



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:50 AM UTC

PDB ID : 2QPE / pdb_00002qpe
Title : An unexpected outcome of surface-engineering an integral membrane protein: Improved crystallization of cytochrome ba3 oxidase from *Thermus thermophilus*
Authors : Liu, B.; Luna, V.M.; Chen, Y.; Stout, C.D.; Fee, J.A.
Deposited on : 2007-07-23
Resolution : 2.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

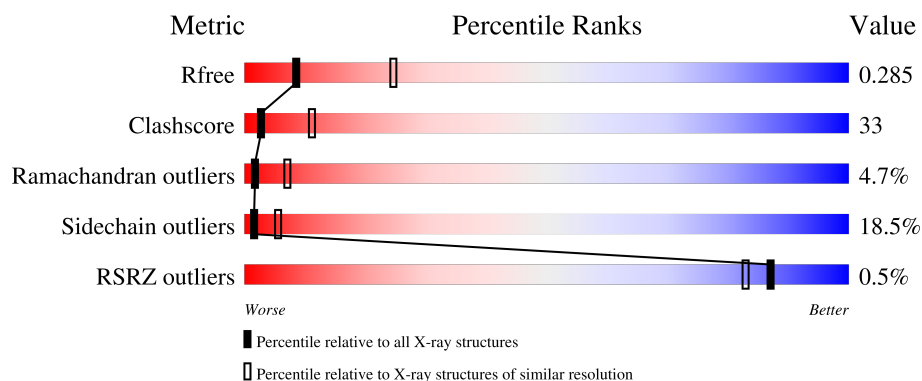
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	% 37% 46% 14% ..
2	B	168	49% 39% 9% ..
3	C	34	35% 38% 24% .

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
6	HAS	A	801	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6077 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
1	A	557	Total	C	N	O	S	0	0	0
			4409	2985	709	699	16			

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	engineered mutation	UNP Q5SJ79

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

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

There is a discrepancy between the modelled and reference sequences:

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

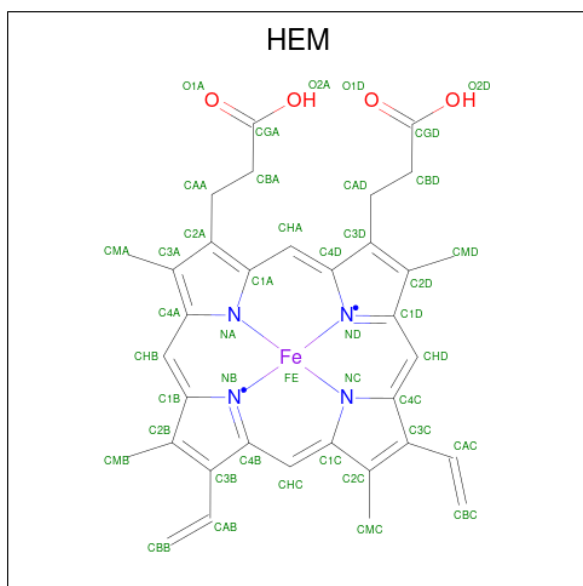
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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

- Molecule 4 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

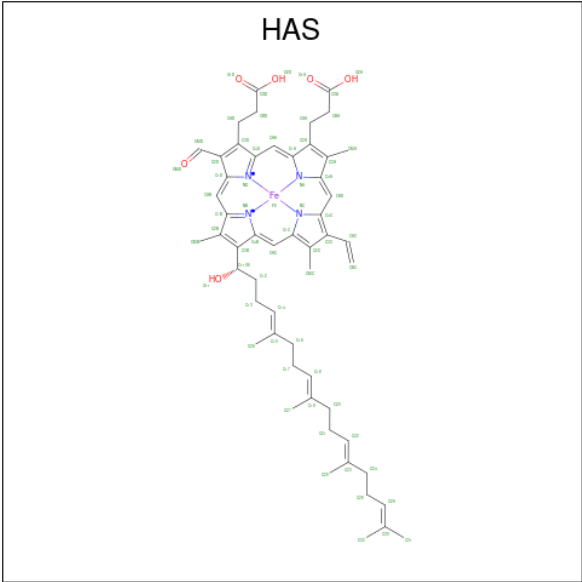
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



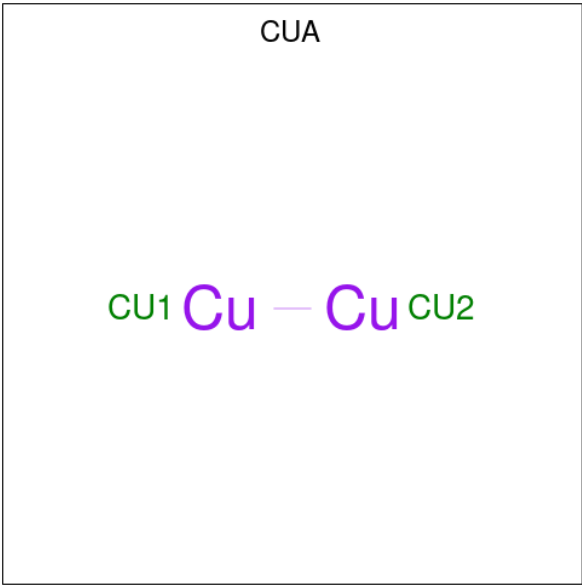
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (CCD ID: HAS) (formula: C₅₄H₆₄FeN₄O₆).



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

- Molecule 7 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

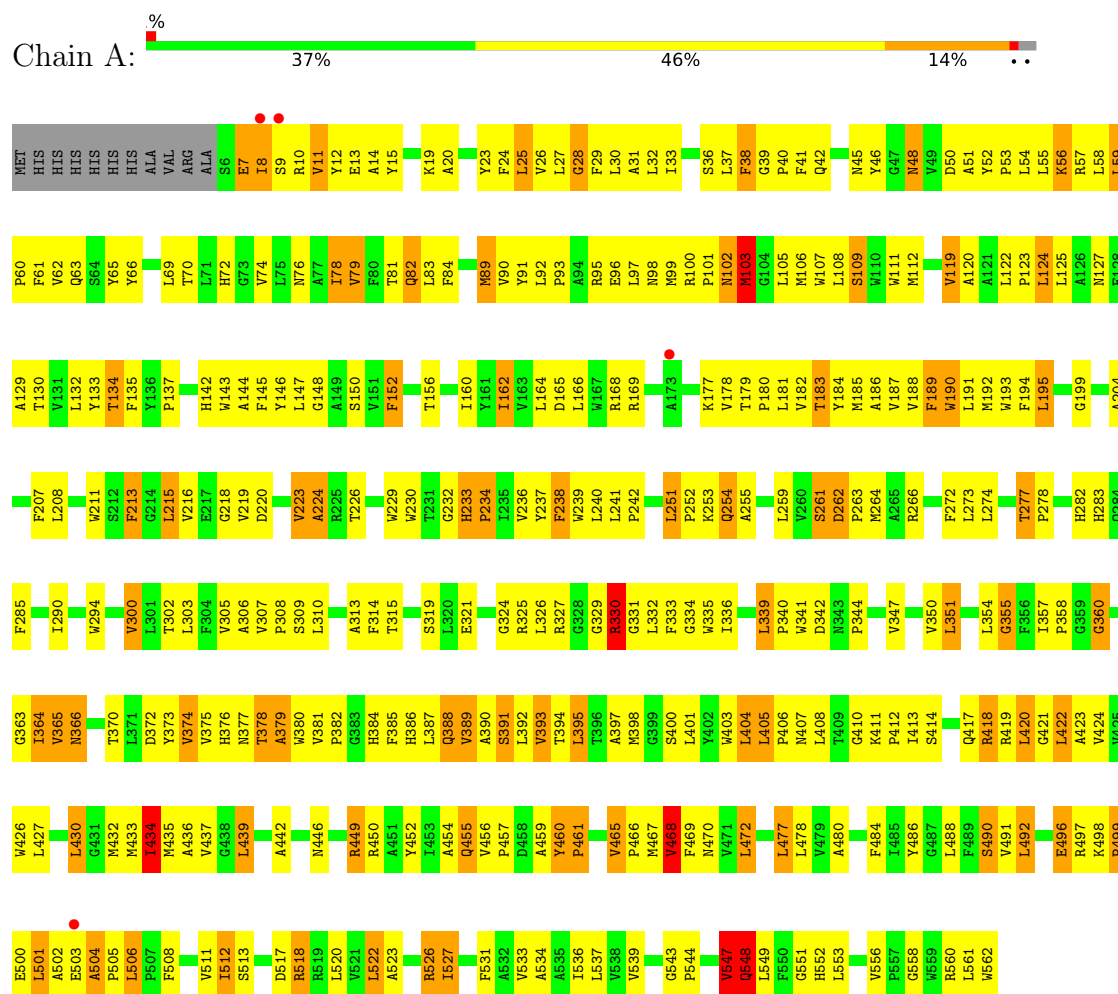


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
7	B	1	2	2	0	0

3 Residue-property plots

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.

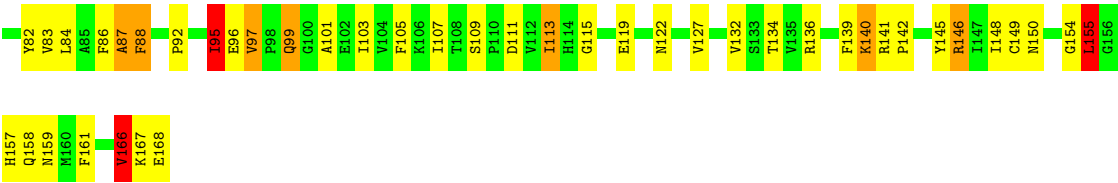
• Molecule 1: Cytochrome c oxidase subunit 1



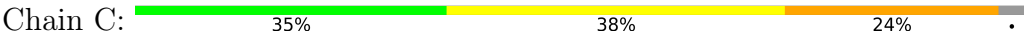
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 





• 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	114.64Å 114.64Å 148.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.99-2.90) 94.7 (19.99-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.302 0.196 , 0.285	Depositor DCC
R_{free} test set	1083 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CUA, HAS, 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	1.21	9/4566 (0.2%)	1.42	35/6266 (0.6%)
2	B	1.19	3/1335 (0.2%)	1.42	13/1822 (0.7%)
3	C	1.27	0/265	1.44	4/359 (1.1%)
All	All	1.20	12/6166 (0.2%)	1.42	52/8447 (0.6%)

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	1
2	B	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	VAL	CA-CB	7.26	1.64	1.54
1	A	119	VAL	CA-CB	6.94	1.64	1.54
1	A	547	VAL	CA-CB	6.38	1.63	1.54
2	B	45	ILE	CA-C	-6.11	1.48	1.53
1	A	378	THR	CA-C	-5.89	1.45	1.52
1	A	90	VAL	CA-CB	5.83	1.62	1.54
1	A	434	ILE	CA-CB	5.48	1.60	1.54
1	A	223	VAL	CA-CB	5.47	1.60	1.54
1	A	357	ILE	CA-C	5.32	1.58	1.52
1	A	162	ILE	CA-CB	5.30	1.59	1.54
2	B	35	TYR	N-CA	-5.29	1.40	1.46
1	A	302	THR	N-CA	5.12	1.52	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	GLY	N-CA-C	9.95	126.12	110.90
1	A	357	ILE	CA-C-N	-9.93	108.35	119.28
1	A	357	ILE	C-N-CA	-9.93	108.35	119.28
2	B	155	LEU	N-CA-C	8.35	122.73	112.54
3	C	12	ILE	N-CA-C	-7.56	105.19	113.43
1	A	103	MET	N-CA-C	7.44	121.46	112.38
1	A	79	VAL	N-CA-C	7.40	118.00	110.82
1	A	330	ARG	CA-C-N	-6.82	115.52	122.27
1	A	330	ARG	C-N-CA	-6.82	115.52	122.27
1	A	262	ASP	N-CA-C	-6.81	103.36	112.55
1	A	460	TYR	CA-C-N	6.78	128.31	119.84
1	A	460	TYR	C-N-CA	6.78	128.31	119.84
1	A	241	LEU	CA-C-N	-6.54	111.80	119.05
1	A	241	LEU	C-N-CA	-6.54	111.80	119.05
2	B	97	VAL	CA-C-N	6.51	126.27	119.76
2	B	97	VAL	C-N-CA	6.51	126.27	119.76
1	A	251	LEU	CA-C-N	-6.37	112.44	119.19
1	A	251	LEU	C-N-CA	-6.37	112.44	119.19
2	B	113	ILE	CB-CA-C	-6.32	101.91	111.33
2	B	166	VAL	N-CA-CB	6.23	117.32	110.53
1	A	393	VAL	N-CA-CB	6.21	117.14	110.62
1	A	66	TYR	N-CA-C	6.13	118.75	111.33
2	B	52	ARG	N-CA-C	6.05	119.14	110.24
1	A	360	GLY	N-CA-C	-6.03	105.20	112.49
1	A	223	VAL	N-CA-CB	5.98	117.40	110.65
1	A	442	ALA	N-CA-C	-5.95	104.88	111.36
1	A	300	VAL	N-CA-CB	5.73	116.87	110.62
1	A	290	ILE	CB-CA-C	5.70	118.66	110.33
1	A	503	GLU	N-CA-C	-5.69	105.00	111.14
1	A	25	LEU	CB-CG-CD1	-5.66	93.71	110.70
1	A	187	VAL	N-CA-C	-5.66	105.59	110.74
2	B	166	VAL	N-CA-C	-5.61	101.49	108.89
1	A	13	GLU	N-CA-C	-5.54	105.50	114.09
2	B	24	ALA	N-CA-C	-5.53	104.95	110.97
2	B	115	GLY	N-CA-C	-5.53	102.67	111.18
1	A	302	THR	N-CA-C	5.48	117.96	111.33
3	C	11	VAL	CA-C-N	-5.44	115.30	122.16
3	C	11	VAL	C-N-CA	-5.44	115.30	122.16
3	C	12	ILE	CB-CA-C	5.41	117.60	110.84
1	A	336	ILE	N-CA-C	5.30	115.52	110.53
1	A	434	ILE	N-CA-CB	5.26	116.34	110.51
1	A	527	ILE	N-CA-C	5.25	115.87	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	ALA	N-CA-C	-5.25	102.28	110.10
1	A	277	THR	CA-C-N	5.23	126.37	119.84
1	A	277	THR	C-N-CA	5.23	126.37	119.84
1	A	468	VAL	N-CA-C	-5.21	105.63	110.53
1	A	38	PHE	N-CA-C	5.19	116.94	111.28
1	A	413	ILE	N-CA-C	5.14	114.70	106.88
2	B	109	SER	CA-C-N	5.13	124.82	119.64
2	B	109	SER	C-N-CA	5.13	124.82	119.64
2	B	95	ILE	N-CA-C	-5.12	99.79	107.37
1	A	351	LEU	N-CA-C	-5.08	105.44	111.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	ILE	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	4515	350	0
2	B	1298	0	1282	62	0
3	C	259	0	279	15	0
4	A	1	0	0	0	0
5	A	43	0	30	7	0
6	A	65	0	61	14	0
7	B	2	0	0	0	0
All	All	6077	0	6167	408	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 33.

All (408) 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:NE2	1:A:237:TYR:CE2	1.71	1.53
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.79	1.27
1:A:385:PHE:CB	6:A:801:HAS:HMA2	1.73	1.18
1:A:385:PHE:CG	6:A:801:HAS:HMA2	1.81	1.16
1:A:410:GLY:CA	1:A:502:ALA:HB2	1.74	1.16
1:A:182:VAL:HG21	1:A:508:PHE:HE2	1.08	1.12
1:A:518:ARG:HH21	1:A:518:ARG:HG3	1.08	1.11
1:A:7:GLU:HB3	1:A:10:ARG:HA	1.30	1.08
1:A:182:VAL:HG21	1:A:508:PHE:CE2	1.91	1.04
1:A:410:GLY:HA2	1:A:502:ALA:CB	1.90	1.01
2:B:142:PRO:HA	2:B:166:VAL:CG2	1.90	1.00
2:B:142:PRO:HA	2:B:166:VAL:HG22	1.48	0.95
1:A:497:ARG:C	1:A:499:PRO:HD3	1.91	0.95
1:A:506:LEU:H	1:A:506:LEU:HD23	1.32	0.94
1:A:385:PHE:HB2	6:A:801:HAS:CMA	1.98	0.93
1:A:410:GLY:HA2	1:A:502:ALA:HB2	0.94	0.93
1:A:430:LEU:O	1:A:434:ILE:HG13	1.70	0.91
1:A:562:TRP:HA	2:B:155:LEU:HD12	1.52	0.91
1:A:518:ARG:HG3	1:A:518:ARG:NH2	1.79	0.91
1:A:76:ASN:HB3	5:A:800:HEM:HBC2	1.53	0.89
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.61	0.89
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.91	0.88
1:A:385:PHE:HB2	6:A:801:HAS:HMA2	1.52	0.88
1:A:412:PRO:HB3	1:A:501:LEU:HD21	1.56	0.87
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.91	0.87
1:A:385:PHE:CB	6:A:801:HAS:CMA	2.53	0.87
1:A:12:TYR:CD1	1:A:19:LYS:HB2	2.10	0.86
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.58	0.85
1:A:20:ALA:HB3	1:A:106:MET:HE2	1.60	0.83
1:A:45:ASN:ND2	1:A:65:TYR:CE1	2.47	0.83
1:A:385:PHE:CG	6:A:801:HAS:CMA	2.61	0.83
1:A:7:GLU:CB	1:A:10:ARG:HA	2.11	0.81
1:A:329:GLY:HA2	1:A:330:ARG:HE	1.43	0.81
1:A:374:VAL:HG12	1:A:375:VAL:HG13	1.63	0.80
1:A:454:ALA:O	1:A:457:PRO:HG3	1.80	0.80
1:A:277:THR:H	1:A:278:PRO:HD2	1.46	0.80
1:A:233:HIS:CE1	1:A:282:HIS:HE1	2.01	0.79
1:A:277:THR:N	1:A:278:PRO:HD2	1.98	0.78
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.19	0.78
1:A:385:PHE:CD2	6:A:801:HAS:HMA2	2.19	0.78
1:A:388:GLN:HB3	6:A:801:HAS:HMC2	1.66	0.78
1:A:162:ILE:O	1:A:165:ASP:HB3	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:HA	1:A:310:LEU:HD12	1.65	0.77
1:A:124:LEU:HD21	1:A:145:PHE:HD1	1.46	0.76
1:A:152:PHE:C	1:A:152:PHE:CD2	2.62	0.76
1:A:152:PHE:C	1:A:152:PHE:HD2	1.95	0.75
1:A:455:GLN:C	1:A:457:PRO:HD3	2.11	0.75
1:A:459:ALA:C	1:A:461:PRO:HD2	2.12	0.75
1:A:410:GLY:CA	1:A:502:ALA:CB	2.60	0.74
1:A:547:VAL:HG12	1:A:548:GLN:N	2.02	0.74
2:B:92:PRO:HD2	2:B:95:ILE:HD11	1.68	0.74
1:A:108:LEU:O	1:A:112:MET:HG3	1.87	0.74
1:A:124:LEU:HD21	1:A:145:PHE:CD1	2.21	0.74
1:A:518:ARG:HH21	1:A:518:ARG:CG	1.95	0.73
1:A:549:LEU:O	1:A:553:LEU:HD23	1.88	0.73
2:B:103:ILE:HD13	2:B:139:PHE:HD1	1.54	0.73
1:A:497:ARG:O	1:A:499:PRO:HD3	1.89	0.73
1:A:63:GLN:CG	1:A:127:ASN:HD22	2.02	0.73
1:A:10:ARG:O	1:A:12:TYR:N	2.22	0.72
1:A:233:HIS:HB3	1:A:234:PRO:CD	2.20	0.72
1:A:52:TYR:O	1:A:56:LYS:HB2	1.90	0.72
1:A:370:THR:HA	1:A:373:TYR:CE1	2.25	0.72
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.72	0.71
1:A:407:ASN:HD21	1:A:506:LEU:CD2	2.03	0.71
1:A:81:THR:HG1	1:A:239:TRP:CD1	2.09	0.71
1:A:107:TRP:O	1:A:111:TRP:HD1	1.73	0.71
1:A:365:VAL:HG12	1:A:366:ASN:N	2.05	0.71
1:A:390:ALA:O	1:A:394:THR:HB	1.91	0.71
1:A:264:MET:HA	1:A:264:MET:HE2	1.73	0.71
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.78	0.70
1:A:331:GLY:H	1:A:334:GLY:HA3	1.57	0.70
1:A:407:ASN:HD21	1:A:506:LEU:HD23	1.56	0.70
1:A:277:THR:N	1:A:278:PRO:CD	2.55	0.70
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.27	0.69
1:A:277:THR:H	1:A:278:PRO:CD	2.05	0.69
1:A:7:GLU:HB3	1:A:10:ARG:CA	2.15	0.69
1:A:220:ASP:OD2	2:B:52:ARG:NH1	2.26	0.69
1:A:20:ALA:CB	1:A:106:MET:HE2	2.22	0.69
1:A:76:ASN:HB3	5:A:800:HEM:CBC	2.21	0.69
1:A:27:LEU:HD23	1:A:83:LEU:CD2	2.23	0.68
1:A:233:HIS:CE1	1:A:282:HIS:CE1	2.80	0.68
1:A:329:GLY:HA2	1:A:330:ARG:NE	2.09	0.68
2:B:97:VAL:O	2:B:166:VAL:HA	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD23	1:A:83:LEU:HD22	1.74	0.68
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.28	0.68
1:A:321:GLU:OE1	1:A:325:ARG:NH2	2.26	0.67
2:B:55:PRO:O	2:B:58:VAL:HG12	1.94	0.67
1:A:499:PRO:HB3	1:A:502:ALA:HB3	1.75	0.66
1:A:14:ALA:O	1:A:100:ARG:NH1	2.29	0.66
1:A:294:TRP:HZ2	1:A:544:PRO:HG2	1.60	0.65
1:A:234:PRO:HG3	1:A:277:THR:HA	1.79	0.65
1:A:97:LEU:HD21	1:A:180:PRO:HG2	1.78	0.65
1:A:152:PHE:CD2	1:A:152:PHE:O	2.50	0.65
2:B:86:PHE:O	2:B:88:PHE:N	2.28	0.65
1:A:233:HIS:CD2	1:A:233:HIS:C	2.74	0.65
1:A:63:GLN:HG3	1:A:127:ASN:HD22	1.60	0.65
1:A:45:ASN:ND2	1:A:65:TYR:HE1	1.96	0.64
1:A:156:THR:O	1:A:160:ILE:HG13	1.98	0.64
1:A:330:ARG:HD2	1:A:330:ARG:N	2.12	0.64
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.33	0.64
1:A:59:LEU:HB2	1:A:61:PHE:HE1	1.62	0.64
1:A:414:SER:OG	1:A:417:GLN:HG3	1.97	0.63
1:A:506:LEU:H	1:A:506:LEU:CD2	2.02	0.63
1:A:435:MET:HG2	1:A:439:LEU:HD22	1.79	0.63
1:A:330:ARG:N	1:A:330:ARG:CD	2.61	0.63
1:A:107:TRP:O	1:A:111:TRP:CD1	2.52	0.62
1:A:213:PHE:HB3	1:A:215:LEU:HD22	1.80	0.62
1:A:120:ALA:O	1:A:123:PRO:HD2	2.00	0.62
1:A:342:ASP:HB2	1:A:418:ARG:HH22	1.64	0.62
1:A:28:GLY:O	1:A:31:ALA:HB3	1.99	0.62
1:A:233:HIS:ND1	1:A:282:HIS:HE1	1.94	0.61
1:A:78:ILE:HG22	1:A:79:VAL:N	2.14	0.61
1:A:233:HIS:CD2	1:A:237:TYR:CD2	2.89	0.61
1:A:366:ASN:HB3	6:A:801:HAS:CMD	2.31	0.61
1:A:366:ASN:HB3	6:A:801:HAS:HMD	1.81	0.61
1:A:477:LEU:HA	1:A:480:ALA:HB3	1.83	0.61
1:A:385:PHE:O	1:A:389:VAL:HG12	2.01	0.61
2:B:142:PRO:HA	2:B:166:VAL:HG21	1.81	0.60
1:A:477:LEU:HD13	5:A:800:HEM:HMB1	1.83	0.60
2:B:83:VAL:HG12	2:B:84:LEU:N	2.17	0.60
1:A:335:TRP:O	1:A:339:LEU:HD22	2.02	0.60
1:A:370:THR:HA	1:A:373:TYR:CD1	2.36	0.60
1:A:56:LYS:O	1:A:60:PRO:HA	2.01	0.60
1:A:386:HIS:CD2	1:A:435:MET:HE1	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:VAL:O	1:A:543:GLY:HA3	2.03	0.59
1:A:102:ASN:OD1	1:A:102:ASN:O	2.21	0.59
1:A:307:VAL:HA	1:A:310:LEU:CD1	2.32	0.59
1:A:385:PHE:HB2	6:A:801:HAS:HMA1	1.84	0.59
1:A:551:GLY:C	1:A:552:HIS:ND1	2.61	0.59
1:A:50:ASP:O	1:A:53:PRO:HD2	2.03	0.58
1:A:388:GLN:N	1:A:388:GLN:HE21	2.00	0.58
1:A:52:TYR:N	1:A:53:PRO:HD2	2.19	0.58
1:A:342:ASP:O	1:A:418:ARG:NH2	2.36	0.58
2:B:92:PRO:HD2	2:B:95:ILE:CD1	2.32	0.58
1:A:233:HIS:HB3	1:A:234:PRO:HD2	1.84	0.58
1:A:547:VAL:CG1	1:A:548:GLN:N	2.67	0.58
1:A:137:PRO:HG2	1:A:224:ALA:CB	2.34	0.58
1:A:137:PRO:CG	1:A:224:ALA:HB1	2.33	0.58
1:A:59:LEU:HB2	1:A:61:PHE:CE1	2.37	0.58
1:A:420:LEU:HD12	1:A:424:VAL:HG23	1.84	0.58
1:A:186:ALA:O	1:A:190:TRP:HD1	1.86	0.57
3:C:26:VAL:O	3:C:27:TYR:C	2.47	0.57
1:A:186:ALA:O	1:A:190:TRP:CD1	2.57	0.57
1:A:400:SER:O	1:A:404:LEU:HB2	2.04	0.57
1:A:523:ALA:O	1:A:526:ARG:HG3	2.03	0.57
1:A:310:LEU:O	1:A:313:ALA:HB3	2.04	0.57
1:A:137:PRO:HG2	1:A:224:ALA:HB1	1.85	0.57
1:A:562:TRP:CA	2:B:155:LEU:HD12	2.30	0.57
1:A:98:ASN:ND2	1:A:98:ASN:O	2.38	0.57
1:A:446:ASN:OD1	2:B:119:GLU:HG3	2.04	0.57
1:A:146:TYR:CD2	1:A:208:LEU:HD13	2.41	0.56
1:A:211:TRP:HZ2	1:A:558:GLY:HA3	1.70	0.56
2:B:32:LEU:O	2:B:35:TYR:HB3	2.06	0.56
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.41	0.56
1:A:261:SER:HB3	1:A:264:MET:HB2	1.87	0.56
1:A:63:GLN:CG	1:A:127:ASN:ND2	2.67	0.56
1:A:377:ASN:HB3	2:B:150:ASN:O	2.06	0.56
2:B:157:HIS:C	2:B:159:ASN:H	2.13	0.56
1:A:119:VAL:HG12	1:A:148:GLY:CA	2.35	0.56
1:A:459:ALA:O	2:B:146:ARG:NH1	2.34	0.56
1:A:220:ASP:HB3	1:A:223:VAL:HG22	1.87	0.55
1:A:91:TYR:CE1	1:A:95:ARG:HD2	2.42	0.55
1:A:191:LEU:HB3	1:A:531:PHE:CD2	2.41	0.55
1:A:410:GLY:HA3	1:A:499:PRO:HG3	1.88	0.55
2:B:86:PHE:CD1	2:B:86:PHE:C	2.86	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:CZ	2:B:14:TYR:HB3	2.43	0.54
1:A:330:ARG:H	1:A:334:GLY:HA3	1.73	0.54
1:A:391:SER:O	1:A:395:LEU:HD12	2.07	0.54
2:B:70:ALA:HB1	2:B:82:TYR:O	2.07	0.54
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.41	0.54
1:A:274:LEU:N	1:A:274:LEU:CD1	2.70	0.54
1:A:388:GLN:NE2	1:A:388:GLN:CA	2.70	0.54
1:A:389:VAL:HG22	5:A:800:HEM:HAC	1.88	0.54
1:A:456:VAL:HG23	1:A:456:VAL:O	2.08	0.54
1:A:547:VAL:HG12	1:A:548:GLN:H	1.72	0.54
1:A:460:TYR:N	1:A:461:PRO:CD	2.70	0.54
2:B:96:GLU:HB3	2:B:167:LYS:NZ	2.22	0.54
2:B:157:HIS:O	2:B:159:ASN:N	2.40	0.54
1:A:27:LEU:O	1:A:28:GLY:C	2.51	0.53
1:A:152:PHE:HD2	1:A:152:PHE:O	1.90	0.53
1:A:344:PRO:HG3	1:A:422:LEU:HG	1.90	0.53
1:A:300:VAL:HG22	2:B:30:ILE:HD13	1.90	0.53
2:B:105:PHE:CZ	2:B:139:PHE:HE1	2.26	0.53
2:B:42:ALA:HB1	2:B:45:ILE:HD12	1.90	0.53
2:B:3:ASP:OD1	3:C:2:GLU:HB3	2.09	0.53
1:A:181:LEU:O	1:A:185:MET:HG3	2.09	0.53
1:A:48:ASN:ND2	1:A:467:MET:HE2	2.24	0.53
1:A:135:PHE:O	1:A:137:PRO:HD3	2.08	0.53
1:A:388:GLN:NE2	1:A:388:GLN:HA	2.24	0.53
1:A:420:LEU:O	1:A:421:GLY:C	2.52	0.53
1:A:106:MET:O	1:A:109:SER:HB3	2.08	0.52
3:C:29:VAL:O	3:C:30:PHE:C	2.51	0.52
1:A:423:ALA:O	1:A:427:LEU:HB2	2.10	0.52
1:A:391:SER:HB2	1:A:395:LEU:HD11	1.92	0.52
1:A:189:PHE:O	1:A:192:MET:N	2.41	0.52
1:A:274:LEU:N	1:A:274:LEU:HD12	2.22	0.52
2:B:105:PHE:HZ	2:B:139:PHE:HE1	1.58	0.52
1:A:426:TRP:O	1:A:430:LEU:HD22	2.11	0.51
3:C:10:ALA:O	3:C:14:VAL:HG23	2.10	0.51
1:A:36:SER:O	1:A:40:PRO:HD3	2.10	0.51
1:A:120:ALA:HB2	1:A:148:GLY:HA3	1.92	0.51
1:A:195:LEU:CD2	1:A:534:ALA:HB1	2.40	0.51
1:A:390:ALA:HB1	1:A:432:MET:HE3	1.92	0.51
1:A:513:SER:O	2:B:5:HIS:CE1	2.63	0.51
1:A:240:LEU:HA	1:A:393:VAL:HG22	1.92	0.51
1:A:398:MET:HG2	1:A:484:PHE:CE1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TYR:N	1:A:53:PRO:CD	2.74	0.51
1:A:332:LEU:CD2	1:A:333:PHE:CE2	2.94	0.51
1:A:433:MET:O	1:A:436:ALA:HB3	2.11	0.51
1:A:7:GLU:O	1:A:10:ARG:HG3	2.11	0.51
1:A:56:LYS:CE	1:A:62:VAL:O	2.59	0.51
1:A:146:TYR:HD2	1:A:208:LEU:HD13	1.76	0.50
1:A:39:GLY:C	5:A:800:HEM:HMB3	2.36	0.50
1:A:46:TYR:CE1	5:A:800:HEM:HBA2	2.46	0.50
1:A:465:VAL:O	1:A:468:VAL:HG23	2.10	0.50
1:A:95:ARG:HA	1:A:95:ARG:CZ	2.41	0.50
1:A:384:HIS:O	1:A:388:GLN:HG2	2.12	0.50
1:A:450:ARG:O	2:B:157:HIS:HD2	1.94	0.50
2:B:113:ILE:HA	2:B:127:VAL:O	2.11	0.50
1:A:101:PRO:HA	1:A:166:LEU:HD11	1.94	0.50
1:A:365:VAL:HG12	1:A:366:ASN:H	1.74	0.50
2:B:157:HIS:C	2:B:159:ASN:N	2.70	0.50
1:A:37:LEU:O	1:A:40:PRO:HD2	2.12	0.50
1:A:379:ALA:O	1:A:382:PRO:HD2	2.12	0.50
1:A:20:ALA:HB3	1:A:106:MET:CE	2.38	0.50
1:A:124:LEU:CD2	1:A:129:ALA:HB3	2.41	0.50
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.78	0.50
1:A:93:PRO:HB3	1:A:183:THR:HA	1.94	0.49
1:A:233:HIS:CB	1:A:234:PRO:CD	2.87	0.49
1:A:459:ALA:C	1:A:461:PRO:CD	2.84	0.49
2:B:145:TYR:CE1	2:B:166:VAL:HG13	2.47	0.49
1:A:385:PHE:HB3	6:A:801:HAS:HMA2	1.82	0.49
1:A:410:GLY:O	1:A:501:LEU:CD1	2.61	0.49
1:A:410:GLY:O	1:A:501:LEU:HD11	2.12	0.49
2:B:99:GLN:O	2:B:99:GLN:HG3	2.10	0.49
1:A:63:GLN:HB2	1:A:127:ASN:ND2	2.28	0.49
1:A:182:VAL:CG2	1:A:508:PHE:HE2	2.00	0.49
1:A:192:MET:HG3	1:A:272:PHE:O	2.12	0.49
1:A:391:SER:C	1:A:395:LEU:HD12	2.38	0.49
2:B:64:TRP:CD1	2:B:83:VAL:O	2.65	0.49
1:A:240:LEU:O	1:A:240:LEU:HG	2.12	0.49
1:A:101:PRO:HB3	1:A:166:LEU:HD11	1.94	0.49
2:B:47:ALA:HB2	2:B:134:THR:HB	1.95	0.49
1:A:459:ALA:O	1:A:461:PRO:HD2	2.12	0.48
1:A:10:ARG:O	1:A:11:VAL:C	2.56	0.48
1:A:262:ASP:O	1:A:263:PRO:C	2.56	0.48
1:A:119:VAL:HG12	1:A:148:GLY:HA2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:O	1:A:366:ASN:C	2.57	0.48
2:B:27:PHE:HA	2:B:30:ILE:HG13	1.95	0.48
1:A:79:VAL:HG13	1:A:152:PHE:HE1	1.79	0.48
1:A:252:PRO:O	1:A:255:ALA:HB3	2.14	0.48
1:A:388:GLN:HE21	1:A:388:GLN:CA	2.26	0.48
1:A:63:GLN:CB	1:A:127:ASN:ND2	2.77	0.48
1:A:262:ASP:N	1:A:263:PRO:HD2	2.28	0.48
1:A:132:LEU:C	1:A:134:THR:H	2.22	0.47
1:A:330:ARG:HD2	1:A:330:ARG:H	1.79	0.47
1:A:488:LEU:CD1	1:A:492:LEU:HD12	2.44	0.47
1:A:373:TYR:OH	2:B:45:ILE:HG12	2.13	0.47
1:A:101:PRO:O	1:A:103:MET:N	2.47	0.47
1:A:41:PHE:CE1	1:A:55:LEU:HD12	2.50	0.47
2:B:83:VAL:HG12	2:B:84:LEU:H	1.79	0.47
1:A:33:ILE:O	1:A:33:ILE:HG22	2.14	0.47
1:A:518:ARG:HA	1:A:518:ARG:HD2	1.69	0.47
2:B:142:PRO:CA	2:B:166:VAL:HG22	2.32	0.47
1:A:41:PHE:CD1	1:A:55:LEU:HD12	2.49	0.47
1:A:450:ARG:O	2:B:157:HIS:CD2	2.67	0.47
1:A:504:ALA:HA	1:A:505:PRO:HD3	1.84	0.47
2:B:63:PRO:HG2	2:B:82:TYR:CD2	2.50	0.47
1:A:193:TRP:CE3	1:A:193:TRP:HA	2.50	0.46
1:A:314:PHE:CD1	2:B:15:GLU:HG2	2.50	0.46
1:A:407:ASN:ND2	1:A:506:LEU:HD22	2.30	0.46
1:A:511:VAL:HG12	1:A:512:ILE:C	2.39	0.46
1:A:78:ILE:O	1:A:82:GLN:HB2	2.15	0.46
1:A:89:MET:HB2	1:A:190:TRP:CZ2	2.50	0.46
1:A:273:LEU:C	1:A:274:LEU:HD12	2.40	0.46
2:B:26:LEU:O	2:B:30:ILE:HG13	2.14	0.46
1:A:79:VAL:HG13	1:A:152:PHE:CE1	2.50	0.46
1:A:101:PRO:O	1:A:103:MET:HG2	2.15	0.46
1:A:192:MET:CG	1:A:273:LEU:HA	2.44	0.46
1:A:340:PRO:C	1:A:342:ASP:H	2.23	0.46
1:A:32:LEU:HA	1:A:76:ASN:ND2	2.30	0.46
1:A:360:GLY:O	1:A:364:ILE:HG13	2.16	0.46
1:A:374:VAL:HG21	3:C:30:PHE:HA	1.98	0.46
2:B:119:GLU:OE2	2:B:146:ARG:NH2	2.46	0.46
1:A:460:TYR:N	1:A:461:PRO:HD2	2.28	0.46
1:A:42:GLN:HG2	1:A:52:TYR:OH	2.16	0.46
1:A:518:ARG:NH2	1:A:518:ARG:CG	2.59	0.46
1:A:12:TYR:CE1	1:A:19:LYS:HB2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:NZ	1:A:62:VAL:O	2.49	0.46
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.51	0.46
1:A:96:GLU:O	1:A:96:GLU:HG2	2.16	0.46
1:A:143:TRP:CE3	1:A:213:PHE:HE2	2.33	0.45
1:A:403:TRP:CZ3	1:A:404:LEU:HD22	2.51	0.45
1:A:385:PHE:CD1	1:A:385:PHE:C	2.94	0.45
1:A:372:ASP:OD1	1:A:376:HIS:HB2	2.17	0.45
3:C:12:ILE:HA	3:C:15:LEU:HB3	1.98	0.45
2:B:148:ILE:HG23	2:B:161:PHE:CE2	2.52	0.45
2:B:101:ALA:O	2:B:103:ILE:HD12	2.16	0.45
1:A:181:LEU:CD1	1:A:266:ARG:HG3	2.46	0.45
1:A:407:ASN:ND2	1:A:506:LEU:CD2	2.77	0.45
1:A:427:LEU:HA	1:A:427:LEU:HD23	1.54	0.45
2:B:154:GLY:O	2:B:157:HIS:HB2	2.16	0.45
1:A:199:GLY:HA3	1:A:230:TRP:HB3	1.99	0.45
1:A:207:PHE:CD1	1:A:219:VAL:HG13	2.52	0.45
1:A:363:GLY:O	1:A:366:ASN:HB2	2.17	0.45
3:C:31:PHE:O	3:C:34:GLY:N	2.44	0.45
1:A:92:LEU:O	1:A:93:PRO:C	2.57	0.45
1:A:404:LEU:O	1:A:408:LEU:HG	2.17	0.44
1:A:439:LEU:HD13	1:A:470:ASN:OD1	2.15	0.44
1:A:548:GLN:O	1:A:551:GLY:N	2.50	0.44
1:A:24:PHE:HZ	1:A:109:SER:OG	2.00	0.44
1:A:355:GLY:HA2	1:A:358:PRO:HD2	1.99	0.44
1:A:81:THR:OG1	1:A:239:TRP:CD1	2.70	0.44
1:A:119:VAL:CG1	1:A:148:GLY:HA2	2.48	0.44
1:A:381:VAL:HG12	1:A:385:PHE:CD2	2.52	0.44
3:C:20:LEU:O	3:C:21:VAL:C	2.60	0.44
1:A:499:PRO:HB3	1:A:502:ALA:CB	2.47	0.44
2:B:74:THR:HG23	2:B:78:GLN:HB3	1.99	0.44
1:A:390:ALA:HB1	1:A:432:MET:CE	2.47	0.44
1:A:488:LEU:HD11	1:A:492:LEU:HD12	1.99	0.44
1:A:41:PHE:HD2	1:A:51:ALA:HB3	1.82	0.44
1:A:146:TYR:CD2	1:A:208:LEU:HB3	2.53	0.44
1:A:69:LEU:HD23	1:A:132:LEU:HD22	2.00	0.43
3:C:6:LYS:HA	3:C:9:LEU:HD12	2.00	0.43
1:A:506:LEU:O	1:A:508:PHE:N	2.49	0.43
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.57	0.43
1:A:112:MET:HB3	1:A:112:MET:HE2	1.76	0.43
1:A:374:VAL:HG23	2:B:122:ASN:ND2	2.34	0.43
1:A:184:TYR:CD1	1:A:527:ILE:HD11	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:CD	1:A:180:PRO:HB2	2.43	0.43
1:A:142:HIS:ND1	1:A:144:ALA:HB3	2.33	0.43
1:A:310:LEU:HB3	2:B:18:TRP:CZ2	2.54	0.43
1:A:69:LEU:HD23	1:A:132:LEU:CD2	2.49	0.43
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.83	0.43
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.80	0.43
1:A:486:TYR:O	1:A:490:SER:HB3	2.19	0.43
1:A:307:VAL:CA	1:A:310:LEU:HD12	2.42	0.42
1:A:324:GLY:HA3	1:A:335:TRP:HB2	2.01	0.42
1:A:401:LEU:O	1:A:405:LEU:HB2	2.19	0.42
1:A:420:LEU:HD12	1:A:420:LEU:O	2.19	0.42
1:A:522:LEU:HD12	1:A:522:LEU:HA	1.51	0.42
2:B:51:GLU:OE2	2:B:132:VAL:HB	2.18	0.42
2:B:107:ILE:HG21	2:B:127:VAL:HG21	2.00	0.42
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.31	0.42
1:A:239:TRP:O	1:A:242:PRO:HD2	2.20	0.42
1:A:378:THR:OG1	1:A:380:TRP:HB3	2.19	0.42
1:A:498:LYS:N	1:A:499:PRO:HD3	2.27	0.42
3:C:16:THR:O	3:C:20:LEU:HG	2.19	0.42
1:A:204:ALA:HA	1:A:208:LEU:HB2	2.01	0.42
1:A:347:VAL:HG12	1:A:351:LEU:HD12	2.00	0.42
1:A:30:LEU:HD23	1:A:30:LEU:HA	2.00	0.42
1:A:188:VAL:O	1:A:189:PHE:O	2.37	0.42
1:A:325:ARG:NH1	1:A:331:GLY:O	2.53	0.42
2:B:105:PHE:HZ	2:B:139:PHE:CE1	2.36	0.42
3:C:27:TYR:O	3:C:28:ALA:C	2.61	0.42
1:A:84:PHE:CE1	1:A:397:ALA:HA	2.54	0.42
1:A:134:THR:O	1:A:135:PHE:C	2.62	0.42
1:A:282:HIS:HA	1:A:285:PHE:CE2	2.54	0.42
1:A:130:THR:O	1:A:130:THR:HG22	2.19	0.42
1:A:342:ASP:HB2	1:A:418:ARG:NH2	2.34	0.42
2:B:24:ALA:O	2:B:28:VAL:HG23	2.20	0.42
1:A:27:LEU:HD23	1:A:83:LEU:HD21	2.01	0.42
1:A:61:PHE:H	1:A:61:PHE:HD1	1.68	0.42
1:A:229:TRP:HZ3	1:A:232:GLY:O	2.02	0.42
1:A:251:LEU:HA	1:A:254:GLN:CG	2.50	0.42
1:A:351:LEU:HD21	1:A:426:TRP:CH2	2.54	0.42
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.72	0.42
1:A:56:LYS:HD3	1:A:62:VAL:O	2.20	0.41
1:A:82:GLN:HG2	1:A:238:PHE:CZ	2.55	0.41
1:A:178:VAL:HG22	1:A:522:LEU:CD1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.86	0.41
1:A:25:LEU:O	1:A:29:PHE:HD1	2.04	0.41
1:A:72:HIS:HE1	5:A:800:HEM:C4B	2.38	0.41
1:A:105:LEU:O	1:A:108:LEU:HB3	2.21	0.41
1:A:306:ALA:O	1:A:310:LEU:HD12	2.20	0.41
2:B:10:ALA:O	2:B:14:TYR:HD1	2.04	0.41
1:A:15:TYR:CZ	1:A:95:ARG:NH1	2.89	0.41
1:A:381:VAL:HB	1:A:382:PRO:HD3	2.03	0.41
1:A:82:GLN:NE2	1:A:156:THR:HG23	2.34	0.41
2:B:140:LYS:HB3	2:B:140:LYS:HE3	1.69	0.41
3:C:31:PHE:O	3:C:32:ALA:C	2.64	0.41
1:A:122:LEU:O	1:A:123:PRO:C	2.63	0.41
1:A:239:TRP:HE3	6:A:801:HAS:HBC2	1.85	0.41
1:A:259:LEU:HG	1:A:261:SER:H	1.85	0.41
1:A:374:VAL:HG11	3:C:26:VAL:HG13	2.02	0.41
1:A:411:LYS:HA	1:A:412:PRO:HD3	1.83	0.41
3:C:24:LEU:HD12	3:C:24:LEU:HA	1.97	0.41
1:A:38:PHE:HE2	1:A:62:VAL:HG21	1.86	0.41
1:A:132:LEU:O	1:A:134:THR:N	2.54	0.41
1:A:223:VAL:O	1:A:226:THR:N	2.53	0.41
1:A:466:PRO:O	1:A:469:PHE:N	2.54	0.41
2:B:40:HIS:CD2	2:B:41:THR:HG23	2.56	0.41
1:A:405:LEU:O	1:A:406:PRO:C	2.63	0.41
1:A:488:LEU:HD11	1:A:492:LEU:CD1	2.51	0.41
2:B:44:VAL:HG11	2:B:122:ASN:C	2.46	0.41
2:B:155:LEU:HD23	2:B:155:LEU:O	2.21	0.41
1:A:192:MET:HG2	1:A:273:LEU:HA	2.03	0.40
1:A:233:HIS:CD2	1:A:234:PRO:N	2.89	0.40
1:A:303:LEU:HD13	2:B:30:ILE:HG12	2.03	0.40
1:A:387:LEU:C	1:A:388:GLN:HE21	2.29	0.40
1:A:417:GLN:HE22	1:A:491:VAL:HA	1.86	0.40
1:A:9:SER:OG	1:A:11:VAL:HG23	2.22	0.40
1:A:184:TYR:CD2	1:A:184:TYR:C	2.99	0.40
1:A:254:GLN:H	1:A:254:GLN:HG2	1.73	0.40
2:B:96:GLU:HB3	2:B:167:LYS:HZ3	1.85	0.40
3:C:15:LEU:C	3:C:15:LEU:HD12	2.46	0.40
1:A:420:LEU:HD12	1:A:420:LEU:C	2.47	0.40
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

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%)	427 (77%)	100 (18%)	28 (5%)	1	6
2	B	164/168 (98%)	139 (85%)	21 (13%)	4 (2%)	4	18
3	C	31/34 (91%)	19 (61%)	9 (29%)	3 (10%)	0	1
All	All	750/770 (97%)	585 (78%)	130 (17%)	35 (5%)	2	7

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	58	LEU
1	A	102	ASN
1	A	189	PHE
1	A	366	ASN
2	B	87	ALA
2	B	88	PHE
3	C	32	ALA
1	A	190	TRP
1	A	365	VAL
1	A	379	ALA
1	A	496	GLU
1	A	526	ARG
2	B	158	GLN
3	C	15	LEU
3	C	16	THR
1	A	109	SER
1	A	341	TRP
1	A	504	ALA
1	A	517	ASP
1	A	461	PRO
1	A	57	ARG
1	A	89	MET
1	A	224	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	392	LEU
1	A	422	LEU
1	A	452	TYR
1	A	548	GLN
2	B	4	GLN
1	A	234	PRO
1	A	233	HIS
1	A	355	GLY
1	A	499	PRO
1	A	547	VAL
1	A	28	GLY

5.3.2 Protein sidechains ⓘ

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%)	368 (81%)	85 (19%)	1	5
2	B	136/138 (99%)	112 (82%)	24 (18%)	2	6
3	C	26/27 (96%)	21 (81%)	5 (19%)	1	5
All	All	615/627 (98%)	501 (82%)	114 (18%)	1	5

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	ILE
1	A	23	TYR
1	A	26	VAL
1	A	48	ASN
1	A	54	LEU
1	A	56	LYS
1	A	59	LEU
1	A	70	THR
1	A	74	VAL
1	A	78	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	GLN
1	A	99	MET
1	A	103	MET
1	A	124	LEU
1	A	125	LEU
1	A	133	TYR
1	A	134	THR
1	A	147	LEU
1	A	150	SER
1	A	152	PHE
1	A	164	LEU
1	A	168	ARG
1	A	169	ARG
1	A	177	LYS
1	A	179	THR
1	A	183	THR
1	A	195	LEU
1	A	213	PHE
1	A	215	LEU
1	A	216	VAL
1	A	236	VAL
1	A	238	PHE
1	A	253	LYS
1	A	254	GLN
1	A	261	SER
1	A	305	VAL
1	A	309	SER
1	A	315	THR
1	A	319	SER
1	A	326	LEU
1	A	327	ARG
1	A	330	ARG
1	A	339	LEU
1	A	350	VAL
1	A	354	LEU
1	A	364	ILE
1	A	374	VAL
1	A	388	GLN
1	A	389	VAL
1	A	391	SER
1	A	395	LEU
1	A	404	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	405	LEU
1	A	418	ARG
1	A	419	ARG
1	A	420	LEU
1	A	430	LEU
1	A	434	ILE
1	A	437	VAL
1	A	439	LEU
1	A	449	ARG
1	A	455	GLN
1	A	465	VAL
1	A	468	VAL
1	A	472	LEU
1	A	477	LEU
1	A	478	LEU
1	A	490	SER
1	A	492	LEU
1	A	496	GLU
1	A	500	GLU
1	A	501	LEU
1	A	506	LEU
1	A	512	ILE
1	A	518	ARG
1	A	520	LEU
1	A	522	LEU
1	A	533	VAL
1	A	536	ILE
1	A	537	LEU
1	A	547	VAL
1	A	548	GLN
1	A	556	VAL
1	A	560	ARG
2	B	6	LYS
2	B	9	LYS
2	B	11	ILE
2	B	12	LEU
2	B	16	LYS
2	B	19	LEU
2	B	23	LEU
2	B	26	LEU
2	B	30	ILE
2	B	39	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	46	PRO
2	B	72	VAL
2	B	77	ASN
2	B	95	ILE
2	B	99	GLN
2	B	111	ASP
2	B	136	ARG
2	B	140	LYS
2	B	141	ARG
2	B	146	ARG
2	B	149	CYS
2	B	155	LEU
2	B	166	VAL
2	B	168	GLU
3	C	2	GLU
3	C	6	LYS
3	C	13	LEU
3	C	21	VAL
3	C	24	LEU

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

Mol	Chain	Res	Type
1	A	48	ASN
1	A	76	ASN
1	A	127	ASN
1	A	254	GLN
1	A	388	GLN
1	A	455	GLN
2	B	4	GLN
2	B	5	HIS
2	B	78	GLN
2	B	91	GLN
2	B	122	ASN
2	B	151	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
7	CUA	B	802	2	0,1,1	-	-	-		
5	HEM	A	800	1	50,50,50	1.86	8 (16%)	67,82,82	1.80	14 (20%)
6	HAS	A	801	1	72,72,72	2.61	23 (31%)	87,109,109	4.00	48 (55%)

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	-	8/14/54/54	-
6	HAS	A	801	1	1/1/8/18	8/42/82/82	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3D-C2D	8.39	1.54	1.36
6	A	801	HAS	C2A-C3A	6.55	1.50	1.36
6	A	801	HAS	CHB-C1D	6.50	1.51	1.38
6	A	801	HAS	CHC-C4B	6.30	1.51	1.38
6	A	801	HAS	CHD-C4A	6.09	1.50	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	FE-NB	6.00	2.13	1.94
6	A	801	HAS	CAC-C3C	-4.99	1.34	1.47
6	A	801	HAS	CHA-C1A	4.86	1.47	1.38
6	A	801	HAS	CHA-C4D	4.83	1.50	1.39
6	A	801	HAS	CHB-C1B	4.71	1.49	1.39
6	A	801	HAS	CHC-C1C	4.35	1.49	1.39
6	A	801	HAS	FE-NC	4.30	2.09	1.95
6	A	801	HAS	FE-ND	4.27	2.08	1.94
6	A	801	HAS	C1A-NA	-4.05	1.32	1.39
6	A	801	HAS	C4A-C3A	3.81	1.52	1.45
6	A	801	HAS	CHD-C4C	3.69	1.47	1.39
6	A	801	HAS	C4A-NA	-3.38	1.33	1.39
6	A	801	HAS	C2D-C3D	3.19	1.44	1.37
5	A	800	HEM	FE-ND	3.13	2.04	1.94
5	A	800	HEM	CMB-C2B	3.08	1.57	1.50
5	A	800	HEM	CMA-C3A	2.99	1.56	1.50
6	A	801	HAS	C4C-NC	-2.93	1.34	1.39
5	A	800	HEM	CAB-C3B	2.92	1.55	1.47
6	A	801	HAS	C1A-C2A	2.46	1.49	1.45
6	A	801	HAS	C4B-C3B	-2.42	1.40	1.44
5	A	800	HEM	FE-NB	2.39	2.02	1.94
5	A	800	HEM	C3C-C2C	-2.37	1.32	1.37
6	A	801	HAS	C1C-NC	-2.29	1.35	1.39
6	A	801	HAS	C2D-C1D	2.28	1.49	1.44
6	A	801	HAS	C1D-ND	-2.25	1.36	1.40
5	A	800	HEM	CMD-C2D	2.21	1.55	1.50

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C3C-C2C-C1C	-15.33	89.10	107.17
6	A	801	HAS	C4C-C3C-C2C	9.30	118.87	107.30
6	A	801	HAS	CBC-CAC-C3C	9.24	173.70	127.53
6	A	801	HAS	CHA-C1A-NA	7.67	132.80	124.45
6	A	801	HAS	CHA-C1A-C2A	-7.64	112.81	124.86
6	A	801	HAS	C2C-C1C-NC	7.54	122.22	110.14
6	A	801	HAS	CHD-C4A-C3A	-7.25	110.42	125.49
6	A	801	HAS	CHC-C1C-C2C	-7.21	106.50	127.43
6	A	801	HAS	CHD-C4A-NA	6.40	131.42	124.45
6	A	801	HAS	C4A-C3A-C2A	-6.02	98.04	106.97
6	A	801	HAS	CHB-C1D-ND	5.85	131.60	124.37
6	A	801	HAS	C2D-C3D-C4D	-5.80	102.23	106.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CBA-CAA-C2A	-5.50	97.32	112.53
6	A	801	HAS	CMC-C2C-C3C	-5.44	113.75	126.55
6	A	801	HAS	OMD-CMD-C2D	-5.30	113.65	125.62
5	A	800	HEM	CAA-CBA-CGA	-5.20	99.88	113.67
6	A	801	HAS	CMC-C2C-C1C	-5.15	117.58	125.42
5	A	800	HEM	C4D-ND-C1D	4.95	111.06	105.21
6	A	801	HAS	CMA-C3A-C2A	-4.92	112.84	126.15
6	A	801	HAS	C1C-CHC-C4B	-4.77	115.04	126.25
6	A	801	HAS	C1A-CHA-C4D	-4.75	115.92	126.02
6	A	801	HAS	C27-C19-C20	4.57	123.17	115.23
6	A	801	HAS	C3C-C4C-NC	-4.32	106.16	109.80
6	A	801	HAS	CAA-C2A-C3A	-4.29	119.84	127.87
6	A	801	HAS	O1A-CGA-CBA	-4.26	109.59	123.09
5	A	800	HEM	CBA-CAA-C2A	4.13	123.95	112.53
6	A	801	HAS	CHC-C4B-NB	4.09	129.43	124.37
5	A	800	HEM	CAD-CBD-CGD	-4.05	102.91	113.67
6	A	801	HAS	CHC-C1C-NC	4.03	131.17	123.86
5	A	800	HEM	CBC-CAC-C3C	-4.02	107.42	127.53
6	A	801	HAS	C1B-CHB-C1D	-4.02	117.00	125.69
6	A	801	HAS	C2A-C1A-NA	3.95	114.13	110.32
6	A	801	HAS	C3D-C4D-ND	3.92	114.14	110.35
6	A	801	HAS	CMB-C2B-C3B	-3.89	122.76	130.28
6	A	801	HAS	C3A-C4A-NA	3.85	116.77	109.64
6	A	801	HAS	C25-C23-C24	3.68	121.61	115.23
5	A	800	HEM	CAA-C2A-C1A	-3.52	118.06	124.94
5	A	800	HEM	C4C-C3C-C2C	3.46	109.81	106.81
6	A	801	HAS	CAD-C3D-C4D	3.43	130.67	124.70
6	A	801	HAS	CHA-C4D-C3D	-3.38	119.85	124.77
5	A	800	HEM	CMA-C3A-C2A	3.26	132.54	125.62
6	A	801	HAS	CHC-C4B-C3B	-3.21	117.70	125.80
6	A	801	HAS	C4C-CHD-C4A	-3.07	115.18	124.66
6	A	801	HAS	CMB-C2B-C1B	3.01	129.73	125.03
5	A	800	HEM	CAA-C2A-C3A	2.97	133.74	127.07
6	A	801	HAS	C1D-ND-C4D	2.90	108.64	105.21
6	A	801	HAS	CHB-C1B-NB	2.75	127.38	124.42
6	A	801	HAS	C31-C30-C29	-2.70	114.56	122.66
6	A	801	HAS	C3B-C4B-NB	2.64	112.87	109.84
6	A	801	HAS	CAA-C2A-C1A	-2.57	119.63	124.85
6	A	801	HAS	O2A-CGA-CBA	2.50	121.90	114.00
6	A	801	HAS	C20-C19-C18	-2.47	115.62	121.17
5	A	800	HEM	C1D-C2D-C3D	-2.32	104.54	106.98
5	A	800	HEM	CMD-C2D-C1D	2.28	128.60	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CHB-C1B-C2B	-2.23	121.51	125.03
6	A	801	HAS	C24-C23-C22	-2.20	116.22	121.17
6	A	801	HAS	C1A-C2A-C3A	-2.09	104.35	107.11
5	A	800	HEM	CMA-C3A-C4A	-2.07	122.26	125.42
5	A	800	HEM	CHD-C4C-NC	2.06	126.70	124.45
5	A	800	HEM	C3B-C2B-C1B	-2.05	104.88	106.41
6	A	801	HAS	C32-C30-C31	2.02	119.24	114.59
6	A	801	HAS	O2D-CGD-CBD	2.01	120.36	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	801	HAS	NA

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	800	HEM	C1A-C2A-CAA-CBA
5	A	800	HEM	C3A-C2A-CAA-CBA
6	A	801	HAS	C1D-C2D-CMD-OMD
6	A	801	HAS	C3D-C2D-CMD-OMD
6	A	801	HAS	C1A-C2A-CAA-CBA
5	A	800	HEM	C4C-C3C-CAC-CBC
5	A	800	HEM	C2C-C3C-CAC-CBC
6	A	801	HAS	CAA-CBA-CGA-O1A
5	A	800	HEM	CAA-CBA-CGA-O1A
5	A	800	HEM	CAD-CBD-CGD-O1D
6	A	801	HAS	CAA-CBA-CGA-O2A
5	A	800	HEM	CAD-CBD-CGD-O2D
6	A	801	HAS	C11-C12-C13-C14
5	A	800	HEM	CAA-CBA-CGA-O2A
6	A	801	HAS	CAD-CBD-CGD-O1D
6	A	801	HAS	CAD-CBD-CGD-O2D

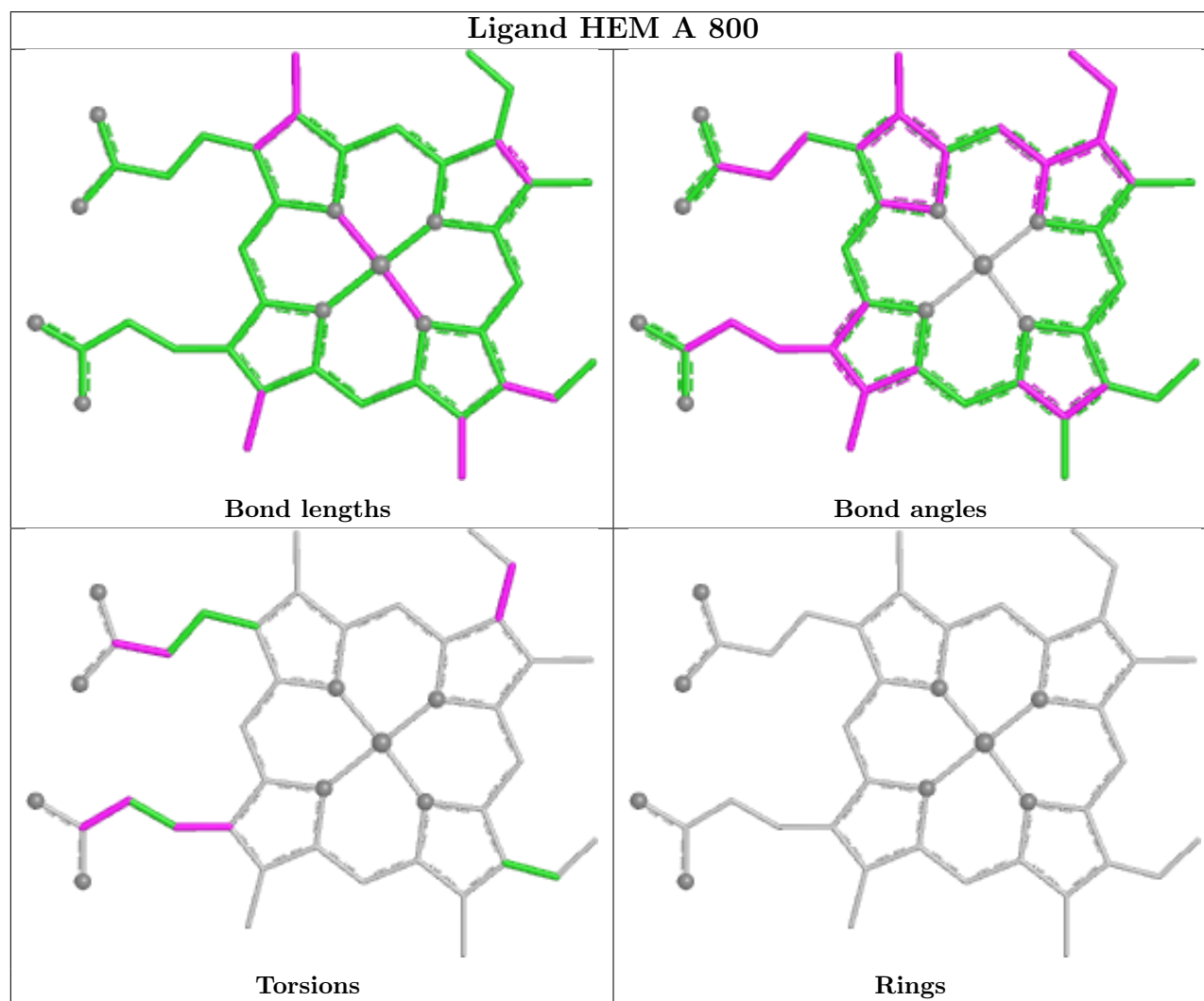
There are no ring outliers.

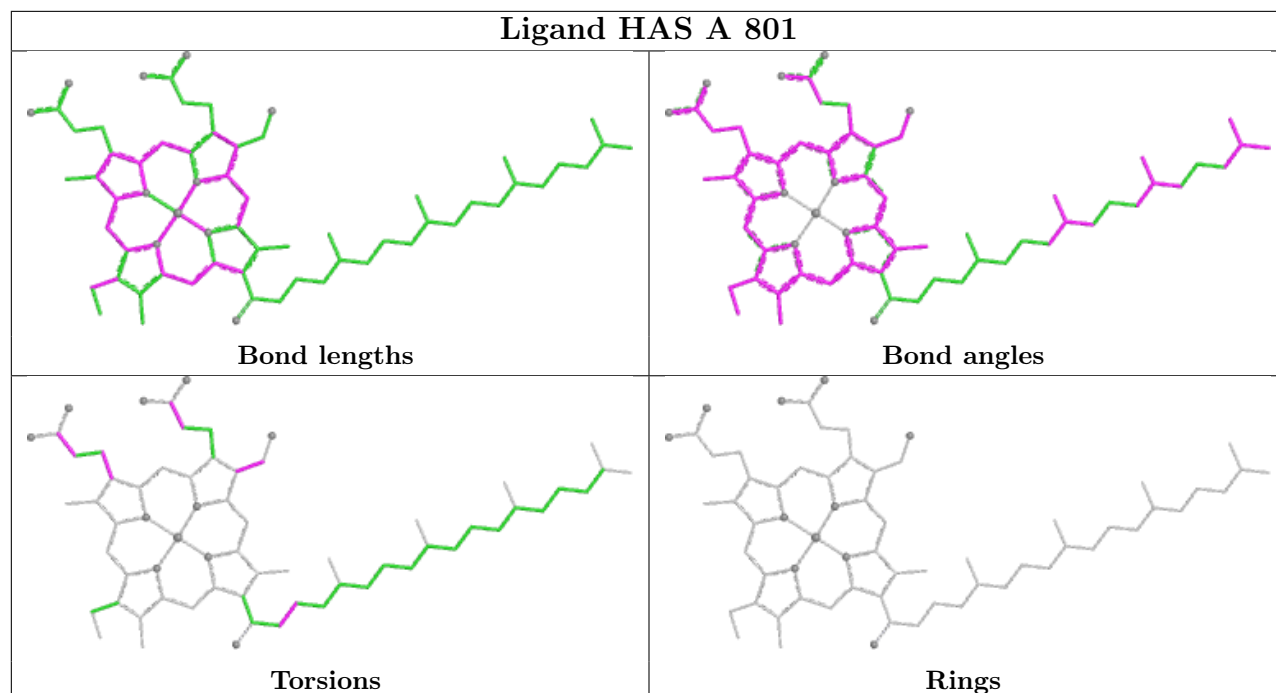
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	7	0
6	A	801	HAS	14	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/568 (98%)	-0.44	4 (0%) 84 79	64, 88, 129, 216	0
2	B	166/168 (98%)	-0.63	0 100 100	71, 88, 124, 174	0
3	C	33/34 (97%)	-0.65	0 100 100	69, 79, 133, 154	0
All	All	756/770 (98%)	-0.49	4 (0%) 87 83	64, 88, 131, 216	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	ALA	3.9
1	A	8	ILE	3.0
1	A	503	GLU	2.4
1	A	9	SER	2.3

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](#)

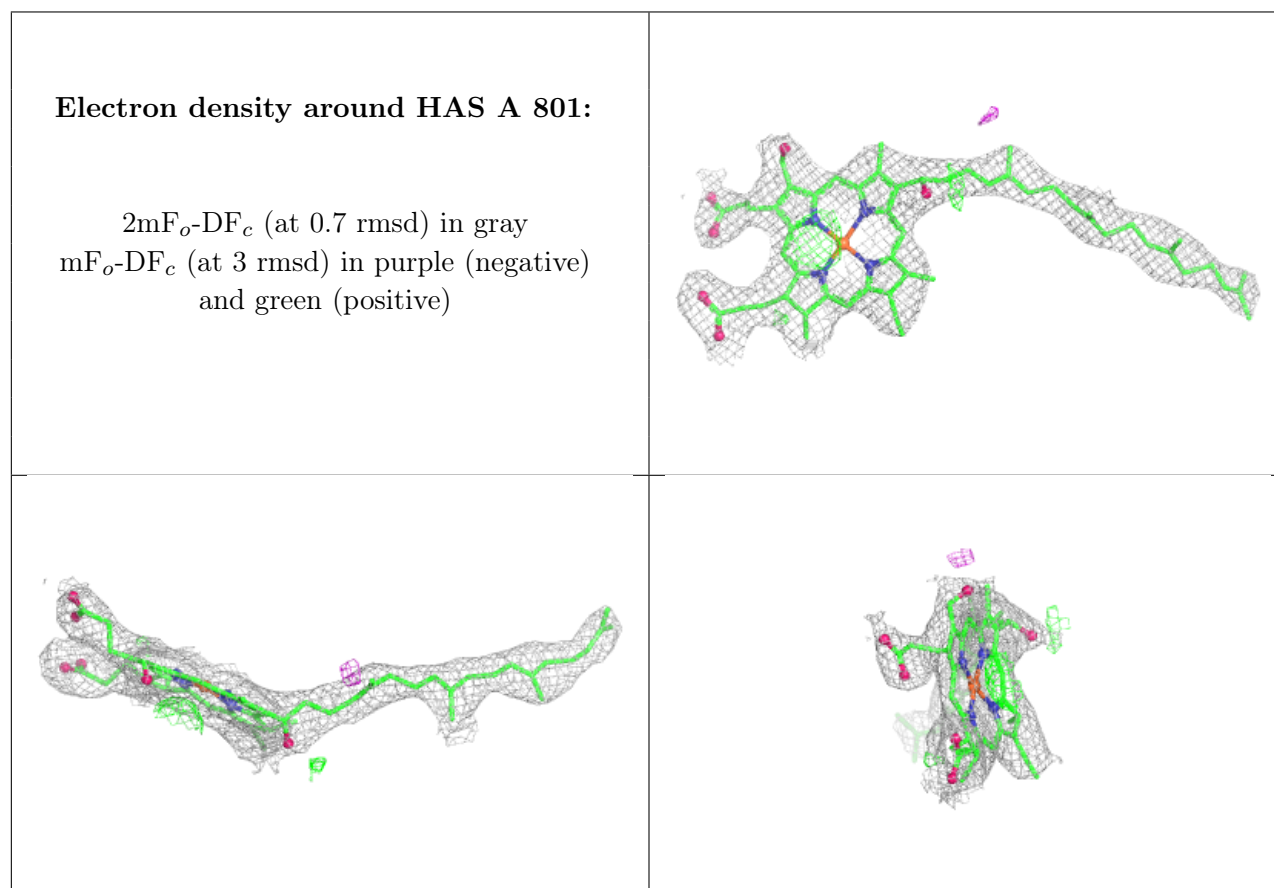
There are no oligosaccharides in this entry.

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, 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.

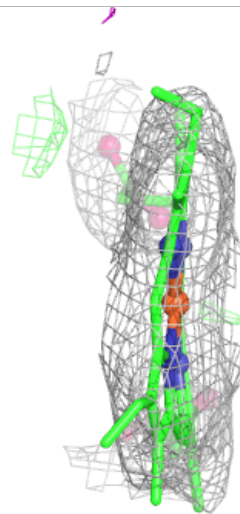
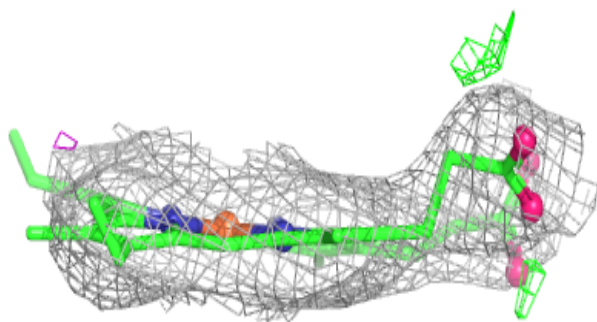
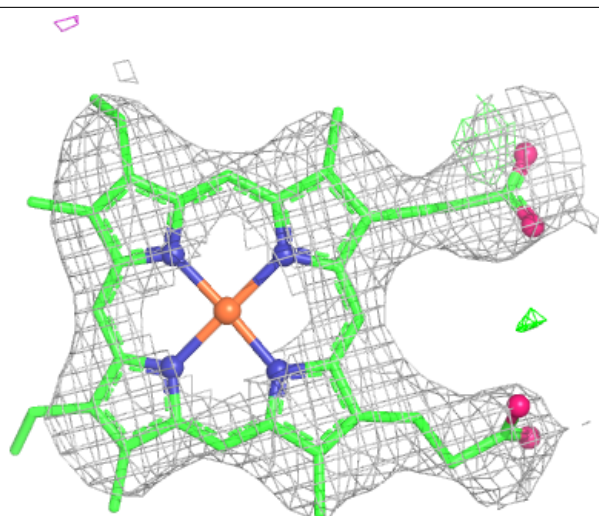
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	HAS	A	801	65/65	0.96	0.09	53,74,87,93	0
5	HEM	A	800	43/43	0.97	0.07	50,68,90,98	0
4	CU1	A	803	1/1	0.98	0.04	84,84,84,84	0
7	CUA	B	802	2/2	0.99	0.02	88,88,88,90	0

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 ⓘ

There are no such residues in this entry.