Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2026 – 08:36 pm BST

PDB ID	:	2UVN / pdb_00002uvn
Title	:	Crystal structure of econazole-bound CYP130 from Mycobacterium tuberculosis
Authors	:	Podust, L.M.; Ortiz de Montellano, P.R.
Deposited on	:	2007-03-12
Resolution	:	3.00 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:

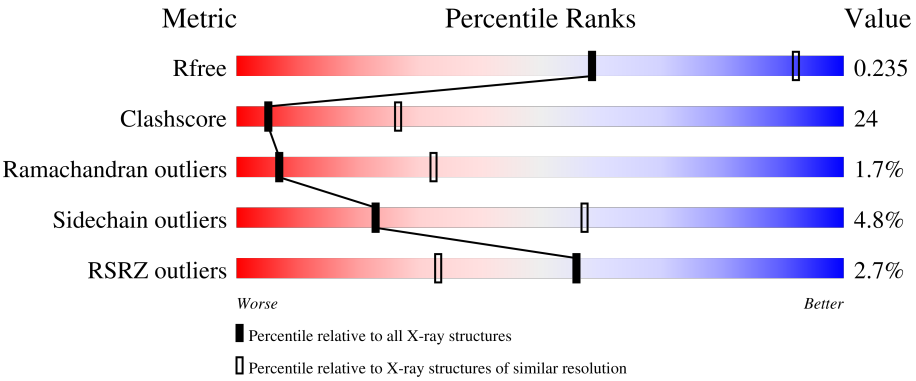
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	414	3% 52% 40%
1	B	414	2% 52% 37% 5% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6364 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.

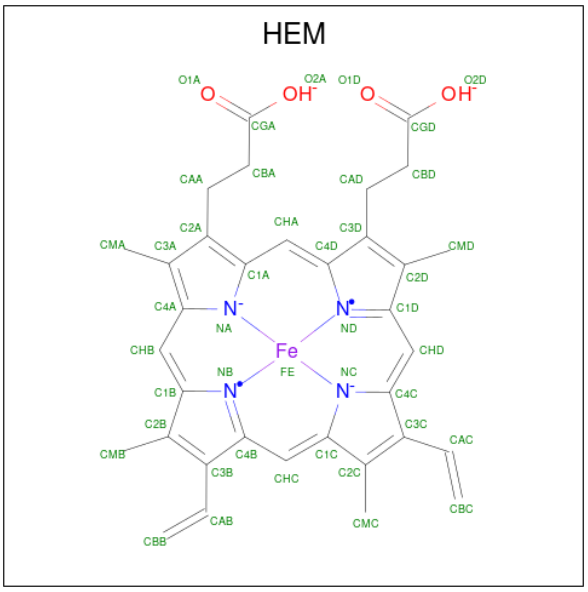
- Molecule 1 is a protein called CYTOCHROME P450 130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3087	1935	559	578	15			
1	B	392	Total	C	N	O	S	0	0	1
			3032	1905	548	564	15			

There are 18 discrepancies between the modelled and reference sequences:

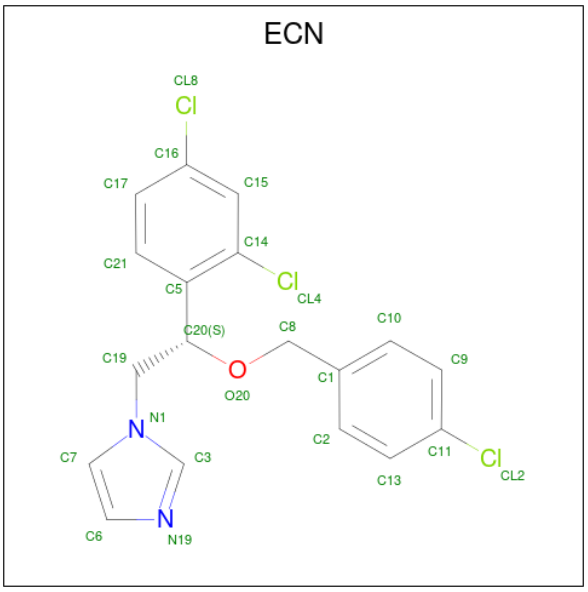
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP Q11062
A	-5	HIS	-	expression tag	UNP Q11062
A	-4	HIS	-	expression tag	UNP Q11062
A	-3	HIS	-	expression tag	UNP Q11062
A	-2	HIS	-	expression tag	UNP Q11062
A	-1	HIS	-	expression tag	UNP Q11062
A	0	HIS	-	expression tag	UNP Q11062
A	406	SER	-	expression tag	UNP Q11062
A	407	ARG	-	expression tag	UNP Q11062
B	-6	MET	-	expression tag	UNP Q11062
B	-5	HIS	-	expression tag	UNP Q11062
B	-4	HIS	-	expression tag	UNP Q11062
B	-3	HIS	-	expression tag	UNP Q11062
B	-2	HIS	-	expression tag	UNP Q11062
B	-1	HIS	-	expression tag	UNP Q11062
B	0	HIS	-	expression tag	UNP Q11062
B	406	SER	-	expression tag	UNP Q11062
B	407	ARG	-	expression tag	UNP Q11062

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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		

- Molecule 3 is 1-[(2S)-2-[(4-CHLOROBENZYL)OXY]-2-(2,4-DICHLOROPHENYL)ETHYL]-1H-IMIDAZOLE (CCD ID: ECN) (formula: $C_{18}H_{15}Cl_3N_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			24	18	3	2	1		

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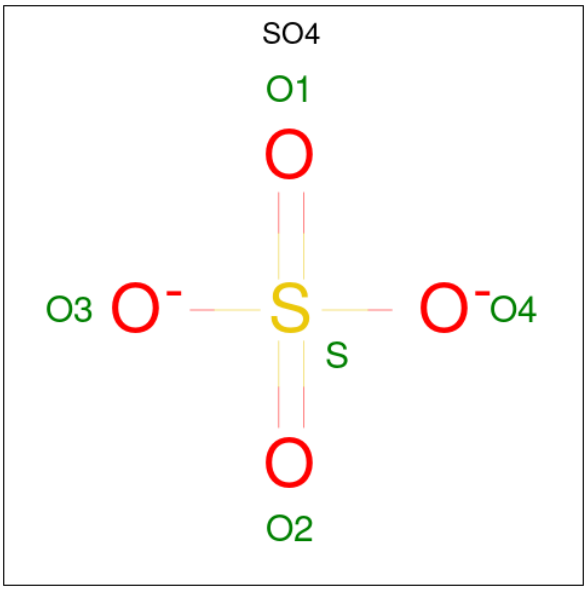
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			24	18	3	2	1		

- Molecule 4 is FLUORIDE ION (CCD ID: F) (formula: F).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	F	0	0
			4	4		
4	B	10	Total	F	0	0
			10	10		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	42	Total O 42 42	0	0
6	B	35	Total O 35 35	0	0

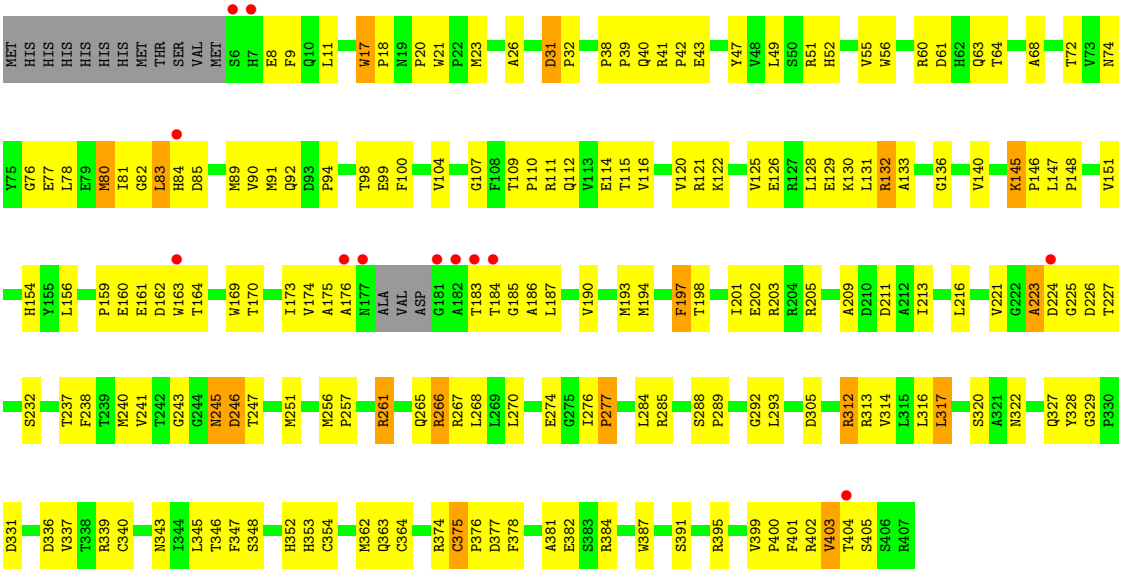
3 Residue-property plots (i)

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: CYTOCHROME P450 130

Chain A:

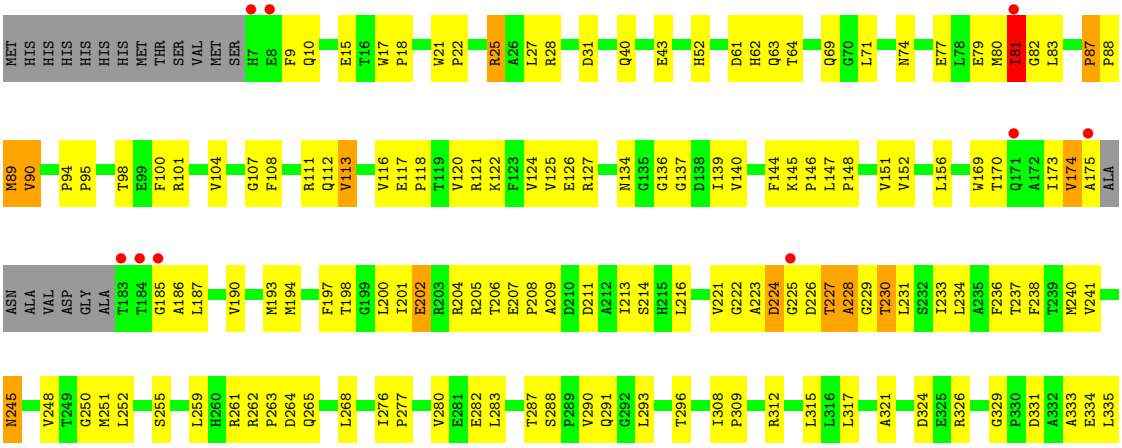




• Molecule 1: CYTOCHROME P450 130

Chain B:






D336
V337
T338
R339
C340
P341
R342
F347
A351
H352
H353
C354
A359
A360
Q363
C364
R365
L368
R374
C375
P376
D377
A381
E382
W387
R394
R395
P396
F401
R402
V403
T404
S405
SER
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.68Å 130.68Å 229.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.67 – 3.00 49.67 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.3 (49.67-3.00) 90.0 (49.67-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.16 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.200 , 0.234 0.202 , 0.235	Depositor DCC
R_{free} test set	4624 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6364	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: ECN, F, HEM, SO4

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	0.46	0/3161	1.00	19/4309 (0.4%)
1	B	0.47	1/3106 (0.0%)	1.01	15/4237 (0.4%)
All	All	0.46	1/6267 (0.0%)	1.00	34/8546 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	THR	C-N	-5.39	1.25	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	GLY	N-CA-C	-8.32	105.51	114.67
1	B	403	VAL	N-CA-C	7.88	114.64	106.21
1	B	329	GLY	CA-C-N	6.86	126.37	119.24
1	B	329	GLY	C-N-CA	6.86	126.37	119.24
1	A	247	THR	N-CA-C	-6.66	103.19	112.45
1	A	94	PRO	N-CA-C	-6.52	104.21	110.47
1	B	31	ASP	CA-C-N	6.29	125.78	119.24
1	B	31	ASP	C-N-CA	6.29	125.78	119.24
1	B	227	THR	N-CA-C	-6.17	97.66	110.80
1	B	334	GLU	N-CA-C	6.15	119.06	109.52
1	B	365	ARG	N-CA-C	-6.04	104.61	111.07
1	A	340	CYS	CA-C-N	5.99	126.30	119.83
1	A	340	CYS	C-N-CA	5.99	126.30	119.83
1	A	198	THR	N-CA-C	-5.92	104.90	111.71
1	A	31	ASP	CA-C-N	5.87	126.28	119.47
1	A	31	ASP	C-N-CA	5.87	126.28	119.47
1	A	329	GLY	CA-C-N	5.67	125.78	119.32
1	A	329	GLY	C-N-CA	5.67	125.78	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	ASP	N-CA-C	5.59	119.73	113.02
1	A	98	THR	N-CA-C	5.56	117.34	111.28
1	A	375	CYS	CA-C-N	5.51	126.73	119.84
1	A	375	CYS	C-N-CA	5.51	126.73	119.84
1	B	90	VAL	N-CA-C	5.50	116.05	108.12
1	B	403	VAL	CB-CA-C	-5.48	107.08	113.22
1	A	328	TYR	N-CA-C	5.47	119.94	112.88
1	A	243	GLY	N-CA-C	5.46	119.28	112.73
1	B	185	GLY	N-CA-C	-5.43	106.33	115.62
1	B	87	PRO	CA-C-N	5.34	126.52	119.84
1	B	87	PRO	C-N-CA	5.34	126.52	119.84
1	B	225	GLY	N-CA-C	-5.33	106.06	114.10
1	A	354	CYS	N-CA-C	5.30	118.16	110.42
1	A	197	PHE	N-CA-C	5.12	116.86	111.28
1	A	132	ARG	N-CA-C	-5.08	105.92	111.82
1	B	351	ALA	N-CA-C	5.06	118.55	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3087	0	3016	159	0
1	B	3032	0	2960	161	0
2	A	43	0	30	6	0
2	B	43	0	30	6	0
3	A	24	0	15	0	0
3	B	24	0	15	0	0
4	A	4	0	0	0	0
4	B	10	0	0	0	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	42	0	0	1	0
6	B	35	0	0	3	0
All	All	6364	0	6066	301	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 24.

All (301) 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:A:312:ARG:HA	1:A:312:ARG:HH11	1.16	1.09
1:A:83:LEU:HD12	1:B:229:GLY:HA2	1.41	1.03
1:A:246:ASP:HB2	1:A:395:ARG:HD3	1.47	0.95
1:B:227:THR:H	1:B:230:THR:HG23	1.38	0.88
1:B:228:ALA:H	1:B:231:LEU:HD13	1.37	0.87
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.38	0.86
1:A:240:MET:HE1	2:A:1408:HEM:HHD	1.57	0.86
1:A:312:ARG:HA	1:A:312:ARG:NH1	1.91	0.84
1:A:84:HIS:HA	1:B:226:ASP:OD2	1.78	0.84
1:B:240:MET:HE1	2:B:1405:HEM:HHD	1.60	0.82
1:A:120:VAL:HG21	1:A:362:MET:HE1	1.61	0.81
1:A:265:GLN:NE2	1:A:337:VAL:HG22	1.97	0.80
1:A:99:GLU:HG2	1:B:81:ILE:HG13	1.62	0.80
1:A:194:MET:HG2	1:B:194:MET:HB3	1.63	0.79
1:A:221:VAL:HG11	1:B:80:MET:HE2	1.63	0.78
1:A:72:THR:O	1:A:313:ARG:HD3	1.85	0.77
1:A:91:MET:HE2	1:A:91:MET:HA	1.69	0.75
1:A:145:LYS:HE3	1:A:145:LYS:O	1.87	0.74
1:B:222:GLY:HA2	1:B:230:THR:HG22	1.69	0.74
1:B:233:ILE:O	1:B:237:THR:HG23	1.88	0.73
1:B:227:THR:O	1:B:229:GLY:N	2.20	0.73
1:B:228:ALA:N	1:B:231:LEU:HD13	2.04	0.72
1:B:27:LEU:HB3	6:B:2006:HOH:O	1.90	0.71
1:A:266:ARG:HD3	1:A:270:LEU:HD11	1.73	0.70
1:A:122:LYS:O	1:A:126:GLU:HG3	1.91	0.70
1:A:145:LYS:NZ	1:A:174:VAL:HG11	2.06	0.69
1:A:111:ARG:O	1:A:115:THR:HG22	1.92	0.69
1:A:403:VAL:C	1:A:405:SER:H	2.02	0.68
1:B:193:MET:HE1	1:B:241:VAL:HG21	1.75	0.68
1:B:207:GLU:N	1:B:208:PRO:HD3	2.09	0.67
1:A:375:CYS:N	1:A:376:PRO:HD3	2.08	0.67
1:B:264:ASP:O	1:B:268:LEU:HD13	1.95	0.67
1:B:120:VAL:HG13	1:B:147:LEU:HD11	1.78	0.66
1:B:226:ASP:OD1	1:B:229:GLY:HA3	1.95	0.66
1:B:227:THR:N	1:B:230:THR:HG23	2.10	0.65
1:B:265:GLN:NE2	1:B:337:VAL:H	1.94	0.65
1:A:213:ILE:HD11	1:A:237:THR:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LYS:O	1:B:126:GLU:HG3	1.97	0.65
1:A:261:ARG:NH1	1:A:382:GLU:OE2	2.30	0.65
1:A:378:PHE:HB2	1:A:401:PHE:CE1	2.32	0.65
1:A:40:GLN:C	1:A:42:PRO:HD3	2.22	0.64
1:A:213:ILE:HD11	1:A:237:THR:HG22	1.80	0.64
1:B:89:MET:HG2	1:B:90:VAL:N	2.11	0.64
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.80	0.64
1:A:8:GLU:HA	1:A:8:GLU:OE1	1.98	0.63
1:A:183:THR:O	1:A:186:ALA:HB3	1.99	0.63
1:A:148:PRO:HA	1:A:363:GLN:HE22	1.64	0.62
1:A:145:LYS:HZ3	1:A:174:VAL:HG11	1.63	0.62
1:A:129:GLU:OE1	1:A:132:ARG:HD3	2.00	0.62
1:A:240:MET:HE3	2:A:1408:HEM:HAC	1.81	0.62
1:A:374:ARG:C	1:A:376:PRO:HD3	2.25	0.61
1:B:251:MET:SD	1:B:364:CYS:SG	2.94	0.61
1:A:240:MET:HE1	2:A:1408:HEM:CHD	2.28	0.61
1:A:197:PHE:O	1:A:201:ILE:HG13	2.01	0.61
1:B:237:THR:O	1:B:241:VAL:HG23	2.01	0.60
1:A:209:ALA:HB3	1:A:211:ASP:OD1	2.01	0.60
1:B:81:ILE:HG22	1:B:82:GLY:N	2.17	0.60
1:B:197:PHE:O	1:B:201:ILE:HG13	2.02	0.60
1:A:312:ARG:HH11	1:A:312:ARG:CA	2.04	0.59
1:B:360:ALA:O	1:B:364:CYS:SG	2.60	0.59
1:B:121:ARG:O	1:B:125:VAL:HG23	2.02	0.59
1:B:230:THR:O	1:B:234:LEU:HG	2.02	0.59
1:A:55:VAL:HG13	1:A:316:LEU:HB3	1.84	0.59
1:A:99:GLU:HG2	1:B:81:ILE:CG1	2.30	0.59
1:B:200:LEU:O	1:B:204:ARG:HG2	2.03	0.59
1:B:250:GLY:CA	1:B:395:ARG:HB3	2.33	0.58
1:A:159:PRO:HG2	1:A:203:ARG:NH1	2.18	0.58
1:B:52:HIS:HA	1:B:321:ALA:HB1	1.84	0.58
1:B:100:PHE:CZ	1:B:104:VAL:HG21	2.38	0.58
1:A:160:GLU:HA	1:A:163:TRP:CD1	2.39	0.58
1:A:381:ALA:HB3	1:A:400:PRO:HB2	1.84	0.58
1:A:80:MET:HE3	1:B:216:LEU:HD13	1.86	0.58
1:A:267:ARG:HA	1:A:270:LEU:HD12	1.86	0.58
1:B:227:THR:H	1:B:230:THR:CG2	2.12	0.57
1:B:108:PHE:HE1	2:B:1405:HEM:HAC	1.68	0.57
1:A:89:MET:HG2	1:A:91:MET:HE3	1.85	0.57
1:B:174:VAL:HG12	1:B:174:VAL:O	2.04	0.57
1:A:145:LYS:H	1:A:146:PRO:HD2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:MET:SD	1:A:364:CYS:HB2	2.44	0.56
1:A:240:MET:CE	2:A:1408:HEM:HAC	2.35	0.56
1:A:18:PRO:HG3	1:A:387:TRP:CD1	2.40	0.56
1:B:61:ASP:OD2	1:B:64:THR:HB	2.06	0.56
1:A:265:GLN:HE21	1:A:337:VAL:HG22	1.71	0.56
1:A:49:LEU:HD12	1:A:316:LEU:CD2	2.36	0.56
1:A:289:PRO:HB2	2:A:1408:HEM:HMB2	1.88	0.56
1:B:193:MET:CE	1:B:241:VAL:HG21	2.36	0.55
1:A:202:GLU:HA	1:A:205:ARG:HD2	1.88	0.55
1:B:204:ARG:HD2	1:B:214:SER:OG	2.06	0.55
1:B:223:ALA:O	1:B:224:ASP:HB3	2.07	0.55
1:B:326:ARG:HH11	1:B:326:ARG:HG3	1.71	0.55
1:A:284:LEU:HD22	1:A:346:THR:HG21	1.89	0.55
1:A:40:GLN:CD	1:A:40:GLN:H	2.15	0.54
1:A:265:GLN:HE22	1:A:337:VAL:HG22	1.71	0.54
1:B:25:ARG:HG2	1:B:25:ARG:NH1	2.15	0.54
1:B:40:GLN:CD	1:B:40:GLN:H	2.14	0.54
1:A:384:ARG:HB2	1:A:400:PRO:HG2	1.89	0.54
1:A:40:GLN:HG2	1:A:41:ARG:HG2	1.89	0.54
1:A:151:VAL:HG21	1:A:363:GLN:CD	2.32	0.54
1:B:17:TRP:N	1:B:18:PRO:CD	2.71	0.54
1:A:61:ASP:OD2	1:A:64:THR:HB	2.08	0.54
1:A:292:GLY:O	1:A:293:LEU:HD23	2.08	0.54
1:B:251:MET:CE	1:B:364:CYS:SG	2.95	0.54
1:A:39:PRO:HG2	1:A:40:GLN:OE1	2.07	0.54
1:B:259:LEU:HD11	1:B:368:LEU:HD11	1.89	0.54
1:A:187:LEU:HG	1:B:205:ARG:HH21	1.72	0.53
1:B:120:VAL:O	1:B:124:VAL:HG23	2.07	0.53
1:A:8:GLU:HG3	1:A:9:PHE:H	1.73	0.53
1:A:80:MET:HG3	1:B:100:PHE:CE1	2.43	0.53
1:B:359:ALA:O	1:B:363:GLN:HG3	2.09	0.53
1:B:347:PHE:HB3	1:B:354:CYS:HB3	1.90	0.53
1:A:227:THR:HG21	1:B:238:PHE:CE2	2.44	0.53
1:B:15:GLU:CD	1:B:15:GLU:H	2.17	0.53
1:B:145:LYS:HB3	1:B:146:PRO:HD3	1.90	0.53
1:B:201:ILE:HD11	1:B:233:ILE:HG21	1.90	0.53
1:A:38:PRO:HB3	1:A:40:GLN:NE2	2.24	0.53
1:B:62:HIS:CD2	1:B:94:PRO:HD2	2.44	0.53
1:A:17:TRP:HA	1:A:17:TRP:CE3	2.44	0.52
1:A:276:ILE:HB	1:A:277:PRO:HD3	1.90	0.52
1:A:125:VAL:HG13	1:A:374:ARG:CZ	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:MET:O	1:B:198:THR:HG23	2.10	0.52
1:A:193:MET:CE	1:A:241:VAL:HG11	2.40	0.52
1:B:117:GLU:HB3	1:B:118:PRO:HD3	1.91	0.52
1:B:25:ARG:HH11	1:B:25:ARG:CG	2.13	0.52
1:B:79:GLU:OE1	1:B:81:ILE:HD12	2.10	0.52
1:B:107:GLY:O	1:B:112:GLN:HG2	2.09	0.52
1:B:248:VAL:HA	1:B:251:MET:HE2	1.92	0.52
1:A:375:CYS:HB3	1:A:403:VAL:HG13	1.91	0.51
1:A:107:GLY:O	1:A:112:GLN:HG2	2.10	0.51
1:A:170:THR:O	1:A:174:VAL:HG23	2.11	0.51
1:A:187:LEU:CD1	1:B:205:ARG:HH21	2.24	0.51
1:B:61:ASP:OD1	1:B:63:GLN:HG2	2.10	0.50
1:B:145:LYS:NZ	1:B:245:ASN:HB3	2.26	0.50
1:B:17:TRP:CZ3	1:B:291:GLN:HG3	2.46	0.50
1:A:81:ILE:HD12	1:A:81:ILE:N	2.26	0.50
1:A:82:GLY:O	1:A:83:LEU:C	2.54	0.50
1:A:404:THR:HG22	1:A:404:THR:O	2.10	0.50
1:B:173:ILE:C	1:B:175:ALA:H	2.20	0.49
1:B:122:LYS:HE2	1:B:126:GLU:OE2	2.11	0.49
1:B:277:PRO:HD2	6:B:2027:HOH:O	2.12	0.49
1:A:223:ALA:O	1:A:225:GLY:N	2.45	0.49
1:A:17:TRP:N	1:A:18:PRO:CD	2.76	0.49
1:A:115:THR:HG23	1:A:154:HIS:CE1	2.47	0.49
1:A:232:SER:OG	1:B:80:MET:HE3	2.12	0.49
1:A:403:VAL:C	1:A:405:SER:N	2.71	0.49
1:B:117:GLU:HG2	1:B:121:ARG:HH12	1.77	0.49
1:B:339:ARG:O	1:B:340:CYS:HB2	2.12	0.49
1:A:131:LEU:HD13	1:A:401:PHE:CD2	2.46	0.49
1:B:137:GLY:O	1:B:401:PHE:HB3	2.13	0.49
1:B:194:MET:HA	1:B:194:MET:HE2	1.94	0.49
1:B:113:VAL:HG22	6:B:2020:HOH:O	2.13	0.49
1:A:40:GLN:O	1:A:42:PRO:HD3	2.13	0.48
1:B:261:ARG:C	1:B:263:PRO:HD3	2.37	0.48
1:A:184:THR:HB	1:B:202:GLU:OE2	2.13	0.48
1:A:274:GLU:O	1:A:277:PRO:HD2	2.12	0.48
1:B:139:ILE:HB	1:B:401:PHE:HB2	1.95	0.48
1:A:130:LYS:O	1:A:133:ALA:HB3	2.13	0.48
1:A:285:ARG:HG2	1:A:322:ASN:HB3	1.95	0.48
1:B:251:MET:HE3	1:B:252:LEU:HG	1.94	0.48
1:B:108:PHE:CE1	2:B:1405:HEM:HAC	2.48	0.48
1:A:120:VAL:HG13	1:A:147:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:TRP:CH2	1:B:291:GLN:HG3	2.49	0.48
1:A:183:THR:OG1	1:B:224:ASP:HA	2.14	0.48
1:B:71:LEU:HD12	1:B:87:PRO:HG3	1.96	0.48
1:A:190:VAL:HG13	1:A:238:PHE:CE2	2.49	0.47
1:A:375:CYS:N	1:A:376:PRO:CD	2.78	0.47
1:B:222:GLY:CA	1:B:230:THR:HG22	2.42	0.47
1:B:326:ARG:HG3	1:B:326:ARG:NH1	2.29	0.47
1:A:83:LEU:O	1:A:85:ASP:N	2.43	0.47
1:A:377:ASP:OD2	1:A:404:THR:HB	2.14	0.47
1:A:156:LEU:HD22	1:A:237:THR:HG22	1.96	0.47
1:B:186:ALA:O	1:B:190:VAL:HG23	2.15	0.47
1:A:331:ASP:CG	1:A:339:ARG:HH22	2.23	0.47
1:B:211:ASP:OD1	1:B:214:SER:OG	2.24	0.47
1:A:384:ARG:HH11	1:A:384:ARG:HB3	1.79	0.47
1:A:23:MET:O	1:A:26:ALA:HB3	2.15	0.46
1:B:89:MET:HB3	1:B:89:MET:HE2	1.68	0.46
1:A:251:MET:CE	1:A:364:CYS:HB2	2.46	0.46
1:A:193:MET:HE3	1:A:241:VAL:HG11	1.98	0.46
1:B:221:VAL:C	1:B:223:ALA:H	2.23	0.46
1:A:194:MET:HG2	1:B:194:MET:CB	2.40	0.46
1:A:20:PRO:HG2	1:A:21:TRP:CZ3	2.51	0.46
1:A:145:LYS:N	1:A:146:PRO:HD2	2.29	0.46
1:A:225:GLY:O	1:A:227:THR:N	2.49	0.46
1:A:32:PRO:HB3	1:A:51:ARG:HD2	1.97	0.46
1:A:174:VAL:HG12	1:A:395:ARG:HH12	1.81	0.46
1:B:15:GLU:CD	1:B:15:GLU:N	2.74	0.46
1:B:402:ARG:O	1:B:402:ARG:HG3	2.15	0.46
1:A:176:ALA:HA	1:A:183:THR:HG22	1.97	0.45
1:A:336:ASP:HB3	1:A:339:ARG:HB2	1.98	0.45
1:A:256:MET:HB2	1:A:257:PRO:CD	2.45	0.45
1:A:305:ASP:OD1	1:A:305:ASP:N	2.47	0.45
1:B:190:VAL:O	1:B:194:MET:HG2	2.16	0.45
1:A:80:MET:HE1	1:B:233:ILE:HA	1.98	0.45
1:A:161:GLU:HG2	1:A:162:ASP:N	2.31	0.45
1:A:47:TYR:HB2	1:A:314:VAL:HG22	1.99	0.45
1:A:74:ASN:ND2	1:A:76:GLY:H	2.15	0.45
1:A:38:PRO:HB3	1:A:40:GLN:HE22	1.80	0.45
1:B:342:ARG:HE	1:B:342:ARG:HA	1.81	0.45
1:B:25:ARG:NH1	1:B:25:ARG:CG	2.74	0.45
1:A:99:GLU:OE2	1:A:99:GLU:HA	2.16	0.45
1:A:241:VAL:O	1:A:245:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:VAL:HB	1:A:405:SER:O	2.16	0.45
1:B:251:MET:HE2	1:B:251:MET:HB3	1.76	0.45
1:B:290:VAL:HG11	2:B:1405:HEM:HMA3	1.98	0.45
1:A:56:TRP:NE1	1:A:60:ARG:HD2	2.32	0.45
1:B:156:LEU:HD22	1:B:213:ILE:HD11	1.98	0.45
1:A:213:ILE:HD11	1:A:237:THR:HG21	1.99	0.44
1:B:80:MET:O	1:B:81:ILE:C	2.60	0.44
1:B:223:ALA:O	1:B:224:ASP:CB	2.65	0.44
1:B:250:GLY:HA2	1:B:396:PRO:HD2	1.98	0.44
1:A:83:LEU:HD12	1:B:229:GLY:CA	2.27	0.44
1:A:121:ARG:O	1:A:125:VAL:HG23	2.18	0.44
1:B:17:TRP:CE3	1:B:394:ARG:HD2	2.53	0.44
1:B:116:VAL:O	1:B:116:VAL:HG22	2.17	0.44
1:B:262:ARG:HG3	1:B:262:ARG:HH11	1.83	0.44
1:B:28:ARG:NE	1:B:324:ASP:HA	2.33	0.44
1:A:169:TRP:O	1:A:173:ILE:HG13	2.17	0.44
1:A:246:ASP:HB2	1:A:395:ARG:CD	2.34	0.44
1:A:347:PHE:O	1:A:348:SER:HB3	2.18	0.44
1:A:109:THR:O	1:A:112:GLN:HB2	2.18	0.44
1:B:336:ASP:O	1:B:338:THR:N	2.50	0.44
1:B:21:TRP:HB2	1:B:22:PRO:HD3	2.00	0.43
1:B:87:PRO:C	1:B:89:MET:H	2.26	0.43
1:B:226:ASP:C	1:B:227:THR:O	2.52	0.43
1:B:352:HIS:O	1:B:353:HIS:C	2.61	0.43
1:A:74:ASN:O	1:A:77:GLU:HB2	2.18	0.43
1:B:101:ARG:NH1	2:B:1405:HEM:O2D	2.46	0.43
1:B:236:PHE:O	1:B:240:MET:HG2	2.18	0.43
1:B:250:GLY:HA3	1:B:395:ARG:HB3	1.98	0.43
1:B:282:GLU:HG2	1:B:335:LEU:HD12	2.00	0.43
1:A:8:GLU:HG3	1:A:9:PHE:N	2.33	0.43
1:A:352:HIS:O	1:A:353:HIS:C	2.60	0.43
1:B:276:ILE:O	1:B:280:VAL:HG23	2.19	0.43
1:B:206:THR:C	1:B:208:PRO:HD3	2.43	0.43
1:B:315:LEU:HG	1:B:317:LEU:CD1	2.48	0.43
1:B:144:PHE:CD1	1:B:252:LEU:HB3	2.54	0.43
1:B:336:ASP:C	1:B:338:THR:N	2.76	0.43
1:A:116:VAL:O	1:A:120:VAL:HG23	2.19	0.43
1:A:402:ARG:HG2	1:A:402:ARG:HH11	1.84	0.43
1:A:100:PHE:CE1	1:A:104:VAL:HG21	2.54	0.43
1:A:403:VAL:O	1:A:405:SER:N	2.50	0.43
1:B:116:VAL:HG22	1:B:120:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:VAL:HG13	1:B:147:LEU:CD1	2.46	0.43
1:A:187:LEU:CG	1:B:205:ARG:HH21	2.32	0.42
1:A:288:SER:O	1:A:289:PRO:C	2.62	0.42
1:A:20:PRO:HG2	1:A:21:TRP:CE3	2.54	0.42
1:B:336:ASP:OD1	1:B:338:THR:HG23	2.19	0.42
1:A:68:ALA:HB2	1:A:92:GLN:HA	2.00	0.42
1:A:317:LEU:HB3	1:A:320:SER:HB3	2.01	0.42
1:A:110:PRO:O	1:A:114:GLU:HG3	2.19	0.42
1:A:140:VAL:HG23	1:A:399:VAL:HB	2.01	0.42
1:B:63:GLN:H	1:B:63:GLN:CD	2.28	0.42
1:B:79:GLU:CD	1:B:81:ILE:HD12	2.45	0.42
1:A:63:GLN:HG3	6:A:2013:HOH:O	2.20	0.42
1:A:90:VAL:O	1:A:90:VAL:HG13	2.19	0.42
1:A:173:ILE:HD12	1:A:193:MET:CE	2.49	0.42
1:A:327:GLN:HE22	1:A:343:ASN:HD22	1.66	0.42
1:B:120:VAL:CG1	1:B:147:LEU:HD11	2.47	0.42
1:B:74:ASN:ND2	1:B:77:GLU:HA	2.35	0.42
1:B:111:ARG:HH11	1:B:111:ARG:HG2	1.84	0.42
1:B:145:LYS:HZ1	1:B:245:ASN:HB3	1.85	0.42
1:B:251:MET:CE	1:B:364:CYS:HG	2.30	0.42
1:A:129:GLU:OE2	1:A:374:ARG:HD3	2.20	0.42
1:B:121:ARG:HB2	1:B:121:ARG:NH1	2.35	0.42
1:B:148:PRO:O	1:B:152:VAL:HG23	2.20	0.42
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.94	0.42
1:B:125:VAL:HG13	1:B:374:ARG:CZ	2.50	0.42
1:B:140:VAL:HA	1:B:144:PHE:HB2	2.02	0.42
1:B:259:LEU:HD23	1:B:259:LEU:HA	1.81	0.42
1:B:287:THR:O	1:B:288:SER:C	2.62	0.42
1:A:55:VAL:HG12	1:A:345:LEU:HD23	2.02	0.41
1:A:160:GLU:O	1:A:163:TRP:HB2	2.20	0.41
1:A:175:ALA:O	1:A:176:ALA:C	2.63	0.41
1:B:375:CYS:HB3	1:B:403:VAL:HG13	2.02	0.41
1:A:173:ILE:HD12	1:A:193:MET:HE2	2.02	0.41
1:B:100:PHE:CE1	1:B:104:VAL:HG21	2.55	0.41
1:B:381:ALA:O	1:B:382:GLU:C	2.61	0.41
1:A:104:VAL:HG23	1:A:216:LEU:HD21	2.01	0.41
1:A:261:ARG:HH11	1:A:382:GLU:CD	2.28	0.41
1:B:18:PRO:HG3	1:B:387:TRP:CD1	2.55	0.41
1:B:151:VAL:HG21	1:B:363:GLN:CD	2.45	0.41
1:B:169:TRP:O	1:B:170:THR:C	2.63	0.41
1:B:255:SER:HB3	1:B:283:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASP:C	1:B:333:ALA:N	2.78	0.41
2:A:1408:HEM:CMA	2:A:1408:HEM:HBA2	2.50	0.41
1:B:95:PRO:O	1:B:98:THR:HB	2.21	0.41
1:B:127:ARG:HH11	1:B:127:ARG:HG3	1.86	0.41
1:A:184:THR:HG22	1:B:202:GLU:OE1	2.21	0.41
1:B:265:GLN:HE21	1:B:337:VAL:H	1.66	0.41
1:A:31:ASP:N	1:A:32:PRO:HD3	2.36	0.41
1:B:251:MET:HE1	1:B:364:CYS:SG	2.60	0.41
1:A:52:HIS:CD2	1:A:327:GLN:HG2	2.56	0.41
1:B:293:LEU:HD12	2:B:1405:HEM:HBA2	2.03	0.41
1:A:11:LEU:HB3	1:A:391:SER:OG	2.22	0.40
1:B:9:PHE:CG	1:B:10:GLN:N	2.89	0.40
1:A:80:MET:HE3	1:B:216:LEU:CD1	2.51	0.40
1:A:136:GLY:HA2	1:A:402:ARG:HA	2.02	0.40
1:B:134:ASN:C	1:B:136:GLY:H	2.28	0.40
1:B:69:GLN:HG3	1:B:296:THR:HG21	2.02	0.40
1:B:308:ILE:HA	1:B:309:PRO:HD3	1.95	0.40
1:B:127:ARG:HD3	1:B:127:ARG:HA	1.84	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	395/414 (95%)	355 (90%)	36 (9%)	4 (1%)	12 45
1	B	388/414 (94%)	346 (89%)	33 (8%)	9 (2%)	5 25
All	All	783/828 (95%)	701 (90%)	69 (9%)	13 (2%)	7 32

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	224	ASP
1	A	226	ASP
1	B	224	ASP
1	A	223	ALA
1	B	81	ILE
1	B	404	THR
1	B	83	LEU
1	B	228	ALA
1	B	337	VAL
1	B	88	PRO
1	B	209	ALA
1	B	174	VAL

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	327/344 (95%)	313 (96%)	14 (4%)	26	60
1	B	321/344 (93%)	304 (95%)	17 (5%)	20	54
All	All	648/688 (94%)	617 (95%)	31 (5%)	23	57

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	TRP
1	A	43	GLU
1	A	78	LEU
1	A	80	MET
1	A	145	LYS
1	A	164	THR
1	A	245	ASN
1	A	261	ARG
1	A	266	ARG
1	A	268	LEU
1	A	277	PRO

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Mol	Chain	Res	Type
1	A	312	ARG
1	A	317	LEU
1	A	403	VAL
1	B	25	ARG
1	B	43	GLU
1	B	81	ILE
1	B	89	MET
1	B	113	VAL
1	B	187	LEU
1	B	202	GLU
1	B	230	THR
1	B	245	ASN
1	B	312	ARG
1	B	338	THR
1	B	342	ARG
1	B	364	CYS
1	B	368	LEU
1	B	377	ASP
1	B	402	ARG
1	B	403	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	74	ASN
1	A	154	HIS
1	A	265	GLN
1	A	343	ASN
1	A	349	HIS
1	A	363	GLN
1	B	40	GLN
1	B	63	GLN
1	B	215	HIS
1	B	245	ASN
1	B	265	GLN
1	B	291	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ECN	B	1406	2	26,26,26	1.69	7 (26%)	35,35,35	1.39	6 (17%)
5	SO4	A	1415	-	4,4,4	0.71	0	6,6,6	0.42	0
5	SO4	A	1413	-	4,4,4	0.59	0	6,6,6	0.36	0
5	SO4	A	1414	-	4,4,4	0.76	0	6,6,6	0.47	0
3	ECN	A	1409	2	26,26,26	1.81	7 (26%)	35,35,35	1.63	6 (17%)
2	HEM	A	1408	3	50,50,50	1.16	5 (10%)	66,82,82	1.06	4 (6%)
2	HEM	B	1405	3	50,50,50	1.12	4 (8%)	66,82,82	1.07	4 (6%)
5	SO4	B	1416	-	4,4,4	0.64	0	6,6,6	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	1405	3	-	4/14/54/54	-
3	ECN	A	1409	2	-	7/13/13/13	0/3/3/3
2	HEM	A	1408	3	-	3/14/54/54	-
3	ECN	B	1406	2	-	7/13/13/13	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1408	HEM	CBC-CAC	3.70	1.48	1.30
3	A	1409	ECN	C13-C2	3.59	1.45	1.38
3	A	1409	ECN	C15-C16	3.47	1.44	1.38
2	B	1405	HEM	CAC-C3C	-3.45	1.38	1.47
3	B	1406	ECN	C14-C5	3.36	1.43	1.39
2	B	1405	HEM	CBB-CAB	3.34	1.46	1.30
3	A	1409	ECN	C13-C11	3.33	1.44	1.38
3	A	1409	ECN	C15-C14	3.10	1.43	1.38
3	B	1406	ECN	C15-C14	3.08	1.43	1.38
3	B	1406	ECN	C13-C2	3.03	1.44	1.38
3	A	1409	ECN	O20-C20	3.02	1.48	1.43
2	A	1408	HEM	CBB-CAB	3.00	1.45	1.30
2	A	1408	HEM	CAC-C3C	-2.86	1.39	1.47
2	B	1405	HEM	CBC-CAC	2.62	1.43	1.30
3	B	1406	ECN	C13-C11	2.61	1.43	1.38
3	B	1406	ECN	C15-C16	2.59	1.42	1.38
3	A	1409	ECN	C21-C5	2.49	1.43	1.39
2	B	1405	HEM	CAB-C3B	-2.47	1.40	1.47
3	A	1409	ECN	C14-C5	2.43	1.42	1.39
2	A	1408	HEM	CAB-C3B	-2.33	1.41	1.47
3	B	1406	ECN	C21-C5	2.14	1.42	1.39
3	B	1406	ECN	O20-C20	2.08	1.47	1.43
2	A	1408	HEM	C4D-C3D	2.02	1.48	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1409	ECN	O20-C20-C19	3.72	113.73	106.33
3	A	1409	ECN	O20-C20-C5	-3.53	106.75	112.08
3	A	1409	ECN	C21-C5-C14	3.24	120.03	116.81
3	A	1409	ECN	C15-C14-C5	-3.06	118.75	122.41
3	B	1406	ECN	O20-C20-C19	3.04	112.38	106.33
3	B	1406	ECN	C15-C14-C5	-2.69	119.20	122.41
3	B	1406	ECN	C21-C5-C14	2.68	119.47	116.81
3	A	1409	ECN	O20-C8-C1	2.53	115.74	109.91
3	A	1409	ECN	C6-N19-C3	2.42	110.08	105.41
2	B	1405	HEM	C2A-C1A-NA	2.38	112.81	110.15
3	B	1406	ECN	O20-C8-C1	2.34	115.30	109.91
2	B	1405	HEM	C4C-NC-C1C	-2.34	103.06	105.35
2	A	1408	HEM	C4A-NA-C1A	-2.33	103.06	105.35
3	B	1406	ECN	C6-N19-C3	2.31	109.87	105.41
2	B	1405	HEM	C4A-NA-C1A	-2.24	103.16	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1405	HEM	C4B-C3B-C2B	-2.19	105.38	107.11
3	B	1406	ECN	O20-C20-C5	-2.17	108.79	112.08
2	A	1408	HEM	C4C-NC-C1C	-2.09	103.30	105.35
2	A	1408	HEM	C4D-ND-C1D	-2.06	102.94	105.07
2	A	1408	HEM	C2D-C1D-ND	2.06	112.35	109.88

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1405	HEM	C2C-C3C-CAC-CBC
3	A	1409	ECN	N1-C19-C20-O20
3	A	1409	ECN	N1-C19-C20-C5
3	A	1409	ECN	C20-C19-N1-C7
3	A	1409	ECN	C20-C19-N1-C3
3	A	1409	ECN	C19-C20-O20-C8
3	A	1409	ECN	C5-C20-O20-C8
3	B	1406	ECN	N1-C19-C20-O20
3	B	1406	ECN	N1-C19-C20-C5
3	B	1406	ECN	C20-C19-N1-C7
3	B	1406	ECN	C20-C19-N1-C3
3	B	1406	ECN	C19-C20-O20-C8
3	B	1406	ECN	C5-C20-O20-C8
2	A	1408	HEM	CAA-CBA-CGA-O1A
2	A	1408	HEM	CAA-CBA-CGA-O2A
3	B	1406	ECN	C1-C8-O20-C20
3	A	1409	ECN	C1-C8-O20-C20
2	B	1405	HEM	CAA-CBA-CGA-O2A
2	B	1405	HEM	CAA-CBA-CGA-O1A
2	B	1405	HEM	C4C-C3C-CAC-CBC
2	A	1408	HEM	C3A-C2A-CAA-CBA

There are no ring outliers.

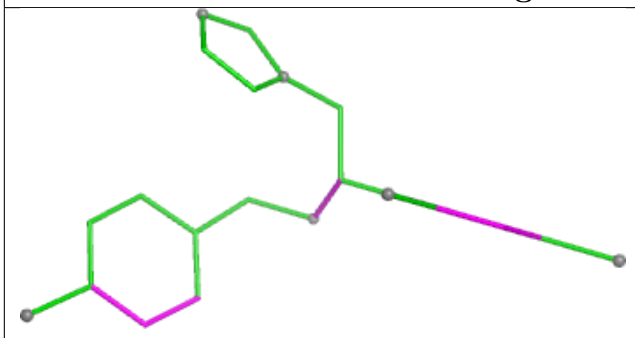
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1408	HEM	6	0
2	B	1405	HEM	6	0

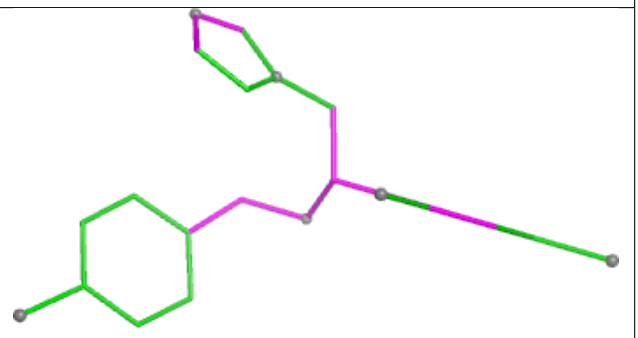
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

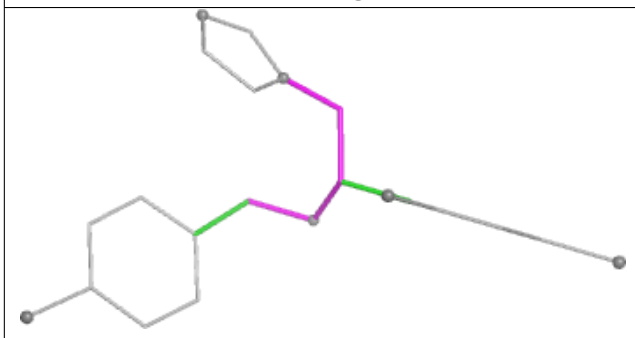
Ligand ECN B 1406



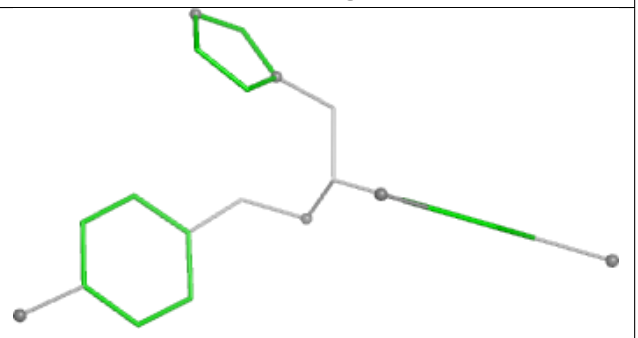
Bond lengths



Bond angles

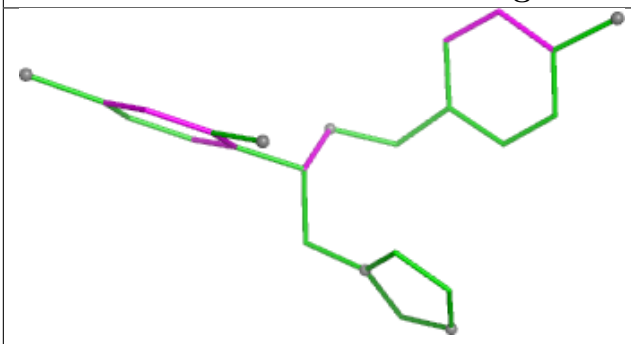


Torsions

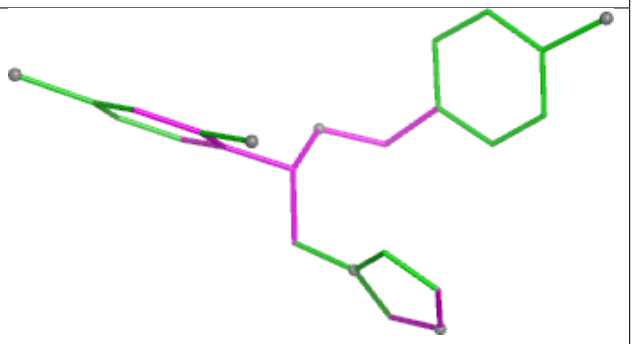


Rings

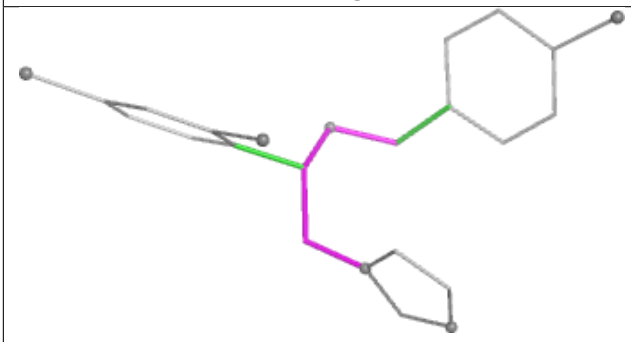
Ligand ECN A 1409



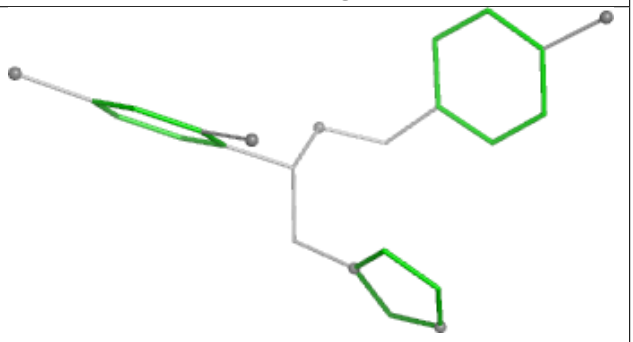
Bond lengths



Bond angles

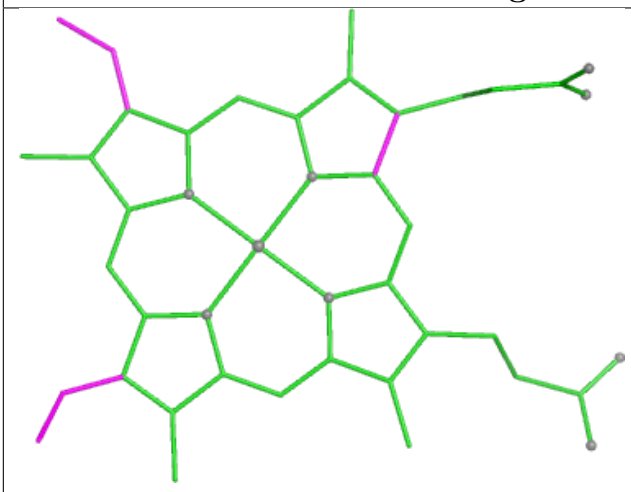


Torsions

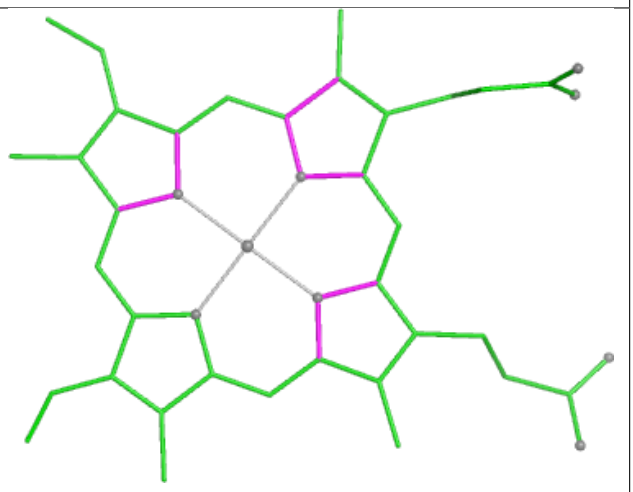


Rings

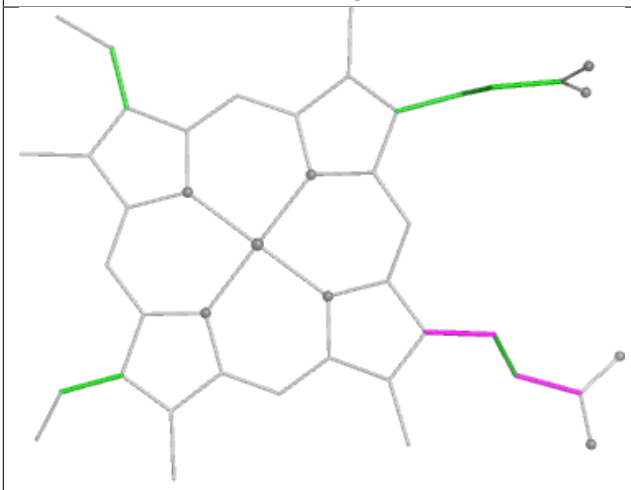
Ligand HEM A 1408



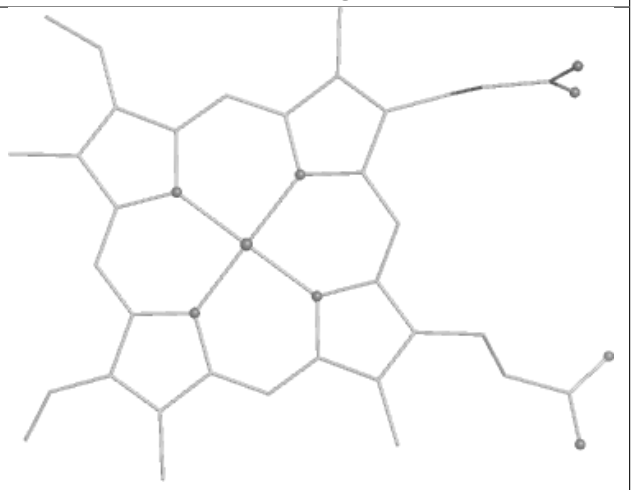
Bond lengths



Bond angles

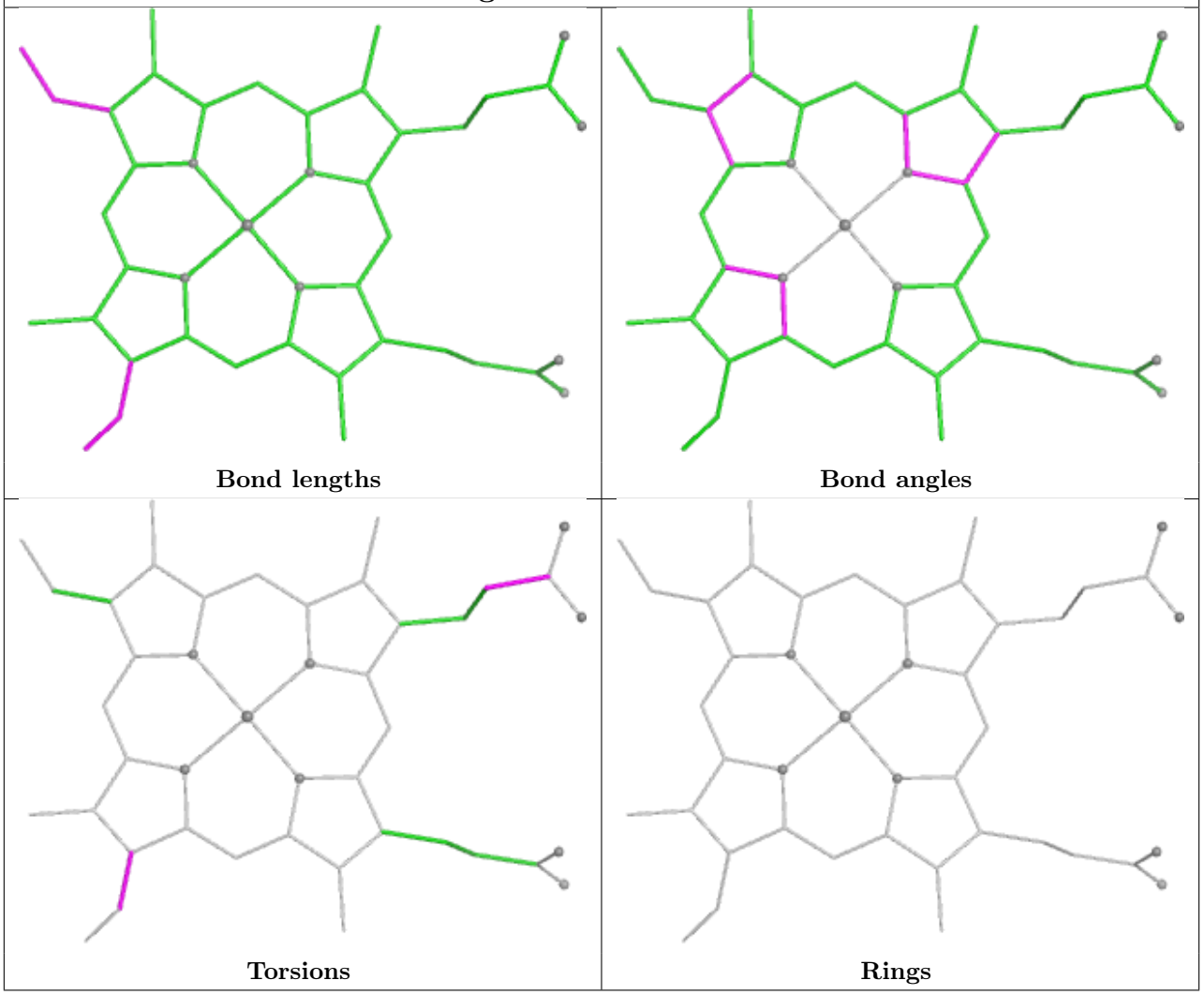


Torsions



Rings

Ligand HEM B 1405



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	399/414 (96%)	-0.13	12 (3%) 52 30	43, 61, 94, 114	0
1	B	392/414 (94%)	-0.06	9 (2%) 61 38	45, 63, 90, 108	0
All	All	791/828 (95%)	-0.10	21 (2%) 56 33	43, 62, 92, 114	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	HIS	4.9
1	B	7	HIS	4.8
1	A	182	ALA	4.8
1	B	175	ALA	4.2
1	A	177	ASN	4.2
1	B	183	THR	4.2
1	A	404	THR	3.6
1	B	81	ILE	3.5
1	B	225	GLY	3.2
1	A	181	GLY	3.2
1	B	8	GLU	3.0
1	A	184	THR	2.8
1	A	6	SER	2.8
1	B	184	THR	2.7
1	A	183	THR	2.6
1	B	185	GLY	2.5
1	A	224	ASP	2.4
1	A	84	HIS	2.2
1	A	163	TRP	2.1
1	A	176	ALA	2.0
1	B	171	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

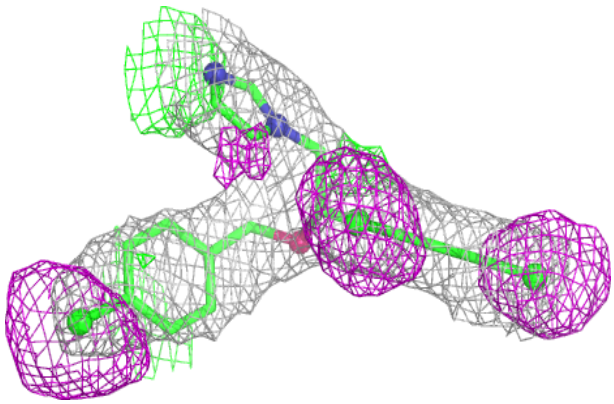
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

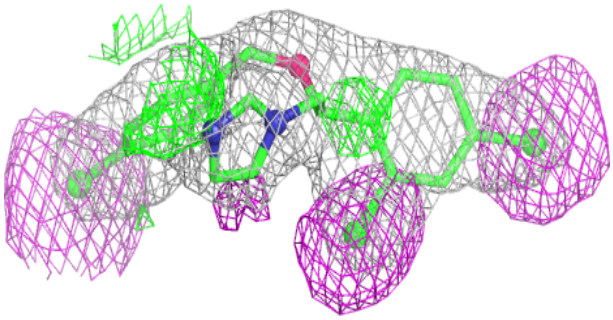
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ECN	B	1406	24/24	0.80	0.20	43,52,60,62	0
5	SO4	A	1415	5/5	0.80	0.14	110,110,110,111	0
3	ECN	A	1409	24/24	0.81	0.18	24,36,46,49	0
4	F	B	1410	1/1	0.82	0.39	53,53,53,53	0
4	F	A	1416	1/1	0.82	0.46	67,67,67,67	0
4	F	B	1408	1/1	0.84	0.33	49,49,49,49	0
4	F	B	1414	1/1	0.86	0.43	57,57,57,57	0
4	F	B	1413	1/1	0.87	0.44	62,62,62,62	0
4	F	A	1411	1/1	0.87	0.37	50,50,50,50	0
4	F	B	1412	1/1	0.87	0.36	47,47,47,47	0
4	F	A	1410	1/1	0.90	0.33	45,45,45,45	0
5	SO4	A	1413	5/5	0.92	0.10	108,108,109,109	0
4	F	B	1417	1/1	0.92	0.33	32,32,32,32	0
5	SO4	B	1416	5/5	0.93	0.15	111,112,112,113	0
4	F	B	1411	1/1	0.95	0.38	37,37,37,37	0
4	F	B	1409	1/1	0.96	0.33	44,44,44,44	0
4	F	B	1407	1/1	0.96	0.18	35,35,35,35	0
4	F	A	1412	1/1	0.96	0.36	49,49,49,49	0
4	F	B	1415	1/1	0.96	0.46	56,56,56,56	0
5	SO4	A	1414	5/5	0.97	0.08	58,60,61,62	0
2	HEM	A	1408	43/43	0.98	0.08	41,47,53,60	0
2	HEM	B	1405	43/43	0.98	0.10	53,61,62,66	0

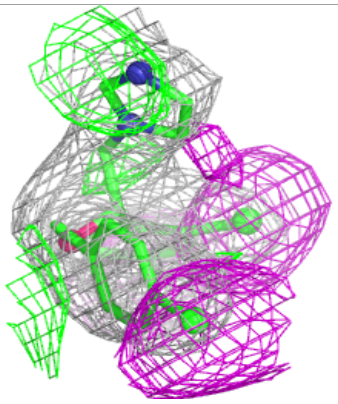
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ECN B 1406:

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

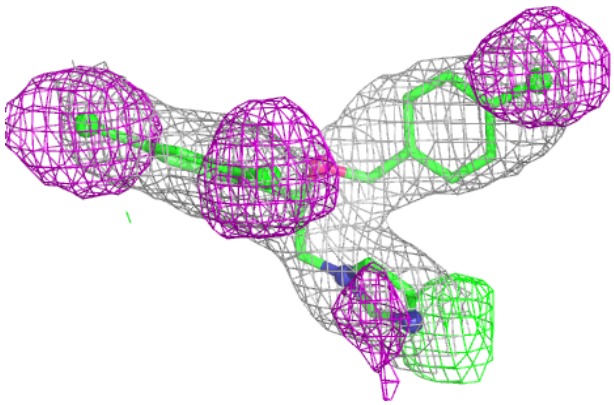


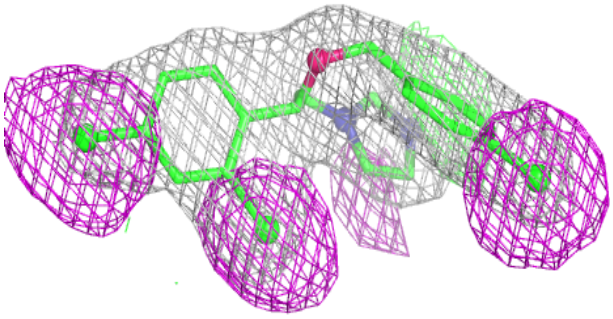


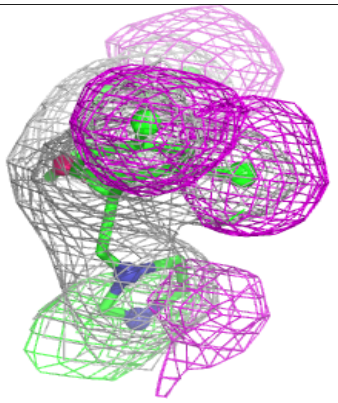


Electron density around ECN A 1409:

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

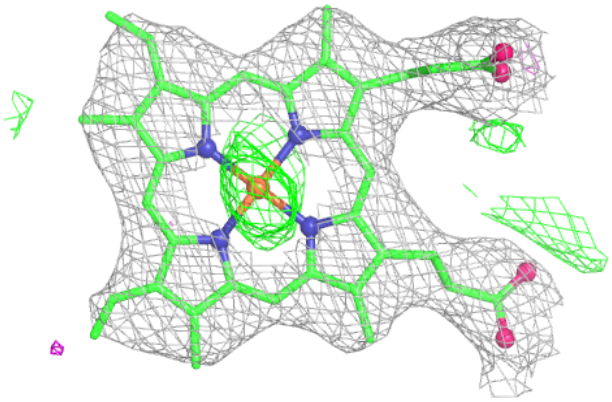


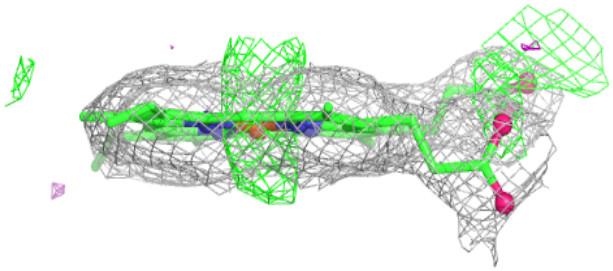


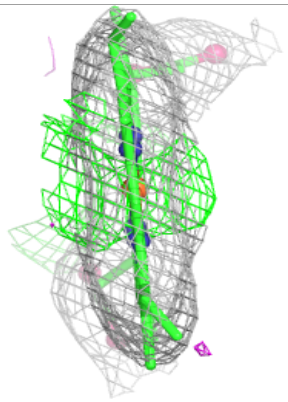


Electron density around HEM A 1408:

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

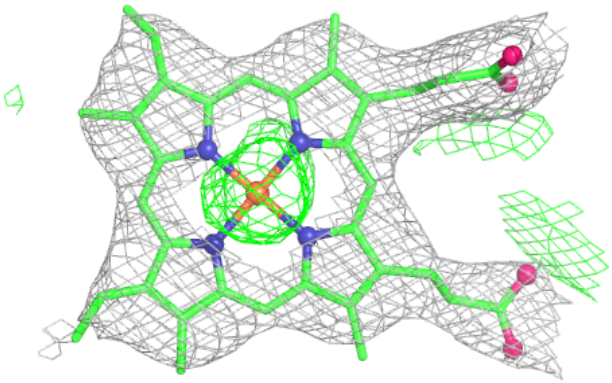


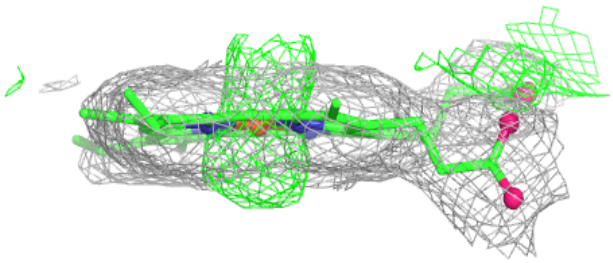


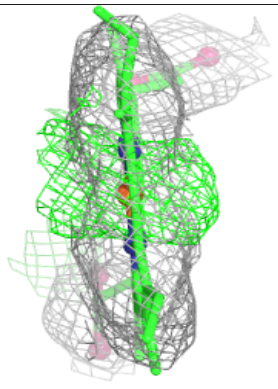


Electron density around HEM B 1405:

$2mF_o$-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.