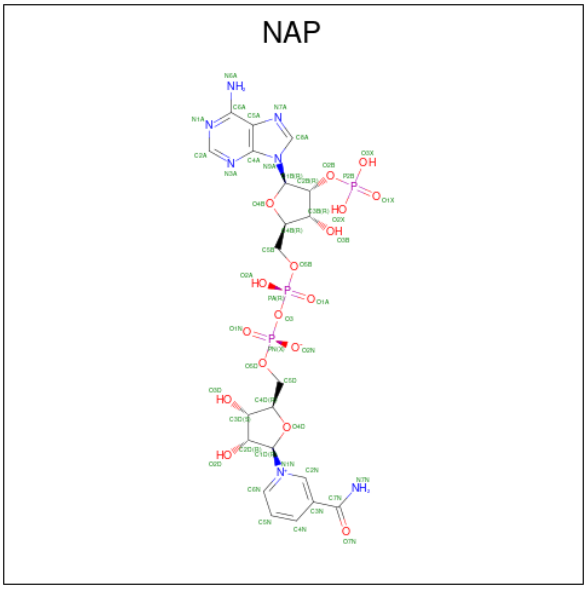
- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

FMN



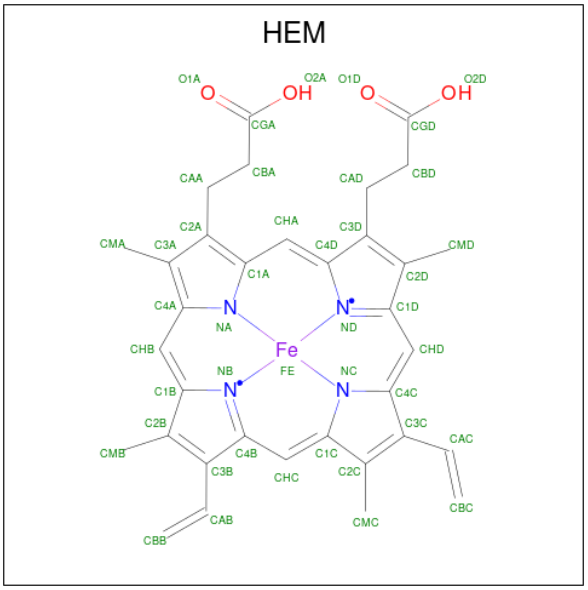
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
4	B	1	31	17	4	9	1	0	0

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
5	B	1	31	10	5	13	3	0	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



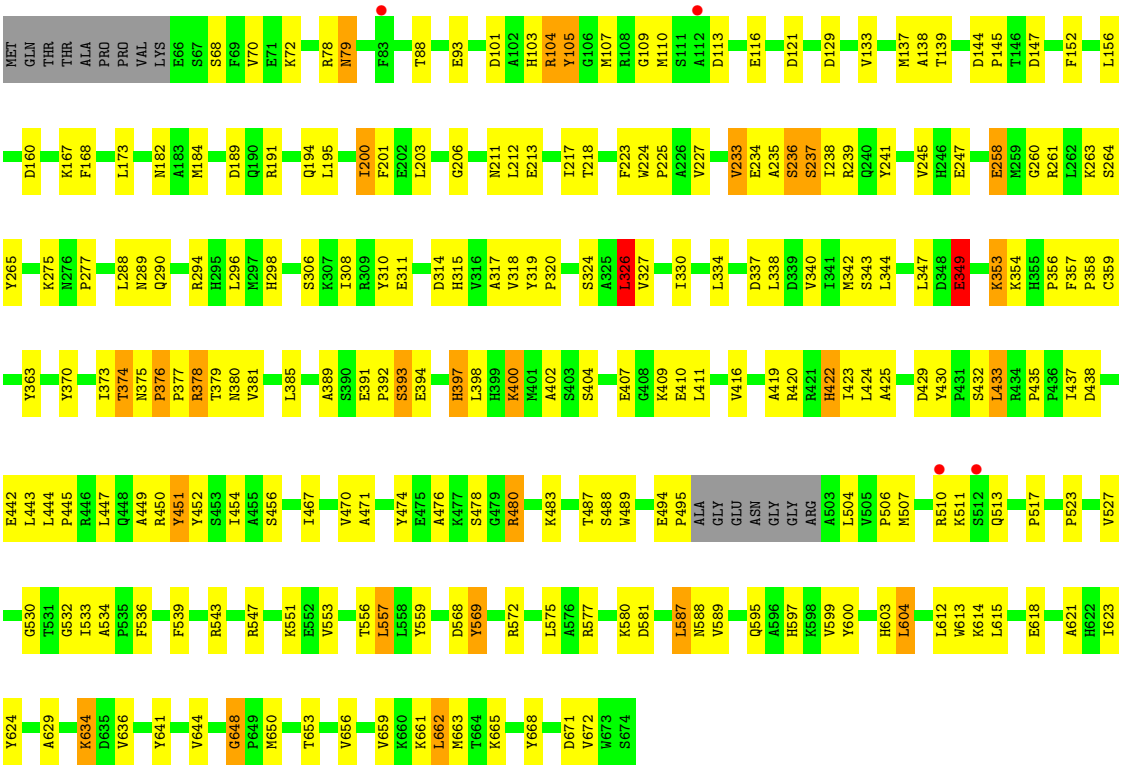
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
6	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
6	D	1	43	34	1	4	4	0	0

3 Residue-property plots (i)

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

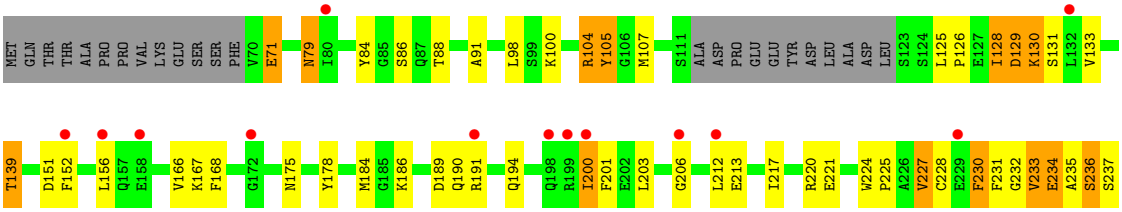
• Molecule 1: NADPH-cytochrome P450 reductase

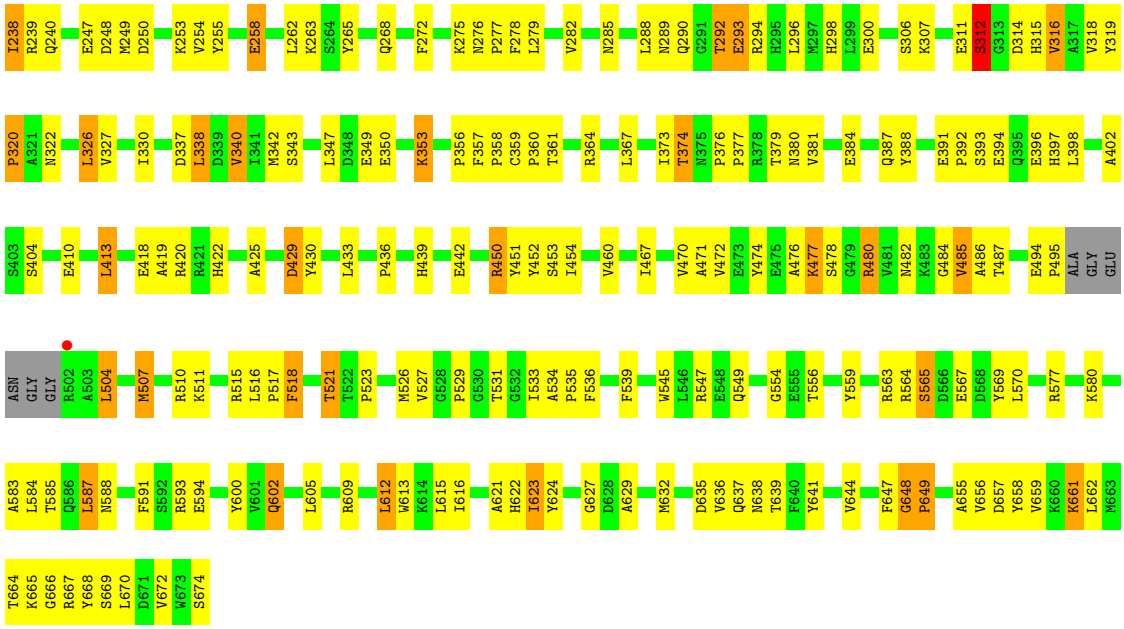
Chain A:



• Molecule 1: NADPH-cytochrome P450 reductase

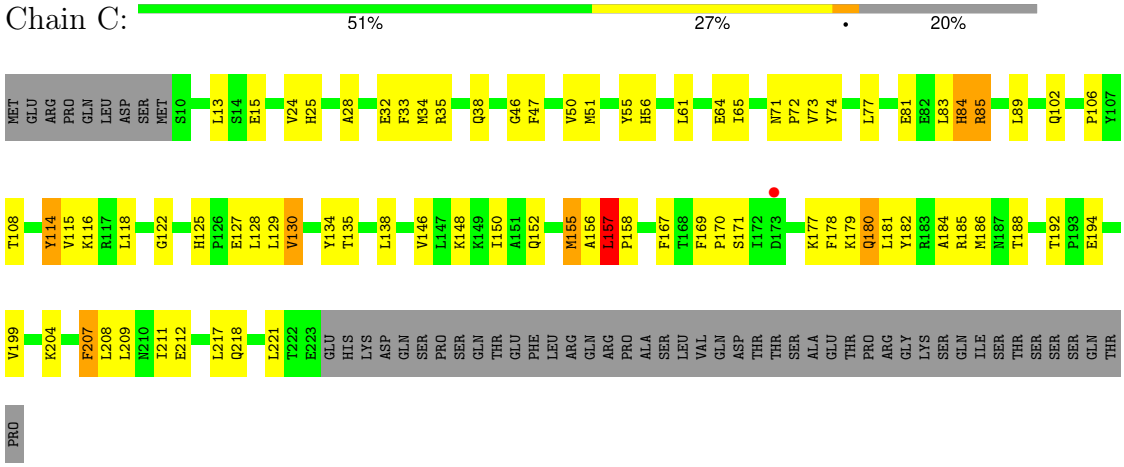
Chain B:





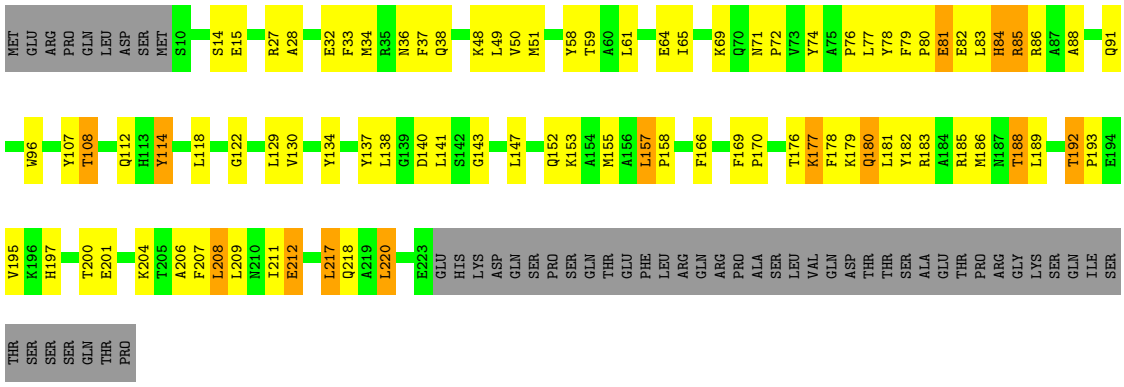
- Molecule 2: Heme oxygenase 1

Chain C:



- Molecule 2: Heme oxygenase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	290.34Å 290.34Å 83.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.34 – 4.30 41.34 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.34-4.30) 100.0 (41.34-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.222 , 0.256 0.215 , 0.250	Depositor DCC
R_{free} test set	1400 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	165.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 168.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13354	wwPDB-VP
Average B, all atoms (Å^2)	235.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAP, HEM, FMN

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	0.56	0/4950	0.83	4/6700 (0.1%)
1	B	0.65	2/4832 (0.0%)	0.87	2/6537 (0.0%)
2	C	0.59	0/1786	0.85	1/2416 (0.0%)
2	D	0.75	0/1786	0.99	2/2416 (0.1%)
All	All	0.63	2/13354 (0.0%)	0.87	9/18069 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	518	PHE	CG-CD2	6.74	1.48	1.38
1	B	518	PHE	CB-CG	5.93	1.61	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	648	GLY	N-CA-C	-9.53	89.27	113.10
1	A	648	GLY	N-CA-C	-6.01	98.07	113.10
1	A	662	LEU	CB-CG-CD1	-6.00	100.80	111.00
2	D	181	LEU	CB-CG-CD2	-5.79	101.15	111.00
1	B	326	LEU	CA-CB-CG	5.68	128.37	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	220	LEU	CA-CB-CG	5.64	128.26	115.30
2	C	157	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	326	LEU	CA-CB-CG	5.08	127.00	115.30
1	A	557	LEU	CB-CG-CD2	-5.00	102.49	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	347	LEU	Peptide
2	D	81	GLU	Peptide

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	4834	0	4679	177	0
1	B	4720	0	4583	227	0
2	C	1742	0	1712	60	0
2	D	1742	0	1712	83	0
3	A	53	0	31	2	0
3	B	53	0	31	4	0
4	A	31	0	19	4	0
4	B	31	0	19	1	0
5	A	31	0	11	0	0
5	B	31	0	11	4	0
6	C	43	0	30	1	0
6	D	43	0	30	1	0
All	All	13354	0	12868	523	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 20.

All (523) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:CYS:HA	1:B:233:VAL:CG1	1.71	1.20
1:B:201:PHE:CE1	1:B:404:SER:HB2	1.88	1.09
1:B:228:CYS:HA	1:B:233:VAL:HG12	1.33	1.08
1:B:201:PHE:HE1	1:B:404:SER:HB2	0.98	1.05
1:B:398:LEU:HD21	1:B:430:TYR:CD2	1.94	1.02
1:A:233:VAL:HG13	1:A:234:GLU:H	1.23	1.01
1:B:233:VAL:HG13	1:B:234:GLU:H	1.20	1.01
1:B:201:PHE:HE1	1:B:404:SER:CB	1.75	0.99
1:A:234:GLU:HG3	1:A:236:SER:HB3	1.47	0.95
2:C:138:LEU:HD21	2:C:182:TYR:CD1	2.02	0.94
1:B:237:SER:O	1:B:238:ILE:HG23	1.65	0.94
1:B:398:LEU:HD21	1:B:430:TYR:CE2	2.04	0.93
2:D:83:LEU:HD22	2:D:137:TYR:HB3	1.53	0.91
2:D:77:LEU:CD1	2:D:130:VAL:HG23	2.01	0.91
1:B:518:PHE:CD2	2:D:76:PRO:HB3	2.06	0.91
1:B:128:ILE:HG22	1:B:128:ILE:O	1.71	0.89
1:B:629:ALA:HB2	1:B:672:VAL:HB	1.54	0.89
1:B:201:PHE:CE1	1:B:404:SER:CB	2.53	0.88
1:A:379:THR:HG23	1:A:402:ALA:HA	1.59	0.84
2:D:138:LEU:HD12	2:D:179:LYS:HG2	1.60	0.84
1:B:233:VAL:HG13	1:B:234:GLU:N	1.90	0.83
1:B:167:LYS:HE3	1:B:230:PHE:HZ	1.43	0.82
1:B:398:LEU:HD11	1:B:433:LEU:HD21	1.60	0.82
1:A:659:VAL:O	1:A:662:LEU:HB2	1.80	0.82
1:A:394:GLU:HG2	1:B:397:HIS:CE1	2.14	0.81
1:B:233:VAL:CG1	1:B:234:GLU:H	1.92	0.81
1:B:494:GLU:HG3	1:B:495:PRO:HD2	1.63	0.81
2:C:155:MET:HB2	2:C:157:LEU:HD22	1.63	0.81
1:B:201:PHE:HD1	1:B:404:SER:HG	1.26	0.80
1:A:317:ALA:HB2	1:A:451:TYR:HD2	1.45	0.80
2:D:155:MET:HB2	2:D:157:LEU:CD2	2.11	0.80
2:D:138:LEU:HD21	2:D:182:TYR:CD1	2.18	0.79
1:A:517:PRO:HD3	1:A:624:TYR:OH	1.84	0.78
1:B:518:PHE:CZ	2:D:76:PRO:HG3	2.19	0.77
1:A:213:GLU:O	1:A:217:ILE:HG13	1.84	0.77
1:A:234:GLU:CG	1:A:236:SER:HB3	2.15	0.77
2:D:77:LEU:HD11	2:D:130:VAL:HG23	1.65	0.77
1:B:156:LEU:HG	1:B:191:ARG:HG2	1.67	0.77
2:C:138:LEU:HD21	2:C:182:TYR:HD1	1.47	0.77
1:B:296:LEU:HD22	1:B:570:LEU:HD21	1.68	0.76
2:C:152:GLN:O	2:C:156:ALA:HA	1.85	0.76
1:B:612:LEU:O	1:B:616:ILE:HG13	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LEU:O	1:B:418:GLU:HG2	1.84	0.76
1:B:337:ASP:O	1:B:340:VAL:HG23	1.86	0.75
1:B:641:TYR:CE1	1:B:656:VAL:HA	2.20	0.75
1:A:156:LEU:HG	1:A:191:ARG:HG2	1.69	0.75
1:B:398:LEU:CD2	1:B:430:TYR:CE2	2.70	0.75
2:D:138:LEU:HD12	2:D:179:LYS:CG	2.17	0.74
1:A:398:LEU:HD11	1:A:433:LEU:HD21	1.68	0.74
1:A:317:ALA:HB2	1:A:451:TYR:CD2	2.23	0.74
1:A:389:ALA:HA	1:A:432:SER:HB3	1.69	0.74
1:A:233:VAL:HG13	1:A:234:GLU:N	2.00	0.74
1:B:600:TYR:HB3	5:B:703:NAP:C2A	2.17	0.74
1:B:228:CYS:CA	1:B:233:VAL:HG12	2.17	0.73
2:D:138:LEU:HD21	2:D:182:TYR:HD1	1.52	0.73
2:D:32:GLU:HB3	2:D:218:GLN:HG2	1.69	0.73
2:C:77:LEU:HD23	2:C:185:ARG:HB3	1.71	0.73
1:A:218:THR:HG23	1:A:378:ARG:HH22	1.53	0.72
1:B:201:PHE:CD1	1:B:404:SER:OG	2.41	0.72
1:B:293:GLU:HG2	1:B:567:GLU:CD	2.09	0.72
1:B:518:PHE:CE2	2:D:76:PRO:HG3	2.25	0.71
1:A:160:ASP:HA	1:A:195:LEU:HD22	1.73	0.71
1:B:201:PHE:HD1	1:B:404:SER:OG	1.73	0.71
2:D:155:MET:HB2	2:D:157:LEU:HD22	1.72	0.70
1:B:237:SER:O	1:B:238:ILE:CG2	2.40	0.70
1:B:391:GLU:HB2	1:B:394:GLU:HG3	1.74	0.70
1:A:569:TYR:CE1	1:A:572:ARG:HA	2.26	0.69
2:D:157:LEU:HB3	2:D:158:PRO:HD3	1.74	0.69
1:B:228:CYS:CA	1:B:233:VAL:CG1	2.62	0.69
1:B:228:CYS:HB3	1:B:234:GLU:HA	1.74	0.69
1:A:139:THR:HG21	1:A:182:ASN:HA	1.74	0.69
1:B:516:LEU:HB3	1:B:517:PRO:HD2	1.73	0.68
1:B:293:GLU:HG2	1:B:567:GLU:OE2	1.91	0.68
1:A:324:SER:O	1:A:327:VAL:HB	1.93	0.68
2:C:157:LEU:HB3	2:C:158:PRO:CD	2.23	0.68
1:B:186:LYS:O	1:B:190:GLN:HG2	1.93	0.68
1:A:349:GLU:OE1	1:A:349:GLU:HA	1.94	0.67
1:B:237:SER:O	1:B:238:ILE:HG12	1.94	0.67
1:B:167:LYS:HE3	1:B:230:PHE:CZ	2.28	0.67
2:C:207:PHE:O	2:C:211:ILE:HG13	1.94	0.67
2:C:128:LEU:HD23	2:C:199:VAL:HG22	1.74	0.67
2:C:46:GLY:HA2	2:C:221:LEU:HD21	1.75	0.67
1:A:527:VAL:HG11	1:A:636:VAL:HG21	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:CZ	1:A:227:VAL:HG21	2.30	0.67
1:B:128:ILE:O	1:B:128:ILE:CG2	2.44	0.66
2:D:207:PHE:O	2:D:211:ILE:HG13	1.95	0.66
1:A:104:ARG:HD3	1:A:238:ILE:HG12	1.78	0.66
2:C:83:LEU:O	2:C:85:ARG:NE	2.28	0.66
1:A:513:GLN:HB2	2:C:177:LYS:HG2	1.77	0.65
2:D:155:MET:HB2	2:D:157:LEU:HD21	1.77	0.65
1:B:190:GLN:O	1:B:194:GLN:HG3	1.97	0.65
1:A:641:TYR:CD1	1:A:659:VAL:HG21	2.32	0.64
1:A:588:ASN:HB3	1:A:604:LEU:HD13	1.79	0.64
2:D:108:THR:HG21	2:D:217:LEU:HD21	1.80	0.64
1:B:602:GLN:HG3	1:B:636:VAL:HG23	1.80	0.63
1:A:577:ARG:HD2	1:A:581:ASP:OD2	1.98	0.63
1:A:653:THR:O	1:A:656:VAL:HG22	1.98	0.63
1:A:160:ASP:HA	1:A:195:LEU:CD2	2.27	0.63
1:B:314:ASP:O	1:B:454:ILE:HG13	1.99	0.62
2:D:143:GLY:O	2:D:147:LEU:HG	1.97	0.62
2:C:77:LEU:HD22	2:C:182:TYR:CE2	2.34	0.62
1:B:451:TYR:CE2	1:B:510:ARG:HD3	2.34	0.62
1:B:623:ILE:HD12	1:B:668:TYR:HD2	1.65	0.62
1:B:379:THR:HG23	1:B:402:ALA:HA	1.80	0.62
1:A:494:GLU:HB2	1:A:495:PRO:HD2	1.81	0.62
1:A:377:PRO:HD2	1:A:416:VAL:CG1	2.29	0.61
1:A:595:GLN:HG2	1:A:597:HIS:O	1.99	0.61
4:A:702:FMN:H2'	4:A:702:FMN:H9	1.81	0.61
1:A:337:ASP:O	1:A:340:VAL:HG23	2.01	0.61
1:B:125:LEU:HD23	1:B:166:VAL:HG13	1.81	0.61
2:C:73:VAL:HB	2:C:127:GLU:HA	1.81	0.61
2:C:155:MET:HB2	2:C:157:LEU:CD2	2.30	0.61
1:A:320:PRO:HG2	1:A:447:LEU:HD21	1.82	0.60
2:C:25:HIS:HA	2:C:207:PHE:CE2	2.36	0.60
1:B:523:PRO:HG2	1:B:621:ALA:HB2	1.84	0.60
2:D:208:LEU:O	2:D:212:GLU:HG2	2.01	0.59
1:A:400:LYS:NZ	1:B:391:GLU:OE1	2.32	0.59
1:A:547:ARG:HG3	1:A:553:VAL:HG21	1.83	0.59
2:D:157:LEU:HB3	2:D:158:PRO:CD	2.32	0.59
1:B:623:ILE:HD12	1:B:668:TYR:CD2	2.37	0.59
1:B:228:CYS:HA	1:B:233:VAL:HG11	1.75	0.59
1:B:429:ASP:OD1	1:B:480:ARG:NH2	2.36	0.59
2:C:128:LEU:HD23	2:C:199:VAL:CG2	2.32	0.59
1:B:217:ILE:O	1:B:221:GLU:HB2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:MET:SD	1:B:507:MET:C	2.81	0.58
1:B:547:ARG:HD2	1:B:583:ALA:HA	1.85	0.58
1:B:511:LYS:HD2	1:B:515:ARG:HH22	1.68	0.58
1:B:613:TRP:CD1	1:B:647:PHE:HB3	2.38	0.58
2:C:77:LEU:CD2	2:C:185:ARG:HB3	2.33	0.58
1:B:288:LEU:HD21	1:B:298:HIS:CB	2.33	0.58
1:B:641:TYR:CD1	1:B:656:VAL:HA	2.38	0.58
1:A:452:TYR:HB3	1:A:467:ILE:HG23	1.86	0.58
1:A:233:VAL:CG1	1:A:234:GLU:H	2.07	0.58
1:A:385:LEU:HB3	1:A:433:LEU:HD11	1.86	0.57
2:C:25:HIS:HA	2:C:207:PHE:HE2	1.67	0.57
1:A:641:TYR:HD1	1:A:659:VAL:HG21	1.68	0.57
2:C:55:TYR:HA	2:C:89:LEU:HD13	1.87	0.57
1:A:289:ASN:HB2	1:A:296:LEU:H	1.69	0.57
1:A:201:PHE:HD1	1:A:404:SER:CB	2.18	0.57
2:C:108:THR:HG21	2:C:217:LEU:HD21	1.87	0.57
2:D:177:LYS:O	2:D:180:GLN:HB2	2.05	0.57
2:C:125:HIS:HB3	2:C:128:LEU:HD12	1.87	0.56
2:D:79:PHE:HB2	2:D:83:LEU:HD12	1.87	0.56
1:A:241:TYR:CE1	1:A:356:PRO:HD3	2.40	0.56
1:A:569:TYR:HE1	1:A:572:ARG:HA	1.68	0.56
1:A:588:ASN:HB3	1:A:604:LEU:CD1	2.34	0.56
1:A:374:THR:O	1:A:422:HIS:HB3	2.05	0.56
1:A:394:GLU:HG2	1:B:397:HIS:HE1	1.68	0.56
1:B:288:LEU:HD21	1:B:298:HIS:HB2	1.88	0.56
1:A:139:THR:HG22	1:A:173:LEU:O	2.05	0.56
2:C:138:LEU:HD21	2:C:182:TYR:CE1	2.40	0.56
1:A:397:HIS:CE1	1:B:394:GLU:HG2	2.41	0.56
1:B:518:PHE:CD2	2:D:76:PRO:CB	2.87	0.56
2:C:157:LEU:HB3	2:C:158:PRO:HD2	1.88	0.56
2:C:34:MET:O	2:C:38:GLN:HG3	2.05	0.56
2:D:74:TYR:CD1	2:D:129:LEU:HD23	2.40	0.56
1:B:494:GLU:HG3	1:B:495:PRO:CD	2.34	0.55
1:A:201:PHE:HD1	1:A:404:SER:HB3	1.71	0.55
1:A:470:VAL:O	1:A:470:VAL:HG13	2.06	0.55
1:A:661:LYS:HE2	2:C:15:GLU:HG2	1.86	0.55
1:B:605:LEU:HD23	1:B:612:LEU:HD21	1.89	0.55
2:D:114:TYR:HE1	2:D:118:LEU:CD1	2.19	0.55
1:A:420:ARG:HD3	1:A:474:TYR:OH	2.07	0.55
1:B:107:MET:HE1	1:B:227:VAL:HG11	1.87	0.55
2:C:114:TYR:CD2	2:C:209:LEU:HB3	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HG	1:B:191:ARG:CG	2.36	0.55
1:B:472:VAL:HB	1:B:484:GLY:HA3	1.89	0.54
1:B:545:TRP:O	1:B:549:GLN:HG2	2.07	0.54
2:D:134:TYR:HB2	2:D:186:MET:HE1	1.88	0.54
1:A:394:GLU:CG	1:B:397:HIS:NE2	2.70	0.54
1:B:518:PHE:CE2	2:D:76:PRO:CB	2.90	0.54
2:D:114:TYR:HE1	2:D:118:LEU:HD11	1.73	0.54
2:D:59:THR:HG23	2:D:86:ARG:HD2	1.90	0.54
1:A:236:SER:O	1:A:237:SER:HB3	2.07	0.54
1:A:288:LEU:HD11	1:A:298:HIS:HB2	1.89	0.54
1:B:450:ARG:NH1	3:B:701:FAD:O2A	2.41	0.53
1:A:363:TYR:CZ	1:A:437:ILE:HG23	2.43	0.53
1:A:235:ALA:HB3	1:A:238:ILE:HD11	1.91	0.53
1:A:641:TYR:CE1	1:A:656:VAL:HA	2.43	0.53
1:B:306:SER:O	1:B:307:LYS:HB2	2.07	0.53
1:B:661:LYS:O	1:B:665:LYS:HG3	2.08	0.53
1:A:471:ALA:HA	1:A:487:THR:HB	1.91	0.53
1:B:125:LEU:N	1:B:126:PRO:HD2	2.23	0.53
2:D:141:LEU:HD11	2:D:178:PHE:CD2	2.43	0.53
1:A:659:VAL:HA	1:A:662:LEU:HD12	1.89	0.53
1:A:237:SER:O	1:A:238:ILE:HG13	2.09	0.53
1:B:130:LYS:HE3	1:B:231:PHE:CD2	2.44	0.53
2:C:130:VAL:HG23	2:C:186:MET:HE2	1.91	0.53
2:C:182:TYR:O	2:C:186:MET:HG3	2.09	0.53
1:A:101:ASP:O	1:A:105:TYR:HB2	2.08	0.53
1:B:238:ILE:O	1:B:238:ILE:HG13	2.07	0.53
2:D:81:GLU:HB2	2:D:82:GLU:OE1	2.08	0.53
2:D:141:LEU:HD11	2:D:178:PHE:HD2	1.74	0.53
2:D:185:ARG:O	2:D:188:THR:HB	2.09	0.53
1:B:107:MET:CE	1:B:227:VAL:HG11	2.38	0.53
1:B:232:GLY:O	1:B:234:GLU:HB2	2.09	0.53
2:D:33:PHE:HB2	2:D:218:GLN:HB2	1.90	0.52
1:A:373:ILE:O	1:A:423:ILE:HG22	2.08	0.52
2:D:34:MET:O	2:D:38:GLN:HG3	2.09	0.52
2:D:50:VAL:HG23	2:D:51:MET:N	2.24	0.52
1:A:487:THR:HG23	3:A:701:FAD:O2P	2.09	0.52
2:D:134:TYR:HB2	2:D:186:MET:CE	2.39	0.52
2:D:83:LEU:O	2:D:85:ARG:NE	2.42	0.52
1:A:200:ILE:O	1:A:404:SER:OG	2.27	0.52
1:B:391:GLU:CB	1:B:394:GLU:HG3	2.39	0.52
1:B:632:MET:SD	1:B:632:MET:C	2.88	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:PHE:CZ	2:C:50:VAL:HG11	2.44	0.52
1:A:557:LEU:HD23	1:A:559:TYR:HE2	1.74	0.52
1:B:237:SER:O	1:B:238:ILE:CB	2.58	0.52
1:B:556:THR:O	1:B:585:THR:HB	2.10	0.52
1:A:394:GLU:HG2	1:B:397:HIS:NE2	2.25	0.52
1:B:322:ASN:HB3	1:B:373:ILE:HD11	1.92	0.52
1:B:529:PRO:HG3	1:B:632:MET:HE2	1.92	0.52
2:D:58:TYR:OH	2:D:140:ASP:OD2	2.24	0.52
1:B:316:VAL:HG12	1:B:454:ILE:HG12	1.92	0.51
1:A:261:ARG:HG3	1:A:264:SER:HB3	1.91	0.51
2:D:14:SER:HB2	2:D:183:ARG:HD3	1.92	0.51
1:B:255:TYR:CZ	1:B:262:LEU:HG	2.45	0.51
1:B:648:GLY:O	1:B:649:PRO:C	2.48	0.51
1:A:385:LEU:HD21	1:A:443:LEU:HD12	1.91	0.51
1:B:107:MET:CE	1:B:227:VAL:CG1	2.88	0.51
1:A:294:ARG:NH2	1:A:568:ASP:OD2	2.44	0.51
1:A:629:ALA:HB2	1:A:672:VAL:HB	1.92	0.51
1:B:278:PHE:CE2	1:B:306:SER:HB3	2.45	0.51
1:B:622:HIS:CE1	1:B:667:ARG:HA	2.46	0.51
1:A:330:ILE:O	1:A:334:LEU:HB2	2.11	0.51
1:A:378:ARG:HB2	1:A:380:ASN:ND2	2.25	0.51
1:B:237:SER:O	1:B:238:ILE:CG1	2.58	0.51
2:C:148:LYS:HB2	2:C:167:PHE:HB3	1.92	0.51
2:D:59:THR:HG23	2:D:86:ARG:CD	2.41	0.51
1:B:128:ILE:HB	1:B:131:SER:HB3	1.93	0.51
1:B:602:GLN:HG3	1:B:636:VAL:CG2	2.41	0.51
1:A:599:VAL:HA	1:A:603:HIS:HD2	1.77	0.50
1:B:518:PHE:CE2	2:D:76:PRO:CG	2.93	0.50
1:A:277:PRO:HG3	1:A:319:TYR:CE2	2.46	0.50
4:A:702:FMN:H2'	4:A:702:FMN:C9	2.40	0.50
1:B:232:GLY:O	1:B:233:VAL:C	2.49	0.50
1:B:507:MET:SD	1:B:507:MET:O	2.70	0.50
2:D:201:GLU:O	2:D:204:LYS:HB2	2.11	0.50
1:B:139:THR:HB	1:B:184:MET:H	1.76	0.50
1:B:86:SER:HB2	1:B:91:ALA:HB3	1.92	0.50
1:A:433:LEU:C	1:A:435:PRO:HD3	2.32	0.50
1:A:530:GLY:O	1:A:533:ILE:HG22	2.11	0.50
1:A:600:TYR:O	1:A:603:HIS:HB2	2.11	0.50
1:A:454:ILE:HG22	1:A:456:SER:H	1.77	0.50
1:B:98:LEU:CD1	1:B:220:ARG:HG3	2.41	0.50
1:B:272:PHE:CG	1:B:278:PHE:HB2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:CE1	1:A:449:ALA:HB2	2.46	0.50
1:A:600:TYR:H	1:A:603:HIS:CD2	2.30	0.50
1:B:349:GLU:HA	1:B:349:GLU:OE1	2.12	0.50
1:B:384:GLU:O	1:B:387:GLN:HG2	2.11	0.50
2:C:138:LEU:HD12	2:C:179:LYS:CG	2.42	0.50
1:A:234:GLU:HG3	1:A:236:SER:CB	2.33	0.50
1:A:661:LYS:HE2	2:C:15:GLU:OE2	2.12	0.50
1:A:393:SER:HB3	1:B:396:GLU:HB2	1.93	0.49
1:B:272:PHE:HD1	1:B:276:ASN:O	1.95	0.49
1:B:343:SER:HA	1:B:359:CYS:SG	2.52	0.49
1:A:480:ARG:HH22	1:B:480:ARG:NH2	2.11	0.49
4:A:702:FMN:H9	4:A:702:FMN:C2'	2.42	0.49
1:B:527:VAL:HG11	1:B:636:VAL:HG21	1.93	0.49
2:C:134:TYR:OH	6:C:300:HEM:HBD2	2.12	0.49
2:D:69:LYS:HD2	2:D:78:TYR:CZ	2.48	0.49
1:B:518:PHE:CE2	2:D:76:PRO:HA	2.48	0.49
2:C:177:LYS:O	2:C:180:GLN:HB2	2.13	0.49
2:D:85:ARG:HG2	2:D:166:PHE:CE1	2.47	0.49
1:A:326:LEU:HD23	1:A:424:LEU:HD23	1.94	0.49
1:B:315:HIS:HB2	1:B:510:ARG:HG3	1.95	0.49
1:A:79:ASN:HD21	1:A:107:MET:HB3	1.78	0.49
2:C:28:ALA:HB2	2:C:211:ILE:HG12	1.94	0.48
2:D:77:LEU:HD11	2:D:130:VAL:CG2	2.41	0.48
1:A:258:GLU:HA	1:A:265:TYR:CZ	2.48	0.48
1:B:79:ASN:HD21	1:B:107:MET:HB3	1.78	0.48
2:C:135:THR:HG23	2:C:207:PHE:CE1	2.48	0.48
2:D:114:TYR:CE1	2:D:118:LEU:HD13	2.47	0.48
1:A:347:LEU:HD23	1:A:347:LEU:HA	1.74	0.48
1:A:389:ALA:CA	1:A:432:SER:HB3	2.43	0.48
1:A:665:LYS:O	2:C:184:ALA:HB2	2.14	0.48
2:D:65:ILE:HG23	2:D:74:TYR:CE2	2.48	0.48
1:B:255:TYR:HA	1:B:258:GLU:OE2	2.14	0.48
1:B:392:PRO:O	1:B:396:GLU:HG2	2.13	0.48
1:A:258:GLU:HA	1:A:265:TYR:CE1	2.49	0.48
1:A:394:GLU:CG	1:B:397:HIS:CE1	2.92	0.48
1:A:613:TRP:HZ3	1:A:644:VAL:HG22	1.79	0.48
1:B:600:TYR:CD2	5:B:703:NAP:C6A	2.97	0.48
1:A:224:TRP:N	1:A:225:PRO:CD	2.77	0.48
1:A:569:TYR:HD1	1:A:569:TYR:O	1.96	0.48
1:A:377:PRO:HD2	1:A:416:VAL:HG13	1.94	0.48
1:B:236:SER:OG	1:B:237:SER:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:PRO:O	2:D:185:ARG:HB3	2.13	0.48
1:B:591:PHE:HB3	1:B:594:GLU:HG3	1.95	0.48
1:B:600:TYR:HB3	1:B:602:GLN:OE1	2.14	0.48
2:D:74:TYR:O	2:D:77:LEU:N	2.39	0.48
1:A:489:TRP:HH2	1:A:506:PRO:HD2	1.79	0.47
1:B:189:ASP:OD2	1:B:203:LEU:HB2	2.13	0.47
1:B:235:ALA:O	1:B:237:SER:O	2.32	0.47
1:B:288:LEU:HD21	1:B:298:HIS:HB3	1.95	0.47
2:C:138:LEU:N	2:C:138:LEU:HD22	2.29	0.47
1:A:385:LEU:CD2	1:A:443:LEU:HD12	2.44	0.47
1:B:374:THR:O	1:B:422:HIS:HB3	2.14	0.47
1:B:388:TYR:CE1	1:B:436:PRO:HD3	2.49	0.47
1:B:600:TYR:CB	5:B:703:NAP:C2A	2.92	0.47
2:D:83:LEU:O	2:D:84:HIS:C	2.53	0.47
1:A:72:LYS:O	1:A:72:LYS:HG3	2.13	0.47
1:A:480:ARG:NH2	1:B:480:ARG:NH2	2.61	0.47
1:A:533:ILE:HD11	1:A:575:LEU:HD11	1.94	0.47
1:B:474:TYR:HE2	1:B:476:ALA:HB2	1.80	0.47
1:B:206:GLY:HA3	1:B:212:LEU:HD12	1.97	0.47
1:B:311:GLU:O	1:B:312:SER:O	2.32	0.47
1:B:644:VAL:HG21	1:B:658:TYR:HD2	1.79	0.47
2:D:134:TYR:HA	2:D:138:LEU:HD23	1.95	0.47
2:D:182:TYR:O	2:D:186:MET:HG3	2.13	0.47
1:B:430:TYR:HB3	1:B:433:LEU:HD23	1.97	0.47
2:D:107:TYR:CZ	2:D:112:GLN:HG2	2.49	0.47
1:A:206:GLY:HA3	1:A:212:LEU:HD12	1.97	0.47
1:B:565:SER:HB3	1:B:594:GLU:OE2	2.15	0.47
1:A:663:MET:HG2	1:A:668:TYR:HB3	1.96	0.47
2:C:177:LYS:O	2:C:180:GLN:CB	2.63	0.47
1:A:78:ARG:CD	1:A:110:MET:HB3	2.45	0.47
2:D:138:LEU:HD12	2:D:179:LYS:HG3	1.95	0.47
1:A:88:THR:HG22	2:C:150:ILE:HD11	1.97	0.47
1:A:419:ALA:O	1:A:476:ALA:HB1	2.15	0.47
1:B:279:LEU:HD23	1:B:504:LEU:HG	1.96	0.47
1:B:624:TYR:HA	1:B:669:SER:O	2.15	0.47
1:B:398:LEU:CD2	1:B:430:TYR:HE2	2.23	0.47
2:C:47:PHE:O	2:C:51:MET:HG2	2.15	0.47
1:A:236:SER:O	1:A:237:SER:CB	2.62	0.46
1:B:487:THR:HG23	3:B:701:FAD:O2P	2.15	0.46
1:B:126:PRO:HD3	1:B:166:VAL:HG22	1.97	0.46
1:B:526:MET:HG2	1:B:536:PHE:CE1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASP:O	1:A:116:GLU:HG2	2.15	0.46
1:B:272:PHE:CD1	1:B:278:PHE:HB2	2.51	0.46
1:B:439:HIS:O	1:B:442:GLU:HB3	2.15	0.46
1:A:629:ALA:HB2	1:A:672:VAL:CG2	2.45	0.46
1:B:175:ASN:HB3	1:B:178:TYR:HD1	1.80	0.46
1:B:472:VAL:HG11	3:B:701:FAD:H52A	1.96	0.46
1:A:201:PHE:CD1	1:A:404:SER:CB	2.99	0.46
1:A:311:GLU:O	1:A:314:ASP:HB2	2.16	0.46
1:A:422:HIS:CE1	1:A:425:ALA:HB2	2.51	0.46
1:B:213:GLU:O	1:B:217:ILE:HG13	2.16	0.46
1:B:298:HIS:CE1	1:B:300:GLU:HG3	2.51	0.46
1:B:559:TYR:CE1	1:B:588:ASN:ND2	2.84	0.46
2:D:77:LEU:HD12	2:D:130:VAL:HG23	1.91	0.46
1:A:138:ALA:HA	1:A:173:LEU:HB2	1.98	0.46
1:B:200:ILE:HD12	1:B:200:ILE:HA	1.73	0.46
2:D:77:LEU:HD22	2:D:182:TYR:CE2	2.50	0.46
2:D:114:TYR:CE1	2:D:118:LEU:CD1	2.99	0.46
1:A:614:LYS:O	1:A:618:GLU:HB2	2.16	0.46
1:B:234:GLU:C	1:B:236:SER:H	2.19	0.46
2:C:56:HIS:HE1	2:C:106:PRO:O	1.99	0.46
1:B:201:PHE:CD1	1:B:404:SER:CB	2.96	0.46
1:B:327:VAL:HG13	1:B:367:LEU:HB3	1.97	0.46
1:B:133:VAL:O	1:B:168:PHE:HA	2.16	0.45
1:B:235:ALA:O	1:B:237:SER:N	2.49	0.45
1:B:523:PRO:HG2	1:B:621:ALA:CB	2.47	0.45
1:A:144:ASP:HB3	1:A:145:PRO:HD2	1.99	0.45
1:B:356:PRO:HG2	1:B:357:PHE:CE2	2.50	0.45
1:A:88:THR:OG1	4:A:702:FMN:O2P	2.24	0.45
1:A:337:ASP:HB3	1:A:340:VAL:CG2	2.47	0.45
1:A:377:PRO:HD2	1:A:416:VAL:HG11	1.98	0.45
1:B:398:LEU:HD21	1:B:430:TYR:HD2	1.69	0.45
1:A:104:ARG:CD	1:A:238:ILE:HG12	2.47	0.45
1:A:523:PRO:HG2	1:A:621:ALA:HB2	1.99	0.45
1:A:587:LEU:HD22	1:A:589:VAL:CG2	2.47	0.45
1:B:452:TYR:HB2	1:B:467:ILE:HD13	1.99	0.45
1:A:358:PRO:HB2	1:A:370:TYR:CE2	2.52	0.45
1:B:233:VAL:CG1	1:B:234:GLU:N	2.59	0.45
1:B:613:TRP:CG	1:B:647:PHE:HB3	2.51	0.45
2:C:181:LEU:O	2:C:181:LEU:HG	2.16	0.45
2:D:50:VAL:CG2	2:D:51:MET:N	2.80	0.45
1:A:233:VAL:CG1	1:A:234:GLU:N	2.73	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ARG:HD2	3:A:701:FAD:N3A	2.32	0.45
1:B:298:HIS:CE1	1:B:300:GLU:CG	2.98	0.45
1:A:315:HIS:HB2	1:A:510:ARG:HG3	1.98	0.45
1:B:564:ARG:HG2	1:B:594:GLU:HG2	1.99	0.45
2:D:61:LEU:O	2:D:65:ILE:HG13	2.17	0.45
1:B:398:LEU:CD1	1:B:433:LEU:HD21	2.38	0.44
2:C:65:ILE:HG23	2:C:74:TYR:CE2	2.52	0.44
1:B:152:PHE:CZ	1:B:156:LEU:HD22	2.52	0.44
1:B:485:VAL:HG12	1:B:486:ALA:N	2.32	0.44
2:C:169:PHE:HA	2:C:170:PRO:HD2	1.79	0.44
1:A:213:GLU:HG3	1:A:217:ILE:HD11	2.00	0.44
1:B:289:ASN:HB2	1:B:296:LEU:H	1.82	0.44
1:B:478:SER:C	1:B:480:ARG:H	2.20	0.44
1:B:563:ARG:HB3	1:B:593:ARG:HD2	1.99	0.44
2:C:32:GLU:HB3	2:C:218:GLN:HG2	1.99	0.44
1:A:349:GLU:OE1	1:A:354:LYS:NZ	2.51	0.44
1:A:513:GLN:HG2	2:C:178:PHE:HA	1.99	0.44
1:B:298:HIS:HE1	1:B:300:GLU:CG	2.31	0.44
1:B:326:LEU:HD22	1:B:373:ILE:HD12	1.99	0.44
1:B:644:VAL:HB	1:B:655:ALA:HB1	1.99	0.44
2:D:61:LEU:HB2	2:D:118:LEU:HD21	1.99	0.44
2:D:80:PRO:O	2:D:84:HIS:HB2	2.17	0.44
1:A:623:ILE:HG21	1:A:668:TYR:CD2	2.52	0.44
1:B:225:PRO:O	1:B:402:ALA:O	2.36	0.44
1:B:228:CYS:HB3	1:B:234:GLU:CA	2.45	0.44
2:C:71:ASN:OD1	2:C:73:VAL:HG22	2.17	0.44
2:C:138:LEU:HD12	2:C:179:LYS:HG2	1.99	0.44
1:A:152:PHE:CZ	1:A:156:LEU:HD22	2.53	0.44
1:B:638:ASN:HA	1:B:641:TYR:CD2	2.53	0.44
1:A:79:ASN:HD22	1:A:79:ASN:H	1.66	0.44
1:A:532:GLY:C	1:A:534:ALA:H	2.21	0.44
2:D:88:ALA:HA	2:D:91:GLN:HG3	2.00	0.44
1:A:239:ARG:HE	1:A:239:ARG:HB3	1.70	0.44
1:B:376:PRO:HA	1:B:377:PRO:HD3	1.74	0.44
1:A:318:VAL:O	1:A:449:ALA:HB1	2.17	0.43
2:C:28:ALA:CB	2:C:211:ILE:HG12	2.48	0.43
2:D:85:ARG:NE	2:D:85:ARG:HA	2.33	0.43
1:B:664:THR:C	1:B:666:GLY:H	2.20	0.43
1:A:237:SER:H	1:A:238:ILE:HD12	1.83	0.43
1:B:531:THR:C	1:B:533:ILE:H	2.22	0.43
1:B:71:GLU:H	1:B:71:GLU:HG3	1.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:VAL:CG2	1:B:658:TYR:HD2	2.31	0.43
1:B:471:ALA:HA	1:B:487:THR:HB	2.01	0.43
1:B:638:ASN:O	1:B:641:TYR:HB2	2.19	0.43
2:C:61:LEU:O	2:C:65:ILE:HG13	2.18	0.43
1:A:201:PHE:CD1	1:A:404:SER:HB3	2.53	0.43
1:A:385:LEU:HD23	1:A:443:LEU:CD1	2.49	0.43
1:A:634:LYS:HB3	1:A:634:LYS:HE2	1.56	0.43
1:B:518:PHE:CE2	2:D:76:PRO:CA	3.02	0.43
2:D:141:LEU:HD23	2:D:141:LEU:HA	1.64	0.43
1:B:254:VAL:HG13	1:B:361:THR:HA	2.00	0.43
1:B:277:PRO:HG3	1:B:319:TYR:CE2	2.54	0.43
2:C:204:LYS:O	2:C:208:LEU:HG	2.18	0.43
2:D:28:ALA:HA	2:D:211:ILE:HG12	2.00	0.43
1:B:84:TYR:O	1:B:84:TYR:CD1	2.72	0.43
1:B:338:LEU:HB3	1:B:364:ARG:HB2	2.00	0.43
1:B:584:LEU:HD23	1:B:587:LEU:HG	2.01	0.43
1:B:659:VAL:O	1:B:662:LEU:HB2	2.18	0.43
2:D:77:LEU:HD23	2:D:77:LEU:HA	1.80	0.43
2:D:155:MET:CB	2:D:157:LEU:HD21	2.45	0.43
1:B:268:GLN:HE22	1:B:278:PHE:HA	1.84	0.42
1:B:516:LEU:HG	1:B:539:PHE:CE1	2.53	0.42
2:D:114:TYR:CD1	2:D:118:LEU:HD13	2.53	0.42
1:A:104:ARG:HD3	1:A:238:ILE:HG21	2.00	0.42
1:A:191:ARG:O	1:A:194:GLN:HB2	2.19	0.42
1:B:638:ASN:HA	1:B:641:TYR:HD2	1.84	0.42
2:C:130:VAL:CG2	2:C:186:MET:HE2	2.49	0.42
1:A:260:GLY:HA3	1:A:275:LYS:O	2.19	0.42
1:A:478:SER:C	1:A:480:ARG:H	2.21	0.42
1:B:422:HIS:CE1	1:B:425:ALA:HB2	2.54	0.42
2:D:206:ALA:O	2:D:209:LEU:HB2	2.19	0.42
1:A:319:TYR:CD1	1:A:449:ALA:HB2	2.54	0.42
1:B:662:LEU:HD23	1:B:667:ARG:HB2	2.00	0.42
1:A:139:THR:HB	1:A:184:MET:HB3	2.01	0.42
1:B:129:ASP:C	1:B:130:LYS:HG3	2.40	0.42
1:B:250:ASP:OD2	1:B:253:LYS:HB2	2.19	0.42
1:B:292:THR:O	1:B:293:GLU:C	2.58	0.42
1:B:600:TYR:HB3	5:B:703:NAP:N1A	2.35	0.42
1:A:139:THR:HB	1:A:184:MET:CB	2.49	0.42
1:A:375:ASN:O	1:A:376:PRO:O	2.37	0.42
1:B:534:ALA:O	1:B:535:PRO:C	2.58	0.42
2:C:138:LEU:HD12	2:C:179:LYS:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:O	1:B:129:ASP:C	2.58	0.42
1:B:139:THR:HG23	4:B:702:FMN:C2	2.49	0.42
1:B:175:ASN:HB3	1:B:178:TYR:CD1	2.54	0.42
1:B:258:GLU:HA	1:B:265:TYR:CZ	2.55	0.42
1:B:319:TYR:HA	1:B:320:PRO:HD3	1.85	0.42
1:B:474:TYR:CE2	1:B:476:ALA:HB2	2.55	0.42
2:D:80:PRO:HA	2:D:84:HIS:CG	2.55	0.42
1:A:70:VAL:HG23	1:A:121:ASP:HB3	2.01	0.42
1:A:613:TRP:CZ3	1:A:644:VAL:HA	2.55	0.42
1:A:648:GLY:O	1:A:650:MET:HG3	2.20	0.42
1:B:296:LEU:HG	1:B:470:VAL:HB	2.02	0.42
1:A:353:LYS:H	1:A:353:LYS:HG2	1.43	0.42
1:A:483:LYS:HD2	1:A:488:SER:OG	2.20	0.42
1:B:420:ARG:HD3	3:B:701:FAD:N3A	2.34	0.42
1:B:353:LYS:H	1:B:353:LYS:HG2	1.70	0.41
2:C:64:GLU:OE1	2:C:122:GLY:HA3	2.20	0.41
1:A:224:TRP:HB2	1:A:225:PRO:HD3	2.02	0.41
1:A:343:SER:OG	1:A:359:CYS:HB3	2.20	0.41
1:B:518:PHE:HE2	2:D:76:PRO:HA	1.85	0.41
2:D:48:LYS:HG2	2:D:96:TRP:CE3	2.55	0.41
1:B:88:THR:O	2:D:153:LYS:HG3	2.20	0.41
2:C:115:VAL:O	2:C:118:LEU:HB2	2.20	0.41
1:A:306:SER:HB2	1:A:308:ILE:HG13	2.01	0.41
1:A:661:LYS:HE2	2:C:15:GLU:CG	2.49	0.41
1:B:516:LEU:HG	1:B:539:PHE:CD1	2.55	0.41
1:B:661:LYS:HG3	2:D:15:GLU:OE1	2.20	0.41
2:C:71:ASN:HA	2:C:72:PRO:HD3	1.87	0.41
1:A:444:LEU:HA	1:A:445:PRO:HD2	1.83	0.41
1:A:543:ARG:HD2	1:A:556:THR:OG1	2.20	0.41
1:B:224:TRP:HB2	1:B:225:PRO:HD3	2.02	0.41
2:D:71:ASN:HA	2:D:72:PRO:HD3	1.90	0.41
1:A:133:VAL:O	1:A:168:PHE:HA	2.21	0.41
1:A:317:ALA:CB	1:A:451:TYR:CD2	3.00	0.41
1:B:627:GLY:O	1:B:672:VAL:HG12	2.20	0.41
1:A:344:LEU:HD21	1:A:438:ASP:HB2	2.02	0.41
1:B:249:MET:CE	1:B:360:PRO:HG2	2.51	0.41
1:B:521:THR:O	1:B:554:GLY:HA3	2.20	0.41
1:A:356:PRO:HG2	1:A:357:PHE:CE2	2.56	0.41
1:A:391:GLU:OE1	1:A:392:PRO:HD2	2.20	0.41
1:B:531:THR:C	1:B:533:ILE:N	2.72	0.41
1:B:587:LEU:HD23	1:B:587:LEU:HA	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:OD2	1:A:203:LEU:HB2	2.21	0.41
1:A:241:TYR:CD2	1:A:442:GLU:HG3	2.55	0.41
1:B:419:ALA:HA	1:B:477:LYS:CG	2.51	0.41
2:D:192:THR:HA	2:D:193:PRO:HD3	1.94	0.41
2:D:197:HIS:O	2:D:200:THR:OG1	2.30	0.41
1:A:277:PRO:HG3	1:A:319:TYR:CD2	2.56	0.41
1:A:337:ASP:HB3	1:A:340:VAL:HG23	2.02	0.41
1:B:565:SER:HA	1:B:591:PHE:CE1	2.55	0.41
2:D:64:GLU:OE1	2:D:122:GLY:HA3	2.21	0.41
1:A:103:HIS:CD2	1:A:109:GLY:H	2.39	0.40
1:A:423:ILE:HG23	1:A:424:LEU:N	2.37	0.40
1:A:536:PHE:O	1:A:539:PHE:HB2	2.21	0.40
1:B:357:PHE:HB2	1:B:358:PRO:HD2	2.02	0.40
1:A:211:ASN:OD1	1:A:213:GLU:HB3	2.21	0.40
1:A:310:TYR:HA	1:A:511:LYS:NZ	2.36	0.40
1:A:569:TYR:CD1	1:A:569:TYR:C	2.95	0.40
1:B:534:ALA:C	1:B:536:PHE:N	2.73	0.40
2:D:169:PHE:HA	2:D:170:PRO:HD2	1.63	0.40
1:A:133:VAL:HG12	1:A:167:LYS:O	2.21	0.40
1:A:430:TYR:HB3	1:A:433:LEU:HD23	2.03	0.40
1:B:477:LYS:H	1:B:477:LYS:HG2	1.71	0.40
6:D:300:HEM:HMD1	6:D:300:HEM:HAD1	1.96	0.40
1:B:104:ARG:HD3	1:B:104:ARG:HA	1.77	0.40
1:B:221:GLU:HG2	1:B:380:ASN:CG	2.42	0.40
2:C:185:ARG:HA	2:C:185:ARG:HD3	1.68	0.40
2:C:209:LEU:O	2:C:212:GLU:HG2	2.21	0.40
1:A:241:TYR:HD2	1:A:442:GLU:HG3	1.87	0.40
1:B:234:GLU:C	1:B:236:SER:N	2.75	0.40
1:B:327:VAL:HA	1:B:330:ILE:HD12	2.04	0.40
2:D:141:LEU:CD1	2:D:178:PHE:HD2	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/618 (97%)	539 (90%)	50 (8%)	9 (2%)	10	46
1	B	582/618 (94%)	509 (88%)	57 (10%)	16 (3%)	5	34
2	C	212/267 (79%)	197 (93%)	13 (6%)	2 (1%)	17	56
2	D	212/267 (79%)	193 (91%)	18 (8%)	1 (0%)	29	68
All	All	1604/1770 (91%)	1438 (90%)	138 (9%)	28 (2%)	9	43

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	VAL
1	A	236	SER
1	A	237	SER
1	A	376	PRO
1	B	230	PHE
1	B	233	VAL
1	B	236	SER
1	B	238	ILE
1	B	128	ILE
1	B	293	GLU
1	B	312	SER
2	C	102	GLN
1	A	349	GLU
1	A	433	LEU
1	B	105	TYR
1	B	240	GLN
2	C	84	HIS
2	D	189	LEU
1	A	68	SER
1	A	147	ASP
1	B	239	ARG
1	B	609	ARG
1	A	671	ASP
1	B	320	PRO
1	B	340	VAL
1	B	282	VAL
1	B	485	VAL
1	B	649	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/528 (98%)	475 (92%)	42 (8%)	11	38
1	B	504/528 (96%)	445 (88%)	59 (12%)	5	23
2	C	183/233 (78%)	164 (90%)	19 (10%)	7	27
2	D	183/233 (78%)	163 (89%)	20 (11%)	6	26
All	All	1387/1522 (91%)	1247 (90%)	140 (10%)	7	28

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	93	GLU
1	A	104	ARG
1	A	105	TYR
1	A	129	ASP
1	A	137	MET
1	A	200	ILE
1	A	245	VAL
1	A	247	GLU
1	A	258	GLU
1	A	263	LYS
1	A	290	GLN
1	A	326	LEU
1	A	338	LEU
1	A	342	MET
1	A	349	GLU
1	A	353	LYS
1	A	374	THR
1	A	378	ARG
1	A	381	VAL
1	A	393	SER
1	A	397	HIS
1	A	400	LYS
1	A	407	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	409	LYS
1	A	410	GLU
1	A	411	LEU
1	A	422	HIS
1	A	429	ASP
1	A	450	ARG
1	A	451	TYR
1	A	480	ARG
1	A	504	LEU
1	A	507	MET
1	A	551	LYS
1	A	569	TYR
1	A	580	LYS
1	A	587	LEU
1	A	604	LEU
1	A	612	LEU
1	A	615	LEU
1	A	634	LYS
1	B	71	GLU
1	B	79	ASN
1	B	100	LYS
1	B	104	ARG
1	B	105	TYR
1	B	129	ASP
1	B	130	LYS
1	B	139	THR
1	B	151	ASP
1	B	200	ILE
1	B	227	VAL
1	B	234	GLU
1	B	247	GLU
1	B	248	ASP
1	B	258	GLU
1	B	263	LYS
1	B	275	LYS
1	B	285	ASN
1	B	290	GLN
1	B	292	THR
1	B	294	ARG
1	B	312	SER
1	B	316	VAL
1	B	318	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	338	LEU
1	B	342	MET
1	B	350	GLU
1	B	353	LYS
1	B	374	THR
1	B	381	VAL
1	B	393	SER
1	B	410	GLU
1	B	413	LEU
1	B	429	ASP
1	B	450	ARG
1	B	453	SER
1	B	460	VAL
1	B	477	LYS
1	B	480	ARG
1	B	482	ASN
1	B	504	LEU
1	B	507	MET
1	B	521	THR
1	B	565	SER
1	B	569	TYR
1	B	577	ARG
1	B	580	LYS
1	B	587	LEU
1	B	602	GLN
1	B	612	LEU
1	B	615	LEU
1	B	623	ILE
1	B	635	ASP
1	B	637	GLN
1	B	639	THR
1	B	657	ASP
1	B	661	LYS
1	B	670	LEU
1	B	674	SER
2	C	13	LEU
2	C	24	VAL
2	C	35	ARG
2	C	81	GLU
2	C	84	HIS
2	C	85	ARG
2	C	114	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	116	LYS
2	C	129	LEU
2	C	130	VAL
2	C	146	VAL
2	C	155	MET
2	C	157	LEU
2	C	171	SER
2	C	180	GLN
2	C	188	THR
2	C	192	THR
2	C	194	GLU
2	C	207	PHE
2	D	27	ARG
2	D	36	ASN
2	D	37	PHE
2	D	49	LEU
2	D	84	HIS
2	D	85	ARG
2	D	108	THR
2	D	114	TYR
2	D	152	GLN
2	D	157	LEU
2	D	176	THR
2	D	177	LYS
2	D	180	GLN
2	D	188	THR
2	D	192	THR
2	D	195	VAL
2	D	208	LEU
2	D	212	GLU
2	D	217	LEU
2	D	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	87	GLN
1	A	198	GLN
1	A	246	HIS
1	A	290	GLN
1	A	298	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	315	HIS
1	A	380	ASN
1	A	395	GLN
1	A	482	ASN
1	A	603	HIS
1	A	622	HIS
1	A	637	GLN
1	B	79	ASN
1	B	87	GLN
1	B	276	ASN
1	B	289	ASN
1	B	290	GLN
1	B	298	HIS
1	B	346	ASN
1	B	380	ASN
1	B	395	GLN
1	B	482	ASN
1	B	617	HIS
1	B	622	HIS
1	B	637	GLN
2	C	36	ASN
2	C	41	GLN
2	C	56	HIS
2	C	68	ASN
2	C	112	GLN
2	C	218	GLN
2	D	36	ASN
2	D	68	ASN
2	D	112	GLN
2	D	132	HIS
2	D	152	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	B	701	-	54,58,58	1.40	9 (16%)	71,89,89	1.66	19 (26%)
6	HEM	D	300	-	42,50,50	1.40	8 (19%)	46,82,82	2.19	11 (23%)
5	NAP	A	703	-	28,33,52	1.19	2 (7%)	40,52,80	1.89	8 (20%)
5	NAP	B	703	-	28,33,52	0.98	1 (3%)	40,52,80	2.22	10 (25%)
6	HEM	C	300	-	42,50,50	1.29	7 (16%)	46,82,82	1.85	10 (21%)
4	FMN	B	702	-	33,33,33	1.74	6 (18%)	48,50,50	1.39	8 (16%)
3	FAD	A	701	-	54,58,58	1.52	9 (16%)	71,89,89	1.60	15 (21%)
4	FMN	A	702	-	33,33,33	1.58	5 (15%)	48,50,50	1.47	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	701	-	-	7/30/50/50	0/6/6/6
6	HEM	D	300	-	-	8/12/54/54	-
5	NAP	A	703	-	-	1/17/37/67	0/3/3/5
5	NAP	B	703	-	-	0/17/37/67	0/3/3/5
6	HEM	C	300	-	-	6/12/54/54	-
4	FMN	B	702	-	-	1/18/18/18	0/3/3/3
3	FAD	A	701	-	-	5/30/50/50	0/6/6/6
4	FMN	A	702	-	-	2/18/18/18	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	FMN	C9A-C5A	6.48	1.51	1.41
4	A	702	FMN	C9A-C5A	5.60	1.50	1.41
3	A	701	FAD	C9A-C5X	4.87	1.49	1.41
3	B	701	FAD	PA-O3P	4.01	1.63	1.59
3	B	701	FAD	C9A-C5X	3.92	1.47	1.41
4	B	702	FMN	C8-C7	3.91	1.50	1.40
3	A	701	FAD	C8-C7	3.88	1.50	1.40
6	D	300	HEM	C1B-NB	-3.78	1.33	1.40
4	A	702	FMN	C8-C7	3.74	1.50	1.40
3	A	701	FAD	O4B-C1B	3.52	1.45	1.40
3	A	701	FAD	P-O3P	3.47	1.63	1.59
5	A	703	NAP	PN-O1N	3.31	1.60	1.50
6	D	300	HEM	CHB-C1B	3.17	1.42	1.34
3	A	701	FAD	C2A-N3A	2.87	1.36	1.32
3	B	701	FAD	C8-C7	2.79	1.47	1.40
6	C	300	HEM	C1B-NB	-2.71	1.35	1.40
6	C	300	HEM	C4D-ND	-2.68	1.35	1.40
6	C	300	HEM	CHB-C1B	2.63	1.41	1.34
4	A	702	FMN	C4A-N5	2.60	1.36	1.30
6	D	300	HEM	C4D-C3D	2.58	1.49	1.45
6	C	300	HEM	FE-NB	2.58	2.12	1.98
3	A	701	FAD	C1'-C2'	2.56	1.56	1.52
4	B	702	FMN	C4A-N5	2.46	1.36	1.30
6	D	300	HEM	C4D-ND	-2.45	1.36	1.40
3	B	701	FAD	P-O3P	2.45	1.62	1.59
4	A	702	FMN	C10-N10	2.44	1.42	1.37
5	A	703	NAP	O4B-C1B	2.40	1.44	1.40
6	C	300	HEM	C3B-C4B	2.39	1.49	1.44
3	B	701	FAD	O2-C2	2.33	1.29	1.24
3	B	701	FAD	C2A-N3A	2.30	1.35	1.32
6	D	300	HEM	FE-NB	2.30	2.10	1.98
3	B	701	FAD	C4X-N5	2.29	1.35	1.30
3	B	701	FAD	C1'-C2'	2.27	1.55	1.52
4	A	702	FMN	C4-N3	-2.21	1.34	1.38
5	B	703	NAP	O4B-C1B	2.20	1.43	1.40
6	D	300	HEM	CHA-C4D	2.17	1.39	1.34
3	A	701	FAD	C5X-N5	-2.16	1.35	1.39
6	C	300	HEM	C4D-C3D	2.14	1.48	1.45
6	C	300	HEM	CHA-C4D	2.13	1.39	1.34
4	B	702	FMN	C10-N10	2.13	1.41	1.37
4	B	702	FMN	C5'-C4'	2.11	1.54	1.51
6	D	300	HEM	C4B-NB	-2.10	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	300	HEM	C3B-C4B	2.08	1.48	1.44
3	A	701	FAD	C6A-C5A	2.06	1.51	1.43
4	B	702	FMN	C4-N3	-2.05	1.35	1.38
3	A	701	FAD	C4X-N5	2.04	1.35	1.30
3	B	701	FAD	C6A-C5A	2.01	1.50	1.43

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	703	NAP	C1B-N9A-C4A	-8.08	112.45	126.64
5	B	703	NAP	N3A-C2A-N1A	-6.34	120.07	128.67
6	D	300	HEM	C1B-NB-C4B	5.82	112.10	105.21
5	A	703	NAP	C1B-N9A-C4A	-5.65	116.71	126.64
6	D	300	HEM	CHD-C1D-ND	5.51	130.37	124.44
6	C	300	HEM	CHD-C1D-ND	5.08	129.90	124.44
3	A	701	FAD	O4B-C1B-N9A	5.08	115.47	108.75
5	A	703	NAP	C4B-O4B-C1B	-4.92	105.42	109.92
6	D	300	HEM	CAD-C3D-C4D	4.91	133.26	124.70
3	B	701	FAD	C4-C4X-N5	4.68	124.68	118.21
6	C	300	HEM	C3B-C4B-NB	-4.42	106.29	109.47
6	D	300	HEM	C3B-C4B-NB	-4.39	106.32	109.47
6	C	300	HEM	C1B-NB-C4B	4.26	110.25	105.21
5	A	703	NAP	O5D-PN-O2N	4.25	123.72	107.80
3	A	701	FAD	O2-C2-N1	-4.08	115.02	121.80
6	D	300	HEM	CHC-C4B-NB	4.05	128.79	124.44
4	A	702	FMN	C4-C4A-N5	3.97	123.69	118.21
3	A	701	FAD	N3A-C2A-N1A	-3.84	123.46	128.67
6	C	300	HEM	CHD-C1D-C2D	-3.75	119.11	125.03
3	B	701	FAD	C9A-C5X-N5	-3.68	118.55	122.45
6	D	300	HEM	CBD-CAD-C3D	3.59	122.47	112.53
3	A	701	FAD	C4-C4X-N5	3.52	123.07	118.21
4	B	702	FMN	C5'-C4'-C3'	3.50	118.83	112.22
5	A	703	NAP	N3A-C2A-N1A	-3.39	124.08	128.67
3	B	701	FAD	O4'-C4'-C3'	3.38	117.16	109.25
3	B	701	FAD	N3A-C2A-N1A	-3.37	124.10	128.67
3	B	701	FAD	C4B-O4B-C1B	-3.25	106.95	109.92
6	D	300	HEM	CAD-C3D-C2D	-3.23	121.82	127.87
4	B	702	FMN	C4-C4A-N5	3.22	122.65	118.21
6	C	300	HEM	CHA-C4D-ND	3.22	128.36	124.37
3	A	701	FAD	O2-C2-N3	3.21	124.74	118.58
6	C	300	HEM	CHC-C4B-NB	3.21	127.88	124.44
4	A	702	FMN	C4A-C10-N10	3.17	121.02	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	703	NAP	O2N-PN-O1N	3.15	123.12	110.83
5	A	703	NAP	C4A-C5A-N7A	-3.12	106.04	109.34
3	B	701	FAD	C5X-N5-C4X	3.11	123.12	118.09
3	B	701	FAD	C4A-C5A-N7A	-3.10	106.06	109.34
3	B	701	FAD	C10-N1-C2	3.09	123.54	116.85
4	B	702	FMN	C4A-C10-N10	3.04	120.83	116.48
5	B	703	NAP	C3B-C2B-C1B	-3.02	97.02	102.81
6	D	300	HEM	CHD-C1D-C2D	-2.96	120.36	125.03
4	A	702	FMN	C4A-C10-N1	-2.90	117.48	124.59
3	B	701	FAD	O2-C2-N3	2.90	124.14	118.58
5	A	703	NAP	C3B-C2B-C1B	-2.89	97.27	102.81
6	D	300	HEM	CBA-CAA-C2A	-2.85	107.75	112.54
5	B	703	NAP	C4B-O4B-C1B	-2.83	107.33	109.92
4	B	702	FMN	O2-C2-N1	-2.63	117.43	121.80
4	A	702	FMN	C10-N1-C2	2.63	122.55	116.85
3	B	701	FAD	C6-C5X-N5	2.61	122.78	118.44
4	A	702	FMN	C10-C4A-N5	-2.61	119.48	124.81
3	A	701	FAD	C4A-C5A-N7A	-2.60	106.59	109.34
5	B	703	NAP	N6A-C6A-N1A	2.60	123.89	118.33
5	B	703	NAP	C2B-C1B-N9A	2.58	118.29	112.56
3	A	701	FAD	O4-C4-C4X	-2.52	119.88	126.53
5	B	703	NAP	O3B-C3B-C4B	-2.48	103.95	111.08
6	C	300	HEM	CHA-C4D-C3D	-2.48	120.65	125.23
3	A	701	FAD	C1B-N9A-C4A	-2.48	122.28	126.64
5	A	703	NAP	O4B-C1B-C2B	2.48	110.84	106.61
3	A	701	FAD	C9A-C5X-N5	-2.47	119.84	122.45
6	C	300	HEM	CBA-CAA-C2A	-2.46	108.40	112.54
3	B	701	FAD	O2-C2-N1	-2.44	117.75	121.80
6	D	300	HEM	O2D-CGD-O1D	-2.44	117.06	123.33
4	A	702	FMN	O2-C2-N1	-2.44	117.75	121.80
6	C	300	HEM	CHB-C1B-NB	2.43	127.39	124.37
3	A	701	FAD	O3'-C3'-C2'	2.43	114.45	108.93
3	A	701	FAD	C5X-C9A-N10	2.41	120.15	117.97
6	D	300	HEM	CAD-CBD-CGD	-2.36	107.41	113.67
5	B	703	NAP	O2A-PA-O1A	2.31	123.19	112.44
4	B	702	FMN	C4A-C10-N1	-2.31	118.94	124.59
3	A	701	FAD	C9-C9A-N10	-2.30	118.77	121.85
3	A	701	FAD	O3B-C3B-C4B	2.28	117.62	111.08
3	B	701	FAD	O4-C4-C4X	-2.27	120.55	126.53
3	B	701	FAD	C10-C4X-N5	-2.27	120.18	124.81
5	B	703	NAP	O3X-P2B-O2X	2.23	116.18	107.80
6	C	300	HEM	O2A-CGA-CBA	2.19	120.92	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	701	FAD	O2A-PA-O3P	2.19	113.18	107.27
4	B	702	FMN	C9A-N10-C10	-2.18	117.43	120.75
4	B	702	FMN	C1'-N10-C9A	2.13	124.78	120.63
3	A	701	FAD	C10-N1-C2	2.05	121.28	116.85
3	B	701	FAD	O2P-P-O1P	2.04	121.94	112.44
3	B	701	FAD	C1'-C2'-C3'	2.03	115.17	109.66
4	B	702	FMN	C10-N1-C2	2.03	121.24	116.85
3	B	701	FAD	C7M-C7-C6	2.03	123.15	119.57
5	A	703	NAP	C5A-C6A-N6A	2.03	123.40	120.31
3	B	701	FAD	C4'-C3'-C2'	2.02	116.93	113.57
3	A	701	FAD	C4'-C3'-C2'	-2.01	110.22	113.57
3	B	701	FAD	O5'-C5'-C4'	2.01	114.74	109.36
4	A	702	FMN	C4-N3-C2	-2.01	122.08	125.64
4	A	702	FMN	C4A-C4-N3	2.01	118.36	113.25

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	FAD	C1'-C2'-C3'-C4'
3	B	701	FAD	C5B-O5B-PA-O2A
3	B	701	FAD	C5B-O5B-PA-O3P
3	B	701	FAD	C3B-C4B-C5B-O5B
3	B	701	FAD	C3'-C4'-C5'-O5'
3	B	701	FAD	O4'-C4'-C5'-O5'
4	A	702	FMN	C2'-C1'-N10-C10
6	C	300	HEM	C2B-C3B-CAB-CBB
6	C	300	HEM	C4B-C3B-CAB-CBB
6	D	300	HEM	C2B-C3B-CAB-CBB
6	D	300	HEM	C4B-C3B-CAB-CBB
3	A	701	FAD	O2'-C2'-C3'-C4'
3	B	701	FAD	O4B-C4B-C5B-O5B
3	A	701	FAD	O2'-C2'-C3'-O3'
6	D	300	HEM	C2D-C3D-CAD-CBD
3	A	701	FAD	C2'-C3'-C4'-O4'
4	A	702	FMN	O2'-C2'-C3'-C4'
6	D	300	HEM	C4D-C3D-CAD-CBD
5	A	703	NAP	C2B-O2B-P2B-O1X
3	B	701	FAD	C5B-O5B-PA-O1A
6	D	300	HEM	CAD-CBD-CGD-O1D
6	D	300	HEM	CAA-CBA-CGA-O2A
6	D	300	HEM	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	702	FMN	C2'-C3'-C4'-C5'
6	C	300	HEM	CAD-CBD-CGD-O2D
6	D	300	HEM	CAA-CBA-CGA-O1A
3	A	701	FAD	C1'-C2'-C3'-O3'
6	C	300	HEM	CAA-CBA-CGA-O2A
6	C	300	HEM	CAD-CBD-CGD-O1D
6	C	300	HEM	CAA-CBA-CGA-O1A

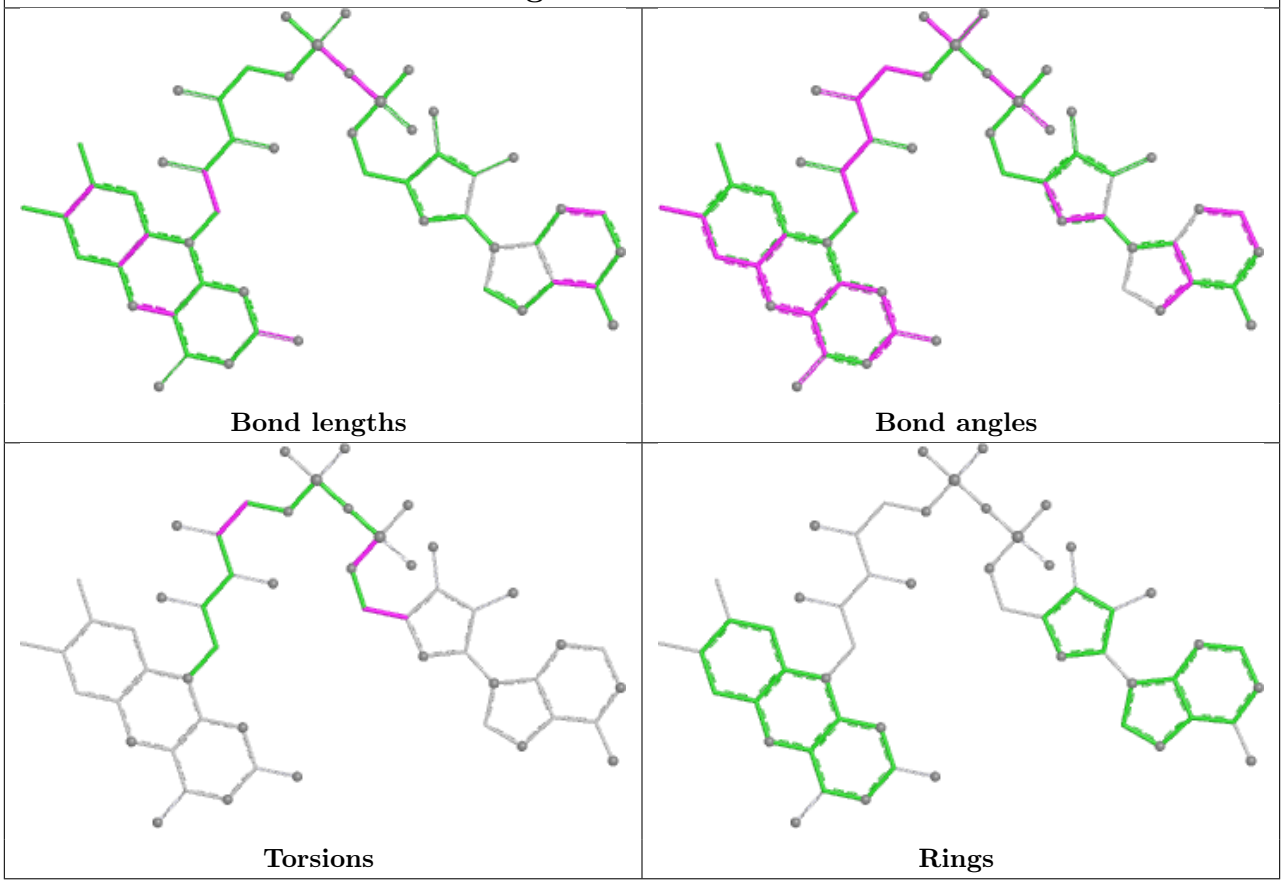
There are no ring outliers.

7 monomers are involved in 17 short contacts:

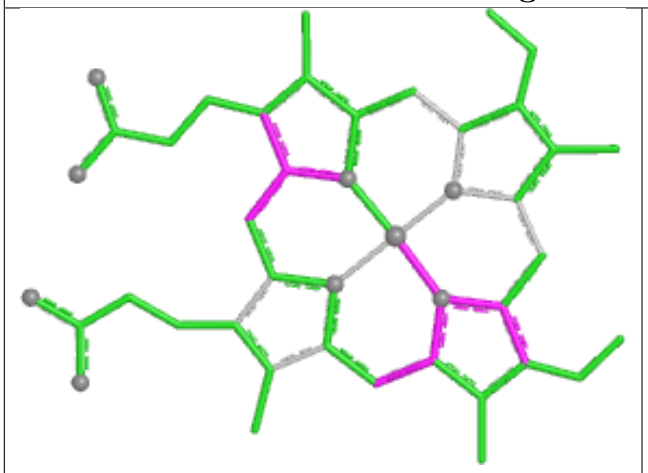
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	FAD	4	0
6	D	300	HEM	1	0
5	B	703	NAP	4	0
6	C	300	HEM	1	0
4	B	702	FMN	1	0
3	A	701	FAD	2	0
4	A	702	FMN	4	0

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.

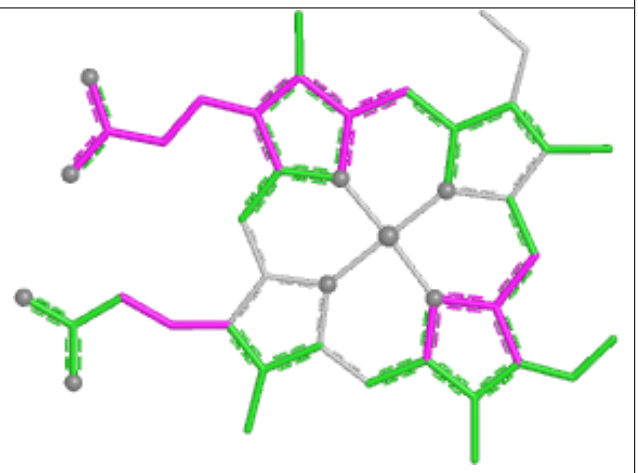
Ligand FAD B 701



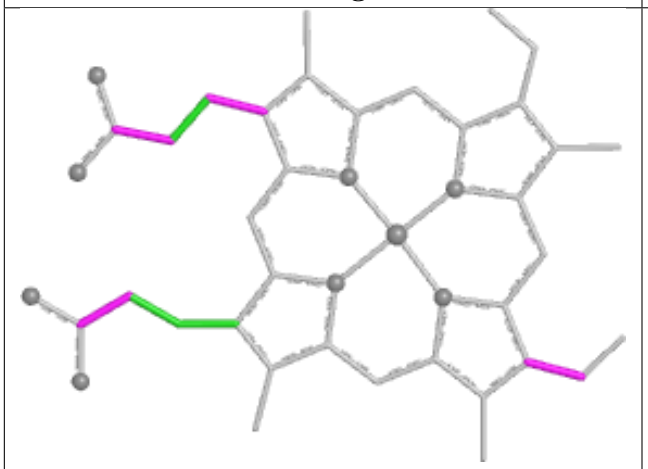
Ligand HEM D 300



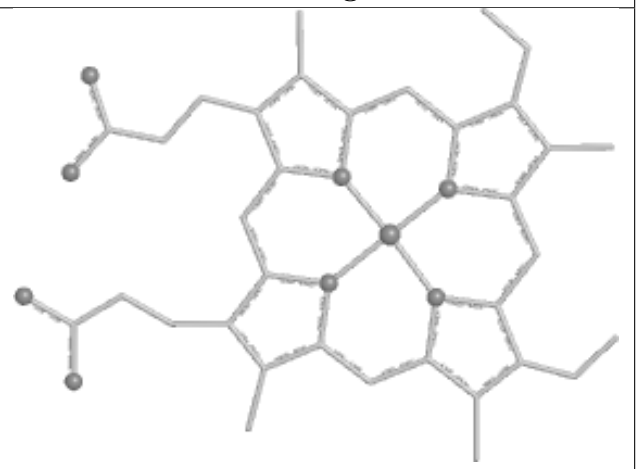
Bond lengths



Bond angles

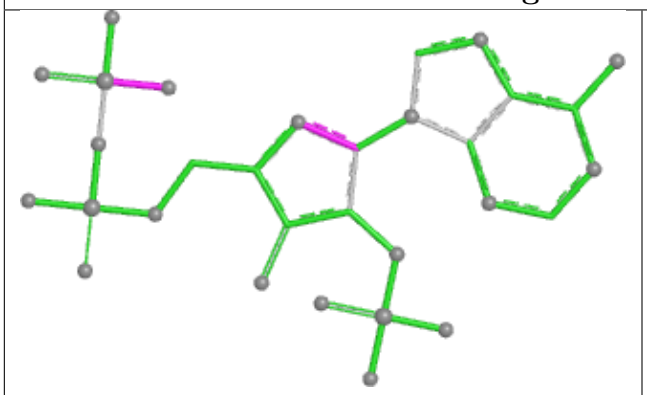


Torsions

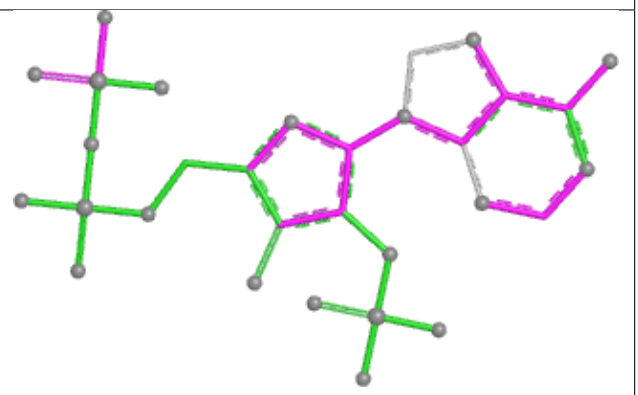


Rings

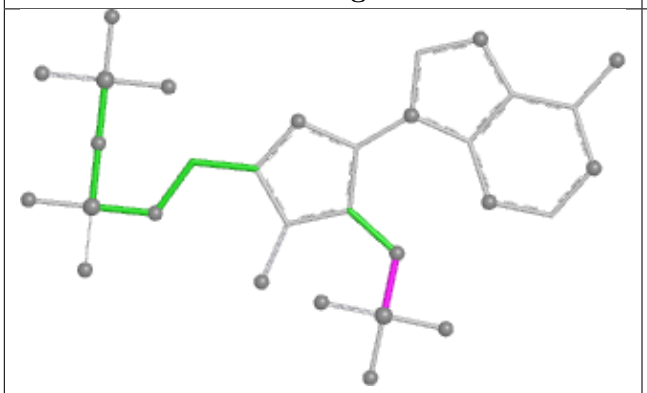
Ligand NAP A 703



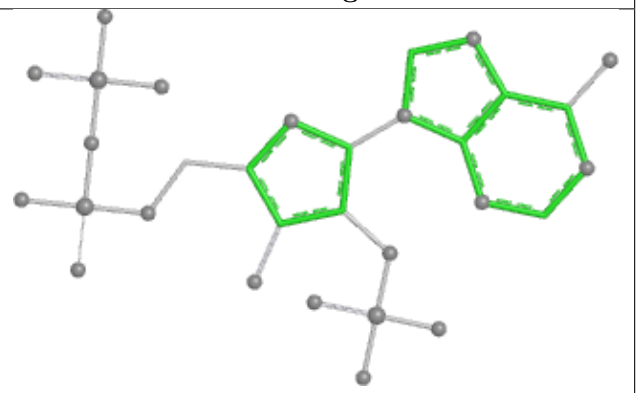
Bond lengths



Bond angles

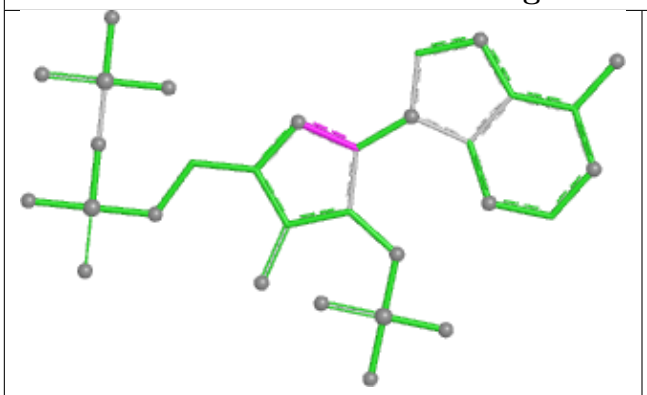


Torsions

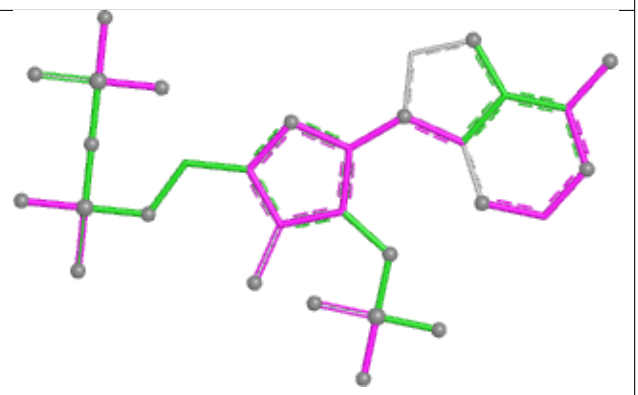


Rings

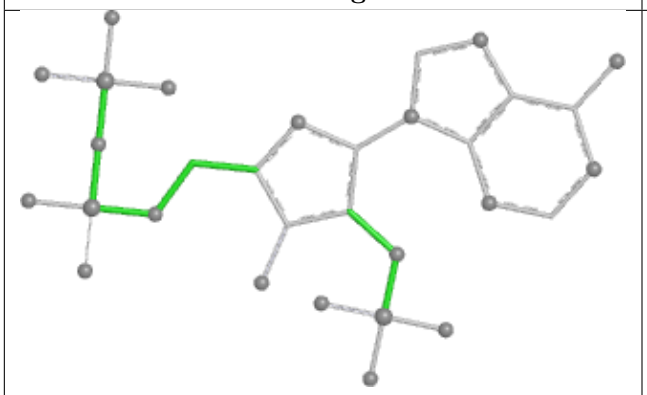
Ligand NAP B 703



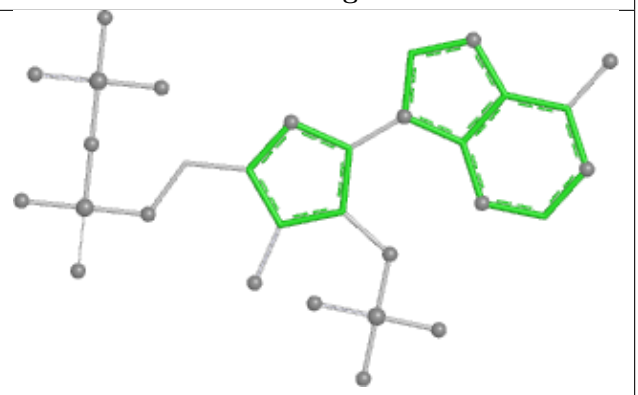
Bond lengths



Bond angles

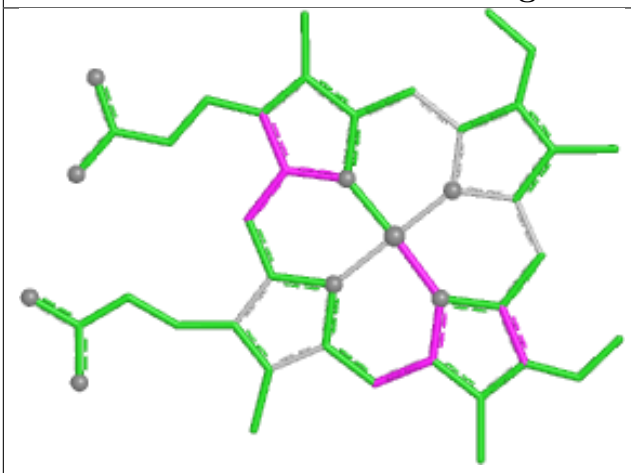


Torsions

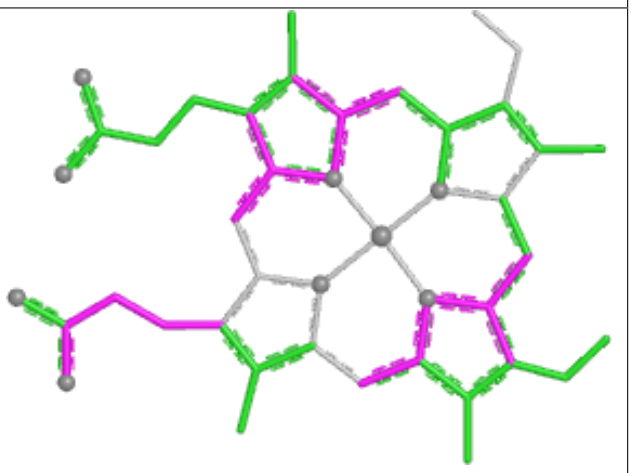


Rings

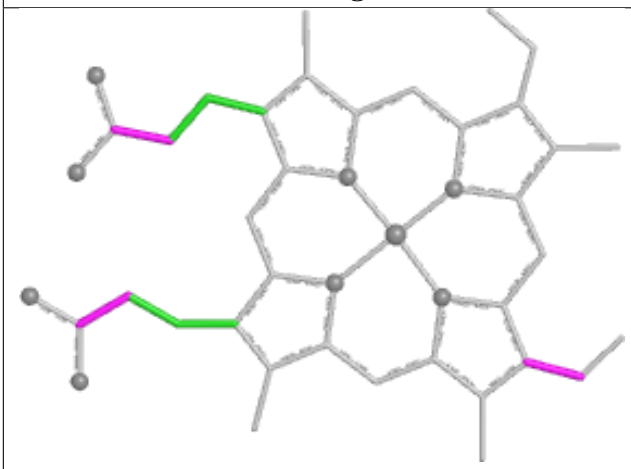
Ligand HEM C 300



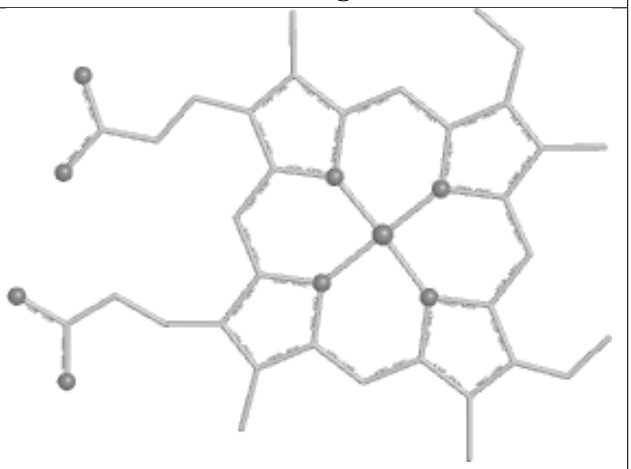
Bond lengths



Bond angles

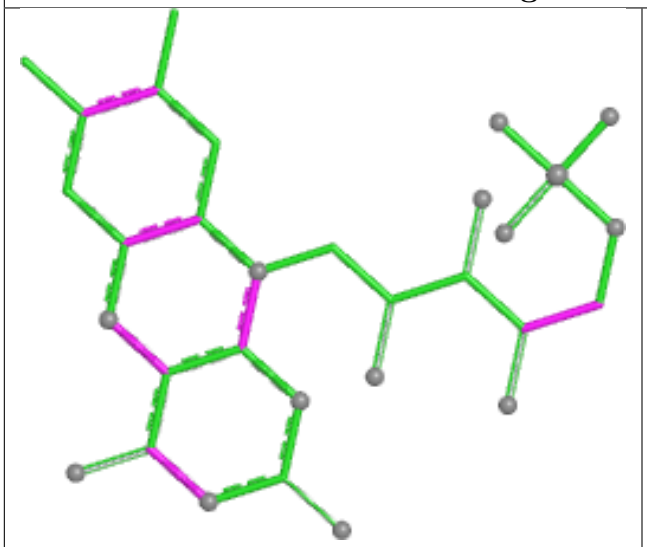


Torsions

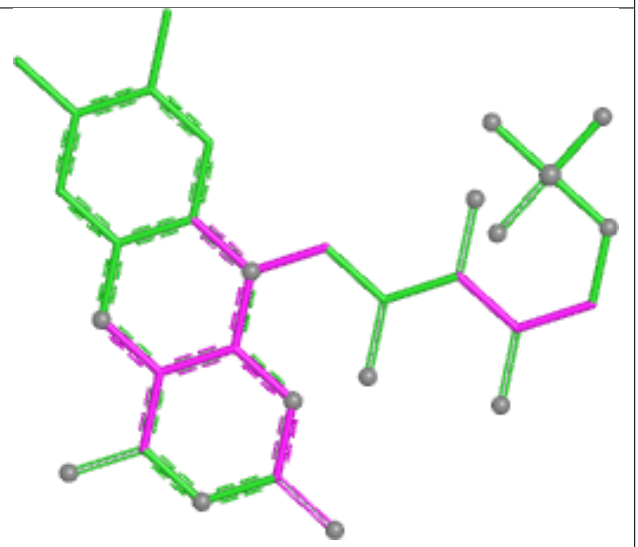


Rings

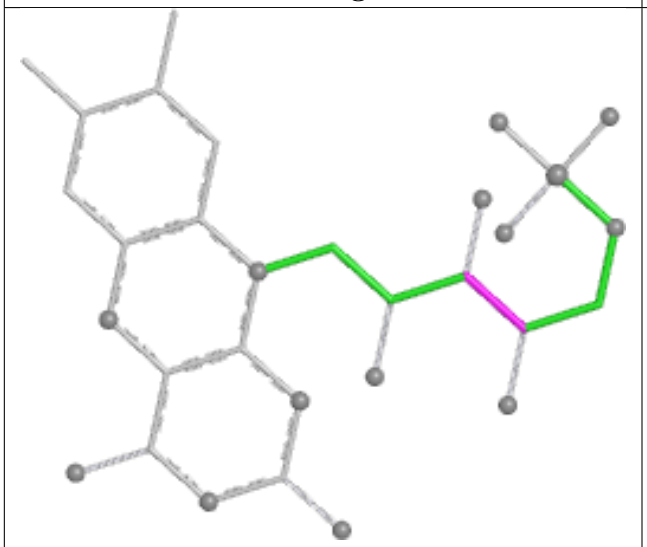
Ligand FMN B 702



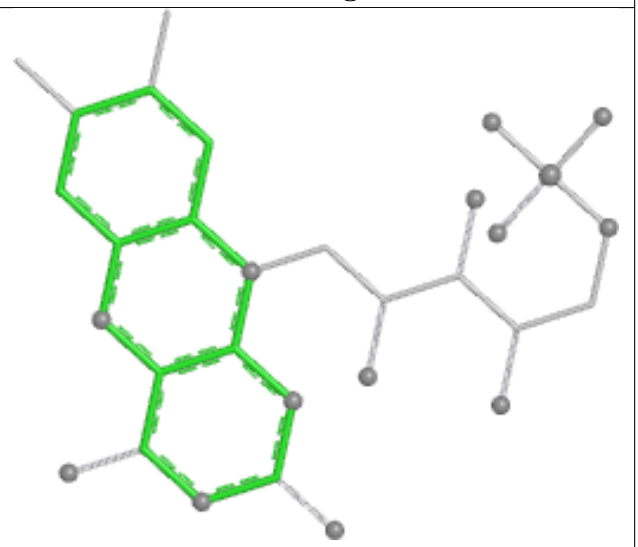
Bond lengths



Bond angles

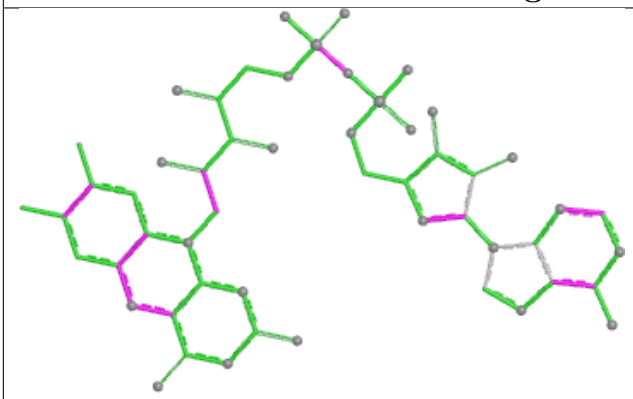


Torsions

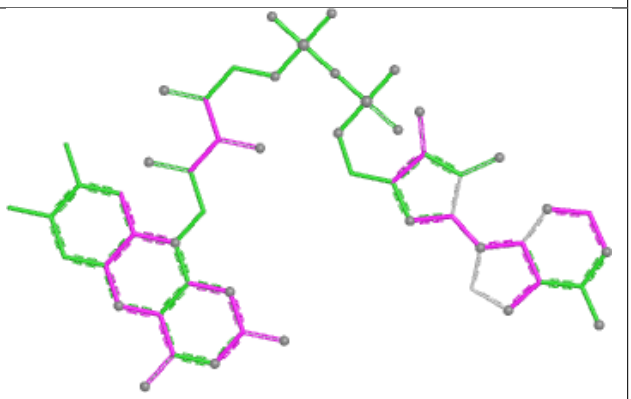


Rings

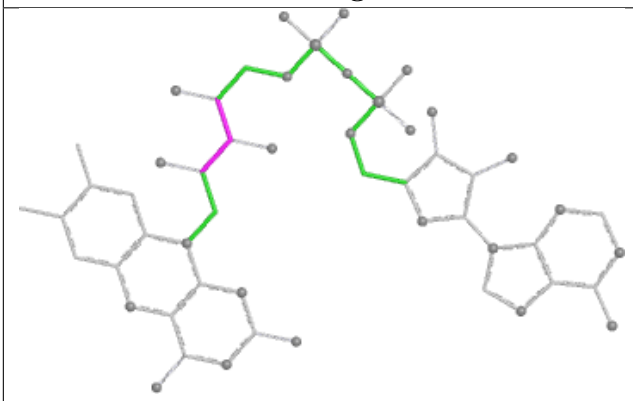
Ligand FAD A 701



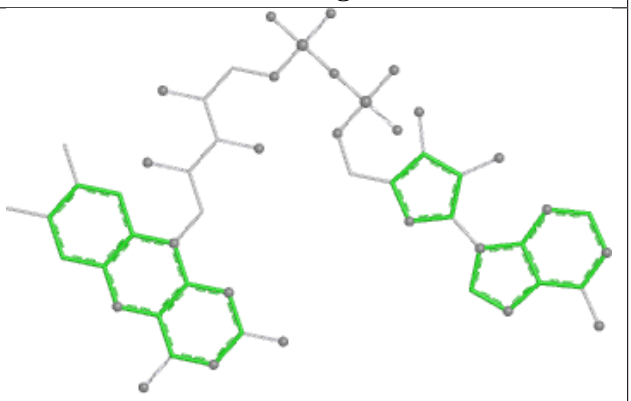
Bond lengths



Bond angles

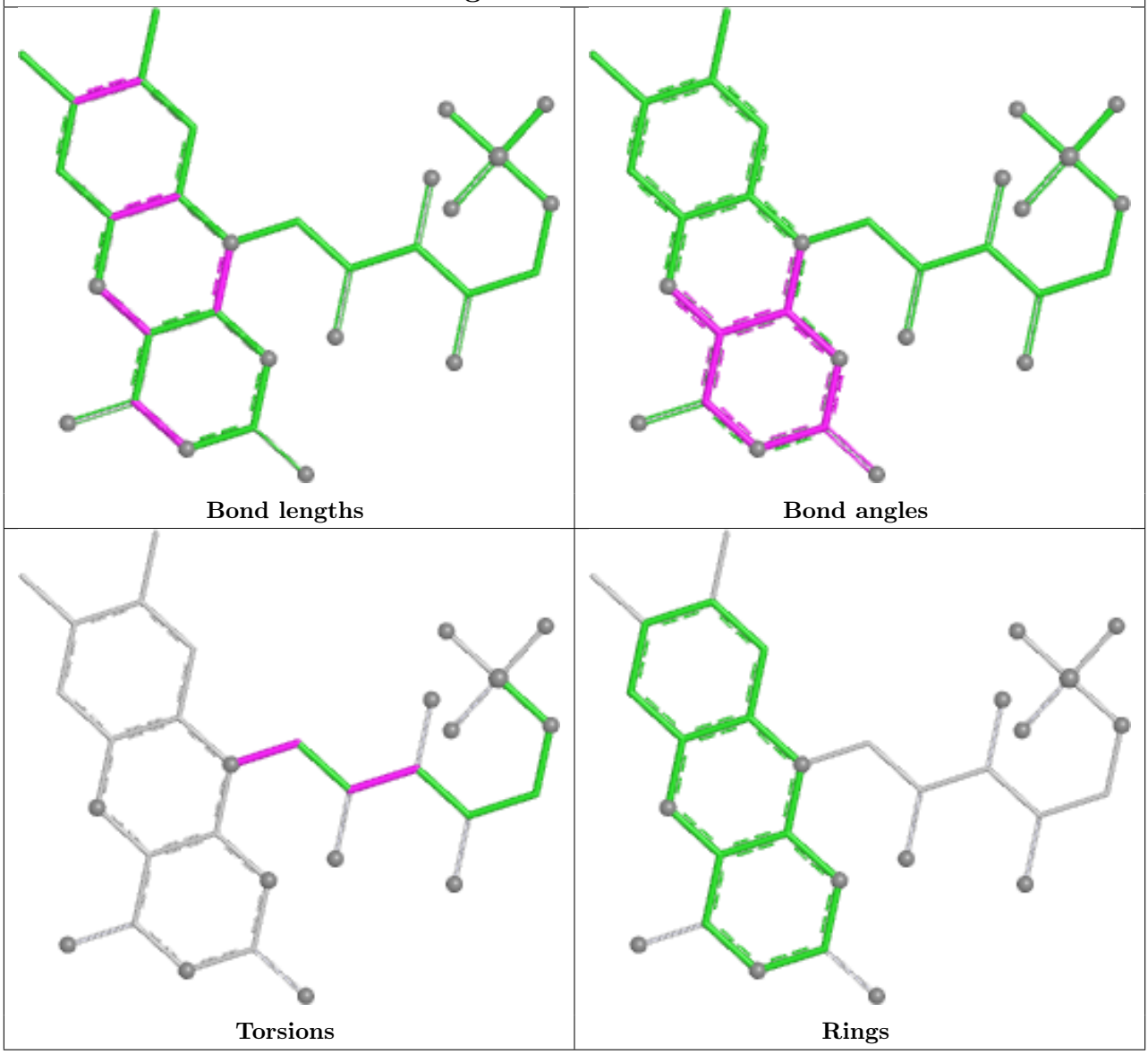


Torsions



Rings

Ligand FMN A 702



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	602/618 (97%)	-0.20	4 (0%) 87 82	145, 232, 340, 408	0
1	B	588/618 (95%)	-0.16	14 (2%) 59 49	96, 213, 423, 500	0
2	C	214/267 (80%)	-0.26	1 (0%) 91 86	142, 241, 303, 345	0
2	D	214/267 (80%)	-0.43	0 100 100	114, 180, 251, 294	0
All	All	1618/1770 (91%)	-0.23	19 (1%) 79 70	96, 221, 375, 500	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	PHE	5.3
1	B	198	GLN	3.4
1	B	502	ARG	3.2
1	B	206	GLY	3.0
1	A	512	SER	2.9
1	B	80	ILE	2.9
1	B	212	LEU	2.9
1	B	191	ARG	2.7
1	B	199	ARG	2.6
1	B	156	LEU	2.5
2	C	173	ASP	2.5
1	A	83	PHE	2.3
1	A	112	ALA	2.3
1	A	510	ARG	2.2
1	B	200	ILE	2.2
1	B	132	LEU	2.2
1	B	229	GLU	2.1
1	B	158	GLU	2.1
1	B	172	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

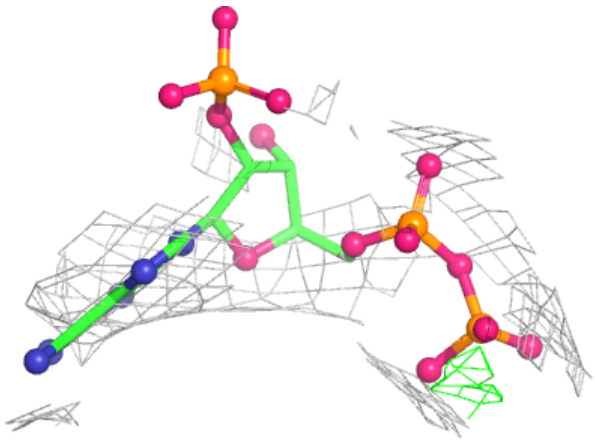
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

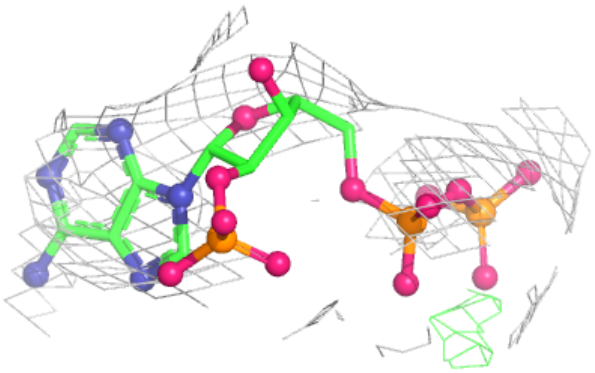
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAP	A	703	31/48	0.68	0.30	154,224,280,288	0
5	NAP	B	703	31/48	0.83	0.24	135,176,209,242	0
6	HEM	C	300	43/43	0.87	0.35	179,251,316,347	0
6	HEM	D	300	43/43	0.88	0.38	165,241,289,365	0
3	FAD	A	701	53/53	0.92	0.24	133,190,255,302	0
3	FAD	B	701	53/53	0.92	0.26	117,159,213,241	0
4	FMN	A	702	31/31	0.93	0.15	245,333,377,395	0
4	FMN	B	702	31/31	0.94	0.17	269,335,425,433	0

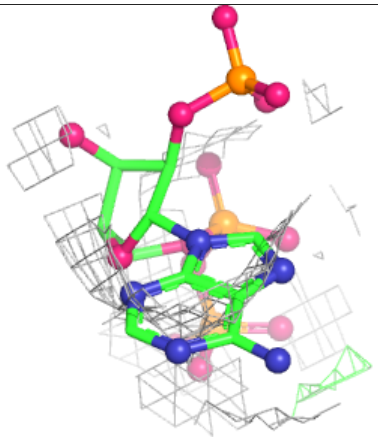
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 703:

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

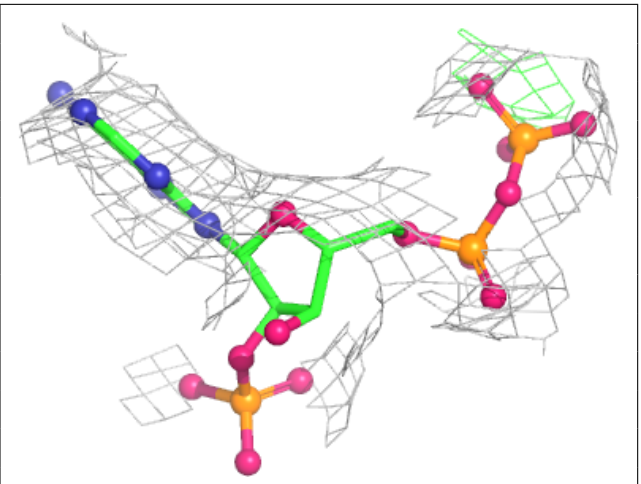


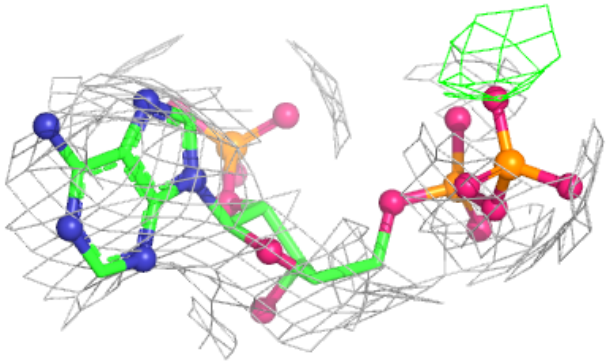


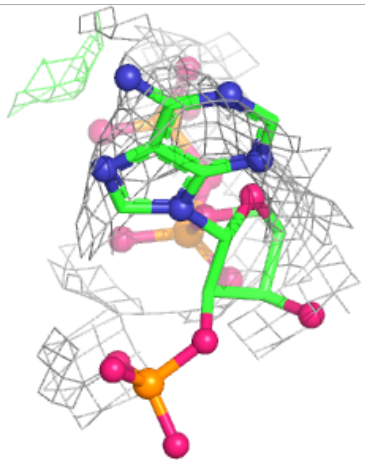


Electron density around NAP B 703:

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

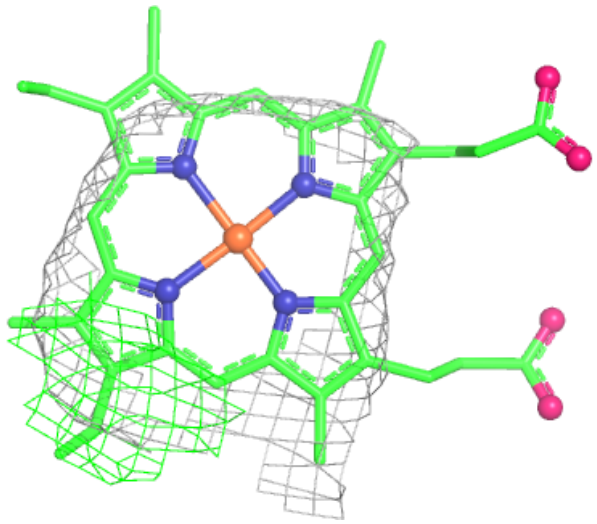


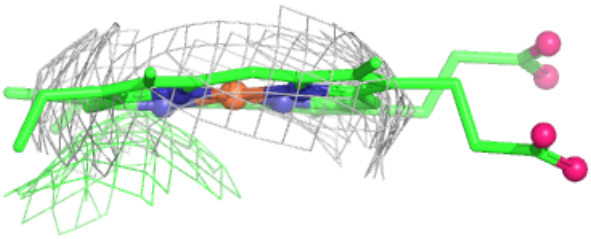


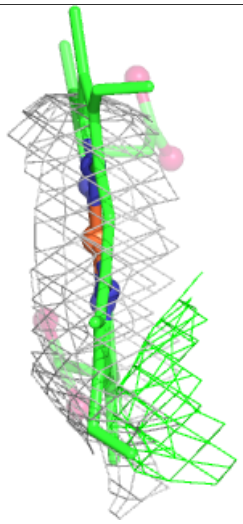


Electron density around HEM C 300:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

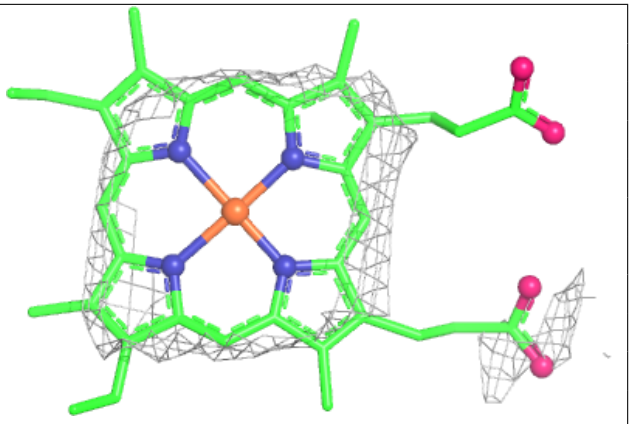


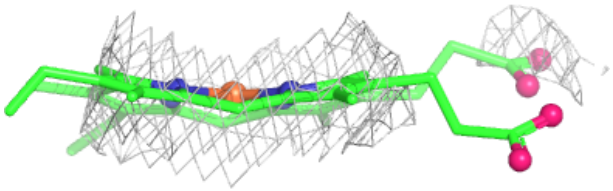


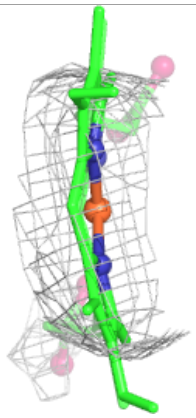


Electron density around HEM D 300:

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

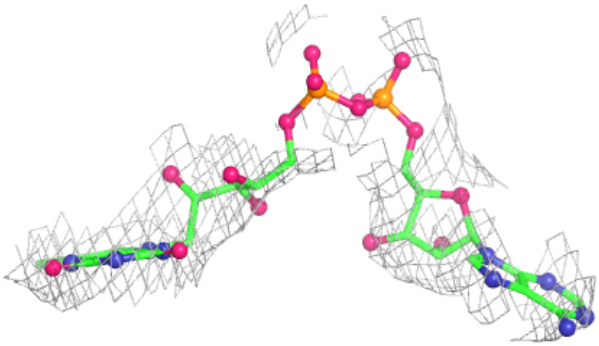


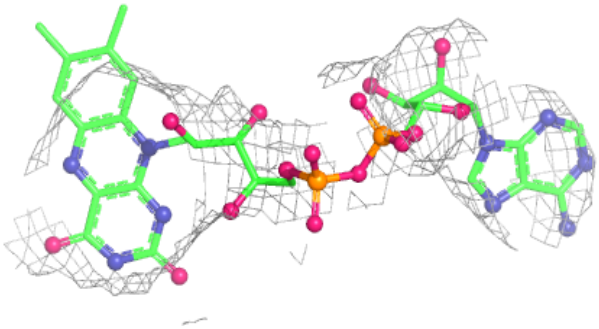


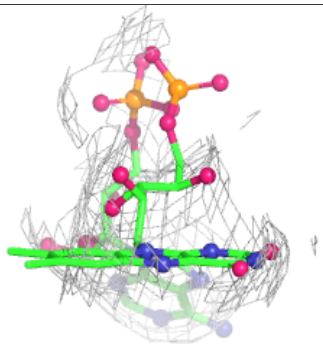


Electron density around FAD A 701:

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

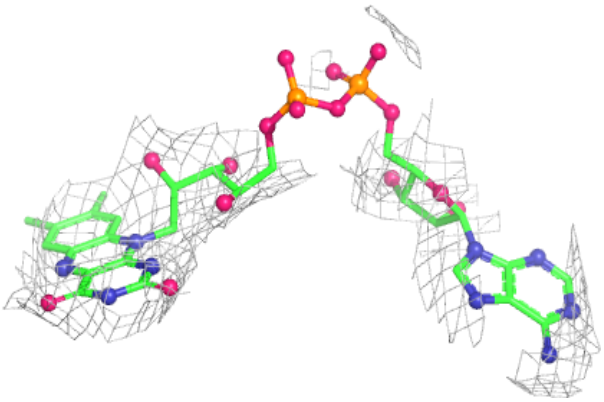


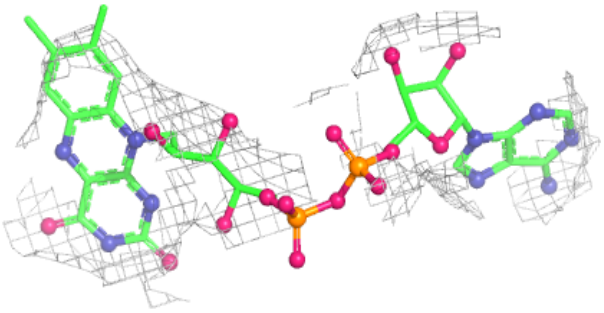


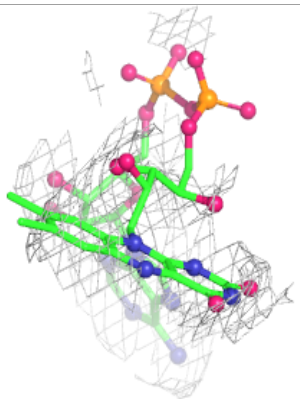


Electron density around FAD B 701:

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

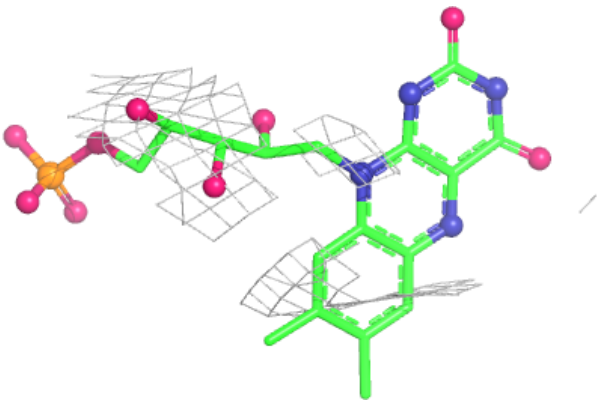


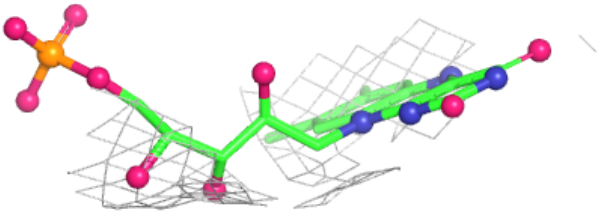


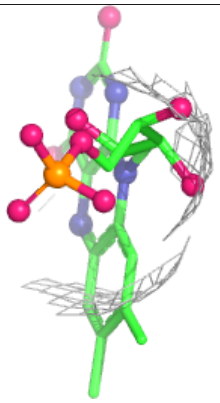


Electron density around FMN A 702:

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

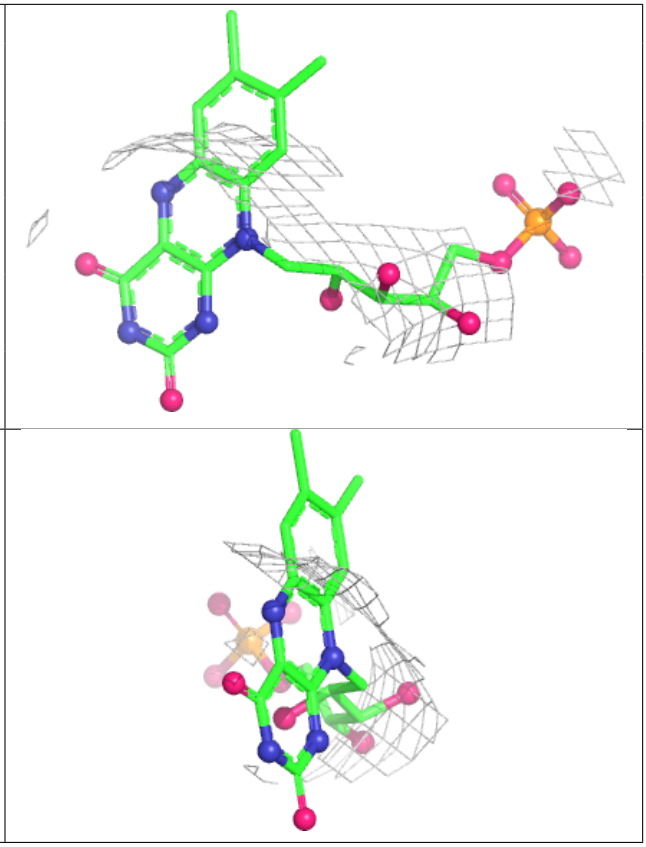






Electron density around FMN B 702:

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



6.5 Other polymers (i)

There are no such residues in this entry.