



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:40 pm BST

PDB ID : 3QJT
Title : The structure of and photolytic induced changes of carbon monoxide binding to the cytochrome ba3-oxidase from *Thermus thermophilus*
Authors : Liu, B.; Zhang, Y.; Sage, J.T.; Doukov, T.; Chen, Y.; Stout, C.D.; Fee, J.A.
Deposited on : 2011-01-30
Resolution : 2.95 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 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 : 2.11
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) : 2.11

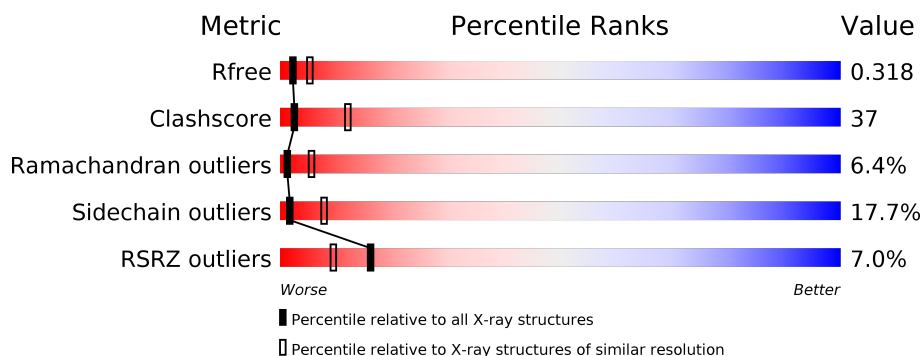
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	568	<div> <div>7%</div> <div> <div></div> <div>36%</div> <div>48%</div> <div>12%</div> <div>• •</div> </div> </div>
2	B	168	<div> <div>5%</div> <div> <div></div> <div>42%</div> <div>46%</div> <div>11%</div> <div>•</div> </div> </div>
3	C	34	<div> <div>9%</div> <div> <div></div> <div>59%</div> <div>26%</div> <div>12%</div> <div>•</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6079 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	4409	2985	709	699	16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	258	ARG	LYS	CONFLICT	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	166	1298	844	217	233	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	GLU	CONFLICT	UNP Q5SJ80

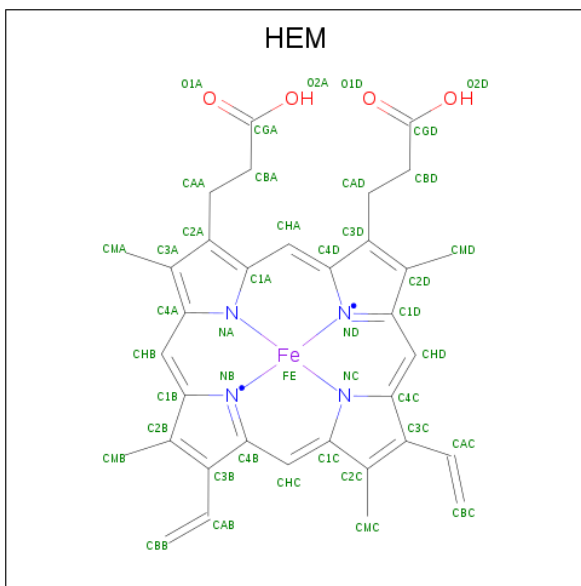
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

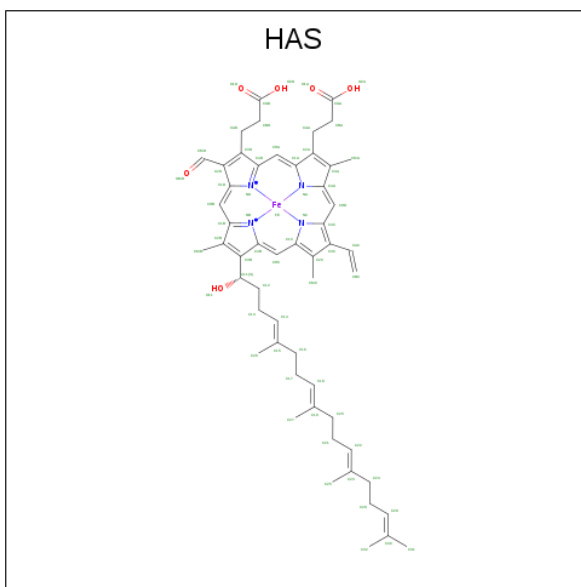
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	33	259	179	39	41	0	0	0

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

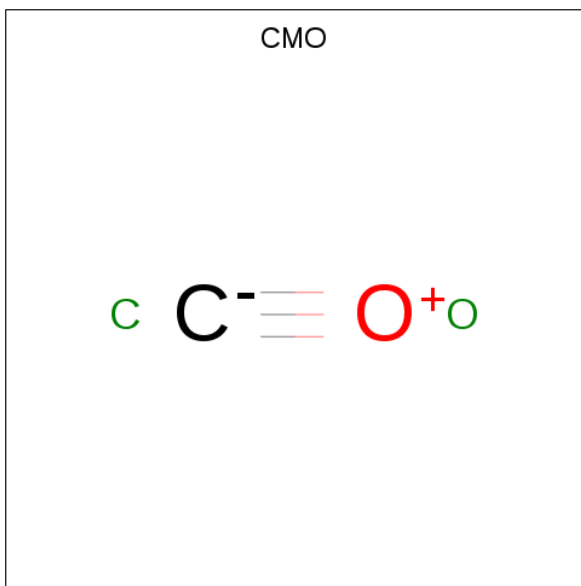
- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





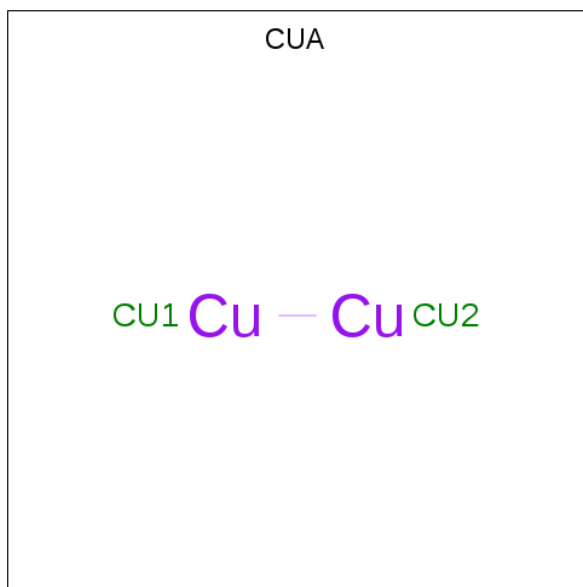
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C O	0	0
			2	1 1		

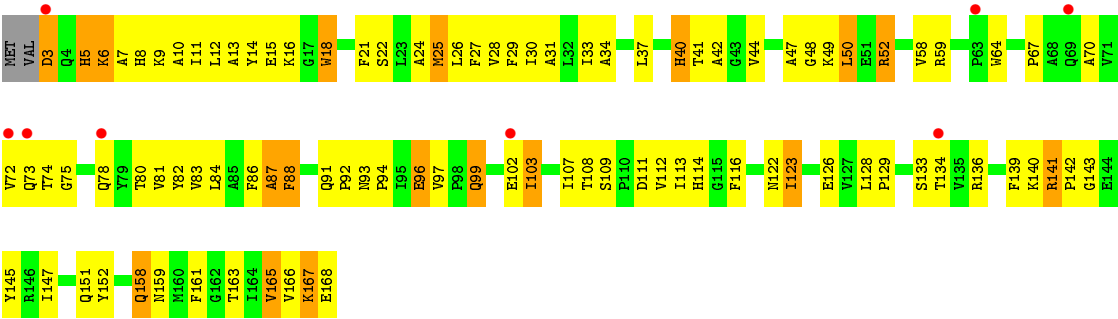
- Molecule 8 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



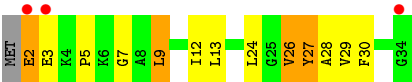
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cu	0	0
			2	2		

- Molecule 1: Cytochrome c oxidase subunit 1





● Molecule 3: Cytochrome c oxidase polypeptide 2A



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.96 Å 114.96 Å 148.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.62 – 2.95 19.62 – 2.95	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.62-2.95) 91.3 (19.62-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.93 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.258 , 0.323 0.258 , 0.318	Depositor DCC
R_{free} test set	976 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	91.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6079	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CMO, HEM, HAS, CUA, CU1

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	0.70	1/4566 (0.0%)	0.88	4/6266 (0.1%)
2	B	0.68	0/1335	0.86	0/1822
3	C	0.61	0/265	0.83	0/359
All	All	0.69	1/6166 (0.0%)	0.87	4/8447 (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	A	0	4
2	B	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	PRO	CA-C	5.56	1.64	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	348	ALA	C-N-CD	5.35	139.64	128.40
1	A	501	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	75	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	504	ALA	N-CA-C	5.07	124.69	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	492	LEU	Peptide
1	A	504	ALA	Peptide
1	A	505	PRO	Peptide
1	A	510	GLU	Peptide
2	B	87	ALA	Peptide

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	4409	0	4516	366	1
2	B	1298	0	1282	102	0
3	C	259	0	279	11	0
4	A	1	0	0	0	0
5	A	43	0	30	9	0
6	A	65	0	61	7	0
7	A	2	0	0	1	0
8	B	2	0	0	0	0
All	All	6079	0	6168	453	1

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 37.

All (453) 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:233:HIS:CD2	1:A:237:TYR:HE2	1.53	1.25
1:A:233:HIS:ND1	1:A:282:HIS:HE1	1.33	1.24
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.14	1.15
1:A:518:ARG:HH21	1:A:518:ARG:HG2	1.05	1.13
1:A:518:ARG:HH21	1:A:518:ARG:CG	1.57	1.13
1:A:233:HIS:NE2	1:A:237:TYR:HE2	1.45	1.13
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.37	1.11
1:A:120:ALA:O	1:A:123:PRO:HD2	1.49	1.11
1:A:34:VAL:O	1:A:37:LEU:HB2	1.54	1.06
2:B:9:LYS:HE2	2:B:9:LYS:HA	1.41	1.02
2:B:74:THR:HG23	2:B:78:GLN:HB3	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:CE1	1:A:282:HIS:HE1	1.85	0.92
2:B:97:VAL:HG11	2:B:103:ILE:HG21	1.51	0.92
1:A:56:LYS:O	1:A:60:PRO:HA	1.69	0.92
1:A:182:VAL:HG21	1:A:508:PHE:CE2	2.06	0.91
1:A:182:VAL:HG21	1:A:508:PHE:HE2	1.33	0.90
1:A:165:ASP:OD2	1:A:169:ARG:HD3	1.74	0.88
1:A:512:ILE:HG21	2:B:8:HIS:HB2	1.54	0.88
1:A:368:SER:HB3	2:B:33:ILE:HD11	1.57	0.87
1:A:225:ARG:NH2	1:A:287:ASP:OD2	2.08	0.87
1:A:233:HIS:CE1	1:A:282:HIS:CE1	2.58	0.86
1:A:506:LEU:HD23	1:A:506:LEU:H	1.40	0.86
1:A:518:ARG:NH2	1:A:518:ARG:HG2	1.81	0.86
1:A:156:THR:O	1:A:160:ILE:HG13	1.76	0.83
2:B:40:HIS:CD2	2:B:41:THR:HG23	2.15	0.82
1:A:92:LEU:HD22	1:A:506:LEU:CD1	2.10	0.82
1:A:518:ARG:CG	1:A:518:ARG:NH2	2.29	0.81
2:B:143:GLY:H	2:B:166:VAL:HG13	1.46	0.81
1:A:413:ILE:HG22	1:A:417:GLN:HB2	1.63	0.81
1:A:418:ARG:HH11	1:A:419:ARG:HH12	1.28	0.80
1:A:97:LEU:HD11	1:A:183:THR:OG1	1.82	0.80
1:A:192:MET:HB2	1:A:273:LEU:HB2	1.62	0.80
1:A:36:SER:N	1:A:76:ASN:HD21	1.79	0.80
1:A:413:ILE:HG22	1:A:417:GLN:CB	2.11	0.80
1:A:417:GLN:HG2	1:A:491:VAL:HG23	1.64	0.80
1:A:406:PRO:HG3	1:A:413:ILE:HD11	1.63	0.80
1:A:284:GLN:HG2	1:A:287:ASP:OD1	1.82	0.80
1:A:368:SER:CB	2:B:33:ILE:HD11	2.11	0.80
1:A:466:PRO:O	1:A:469:PHE:HB2	1.85	0.77
1:A:310:LEU:HD13	2:B:22:SER:OG	1.85	0.77
1:A:32:LEU:O	1:A:36:SER:HB2	1.86	0.76
1:A:418:ARG:HH11	1:A:419:ARG:NH1	1.84	0.76
1:A:463:ALA:O	1:A:467:MET:HB2	1.87	0.75
1:A:280:GLY:HA3	1:A:542:TYR:OH	1.87	0.74
1:A:518:ARG:HH21	1:A:518:ARG:HG3	1.52	0.74
1:A:241:LEU:HA	1:A:244:TYR:HB2	1.71	0.73
1:A:9:SER:C	1:A:11:VAL:H	1.90	0.73
1:A:221:PRO:HA	1:A:224:ALA:HB3	1.69	0.73
1:A:96:GLU:HG2	1:A:96:GLU:O	1.88	0.72
2:B:111:ASP:OD2	2:B:112:VAL:HG22	1.90	0.72
2:B:86:PHE:O	2:B:88:PHE:N	2.20	0.72
1:A:250:ILE:HD13	1:A:403:TRP:CH2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:TYR:O	3:C:30:PHE:HB3	1.89	0.72
1:A:291:ASP:OD2	1:A:293:THR:HB	1.88	0.72
1:A:24:PHE:CE2	1:A:86:GLN:HB2	2.25	0.71
1:A:178:VAL:HG12	1:A:179:THR:N	2.05	0.71
1:A:78:ILE:O	1:A:82:GLN:HB2	1.91	0.71
1:A:337:ARG:O	1:A:337:ARG:HG3	1.89	0.71
1:A:506:LEU:HD23	1:A:506:LEU:N	2.05	0.71
1:A:12:TYR:HB3	1:A:19:LYS:HD2	1.71	0.70
1:A:389:VAL:HB	6:A:801:HAS:HBC2	1.74	0.70
2:B:40:HIS:HD2	2:B:41:THR:N	1.89	0.70
1:A:500:GLU:CD	1:A:501:LEU:H	1.95	0.70
2:B:158:GLN:N	2:B:158:GLN:NE2	2.41	0.69
1:A:233:HIS:O	1:A:234:PRO:C	2.29	0.69
1:A:500:GLU:CG	1:A:501:LEU:H	2.03	0.69
1:A:253:LYS:O	1:A:255:ALA:N	2.27	0.68
1:A:85:ALA:O	1:A:89:MET:HB2	1.94	0.68
1:A:271:LEU:O	1:A:275:LEU:HD12	1.94	0.67
1:A:253:LYS:C	1:A:255:ALA:H	1.95	0.67
1:A:264:MET:SD	2:B:15:GLU:HG2	2.35	0.67
2:B:8:HIS:HA	2:B:11:ILE:HD12	1.76	0.67
1:A:282:HIS:HA	1:A:285:PHE:CE1	2.31	0.66
2:B:27:PHE:O	2:B:31:ALA:N	2.25	0.66
2:B:74:THR:CG2	2:B:78:GLN:HB3	2.25	0.66
2:B:40:HIS:CD2	2:B:41:THR:CG2	2.77	0.66
1:A:122:LEU:O	1:A:123:PRO:C	2.34	0.66
1:A:189:PHE:CE1	1:A:242:PRO:HD3	2.29	0.66
2:B:40:HIS:HD2	2:B:41:THR:HG23	1.57	0.66
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.31	0.66
1:A:201:VAL:O	1:A:205:VAL:HG23	1.96	0.65
1:A:261:SER:OG	1:A:263:PRO:HD2	1.96	0.65
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.31	0.65
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.09	0.65
2:B:59:ARG:O	2:B:59:ARG:HG3	1.97	0.64
1:A:178:VAL:CG1	1:A:179:THR:N	2.59	0.64
1:A:195:LEU:O	1:A:198:LEU:HD12	1.97	0.64
1:A:389:VAL:HG13	5:A:800:HEM:HBC2	1.79	0.64
1:A:418:ARG:NH1	1:A:419:ARG:HH12	1.94	0.64
1:A:503:GLU:O	1:A:504:ALA:HB2	1.96	0.64
1:A:407:ASN:ND2	1:A:504:ALA:HB3	2.13	0.64
1:A:120:ALA:HB2	1:A:148:GLY:HA3	1.78	0.64
2:B:158:GLN:HE21	2:B:159:ASN:N	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:GLU:HA	2:B:165:VAL:O	1.98	0.64
1:A:131:VAL:HG23	1:A:135:PHE:HA	1.80	0.63
1:A:52:TYR:N	1:A:53:PRO:CD	2.61	0.63
1:A:36:SER:H	1:A:76:ASN:HD21	1.45	0.63
1:A:386:HIS:CE1	5:A:800:HEM:C1A	2.88	0.62
1:A:95:ARG:HH11	1:A:505:PRO:HD3	1.64	0.62
2:B:147:ILE:O	2:B:161:PHE:HA	1.98	0.62
2:B:9:LYS:HE2	2:B:9:LYS:CA	2.25	0.62
1:A:32:LEU:HB2	1:A:80:PHE:CD1	2.34	0.62
2:B:8:HIS:HA	2:B:11:ILE:CD1	2.31	0.61
2:B:9:LYS:HA	2:B:9:LYS:CE	2.21	0.61
1:A:285:PHE:O	1:A:295:LYS:NZ	2.31	0.61
2:B:97:VAL:CG1	2:B:103:ILE:HG21	2.28	0.61
1:A:194:PHE:HA	1:A:197:SER:OG	2.01	0.61
1:A:215:LEU:O	1:A:216:VAL:HG13	2.01	0.61
1:A:300:VAL:HG13	2:B:30:ILE:CD1	2.31	0.61
1:A:40:PRO:HA	1:A:43:ALA:HB3	1.81	0.61
1:A:59:LEU:HB3	1:A:61:PHE:CE1	2.36	0.61
1:A:106:MET:HG3	1:A:106:MET:O	2.00	0.60
1:A:213:PHE:HB3	1:A:215:LEU:HD13	1.82	0.60
1:A:255:ALA:HB2	1:A:346:PHE:CD1	2.36	0.60
2:B:40:HIS:CD2	2:B:41:THR:N	2.69	0.60
1:A:310:LEU:O	1:A:313:ALA:HB3	2.01	0.60
1:A:462:HIS:N	1:A:462:HIS:ND1	2.50	0.60
1:A:518:ARG:NH2	1:A:518:ARG:HG3	2.13	0.60
1:A:288:PRO:HB3	2:B:133:SER:HA	1.82	0.60
1:A:410:GLY:HA2	1:A:502:ALA:HB2	1.84	0.59
1:A:209:LEU:O	1:A:213:PHE:HB2	2.02	0.59
3:C:26:VAL:O	3:C:29:VAL:N	2.34	0.59
1:A:496:GLU:C	1:A:498:LYS:H	2.05	0.59
2:B:18:TRP:HA	2:B:18:TRP:CE3	2.37	0.59
1:A:9:SER:C	1:A:11:VAL:N	2.55	0.59
1:A:386:HIS:HE1	5:A:800:HEM:C1A	2.21	0.59
1:A:554:ASN:HD22	2:B:52:ARG:CG	2.16	0.59
2:B:12:LEU:O	2:B:16:LYS:HG3	2.03	0.59
1:A:330:ARG:HD2	1:A:331:GLY:H	1.68	0.58
1:A:500:GLU:CG	1:A:501:LEU:N	2.66	0.58
2:B:158:GLN:N	2:B:158:GLN:HE21	2.01	0.58
1:A:463:ALA:O	1:A:465:VAL:N	2.37	0.58
3:C:26:VAL:O	3:C:28:ALA:N	2.36	0.58
1:A:512:ILE:CG2	2:B:8:HIS:HB2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:HG23	1:A:135:PHE:HB3	1.86	0.58
1:A:156:THR:CB	1:A:193:TRP:HE1	2.16	0.58
2:B:40:HIS:HD2	2:B:41:THR:CG2	2.15	0.58
1:A:12:TYR:CD1	1:A:19:LYS:HB2	2.39	0.58
1:A:506:LEU:CD2	1:A:506:LEU:H	2.14	0.58
1:A:227:LEU:O	1:A:230:TRP:HB3	2.04	0.57
1:A:413:ILE:HG22	1:A:417:GLN:HB3	1.84	0.57
1:A:414:SER:N	1:A:417:GLN:OE1	2.37	0.57
1:A:330:ARG:HD2	1:A:330:ARG:N	2.20	0.57
1:A:120:ALA:O	1:A:123:PRO:CD	2.39	0.57
1:A:131:VAL:HG23	1:A:135:PHE:CB	2.35	0.57
1:A:466:PRO:O	1:A:469:PHE:N	2.38	0.57
1:A:220:ASP:OD2	2:B:52:ARG:NH1	2.38	0.57
1:A:233:HIS:HD2	1:A:237:TYR:CE2	2.13	0.57
1:A:42:GLN:OE1	1:A:69:LEU:HA	2.04	0.57
1:A:106:MET:HA	1:A:162:ILE:HD11	1.86	0.57
1:A:321:GLU:OE2	3:C:5:PRO:HA	2.05	0.56
1:A:178:VAL:CG1	1:A:179:THR:H	2.18	0.56
1:A:239:TRP:HE3	6:A:801:HAS:CBC	2.19	0.56
1:A:430:LEU:O	1:A:434:ILE:HG13	2.06	0.56
1:A:281:PHE:O	1:A:284:GLN:N	2.36	0.56
3:C:9:LEU:HA	3:C:12:ILE:CG1	2.36	0.56
1:A:165:ASP:OD2	1:A:169:ARG:CD	2.52	0.56
1:A:112:MET:HB2	1:A:155:SER:HB2	1.88	0.55
1:A:307:VAL:HA	1:A:310:LEU:HD12	1.87	0.55
1:A:21:THR:O	1:A:24:PHE:N	2.39	0.55
1:A:76:ASN:HB3	5:A:800:HEM:HAC	1.88	0.55
2:B:67:PRO:HB3	2:B:91:GLN:HG2	1.88	0.55
1:A:233:HIS:HE2	1:A:237:TYR:HH	1.54	0.55
2:B:80:THR:HG21	2:B:82:TYR:CE1	2.42	0.55
6:A:801:HAS:C1D	7:A:563:CMO:C	2.69	0.55
2:B:18:TRP:HA	2:B:18:TRP:HE3	1.70	0.54
2:B:6:LYS:O	2:B:7:ALA:C	2.45	0.54
3:C:26:VAL:O	3:C:27:TYR:C	2.46	0.54
3:C:9:LEU:HA	3:C:12:ILE:HG12	1.89	0.54
1:A:79:VAL:HA	1:A:152:PHE:HZ	1.71	0.54
1:A:211:TRP:HZ2	1:A:558:GLY:HA2	1.72	0.54
1:A:163:VAL:HG21	1:A:190:TRP:CD1	2.42	0.54
2:B:10:ALA:O	2:B:14:TYR:HD1	1.90	0.54
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.88	0.54
1:A:173:ALA:C	1:A:175:PRO:HD3	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLY:HA3	1:A:392:LEU:HD12	1.89	0.54
1:A:463:ALA:HB3	1:A:467:MET:HE1	1.90	0.54
1:A:92:LEU:HD22	1:A:506:LEU:HD13	1.87	0.54
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.43	0.54
1:A:253:LYS:C	1:A:255:ALA:N	2.60	0.54
1:A:282:HIS:NE2	1:A:283:HIS:CD2	2.76	0.54
1:A:390:ALA:O	1:A:394:THR:HB	2.09	0.54
1:A:68:GLY:O	1:A:70:THR:N	2.41	0.54
2:B:143:GLY:N	2:B:166:VAL:HG13	2.20	0.54
1:A:192:MET:HG3	1:A:273:LEU:HA	1.90	0.53
1:A:281:PHE:O	1:A:282:HIS:C	2.46	0.53
1:A:290:ILE:O	1:A:295:LYS:HE3	2.08	0.53
1:A:23:TYR:HD1	1:A:107:TRP:HH2	1.56	0.53
1:A:40:PRO:HA	1:A:43:ALA:CB	2.39	0.53
1:A:95:ARG:C	1:A:97:LEU:H	2.12	0.53
2:B:50:LEU:HD22	2:B:52:ARG:CZ	2.39	0.53
1:A:24:PHE:CD2	1:A:86:GLN:HB2	2.43	0.53
1:A:311:MET:O	1:A:314:PHE:N	2.36	0.53
1:A:41:PHE:CE2	1:A:55:LEU:HB2	2.44	0.52
1:A:138:PRO:HG3	2:B:129:PRO:HG2	1.90	0.52
1:A:420:LEU:O	1:A:421:GLY:C	2.47	0.52
1:A:506:LEU:O	1:A:508:PHE:N	2.42	0.52
1:A:82:GLN:NE2	1:A:86:GLN:OE1	2.43	0.52
1:A:64:SER:HB2	1:A:67:GLN:H	1.74	0.52
1:A:252:PRO:O	1:A:257:GLY:N	2.43	0.52
2:B:74:THR:HG23	2:B:78:GLN:CB	2.30	0.52
1:A:401:LEU:O	1:A:405:LEU:HB2	2.10	0.52
1:A:95:ARG:HA	1:A:95:ARG:NH2	2.25	0.52
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.40	0.52
1:A:314:PHE:CZ	2:B:14:TYR:HB3	2.45	0.52
2:B:158:GLN:NE2	2:B:158:GLN:H	2.05	0.52
1:A:213:PHE:HB3	1:A:215:LEU:CD1	2.40	0.52
1:A:447:VAL:HG11	1:A:453:ILE:HD13	1.91	0.51
1:A:200:LEU:HB2	1:A:231:THR:HG21	1.92	0.51
1:A:330:ARG:N	1:A:330:ARG:CD	2.74	0.51
1:A:400:SER:HA	1:A:403:TRP:HE1	1.76	0.51
2:B:29:PHE:O	2:B:30:ILE:C	2.47	0.51
1:A:327:ARG:HB2	1:A:338:ALA:HB1	1.93	0.51
1:A:463:ALA:HB3	1:A:467:MET:CE	2.40	0.51
1:A:230:TRP:O	1:A:234:PRO:HD2	2.11	0.51
1:A:92:LEU:HD23	1:A:92:LEU:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ALA:O	2:B:16:LYS:HB2	2.11	0.51
1:A:456:VAL:O	1:A:456:VAL:HG23	2.12	0.50
1:A:156:THR:O	1:A:160:ILE:CG1	2.54	0.50
1:A:189:PHE:HE1	1:A:242:PRO:HD3	1.75	0.50
1:A:196:ALA:CB	1:A:234:PRO:HG2	2.42	0.50
1:A:27:LEU:HB3	1:A:83:LEU:HD13	1.92	0.50
1:A:21:THR:O	1:A:24:PHE:HB2	2.11	0.50
1:A:463:ALA:HB1	1:A:467:MET:HE3	1.94	0.50
1:A:234:PRO:O	1:A:237:TYR:N	2.45	0.50
1:A:463:ALA:CB	1:A:467:MET:CE	2.90	0.50
1:A:300:VAL:HG13	2:B:30:ILE:HD13	1.92	0.50
1:A:504:ALA:O	1:A:506:LEU:HD23	2.12	0.50
2:B:113:ILE:CG2	2:B:151:GLN:HG2	2.42	0.49
2:B:83:VAL:HB	2:B:107:ILE:HG12	1.94	0.49
1:A:406:PRO:O	1:A:408:LEU:N	2.45	0.49
2:B:34:ALA:HA	2:B:37:LEU:HB2	1.93	0.49
1:A:91:TYR:CZ	1:A:95:ARG:HD3	2.48	0.49
1:A:12:TYR:CB	1:A:19:LYS:HD2	2.41	0.49
1:A:67:GLN:HA	1:A:130:THR:HG23	1.93	0.49
1:A:366:ASN:HB3	6:A:801:HAS:HMD	1.94	0.49
1:A:192:MET:O	1:A:195:LEU:N	2.46	0.49
1:A:379:ALA:HA	1:A:382:PRO:HG2	1.93	0.49
1:A:101:PRO:O	1:A:103:MET:HG2	2.13	0.49
1:A:23:TYR:HD1	1:A:107:TRP:CH2	2.31	0.49
1:A:185:MET:O	1:A:188:VAL:HG22	2.13	0.49
1:A:350:VAL:O	1:A:354:LEU:HD22	2.13	0.49
2:B:40:HIS:HD2	2:B:41:THR:H	1.60	0.49
1:A:102:ASN:OD1	1:A:105:LEU:HB2	2.13	0.49
2:B:113:ILE:HG22	2:B:151:GLN:HG2	1.95	0.49
1:A:526:ARG:HB3	1:A:529:PHE:HB3	1.95	0.48
1:A:59:LEU:HD23	1:A:59:LEU:N	2.27	0.48
1:A:82:GLN:O	1:A:86:GLN:HG3	2.12	0.48
2:B:107:ILE:HD11	2:B:116:PHE:CE2	2.48	0.48
2:B:64:TRP:CZ2	2:B:82:TYR:HD2	2.31	0.48
1:A:149:ALA:O	1:A:153:VAL:HB	2.12	0.48
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.48	0.48
1:A:247:ILE:HD13	1:A:353:LEU:HD11	1.95	0.48
1:A:316:VAL:O	1:A:317:ALA:C	2.51	0.48
2:B:97:VAL:O	2:B:166:VAL:HA	2.13	0.48
1:A:131:VAL:CG2	1:A:135:PHE:HB3	2.42	0.48
1:A:418:ARG:NH1	1:A:419:ARG:NH1	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLU:C	1:A:498:LYS:N	2.67	0.48
1:A:552:HIS:HD1	1:A:552:HIS:N	2.11	0.48
1:A:552:HIS:ND1	1:A:552:HIS:N	2.61	0.48
1:A:81:THR:HB	1:A:239:TRP:CD1	2.48	0.48
1:A:87:ALA:O	1:A:88:ILE:C	2.51	0.48
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.50	0.47
1:A:156:THR:HB	1:A:193:TRP:HE1	1.78	0.47
1:A:288:PRO:HG3	2:B:133:SER:OG	2.14	0.47
2:B:3:ASP:OD1	3:C:2:GLU:N	2.47	0.47
1:A:449:ARG:NH1	6:A:801:HAS:CGA	2.77	0.47
1:A:24:PHE:HE2	1:A:86:GLN:CD	2.18	0.47
2:B:140:LYS:O	2:B:141:ARG:CB	2.61	0.47
1:A:158:VAL:O	1:A:161:TYR:HB3	2.14	0.47
1:A:301:LEU:O	1:A:304:PHE:HB2	2.15	0.47
1:A:386:HIS:HE1	5:A:800:HEM:C4D	2.33	0.47
1:A:91:TYR:OH	1:A:95:ARG:HD3	2.14	0.47
1:A:321:GLU:OE1	3:C:7:GLY:N	2.47	0.47
2:B:18:TRP:O	2:B:22:SER:HB3	2.15	0.47
1:A:24:PHE:CD1	1:A:110:TRP:HD1	2.33	0.47
1:A:330:ARG:HD2	1:A:334:GLY:HA3	1.97	0.47
1:A:68:GLY:O	1:A:69:LEU:C	2.53	0.47
2:B:109:SER:HB3	2:B:129:PRO:HA	1.97	0.47
1:A:38:PHE:O	1:A:41:PHE:HB2	2.15	0.47
1:A:32:LEU:HG	1:A:32:LEU:O	2.15	0.46
1:A:52:TYR:N	1:A:53:PRO:HD3	2.30	0.46
1:A:23:TYR:CD1	1:A:107:TRP:HH2	2.33	0.46
1:A:184:TYR:HE1	1:A:527:ILE:HD11	1.80	0.46
1:A:74:VAL:HG22	1:A:78:ILE:HD12	1.96	0.46
1:A:370:THR:HA	1:A:373:TYR:CD1	2.51	0.46
2:B:47:ALA:HB2	2:B:134:THR:HB	1.95	0.46
1:A:356:PHE:CD1	1:A:388:GLN:NE2	2.84	0.46
1:A:387:LEU:O	1:A:391:SER:HB3	2.15	0.46
1:A:518:ARG:O	1:A:522:LEU:HB2	2.16	0.46
1:A:121:ALA:O	1:A:125:LEU:HG	2.16	0.46
1:A:137:PRO:HG2	1:A:224:ALA:HB1	1.97	0.46
1:A:379:ALA:HB1	1:A:439:LEU:HD12	1.98	0.46
1:A:233:HIS:C	1:A:233:HIS:CD2	2.88	0.46
1:A:532:ALA:O	1:A:536:ILE:N	2.47	0.46
1:A:242:PRO:O	1:A:246:ILE:HG13	2.16	0.46
1:A:52:TYR:CD1	1:A:52:TYR:N	2.83	0.46
2:B:113:ILE:CG2	2:B:114:HIS:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASN:HD22	2:B:52:ARG:HG2	1.81	0.46
1:A:23:TYR:C	1:A:110:TRP:HE1	2.18	0.46
1:A:397:ALA:O	1:A:400:SER:HB3	2.15	0.46
1:A:159:SER:HA	1:A:162:ILE:HD12	1.99	0.45
1:A:292:PRO:HD3	2:B:48:GLY:HA2	1.97	0.45
1:A:300:VAL:HG13	2:B:30:ILE:HD11	1.98	0.45
2:B:99:GLN:HG2	2:B:168:GLU:O	2.16	0.45
1:A:66:TYR:CD2	2:B:152:TYR:CE1	3.04	0.45
1:A:68:GLY:C	1:A:70:THR:N	2.68	0.45
1:A:9:SER:O	1:A:9:SER:OG	2.31	0.45
1:A:339:LEU:HB3	1:A:346:PHE:CE2	2.51	0.45
1:A:554:ASN:HD22	2:B:52:ARG:HG3	1.80	0.45
1:A:112:MET:CB	1:A:155:SER:HB2	2.46	0.45
1:A:234:PRO:HG3	1:A:277:THR:HA	1.98	0.45
1:A:270:LEU:O	1:A:274:LEU:HD13	2.17	0.45
1:A:76:ASN:O	1:A:80:PHE:HB3	2.16	0.45
1:A:209:LEU:N	1:A:210:PRO:HD2	2.31	0.45
1:A:343:ASN:HA	1:A:344:PRO:HD2	1.85	0.45
1:A:398:MET:O	1:A:401:LEU:HB2	2.16	0.45
1:A:517:ASP:O	1:A:521:VAL:HG23	2.16	0.45
2:B:142:PRO:HG3	2:B:168:GLU:OE1	2.16	0.45
1:A:123:PRO:HG3	1:A:144:ALA:HB3	1.98	0.45
1:A:233:HIS:NE2	1:A:237:TYR:OH	2.41	0.45
1:A:445:LEU:O	1:A:446:ASN:HB2	2.17	0.45
2:B:40:HIS:C	2:B:42:ALA:H	2.21	0.45
1:A:131:VAL:HG23	1:A:135:PHE:CA	2.45	0.45
1:A:342:ASP:HB2	1:A:418:ARG:NH2	2.31	0.44
2:B:167:LYS:O	2:B:168:GLU:C	2.56	0.44
1:A:427:LEU:HB3	1:A:480:ALA:HB2	1.99	0.44
1:A:134:THR:HA	1:A:228:PHE:CZ	2.52	0.44
1:A:32:LEU:HB2	1:A:80:PHE:CG	2.52	0.44
1:A:513:SER:HB3	2:B:5:HIS:CE1	2.53	0.44
1:A:236:VAL:HA	1:A:239:TRP:CE3	2.53	0.44
1:A:442:ALA:HB1	1:A:447:VAL:CG2	2.47	0.44
2:B:103:ILE:HG13	2:B:139:PHE:CE1	2.53	0.44
1:A:131:VAL:CG2	1:A:135:PHE:CB	2.96	0.44
1:A:20:ALA:O	1:A:21:THR:C	2.56	0.44
1:A:331:GLY:O	1:A:332:LEU:C	2.55	0.44
1:A:332:LEU:HG	1:A:333:PHE:CE1	2.52	0.44
1:A:65:TYR:OH	5:A:800:HEM:O1A	2.34	0.44
2:B:107:ILE:CD1	2:B:116:PHE:CD2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HA	1:A:162:ILE:CD1	2.48	0.44
1:A:9:SER:O	1:A:11:VAL:N	2.50	0.44
1:A:141:GLY:O	1:A:142:HIS:C	2.56	0.44
1:A:196:ALA:HB2	1:A:234:PRO:HG2	1.99	0.44
1:A:92:LEU:HD13	1:A:250:ILE:HD11	2.00	0.44
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.89	0.44
1:A:339:LEU:HG	1:A:346:PHE:CZ	2.53	0.44
1:A:88:ILE:HG22	1:A:89:MET:SD	2.58	0.44
1:A:369:PHE:HB3	1:A:370:THR:H	1.31	0.43
1:A:385:PHE:HB3	6:A:801:HAS:C3A	2.48	0.43
1:A:386:HIS:HE1	5:A:800:HEM:CHA	2.30	0.43
1:A:30:LEU:O	1:A:34:VAL:HG23	2.18	0.43
2:B:128:LEU:O	2:B:129:PRO:C	2.55	0.43
2:B:59:ARG:CG	2:B:59:ARG:O	2.66	0.43
1:A:29:PHE:HE2	1:A:398:MET:HA	1.82	0.43
1:A:38:PHE:O	1:A:39:GLY:C	2.57	0.43
1:A:52:TYR:HH	1:A:65:TYR:HD1	1.64	0.43
2:B:141:ARG:HE	2:B:141:ARG:HB3	1.50	0.43
1:A:311:MET:O	1:A:312:THR:C	2.56	0.43
1:A:330:ARG:H	1:A:330:ARG:HD2	1.81	0.43
1:A:400:SER:HA	1:A:403:TRP:NE1	2.34	0.43
1:A:476:VAL:O	1:A:479:VAL:HB	2.19	0.43
2:B:109:SER:HB3	2:B:129:PRO:CA	2.48	0.43
1:A:116:GLY:O	1:A:117:LEU:C	2.55	0.43
1:A:412:PRO:C	1:A:413:ILE:HD13	2.39	0.43
1:A:463:ALA:O	1:A:464:ALA:C	2.56	0.43
2:B:21:PHE:O	2:B:24:ALA:HB3	2.19	0.43
2:B:70:ALA:O	2:B:81:VAL:HA	2.18	0.43
2:B:91:GLN:HA	2:B:92:PRO:HA	1.74	0.43
1:A:66:TYR:OH	2:B:158:GLN:HB3	2.18	0.43
1:A:239:TRP:CE3	1:A:389:VAL:HG21	2.53	0.43
1:A:422:LEU:HD12	1:A:422:LEU:H	1.83	0.43
2:B:93:ASN:HA	2:B:94:PRO:HA	1.77	0.43
1:A:115:ILE:O	1:A:119:VAL:HG23	2.18	0.43
2:B:107:ILE:HG22	2:B:108:THR:N	2.34	0.43
1:A:196:ALA:HB2	1:A:234:PRO:CG	2.48	0.42
1:A:260:VAL:HB	2:B:11:ILE:HD13	2.01	0.42
1:A:311:MET:HA	2:B:18:TRP:CD1	2.54	0.42
1:A:388:GLN:HA	1:A:388:GLN:NE2	2.35	0.42
1:A:197:SER:O	1:A:201:VAL:HB	2.18	0.42
1:A:413:ILE:CG2	1:A:417:GLN:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HG12	1:A:246:ILE:HD11	2.01	0.42
2:B:86:PHE:HE2	2:B:91:GLN:HB2	1.85	0.42
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.54	0.42
1:A:331:GLY:O	1:A:334:GLY:N	2.53	0.42
1:A:482:LEU:N	1:A:482:LEU:HD23	2.35	0.42
1:A:503:GLU:O	1:A:504:ALA:CB	2.64	0.42
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.55	0.42
2:B:122:ASN:O	2:B:123:ILE:C	2.58	0.42
1:A:23:TYR:HA	1:A:23:TYR:HD2	1.75	0.42
1:A:342:ASP:HB2	1:A:418:ARG:HH21	1.85	0.42
1:A:290:ILE:O	1:A:290:ILE:HG22	2.20	0.42
1:A:48:ASN:HD21	1:A:457:PRO:HA	1.85	0.42
1:A:44:LEU:C	1:A:47:GLY:H	2.23	0.42
1:A:386:HIS:CE1	5:A:800:HEM:C4D	3.07	0.42
1:A:122:LEU:HB2	1:A:123:PRO:HD3	2.02	0.42
1:A:24:PHE:CE2	1:A:86:GLN:CB	2.99	0.42
1:A:404:LEU:HA	1:A:404:LEU:HD12	1.82	0.42
1:A:427:LEU:HA	1:A:427:LEU:HD23	1.58	0.42
1:A:464:ALA:O	1:A:467:MET:HB3	2.19	0.42
2:B:13:ALA:HA	2:B:16:LYS:HG3	2.02	0.42
2:B:14:TYR:O	2:B:15:GLU:C	2.59	0.42
2:B:158:GLN:HE21	2:B:158:GLN:CA	2.31	0.42
1:A:36:SER:N	1:A:76:ASN:ND2	2.59	0.41
2:B:64:TRP:CE2	2:B:82:TYR:HD2	2.38	0.41
1:A:111:TRP:O	1:A:115:ILE:HG13	2.20	0.41
1:A:250:ILE:O	1:A:251:LEU:C	2.58	0.41
1:A:25:LEU:HD11	1:A:404:LEU:HD23	2.03	0.41
1:A:229:TRP:CE3	1:A:229:TRP:HA	2.54	0.41
1:A:229:TRP:CE3	1:A:283:HIS:CD2	3.08	0.41
2:B:103:ILE:HG13	2:B:139:PHE:HE1	1.84	0.41
1:A:20:ALA:HB3	1:A:106:MET:CE	2.51	0.41
1:A:95:ARG:C	1:A:97:LEU:N	2.73	0.41
1:A:232:GLY:O	1:A:235:ILE:HG22	2.21	0.41
1:A:321:GLU:O	1:A:325:ARG:HG2	2.21	0.41
1:A:38:PHE:CE1	1:A:71:LEU:CB	3.04	0.41
1:A:465:VAL:HG13	1:A:466:PRO:HD2	2.03	0.41
1:A:545:THR:O	1:A:548:GLN:HB2	2.20	0.41
2:B:25:MET:O	2:B:28:VAL:HB	2.20	0.41
1:A:221:PRO:HA	1:A:224:ALA:CB	2.47	0.41
1:A:243:ALA:HA	1:A:396:THR:HG21	2.02	0.41
1:A:435:MET:HG2	1:A:439:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:VAL:O	1:A:466:PRO:C	2.58	0.41
1:A:281:PHE:HA	1:A:284:GLN:HB2	2.03	0.41
1:A:297:ILE:HG22	1:A:298:HIS:N	2.35	0.41
1:A:79:VAL:O	1:A:83:LEU:HG	2.21	0.41
2:B:37:LEU:HA	2:B:37:LEU:HD12	1.78	0.41
1:A:351:LEU:HA	1:A:354:LEU:HD23	2.02	0.41
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.88	0.41
1:A:296:MET:O	1:A:299:SER:HB3	2.20	0.41
1:A:388:GLN:HA	1:A:388:GLN:HE21	1.86	0.41
2:B:75:GLY:N	2:B:78:GLN:HB2	2.36	0.41
1:A:120:ALA:O	1:A:121:ALA:C	2.60	0.41
1:A:339:LEU:HG	1:A:346:PHE:HZ	1.85	0.41
1:A:447:VAL:CG1	1:A:453:ILE:HD13	2.51	0.41
2:B:27:PHE:HA	2:B:30:ILE:HB	2.03	0.41
1:A:120:ALA:O	1:A:122:LEU:N	2.54	0.40
1:A:137:PRO:CG	1:A:224:ALA:HB1	2.50	0.40
1:A:339:LEU:HA	1:A:340:PRO:HD3	1.72	0.40
1:A:89:MET:HB3	1:A:190:TRP:HE1	1.85	0.40
1:A:439:LEU:HD12	1:A:439:LEU:HA	1.84	0.40
1:A:20:ALA:HB3	1:A:106:MET:HE2	2.03	0.40
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.36	0.40
1:A:245:ALA:O	1:A:246:ILE:C	2.60	0.40
1:A:26:VAL:O	1:A:27:LEU:C	2.60	0.40
1:A:363:GLY:O	1:A:367:ALA:HB2	2.21	0.40
2:B:73:GLN:NE2	2:B:75:GLY:O	2.46	0.40
1:A:321:GLU:OE1	3:C:7:GLY:HA3	2.21	0.40
1:A:243:ALA:CB	1:A:396:THR:HG21	2.51	0.40
1:A:406:PRO:C	1:A:408:LEU:N	2.75	0.40
1:A:446:ASN:HA	1:A:446:ASN:HD22	1.67	0.40
1:A:488:LEU:HD12	1:A:488:LEU:HA	1.77	0.40
3:C:2:GLU:CD	3:C:3:GLU:H	2.24	0.40
1:A:449:ARG:HD2	1:A:450:ARG:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:PRO:CA	1:A:499:PRO:O[7_555]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/568 (98%)	411 (74%)	103 (19%)	41 (7%)	1	4
2	B	164/168 (98%)	123 (75%)	36 (22%)	5 (3%)	4	20
3	C	31/34 (91%)	25 (81%)	4 (13%)	2 (6%)	1	5
All	All	750/770 (97%)	559 (74%)	143 (19%)	48 (6%)	1	5

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ALA
1	A	121	ALA
1	A	377	ASN
1	A	421	GLY
1	A	464	ALA
1	A	499	PRO
1	A	501	LEU
2	B	87	ALA
2	B	88	PHE
2	B	141	ARG
3	C	26	VAL
3	C	27	TYR
1	A	10	ARG
1	A	39	GLY
1	A	88	ILE
1	A	205	VAL
1	A	407	ASN
1	A	439	LEU
1	A	500	GLU
1	A	69	LEU
1	A	133	TYR
1	A	251	LEU
1	A	254	GLN
1	A	467	MET

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Mol	Chain	Res	Type
1	A	497	ARG
1	A	502	ALA
1	A	506	LEU
2	B	49	LYS
1	A	178	VAL
1	A	185	MET
1	A	129	ALA
1	A	135	PHE
1	A	199	GLY
1	A	245	ALA
1	A	355	GLY
1	A	503	GLU
1	A	505	PRO
1	A	517	ASP
1	A	317	ALA
1	A	406	PRO
1	A	411	LYS
1	A	279	VAL
1	A	465	VAL
1	A	308	PRO
1	A	316	VAL
2	B	123	ILE
1	A	16	PRO
1	A	291	ASP

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	453/462 (98%)	372 (82%)	81 (18%)	2	7
2	B	136/138 (99%)	112 (82%)	24 (18%)	2	8
3	C	26/27 (96%)	22 (85%)	4 (15%)	2	11
All	All	615/627 (98%)	506 (82%)	109 (18%)	2	8

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	36	SER
1	A	54	LEU
1	A	59	LEU
1	A	63	GLN
1	A	64	SER
1	A	69	LEU
1	A	82	GLN
1	A	89	MET
1	A	95	ARG
1	A	98	ASN
1	A	102	ASN
1	A	133	TYR
1	A	153	VAL
1	A	155	SER
1	A	168	ARG
1	A	174	ASN
1	A	195	LEU
1	A	198	LEU
1	A	206	LEU
1	A	213	PHE
1	A	217	GLU
1	A	223	VAL
1	A	225	ARG
1	A	230	TRP
1	A	246	ILE
1	A	249	THR
1	A	254	GLN
1	A	271	LEU
1	A	273	LEU
1	A	275	LEU
1	A	279	VAL
1	A	297	ILE
1	A	305	VAL
1	A	311	MET
1	A	315	THR
1	A	330	ARG
1	A	337	ARG
1	A	339	LEU
1	A	342	ASP
1	A	354	LEU
1	A	368	SER
1	A	369	PHE

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Mol	Chain	Res	Type
1	A	370	THR
1	A	400	SER
1	A	401	LEU
1	A	405	LEU
1	A	413	ILE
1	A	419	ARG
1	A	422	LEU
1	A	430	LEU
1	A	439	LEU
1	A	440	HIS
1	A	449	ARG
1	A	452	TYR
1	A	462	HIS
1	A	465	VAL
1	A	467	MET
1	A	472	LEU
1	A	478	LEU
1	A	482	LEU
1	A	491	VAL
1	A	492	LEU
1	A	497	ARG
1	A	503	GLU
1	A	506	LEU
1	A	511	VAL
1	A	517	ASP
1	A	518	ARG
1	A	519	ARG
1	A	522	LEU
1	A	525	ASP
1	A	527	ILE
1	A	533	VAL
1	A	536	ILE
1	A	548	GLN
1	A	549	LEU
1	A	550	PHE
1	A	552	HIS
1	A	553	LEU
1	A	556	VAL
2	B	3	ASP
2	B	5	HIS
2	B	6	LYS
2	B	18	TRP

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Mol	Chain	Res	Type
2	B	25	MET
2	B	26	LEU
2	B	40	HIS
2	B	44	VAL
2	B	50	LEU
2	B	52	ARG
2	B	58	VAL
2	B	72	VAL
2	B	84	LEU
2	B	96	GLU
2	B	99	GLN
2	B	102	GLU
2	B	103	ILE
2	B	126	GLU
2	B	136	ARG
2	B	145	TYR
2	B	158	GLN
2	B	163	THR
2	B	165	VAL
2	B	167	LYS
3	C	2	GLU
3	C	9	LEU
3	C	13	LEU
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	82	GLN
1	A	98	ASN
1	A	254	GLN
1	A	388	GLN
1	A	446	ASN
2	B	5	HIS
2	B	40	HIS
2	B	117	HIS
2	B	122	ASN
2	B	158	GLN
2	B	159	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
5	HEM	A	800	1	27,50,50	2.28	6 (22%)	17,82,82	1.23	1 (5%)
6	HAS	A	801	1,7	56,72,72	3.66	18 (32%)	50,109,109	3.72	26 (52%)
7	CMO	A	563	4,6	0,1,1	0.00	-	-		
8	CUA	B	802	2	0,1,1	0.00	-	-		

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
5	HEM	A	800	1	-	0/6/54/54	-
6	HAS	A	801	1,7	-	5/35/122/122	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C1B-NB	-12.07	1.33	1.49
6	A	801	HAS	C1D-ND	-10.43	1.35	1.49
6	A	801	HAS	C4B-NB	-8.91	1.37	1.49
6	A	801	HAS	C1D-C2D	-8.78	1.37	1.51
6	A	801	HAS	C4D-ND	-8.64	1.37	1.49
6	A	801	HAS	C3C-CAC	-7.82	1.32	1.47
6	A	801	HAS	C1A-C2A	7.05	1.47	1.38
6	A	801	HAS	C4A-C3A	5.63	1.45	1.38
5	A	800	HEM	C3D-C2D	5.53	1.54	1.37
5	A	800	HEM	C3B-C2B	-5.19	1.33	1.40
6	A	801	HAS	C2B-C3B	4.59	1.38	1.34
5	A	800	HEM	C3C-C2C	-4.56	1.34	1.40
6	A	801	HAS	C3C-C2C	-4.35	1.34	1.40
6	A	801	HAS	CHD-C4A	-4.09	1.46	1.51
5	A	800	HEM	C3C-CAC	3.79	1.55	1.47
5	A	800	HEM	C3B-CAB	3.63	1.55	1.47
6	A	801	HAS	C2A-C3A	3.24	1.47	1.37
6	A	801	HAS	C3D-C2D	3.05	1.37	1.34
6	A	801	HAS	CHD-C4C	-2.77	1.48	1.51
6	A	801	HAS	FE-NA	2.58	2.14	1.95
6	A	801	HAS	C1C-C2C	2.54	1.41	1.38
6	A	801	HAS	CMD-C2D	2.46	1.49	1.44
5	A	800	HEM	CAD-C3D	2.18	1.56	1.52
6	A	801	HAS	FE-NC	2.12	2.11	1.95

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CHB-C1B-NB	11.24	124.91	110.94
6	A	801	HAS	CHB-C1D-ND	10.48	123.96	110.94
6	A	801	HAS	CHC-C4B-NB	8.01	125.86	110.75
6	A	801	HAS	CHA-C4D-ND	7.86	125.57	110.75
6	A	801	HAS	CHC-C1C-C2C	-6.03	119.02	129.45
6	A	801	HAS	C4C-CHD-C4A	5.54	126.38	112.87
6	A	801	HAS	C25-C23-C24	4.97	123.63	115.27
6	A	801	HAS	CHD-C4A-C3A	-4.79	121.52	129.53
6	A	801	HAS	OMD-CMD-C2D	-4.49	118.71	124.39
6	A	801	HAS	CAA-CBA-CGA	-4.34	105.39	112.67
6	A	801	HAS	C21-C22-C23	-4.17	117.62	127.66
6	A	801	HAS	C27-C19-C20	4.06	122.10	115.27
6	A	801	HAS	C1D-CHB-C1B	3.92	127.47	116.15
6	A	801	HAS	CAD-CBD-CGD	-3.44	106.90	112.67
6	A	801	HAS	C4C-C3C-C2C	3.43	109.67	104.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C12-C13-C14	-3.38	103.30	112.23
6	A	801	HAS	CMA-C3A-C2A	3.20	130.98	124.94
6	A	801	HAS	C4A-C3A-C2A	-2.96	102.66	105.81
6	A	801	HAS	C26-C15-C16	2.88	120.12	115.27
5	A	800	HEM	CBA-CAA-C2A	-2.79	107.34	112.49
6	A	801	HAS	CAA-C2A-C1A	-2.73	125.38	127.30
6	A	801	HAS	CBD-CAD-C3D	-2.71	109.56	114.35
6	A	801	HAS	CHD-C4C-C3C	-2.58	126.22	129.61
6	A	801	HAS	C20-C19-C18	-2.47	116.11	121.12
6	A	801	HAS	C32-C30-C31	2.34	119.78	114.60
6	A	801	HAS	CHB-C1B-C2B	2.32	121.94	114.70
6	A	801	HAS	C25-C23-C22	-2.05	118.42	123.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	HAS	C1D-C2D-CMD-OMD
6	A	801	HAS	C25-C23-C24-C28
6	A	801	HAS	C22-C23-C24-C28
6	A	801	HAS	C3D-C2D-CMD-OMD
6	A	801	HAS	C3B-C11-C12-C13

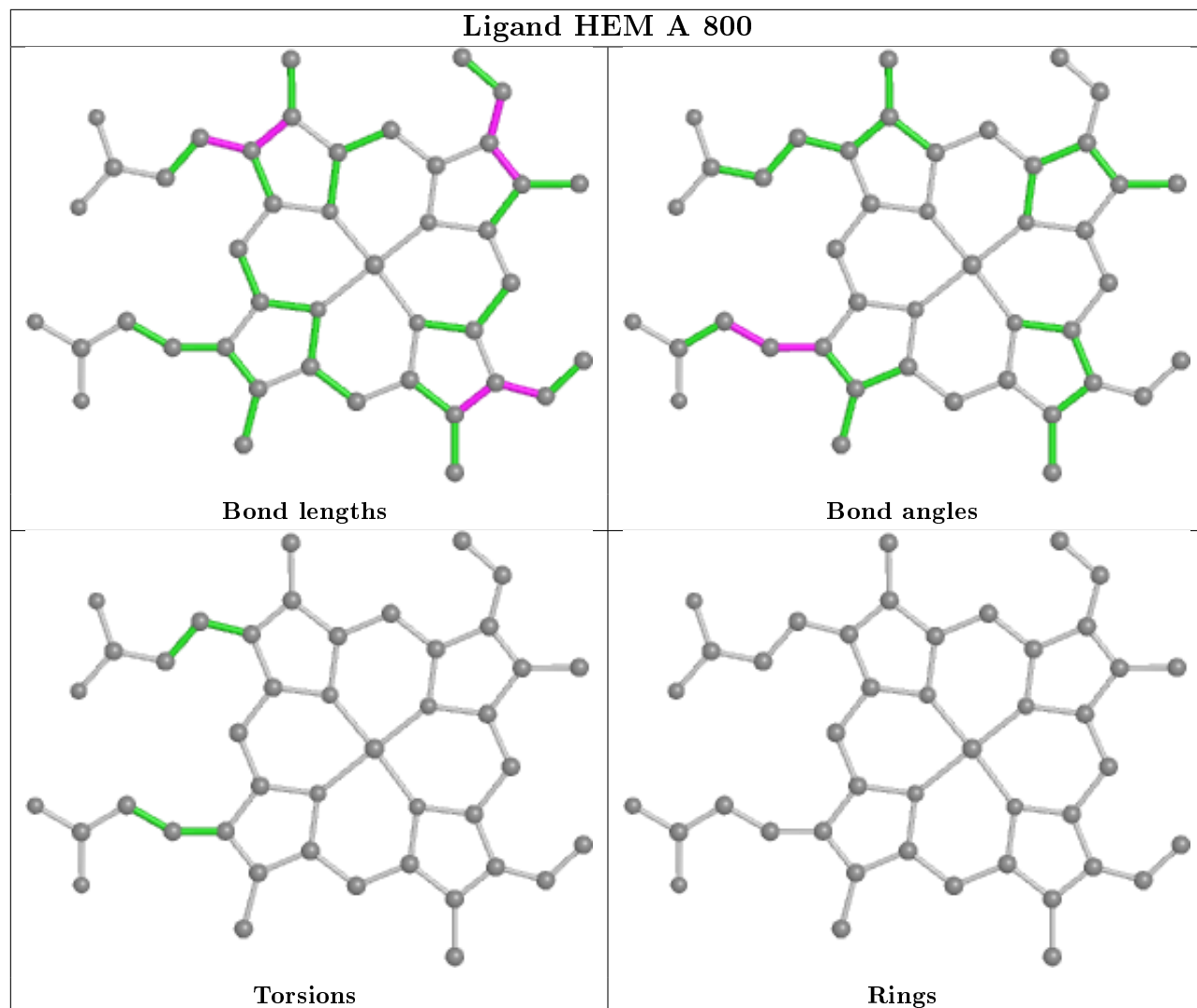
There are no ring outliers.

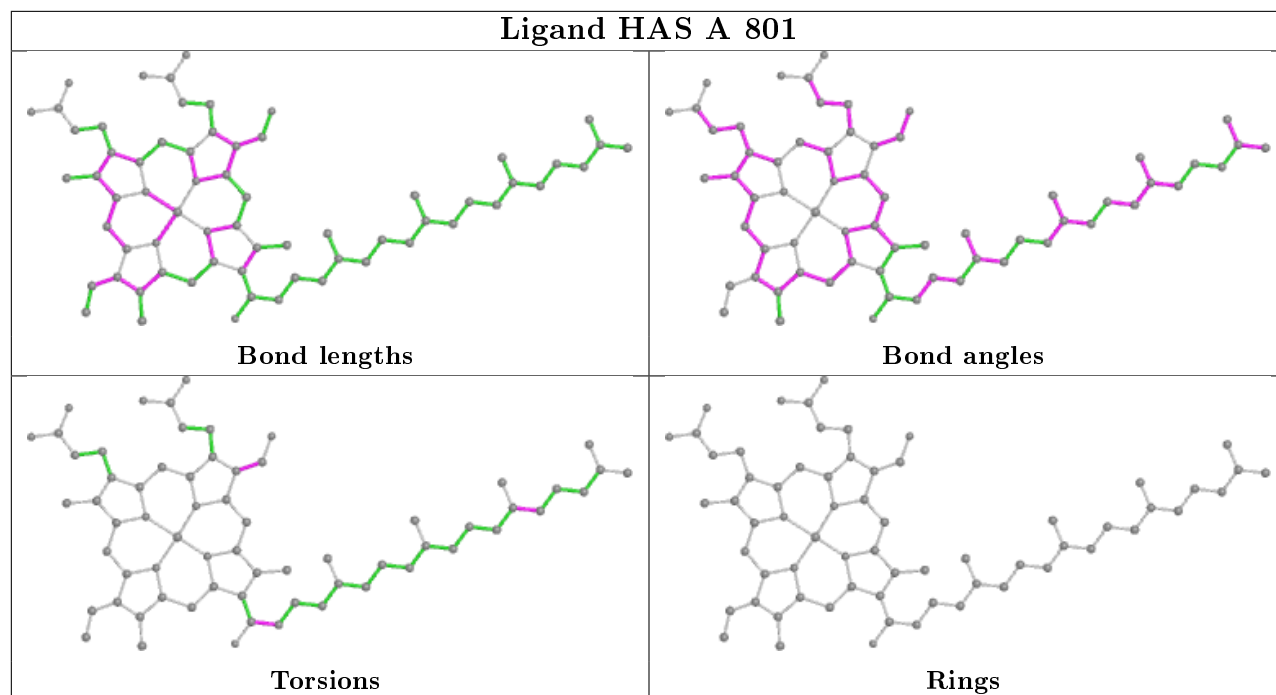
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	9	0
6	A	801	HAS	7	0
7	A	563	CMO	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/568 (98%)	0.28	42 (7%) 14 8	54, 74, 98, 128	1 (0%)
2	B	166/168 (98%)	0.13	8 (4%) 30 19	57, 73, 99, 116	0
3	C	33/34 (97%)	-0.05	3 (9%) 9 5	60, 81, 138, 184	0
All	All	756/770 (98%)	0.23	53 (7%) 16 9	54, 74, 100, 184	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	PRO	7.7
1	A	9	SER	6.9
1	A	505	PRO	6.7
1	A	514	GLY	6.4
1	A	497	ARG	6.1
1	A	6	SER	5.8
1	A	495	ARG	4.7
1	A	11	VAL	4.4
3	C	34	GLY	4.3
1	A	8	ILE	4.3
1	A	504	ALA	4.1
1	A	7	GLU	3.9
1	A	214	GLY	3.9
1	A	217	GLU	3.8
1	A	496	GLU	3.5
1	A	513	SER	3.4
1	A	215	LEU	3.3
2	B	102	GLU	3.1
1	A	15	TYR	3.0
2	B	3	ASP	3.0
1	A	57	ARG	2.8
1	A	10	ARG	2.8
1	A	104	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	177	LYS	2.8
1	A	523	ALA	2.8
1	A	517	ASP	2.7
3	C	3	GLU	2.7
1	A	12	TYR	2.6
1	A	498	LYS	2.6
1	A	412	PRO	2.5
1	A	165	ASP	2.5
2	B	134	THR	2.5
1	A	368	SER	2.4
2	B	78	GLN	2.4
1	A	502	ALA	2.4
1	A	462	HIS	2.3
2	B	63	PRO	2.3
1	A	539	VAL	2.3
1	A	168	ARG	2.2
3	C	2	GLU	2.2
1	A	418	ARG	2.2
1	A	519	ARG	2.2
2	B	72	VAL	2.2
1	A	528	GLY	2.2
1	A	371	LEU	2.2
1	A	522	LEU	2.1
2	B	73	GLN	2.1
1	A	370	THR	2.1
1	A	332	LEU	2.0
2	B	69	GLN	2.0
1	A	499	PRO	2.0
1	A	50	ASP	2.0
1	A	97	LEU	2.0

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 ⓘ

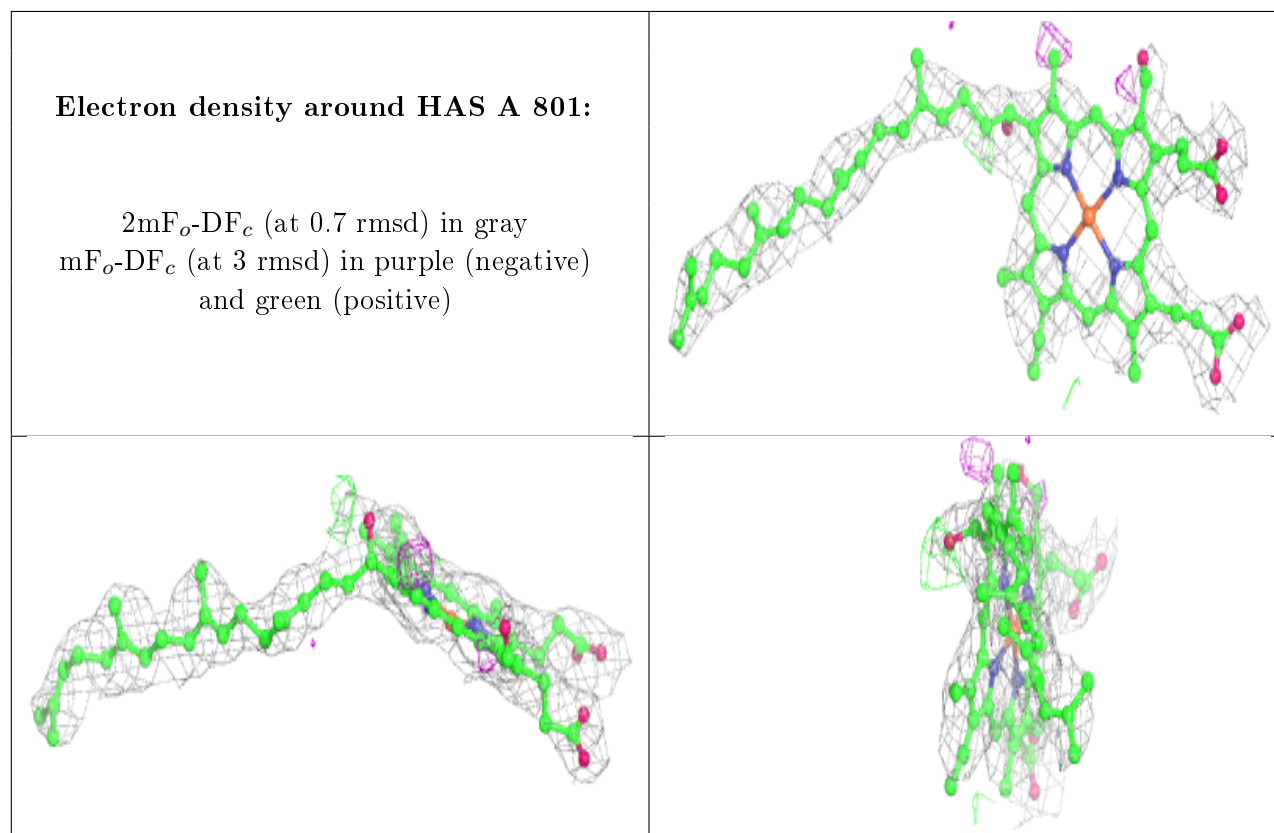
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

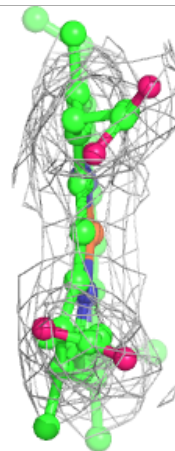
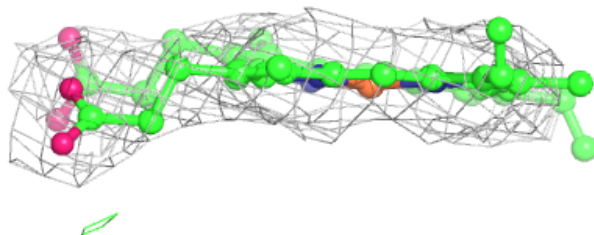
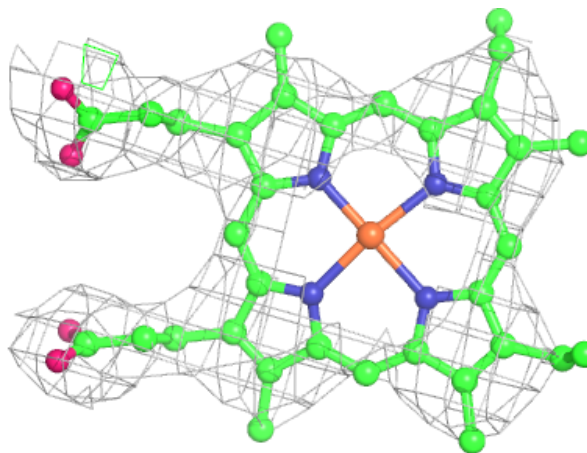
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	HAS	A	801	65/65	0.94	0.18	46,51,55,57	0
8	CUA	B	802	2/2	0.96	0.06	56,56,56,57	0
5	HEM	A	800	43/43	0.97	0.14	50,54,58,59	0
4	CU1	A	803	1/1	0.99	0.05	57,57,57,57	0
7	CMO	A	563	2/2	1.00	0.07	53,53,53,71	0

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)



6.5 Other polymers [i](#)

There are no such residues in this entry.