Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 01:36 PM EST

PDB ID	:	3VLL
Title	:	Crystal Structure Analysis of the Ser305Ala variant of KatG from HALOARCULA MARISMORTUI Complexes with Inhibitor SHA
Authors	:	Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on	:	2011-12-01
Resolution	:	2.00 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 ⓘ symbol.

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

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

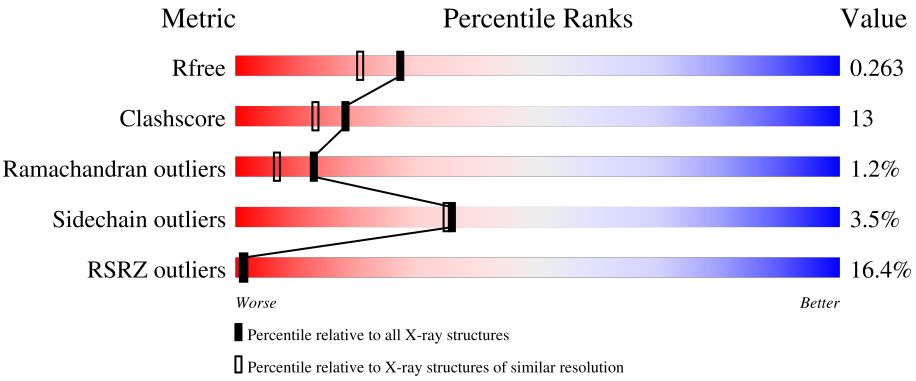
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	737	13% 75% 19% • 5%
1	B	737	19% 69% 25% • •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SHA	A	801	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11483 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.

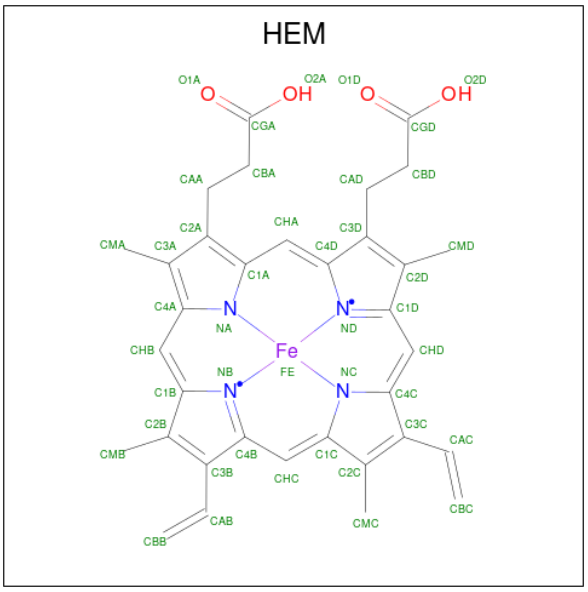
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	0	0
			5542	3469	929	1126	18			
1	B	710	Total	C	N	O	S	0	0	0
			5591	3497	941	1134	19			

There are 14 discrepancies between the modelled and reference sequences:

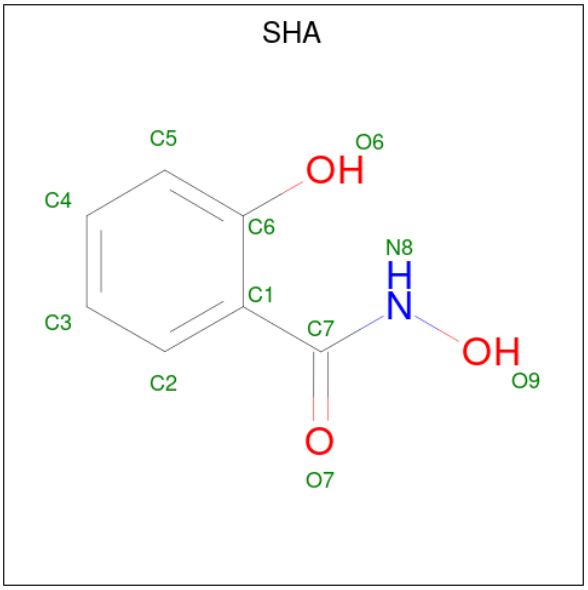
Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	SER	engineered mutation	UNP O59651
A	732	HIS	-	expression tag	UNP O59651
A	733	HIS	-	expression tag	UNP O59651
A	734	HIS	-	expression tag	UNP O59651
A	735	HIS	-	expression tag	UNP O59651
A	736	HIS	-	expression tag	UNP O59651
A	737	HIS	-	expression tag	UNP O59651
B	305	ALA	SER	engineered mutation	UNP O59651
B	732	HIS	-	expression tag	UNP O59651
B	733	HIS	-	expression tag	UNP O59651
B	734	HIS	-	expression tag	UNP O59651
B	735	HIS	-	expression tag	UNP O59651
B	736	HIS	-	expression tag	UNP O59651
B	737	HIS	-	expression tag	UNP O59651

- 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		

- Molecule 3 is SALICYLHYDROXAMIC ACID (three-letter code: SHA) (formula: $C_7H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is water.

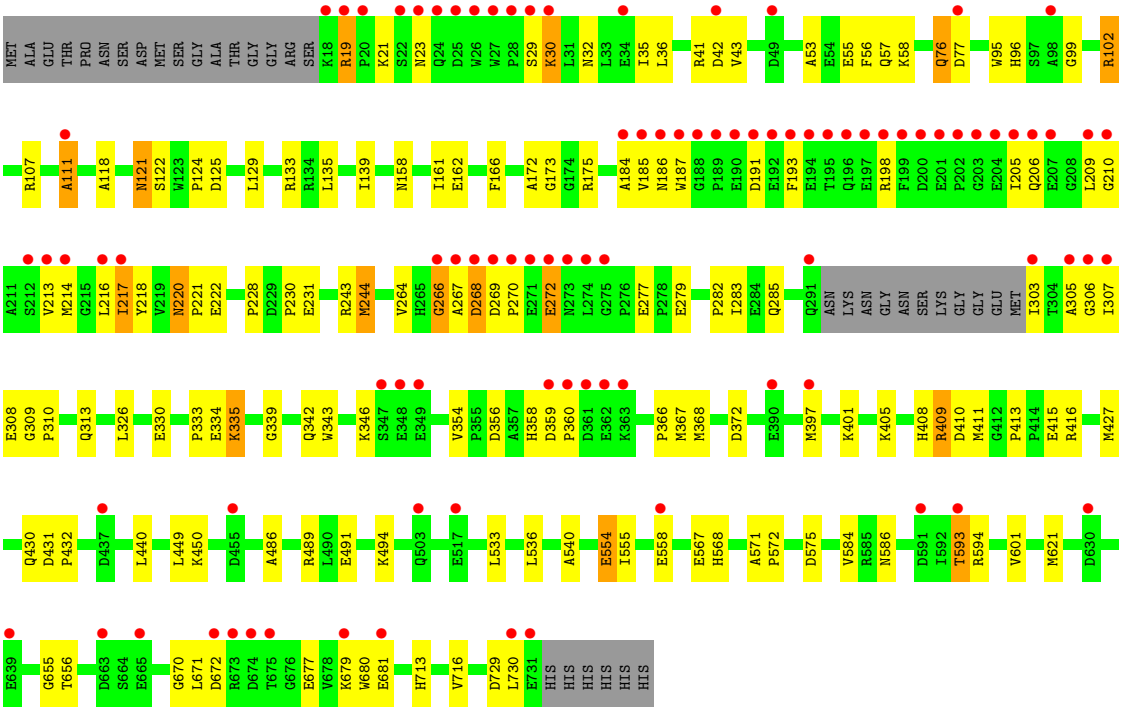
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	149	Total O 149 149	0	0
4	B	93	Total O 93 93	0	0

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.

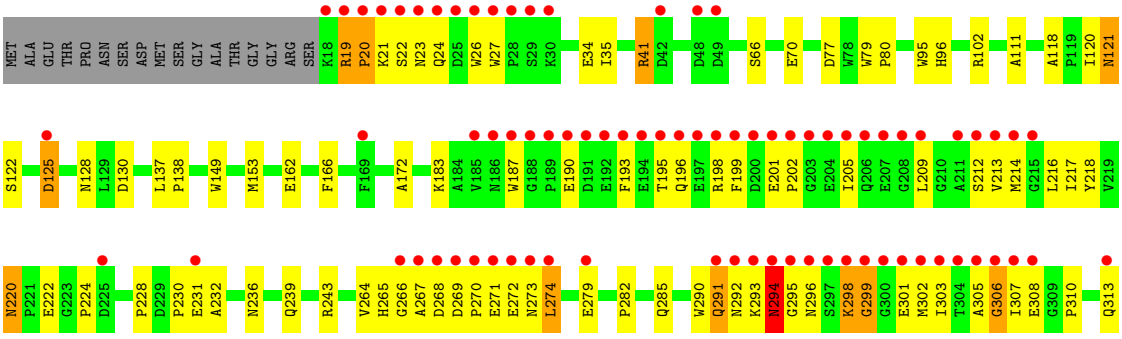
• Molecule 1: Catalase-peroxidase 2

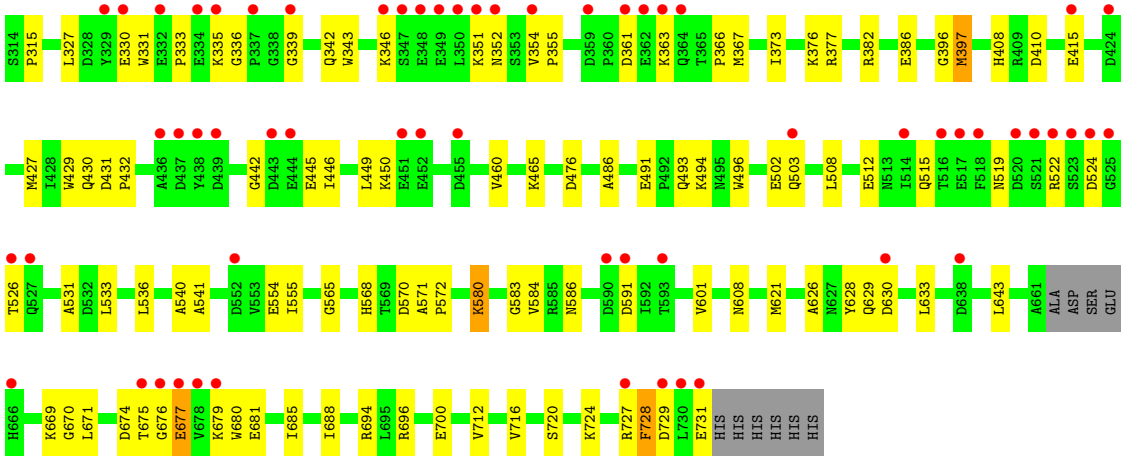
Chain A:



• Molecule 1: Catalase-peroxidase 2

Chain B:




S314 P315 L327 D328 Y329 E330 W331 E332 P333 E334 K335 G336 P337 G338 G339 Q342 W343 K346 S347 E348 E349 L350 K351 N352 S353 V354 P355 D359 P360 D361 E362 K363 Q364 T365 P366 M367 I373 K376 R377 R382 E386 G396 M397 H408 R409 D410 E415 D424
M427 I428 W429 Q430 D431 P432 A436 D437 Y438 D439 G442 D443 E444 E445 I446 L449 K450 E451 E452 D455 V460 K465 D476 A486 E491 P492 Q493 K494 M495 W496 E502 Q503 L508 E512 N513 I514 Q515 T516 E517 F518 N519 D520 S521 R522 S523 D524 G525
T526 Q527 A531 D532 L533 L536 A540 A541 D552 V553 E554 I555 G565 H568 T569 D570 A571 P572 K580 G583 V584 R585 N586 D590 D591 I592 T593 V601 N608 M621 A626 N627 Y628 Q629 D630 L633 D638 L643 A661 ALA ASP SER GLU
H666 K669 G670 L671 D674 T675 G676 E677 V678 K679 W680 E681 I685 I688 R694 L695 R696 E700 V712 V716 S720 K724 R727 F728 D729 L730 E731 HIS 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	150.19Å 76.32Å 140.24Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	48.36 – 2.00 48.36 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.36-2.00) 96.2 (48.36-1.79)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.271 0.240 , 0.263	Depositor DCC
R_{free} test set	7133 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11483	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: SHA, 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	0.39	1/5677 (0.0%)	0.56	0/7716
1	B	0.31	0/5726	0.52	0/7778
All	All	0.35	1/11403 (0.0%)	0.55	0/15494

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	ILE	C-N	10.20	1.57	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5542	0	5191	135	0
1	B	5591	0	5244	165	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	11	0	6	1	0
3	B	11	0	6	1	0
4	A	149	0	0	1	0
4	B	93	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11483	0	10507	291	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 13.

All (291) 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:95:TRP:CH2	1:A:218:TYR:HE1	1.08	1.66
1:B:95:TRP:CH2	1:B:218:TYR:HE1	1.10	1.62
1:A:95:TRP:HH2	1:A:218:TYR:CE1	1.01	1.62
1:B:95:TRP:HH2	1:B:218:TYR:CE1	1.11	1.60
1:A:95:TRP:CH2	1:A:218:TYR:CE1	1.87	1.46
1:B:95:TRP:CH2	1:B:218:TYR:CE1	1.96	1.22
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.41	0.98
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.45	0.97
1:A:270:PRO:HG3	1:A:305:ALA:HA	1.48	0.94
1:A:310:PRO:HG3	1:A:354:VAL:HG11	1.51	0.92
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.49	0.92
1:A:95:TRP:HH2	1:A:218:TYR:CD1	1.87	0.91
1:A:427:MET:H	1:A:430:GLN:HE21	1.17	0.91
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.52	0.90
1:A:267:ALA:H	1:A:303:ILE:HG12	1.36	0.88
1:A:95:TRP:CZ3	1:A:218:TYR:HE1	1.91	0.86
1:A:427:MET:H	1:A:430:GLN:NE2	1.74	0.85
1:A:672:ASP:HB2	1:A:679:LYS:HD3	1.56	0.84
1:A:266:GLY:HA2	1:A:303:ILE:HA	1.59	0.83
1:A:172:ALA:H	1:A:408:HIS:HE1	1.27	0.81
1:B:310:PRO:HG3	1:B:354:VAL:HG11	1.61	0.81
1:B:19:ARG:HD3	1:B:19:ARG:H	1.47	0.80
1:A:95:TRP:CH2	1:A:218:TYR:CD1	2.68	0.77
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.67	0.77
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.66	0.76
1:B:670:GLY:O	1:B:679:LYS:HB3	1.84	0.76
1:B:270:PRO:HB3	1:B:306:GLY:HA3	1.67	0.76
1:A:43:VAL:HG21	1:B:694:ARG:NH2	2.00	0.76
1:A:326:LEU:HD13	1:A:368:MET:HE2	1.68	0.75
1:B:282:PRO:HD2	1:B:285:GLN:NE2	2.02	0.74
1:B:95:TRP:CZ2	1:B:218:TYR:CE1	2.72	0.74
1:A:397:MET:HE2	1:A:401:LYS:HG3	1.69	0.74
1:A:217:ILE:HG23	1:A:218:TYR:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:H	1:B:274:LEU:HD12	1.52	0.74
1:A:264:VAL:HG21	1:A:307:ILE:HG22	1.68	0.73
1:B:269:ASP:HB3	1:B:272:GLU:HB2	1.70	0.73
1:A:267:ALA:N	1:A:303:ILE:HG12	2.04	0.72
1:B:679:LYS:HG2	1:B:680:TRP:H	1.54	0.72
1:A:191:ASP:HA	1:B:21:LYS:NZ	2.03	0.72
1:B:266:GLY:HA2	1:B:303:ILE:HG23	1.74	0.70
1:B:565:GLY:H	1:B:568:HIS:HD2	1.39	0.70
1:B:583:GLY:HA2	1:B:685:ILE:HD13	1.73	0.70
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.74	0.69
1:A:269:ASP:HB3	1:A:272:GLU:OE1	1.93	0.69
1:B:172:ALA:H	1:B:408:HIS:HE1	1.41	0.69
1:B:265:HIS:HB3	1:B:303:ILE:HA	1.74	0.69
1:B:273:ASN:HB3	1:B:293:LYS:H	1.58	0.68
1:A:326:LEU:HD13	1:A:368:MET:CE	2.23	0.67
1:A:567:GLU:HG2	1:A:568:HIS:CD2	2.31	0.66
1:B:190:GLU:HG2	1:B:196:GLN:HA	1.77	0.65
1:A:41:ARG:HG2	1:B:41:ARG:HD2	1.79	0.65
1:A:671:LEU:O	1:A:672:ASP:HB3	1.96	0.65
1:B:633:LEU:HD23	1:B:681:GLU:HG3	1.79	0.65
1:A:23:ASN:HD22	1:A:30:LYS:HD3	1.62	0.65
1:B:121:ASN:HD22	1:B:122:SER:N	1.95	0.64
1:B:727:ARG:HB3	1:B:727:ARG:HH21	1.62	0.64
1:A:53:ALA:O	1:A:57:GLN:HG3	1.98	0.64
1:A:335:LYS:HB3	1:A:335:LYS:HZ3	1.63	0.64
1:A:593:THR:HG23	1:A:594:ARG:H	1.61	0.64
1:B:580:LYS:HD3	1:B:580:LYS:H	1.64	0.63
1:B:491:GLU:CD	1:B:494:LYS:HE2	2.18	0.63
1:A:656:THR:HA	1:A:672:ASP:HA	1.80	0.62
1:B:220:ASN:HD22	1:B:222:GLU:H	1.45	0.61
1:B:239:GLN:HE21	1:B:243:ARG:HH21	1.47	0.61
1:A:191:ASP:HA	1:B:21:LYS:HZ3	1.63	0.61
1:B:460:VAL:HG13	1:B:541:ALA:HB1	1.82	0.60
1:A:655:GLY:O	1:A:672:ASP:HA	2.01	0.60
1:A:111:ALA:O	1:A:175:ARG:HB3	2.02	0.60
1:B:727:ARG:HB3	1:B:727:ARG:NH2	2.17	0.60
1:A:186:ASN:HB2	1:B:20:PRO:HG3	1.83	0.60
1:B:580:LYS:HD3	1:B:580:LYS:N	2.16	0.60
1:B:580:LYS:H	1:B:580:LYS:CD	2.15	0.60
1:B:290:TRP:O	1:B:292:ASN:N	2.35	0.59
1:A:205:ILE:HB	1:A:243:ARG:HH12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLY:O	1:A:308:GLU:HB2	2.03	0.58
1:B:376:LYS:O	1:B:382:ARG:HD3	2.02	0.58
1:B:294:ASN:O	1:B:302:MET:HA	2.03	0.58
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.84	0.58
1:A:99:GLY:C	1:A:217:ILE:HD11	2.24	0.58
1:A:270:PRO:HD3	1:A:306:GLY:H	1.69	0.58
1:A:368:MET:CE	1:A:372:ASP:HB3	2.34	0.58
1:A:397:MET:CE	1:A:401:LYS:HG3	2.32	0.58
1:B:196:GLN:HB3	1:B:213:VAL:HG22	1.86	0.58
1:B:266:GLY:O	1:B:308:GLU:HB2	2.03	0.58
1:B:327:LEU:HD22	1:B:382:ARG:NH2	2.18	0.57
1:B:503:GLN:HG3	4:B:954:HOH:O	2.03	0.57
1:A:121:ASN:HD22	1:A:122:SER:N	2.01	0.57
1:B:198:ARG:HD2	1:B:212:SER:C	2.25	0.57
1:B:231:GLU:OE1	1:B:377:ARG:HD2	2.05	0.56
1:B:335:LYS:HD2	1:B:339:GLY:HA2	1.86	0.56
1:B:354:VAL:HG21	1:B:366:PRO:HG3	1.86	0.56
1:B:111:ALA:HB2	1:B:410:ASP:OD2	2.05	0.56
1:B:213:VAL:HB	1:B:216:LEU:CD1	2.35	0.56
1:A:95:TRP:CZ3	1:A:218:TYR:CE1	2.76	0.56
1:A:107:ARG:HD3	1:A:185:VAL:HG22	1.87	0.56
1:B:580:LYS:H	1:B:580:LYS:HZ2	1.53	0.56
1:A:111:ALA:HB2	1:A:410:ASP:OD2	2.06	0.56
1:B:149:TRP:O	1:B:153:MET:HG3	2.05	0.56
1:B:450:LYS:HZ2	1:B:536:LEU:HD11	1.71	0.56
1:B:570:ASP:OD1	1:B:572:PRO:HD2	2.05	0.56
1:B:427:MET:HG2	1:B:430:GLN:HE21	1.71	0.55
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.88	0.55
1:B:431:ASP:N	1:B:432:PRO:HD3	2.22	0.54
1:A:567:GLU:HG2	1:A:568:HIS:HD2	1.71	0.54
1:B:230:PRO:HB2	1:B:377:ARG:HG3	1.90	0.54
1:B:95:TRP:CH2	1:B:218:TYR:CD1	2.86	0.54
1:B:199:PHE:HB3	1:B:205:ILE:HA	1.90	0.54
1:A:220:ASN:HD22	1:A:220:ASN:C	2.10	0.54
1:B:120:ILE:HD11	1:B:187:TRP:CZ2	2.43	0.54
1:A:270:PRO:HG3	1:A:305:ALA:CA	2.30	0.53
1:A:43:VAL:HG21	1:B:694:ARG:HH22	1.72	0.53
1:B:450:LYS:HZ2	1:B:450:LYS:HB2	1.74	0.53
1:B:273:ASN:O	1:B:292:ASN:HA	2.09	0.53
1:B:427:MET:HG2	1:B:430:GLN:NE2	2.23	0.53
1:B:220:ASN:ND2	1:B:222:GLU:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLN:HG3	1:A:135:LEU:CD2	2.40	0.52
1:A:96:HIS:CE1	1:A:125:ASP:O	2.62	0.52
1:A:217:ILE:CG2	1:A:218:TYR:N	2.69	0.52
1:A:670:GLY:O	1:A:679:LYS:O	2.26	0.52
1:A:405:LYS:O	1:A:409:ARG:HB2	2.09	0.52
1:B:307:ILE:N	1:B:307:ILE:HD12	2.25	0.52
1:B:476:ASP:CG	1:B:608:ASN:HD21	2.13	0.52
1:B:450:LYS:HG3	1:B:540:ALA:HB2	1.92	0.52
1:A:32:ASN:ND2	1:A:35:ILE:HG23	2.24	0.52
1:B:125:ASP:OD2	1:B:217:ILE:HG12	2.09	0.51
1:A:124:PRO:HG2	1:A:193:PHE:HB3	1.93	0.51
1:B:450:LYS:NZ	1:B:536:LEU:HD11	2.25	0.51
1:B:676:GLY:O	1:B:677:GLU:HB2	2.10	0.51
1:A:282:PRO:HD2	1:A:285:GLN:NE2	2.25	0.50
1:B:333:PRO:HG3	1:B:343:TRP:CZ2	2.46	0.50
1:B:354:VAL:CG2	1:B:366:PRO:HG3	2.41	0.50
1:A:216:LEU:HD22	3:A:801:SHA:O6	2.11	0.50
1:A:268:ASP:O	1:A:306:GLY:HA2	2.12	0.50
1:A:308:GLU:H	1:A:342:GLN:HE22	1.59	0.50
1:B:427:MET:CG	1:B:430:GLN:HE21	2.25	0.50
1:B:118:ALA:HB2	1:B:279:GLU:CD	2.31	0.50
1:B:508:LEU:O	1:B:512:GLU:HG3	2.10	0.50
1:B:555:ILE:HG12	1:B:716:VAL:HG13	1.94	0.50
1:A:139:ILE:HG13	4:A:1025:HOH:O	2.12	0.49
1:A:558:GLU:OE1	1:A:730:LEU:HD22	2.12	0.49
1:A:217:ILE:HG23	1:A:218:TYR:H	1.73	0.49
1:B:125:ASP:CG	1:B:216:LEU:HA	2.32	0.49
1:B:696:ARG:O	1:B:700:GLU:HG3	2.12	0.49
1:A:335:LYS:HB3	1:A:335:LYS:NZ	2.27	0.49
1:B:330:GLU:HB3	1:B:346:LYS:HD3	1.93	0.49
1:A:35:ILE:HB	1:A:184:ALA:HB2	1.95	0.49
1:B:162:GLU:HA	1:B:166:PHE:O	2.11	0.49
1:B:291:GLN:O	1:B:293:LYS:HE3	2.13	0.49
1:A:220:ASN:ND2	1:A:222:GLU:H	2.11	0.48
1:A:307:ILE:HA	1:A:342:GLN:NE2	2.29	0.48
1:B:34:GLU:CD	1:B:183:LYS:HE2	2.33	0.48
1:A:554:GLU:OE1	1:A:554:GLU:HA	2.13	0.48
1:B:230:PRO:CB	1:B:377:ARG:HG3	2.43	0.48
1:A:102:ARG:HD3	1:A:107:ARG:O	2.14	0.48
1:A:122:SER:HB3	1:A:277:GLU:HG3	1.95	0.48
1:B:193:PHE:O	1:B:195:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LYS:HG2	1:B:352:ASN:ND2	2.28	0.47
1:B:382:ARG:NH2	1:B:386:GLU:OE1	2.47	0.47
1:B:679:LYS:HG2	1:B:680:TRP:N	2.25	0.47
1:A:198:ARG:NH1	1:A:209:LEU:HD13	2.30	0.47
1:A:264:VAL:HG22	1:A:309:GLY:O	2.15	0.47
1:A:413:PRO:HB2	1:A:415:GLU:OE1	2.14	0.47
1:A:335:LYS:HZ3	1:A:339:GLY:HA2	1.80	0.47
1:A:431:ASP:N	1:A:432:PRO:HD3	2.30	0.47
1:A:220:ASN:HD22	1:A:221:PRO:N	2.12	0.47
1:B:80:PRO:HD2	1:B:296:ASN:O	2.15	0.47
1:A:161:ILE:CG2	1:A:166:PHE:HB3	2.45	0.46
1:A:270:PRO:HB3	1:A:303:ILE:HG22	1.97	0.46
1:A:415:GLU:H	1:A:415:GLU:CD	2.19	0.46
1:A:161:ILE:HG22	1:A:166:PHE:HB3	1.96	0.46
1:A:401:LYS:HE3	1:A:427:MET:CE	2.45	0.46
1:B:271:GLU:HA	1:B:274:LEU:HD13	1.96	0.46
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.97	0.46
1:B:265:HIS:HB3	1:B:303:ILE:CA	2.45	0.46
1:A:32:ASN:ND2	1:A:35:ILE:CG2	2.78	0.46
1:B:486:ALA:HB2	1:B:531:ALA:HB2	1.98	0.46
1:B:676:GLY:O	1:B:677:GLU:CB	2.63	0.46
1:A:56:PHE:CZ	1:A:173:GLY:HA3	2.51	0.46
1:B:224:PRO:HG3	1:B:236:ASN:HD22	1.80	0.46
1:B:522:ARG:HG3	1:B:526:THR:O	2.15	0.46
1:A:41:ARG:HD2	1:A:41:ARG:O	2.16	0.46
1:A:55:GLU:HA	1:A:58:LYS:HD3	1.96	0.46
1:A:334:GLU:O	1:A:334:GLU:HG3	2.16	0.46
1:B:352:ASN:O	1:B:363:LYS:HD2	2.15	0.46
1:A:440:LEU:HD22	1:A:440:LEU:N	2.31	0.46
1:B:22:SER:HB3	1:B:24:GLN:NE2	2.30	0.46
1:B:449:LEU:HD22	1:B:533:LEU:HD21	1.98	0.45
1:A:96:HIS:HE1	1:A:125:ASP:O	1.98	0.45
1:B:720:SER:O	1:B:724:LYS:HG2	2.15	0.45
1:A:198:ARG:HG3	1:A:205:ILE:HG23	1.99	0.45
1:A:214:MET:C	1:A:216:LEU:H	2.20	0.45
1:B:352:ASN:HB3	1:B:363:LYS:HB3	1.96	0.45
1:A:335:LYS:NZ	1:A:339:GLY:HA2	2.31	0.45
1:A:491:GLU:HG2	1:A:494:LYS:HE2	1.98	0.45
1:B:198:ARG:HD2	1:B:212:SER:O	2.17	0.45
1:B:354:VAL:HG13	1:B:355:PRO:HD2	1.97	0.45
1:A:210:GLY:O	1:A:244:MET:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:O	1:A:230:PRO:HD3	2.16	0.45
1:A:368:MET:HE3	1:A:372:ASP:HB3	1.98	0.45
1:A:427:MET:N	1:A:430:GLN:HE21	1.99	0.45
1:B:313:GLN:C	1:B:315:PRO:HD3	2.37	0.45
1:B:19:ARG:HD3	1:B:19:ARG:N	2.25	0.44
1:B:307:ILE:HG23	1:B:342:GLN:CD	2.38	0.44
1:B:515:GLN:HG2	1:B:519:ASN:ND2	2.32	0.44
1:B:628:TYR:CE1	1:B:629:GLN:HG3	2.51	0.44
1:B:95:TRP:CZ2	1:B:218:TYR:CD1	3.03	0.44
1:B:121:ASN:HD22	1:B:121:ASN:C	2.19	0.44
1:A:283:ILE:HD11	1:B:688:ILE:N	2.33	0.44
1:B:137:LEU:HB3	1:B:138:PRO:HD3	2.00	0.44
1:B:66:SER:O	1:B:70:GLU:HG3	2.18	0.44
1:B:202:PRO:HG2	1:B:232:ALA:HB1	1.99	0.44
1:B:209:LEU:O	1:B:243:ARG:HD3	2.18	0.44
1:B:267:ALA:H	1:B:303:ILE:CD1	2.30	0.44
1:A:354:VAL:CG2	1:A:366:PRO:HG3	2.48	0.44
1:A:449:LEU:HD22	1:A:533:LEU:HD21	1.99	0.44
1:B:23:ASN:HA	1:B:26:TRP:HD1	1.83	0.44
1:B:79:TRP:CE3	1:B:296:ASN:HA	2.53	0.44
1:B:228:PRO:O	1:B:230:PRO:HD3	2.18	0.44
1:B:728:PHE:HA	1:B:731:GLU:CD	2.39	0.44
1:A:118:ALA:HB2	1:A:279:GLU:HG3	1.99	0.44
1:B:121:ASN:C	1:B:121:ASN:ND2	2.72	0.44
1:B:643:LEU:HD23	1:B:712:VAL:HG13	2.00	0.44
1:A:19:ARG:H	1:A:19:ARG:HD3	1.83	0.43
1:B:264:VAL:HG21	1:B:307:ILE:HG22	1.99	0.43
1:B:268:ASP:HB3	1:B:273:ASN:ND2	2.33	0.43
1:B:196:GLN:CG	1:B:213:VAL:HG22	2.48	0.43
1:B:213:VAL:HB	1:B:216:LEU:HG	2.00	0.43
1:B:128:ASN:HA	1:B:130:ASP:OD2	2.17	0.43
1:A:205:ILE:HG22	1:A:206:GLN:N	2.33	0.43
1:B:669:LYS:HA	1:B:669:LYS:HD3	1.86	0.43
1:A:356:ASP:HB3	1:A:359:ASP:O	2.18	0.43
1:B:427:MET:HB3	1:B:429:TRP:CD1	2.54	0.43
1:A:121:ASN:HD22	1:A:121:ASN:C	2.19	0.43
1:B:310:PRO:CG	1:B:354:VAL:HG11	2.39	0.43
1:A:118:ALA:HB2	1:A:279:GLU:CG	2.49	0.43
1:A:679:LYS:O	1:A:680:TRP:CB	2.66	0.43
1:B:415:GLU:HG2	1:B:729:ASP:HA	2.01	0.43
1:B:442:GLY:O	1:B:446:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:GLN:HG2	1:B:496:TRP:CH2	2.54	0.43
1:A:555:ILE:HG12	1:A:716:VAL:HG13	2.01	0.42
1:B:427:MET:HB3	1:B:429:TRP:NE1	2.34	0.42
1:A:43:VAL:HG21	1:B:694:ARG:HH21	1.78	0.42
1:B:190:GLU:OE2	1:B:196:GLN:HA	2.20	0.42
1:B:224:PRO:HG3	1:B:236:ASN:ND2	2.34	0.42
1:B:331:TRP:HB3	1:B:343:TRP:HB3	2.00	0.42
1:A:41:ARG:HB3	1:B:41:ARG:HB3	2.01	0.42
1:B:580:LYS:CD	1:B:580:LYS:N	2.80	0.42
1:A:129:LEU:O	1:A:133:ARG:HG3	2.19	0.42
1:A:536:LEU:HD23	1:A:536:LEU:O	2.20	0.42
1:B:298:LYS:O	1:B:299:GLY:C	2.57	0.42
1:B:26:TRP:HB2	1:B:27:TRP:CE3	2.54	0.42
1:B:291:GLN:OE1	1:B:291:GLN:HA	2.19	0.42
1:B:96:HIS:NE2	3:B:801:SHA:N8	2.68	0.42
1:B:198:ARG:CZ	1:B:209:LEU:HD13	2.49	0.42
1:B:445:GLU:OE1	1:B:526:THR:HG21	2.19	0.42
1:A:185:VAL:HG11	1:A:187:TRP:CZ2	2.55	0.42
1:A:567:GLU:H	1:A:567:GLU:CD	2.23	0.42
1:B:515:GLN:HG2	1:B:519:ASN:HD21	1.85	0.42
1:A:118:ALA:HB2	1:A:279:GLU:CD	2.39	0.41
1:A:486:ALA:O	1:A:489:ARG:HG2	2.20	0.41
1:B:301:GLU:H	1:B:301:GLU:HG2	1.61	0.41
1:B:397:MET:HA	1:B:397:MET:CE	2.50	0.41
1:A:397:MET:HE2	1:A:397:MET:O	2.19	0.41
1:B:172:ALA:N	1:B:408:HIS:HE1	2.13	0.41
1:B:220:ASN:HD22	1:B:220:ASN:C	2.22	0.41
1:B:352:ASN:HB3	1:B:363:LYS:CB	2.51	0.41
1:A:118:ALA:HA	1:A:121:ASN:ND2	2.35	0.41
1:A:220:ASN:HD22	1:A:222:GLU:H	1.69	0.41
1:A:411:MET:O	1:A:416:ARG:HD3	2.20	0.41
1:B:343:TRP:CD2	1:B:373:ILE:HG13	2.56	0.41
1:B:465:LYS:NZ	1:B:630:ASP:OD2	2.54	0.41
1:B:502:GLU:HG2	1:B:503:GLN:N	2.36	0.41
1:A:231:GLU:H	1:A:231:GLU:CD	2.24	0.41
1:A:330:GLU:HB2	1:A:346:LYS:HD2	2.02	0.41
1:A:333:PRO:HG3	1:A:343:TRP:CH2	2.56	0.41
1:A:358:HIS:O	1:A:360:PRO:HD3	2.21	0.41
1:B:196:GLN:HG2	1:B:213:VAL:HG22	2.03	0.41
1:B:310:PRO:O	1:B:366:PRO:HA	2.21	0.41
1:A:121:ASN:C	1:A:121:ASN:ND2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:H	1:B:274:LEU:CD1	2.29	0.41
1:B:330:GLU:CB	1:B:346:LYS:HD3	2.50	0.41
1:B:674:ASP:O	1:B:677:GLU:OE1	2.38	0.41
1:A:217:ILE:CG2	1:A:218:TYR:H	2.32	0.41
1:A:450:LYS:HG3	1:A:540:ALA:HB2	2.02	0.41
1:A:35:ILE:HG13	1:A:36:LEU:N	2.35	0.40
1:A:158:ASN:O	1:A:162:GLU:HG3	2.22	0.40
1:A:270:PRO:HD3	1:A:306:GLY:N	2.34	0.40
1:A:368:MET:HE1	1:A:372:ASP:HB3	2.04	0.40
1:B:294:ASN:HD22	1:B:294:ASN:HA	1.56	0.40
1:B:621:MET:HG3	1:B:626:ALA:HB3	2.04	0.40
1:B:166:PHE:HZ	1:B:396:GLY:O	2.05	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	699/737 (95%)	665 (95%)	30 (4%)	4 (1%)	25 19
1	B	706/737 (96%)	650 (92%)	43 (6%)	13 (2%)	8 3
All	All	1405/1474 (95%)	1315 (94%)	73 (5%)	17 (1%)	13 7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	LYS
1	B	305	ALA
1	A	268	ASP
1	B	291	GLN
1	B	591	ASP
1	B	677	GLU

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Mol	Chain	Res	Type
1	A	111	ALA
1	B	294	ASN
1	B	299	GLY
1	B	524	ASP
1	B	274	LEU
1	B	306	GLY
1	A	29	SER
1	B	20	PRO
1	B	336	GLY
1	B	295	GLY
1	A	266	GLY

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	581/607 (96%)	559 (96%)	22 (4%)	33	31
1	B	586/607 (96%)	567 (97%)	19 (3%)	39	38
All	All	1167/1214 (96%)	1126 (96%)	41 (4%)	36	35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	21	LYS
1	A	30	LYS
1	A	42	ASP
1	A	76	GLN
1	A	77	ASP
1	A	102	ARG
1	A	121	ASN
1	A	220	ASN
1	A	244	MET
1	A	272	GLU
1	A	335	LYS

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Mol	Chain	Res	Type
1	A	367	MET
1	A	409	ARG
1	A	554	GLU
1	A	575	ASP
1	A	586	ASN
1	A	593	THR
1	A	677	GLU
1	A	681	GLU
1	A	713	HIS
1	A	729	ASP
1	B	19	ARG
1	B	41	ARG
1	B	77	ASP
1	B	102	ARG
1	B	121	ASN
1	B	125	ASP
1	B	201	GLU
1	B	214	MET
1	B	220	ASN
1	B	294	ASN
1	B	361	ASP
1	B	367	MET
1	B	397	MET
1	B	554	GLU
1	B	580	LYS
1	B	586	ASN
1	B	671	LEU
1	B	675	THR
1	B	728	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	38	GLN
1	A	57	GLN
1	A	121	ASN
1	A	145	GLN
1	A	220	ASN
1	A	227	ASN
1	A	273	ASN
1	A	285	GLN

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Mol	Chain	Res	Type
1	A	286	GLN
1	A	324	ASN
1	A	342	GLN
1	A	352	ASN
1	A	389	GLN
1	A	408	HIS
1	A	430	GLN
1	A	513	ASN
1	A	515	GLN
1	A	527	GLN
1	A	568	HIS
1	A	586	ASN
1	B	24	GLN
1	B	121	ASN
1	B	196	GLN
1	B	220	ASN
1	B	285	GLN
1	B	286	GLN
1	B	313	GLN
1	B	324	ASN
1	B	352	ASN
1	B	358	HIS
1	B	389	GLN
1	B	408	HIS
1	B	430	GLN
1	B	513	ASN
1	B	515	GLN
1	B	568	HIS
1	B	586	ASN
1	B	603	ASN
1	B	608	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	SHA	B	801	-	11,11,11	1.60	2 (18%)	13,14,14	0.60	0
2	HEM	B	800	1	41,50,50	2.41	12 (29%)	45,82,82	9.61	33 (73%)
2	HEM	A	800	1	41,50,50	2.09	13 (31%)	45,82,82	8.33	31 (68%)
3	SHA	A	801	-	11,11,11	1.71	3 (27%)	13,14,14	0.57	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
3	SHA	B	801	-	-	1/6/6/6	0/1/1/1
2	HEM	B	800	1	-	3/12/54/54	-
2	HEM	A	800	1	-	2/12/54/54	-
3	SHA	A	801	-	-	1/6/6/6	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	FE-NB	8.37	2.38	1.96
2	A	800	HEM	CBB-CAB	5.20	1.56	1.30
2	B	800	HEM	CBB-CAB	4.94	1.54	1.30
2	B	800	HEM	FE-ND	4.69	2.20	1.96
2	B	800	HEM	C3C-C2C	-4.68	1.33	1.40
2	A	800	HEM	FE-ND	4.27	2.18	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HEM	C3C-C2C	-4.14	1.34	1.40
2	B	800	HEM	CBD-CGD	-4.13	1.41	1.50
2	A	800	HEM	CBD-CGD	-4.10	1.41	1.50
2	B	800	HEM	CBC-CAC	4.06	1.56	1.29
2	A	800	HEM	CBC-CAC	4.03	1.56	1.29
2	A	800	HEM	FE-NB	4.03	2.16	1.96
2	B	800	HEM	CBA-CGA	-3.98	1.41	1.50
2	A	800	HEM	CBA-CGA	-3.85	1.41	1.50
3	B	801	SHA	C1-C6	3.40	1.46	1.40
3	A	801	SHA	C1-C6	3.37	1.46	1.40
3	B	801	SHA	C7-N8	3.16	1.36	1.32
3	A	801	SHA	C7-N8	2.89	1.36	1.32
2	B	800	HEM	C3C-CAC	2.54	1.53	1.47
2	A	800	HEM	O1A-CGA	2.48	1.30	1.22
2	A	800	HEM	C3C-CAC	2.40	1.52	1.47
2	B	800	HEM	C4D-ND	-2.39	1.36	1.40
2	B	800	HEM	CBD-CAD	2.29	1.59	1.52
2	B	800	HEM	O1A-CGA	2.28	1.29	1.22
2	A	800	HEM	CHB-C1B	2.27	1.40	1.35
2	A	800	HEM	CBD-CAD	2.25	1.59	1.52
2	A	800	HEM	C4D-ND	-2.15	1.36	1.40
2	B	800	HEM	CHA-C4D	2.12	1.40	1.35
3	A	801	SHA	C2-C1	2.12	1.43	1.39
2	A	800	HEM	CHA-C4D	2.11	1.40	1.35

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	800	HEM	C4B-CHC-C1C	33.50	166.77	122.56
2	B	800	HEM	C4C-CHD-C1D	29.16	161.04	122.56
2	A	800	HEM	C4C-CHD-C1D	25.33	155.99	122.56
2	A	800	HEM	C4B-CHC-C1C	24.29	154.61	122.56
2	B	800	HEM	CHC-C4B-NB	-18.23	104.62	124.43
2	B	800	HEM	CHC-C4B-C3B	17.70	151.66	124.57
2	A	800	HEM	CHC-C4B-NB	-17.10	105.85	124.43
2	B	800	HEM	CHB-C1B-NB	-15.95	104.68	124.38
2	A	800	HEM	CHA-C4D-ND	-15.52	105.21	124.38
2	B	800	HEM	CHD-C1D-ND	-15.48	107.61	124.43
2	A	800	HEM	CHB-C1B-NB	-13.50	107.70	124.38
2	A	800	HEM	CHD-C1D-ND	-12.50	110.85	124.43
2	A	800	HEM	CHA-C4D-C3D	11.68	147.24	125.33
2	B	800	HEM	CHA-C4D-ND	-11.64	110.00	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	HEM	CHC-C4B-C3B	11.27	141.83	124.57
2	B	800	HEM	CHD-C1D-C2D	11.27	142.58	124.98
2	B	800	HEM	CHA-C4D-C3D	10.92	145.82	125.33
2	A	800	HEM	C3B-C2B-C1B	-10.39	98.78	106.49
2	A	800	HEM	C4A-C3A-C2A	-9.17	100.61	107.00
2	B	800	HEM	O2D-CGD-O1D	-8.72	101.56	123.30
2	A	800	HEM	C2B-C1B-NB	8.55	119.97	109.84
2	B	800	HEM	C4B-C3B-C2B	8.42	113.80	107.11
2	A	800	HEM	CAD-C3D-C4D	-7.78	111.07	124.66
2	A	800	HEM	C1D-C2D-C3D	-7.51	99.07	106.96
2	B	800	HEM	C3D-C4D-ND	-6.93	102.45	110.17
2	B	800	HEM	CAD-C3D-C4D	-6.88	112.64	124.66
2	B	800	HEM	O1D-CGD-CBD	6.84	145.05	123.08
2	B	800	HEM	C4A-C3A-C2A	-6.43	102.53	107.00
2	A	800	HEM	CMD-C2D-C1D	6.35	134.70	125.04
2	A	800	HEM	O2A-CGA-O1A	-5.97	108.41	123.30
2	B	800	HEM	C4D-ND-C1D	5.93	111.19	105.07
2	B	800	HEM	CHB-C1B-C2B	5.86	142.94	126.72
2	B	800	HEM	C3B-C2B-C1B	-5.84	102.15	106.49
2	A	800	HEM	C1B-NB-C4B	-5.66	99.23	105.07
2	B	800	HEM	O2A-CGA-O1A	-5.55	109.46	123.30
2	A	800	HEM	O2D-CGD-O1D	-5.41	109.82	123.30
2	A	800	HEM	CHD-C1D-C2D	5.37	133.37	124.98
2	A	800	HEM	O2A-CGA-CBA	5.30	131.05	114.03
2	B	800	HEM	C4D-C3D-C2D	5.17	114.42	106.90
2	A	800	HEM	C4D-C3D-C2D	4.88	114.01	106.90
2	A	800	HEM	C4B-C3B-C2B	4.87	110.98	107.11
2	A	800	HEM	CMC-C2C-C3C	4.78	133.63	124.68
2	B	800	HEM	CMA-C3A-C2A	4.69	133.78	124.94
2	B	800	HEM	C1D-C2D-C3D	-4.60	102.12	106.96
2	A	800	HEM	C2D-C1D-ND	4.55	115.34	109.88
2	B	800	HEM	CMC-C2C-C3C	4.34	132.79	124.68
2	A	800	HEM	CAA-CBA-CGA	-4.07	102.35	113.76
2	B	800	HEM	C1B-NB-C4B	4.01	109.22	105.07
2	A	800	HEM	CAD-C3D-C2D	3.73	134.82	127.88
2	B	800	HEM	CMB-C2B-C3B	3.53	136.95	128.30
2	A	800	HEM	C3D-C4D-ND	-3.44	106.34	110.17
2	B	800	HEM	CMB-C2B-C1B	-3.33	119.97	125.04
2	A	800	HEM	CMB-C2B-C3B	3.24	136.24	128.30
2	B	800	HEM	CMA-C3A-C4A	-3.14	123.64	128.46
2	B	800	HEM	CAA-CBA-CGA	-3.13	104.97	113.76
2	B	800	HEM	CBA-CAA-C2A	2.93	117.62	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	HEM	O1D-CGD-CBD	2.92	132.46	123.08
2	A	800	HEM	CMA-C3A-C2A	2.79	130.19	124.94
2	B	800	HEM	CMD-C2D-C1D	2.78	129.28	125.04
2	B	800	HEM	CAD-C3D-C2D	2.66	132.84	127.88
2	B	800	HEM	O2A-CGA-CBA	2.65	122.53	114.03
2	A	800	HEM	CBA-CAA-C2A	2.61	117.07	112.62
2	B	800	HEM	CAD-CBD-CGD	-2.43	108.38	113.60
2	A	800	HEM	CBB-CAB-C3B	2.07	137.90	127.62

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	SHA	C2-C1-C7-N8
3	B	801	SHA	C2-C1-C7-N8
2	A	800	HEM	CAA-CBA-CGA-O2A
2	B	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	C2B-C3B-CAB-CBB

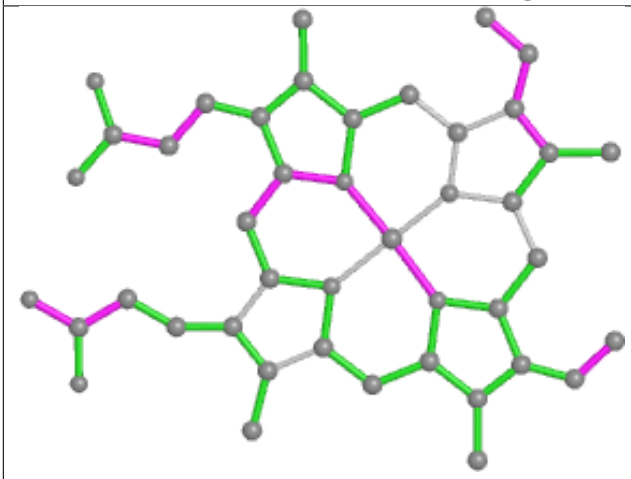
There are no ring outliers.

2 monomers are involved in 2 short contacts:

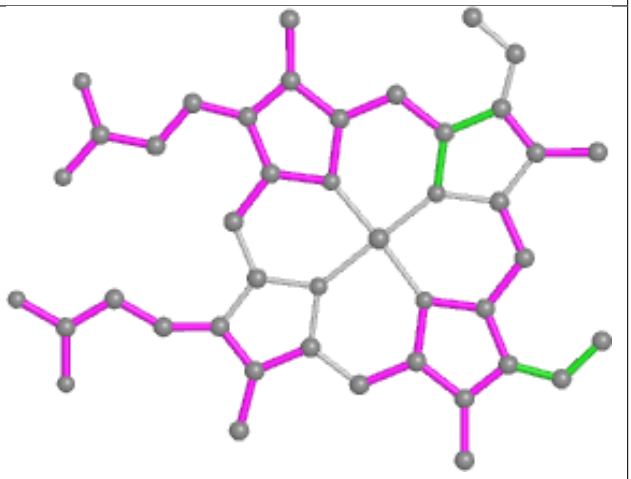
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	SHA	1	0
3	A	801	SHA	1	0

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.

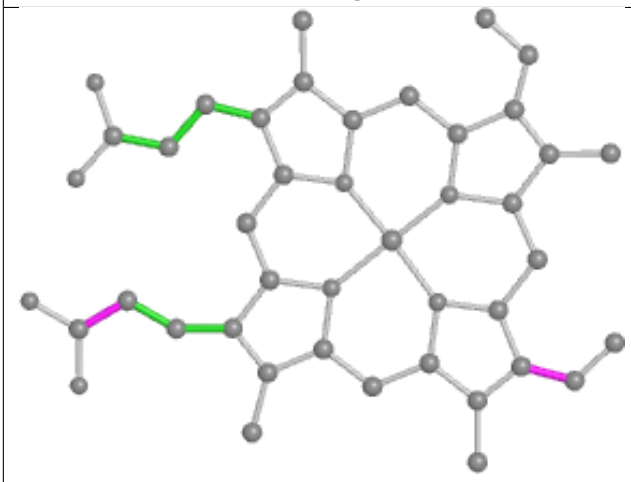
Ligand HEM B 800



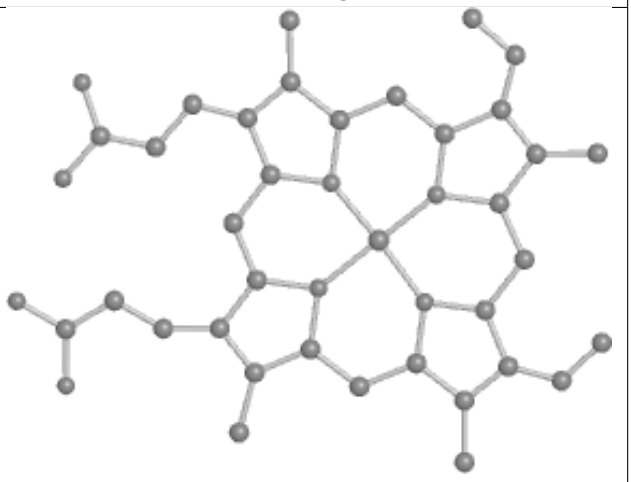
Bond lengths



Bond angles

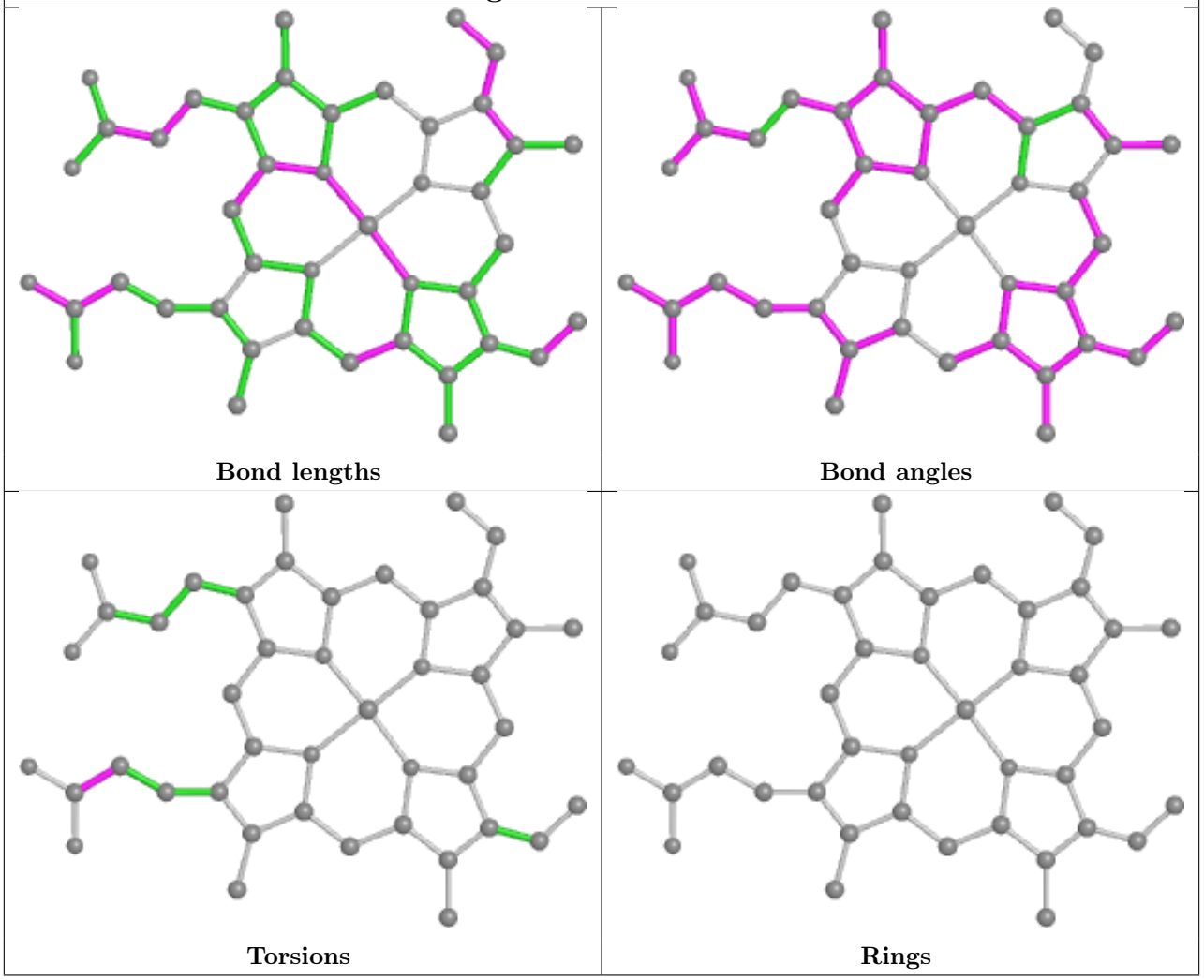


Torsions



Rings

Ligand HEM A 800



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	703/737 (95%)	0.77	93 (13%)	3 2	16, 27, 68, 78	0
1	B	710/737 (96%)	1.27	139 (19%)	1 0	17, 35, 72, 80	0
All	All	1413/1474 (95%)	1.02	232 (16%)	1 1	16, 31, 70, 80	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	SER	16.9
1	A	267	ALA	13.4
1	A	273	ASN	13.3
1	B	296	ASN	13.2
1	B	300	GLY	13.1
1	B	20	PRO	12.8
1	A	26	TRP	12.8
1	B	305	ALA	12.6
1	A	272	GLU	12.3
1	B	273	ASN	11.9
1	A	188	GLY	11.7
1	A	19	ARG	11.6
1	B	299	GLY	11.1
1	B	298	LYS	10.8
1	B	730	LEU	10.7
1	B	193	PHE	10.7
1	A	25	ASP	10.6
1	B	26	TRP	10.2
1	A	305	ALA	10.1
1	A	192	GLU	9.9
1	B	195	THR	9.9
1	A	28	PRO	9.8
1	B	675	THR	9.8
1	B	303	ILE	9.7

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Mol	Chain	Res	Type	RSRZ
1	B	189	PRO	9.6
1	A	270	PRO	9.6
1	A	20	PRO	9.5
1	A	27	TRP	9.3
1	B	269	ASP	9.1
1	B	270	PRO	9.0
1	B	307	ILE	8.5
1	B	294	ASN	8.5
1	B	192	GLU	8.4
1	A	204	GLU	8.3
1	B	295	GLY	8.3
1	A	29	SER	8.3
1	B	191	ASP	8.3
1	A	730	LEU	8.1
1	A	361	ASP	8.0
1	B	306	GLY	8.0
1	B	292	ASN	7.9
1	A	189	PRO	7.9
1	B	268	ASP	7.8
1	B	200	ASP	7.8
1	B	267	ALA	7.7
1	B	678	VAL	7.7
1	B	677	GLU	7.7
1	A	195	THR	7.5
1	B	293	LYS	7.5
1	B	272	GLU	7.5
1	A	274	LEU	7.3
1	B	196	GLN	7.2
1	B	187	TRP	7.1
1	B	197	GLU	7.0
1	B	266	GLY	7.0
1	A	269	ASP	6.8
1	A	202	PRO	6.8
1	A	199	PHE	6.7
1	B	25	ASP	6.5
1	A	191	ASP	6.5
1	B	337	PRO	6.5
1	B	22	SER	6.4
1	A	207	GLU	6.4
1	B	523	SER	6.4
1	B	214	MET	6.4
1	B	729	ASP	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	187	TRP	6.3
1	A	360	PRO	6.3
1	B	28	PRO	6.3
1	B	590	ASP	6.3
1	A	303	ILE	6.2
1	B	524	ASP	6.2
1	B	362	GLU	6.2
1	B	676	GLY	6.1
1	A	675	THR	6.1
1	B	349	GLU	6.1
1	A	271	GLU	6.0
1	B	301	GLU	6.0
1	A	731	GLU	6.0
1	A	203	GLY	5.9
1	B	207	GLU	5.9
1	A	663	ASP	5.9
1	B	274	LEU	5.9
1	A	674	ASP	5.8
1	A	200	ASP	5.8
1	B	731	GLU	5.7
1	B	205	ILE	5.6
1	A	291	GLN	5.6
1	B	27	TRP	5.6
1	A	209	LEU	5.6
1	B	302	MET	5.6
1	B	437	ASP	5.5
1	B	19	ARG	5.5
1	B	21	LYS	5.4
1	B	213	VAL	5.4
1	B	188	GLY	5.3
1	B	190	GLU	5.3
1	A	193	PHE	5.3
1	A	213	VAL	5.1
1	B	339	GLY	5.0
1	B	18	LYS	5.0
1	A	206	GLN	5.0
1	A	205	ILE	4.9
1	A	194	GLU	4.8
1	A	266	GLY	4.8
1	A	437	ASP	4.8
1	B	24	GLN	4.7
1	B	23	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLU	4.6
1	B	185	VAL	4.6
1	B	334	GLU	4.5
1	B	202	PRO	4.5
1	B	361	ASP	4.5
1	B	208	GLY	4.4
1	B	42	ASP	4.4
1	A	201	GLU	4.3
1	B	212	SER	4.2
1	B	346	LYS	4.2
1	B	194	GLU	4.2
1	B	203	GLY	4.2
1	B	521	SER	4.2
1	B	424	ASP	4.1
1	A	190	GLU	4.0
1	B	209	LEU	4.0
1	B	516	THR	4.0
1	A	216	LEU	3.9
1	A	348	GLU	3.9
1	B	451	GLU	3.8
1	A	23	ASN	3.8
1	B	443	ASP	3.8
1	B	201	GLU	3.7
1	A	349	GLU	3.7
1	A	673	ARG	3.7
1	B	29	SER	3.7
1	A	197	GLU	3.7
1	B	199	PHE	3.7
1	A	347	SER	3.6
1	B	198	ARG	3.5
1	B	304	THR	3.5
1	A	198	ARG	3.5
1	A	359	ASP	3.4
1	B	350	LEU	3.4
1	B	455	ASP	3.4
1	A	22	SER	3.4
1	B	522	ARG	3.4
1	A	212	SER	3.4
1	B	354	VAL	3.4
1	B	444	GLU	3.3
1	B	638	ASP	3.3
1	A	184	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	42	ASP	3.3
1	A	593	THR	3.3
1	B	347	SER	3.3
1	B	514	ILE	3.3
1	A	672	ASP	3.2
1	B	520	ASP	3.2
1	B	348	GLU	3.2
1	B	329	TYR	3.2
1	B	271	GLU	3.1
1	B	291	GLN	3.1
1	A	665	GLU	3.1
1	B	215	GLY	3.0
1	A	185	VAL	3.0
1	A	30	LYS	3.0
1	B	48	ASP	3.0
1	A	306	GLY	2.9
1	A	517	GLU	2.9
1	B	593	THR	2.9
1	A	18	LYS	2.9
1	B	204	GLU	2.9
1	B	630	ASP	2.9
1	A	196	GLN	2.9
1	A	214	MET	2.9
1	B	211	ALA	2.8
1	A	217	ILE	2.8
1	B	517	GLU	2.8
1	B	279	GLU	2.8
1	B	525	GLY	2.7
1	B	552	ASP	2.7
1	B	206	GLN	2.7
1	B	727	ARG	2.7
1	B	30	LYS	2.7
1	A	111	ALA	2.6
1	B	169	PHE	2.6
1	B	518	PHE	2.6
1	B	503	GLN	2.6
1	B	526	THR	2.5
1	A	186	ASN	2.5
1	B	231	GLU	2.5
1	B	679	LYS	2.5
1	B	351	LYS	2.5
1	A	24	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	436	ALA	2.5
1	B	364	GLN	2.5
1	A	268	ASP	2.4
1	B	308	GLU	2.4
1	B	225	ASP	2.4
1	B	186	ASN	2.4
1	B	363	LYS	2.4
1	A	390	GLU	2.4
1	B	359	ASP	2.4
1	B	313	GLN	2.4
1	A	77	ASP	2.4
1	A	503	GLN	2.3
1	A	307	ILE	2.3
1	B	332	GLU	2.3
1	B	49	ASP	2.3
1	B	335	LYS	2.3
1	B	438	TYR	2.3
1	B	415	GLU	2.3
1	B	591	ASP	2.3
1	A	98	ALA	2.2
1	A	275	GLY	2.2
1	A	363	LYS	2.2
1	B	527	GLN	2.2
1	A	34	GLU	2.1
1	A	630	ASP	2.1
1	A	558	GLU	2.1
1	A	681	GLU	2.1
1	B	352	ASN	2.1
1	A	455	ASP	2.1
1	B	439	ASP	2.1
1	A	210	GLY	2.1
1	A	679	LYS	2.1
1	A	49	ASP	2.0
1	A	397	MET	2.0
1	B	330	GLU	2.0
1	B	452	GLU	2.0
1	A	591	ASP	2.0
1	A	639	GLU	2.0
1	B	666	HIS	2.0
1	B	125	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

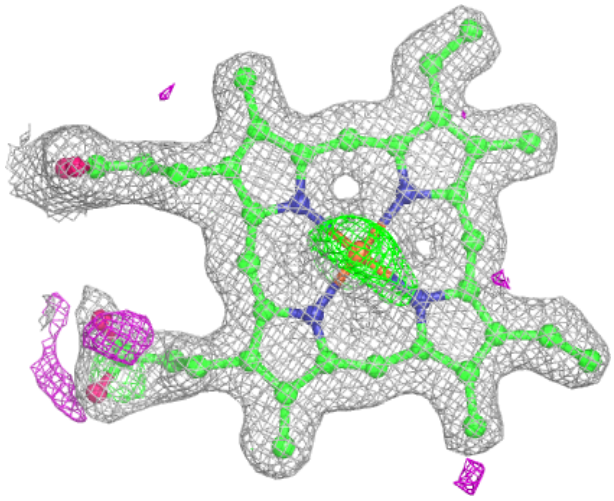
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

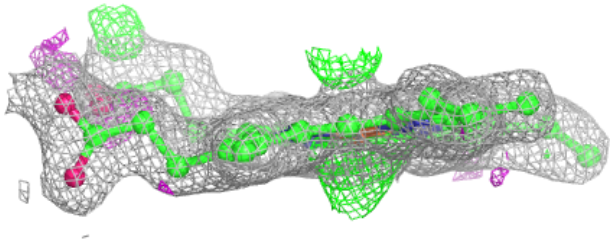
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SHA	A	801	11/11	0.47	0.53	52,52,52,53	11
3	SHA	B	801	11/11	0.67	0.25	49,51,51,51	11
2	HEM	A	800	43/43	0.96	0.15	15,21,30,39	0
2	HEM	B	800	43/43	0.96	0.12	21,29,36,39	0

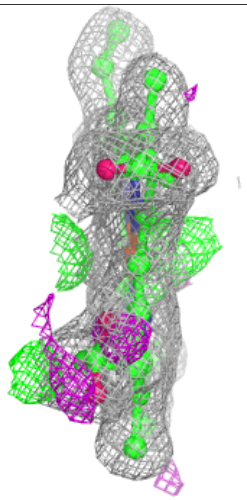
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 800:

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

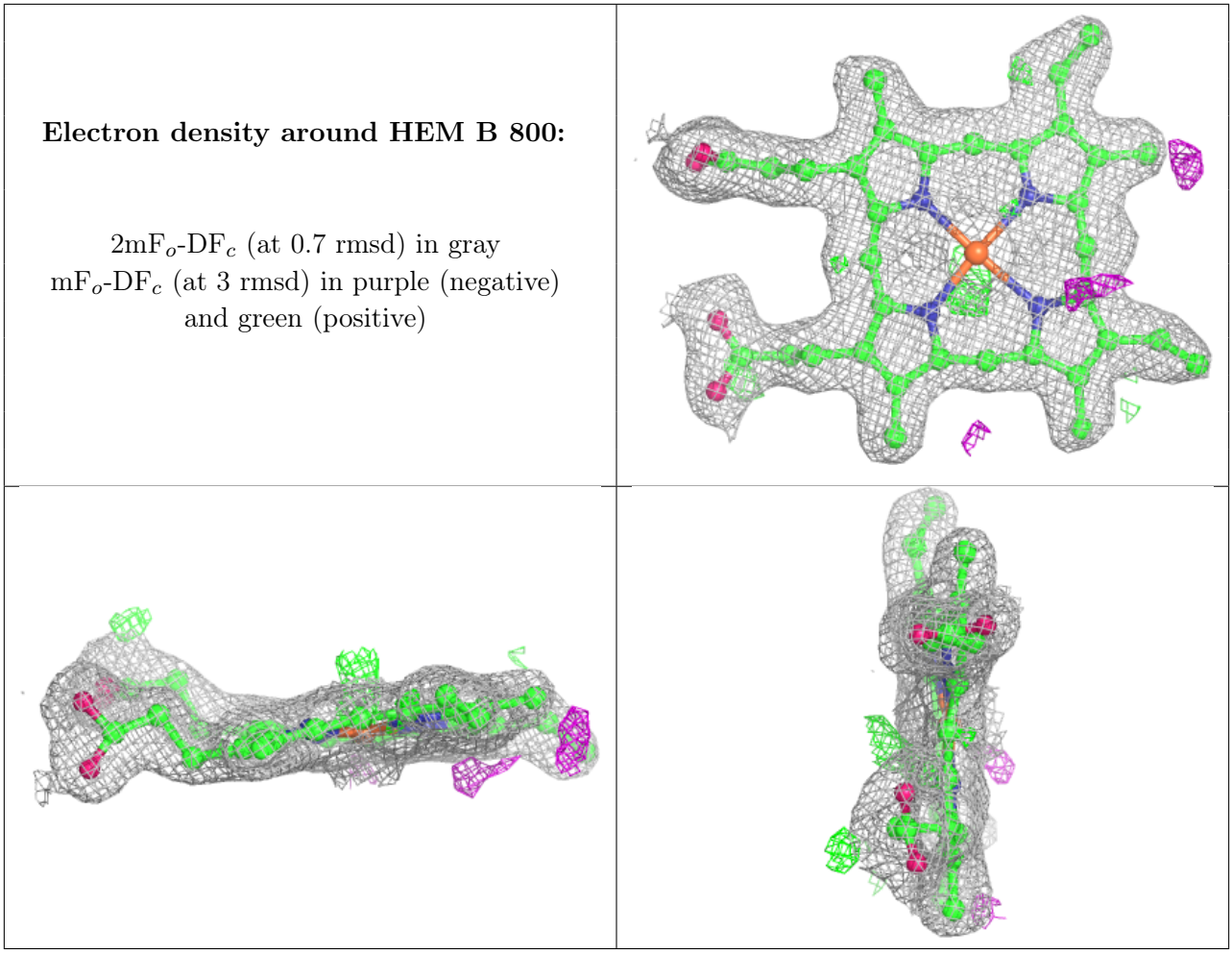






Electron density around HEM B 800:

$2mF_o$-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

There are no such residues in this entry.