Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 12:55 am GMT

PDB ID	:	4BMM
Title	:	Crystal structure of Trypanosoma cruzi CYP51 bound to the inhibitor (R)-N-(3-(1H-indol-3-yl)-1-oxo-1-(pyridin-4-ylamino)propan-2-yl)-2',3, 5'-trifluoro-(1,1'-biphenyl)-4-carboxamide
Authors	:	Choi, J.Y.; Calvet, C.M.; Gunatilleke, S.S.; Roush, W.R.; McKerrow, J.H.; Podust, L.M.
Deposited on	:	2013-05-09
Resolution	:	2.84 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 (1)) were used in the production of this report:

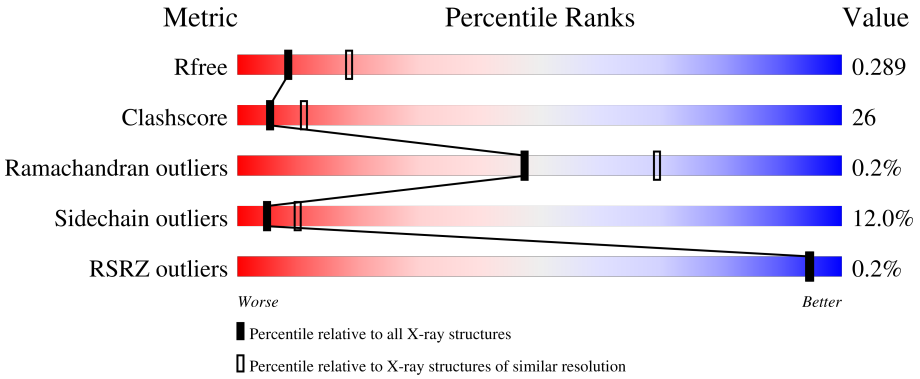
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	467	53% 35% 6% 6%
1	B	467	52% 37% 6% 5%
1	C	467	57% 32% 6% 6%
1	D	467	53% 36% 5% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14088 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 STEROL 14-ALPHA DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3431	2203	590	610	28			
1	B	442	Total	C	N	O	S	0	0	0
			3432	2205	596	603	28			
1	C	440	Total	C	N	O	S	0	0	0
			3415	2193	595	599	28			
1	D	442	Total	C	N	O	S	0	0	0
			3448	2219	591	610	28			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	expression tag	UNP Q7Z1V1
A	22	ALA	-	expression tag	UNP Q7Z1V1
A	23	LYS	-	expression tag	UNP Q7Z1V1
A	24	LYS	-	expression tag	UNP Q7Z1V1
A	25	THR	-	expression tag	UNP Q7Z1V1
A	26	SER	-	expression tag	UNP Q7Z1V1
A	27	SER	-	expression tag	UNP Q7Z1V1
A	28	LYS	-	expression tag	UNP Q7Z1V1
A	29	GLY	-	expression tag	UNP Q7Z1V1
A	30	LYS	-	expression tag	UNP Q7Z1V1
A	31	LEU	-	expression tag	UNP Q7Z1V1
A	482	HIS	-	expression tag	UNP Q7Z1V1
A	483	HIS	-	expression tag	UNP Q7Z1V1
A	484	HIS	-	expression tag	UNP Q7Z1V1
A	485	HIS	-	expression tag	UNP Q7Z1V1
A	486	HIS	-	expression tag	UNP Q7Z1V1
A	487	HIS	-	expression tag	UNP Q7Z1V1
B	21	MET	-	expression tag	UNP Q7Z1V1
B	22	ALA	-	expression tag	UNP Q7Z1V1
B	23	LYS	-	expression tag	UNP Q7Z1V1
B	24	LYS	-	expression tag	UNP Q7Z1V1

Continued on next page...

Continued from previous page...

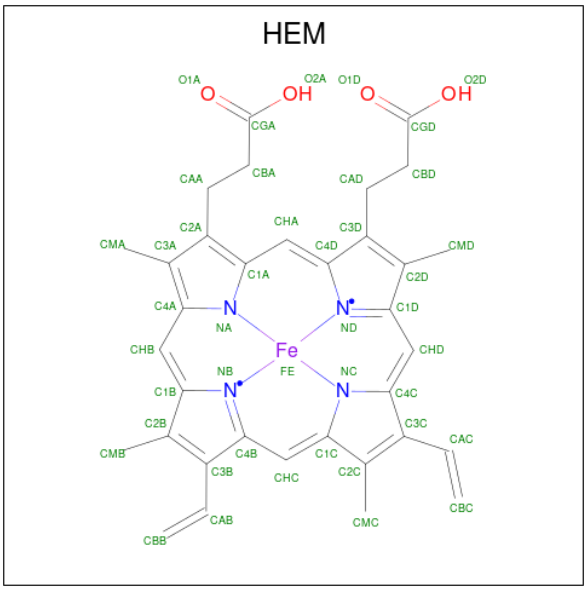
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	THR	-	expression tag	UNP Q7Z1V1
B	26	SER	-	expression tag	UNP Q7Z1V1
B	27	SER	-	expression tag	UNP Q7Z1V1
B	28	LYS	-	expression tag	UNP Q7Z1V1
B	29	GLY	-	expression tag	UNP Q7Z1V1
B	30	LYS	-	expression tag	UNP Q7Z1V1
B	31	LEU	-	expression tag	UNP Q7Z1V1
B	482	HIS	-	expression tag	UNP Q7Z1V1
B	483	HIS	-	expression tag	UNP Q7Z1V1
B	484	HIS	-	expression tag	UNP Q7Z1V1
B	485	HIS	-	expression tag	UNP Q7Z1V1
B	486	HIS	-	expression tag	UNP Q7Z1V1
B	487	HIS	-	expression tag	UNP Q7Z1V1
C	21	MET	-	expression tag	UNP Q7Z1V1
C	22	ALA	-	expression tag	UNP Q7Z1V1
C	23	LYS	-	expression tag	UNP Q7Z1V1
C	24	LYS	-	expression tag	UNP Q7Z1V1
C	25	THR	-	expression tag	UNP Q7Z1V1
C	26	SER	-	expression tag	UNP Q7Z1V1
C	27	SER	-	expression tag	UNP Q7Z1V1
C	28	LYS	-	expression tag	UNP Q7Z1V1
C	29	GLY	-	expression tag	UNP Q7Z1V1
C	30	LYS	-	expression tag	UNP Q7Z1V1
C	31	LEU	-	expression tag	UNP Q7Z1V1
C	482	HIS	-	expression tag	UNP Q7Z1V1
C	483	HIS	-	expression tag	UNP Q7Z1V1
C	484	HIS	-	expression tag	UNP Q7Z1V1
C	485	HIS	-	expression tag	UNP Q7Z1V1
C	486	HIS	-	expression tag	UNP Q7Z1V1
C	487	HIS	-	expression tag	UNP Q7Z1V1
D	21	MET	-	expression tag	UNP Q7Z1V1
D	22	ALA	-	expression tag	UNP Q7Z1V1
D	23	LYS	-	expression tag	UNP Q7Z1V1
D	24	LYS	-	expression tag	UNP Q7Z1V1
D	25	THR	-	expression tag	UNP Q7Z1V1
D	26	SER	-	expression tag	UNP Q7Z1V1
D	27	SER	-	expression tag	UNP Q7Z1V1
D	28	LYS	-	expression tag	UNP Q7Z1V1
D	29	GLY	-	expression tag	UNP Q7Z1V1
D	30	LYS	-	expression tag	UNP Q7Z1V1
D	31	LEU	-	expression tag	UNP Q7Z1V1
D	482	HIS	-	expression tag	UNP Q7Z1V1

Continued on next page...

Continued from previous page...

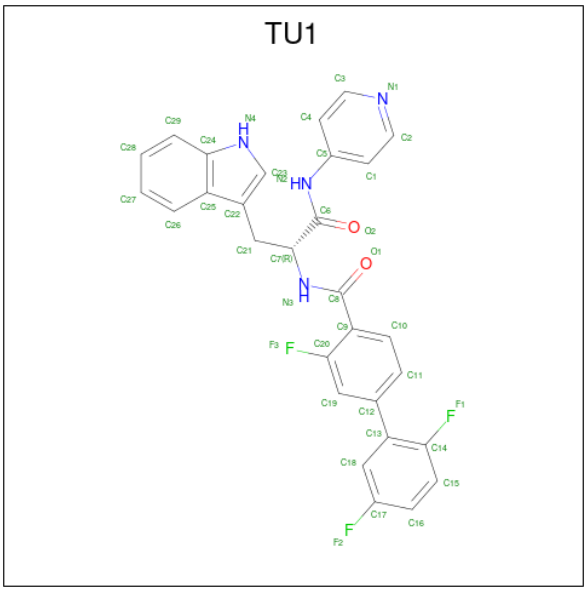
Chain	Residue	Modelled	Actual	Comment	Reference
D	483	HIS	-	expression tag	UNP Q7Z1V1
D	484	HIS	-	expression tag	UNP Q7Z1V1
D	485	HIS	-	expression tag	UNP Q7Z1V1
D	486	HIS	-	expression tag	UNP Q7Z1V1
D	487	HIS	-	expression tag	UNP Q7Z1V1

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is 4-[2,5-bis(fluoranyl)phenyl]-2-fluoranyl-N-[(2R)-3-(1H-indol-3-yl)-1-oxidanylidene-1-(pyridin-4-ylamino)propan-2-yl]benzamide (three-letter code: TU1) (formula: $C_{29}H_{21}F_3N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O 38 29 3 4 2	0	0
3	B	1	Total C F N O 38 29 3 4 2	0	0
3	C	1	Total C F N O 38 29 3 4 2	0	0
3	D	1	Total C F N O 38 29 3 4 2	0	0

- Molecule 4 is water.

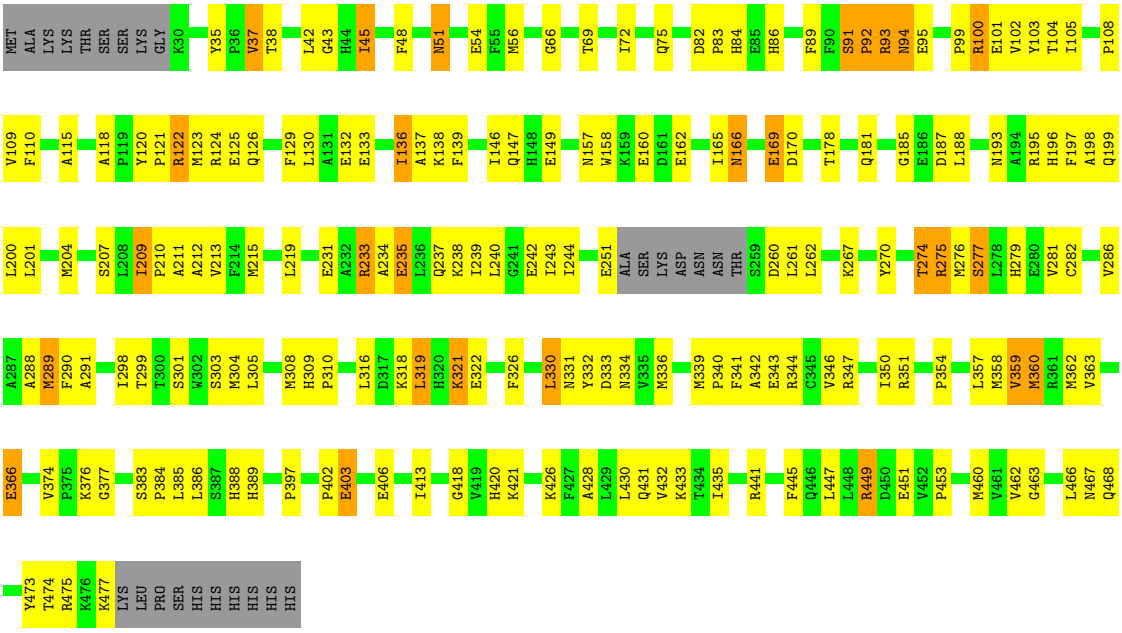
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	6	Total O 6 6	0	0
4	B	1	Total O 1 1	0	0
4	C	9	Total O 9 9	0	0
4	C	2	Total O 2 2	0	0
4	D	7	Total O 7 7	0	0

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.

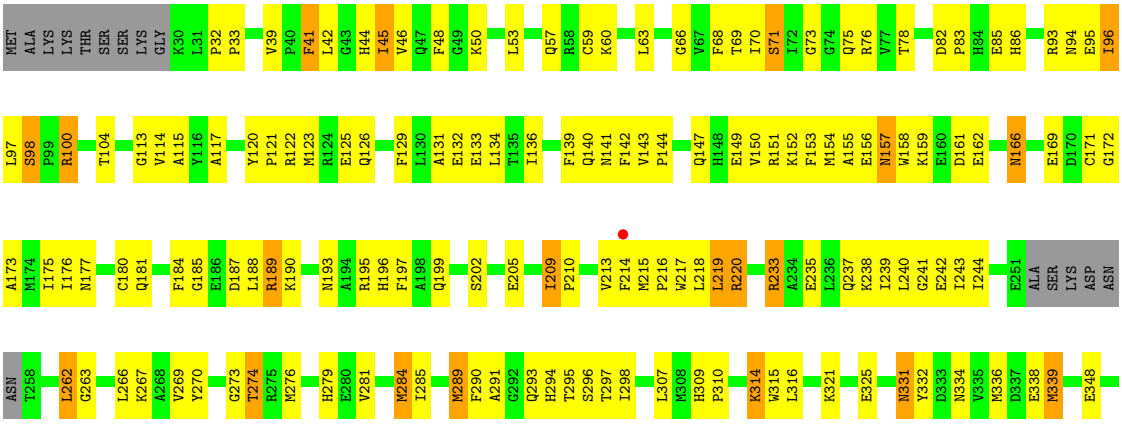
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

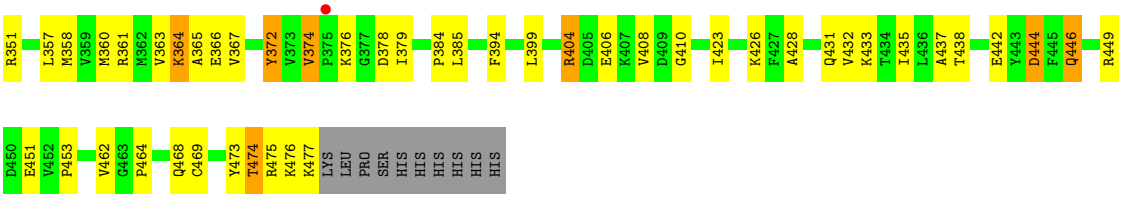
Chain A:



• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

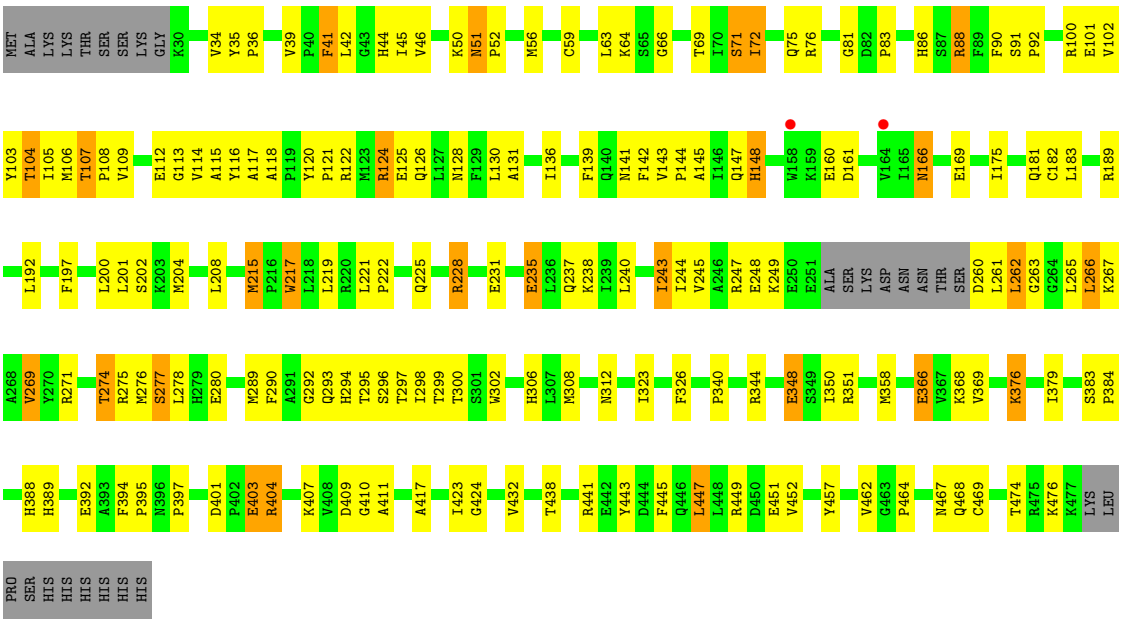
Chain B:





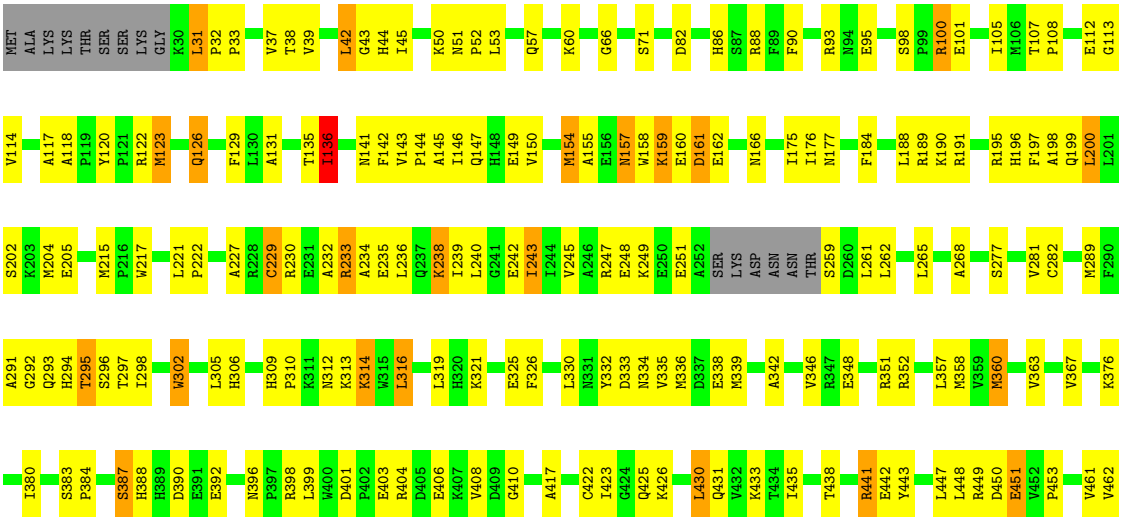
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

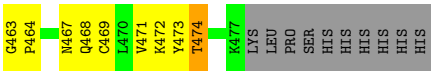
Chain C:



• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain D:




G463
P464
N467
Q468
C469
L470
V471
K472
Y473
T474
K477
LYS
LEU
PRO
SER
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	272.47Å 66.45Å 122.22Å 90.00° 110.65° 90.00°	Depositor
Resolution (Å)	114.63 – 2.84 114.37 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.7 (114.63-2.84) 99.7 (114.37-2.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.189 , 0.290 0.189 , 0.289	Depositor DCC
R_{free} test set	2469 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14088	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TU1, HEM

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	0.54	0/3515	0.73	0/4770
1	B	0.53	0/3516	0.71	0/4770
1	C	0.49	0/3497	0.70	1/4739 (0.0%)
1	D	0.59	1/3531 (0.0%)	0.77	2/4785 (0.0%)
All	All	0.54	1/14059 (0.0%)	0.73	3/19064 (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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	33	PRO	N-CD	5.11	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	107	THR	C-N-CD	6.41	141.86	128.40
1	D	32	PRO	C-N-CD	5.87	140.72	128.40
1	D	31	LEU	C-N-CD	5.40	139.75	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	39	VAL	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	3431	0	3347	167	0
1	B	3432	0	3356	166	0
1	C	3415	0	3348	194	0
1	D	3448	0	3402	177	0
2	A	43	0	30	11	0
2	B	43	0	30	6	0
2	C	43	0	30	8	0
2	D	43	0	30	13	0
3	A	38	0	21	7	0
3	B	38	0	21	2	0
3	C	38	0	21	2	0
3	D	38	0	21	5	0
4	A	13	0	0	1	0
4	B	7	0	0	0	0
4	C	11	0	0	0	0
4	D	7	0	0	0	0
All	All	14088	0	13657	726	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 26.

All (726) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:GLU:O	1:D:239:ILE:HG13	1.40	1.17
1:A:109:VAL:HG13	1:A:204:MET:CE	1.79	1.11
1:B:215:MET:HB2	1:B:218:LEU:HD12	1.24	1.10
1:A:109:VAL:HG13	1:A:204:MET:HE2	1.08	1.08
1:D:162:GLU:HB3	1:D:474:THR:HG23	1.38	1.04
1:A:475:ARG:CD	1:A:477:LYS:CB	2.36	1.03
1:C:269:VAL:CG1	1:C:275:ARG:HA	1.87	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:PRO:O	1:B:219:LEU:N	1.90	1.03
1:C:237:GLN:CG	1:C:278:LEU:HD21	1.91	1.00
1:C:237:GLN:HG3	1:C:278:LEU:HD21	1.46	0.98
1:A:109:VAL:CG1	1:A:204:MET:HE2	1.93	0.98
1:C:269:VAL:HG13	1:C:275:ARG:HG2	1.45	0.97
1:C:269:VAL:HG12	1:C:275:ARG:HA	1.48	0.96
1:D:227:ALA:HB1	1:D:230:ARG:HB2	1.44	0.95
1:B:44:HIS:HD2	1:B:71:SER:H	1.05	0.94
1:B:215:MET:HB2	1:B:218:LEU:CD1	1.96	0.94
1:D:233:ARG:HG2	1:D:233:ARG:HH11	1.30	0.94
1:C:366:GLU:HB3	1:C:376:LYS:HE2	1.50	0.93
1:B:442:GLU:O	1:B:476:LYS:HB2	1.69	0.91
1:A:102:VAL:HG23	1:A:103:TYR:CD1	2.07	0.90
1:A:122:ARG:O	1:A:126:GLN:HG3	1.71	0.90
1:C:244:ILE:HG22	1:C:248:GLU:CG	2.03	0.88
1:C:104:THR:O	1:C:107:THR:N	2.07	0.87
1:C:244:ILE:O	1:C:248:GLU:HG2	1.74	0.87
1:C:269:VAL:CG1	1:C:275:ARG:CA	2.53	0.86
1:A:363:VAL:HG12	1:A:376:LYS:HA	1.56	0.86
1:C:113:GLY:O	1:C:118:ALA:HB2	1.75	0.86
1:D:44:HIS:CD2	1:D:71:SER:H	1.93	0.86
1:B:73:GLY:HA3	1:B:215:MET:CE	2.05	0.85
1:C:109:VAL:HG21	1:C:208:LEU:HD21	1.58	0.85
1:B:220:ARG:HG2	1:B:220:ARG:HH11	1.42	0.85
1:D:161:ASP:O	1:D:474:THR:HG22	1.77	0.84
1:B:281:VAL:O	1:B:285:ILE:HG13	1.77	0.84
1:C:260:ASP:OD1	1:C:261:LEU:N	2.10	0.84
1:C:269:VAL:HG12	1:C:275:ARG:CA	2.09	0.83
1:A:467:ASN:OD1	1:A:468:GLN:HG3	1.79	0.83
1:B:357:LEU:HD21	1:B:462:VAL:HG21	1.59	0.82
1:C:269:VAL:HG13	1:C:275:ARG:HA	1.61	0.82
1:A:42:LEU:O	1:A:45:ILE:CG2	2.28	0.82
1:A:270:TYR:CZ	1:A:276:MET:HG2	2.15	0.82
1:B:98:SER:HB2	1:B:120:TYR:OH	1.80	0.82
1:A:237:GLN:HE21	1:A:279:HIS:HA	1.44	0.81
1:B:209:ILE:HD12	1:B:209:ILE:H	1.43	0.81
1:B:263:GLY:HA2	1:B:266:LEU:HD12	1.61	0.81
1:D:200:LEU:HD23	1:D:232:ALA:HB1	1.61	0.81
1:D:443:TYR:HE2	1:D:473:TYR:CD2	2.00	0.80
1:C:69:THR:HG21	1:C:76:ARG:HH11	1.47	0.80
1:A:139:PHE:CD2	1:A:430:LEU:HD22	2.17	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:HIS:O	1:D:199:GLN:HB2	1.81	0.79
1:A:282:CYS:O	1:A:286:VAL:HG23	1.83	0.79
1:D:342:ALA:O	1:D:346:VAL:HG23	1.82	0.79
1:B:240:LEU:O	1:B:244:ILE:HG13	1.83	0.79
1:C:269:VAL:HG13	1:C:275:ARG:CG	2.11	0.79
1:C:262:LEU:HD12	1:C:262:LEU:O	1.82	0.79
1:D:298:ILE:HD13	1:D:463:GLY:CA	2.13	0.79
2:A:1450:HEM:HBC2	2:A:1450:HEM:HHD	1.66	0.78
1:B:262:LEU:HD23	1:B:263:GLY:N	1.99	0.78
1:C:136:ILE:O	1:C:139:PHE:HB2	1.84	0.78
1:B:100:ARG:O	1:B:104:THR:HG23	1.84	0.78
1:B:44:HIS:CD2	1:B:71:SER:H	1.98	0.78
1:A:270:TYR:OH	1:A:276:MET:HG2	1.83	0.78
1:B:270:TYR:OH	1:B:276:MET:HG2	1.84	0.77
1:C:260:ASP:OD2	1:C:262:LEU:HB3	1.83	0.77
1:A:42:LEU:O	1:A:45:ILE:HG23	1.83	0.77
1:D:188:LEU:HD13	1:D:243:ILE:HD12	1.67	0.77
1:C:269:VAL:CG1	1:C:275:ARG:CG	2.63	0.77
1:C:244:ILE:HG22	1:C:248:GLU:HG2	1.67	0.76
1:B:307:LEU:O	1:B:316:LEU:HD22	1.86	0.76
1:B:363:VAL:HG12	1:B:376:LYS:HA	1.68	0.76
1:B:129:PHE:O	1:B:133:GLU:HG2	1.87	0.75
1:A:211:ALA:HB2	1:C:221:LEU:HD11	1.67	0.75
1:D:44:HIS:HD2	1:D:71:SER:H	1.34	0.75
1:D:200:LEU:HD23	1:D:232:ALA:CB	2.15	0.75
2:D:1450:HEM:HBB2	2:D:1450:HEM:HMB2	1.67	0.75
1:A:94:ASN:H	1:A:94:ASN:HD22	1.35	0.75
2:C:1450:HEM:HBC2	2:C:1450:HEM:HHD	1.69	0.74
1:D:204:MET:HA	1:D:229:CYS:HB2	1.68	0.74
1:D:200:LEU:HD23	1:D:232:ALA:CA	2.17	0.74
1:A:270:TYR:HD2	1:A:274:THR:O	1.71	0.73
1:B:73:GLY:HA3	1:B:215:MET:HE1	1.70	0.73
1:C:113:GLY:H	1:C:117:ALA:HB1	1.53	0.73
1:B:98:SER:OG	1:B:100:ARG:CG	2.37	0.73
1:A:133:GLU:HB3	1:A:261:LEU:HD12	1.70	0.73
1:A:210:PRO:HG3	1:A:460:MET:CE	2.18	0.73
1:C:107:THR:HG22	1:C:108:PRO:CD	2.19	0.73
1:D:162:GLU:CB	1:D:474:THR:HG23	2.14	0.73
1:C:69:THR:HG21	1:C:76:ARG:NH1	2.04	0.73
1:D:93:ARG:NH1	1:D:95:GLU:HB2	2.04	0.72
1:D:197:PHE:CE2	1:D:289:MET:HG3	2.25	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:GLU:O	1:D:251:GLU:HG2	1.88	0.72
1:A:83:PRO:HA	1:A:86:HIS:CD2	2.25	0.72
1:D:316:LEU:HD12	1:D:316:LEU:O	1.89	0.72
1:B:172:GLY:HA2	1:B:297:THR:OG1	1.90	0.72
1:A:237:GLN:NE2	1:A:279:HIS:HA	2.04	0.71
1:C:90:PHE:CG	1:C:417:ALA:HB3	2.26	0.71
1:C:269:VAL:HG12	1:C:274:THR:C	2.11	0.71
1:D:293:GLN:HG3	1:D:294:HIS:N	2.05	0.71
1:B:115:ALA:O	1:B:123:MET:HG3	1.91	0.71
1:C:269:VAL:CG1	1:C:275:ARG:HG2	2.19	0.71
1:D:357:LEU:O	1:D:384:PRO:HD2	1.90	0.71
1:C:237:GLN:NE2	1:C:278:LEU:CD2	2.54	0.71
1:B:73:GLY:HA3	1:B:215:MET:HE3	1.72	0.70
1:B:294:HIS:O	1:B:297:THR:HG22	1.91	0.70
1:A:210:PRO:HG3	1:A:460:MET:HE3	1.74	0.70
1:D:162:GLU:HB3	1:D:474:THR:CG2	2.21	0.70
1:C:90:PHE:HD2	1:C:417:ALA:O	1.74	0.70
1:C:277:SER:OG	1:C:280:GLU:HG3	1.90	0.70
1:D:86:HIS:NE2	1:D:387:SER:OG	2.25	0.70
1:B:166:ASN:HD22	1:B:169:GLU:H	1.38	0.69
1:B:210:PRO:O	1:B:213:VAL:HG23	1.92	0.69
1:C:107:THR:HG22	1:C:108:PRO:HD3	1.72	0.69
1:C:237:GLN:NE2	1:C:278:LEU:HD23	2.08	0.69
1:A:109:VAL:HG22	1:A:204:MET:HB3	1.74	0.69
1:B:291:ALA:HB1	3:B:1460:TU1:HA	1.74	0.69
1:A:270:TYR:CE2	1:A:276:MET:HG2	2.27	0.69
1:C:90:PHE:CD2	1:C:417:ALA:O	2.46	0.69
1:D:233:ARG:HG2	1:D:233:ARG:NH1	2.02	0.69
1:B:187:ASP:OD1	1:B:188:LEU:N	2.27	0.68
1:C:104:THR:O	1:C:108:PRO:HD2	1.94	0.68
1:C:122:ARG:HA	1:C:125:GLU:HG3	1.76	0.68
1:C:201:LEU:HD22	1:C:290:PHE:HD1	1.57	0.68
1:C:269:VAL:HG12	1:C:275:ARG:N	2.09	0.68
1:B:348:GLU:OE1	1:B:348:GLU:HA	1.93	0.68
2:A:1450:HEM:HMB2	2:A:1450:HEM:HBB2	1.75	0.68
1:C:136:ILE:HG23	1:C:139:PHE:CD2	2.29	0.67
1:A:66:GLY:HA3	1:A:82:ASP:HB2	1.75	0.67
1:C:269:VAL:HG12	1:C:274:THR:O	1.95	0.67
1:B:98:SER:OG	1:B:100:ARG:HG3	1.94	0.67
1:C:244:ILE:O	1:C:248:GLU:CG	2.43	0.67
1:B:220:ARG:HG2	1:B:220:ARG:NH1	2.09	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:HB3	1:B:120:TYR:CE1	2.29	0.66
1:D:443:TYR:CE2	1:D:473:TYR:CD2	2.82	0.66
1:C:290:PHE:O	1:C:293:GLN:HG2	1.95	0.66
1:D:351:ARG:NH1	1:D:388:HIS:O	2.27	0.66
1:B:332:TYR:CZ	1:B:336:MET:HG3	2.30	0.66
1:B:366:GLU:HA	1:B:374:VAL:O	1.96	0.66
1:A:210:PRO:CG	1:A:460:MET:HE3	2.25	0.65
1:B:262:LEU:HD23	1:B:263:GLY:H	1.59	0.65
1:D:141:ASN:O	1:D:144:PRO:HD2	1.95	0.65
1:C:175:ILE:HD12	1:C:296:SER:HB3	1.78	0.65
1:B:449:ARG:NH1	1:B:451:GLU:O	2.29	0.65
1:A:240:LEU:O	1:A:244:ILE:HG13	1.95	0.65
1:B:69:THR:HG23	1:B:78:THR:OG1	1.97	0.65
1:B:291:ALA:HB1	3:B:1460:TU1:C2	2.25	0.65
2:C:1450:HEM:HBB2	2:C:1450:HEM:HMB2	1.79	0.65
1:D:467:ASN:OD1	1:D:468:GLN:N	2.30	0.65
1:B:166:ASN:ND2	1:B:169:GLU:H	1.95	0.65
1:C:105:ILE:HG22	1:C:219:LEU:HD11	1.79	0.65
1:B:98:SER:OG	1:B:100:ARG:HG2	1.97	0.64
1:D:195:ARG:HA	1:D:195:ARG:NE	2.12	0.64
1:B:365:ALA:O	1:B:367:VAL:HG13	1.97	0.64
1:B:215:MET:CB	1:B:218:LEU:CD1	2.73	0.64
1:B:431:GLN:O	1:B:435:ILE:HG13	1.97	0.64
1:D:155:ALA:O	1:D:159:LYS:HD3	1.97	0.64
1:B:233:ARG:HH12	1:B:279:HIS:CE1	2.16	0.64
1:C:35:TYR:CD1	1:C:36:PRO:HD2	2.33	0.64
2:D:1450:HEM:HHD	2:D:1450:HEM:HBC2	1.80	0.64
1:D:261:LEU:HD11	1:D:265:LEU:HD11	1.79	0.63
1:D:360:MET:SD	3:D:1460:TU1:H15	2.38	0.63
1:B:83:PRO:HA	1:B:86:HIS:CD2	2.33	0.63
1:A:99:PRO:O	1:A:102:VAL:HG22	1.98	0.63
1:A:110:PHE:O	1:A:233:ARG:NH2	2.31	0.63
1:A:94:ASN:H	1:A:94:ASN:ND2	1.97	0.63
1:B:75:GLN:HG3	1:B:76:ARG:O	1.99	0.62
1:B:76:ARG:HB3	1:B:378:ASP:OD1	1.99	0.62
1:B:147:GLN:NE2	1:B:151:ARG:NH1	2.47	0.62
2:B:1450:HEM:HBC2	2:B:1450:HEM:HHD	1.82	0.62
1:C:278:LEU:HD23	1:C:278:LEU:C	2.19	0.62
1:B:428:ALA:O	1:B:432:VAL:HG23	1.99	0.62
1:C:50:LYS:HG3	1:C:51:ASN:N	2.15	0.62
1:A:305:LEU:HD23	1:A:447:LEU:HD13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:MET:HG2	1:B:158:TRP:CE3	2.35	0.62
1:B:209:ILE:HD12	1:B:209:ILE:N	2.15	0.62
1:C:35:TYR:CD2	1:C:59:CYS:SG	2.93	0.61
1:C:63:LEU:O	1:C:64:LYS:HB2	2.00	0.61
1:C:244:ILE:CG2	1:C:248:GLU:CD	2.69	0.61
1:D:319:LEU:O	1:D:319:LEU:HD12	2.01	0.61
1:D:142:PHE:O	1:D:146:ILE:HG13	1.99	0.61
1:D:239:ILE:O	1:D:243:ILE:HG13	2.01	0.61
1:C:237:GLN:CG	1:C:278:LEU:CD2	2.75	0.61
1:D:120:TYR:HD1	1:D:123:MET:HE2	1.66	0.61
1:D:351:ARG:O	1:D:388:HIS:ND1	2.33	0.61
1:C:389:HIS:CD2	1:C:397:PRO:HB2	2.35	0.61
2:A:1450:HEM:C1A	3:A:1460:TU1:H3	2.36	0.61
1:C:447:LEU:O	1:C:449:ARG:N	2.31	0.61
1:A:277:SER:OG	1:A:279:HIS:HB3	2.00	0.61
1:D:122:ARG:O	1:D:126:GLN:HG3	2.01	0.61
1:D:147:GLN:NE2	1:D:330:LEU:HD12	2.16	0.61
1:D:245:VAL:O	1:D:249:LYS:HB2	2.00	0.61
1:C:244:ILE:C	1:C:248:GLU:HG2	2.20	0.61
1:B:215:MET:CB	1:B:218:LEU:HD12	2.14	0.60
1:C:83:PRO:HA	1:C:86:HIS:CE1	2.36	0.60
2:D:1450:HEM:HBD2	2:D:1450:HEM:HHA	1.83	0.60
1:A:136:ILE:HD12	1:A:137:ALA:H	1.65	0.60
1:C:244:ILE:HG23	1:C:248:GLU:CD	2.21	0.60
1:D:348:GLU:OE1	1:D:348:GLU:HA	2.01	0.60
1:D:161:ASP:O	1:D:474:THR:CG2	2.49	0.60
1:C:237:GLN:HE21	1:C:278:LEU:HD23	1.66	0.60
1:C:104:THR:O	1:C:107:THR:HG22	2.01	0.60
1:C:105:ILE:O	1:C:108:PRO:HG2	2.02	0.60
1:C:109:VAL:CG2	1:C:208:LEU:HD21	2.29	0.60
1:B:139:PHE:HA	1:B:142:PHE:CD2	2.37	0.60
2:D:1450:HEM:HBB2	2:D:1450:HEM:CMB	2.30	0.60
1:A:351:ARG:HD2	1:A:351:ARG:O	2.01	0.60
1:B:120:TYR:HB2	1:B:121:PRO:CD	2.32	0.59
1:D:261:LEU:CD1	1:D:265:LEU:HD11	2.32	0.59
1:A:198:ALA:HA	1:A:201:LEU:HD12	1.84	0.59
1:B:451:GLU:HA	1:B:451:GLU:OE1	2.02	0.59
1:C:66:GLY:O	1:C:81:GLY:N	2.34	0.59
1:D:233:ARG:NH1	1:D:282:CYS:SG	2.69	0.59
1:A:110:PHE:C	1:A:233:ARG:HH21	2.04	0.59
1:C:42:LEU:HD13	1:C:42:LEU:O	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:MET:HB2	1:C:445:PHE:O	2.02	0.59
1:A:187:ASP:OD1	1:A:188:LEU:N	2.33	0.59
1:A:366:GLU:HA	1:A:374:VAL:O	2.03	0.59
1:D:464:PRO:HB2	1:D:469:CYS:SG	2.42	0.59
2:D:1450:HEM:C1A	3:D:1460:TU1:H3	2.37	0.59
1:A:102:VAL:HG23	1:A:103:TYR:CE1	2.37	0.59
1:C:100:ARG:CZ	1:C:118:ALA:O	2.51	0.59
1:C:197:PHE:CE2	1:C:289:MET:HG3	2.38	0.59
1:B:293:GLN:HG3	1:B:294:HIS:N	2.17	0.59
1:B:33:PRO:HB2	1:B:63:LEU:HD13	1.84	0.59
1:D:53:LEU:O	1:D:57:GLN:HG3	2.04	0.58
1:D:154:MET:O	1:D:158:TRP:N	2.36	0.58
1:D:200:LEU:CD2	1:D:232:ALA:O	2.51	0.58
1:C:269:VAL:HG11	1:C:275:ARG:HG3	1.85	0.58
1:D:136:ILE:HD13	1:D:136:ILE:N	2.18	0.58
1:D:330:LEU:HD23	1:D:334:ASN:HD22	1.69	0.58
1:C:262:LEU:HD12	1:C:262:LEU:C	2.23	0.58
1:A:124:ARG:O	1:A:125:GLU:C	2.41	0.58
1:D:245:VAL:HG12	1:D:249:LYS:HD2	1.86	0.58
1:C:443:TYR:O	1:C:476:LYS:HD2	2.03	0.58
1:B:60:LYS:HG3	1:B:66:GLY:HA2	1.85	0.58
1:A:100:ARG:HG3	1:A:101:GLU:OE1	2.04	0.57
1:B:270:TYR:HD1	1:B:274:THR:O	1.86	0.57
1:C:276:MET:HG2	1:C:280:GLU:OE1	2.04	0.57
1:B:82:ASP:O	1:B:85:GLU:N	2.32	0.57
1:C:447:LEU:HD11	1:C:449:ARG:HB2	1.87	0.57
1:D:154:MET:HE1	1:D:438:THR:HG22	1.87	0.57
1:A:204:MET:O	1:A:207:SER:OG	2.19	0.57
1:A:149:GLU:HB3	1:A:178:THR:HG22	1.87	0.57
1:D:200:LEU:HD23	1:D:232:ALA:HA	1.86	0.57
1:C:201:LEU:CD2	1:C:290:PHE:HD1	2.17	0.57
1:D:227:ALA:HB1	1:D:230:ARG:CB	2.28	0.57
1:B:149:GLU:OE1	1:B:149:GLU:HA	2.05	0.56
1:C:142:PHE:HE1	1:C:182:CYS:O	1.88	0.56
1:D:309:HIS:CD2	1:D:310:PRO:HD2	2.40	0.56
1:A:342:ALA:O	1:A:346:VAL:HG23	2.06	0.56
1:B:141:ASN:O	1:B:144:PRO:HD2	2.05	0.56
1:C:215:MET:HB3	1:C:217:TRP:CZ2	2.41	0.56
1:A:147:GLN:NE2	1:A:330:LEU:HG	2.21	0.56
1:B:270:TYR:O	1:B:273:GLY:N	2.38	0.56
1:D:293:GLN:HG3	1:D:294:HIS:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:TYR:N	1:C:121:PRO:CD	2.69	0.56
2:D:1450:HEM:HHA	2:D:1450:HEM:CBD	2.35	0.56
1:D:306:HIS:O	1:D:312:ASN:ND2	2.39	0.56
1:A:431:GLN:O	1:A:435:ILE:HG13	2.06	0.55
1:B:120:TYR:CB	1:B:121:PRO:CD	2.84	0.55
1:B:295:THR:HG23	2:B:1450:HEM:CAB	2.36	0.55
1:C:107:THR:CG2	1:C:108:PRO:CD	2.84	0.55
1:B:33:PRO:HD3	1:B:372:TYR:CE2	2.40	0.55
1:C:175:ILE:HG13	1:C:297:THR:OG1	2.06	0.55
1:D:406:GLU:OE2	1:D:410:GLY:N	2.35	0.55
1:A:197:PHE:CE2	1:A:289:MET:HG2	2.41	0.55
1:B:331:ASN:H	1:B:334:ASN:ND2	2.04	0.55
1:A:72:ILE:O	1:A:75:GLN:HB3	2.07	0.55
1:C:113:GLY:N	1:C:117:ALA:HB1	2.20	0.55
1:C:263:GLY:O	1:C:267:LYS:HG3	2.07	0.55
1:D:197:PHE:HE2	1:D:289:MET:HG3	1.69	0.55
1:B:143:VAL:HG21	1:B:332:TYR:HA	1.87	0.55
1:C:103:TYR:HE2	3:C:1460:TU1:HC	1.55	0.55
1:D:261:LEU:HD12	1:D:261:LEU:O	2.06	0.55
1:B:149:GLU:HG2	1:B:177:ASN:HB3	1.88	0.55
1:B:270:TYR:CZ	1:B:276:MET:HG2	2.41	0.55
1:B:42:LEU:O	1:B:45:ILE:HG23	2.07	0.55
1:C:42:LEU:HD11	1:C:46:VAL:HG23	1.89	0.55
1:D:302:TRP:CD2	1:D:464:PRO:HG3	2.42	0.55
1:B:291:ALA:O	1:B:295:THR:HG22	2.08	0.54
1:A:286:VAL:O	1:A:290:PHE:HB2	2.08	0.54
1:D:120:TYR:HD1	1:D:123:MET:CE	2.20	0.54
1:B:150:VAL:HG12	1:B:154:MET:CE	2.38	0.54
1:B:153:PHE:O	1:B:157:ASN:N	2.39	0.54
1:A:100:ARG:HG3	1:A:101:GLU:N	2.22	0.54
1:A:157:ASN:O	1:A:158:TRP:HD1	1.91	0.54
1:B:233:ARG:HH12	1:B:279:HIS:HE1	1.55	0.54
1:C:45:ILE:O	1:C:45:ILE:HD12	2.08	0.54
1:A:389:HIS:CD2	1:A:397:PRO:HB2	2.42	0.54
1:A:418:GLY:O	1:A:421:LYS:HG2	2.07	0.54
1:C:183:LEU:O	1:C:261:LEU:HB3	2.07	0.54
1:A:322:GLU:OE2	1:A:340:PRO:HD2	2.08	0.54
1:B:32:PRO:HA	1:B:372:TYR:CD2	2.42	0.54
2:C:1450:HEM:HBB2	2:C:1450:HEM:CMB	2.38	0.54
1:D:38:THR:HG22	1:D:39:VAL:HG23	1.90	0.54
1:D:448:LEU:HD23	1:D:448:LEU:N	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLY:N	1:A:260:ASP:OD2	2.40	0.54
1:A:420:HIS:HA	2:A:1450:HEM:O1D	2.08	0.54
1:B:334:ASN:HA	1:B:338:GLU:HB2	1.90	0.54
1:D:200:LEU:CD2	1:D:232:ALA:HA	2.37	0.54
1:B:184:PHE:O	1:B:189:ARG:NH1	2.41	0.54
1:A:332:TYR:CE2	1:A:336:MET:HG3	2.43	0.53
1:D:351:ARG:O	1:D:351:ARG:HD2	2.08	0.53
1:B:152:LYS:O	1:B:156:GLU:HB2	2.09	0.53
1:C:131:ALA:HA	1:C:423:ILE:HD12	1.91	0.53
2:C:1450:HEM:C1A	3:C:1460:TU1:H3	2.43	0.53
1:A:299:THR:HG21	1:A:350:ILE:HD11	1.91	0.53
1:C:107:THR:CG2	1:C:108:PRO:HD3	2.37	0.53
1:C:351:ARG:HD2	1:C:351:ARG:O	2.09	0.53
1:A:357:LEU:HD22	1:A:385:LEU:HD13	1.91	0.53
1:B:96:ILE:O	1:B:97:LEU:HD23	2.08	0.53
1:D:160:GLU:HB2	1:D:162:GLU:O	2.09	0.53
1:B:120:TYR:HB2	1:B:121:PRO:HD3	1.90	0.53
1:A:210:PRO:HG3	1:A:460:MET:HE1	1.91	0.53
1:D:316:LEU:HD12	1:D:316:LEU:C	2.29	0.53
1:B:131:ALA:O	1:B:134:LEU:N	2.37	0.53
1:C:35:TYR:CD1	1:C:36:PRO:CD	2.91	0.53
1:C:298:ILE:HD13	1:C:462:VAL:O	2.09	0.53
1:A:130:LEU:HD11	1:A:288:ALA:HB2	1.91	0.52
1:C:124:ARG:NH1	1:C:128:ASN:OD1	2.39	0.52
1:C:142:PHE:O	1:C:145:ALA:HB3	2.09	0.52
1:D:184:PHE:O	1:D:189:ARG:NH1	2.42	0.52
1:A:449:ARG:HH11	1:A:449:ARG:HB3	1.74	0.52
1:D:239:ILE:O	1:D:243:ILE:CG1	2.58	0.52
1:D:313:LYS:HA	1:D:316:LEU:HB3	1.91	0.52
1:D:449:ARG:NH1	1:D:451:GLU:O	2.41	0.52
1:A:166:ASN:ND2	1:A:169:GLU:H	2.07	0.52
1:A:210:PRO:HB3	1:A:460:MET:CE	2.40	0.52
1:B:175:ILE:HG13	1:B:297:THR:HA	1.89	0.52
1:B:149:GLU:CG	1:B:177:ASN:HB3	2.40	0.52
1:D:136:ILE:HD13	1:D:136:ILE:H	1.73	0.52
1:A:331:ASN:OD1	1:A:333:ASP:N	2.42	0.52
1:A:197:PHE:O	1:A:201:LEU:HD12	2.10	0.52
1:A:291:ALA:HB1	3:A:1460:TU1:C2	2.40	0.52
1:D:247:ARG:NH1	1:D:262:LEU:HD23	2.25	0.52
1:D:450:ASP:O	1:D:451:GLU:OE1	2.28	0.52
1:A:158:TRP:NE1	1:A:165:ILE:HG21	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:O	1:B:176:ILE:HG22	2.09	0.52
1:C:125:GLU:OE1	1:C:271:ARG:HD2	2.09	0.52
1:D:335:VAL:HG12	1:D:433:LYS:HE2	1.91	0.52
1:A:298:ILE:HD13	1:A:463:GLY:CA	2.40	0.52
1:B:59:CYS:HB3	1:B:68:PHE:CE2	2.45	0.52
1:B:180:CYS:O	1:B:181:GLN:C	2.47	0.52
2:B:1450:HEM:HBB2	2:B:1450:HEM:HMB2	1.92	0.52
1:A:42:LEU:O	1:A:45:ILE:HG22	2.06	0.51
1:C:122:ARG:O	1:C:126:GLN:CG	2.57	0.51
1:B:69:THR:HA	1:B:78:THR:HA	1.92	0.51
1:C:237:GLN:HG2	1:C:278:LEU:HD21	1.89	0.51
1:B:464:PRO:HB2	1:B:469:CYS:SG	2.50	0.51
1:D:142:PHE:O	1:D:145:ALA:HB3	2.10	0.51
1:A:132:GLU:O	1:A:138:LYS:NZ	2.44	0.51
1:B:215:MET:O	1:B:218:LEU:HB2	2.09	0.51
1:B:238:LYS:O	1:B:242:GLU:HG3	2.10	0.51
1:B:339:MET:CE	1:B:437:ALA:HB2	2.41	0.51
1:C:72:ILE:O	1:C:75:GLN:N	2.43	0.51
1:C:197:PHE:HE2	1:C:289:MET:HG3	1.75	0.51
1:C:244:ILE:O	1:C:248:GLU:N	2.27	0.51
1:C:451:GLU:OE1	1:C:451:GLU:HA	2.10	0.51
1:C:221:LEU:HB2	1:C:222:PRO:CD	2.40	0.51
1:D:298:ILE:HD13	1:D:463:GLY:HA2	1.91	0.51
1:D:422:CYS:HB2	2:D:1450:HEM:NA	2.25	0.51
1:A:48:PHE:HZ	1:A:358:MET:CE	2.23	0.51
1:B:83:PRO:HB2	1:B:408:VAL:HG11	1.92	0.51
1:D:42:LEU:C	1:D:42:LEU:HD12	2.30	0.51
1:C:394:PHE:HA	1:C:404:ARG:HH12	1.76	0.51
1:A:304:MET:O	1:A:308:MET:HG2	2.11	0.51
1:B:93:ARG:CB	1:B:95:GLU:HG2	2.41	0.51
1:D:86:HIS:CE1	1:D:387:SER:OG	2.64	0.51
1:D:392:GLU:HG2	1:D:408:VAL:CG2	2.41	0.51
1:B:294:HIS:C	1:B:297:THR:HG22	2.32	0.51
1:A:102:VAL:HG23	1:A:103:TYR:HD1	1.71	0.50
1:C:231:GLU:O	1:C:235:GLU:HB2	2.12	0.50
1:A:102:VAL:C	1:A:103:TYR:HD1	2.14	0.50
1:C:114:VAL:N	1:C:117:ALA:HB3	2.27	0.50
1:C:348:GLU:OE1	1:C:351:ARG:HB3	2.12	0.50
1:D:42:LEU:HD13	1:D:45:ILE:HG22	1.92	0.50
1:D:175:ILE:HG13	1:D:297:THR:HA	1.93	0.50
1:A:136:ILE:HD12	1:A:136:ILE:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ARG:HA	1:C:116:TYR:HB3	1.94	0.50
1:B:316:LEU:O	1:B:316:LEU:HD12	2.11	0.50
1:C:237:GLN:CD	1:C:278:LEU:CD2	2.80	0.50
1:A:122:ARG:HG2	1:A:126:GLN:NE2	2.26	0.50
1:A:344:ARG:HD3	1:A:402:PRO:O	2.12	0.50
1:C:464:PRO:HB2	1:C:469:CYS:SG	2.52	0.50
1:A:209:ILE:HD12	1:A:209:ILE:N	2.26	0.50
1:B:97:LEU:CD2	1:B:363:VAL:HG22	2.42	0.50
1:D:129:PHE:CE1	1:D:268:ALA:HB1	2.46	0.50
1:A:354:PRO:HG3	1:A:384:PRO:C	2.33	0.49
1:D:443:TYR:CE2	1:D:473:TYR:HD2	2.28	0.49
1:A:305:LEU:HD22	1:A:453:PRO:CD	2.42	0.49
1:D:305:LEU:HD13	1:D:453:PRO:HD2	1.93	0.49
1:A:162:GLU:HA	1:A:473:TYR:O	2.11	0.49
1:A:195:ARG:O	1:A:199:GLN:HG3	2.12	0.49
1:C:240:LEU:O	1:C:243:ILE:HG22	2.12	0.49
1:C:269:VAL:CG1	1:C:275:ARG:N	2.73	0.49
1:B:53:LEU:O	1:B:57:GLN:HG3	2.12	0.49
1:B:147:GLN:NE2	1:B:151:ARG:HH12	2.09	0.49
1:D:113:GLY:H	1:D:117:ALA:HB1	1.77	0.49
1:A:384:PRO:O	1:A:388:HIS:HB2	2.13	0.49
1:B:115:ALA:C	1:B:123:MET:HG3	2.32	0.49
2:D:1450:HEM:HMD3	3:D:1460:TU1:H28	1.94	0.49
1:A:105:ILE:O	1:A:108:PRO:HD2	2.13	0.49
1:B:294:HIS:HA	1:B:297:THR:HG22	1.95	0.49
1:C:121:PRO:O	1:C:125:GLU:HG2	2.13	0.49
1:C:302:TRP:O	1:C:306:HIS:CD2	2.65	0.49
1:A:322:GLU:OE1	1:A:341:PHE:HB3	2.13	0.49
1:A:351:ARG:O	1:A:388:HIS:HB3	2.13	0.49
1:B:351:ARG:HD3	1:B:394:PHE:CD1	2.47	0.49
1:C:340:PRO:O	1:C:344:ARG:HG3	2.12	0.49
1:B:293:GLN:CG	1:B:294:HIS:N	2.76	0.49
1:D:291:ALA:HB2	3:D:1460:TU1:H27	1.95	0.49
1:D:298:ILE:HD13	1:D:463:GLY:HA3	1.92	0.49
1:C:292:GLY:O	1:C:293:GLN:C	2.52	0.49
1:D:98:SER:OG	1:D:101:GLU:OE1	2.31	0.49
1:B:162:GLU:HB3	1:B:474:THR:HG23	1.95	0.48
1:C:113:GLY:H	1:C:117:ALA:CB	2.25	0.48
1:B:291:ALA:O	1:B:295:THR:CG2	2.61	0.48
1:C:103:TYR:O	1:C:106:MET:HB2	2.14	0.48
1:D:351:ARG:HD2	1:D:351:ARG:C	2.34	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1450:HEM:HBC2	2:B:1450:HEM:CHD	2.43	0.48
1:C:52:PRO:O	1:C:56:MET:HG3	2.13	0.48
1:C:90:PHE:CD2	1:C:417:ALA:HB3	2.48	0.48
2:C:1450:HEM:HHA	2:C:1450:HEM:CBD	2.43	0.48
1:D:136:ILE:H	1:D:136:ILE:CD1	2.27	0.48
1:A:237:GLN:HE21	1:A:279:HIS:CA	2.21	0.48
1:B:95:GLU:O	1:B:364:LYS:HG3	2.13	0.48
1:D:277:SER:O	1:D:281:VAL:HG23	2.14	0.48
1:C:269:VAL:HG11	1:C:275:ARG:CG	2.37	0.48
1:D:200:LEU:CD2	1:D:232:ALA:CA	2.89	0.48
1:D:442:GLU:O	1:D:443:TYR:CD1	2.67	0.48
1:A:234:ALA:O	1:A:238:LYS:HB2	2.13	0.48
1:A:384:PRO:O	1:A:388:HIS:CG	2.67	0.48
2:A:1450:HEM:HBC2	2:A:1450:HEM:CHD	2.40	0.48
1:B:114:VAL:CG1	1:B:284:MET:HE2	2.43	0.48
1:C:447:LEU:CD1	1:C:449:ARG:HB2	2.43	0.48
1:D:90:PHE:CG	1:D:417:ALA:HB3	2.48	0.48
1:A:105:ILE:HG22	1:A:219:LEU:HD11	1.96	0.48
1:B:239:ILE:O	1:B:243:ILE:HG12	2.14	0.48
1:C:394:PHE:HA	1:C:404:ARG:NH1	2.28	0.48
1:A:316:LEU:HD12	1:A:316:LEU:O	2.13	0.48
1:D:261:LEU:HD12	1:D:261:LEU:C	2.34	0.48
1:C:104:THR:C	1:C:107:THR:H	2.11	0.47
1:C:201:LEU:HD22	1:C:290:PHE:CD1	2.45	0.47
1:B:339:MET:HE1	1:B:437:ALA:HB2	1.95	0.47
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.14	0.47
1:C:244:ILE:HG22	1:C:248:GLU:CD	2.34	0.47
1:D:66:GLY:HA3	1:D:82:ASP:HB2	1.96	0.47
1:D:126:GLN:HA	1:D:129:PHE:HD2	1.79	0.47
1:C:42:LEU:HD13	1:C:42:LEU:C	2.34	0.47
1:C:101:GLU:O	1:C:104:THR:OG1	2.32	0.47
1:C:306:HIS:O	1:C:312:ASN:ND2	2.34	0.47
1:C:401:ASP:O	1:C:403:GLU:N	2.47	0.47
1:C:245:VAL:O	1:C:249:LYS:N	2.42	0.47
1:C:384:PRO:O	1:C:388:HIS:CG	2.67	0.47
1:D:292:GLY:O	1:D:296:SER:HB2	2.15	0.47
1:D:351:ARG:HD2	1:D:388:HIS:HB3	1.96	0.47
1:A:428:ALA:O	1:A:432:VAL:HG23	2.14	0.47
1:A:82:ASP:OD1	1:A:84:HIS:HB2	2.14	0.47
1:B:220:ARG:NH1	1:B:220:ARG:CG	2.78	0.47
1:C:189:ARG:HA	1:C:192:LEU:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:LEU:HB2	1:C:222:PRO:HD2	1.97	0.47
1:C:447:LEU:HD11	1:C:449:ARG:CB	2.44	0.47
1:D:93:ARG:NH1	1:D:95:GLU:CB	2.76	0.47
1:D:200:LEU:HD22	1:D:232:ALA:O	2.13	0.47
1:A:332:TYR:CZ	1:A:336:MET:HG3	2.50	0.47
1:C:105:ILE:HG13	1:C:106:MET:N	2.29	0.47
1:C:122:ARG:O	1:C:126:GLN:HG2	2.13	0.47
1:C:392:GLU:O	1:C:407:LYS:HB2	2.15	0.47
1:A:37:VAL:HG12	1:A:43:GLY:HA2	1.96	0.47
1:D:401:ASP:O	1:D:404:ARG:HG2	2.15	0.47
1:B:161:ASP:O	1:B:475:ARG:N	2.38	0.47
1:D:114:VAL:N	1:D:117:ALA:HB3	2.30	0.47
1:D:294:HIS:HB3	1:D:461:VAL:HG11	1.97	0.47
1:B:196:HIS:HA	1:B:199:GLN:HG3	1.96	0.46
1:B:314:LYS:CG	1:B:315:TRP:N	2.78	0.46
1:D:175:ILE:HD12	1:D:296:SER:HB3	1.97	0.46
1:A:91:SER:O	1:A:92:PRO:C	2.53	0.46
1:B:45:ILE:HG13	1:B:46:VAL:N	2.30	0.46
1:B:120:TYR:CB	1:B:121:PRO:HD3	2.45	0.46
1:C:41:PHE:CD1	1:C:42:LEU:N	2.83	0.46
1:C:34:VAL:HG22	1:C:69:THR:HB	1.98	0.46
1:D:176:ILE:HG12	1:D:198:ALA:HB2	1.96	0.46
1:D:229:CYS:O	1:D:232:ALA:HB3	2.14	0.46
1:D:313:LYS:O	1:D:314:LYS:C	2.54	0.46
1:A:166:ASN:ND2	1:A:166:ASN:C	2.69	0.46
1:A:212:ALA:HB1	1:A:219:LEU:HG	1.97	0.46
1:D:129:PHE:CD1	1:D:268:ALA:HB1	2.50	0.46
1:A:467:ASN:OD1	1:A:468:GLN:N	2.49	0.46
1:D:262:LEU:HA	1:D:265:LEU:HD12	1.98	0.46
1:A:136:ILE:CD1	1:A:137:ALA:N	2.79	0.46
1:D:293:GLN:CG	1:D:294:HIS:N	2.78	0.46
1:A:298:ILE:HD13	1:A:462:VAL:C	2.35	0.46
1:A:466:LEU:HD12	1:A:466:LEU:O	2.16	0.46
1:A:473:TYR:C	1:A:473:TYR:CD1	2.89	0.46
1:B:41:PHE:O	1:B:73:GLY:HA2	2.16	0.46
1:C:143:VAL:N	1:C:144:PRO:CD	2.79	0.46
1:D:309:HIS:CG	1:D:310:PRO:HD2	2.51	0.46
1:D:358:MET:HG3	1:D:383:SER:HB2	1.96	0.46
1:A:213:VAL:HG12	1:A:360:MET:CE	2.46	0.46
1:B:475:ARG:HD2	1:B:477:LYS:CB	2.46	0.46
1:C:90:PHE:CD1	1:C:417:ALA:HB3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:HIS:CE1	1:C:411:ALA:HA	2.52	0.45
1:A:231:GLU:O	1:A:235:GLU:N	2.42	0.45
1:C:447:LEU:HD21	1:C:451:GLU:O	2.15	0.45
1:D:50:LYS:HG3	1:D:51:ASN:H	1.80	0.45
1:D:197:PHE:CZ	1:D:289:MET:HG3	2.51	0.45
1:A:93:ARG:HD2	1:A:95:GLU:OE1	2.17	0.45
2:A:1450:HEM:HBD2	2:A:1450:HEM:HHA	1.98	0.45
1:B:357:LEU:O	1:B:384:PRO:HD2	2.15	0.45
1:C:121:PRO:O	1:C:125:GLU:CG	2.65	0.45
1:C:299:THR:HG21	1:C:350:ILE:HD11	1.98	0.45
1:D:450:ASP:C	1:D:451:GLU:OE1	2.55	0.45
1:B:113:GLY:H	1:B:117:ALA:HB1	1.81	0.45
1:C:175:ILE:HG13	1:C:297:THR:HA	1.97	0.45
1:D:351:ARG:O	1:D:388:HIS:HB3	2.16	0.45
1:B:309:HIS:CD2	1:B:310:PRO:HD2	2.52	0.45
1:C:75:GLN:HG3	1:C:76:ARG:N	2.31	0.45
1:C:113:GLY:N	1:C:117:ALA:CB	2.79	0.45
1:D:234:ALA:O	1:D:238:LYS:HB2	2.16	0.45
1:A:89:PHE:CD1	1:A:89:PHE:C	2.90	0.45
1:C:91:SER:O	1:C:92:PRO:C	2.55	0.45
1:C:237:GLN:HE21	1:C:278:LEU:CD2	2.25	0.45
1:B:270:TYR:CE1	1:B:276:MET:HG2	2.52	0.45
1:C:114:VAL:O	1:C:115:ALA:HB3	2.17	0.45
1:C:243:ILE:O	1:C:243:ILE:HD13	2.16	0.45
1:C:395:PRO:O	1:C:404:ARG:NH2	2.49	0.45
1:A:109:VAL:CG2	1:A:204:MET:HB3	2.43	0.45
1:B:75:GLN:HG2	1:B:379:ILE:HG13	1.99	0.45
1:A:341:PHE:O	1:A:344:ARG:HB2	2.16	0.45
1:B:44:HIS:HD2	1:B:71:SER:N	1.90	0.45
1:B:294:HIS:CA	1:B:297:THR:HG22	2.47	0.45
1:C:175:ILE:HG13	1:C:297:THR:CA	2.47	0.45
1:D:471:VAL:HG12	1:D:472:LYS:N	2.32	0.45
1:C:130:LEU:HD12	1:C:130:LEU:O	2.17	0.45
1:D:143:VAL:N	1:D:144:PRO:CD	2.80	0.45
1:D:326:PHE:O	1:D:441:ARG:NH2	2.48	0.45
1:A:125:GLU:O	1:A:129:PHE:CD2	2.70	0.44
1:B:372:TYR:CD1	1:B:372:TYR:N	2.85	0.44
1:C:52:PRO:HD2	1:C:457:TYR:CD2	2.53	0.44
1:D:363:VAL:HG12	1:D:376:LYS:HA	1.99	0.44
1:B:197:PHE:CE2	1:B:289:MET:HG3	2.52	0.44
1:B:314:LYS:HG2	1:B:315:TRP:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:HE22	1:A:330:LEU:HG	1.83	0.44
1:C:260:ASP:CG	1:C:262:LEU:H	2.20	0.44
1:B:217:TRP:HB2	1:D:42:LEU:HD23	1.99	0.44
1:C:106:MET:HE3	1:C:106:MET:HA	1.99	0.44
1:D:236:LEU:O	1:D:240:LEU:HG	2.17	0.44
1:D:431:GLN:O	1:D:435:ILE:HG13	2.18	0.44
1:B:357:LEU:HD22	1:B:385:LEU:HD22	2.00	0.44
1:C:237:GLN:CD	1:C:278:LEU:HD21	2.38	0.44
1:C:441:ARG:O	1:C:476:LYS:HD3	2.18	0.44
1:D:336:MET:HG2	1:D:430:LEU:CD1	2.47	0.44
1:B:202:SER:O	1:B:205:GLU:N	2.50	0.44
1:A:344:ARG:HH11	1:A:403:GLU:HA	1.82	0.44
1:B:97:LEU:HD22	1:B:363:VAL:HG22	1.99	0.44
1:D:122:ARG:O	1:D:126:GLN:CG	2.65	0.44
1:C:269:VAL:HG13	1:C:275:ARG:CA	2.33	0.44
1:C:323:ILE:HA	1:C:326:PHE:CE2	2.52	0.44
1:A:357:LEU:HD21	1:A:462:VAL:HG21	2.00	0.43
1:C:131:ALA:CA	1:C:423:ILE:HD12	2.47	0.43
1:C:424:GLY:HA3	2:C:1450:HEM:C3C	2.53	0.43
1:D:131:ALA:O	1:D:135:THR:HG23	2.18	0.43
1:D:396:ASN:ND2	1:D:399:LEU:HD22	2.33	0.43
2:A:1450:HEM:HBB2	2:A:1450:HEM:CMB	2.46	0.43
1:B:444:ASP:O	1:B:473:TYR:HA	2.18	0.43
1:C:44:HIS:CD2	1:C:71:SER:H	2.36	0.43
1:C:105:ILE:O	1:C:108:PRO:HD2	2.18	0.43
1:C:228:ARG:H	1:C:228:ARG:HG2	1.53	0.43
1:D:143:VAL:O	1:D:144:PRO:C	2.54	0.43
1:A:166:ASN:ND2	1:A:166:ASN:O	2.50	0.43
1:A:209:ILE:HD12	1:A:209:ILE:H	1.82	0.43
1:A:354:PRO:HG3	1:A:385:LEU:N	2.33	0.43
1:D:44:HIS:HD2	1:D:71:SER:N	2.08	0.43
1:A:103:TYR:CD1	1:A:103:TYR:N	2.87	0.43
1:A:449:ARG:HE	1:A:468:GLN:HG2	1.83	0.43
1:B:162:GLU:HA	1:B:473:TYR:O	2.19	0.43
1:B:363:VAL:HG12	1:B:376:LYS:CA	2.43	0.43
1:C:105:ILE:CG1	1:C:106:MET:N	2.82	0.43
1:D:107:THR:HB	1:D:108:PRO:HD3	1.99	0.43
1:D:136:ILE:N	1:D:136:ILE:CD1	2.82	0.43
1:A:239:ILE:O	1:A:243:ILE:N	2.47	0.43
1:B:446:GLN:HE21	1:B:446:GLN:HB3	1.70	0.43
1:D:238:LYS:O	1:D:242:GLU:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TRP:HE1	1:A:165:ILE:HG21	1.83	0.43
1:B:453:PRO:HB3	1:B:468:GLN:HB2	2.00	0.43
1:C:122:ARG:O	1:C:126:GLN:HG3	2.18	0.43
1:C:142:PHE:CE1	1:C:182:CYS:O	2.71	0.43
1:D:339:MET:CE	1:D:342:ALA:CB	2.97	0.43
1:A:91:SER:HB2	1:A:92:PRO:HD3	2.01	0.43
1:A:211:ALA:HB2	1:C:221:LEU:CD1	2.43	0.43
1:A:305:LEU:HD22	1:A:453:PRO:HD3	2.01	0.43
1:C:88:ARG:HD3	1:C:369:VAL:HA	2.01	0.43
1:D:157:ASN:HD22	1:D:157:ASN:N	2.17	0.43
1:A:298:ILE:HD13	1:A:463:GLY:N	2.34	0.43
1:A:308:MET:HE2	1:A:445:PHE:HB2	2.01	0.43
1:A:322:GLU:OE2	1:A:339:MET:HA	2.18	0.43
1:A:363:VAL:O	1:A:377:GLY:N	2.29	0.43
3:A:1460:TU1:F2	1:C:222:PRO:HD2	2.08	0.43
1:B:48:PHE:CD1	1:B:48:PHE:C	2.91	0.43
1:D:235:GLU:HG2	1:D:239:ILE:HD11	2.01	0.43
1:D:240:LEU:HA	1:D:243:ILE:HG13	2.01	0.43
1:C:86:HIS:ND1	1:C:410:GLY:O	2.52	0.43
1:D:100:ARG:HG3	1:D:101:GLU:N	2.33	0.43
1:D:147:GLN:NE2	1:D:330:LEU:HB2	2.34	0.43
1:C:166:ASN:HD22	1:C:169:GLU:H	1.67	0.42
1:A:330:LEU:HA	1:A:334:ASN:HD22	1.84	0.42
1:A:477:LYS:O	4:A:2013:HOH:O	2.21	0.42
1:C:91:SER:HB2	1:C:92:PRO:HD3	2.00	0.42
1:D:396:ASN:ND2	1:D:399:LEU:CD2	2.82	0.42
1:C:401:ASP:C	1:C:403:GLU:H	2.22	0.42
1:D:423:ILE:HD11	2:D:1450:HEM:HMD2	1.99	0.42
1:B:423:ILE:HD11	2:B:1450:HEM:HMD2	2.00	0.42
1:C:105:ILE:C	1:C:108:PRO:HD2	2.39	0.42
1:D:157:ASN:N	1:D:157:ASN:ND2	2.68	0.42
1:D:380:ILE:HG23	1:D:380:ILE:O	2.19	0.42
1:A:109:VAL:HG13	1:A:204:MET:HE1	1.87	0.42
1:A:451:GLU:OE1	1:A:451:GLU:HA	2.19	0.42
1:D:112:GLU:O	1:D:114:VAL:HG23	2.20	0.42
1:D:205:GLU:CD	1:D:294:HIS:HE2	2.23	0.42
1:D:313:LYS:O	1:D:316:LEU:N	2.53	0.42
1:A:48:PHE:CZ	1:A:358:MET:CE	3.03	0.42
1:A:147:GLN:HE22	1:A:330:LEU:H	1.67	0.42
1:A:237:GLN:NE2	1:A:279:HIS:CA	2.77	0.42
1:A:343:GLU:HG2	1:A:347:ARG:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:THR:HB	2:C:1450:HEM:CAB	2.50	0.42
1:A:331:ASN:OD1	1:A:331:ASN:C	2.58	0.42
1:B:155:ALA:O	1:B:159:LYS:HG2	2.19	0.42
1:C:423:ILE:HG12	2:C:1450:HEM:CMD	2.50	0.42
1:C:447:LEU:C	1:C:449:ARG:N	2.73	0.42
1:A:363:VAL:CG1	1:A:376:LYS:HA	2.40	0.42
1:B:121:PRO:O	1:B:125:GLU:HG3	2.20	0.42
1:C:200:LEU:O	1:C:204:MET:HG3	2.19	0.42
1:A:109:VAL:CG1	1:A:204:MET:CE	2.70	0.42
1:B:136:ILE:CG2	1:B:332:TYR:OH	2.68	0.42
1:B:295:THR:CG2	1:B:296:SER:N	2.83	0.42
1:B:406:GLU:OE1	1:B:410:GLY:N	2.53	0.42
1:C:142:PHE:CE1	1:C:182:CYS:HB3	2.55	0.42
1:D:245:VAL:O	1:D:249:LYS:N	2.43	0.42
1:D:298:ILE:HD13	1:D:462:VAL:C	2.40	0.42
1:A:146:ILE:O	1:A:147:GLN:C	2.58	0.42
1:B:59:CYS:CB	1:B:68:PHE:CE2	3.03	0.42
1:B:114:VAL:CG1	1:B:284:MET:CE	2.97	0.42
1:B:361:ARG:HH22	2:B:1450:HEM:CGA	2.32	0.42
1:B:399:LEU:O	1:B:404:ARG:NH2	2.52	0.42
1:C:35:TYR:CD1	1:C:36:PRO:N	2.88	0.42
1:C:139:PHE:HA	1:C:142:PHE:CD2	2.55	0.42
1:D:149:GLU:CG	1:D:177:ASN:HB3	2.49	0.42
1:D:422:CYS:HA	2:D:1450:HEM:C4D	2.54	0.42
1:A:136:ILE:CD1	1:A:137:ALA:H	2.30	0.41
2:A:1450:HEM:C4D	3:A:1460:TU1:H3	2.55	0.41
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.84	0.41
1:C:266:LEU:O	1:C:267:LYS:C	2.58	0.41
1:D:126:GLN:O	1:D:129:PHE:HB2	2.20	0.41
1:D:467:ASN:OD1	1:D:468:GLN:HG3	2.19	0.41
1:A:51:ASN:HB3	1:A:54:GLU:HB3	2.02	0.41
1:A:262:LEU:O	1:A:262:LEU:HD12	2.21	0.41
1:A:270:TYR:CE2	1:A:276:MET:CG	3.02	0.41
1:B:185:GLY:O	1:B:188:LEU:N	2.52	0.41
1:B:262:LEU:CD2	1:B:263:GLY:N	2.77	0.41
1:B:263:GLY:O	1:B:267:LYS:HG3	2.21	0.41
1:C:181:GLN:OE1	1:C:189:ARG:NE	2.53	0.41
1:C:243:ILE:O	1:C:247:ARG:CG	2.68	0.41
2:A:1450:HEM:CHA	3:A:1460:TU1:H3	2.50	0.41
1:C:278:LEU:HD23	1:C:278:LEU:O	2.20	0.41
1:D:50:LYS:HG3	1:D:51:ASN:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ASN:HA	1:D:52:PRO:HD3	1.87	0.41
1:D:221:LEU:HB3	1:D:222:PRO:HD2	2.01	0.41
1:D:352:ARG:NH2	1:D:398:ARG:O	2.53	0.41
1:A:118:ALA:HB1	1:A:122:ARG:HB3	2.02	0.41
1:A:319:LEU:O	1:A:322:GLU:HB3	2.20	0.41
1:C:358:MET:HE2	1:C:383:SER:HB2	2.02	0.41
1:D:451:GLU:OE1	1:D:451:GLU:HA	2.20	0.41
1:A:56:MET:HB3	1:A:386:LEU:HD13	2.02	0.41
1:A:326:PHE:O	1:A:441:ARG:NH2	2.53	0.41
1:B:269:VAL:HG12	1:B:273:GLY:HA2	2.02	0.41
1:D:215:MET:HB3	1:D:217:TRP:CE2	2.55	0.41
1:D:302:TRP:CE3	1:D:302:TRP:HA	2.56	0.41
1:D:351:ARG:C	1:D:351:ARG:CD	2.89	0.41
1:A:166:ASN:HD22	1:A:169:GLU:H	1.68	0.41
1:C:467:ASN:OD1	1:C:468:GLN:N	2.54	0.41
1:A:362:MET:CE	1:A:377:GLY:HA2	2.51	0.41
1:B:150:VAL:HG12	1:B:154:MET:HE3	2.02	0.41
1:B:157:ASN:O	1:B:158:TRP:HD1	2.04	0.41
1:D:422:CYS:HB2	2:D:1450:HEM:C1A	2.56	0.41
1:A:339:MET:N	1:A:340:PRO:CD	2.84	0.41
1:D:233:ARG:HH11	1:D:233:ARG:CG	2.16	0.41
1:A:133:GLU:CB	1:A:261:LEU:HD12	2.47	0.41
1:A:275:ARG:HE	1:A:275:ARG:HB2	1.80	0.41
1:A:318:LYS:O	1:A:321:LYS:HB3	2.21	0.41
1:A:420:HIS:ND1	2:A:1450:HEM:O1D	2.54	0.41
2:A:1450:HEM:NA	3:A:1460:TU1:H3	2.36	0.41
1:B:217:TRP:CZ3	1:B:218:LEU:HD23	2.55	0.41
1:B:315:TRP:CE3	1:B:315:TRP:HA	2.56	0.41
1:C:147:GLN:O	1:C:148:HIS:C	2.60	0.41
1:D:43:GLY:HA3	1:D:71:SER:O	2.20	0.41
1:D:146:ILE:O	1:D:150:VAL:HG23	2.21	0.41
1:D:425:GLN:O	1:D:426:LYS:C	2.60	0.41
2:D:1450:HEM:NA	3:D:1460:TU1:C3	2.83	0.41
1:A:385:LEU:HD12	1:A:385:LEU:HA	1.93	0.41
1:B:197:PHE:CE2	1:B:289:MET:CG	3.03	0.41
1:C:104:THR:O	1:C:107:THR:CB	2.69	0.41
1:C:142:PHE:O	1:C:145:ALA:N	2.54	0.41
1:C:300:THR:HA	1:C:432:VAL:HG13	2.03	0.41
1:D:126:GLN:HA	1:D:129:PHE:CD2	2.56	0.41
1:D:332:TYR:CD1	1:D:332:TYR:C	2.94	0.41
1:A:115:ALA:O	1:A:123:MET:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:HG21	1:B:332:TYR:OH	2.21	0.40
1:B:294:HIS:HA	1:B:297:THR:CG2	2.51	0.40
1:D:113:GLY:O	1:D:118:ALA:HB2	2.21	0.40
1:A:120:TYR:N	1:A:121:PRO:HD2	2.36	0.40
1:A:196:HIS:O	1:A:200:LEU:HD12	2.21	0.40
1:C:293:GLN:HG3	1:C:294:HIS:N	2.36	0.40
1:A:101:GLU:OE1	1:A:101:GLU:N	2.55	0.40
1:A:276:MET:CE	1:A:281:VAL:HG22	2.52	0.40
1:A:309:HIS:CG	1:A:310:PRO:HD2	2.56	0.40
1:A:389:HIS:HA	1:A:397:PRO:HB3	2.03	0.40
1:B:114:VAL:HG13	1:B:284:MET:CE	2.51	0.40
1:B:241:GLY:O	1:B:244:ILE:N	2.55	0.40
1:C:358:MET:CE	1:C:383:SER:HB2	2.51	0.40
1:D:294:HIS:O	1:D:298:ILE:HG13	2.21	0.40
1:A:359:VAL:C	1:A:360:MET:HG2	2.41	0.40
1:B:166:ASN:ND2	1:B:166:ASN:C	2.74	0.40
1:D:295:THR:HB	2:D:1450:HEM:CAB	2.52	0.40
1:A:291:ALA:HB2	3:A:1460:TU1:H27	2.04	0.40
1:B:122:ARG:O	1:B:126:GLN:HG3	2.22	0.40
1:B:153:PHE:CD1	1:B:153:PHE:C	2.95	0.40
1:C:183:LEU:HB3	1:C:261:LEU:HD22	2.04	0.40
1:D:60:LYS:NZ	1:D:390:ASP:OD1	2.50	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	437/467 (94%)	403 (92%)	32 (7%)	2 (0%)	29 51
1	B	438/467 (94%)	424 (97%)	13 (3%)	1 (0%)	47 69
1	C	436/467 (93%)	403 (92%)	33 (8%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	438/467 (94%)	414 (94%)	23 (5%)	1 (0%)	47 69
All	All	1749/1868 (94%)	1644 (94%)	101 (6%)	4 (0%)	47 69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	B	39	VAL
1	A	92	PRO
1	D	136	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	356/408 (87%)	312 (88%)	44 (12%)	4 9
1	B	354/408 (87%)	307 (87%)	47 (13%)	4 7
1	C	351/408 (86%)	311 (89%)	40 (11%)	5 11
1	D	359/408 (88%)	319 (89%)	40 (11%)	6 12
All	All	1420/1632 (87%)	1249 (88%)	171 (12%)	5 10

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	TYR
1	A	37	VAL
1	A	38	THR
1	A	45	ILE
1	A	51	ASN
1	A	69	THR
1	A	93	ARG
1	A	94	ASN
1	A	100	ARG
1	A	104	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	122	ARG
1	A	136	ILE
1	A	166	ASN
1	A	169	GLU
1	A	170	ASP
1	A	181	GLN
1	A	193	ASN
1	A	209	ILE
1	A	215	MET
1	A	233	ARG
1	A	235	GLU
1	A	242	GLU
1	A	251	GLU
1	A	267	LYS
1	A	274	THR
1	A	275	ARG
1	A	277	SER
1	A	289	MET
1	A	301	SER
1	A	303	SER
1	A	319	LEU
1	A	321	LYS
1	A	330	LEU
1	A	359	VAL
1	A	360	MET
1	A	366	GLU
1	A	383	SER
1	A	403	GLU
1	A	406	GLU
1	A	413	ILE
1	A	426	LYS
1	A	433	LYS
1	A	449	ARG
1	A	474	THR
1	B	41	PHE
1	B	45	ILE
1	B	50	LYS
1	B	70	ILE
1	B	71	SER
1	B	96	ILE
1	B	98	SER
1	B	100	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	132	GLU
1	B	140	GLN
1	B	157	ASN
1	B	166	ASN
1	B	171	CYS
1	B	189	ARG
1	B	190	LYS
1	B	193	ASN
1	B	195	ARG
1	B	209	ILE
1	B	214	PHE
1	B	219	LEU
1	B	220	ARG
1	B	233	ARG
1	B	235	GLU
1	B	237	GLN
1	B	262	LEU
1	B	274	THR
1	B	284	MET
1	B	289	MET
1	B	290	PHE
1	B	298	ILE
1	B	314	LYS
1	B	321	LYS
1	B	325	GLU
1	B	331	ASN
1	B	339	MET
1	B	358	MET
1	B	360	MET
1	B	364	LYS
1	B	372	TYR
1	B	374	VAL
1	B	404	ARG
1	B	426	LYS
1	B	433	LYS
1	B	438	THR
1	B	444	ASP
1	B	446	GLN
1	B	474	THR
1	C	41	PHE
1	C	51	ASN
1	C	71	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	72	ILE
1	C	88	ARG
1	C	102	VAL
1	C	104	THR
1	C	112	GLU
1	C	124	ARG
1	C	141	ASN
1	C	148	HIS
1	C	160	GLU
1	C	161	ASP
1	C	166	ASN
1	C	202	SER
1	C	215	MET
1	C	217	TRP
1	C	225	GLN
1	C	228	ARG
1	C	235	GLU
1	C	238	LYS
1	C	243	ILE
1	C	262	LEU
1	C	265	LEU
1	C	266	LEU
1	C	269	VAL
1	C	274	THR
1	C	277	SER
1	C	348	GLU
1	C	366	GLU
1	C	368	LYS
1	C	376	LYS
1	C	379	ILE
1	C	403	GLU
1	C	404	ARG
1	C	409	ASP
1	C	438	THR
1	C	447	LEU
1	C	452	VAL
1	C	474	THR
1	D	31	LEU
1	D	37	VAL
1	D	42	LEU
1	D	88	ARG
1	D	100	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	105	ILE
1	D	123	MET
1	D	126	GLN
1	D	136	ILE
1	D	154	MET
1	D	157	ASN
1	D	159	LYS
1	D	161	ASP
1	D	166	ASN
1	D	190	LYS
1	D	191	ARG
1	D	200	LEU
1	D	202	SER
1	D	229	CYS
1	D	233	ARG
1	D	238	LYS
1	D	243	ILE
1	D	259	SER
1	D	295	THR
1	D	302	TRP
1	D	314	LYS
1	D	316	LEU
1	D	321	LYS
1	D	325	GLU
1	D	333	ASP
1	D	338	GLU
1	D	360	MET
1	D	367	VAL
1	D	387	SER
1	D	403	GLU
1	D	430	LEU
1	D	441	ARG
1	D	447	LEU
1	D	451	GLU
1	D	474	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	94	ASN
1	A	140	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	237	GLN
1	A	334	ASN
1	B	44	HIS
1	B	94	ASN
1	B	140	GLN
1	B	148	HIS
1	B	166	ASN
1	B	193	ASN
1	B	279	HIS
1	B	293	GLN
1	B	331	ASN
1	B	334	ASN
1	B	446	GLN
1	B	458	HIS
1	C	44	HIS
1	C	166	ASN
1	C	237	GLN
1	C	306	HIS
1	D	44	HIS
1	D	47	GLN
1	D	84	HIS
1	D	148	HIS
1	D	157	ASN
1	D	166	ASN
1	D	334	ASN
1	D	396	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	TU1	C	1460	2	41,42,42	1.99	3 (7%)	55,59,59	2.00	16 (29%)
2	HEM	B	1450	3,1	41,50,50	1.38	6 (14%)	45,82,82	1.94	11 (24%)
3	TU1	B	1460	2	41,42,42	1.97	6 (14%)	55,59,59	2.14	23 (41%)
3	TU1	A	1460	2	41,42,42	1.86	5 (12%)	55,59,59	1.65	11 (20%)
2	HEM	C	1450	3,1	41,50,50	1.34	6 (14%)	45,82,82	1.92	8 (17%)
3	TU1	D	1460	2	41,42,42	1.86	4 (9%)	55,59,59	1.61	9 (16%)
2	HEM	D	1450	3,1	41,50,50	1.43	6 (14%)	45,82,82	2.10	13 (28%)
2	HEM	A	1450	3,1	41,50,50	1.46	5 (12%)	45,82,82	2.29	14 (31%)

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	TU1	C	1460	2	-	0/23/24/24	0/5/5/5
2	HEM	B	1450	3,1	-	0/12/54/54	-
3	TU1	B	1460	2	-	0/23/24/24	0/5/5/5
3	TU1	A	1460	2	-	0/23/24/24	0/5/5/5
2	HEM	C	1450	3,1	-	4/12/54/54	-
3	TU1	D	1460	2	-	1/23/24/24	0/5/5/5
2	HEM	D	1450	3,1	-	4/12/54/54	-
2	HEM	A	1450	3,1	-	6/12/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1460	TU1	C13-C14	8.52	1.50	1.39
3	C	1460	TU1	C13-C14	8.35	1.50	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1460	TU1	C13-C14	7.52	1.49	1.39
3	B	1460	TU1	C9-C20	7.38	1.49	1.38
3	A	1460	TU1	C13-C14	7.24	1.49	1.39
3	A	1460	TU1	C9-C20	7.09	1.48	1.38
3	C	1460	TU1	C9-C20	7.05	1.48	1.38
3	D	1460	TU1	C9-C20	5.72	1.46	1.38
2	D	1450	HEM	C1B-NB	-4.42	1.32	1.40
2	C	1450	HEM	C1B-NB	-4.24	1.33	1.40
2	A	1450	HEM	C1B-NB	-4.11	1.33	1.40
2	B	1450	HEM	C1B-NB	-3.73	1.33	1.40
2	A	1450	HEM	C4B-NB	-3.42	1.31	1.38
3	B	1460	TU1	C5-N2	-3.27	1.35	1.41
3	D	1460	TU1	C5-N2	-3.21	1.35	1.41
2	B	1450	HEM	C4D-ND	-3.14	1.34	1.40
2	B	1450	HEM	C4B-NB	-3.13	1.32	1.38
2	A	1450	HEM	C4D-C3D	3.02	1.50	1.45
2	D	1450	HEM	C4B-NB	-2.80	1.33	1.38
3	A	1460	TU1	C29-C24	-2.75	1.37	1.41
2	D	1450	HEM	C4D-ND	-2.75	1.35	1.40
3	C	1460	TU1	C5-N2	-2.56	1.36	1.41
2	C	1450	HEM	FE-NB	2.39	2.08	1.96
3	A	1460	TU1	C5-N2	-2.38	1.36	1.41
3	B	1460	TU1	C29-C24	-2.38	1.37	1.41
2	C	1450	HEM	C4D-ND	-2.36	1.36	1.40
2	C	1450	HEM	C4D-C3D	2.34	1.49	1.45
2	C	1450	HEM	CHB-C1B	2.31	1.40	1.35
2	B	1450	HEM	CHB-C1B	2.30	1.40	1.35
2	B	1450	HEM	FE-NB	2.26	2.08	1.96
2	A	1450	HEM	C4D-ND	-2.21	1.36	1.40
2	D	1450	HEM	C3C-C2C	-2.21	1.37	1.40
2	A	1450	HEM	C3C-C2C	-2.15	1.37	1.40
3	B	1460	TU1	C26-C25	-2.14	1.37	1.42
2	D	1450	HEM	C1D-ND	-2.14	1.34	1.38
3	A	1460	TU1	C26-C25	-2.12	1.37	1.42
2	C	1450	HEM	C4B-NB	-2.04	1.34	1.38
2	D	1450	HEM	FE-NB	2.04	2.07	1.96
3	D	1460	TU1	C24-N4	-2.03	1.32	1.38
3	B	1460	TU1	C18-C17	2.01	1.41	1.37
2	B	1450	HEM	C1A-CHA	-2.00	1.35	1.41

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1450	HEM	CAD-C3D-C4D	6.42	135.87	124.66
2	A	1450	HEM	C1B-NB-C4B	5.79	111.05	105.07
2	D	1450	HEM	C1B-NB-C4B	5.63	110.89	105.07
2	B	1450	HEM	C1B-NB-C4B	5.54	110.80	105.07
3	B	1460	TU1	C26-C25-C24	5.05	124.87	118.17
3	C	1460	TU1	C19-C20-C9	-4.96	118.23	123.53
2	C	1450	HEM	CAD-C3D-C4D	4.95	133.31	124.66
2	A	1450	HEM	CHC-C4B-NB	4.91	129.77	124.43
2	D	1450	HEM	CHC-C4B-NB	4.87	129.72	124.43
3	B	1460	TU1	C11-C12-C13	-4.81	113.11	120.91
2	D	1450	HEM	CAD-C3D-C4D	4.75	132.97	124.66
2	D	1450	HEM	CHD-C1D-ND	4.74	129.58	124.43
2	C	1450	HEM	CHC-C4B-NB	4.73	129.57	124.43
2	C	1450	HEM	C1B-NB-C4B	4.71	109.94	105.07
2	B	1450	HEM	CHC-C4B-NB	4.67	129.50	124.43
3	C	1460	TU1	C11-C12-C13	-4.64	113.40	120.91
2	A	1450	HEM	CHD-C1D-ND	4.59	129.41	124.43
2	C	1450	HEM	CHD-C1D-ND	4.57	129.40	124.43
3	A	1460	TU1	C19-C20-C9	-4.42	118.82	123.53
2	B	1450	HEM	CHD-C1D-ND	4.39	129.21	124.43
3	C	1460	TU1	C15-C14-C13	-4.26	118.09	123.30
2	D	1450	HEM	CBA-CAA-C2A	-4.20	105.45	112.62
3	D	1460	TU1	C9-C8-N3	4.07	124.34	116.80
3	C	1460	TU1	C19-C12-C13	4.07	127.34	120.61
3	C	1460	TU1	C9-C8-N3	4.01	124.22	116.80
3	B	1460	TU1	C19-C20-C9	-3.97	119.30	123.53
2	C	1450	HEM	CHD-C1D-C2D	-3.97	118.78	124.98
3	B	1460	TU1	C21-C22-C25	-3.96	120.09	126.25
2	A	1450	HEM	CAD-C3D-C2D	-3.91	120.59	127.88
3	B	1460	TU1	C19-C12-C13	3.69	126.72	120.61
3	D	1460	TU1	C19-C20-C9	-3.68	119.61	123.53
3	D	1460	TU1	C15-C14-C13	-3.66	118.83	123.30
3	B	1460	TU1	C21-C22-C23	3.64	132.46	127.97
2	A	1450	HEM	O2D-CGD-O1D	-3.63	114.25	123.30
3	D	1460	TU1	O1-C8-C9	-3.56	114.50	121.01
3	A	1460	TU1	C15-C14-C13	-3.54	118.98	123.30
2	A	1450	HEM	CHD-C1D-C2D	-3.53	119.47	124.98
3	A	1460	TU1	C26-C25-C24	3.46	122.76	118.17
3	A	1460	TU1	C9-C8-N3	3.38	123.06	116.80
2	D	1450	HEM	CAD-C3D-C2D	-3.33	121.68	127.88
2	A	1450	HEM	O2D-CGD-CBD	3.31	124.66	114.03
3	B	1460	TU1	C15-C16-C17	3.28	121.75	118.36
3	C	1460	TU1	C22-C21-C7	-3.25	107.09	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1460	TU1	C12-C13-C14	3.21	127.91	122.69
3	B	1460	TU1	C21-C7-C6	3.19	118.52	110.25
3	B	1460	TU1	C15-C14-C13	-3.19	119.41	123.30
3	B	1460	TU1	C21-C7-N3	-3.12	104.22	110.79
2	B	1450	HEM	CAD-CBD-CGD	-3.09	106.94	113.60
2	B	1450	HEM	C4B-CHC-C1C	3.09	126.64	122.56
3	A	1460	TU1	C11-C12-C13	-3.09	115.91	120.91
2	C	1450	HEM	CAD-C3D-C2D	-3.05	122.19	127.88
3	D	1460	TU1	F1-C14-C13	3.04	123.47	118.89
2	B	1450	HEM	CHD-C1D-C2D	-2.93	120.40	124.98
2	A	1450	HEM	CAA-CBA-CGA	-2.93	105.55	113.76
2	D	1450	HEM	CHD-C1D-C2D	-2.92	120.42	124.98
3	C	1460	TU1	C15-C16-C17	2.90	121.36	118.36
2	A	1450	HEM	CBD-CAD-C3D	2.83	120.48	112.63
3	B	1460	TU1	C27-C26-C25	-2.81	116.99	120.89
3	C	1460	TU1	C26-C25-C24	2.78	121.86	118.17
3	B	1460	TU1	C29-C24-C25	-2.75	115.73	120.76
3	A	1460	TU1	C27-C26-C25	-2.73	117.11	120.89
3	D	1460	TU1	C15-C16-C17	2.72	121.18	118.36
3	B	1460	TU1	F2-C17-C18	2.69	122.09	118.25
2	D	1450	HEM	CMD-C2D-C1D	2.68	129.12	125.04
2	B	1450	HEM	CHA-C4D-C3D	-2.67	120.32	125.33
2	B	1450	HEM	CHA-C4D-ND	2.65	127.66	124.38
2	D	1450	HEM	CHA-C4D-ND	2.65	127.66	124.38
3	C	1460	TU1	O1-C8-C9	-2.64	116.19	121.01
3	D	1460	TU1	F3-C20-C19	2.63	123.83	118.61
2	B	1450	HEM	O2D-CGD-CBD	2.57	122.29	114.03
2	A	1450	HEM	C4B-CHC-C1C	2.51	125.87	122.56
3	C	1460	TU1	O2-C6-N2	2.49	129.29	123.93
3	C	1460	TU1	C16-C17-C18	-2.49	120.05	123.29
3	B	1460	TU1	C9-C8-N3	2.43	121.30	116.80
3	C	1460	TU1	C18-C13-C12	-2.42	114.07	118.58
3	A	1460	TU1	C11-C12-C19	2.42	121.59	118.16
3	A	1460	TU1	C15-C16-C17	2.38	120.83	118.36
2	B	1450	HEM	C2C-C3C-C4C	2.38	108.56	106.90
3	B	1460	TU1	C12-C13-C14	-2.36	118.85	122.69
3	B	1460	TU1	O2-C6-N2	2.34	128.95	123.93
3	D	1460	TU1	C20-C9-C8	-2.33	119.70	125.09
2	D	1450	HEM	CHB-C1B-NB	2.33	127.26	124.38
2	C	1450	HEM	CBD-CAD-C3D	2.33	119.09	112.63
3	C	1460	TU1	F1-C14-C13	2.32	122.39	118.89
3	D	1460	TU1	C27-C26-C25	-2.32	117.68	120.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1460	TU1	C1-C5-N2	2.31	128.19	120.40
2	A	1450	HEM	C4D-C3D-C2D	-2.30	103.54	106.90
2	D	1450	HEM	CHA-C4D-C3D	-2.26	121.08	125.33
2	C	1450	HEM	O2D-CGD-O1D	-2.22	117.76	123.30
3	B	1460	TU1	C27-C28-C29	2.19	123.51	120.44
3	C	1460	TU1	C1-C5-N2	2.19	127.75	120.40
2	B	1450	HEM	C3C-C4C-NC	-2.18	106.83	110.94
3	A	1460	TU1	C7-N3-C8	-2.17	116.30	121.60
3	B	1460	TU1	C10-C9-C20	2.16	119.12	116.67
3	A	1460	TU1	C22-C21-C7	-2.15	109.24	113.45
3	B	1460	TU1	C26-C25-C22	-2.14	130.49	134.42
3	B	1460	TU1	O1-C8-N3	-2.13	118.54	122.45
2	D	1450	HEM	CAD-CBD-CGD	-2.12	109.04	113.60
3	C	1460	TU1	C27-C26-C25	-2.12	117.96	120.89
3	B	1460	TU1	C18-C13-C12	2.09	122.48	118.58
2	A	1450	HEM	CMA-C3A-C4A	-2.08	125.26	128.46
2	A	1450	HEM	CHB-C1B-NB	2.07	126.94	124.38
3	B	1460	TU1	C4-C5-N2	-2.06	113.46	120.40
2	D	1450	HEM	C3C-C4C-NC	-2.04	107.09	110.94
3	B	1460	TU1	C1-C5-N2	2.02	127.20	120.40

There are no chirality outliers.

All (15) torsion outliers are listed below:

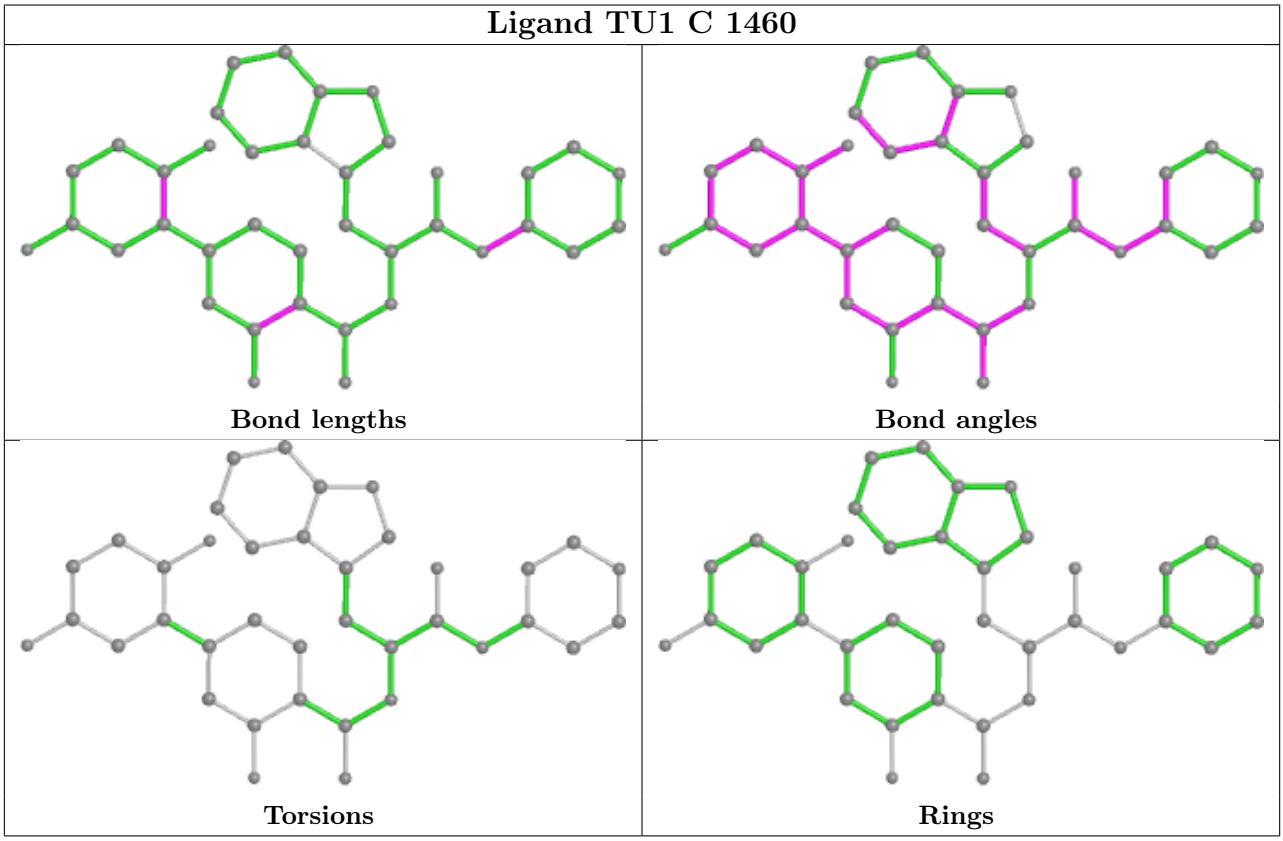
Mol	Chain	Res	Type	Atoms
2	A	1450	HEM	C3A-C2A-CAA-CBA
2	A	1450	HEM	C2D-C3D-CAD-CBD
2	A	1450	HEM	C4D-C3D-CAD-CBD
2	C	1450	HEM	C2D-C3D-CAD-CBD
2	C	1450	HEM	C4D-C3D-CAD-CBD
2	D	1450	HEM	C2D-C3D-CAD-CBD
2	D	1450	HEM	C4D-C3D-CAD-CBD
2	A	1450	HEM	C1A-C2A-CAA-CBA
3	D	1460	TU1	O1-C8-C9-C20
2	C	1450	HEM	CAD-CBD-CGD-O2D
2	C	1450	HEM	CAD-CBD-CGD-O1D
2	D	1450	HEM	CAD-CBD-CGD-O2D
2	A	1450	HEM	CAD-CBD-CGD-O1D
2	A	1450	HEM	CAD-CBD-CGD-O2D
2	D	1450	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

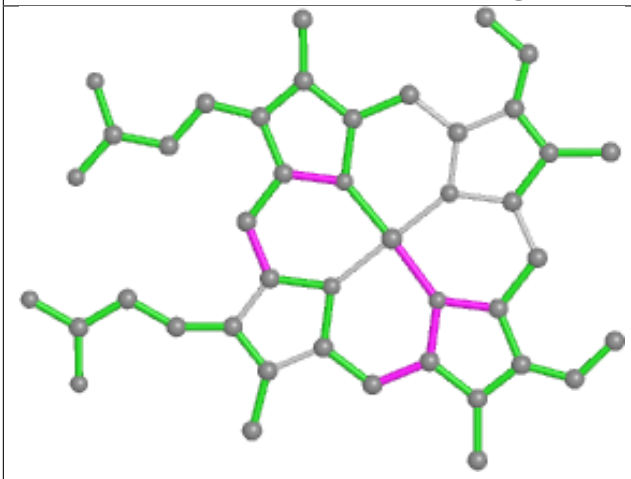
8 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1460	TU1	2	0
2	B	1450	HEM	6	0
3	B	1460	TU1	2	0
3	A	1460	TU1	7	0
2	C	1450	HEM	8	0
3	D	1460	TU1	5	0
2	D	1450	HEM	13	0
2	A	1450	HEM	11	0

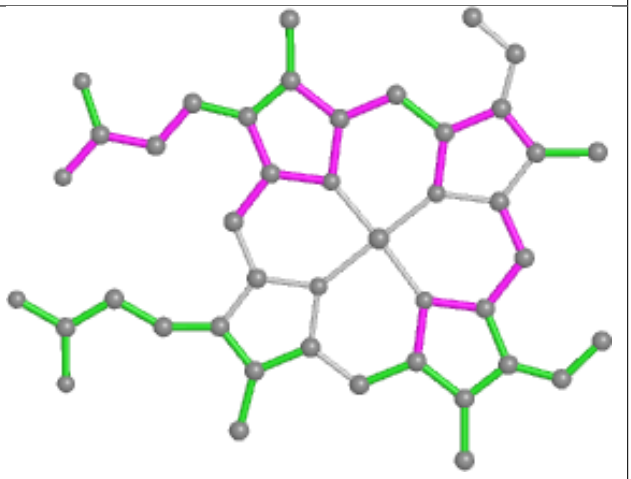
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



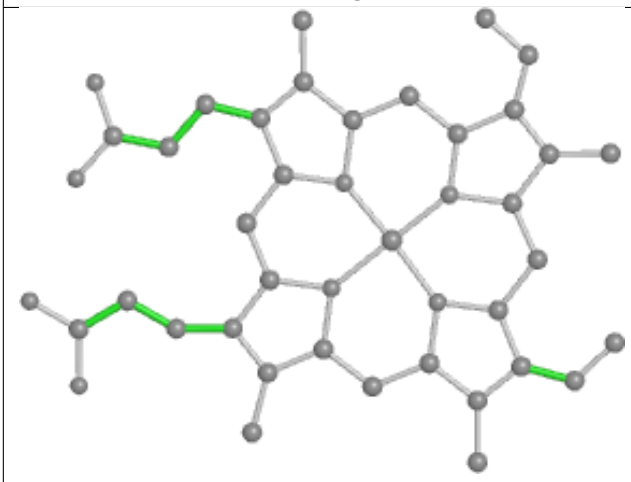
Ligand HEM B 1450



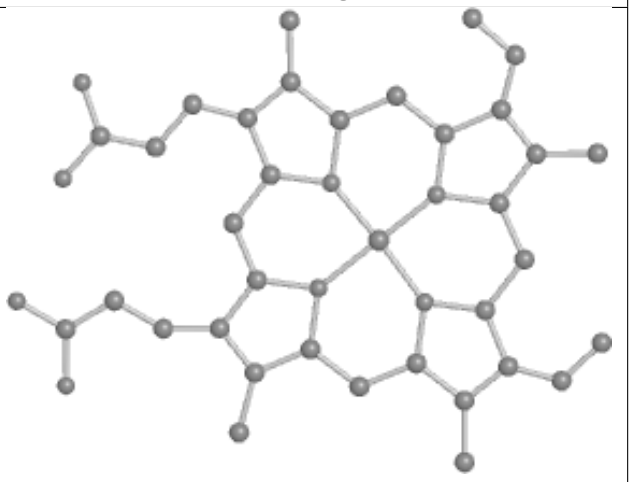
Bond lengths



Bond angles

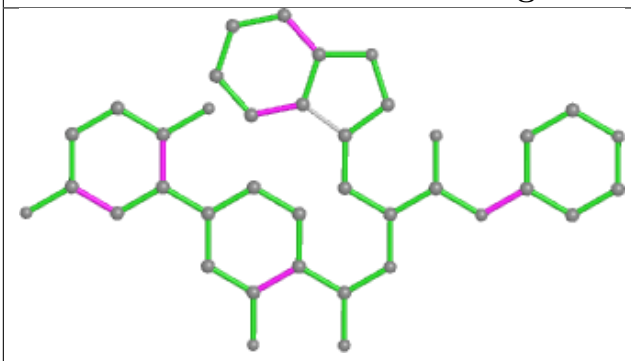


Torsions

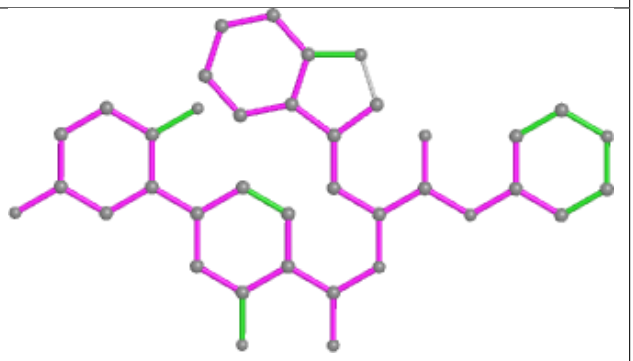


Rings

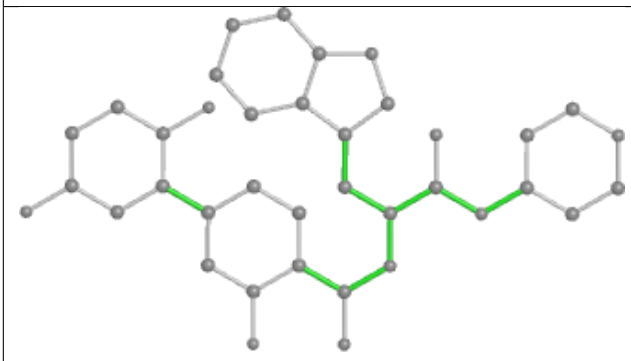
Ligand TU1 B 1460



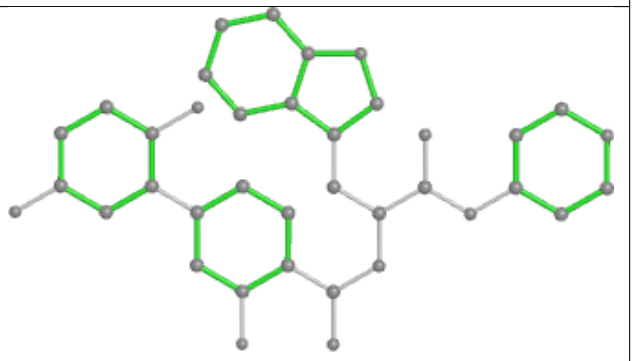
Bond lengths



Bond angles

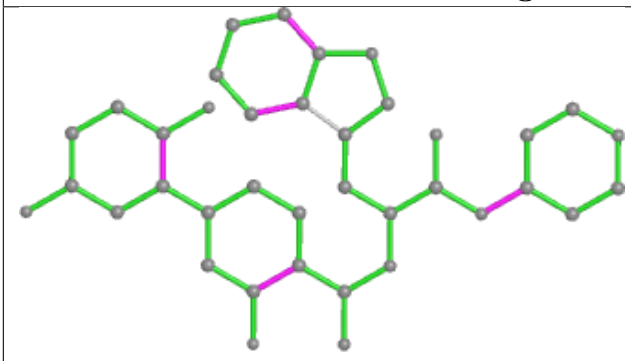


Torsions

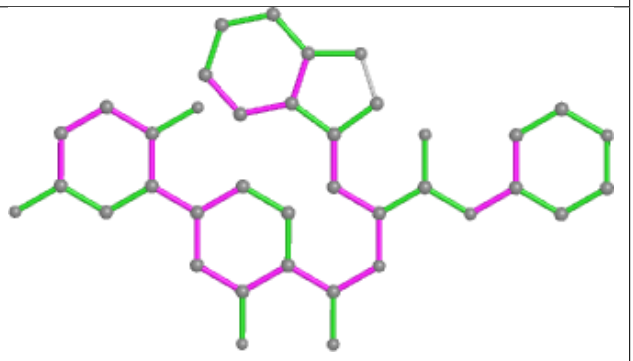


Rings

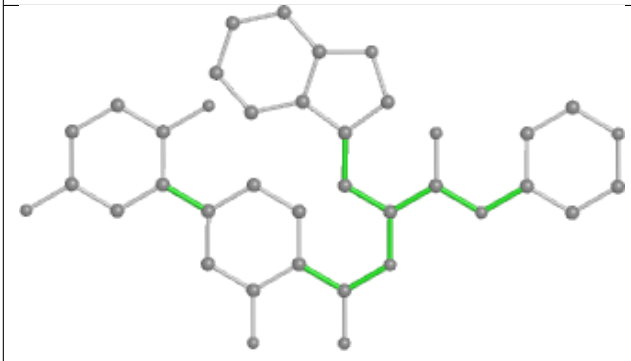
Ligand TU1 A 1460



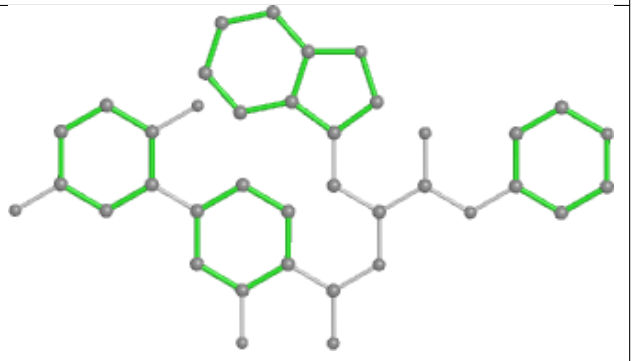
Bond lengths



Bond angles

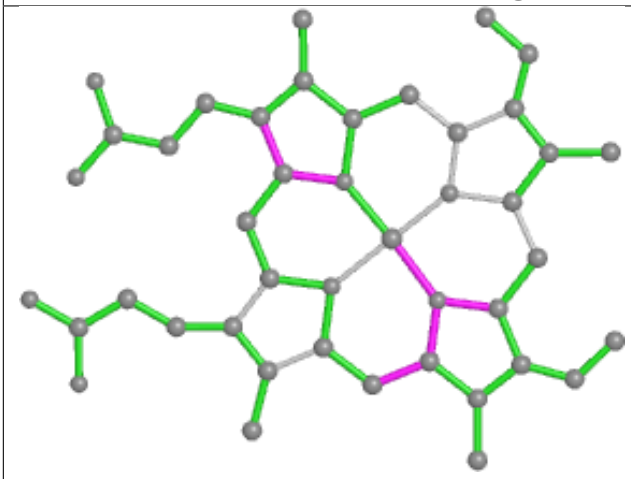


Torsions

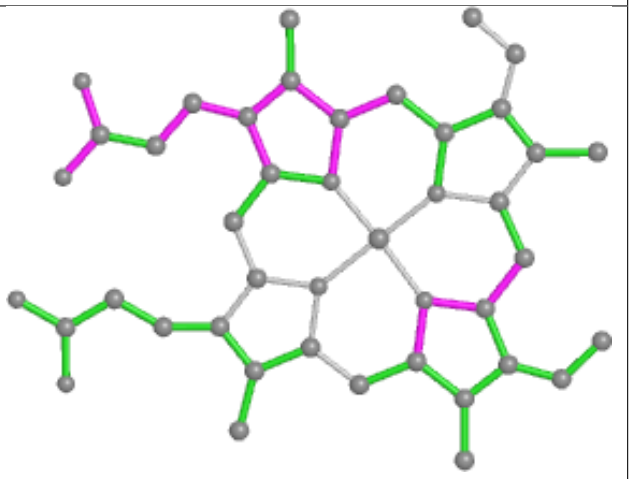


Rings

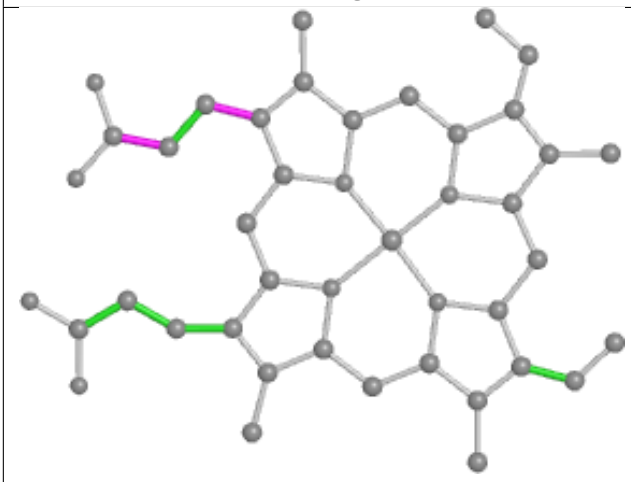
Ligand HEM C 1450



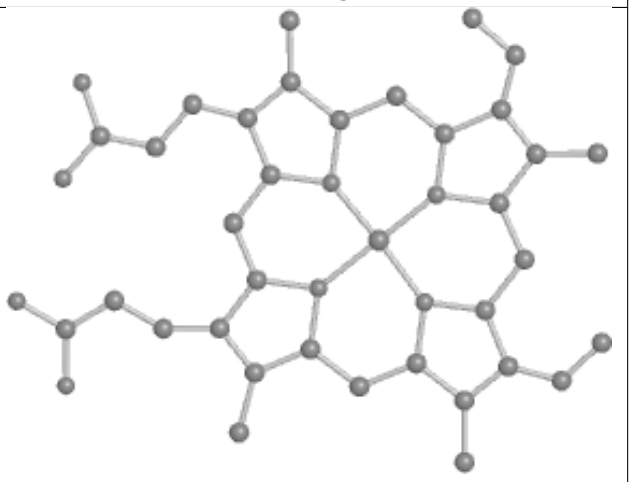
Bond lengths



Bond angles

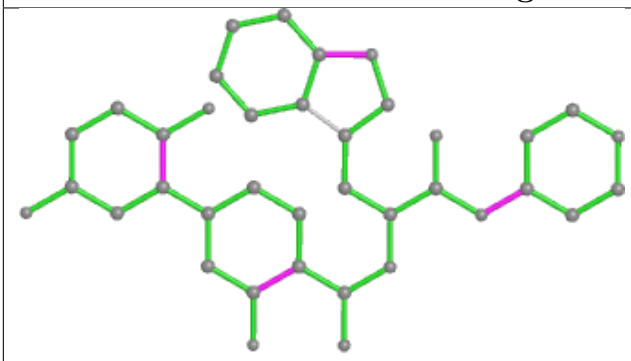


Torsions

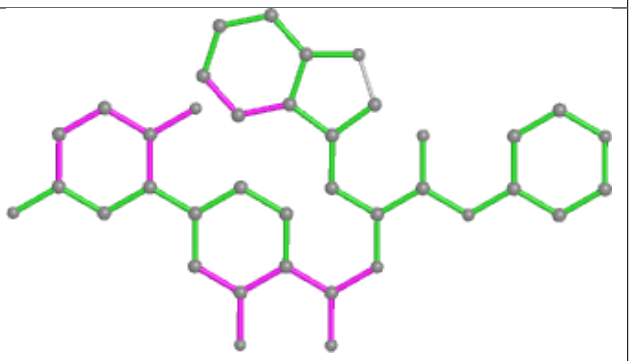


Rings

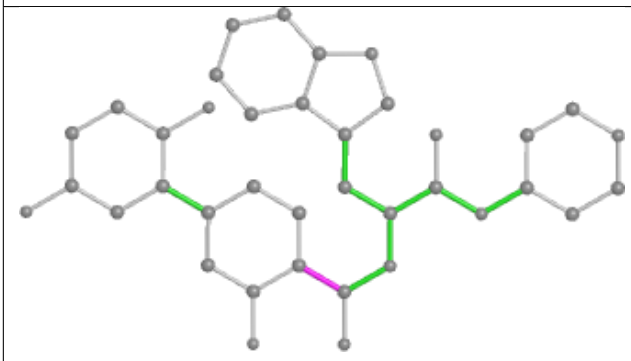
Ligand TU1 D 1460



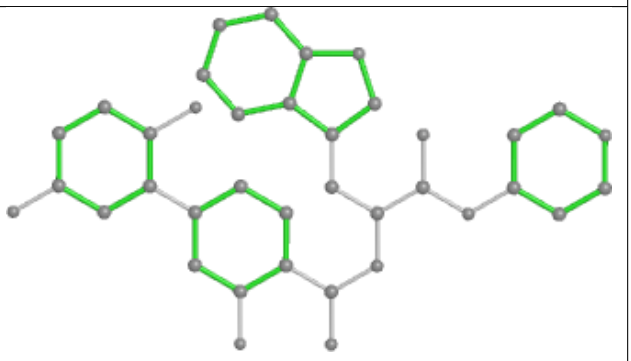
Bond lengths



Bond angles

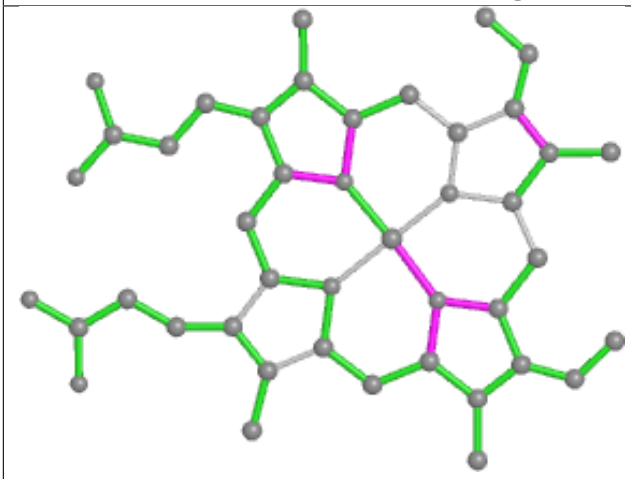


Torsions

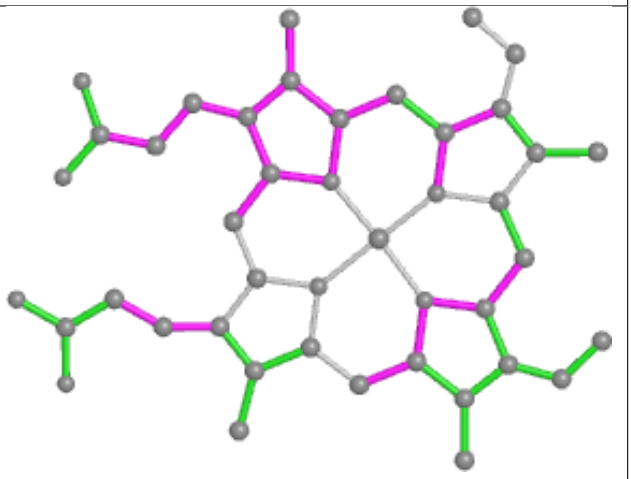


Rings

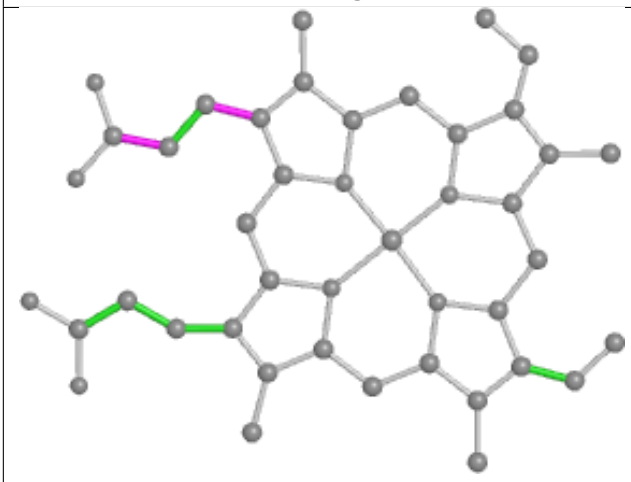
Ligand HEM D 1450



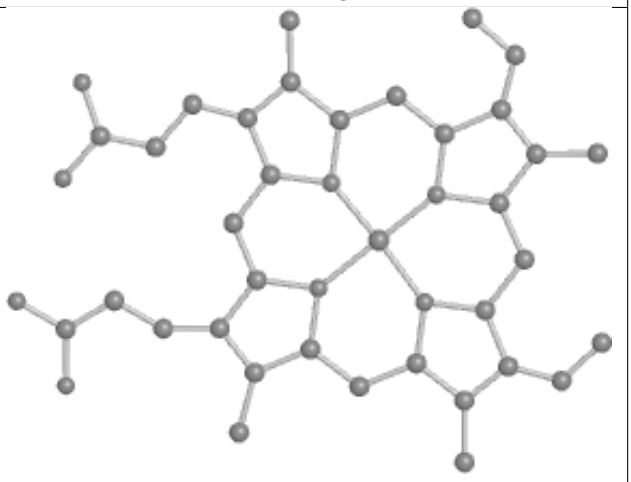
Bond lengths



Bond angles

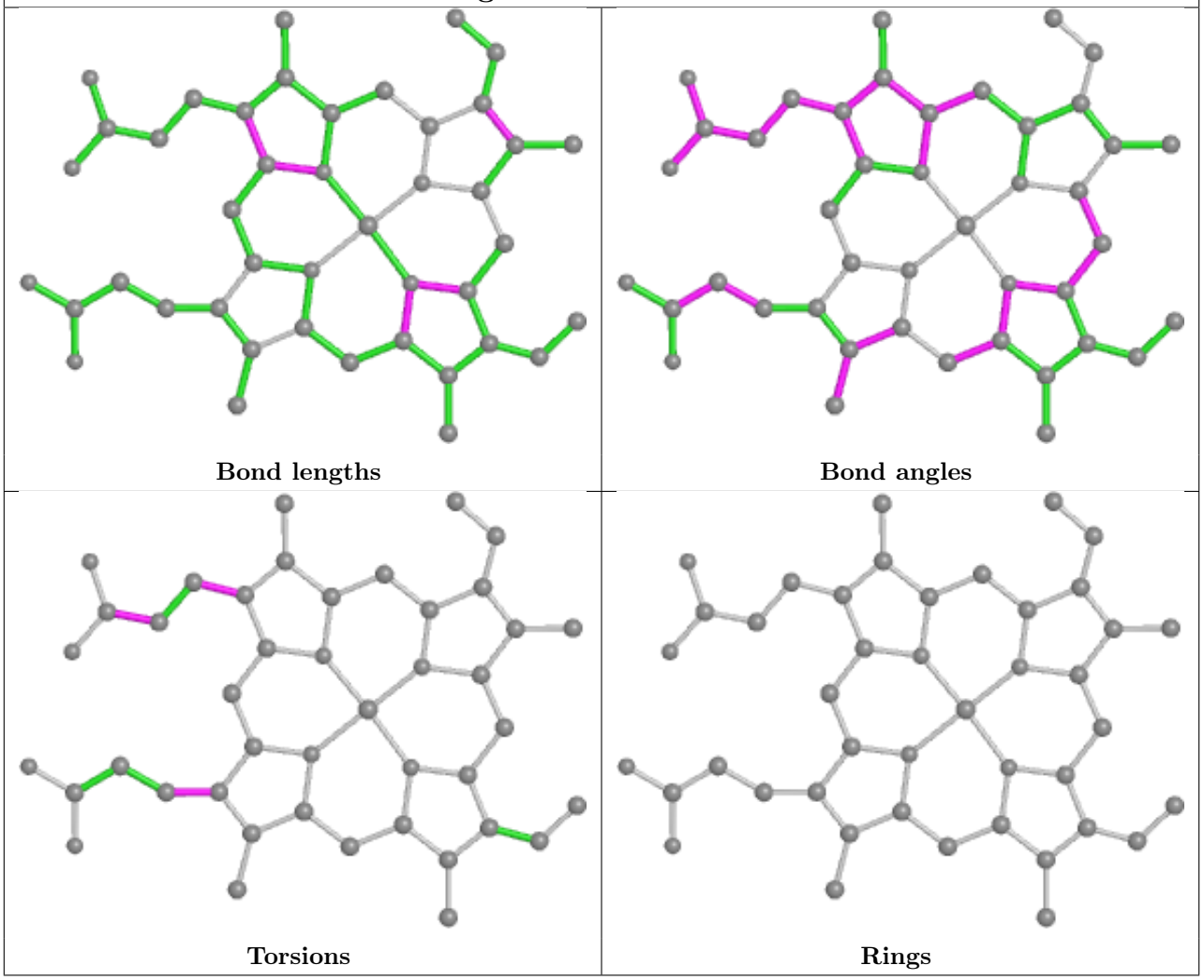


Torsions



Rings

Ligand HEM A 1450



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	441/467 (94%)	-0.51	0 100 100	47, 69, 109, 142	0
1	B	442/467 (94%)	-0.51	2 (0%) 91 89	57, 80, 114, 146	0
1	C	440/467 (94%)	-0.38	2 (0%) 91 89	60, 88, 128, 180	0
1	D	442/467 (94%)	-0.52	0 100 100	46, 68, 107, 140	0
All	All	1765/1868 (94%)	-0.48	4 (0%) 95 94	46, 77, 118, 180	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	PHE	4.1
1	C	158	TRP	2.4
1	B	375	PRO	2.2
1	C	164	VAL	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

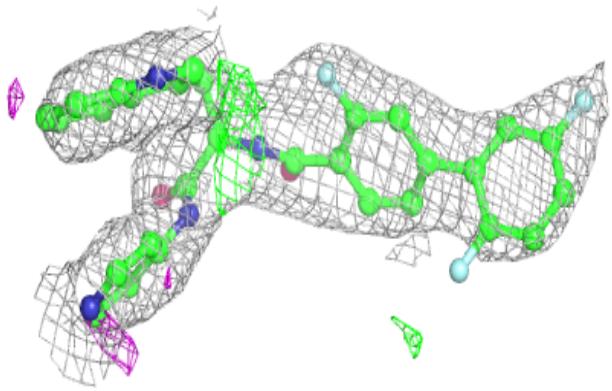
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

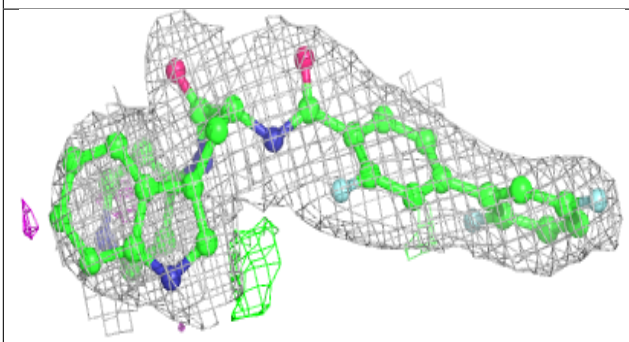
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TU1	B	1460	38/38	0.94	0.19	60,67,85,107	0
3	TU1	A	1460	38/38	0.95	0.24	51,55,77,99	0
3	TU1	C	1460	38/38	0.96	0.22	59,64,91,120	0
3	TU1	D	1460	38/38	0.97	0.17	51,55,67,82	0
2	HEM	A	1450	43/43	0.98	0.20	47,51,56,64	0
2	HEM	B	1450	43/43	0.98	0.18	56,59,62,68	0
2	HEM	C	1450	43/43	0.98	0.20	60,62,68,71	0
2	HEM	D	1450	43/43	0.98	0.19	50,52,55,59	0

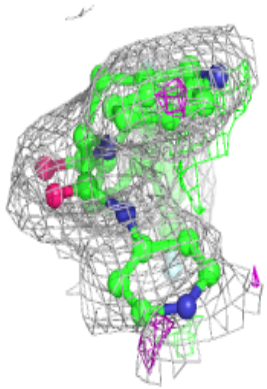
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TU1 B 1460:

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

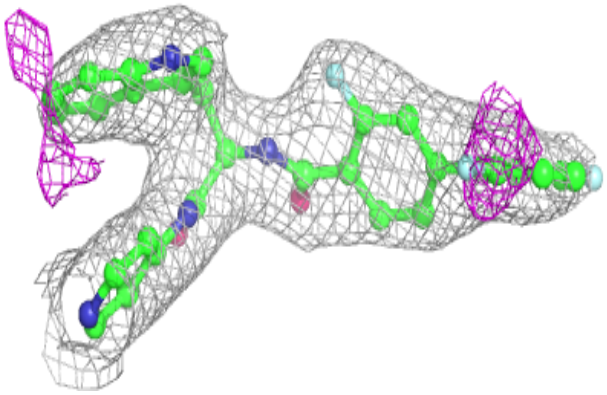


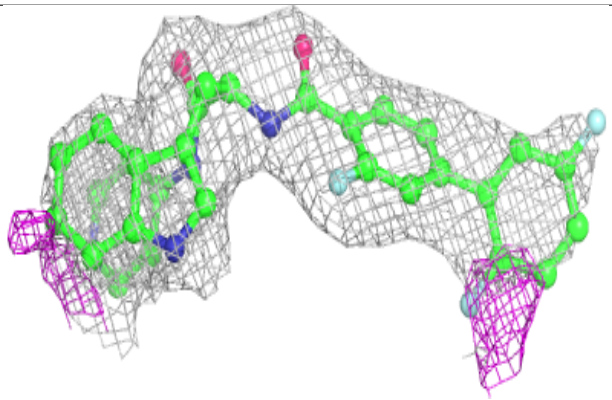


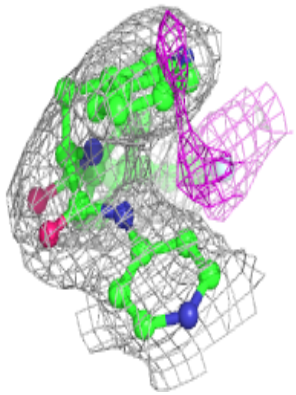


Electron density around TU1 A 1460:

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

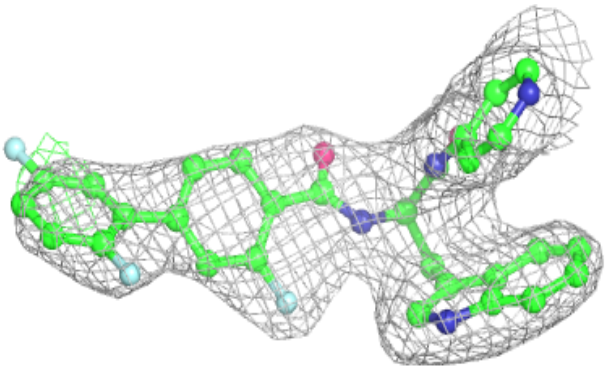


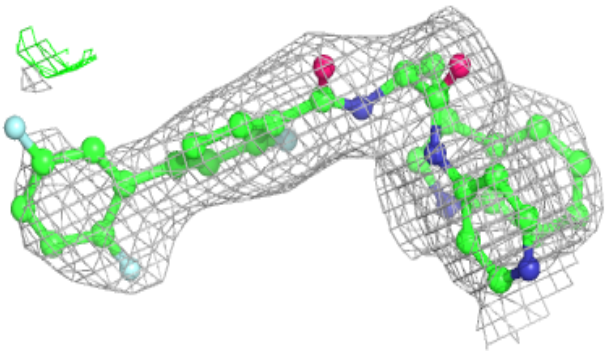


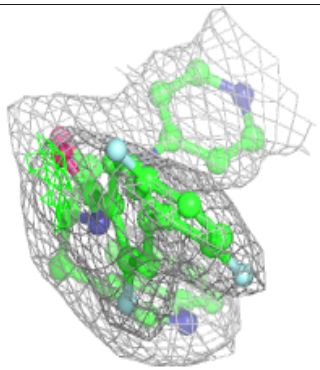


Electron density around TU1 C 1460:

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

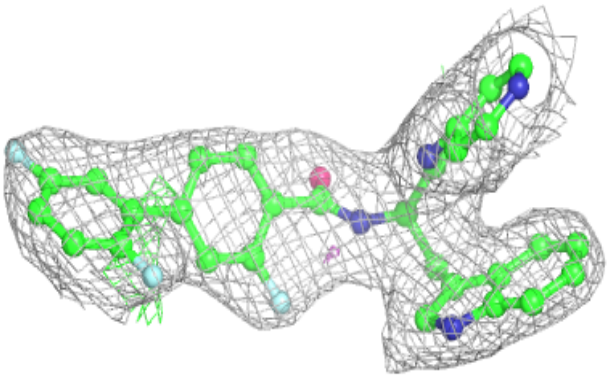


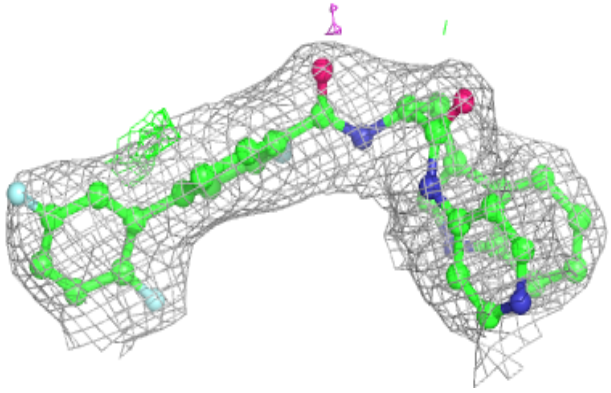


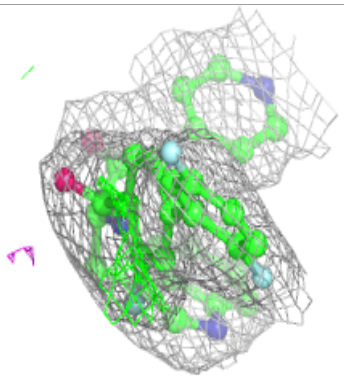


Electron density around TU1 D 1460:

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

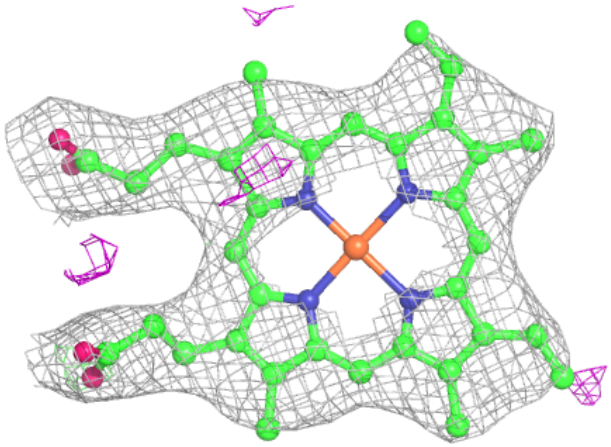


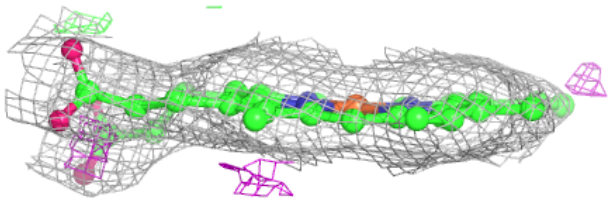


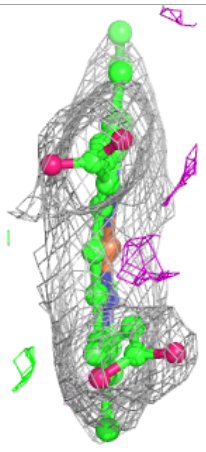


Electron density around HEM A 1450:

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

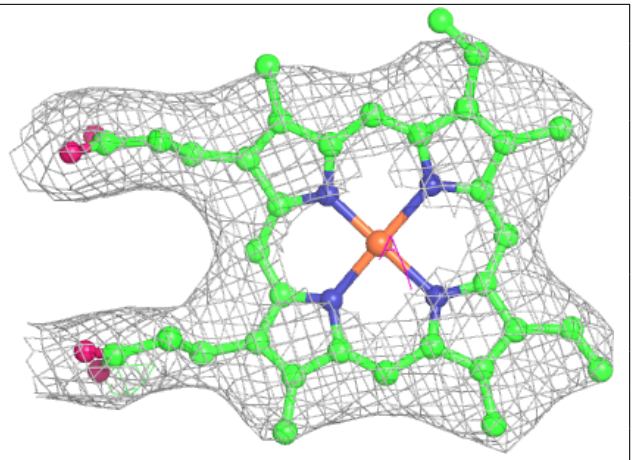


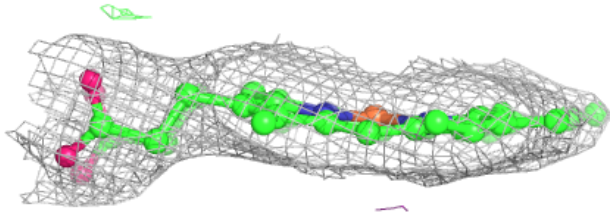


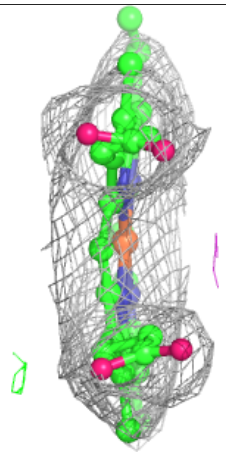


Electron density around HEM B 1450:

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

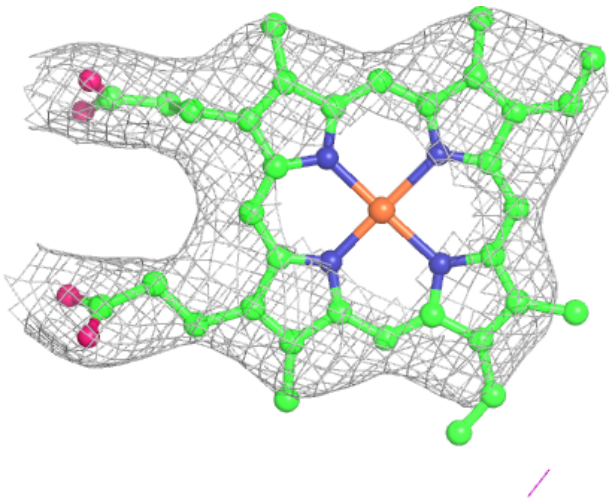


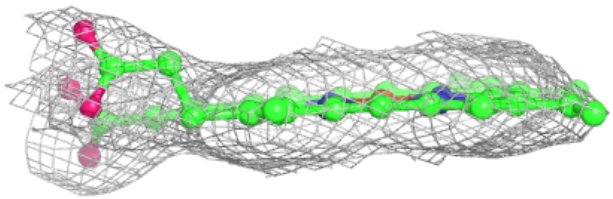


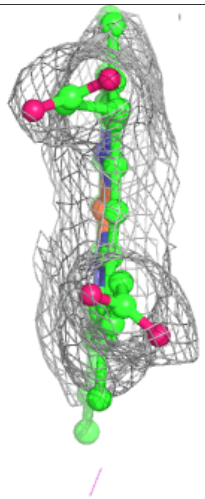


Electron density around HEM C 1450:

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

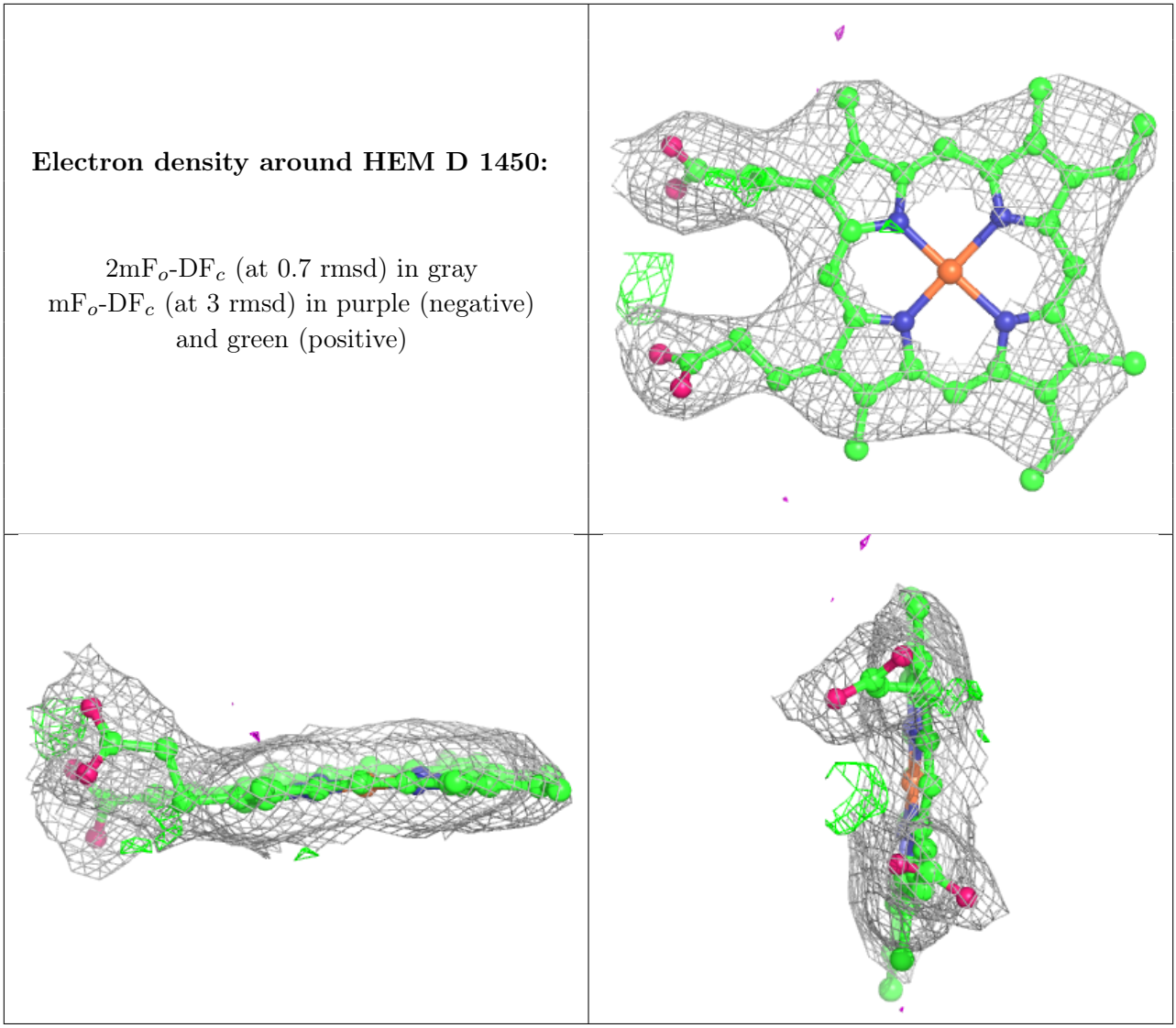






Electron density around HEM D 1450:

$2mF_o$-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.