



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:05 pm BST

PDB ID : 1MBD
Title : X-ray structure of sperm whale deoxymoglobin refined at 1.4Å resolution
Authors : Phillips, S.E.V.
Deposited on : 1981-08-27
Resolution : 1.40 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

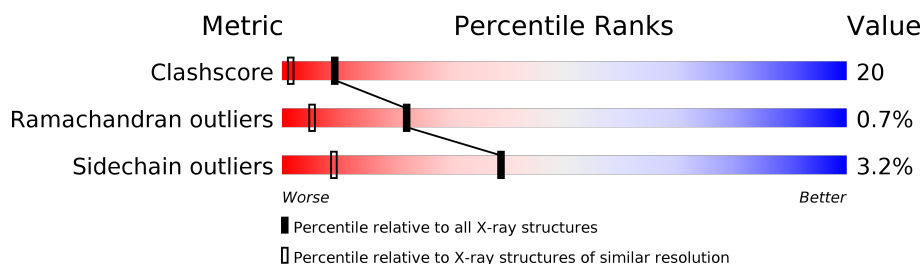
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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))
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	153	<div> <div></div> <div>32%</div> <div>39%</div> <div>21%</div> <div>8%</div> </div>

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
2	SO4	A	154	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1666 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 MYOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	4	0
			1230	795	216	217	2			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is water.

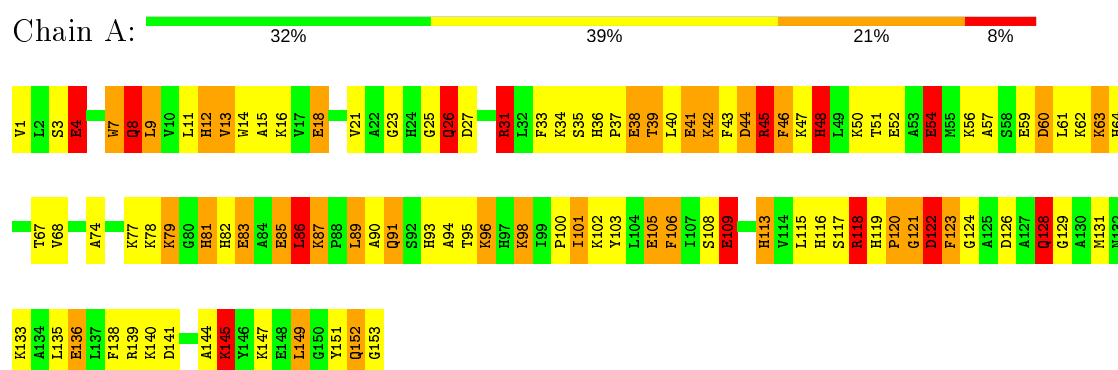
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	388	Total	O	0	0
			388	388		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

• Molecule 1: MYOGLOBIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.66Å 31.12Å 35.06Å 90.00° 105.78° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CONSTRAINED RECIPROCAL-SPACE LEAST-SQUARES	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1666	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	2.18	43/1281 (3.4%)	3.00	102/1721 (5.9%)

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	15

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	HIS	CE1-NE2	9.20	1.53	1.32
1	A	41	GLU	CD-OE2	-9.09	1.15	1.25
1	A	109	GLU	CD-OE1	-8.74	1.16	1.25
1	A	105	GLU	CG-CD	7.94	1.63	1.51
1	A	83	GLU	CD-OE2	-7.18	1.17	1.25
1	A	4	GLU	CD-OE2	-7.10	1.17	1.25
1	A	81	HIS	CE1-NE2	6.99	1.48	1.32
1	A	91	GLN	C-N	6.94	1.50	1.34
1	A	81	HIS	CG-CD2	6.82	1.47	1.35
1	A	14	TRP	CG-CD1	6.47	1.45	1.36
1	A	25	GLY	N-CA	6.47	1.55	1.46
1	A	108	SER	CA-CB	-6.45	1.43	1.52
1	A	81	HIS	CG-ND1	6.23	1.52	1.38
1	A	118	ARG	NE-CZ	6.22	1.41	1.33
1	A	4	GLU	CD-OE1	6.14	1.32	1.25
1	A	147	LYS	CD-CE	6.11	1.66	1.51
1	A	45	ARG	CB-CG	-5.95	1.36	1.52
1	A	83	GLU	CG-CD	5.94	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	HIS	ND1-CE1	5.87	1.49	1.34
1	A	86[A]	LEU	CA-C	-5.87	1.37	1.52
1	A	86[B]	LEU	CA-C	-5.87	1.37	1.52
1	A	14	TRP	NE1-CE2	-5.82	1.29	1.37
1	A	121	GLY	N-CA	5.80	1.54	1.46
1	A	12	HIS	CE1-NE2	5.79	1.46	1.32
1	A	23	GLY	N-CA	-5.69	1.37	1.46
1	A	45	ARG	CZ-NH2	5.69	1.40	1.33
1	A	38	GLU	CD-OE2	5.60	1.31	1.25
1	A	120	PRO	C-N	-5.58	1.23	1.33
1	A	105	GLU	CD-OE2	-5.57	1.19	1.25
1	A	123	PHE	CE2-CZ	-5.56	1.26	1.37
1	A	45	ARG	CZ-NH1	5.52	1.40	1.33
1	A	121	GLY	C-N	-5.47	1.21	1.34
1	A	31	ARG	CD-NE	5.45	1.55	1.46
1	A	118	ARG	CD-NE	-5.33	1.37	1.46
1	A	9	LEU	CA-CB	-5.27	1.41	1.53
1	A	145	LYS	CD-CE	5.27	1.64	1.51
1	A	85	GLU	CD-OE1	-5.27	1.19	1.25
1	A	98	LYS	CB-CG	-5.26	1.38	1.52
1	A	98	LYS	C-N	-5.16	1.22	1.34
1	A	81	HIS	N-CA	5.12	1.56	1.46
1	A	124	GLY	N-CA	5.07	1.53	1.46
1	A	68	VAL	CA-C	-5.04	1.39	1.52
1	A	96	LYS	CG-CD	5.03	1.69	1.52

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ARG	NE-CZ-NH2	-52.76	93.92	120.30
1	A	31	ARG	NE-CZ-NH1	-16.88	111.86	120.30
1	A	118	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	A	26	GLN	OE1-CD-NE2	-13.79	90.19	121.90
1	A	139	ARG	NE-CZ-NH2	13.18	126.89	120.30
1	A	109	GLU	OE1-CD-OE2	-13.10	107.58	123.30
1	A	126	ASP	CB-CG-OD1	-12.61	106.95	118.30
1	A	86[A]	LEU	CD1-CG-CD2	-12.54	72.87	110.50
1	A	86[B]	LEU	CD1-CG-CD2	-12.54	72.87	110.50
1	A	106	PHE	CB-CG-CD2	-12.18	112.27	120.80
1	A	118	ARG	CD-NE-CZ	11.69	139.97	123.60
1	A	118	ARG	NH1-CZ-NH2	11.69	132.25	119.40
1	A	1	VAL	N-CA-CB	-11.20	86.86	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	GLU	CG-CD-OE2	-10.95	96.40	118.30
1	A	45	ARG	NE-CZ-NH2	10.09	125.35	120.30
1	A	139	ARG	NE-CZ-NH1	-10.08	115.26	120.30
1	A	52	GLU	OE1-CD-OE2	9.96	135.25	123.30
1	A	113	HIS	CG-ND1-CE1	-9.94	92.78	105.70
1	A	45	ARG	NH1-CZ-NH2	-9.82	108.60	119.40
1	A	115	LEU	CB-CG-CD1	9.72	127.52	111.00
1	A	138	PHE	CB-CG-CD2	-9.27	114.31	120.80
1	A	83	GLU	OE1-CD-OE2	-8.96	112.55	123.30
1	A	4	GLU	CG-CD-OE1	8.95	136.20	118.30
1	A	64	HIS	CG-ND1-CE1	-8.68	94.41	105.70
1	A	91	GLN	O-C-N	-8.55	109.02	122.70
1	A	89[A]	LEU	CD1-CG-CD2	-8.52	84.95	110.50
1	A	89[B]	LEU	CD1-CG-CD2	-8.52	84.95	110.50
1	A	128	GLN	CG-CD-OE1	-8.51	104.58	121.60
1	A	13[A]	VAL	CG1-CB-CG2	-8.45	97.38	110.90
1	A	13[B]	VAL	CG1-CB-CG2	-8.45	97.38	110.90
1	A	145	LYS	CB-CG-CD	8.30	133.19	111.60
1	A	139	ARG	CD-NE-CZ	8.24	135.13	123.60
1	A	18	GLU	O-C-N	8.19	135.80	122.70
1	A	147	LYS	CD-CE-NZ	-8.15	92.94	111.70
1	A	45	ARG	N-CA-CB	-8.07	96.07	110.60
1	A	86[A]	LEU	O-C-N	-8.03	109.86	122.70
1	A	86[B]	LEU	O-C-N	-8.03	109.86	122.70
1	A	38	GLU	OE1-CD-OE2	-7.73	114.02	123.30
1	A	122	ASP	N-CA-CB	7.71	124.47	110.60
1	A	83	GLU	CG-CD-OE1	7.66	133.62	118.30
1	A	87	LYS	CB-CG-CD	-7.66	91.68	111.60
1	A	18	GLU	OE1-CD-OE2	7.50	132.29	123.30
1	A	91	GLN	CA-C-O	7.42	135.69	120.10
1	A	144	ALA	O-C-N	-7.29	111.04	122.70
1	A	31	ARG	CG-CD-NE	-7.09	96.92	111.80
1	A	87	LYS	CA-CB-CG	-7.01	97.98	113.40
1	A	96	LYS	CD-CE-NZ	6.82	127.39	111.70
1	A	118	ARG	O-C-N	-6.70	111.98	122.70
1	A	109	GLU	CG-CD-OE2	6.68	131.66	118.30
1	A	63	LYS	CB-CG-CD	-6.64	94.33	111.60
1	A	122	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	86[A]	LEU	CA-C-O	6.58	133.91	120.10
1	A	86[B]	LEU	CA-C-O	6.58	133.91	120.10
1	A	113	HIS	ND1-CG-CD2	6.58	118.01	108.80
1	A	101	ILE	O-C-N	-6.51	112.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	CB-CG-CD2	6.50	125.35	120.80
1	A	64	HIS	ND1-CE1-NE2	6.48	124.16	109.90
1	A	87	LYS	O-C-N	-6.43	108.88	121.10
1	A	27	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	A	31	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	A	64	HIS	ND1-CG-CD2	6.24	117.53	108.80
1	A	131	MET	CG-SD-CE	-6.22	90.25	100.20
1	A	106	PHE	CD1-CG-CD2	6.15	126.29	118.30
1	A	4	GLU	CB-CA-C	6.02	122.43	110.40
1	A	27	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	126	ASP	N-CA-CB	5.95	121.32	110.60
1	A	21	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	A	13[A]	VAL	CA-CB-CG1	5.91	119.76	110.90
1	A	13[B]	VAL	CA-CB-CG1	5.91	119.76	110.90
1	A	68	VAL	O-C-N	-5.91	113.25	122.70
1	A	54	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	A	89[A]	LEU	CB-CG-CD1	-5.90	100.96	111.00
1	A	89[B]	LEU	CB-CG-CD1	-5.90	100.96	111.00
1	A	7	TRP	CG-CD2-CE3	5.86	139.17	133.90
1	A	81	HIS	CG-ND1-CE1	-5.85	98.09	105.70
1	A	41	GLU	O-C-N	-5.80	113.42	122.70
1	A	60	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	27	ASP	OD1-CG-OD2	5.76	134.25	123.30
1	A	98	LYS	CD-CE-NZ	-5.75	98.47	111.70
1	A	63	LYS	CD-CE-NZ	-5.75	98.48	111.70
1	A	89[A]	LEU	CB-CG-CD2	5.72	120.72	111.00
1	A	89[B]	LEU	CB-CG-CD2	5.72	120.72	111.00
1	A	126	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	44	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	48	HIS	O-C-N	-5.55	113.82	122.70
1	A	90	ALA	N-CA-CB	-5.54	102.35	110.10
1	A	8	GLN	OE1-CD-NE2	-5.49	109.28	121.90
1	A	149	LEU	O-C-N	-5.48	113.89	123.20
1	A	45	ARG	O-C-N	-5.44	114.00	122.70
1	A	116	HIS	CB-CG-CD2	-5.43	113.96	130.80
1	A	8	GLN	O-C-N	-5.42	114.03	122.70
1	A	41	GLU	CB-CG-CD	-5.34	99.78	114.20
1	A	94	ALA	N-CA-CB	-5.33	102.64	110.10
1	A	138	PHE	CB-CG-CD1	5.27	124.49	120.80
1	A	7	TRP	N-CA-CB	5.27	120.09	110.60
1	A	39	THR	CA-CB-CG2	5.24	119.73	112.40
1	A	129	GLY	O-C-N	-5.21	114.36	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	LYS	CB-CG-CD	-5.20	98.09	111.60
1	A	43	PHE	CB-CG-CD1	5.12	124.39	120.80
1	A	120	PRO	O-C-N	-5.08	114.56	123.20
1	A	79	LYS	O-C-N	5.08	131.83	123.20
1	A	60	ASP	OD1-CG-OD2	5.04	132.88	123.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	GLU	Sidechain
1	A	118	ARG	Sidechain
1	A	122	ASP	Sidechain,Mainchain
1	A	128	GLN	Sidechain
1	A	136	GLU	Sidechain
1	A	26	GLN	Sidechain
1	A	31	ARG	Sidechain
1	A	4	GLU	Sidechain
1	A	42	LYS	Mainchain
1	A	45	ARG	Sidechain
1	A	48	HIS	Mainchain
1	A	54	GLU	Sidechain
1	A	67	THR	Mainchain
1	A	8	GLN	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1230	0	1257	50	251
2	A	5	0	0	0	2
3	A	43	0	30	1	0
4	A	388	0	0	31	246
All	All	1666	0	1287	51	306

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 20.

All (51) 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:61:LEU:HG	4:A:528:HOH:O	1.16	1.27
1:A:26:GLN:CD	4:A:328:HOH:O	1.86	1.12
1:A:91:GLN:O	4:A:321:HOH:O	1.66	1.12
1:A:98:LYS:NZ	1:A:151[B]:TYR:HE1	1.48	1.12
1:A:86[B]:LEU:CD2	1:A:86[B]:LEU:CD1	2.31	1.08
1:A:34:LYS:HE3	4:A:332:HOH:O	1.53	1.07
1:A:98:LYS:NZ	1:A:151[B]:TYR:CE1	2.35	0.95
1:A:140:LYS:HE3	4:A:525:HOH:O	1.64	0.94
1:A:122:ASP:CG	4:A:350:HOH:O	2.08	0.91
1:A:91:GLN:NE2	4:A:276:HOH:O	2.07	0.87
1:A:34:LYS:NZ	4:A:286:HOH:O	2.10	0.84
1:A:153:GLY:N	4:A:539:HOH:O	2.10	0.82
1:A:8:GLN:OE1	4:A:541:HOH:O	1.98	0.81
1:A:34:LYS:HD3	4:A:287:HOH:O	1.81	0.79
1:A:83:GLU:OE2	4:A:248:HOH:O	2.05	0.73
1:A:109:GLU:OE1	4:A:543:HOH:O	2.08	0.72
1:A:153:GLY:CA	4:A:539:HOH:O	2.36	0.72
1:A:153:GLY:HA3	4:A:539:HOH:O	1.90	0.71
1:A:98:LYS:HZ3	1:A:151[B]:TYR:HE1	1.39	0.70
1:A:26:GLN:NE2	4:A:328:HOH:O	2.14	0.69
1:A:86[B]:LEU:CD1	1:A:86[B]:LEU:HD22	2.21	0.68
1:A:113:HIS:ND1	4:A:508:HOH:O	2.29	0.65
1:A:26:GLN:OE1	1:A:62:LYS:HD2	2.00	0.61
1:A:60:ASP:OD1	4:A:296:HOH:O	2.17	0.59
1:A:86[B]:LEU:HD13	1:A:86[B]:LEU:HD22	1.83	0.59
1:A:141:ASP:O	1:A:145:LYS:HE2	2.03	0.58
1:A:145:LYS:HE3	4:A:365:HOH:O	2.02	0.58
1:A:121:GLY:C	4:A:350:HOH:O	2.47	0.53
1:A:140:LYS:CE	4:A:525:HOH:O	2.40	0.52
1:A:95:THR:OG1	4:A:321:HOH:O	1.91	0.52
1:A:81:HIS:HD2	4:A:307:HOH:O	1.92	0.51
1:A:31:ARG:NH2	4:A:338:HOH:O	2.43	0.50
1:A:83:GLU:CD	1:A:83:GLU:H	2.14	0.50
1:A:83:GLU:HG3	4:A:248:HOH:O	2.12	0.48
1:A:109:GLU:HG3	4:A:355:HOH:O	2.13	0.48
1:A:82:HIS:CD2	1:A:86[B]:LEU:HD22	2.49	0.47
1:A:83:GLU:OE1	4:A:196:HOH:O	2.20	0.47
1:A:78:LYS:HE3	1:A:85:GLU:OE2	2.15	0.47
1:A:13[B]:VAL:HG22	1:A:122:ASP:O	2.16	0.46
1:A:13[A]:VAL:HG12	1:A:122:ASP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:C	4:A:321:HOH:O	2.34	0.46
1:A:149:LEU:HD11	4:A:230:HOH:O	2.17	0.45
1:A:101:ILE:HG12	1:A:152:GLN:HE22	1.83	0.43
1:A:119:HIS:N	1:A:120:PRO:CD	2.83	0.42
3:A:155:HEM:HMC1	3:A:155:HEM:HBC2	2.01	0.42
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.85	0.41
1:A:15:ALA:O	4:A:329:HOH:O	2.22	0.41
1:A:128:GLN:OE1	4:A:225:HOH:O	2.22	0.40
1:A:141:ASP:O	1:A:145:LYS:CE	2.68	0.40

All (306) 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:39:THR:N	4:A:453:HOH:O[1_554]	0.18	2.02
4:A:538:HOH:O	4:A:542:HOH:O[2_555]	0.28	1.92
1:A:153:GLY:C	4:A:353:HOH:O[2_555]	0.33	1.87
1:A:4:GLU:CD	1:A:36:HIS:N[1_556]	0.48	1.72
1:A:4:GLU:CG	1:A:35:SER:C[1_556]	0.50	1.70
1:A:4:GLU:OE1	1:A:36:HIS:CA[1_556]	0.59	1.61
1:A:4:GLU:CB	1:A:35:SER:O[1_556]	0.60	1.60
1:A:39:THR:CG2	4:A:460:HOH:O[1_554]	0.62	1.58
1:A:119:HIS:CG	4:A:412:HOH:O[2_646]	0.63	1.57
1:A:50:LYS:CG	1:A:77:LYS:CE[1_554]	0.69	1.51
1:A:117:SER:C	4:A:447:HOH:O[2_645]	0.72	1.48
1:A:106:PHE:CD1	4:A:359:HOH:O[1_554]	0.73	1.47
1:A:63:LYS:CG	4:A:493:HOH:O[2_655]	0.74	1.46
1:A:117:SER:O	4:A:447:HOH:O[2_645]	0.78	1.42
4:A:189:HOH:O	4:A:336:HOH:O[1_554]	0.79	1.41
2:A:154:SO4:O2	4:A:357:HOH:O[2_655]	0.82	1.38
4:A:193:HOH:O	4:A:487:HOH:O[1_554]	0.84	1.36
1:A:4:GLU:OE2	1:A:36:HIS:N[1_556]	0.90	1.30
4:A:166:HOH:O	4:A:294:HOH:O[1_554]	0.93	1.27
1:A:40:LEU:N	4:A:432:HOH:O[1_554]	0.95	1.25
4:A:311:HOH:O	4:A:423:HOH:O[2_645]	0.96	1.24
1:A:121:GLY:O	4:A:473:HOH:O[2_646]	0.98	1.22
1:A:37:PRO:CA	1:A:79:LYS:CE[1_554]	1.00	1.20
1:A:153:GLY:OXT	4:A:540:HOH:O[2_555]	1.01	1.19
1:A:26:GLN:CB	4:A:269:HOH:O[2_645]	1.01	1.19
1:A:54:GLU:CD	4:A:433:HOH:O[1_554]	1.02	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:SER:O	4:A:259:HOH:O[1_556]	1.02	1.18
1:A:12:HIS:N	4:A:292:HOH:O[1_556]	1.03	1.17
1:A:122:ASP:CA	4:A:462:HOH:O[2_646]	1.04	1.16
1:A:47:LYS:O	4:A:406:HOH:O[1_554]	1.05	1.15
1:A:40:LEU:CD1	4:A:420:HOH:O[1_554]	1.06	1.14
1:A:122:ASP:N	4:A:318:HOH:O[2_646]	1.06	1.14
1:A:63:LYS:NZ	4:A:481:HOH:O[2_655]	1.06	1.14
1:A:4:GLU:CG	1:A:35:SER:O[1_556]	1.06	1.14
1:A:98:LYS:O	4:A:397:HOH:O[1_554]	1.07	1.13
1:A:153:GLY:O	4:A:353:HOH:O[2_555]	1.07	1.13
4:A:203:HOH:O	4:A:368:HOH:O[2_646]	1.08	1.12
4:A:333:HOH:O	4:A:489:HOH:O[2_655]	1.09	1.11
4:A:237:HOH:O	4:A:530:HOH:O[2_646]	1.10	1.10
1:A:54:GLU:CG	4:A:433:HOH:O[1_554]	1.12	1.08
1:A:50:LYS:CB	1:A:77:LYS:CE[1_554]	1.13	1.07
1:A:47:LYS:CA	4:A:391:HOH:O[1_554]	1.14	1.06
1:A:42:LYS:CG	4:A:175:HOH:O[1_554]	1.14	1.06
1:A:50:LYS:CG	1:A:77:LYS:NZ[1_554]	1.14	1.06
1:A:40:LEU:CG	4:A:420:HOH:O[1_554]	1.14	1.06
4:A:279:HOH:O	4:A:426:HOH:O[1_554]	1.15	1.05
1:A:119:HIS:CB	4:A:412:HOH:O[2_646]	1.15	1.05
1:A:4:GLU:OE1	1:A:36:HIS:CB[1_556]	1.16	1.04
1:A:50:LYS:N	4:A:238:HOH:O[1_554]	1.16	1.04
4:A:180:HOH:O	4:A:470:HOH:O[2_556]	1.20	1.00
1:A:47:LYS:N	4:A:391:HOH:O[1_554]	1.21	0.99
4:A:468:HOH:O	4:A:512:HOH:O[2_656]	1.21	0.99
1:A:57:ALA:CB	4:A:244:HOH:O[2_655]	1.21	0.99
1:A:123:PHE:CB	4:A:439:HOH:O[2_646]	1.23	0.97
1:A:41:GLU:OE2	1:A:78:LYS:CG[1_554]	1.24	0.96
1:A:44:ASP:O	4:A:367:HOH:O[1_554]	1.25	0.95
1:A:8:GLN:O	4:A:251:HOH:O[1_556]	1.25	0.95
4:A:296:HOH:O	4:A:486:HOH:O[2_655]	1.26	0.94
4:A:224:HOH:O	4:A:524:HOH:O[1_565]	1.26	0.94
1:A:39:THR:CA	4:A:453:HOH:O[1_554]	1.27	0.93
4:A:209:HOH:O	4:A:280:HOH:O[2_645]	1.28	0.92
1:A:8:GLN:OE1	4:A:186:HOH:O[1_556]	1.28	0.92
1:A:4:GLU:CD	1:A:35:SER:C[1_556]	1.29	0.91
1:A:4:GLU:CD	1:A:36:HIS:CA[1_556]	1.30	0.90
1:A:101:ILE:CG1	4:A:437:HOH:O[1_554]	1.30	0.90
4:A:217:HOH:O	4:A:325:HOH:O[2_655]	1.33	0.87
4:A:454:HOH:O	4:A:512:HOH:O[2_656]	1.34	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:HIS:ND1	4:A:203:HOH:O[2_655]	1.34	0.86
1:A:74:ALA:O	4:A:220:HOH:O[1_556]	1.34	0.86
1:A:153:GLY:OXT	4:A:353:HOH:O[2_555]	1.34	0.86
1:A:41:GLU:OE2	1:A:78:LYS:CD[1_554]	1.35	0.85
1:A:48:HIS:CB	4:A:385:HOH:O[1_554]	1.35	0.85
1:A:8:GLN:C	4:A:251:HOH:O[1_556]	1.35	0.85
1:A:123:PHE:N	4:A:451:HOH:O[2_646]	1.36	0.84
1:A:120:PRO:CG	4:A:476:HOH:O[2_645]	1.36	0.84
1:A:38:GLU:N	4:A:526:HOH:O[1_554]	1.36	0.84
1:A:122:ASP:OD2	4:A:454:HOH:O[2_646]	1.36	0.84
1:A:102:LYS:O	4:A:479:HOH:O[1_554]	1.36	0.84
1:A:16:LYS:CE	4:A:410:HOH:O[2_646]	1.38	0.82
4:A:309:HOH:O	4:A:421:HOH:O[1_554]	1.38	0.82
1:A:40:LEU:CA	4:A:432:HOH:O[1_554]	1.39	0.81
1:A:51:THR:OG1	4:A:466:HOH:O[1_554]	1.39	0.81
4:A:170:HOH:O	4:A:214:HOH:O[2_556]	1.40	0.80
1:A:16:LYS:NZ	4:A:399:HOH:O[2_646]	1.40	0.80
1:A:50:LYS:CD	1:A:77:LYS:CE[1_554]	1.41	0.79
1:A:38:GLU:C	4:A:453:HOH:O[1_554]	1.42	0.78
1:A:38:GLU:CB	4:A:526:HOH:O[1_554]	1.42	0.78
1:A:13[A]:VAL:CG2	4:A:395:HOH:O[2_646]	1.43	0.77
1:A:103:TYR:CG	4:A:435:HOH:O[1_554]	1.43	0.77
4:A:250:HOH:O	4:A:308:HOH:O[1_554]	1.43	0.77
4:A:184:HOH:O	4:A:228:HOH:O[2_645]	1.44	0.76
1:A:63:LYS:CE	4:A:481:HOH:O[2_655]	1.45	0.75
1:A:38:GLU:CA	4:A:526:HOH:O[1_554]	1.45	0.75
1:A:41:GLU:OE1	1:A:78:LYS:CA[1_554]	1.46	0.74
1:A:41:GLU:N	4:A:174:HOH:O[1_554]	1.46	0.74
1:A:50:LYS:CG	1:A:77:LYS:CD[1_554]	1.47	0.73
1:A:123:PHE:CA	4:A:451:HOH:O[2_646]	1.47	0.73
1:A:4:GLU:CA	1:A:35:SER:O[1_556]	1.48	0.72
1:A:37:PRO:CB	1:A:79:LYS:CE[1_554]	1.49	0.71
1:A:16:LYS:CD	4:A:410:HOH:O[2_646]	1.50	0.70
1:A:103:TYR:CD1	4:A:435:HOH:O[1_554]	1.50	0.70
1:A:103:TYR:CD2	4:A:435:HOH:O[1_554]	1.51	0.69
1:A:122:ASP:C	4:A:451:HOH:O[2_646]	1.51	0.69
1:A:48:HIS:CG	4:A:203:HOH:O[2_655]	1.52	0.68
1:A:37:PRO:CB	1:A:79:LYS:CG[1_554]	1.52	0.68
1:A:38:GLU:CG	4:A:467:HOH:O[1_554]	1.52	0.68
1:A:4:GLU:CG	1:A:35:SER:CA[1_556]	1.53	0.67
1:A:15:ALA:N	4:A:377:HOH:O[2_646]	1.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:O	4:A:302:HOH:O[2_655]	1.54	0.66
1:A:56:LYS:NZ	1:A:59:GLU:CG[2_645]	1.54	0.66
1:A:9:LEU:N	4:A:251:HOH:O[1_556]	1.56	0.64
1:A:119:HIS:ND1	4:A:412:HOH:O[2_646]	1.56	0.64
1:A:103:TYR:N	4:A:457:HOH:O[1_554]	1.56	0.64
1:A:122:ASP:N	4:A:462:HOH:O[2_646]	1.57	0.63
4:A:492:HOH:O	4:A:521:HOH:O[2_656]	1.57	0.63
4:A:243:HOH:O	4:A:507:HOH:O[1_556]	1.57	0.63
1:A:60:ASP:CA	4:A:302:HOH:O[2_655]	1.57	0.63
1:A:121:GLY:C	4:A:473:HOH:O[2_646]	1.58	0.62
1:A:106:PHE:CE1	4:A:359:HOH:O[1_554]	1.58	0.62
1:A:4:GLU:OE2	1:A:35:SER:C[1_556]	1.58	0.62
1:A:13[B]:VAL:CG1	4:A:402:HOH:O[2_646]	1.59	0.61
1:A:16:LYS:CD	4:A:399:HOH:O[2_646]	1.59	0.61
1:A:13[B]:VAL:CG1	4:A:416:HOH:O[2_646]	1.60	0.60
1:A:16:LYS:CE	4:A:399:HOH:O[2_646]	1.61	0.59
1:A:4:GLU:OE1	1:A:36:HIS:N[1_556]	1.62	0.58
1:A:41:GLU:OE1	1:A:78:LYS:CB[1_554]	1.63	0.57
1:A:91:GLN:OE1	1:A:153:GLY:O[2_555]	1.63	0.57
1:A:48:HIS:ND1	4:A:368:HOH:O[1_554]	1.63	0.57
4:A:337:HOH:O	4:A:541:HOH:O[1_554]	1.64	0.56
1:A:39:THR:C	4:A:432:HOH:O[1_554]	1.65	0.55
4:A:426:HOH:O	4:A:529:HOH:O[1_556]	1.65	0.55
1:A:118:ARG:O	4:A:429:HOH:O[2_645]	1.66	0.54
1:A:136:GLU:OE2	4:A:539:HOH:O[2_545]	1.66	0.54
1:A:37:PRO:CA	1:A:79:LYS:CD[1_554]	1.67	0.53
4:A:159:HOH:O	4:A:417:HOH:O[2_646]	1.68	0.52
1:A:41:GLU:CD	1:A:78:LYS:CD[1_554]	1.69	0.51
1:A:40:LEU:CB	4:A:444:HOH:O[1_554]	1.70	0.50
1:A:123:PHE:CA	4:A:439:HOH:O[2_646]	1.70	0.50
1:A:33:PHE:O	1:A:79:LYS:NZ[1_554]	1.70	0.50
1:A:37:PRO:N	1:A:79:LYS:CE[1_554]	1.70	0.50
1:A:102:LYS:CA	4:A:484:HOH:O[1_554]	1.70	0.50
1:A:117:SER:CA	4:A:447:HOH:O[2_645]	1.70	0.50
1:A:103:TYR:CA	4:A:457:HOH:O[1_554]	1.70	0.50
1:A:47:LYS:C	4:A:406:HOH:O[1_554]	1.71	0.49
1:A:117:SER:O	4:A:465:HOH:O[2_645]	1.71	0.49
4:A:468:HOH:O	4:A:517:HOH:O[2_656]	1.72	0.48
1:A:3:SER:C	4:A:259:HOH:O[1_556]	1.72	0.48
1:A:44:ASP:C	4:A:367:HOH:O[1_554]	1.72	0.48
1:A:54:GLU:OE2	4:A:238:HOH:O[1_554]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:CD	1:A:78:LYS:NZ[1_554]	1.72	0.48
1:A:103:TYR:OH	4:A:461:HOH:O[1_554]	1.73	0.47
1:A:4:GLU:CG	1:A:36:HIS:N[1_556]	1.73	0.47
1:A:122:ASP:O	4:A:451:HOH:O[2_646]	1.74	0.46
1:A:103:TYR:CE1	4:A:435:HOH:O[1_554]	1.74	0.46
1:A:103:TYR:CZ	4:A:461:HOH:O[1_554]	1.74	0.46
1:A:41:GLU:CD	1:A:78:LYS:CG[1_554]	1.74	0.46
4:A:181:HOH:O	4:A:371:HOH:O[2_646]	1.75	0.45
4:A:276:HOH:O	4:A:316:HOH:O[1_565]	1.75	0.45
1:A:4:GLU:CB	1:A:35:SER:C[1_556]	1.76	0.44
1:A:39:THR:CB	4:A:460:HOH:O[1_554]	1.77	0.43
1:A:16:LYS:CG	4:A:410:HOH:O[2_646]	1.78	0.42
1:A:153:GLY:CA	4:A:353:HOH:O[2_555]	1.78	0.42
4:A:270:HOH:O	4:A:465:HOH:O[2_655]	1.78	0.42
1:A:41:GLU:CD	1:A:78:LYS:CB[1_554]	1.79	0.41
1:A:47:LYS:CE	1:A:78:LYS:NZ[1_554]	1.79	0.41
1:A:12:HIS:CE1	4:A:417:HOH:O[2_646]	1.79	0.41
1:A:103:TYR:CE2	4:A:435:HOH:O[1_554]	1.79	0.41
1:A:50:LYS:NZ	4:A:308:HOH:O[1_554]	1.79	0.41
1:A:121:GLY:O	4:A:462:HOH:O[2_646]	1.81	0.39
4:A:315:HOH:O	4:A:347:HOH:O[2_545]	1.81	0.39
1:A:59:GLU:C	4:A:302:HOH:O[2_655]	1.81	0.39
1:A:48:HIS:CA	4:A:385:HOH:O[1_554]	1.81	0.39
1:A:103:TYR:CB	4:A:457:HOH:O[1_554]	1.81	0.39
1:A:36:HIS:CB	4:A:295:HOH:O[1_554]	1.82	0.38
1:A:121:GLY:C	4:A:318:HOH:O[2_646]	1.82	0.38
1:A:40:LEU:O	4:A:400:HOH:O[1_554]	1.82	0.38
1:A:60:ASP:N	4:A:302:HOH:O[2_655]	1.82	0.38
1:A:40:LEU:C	4:A:432:HOH:O[1_554]	1.83	0.37
1:A:47:LYS:CG	4:A:382:HOH:O[1_554]	1.83	0.37
1:A:4:GLU:OE2	1:A:36:HIS:CA[1_556]	1.83	0.37
1:A:121:GLY:C	4:A:462:HOH:O[2_646]	1.84	0.36
1:A:122:ASP:CA	4:A:318:HOH:O[2_646]	1.84	0.36
1:A:118:ARG:N	4:A:447:HOH:O[2_645]	1.85	0.35
1:A:47:LYS:C	4:A:391:HOH:O[1_554]	1.85	0.35
4:A:533:HOH:O	4:A:535:HOH:O[2_646]	1.85	0.35
1:A:41:GLU:N	4:A:432:HOH:O[1_554]	1.85	0.35
4:A:207:HOH:O	4:A:514:HOH:O[1_564]	1.85	0.35
1:A:50:LYS:CB	1:A:77:LYS:NZ[1_554]	1.85	0.35
4:A:170:HOH:O	4:A:483:HOH:O[2_556]	1.86	0.34
1:A:41:GLU:CG	1:A:81:HIS:O[1_554]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:CG	4:A:520:HOH:O[1_564]	1.86	0.34
1:A:119:HIS:CD2	4:A:412:HOH:O[2_646]	1.86	0.34
1:A:103:TYR:CZ	4:A:435:HOH:O[1_554]	1.87	0.33
1:A:122:ASP:CB	4:A:428:HOH:O[2_646]	1.87	0.33
4:A:228:HOH:O	4:A:490:HOH:O[2_655]	1.88	0.32
1:A:45:ARG:C	4:A:367:HOH:O[1_554]	1.88	0.32
1:A:54:GLU:OE1	4:A:458:HOH:O[1_554]	1.88	0.32
1:A:37:PRO:CB	1:A:79:LYS:CD[1_554]	1.88	0.32
1:A:37:PRO:N	1:A:79:LYS:NZ[1_554]	1.89	0.31
1:A:54:GLU:CB	4:A:433:HOH:O[1_554]	1.89	0.31
1:A:100:PRO:O	4:A:457:HOH:O[1_554]	1.89	0.31
1:A:34:LYS:NZ	4:A:211:HOH:O[1_554]	1.89	0.31
1:A:105:GLU:CB	4:A:479:HOH:O[1_554]	1.90	0.30
1:A:18:GLU:OE2	4:A:529:HOH:O[1_556]	1.91	0.29
1:A:40:LEU:CG	4:A:312:HOH:O[1_554]	1.91	0.29
1:A:11:LEU:C	4:A:292:HOH:O[1_556]	1.92	0.28
1:A:7:TRP:CB	1:A:37:PRO:CG[1_556]	1.92	0.28
1:A:51:THR:CG2	4:A:272:HOH:O[1_554]	1.92	0.28
1:A:54:GLU:OE2	4:A:433:HOH:O[1_554]	1.93	0.27
1:A:37:PRO:CB	1:A:79:LYS:CB[1_554]	1.93	0.27
1:A:37:PRO:CG	1:A:79:LYS:CE[1_554]	1.93	0.27
4:A:207:HOH:O	4:A:516:HOH:O[1_564]	1.94	0.26
1:A:4:GLU:OE1	1:A:36:HIS:CG[1_556]	1.94	0.26
1:A:37:PRO:CA	1:A:79:LYS:NZ[1_554]	1.94	0.26
1:A:38:GLU:CB	1:A:81:HIS:CE1[1_554]	1.94	0.26
1:A:41:GLU:CB	4:A:174:HOH:O[1_554]	1.95	0.25
1:A:4:GLU:CD	1:A:35:SER:O[1_556]	1.96	0.24
1:A:8:GLN:CA	4:A:187:HOH:O[1_556]	1.97	0.23
1:A:38:GLU:O	1:A:81:HIS:ND1[1_554]	1.97	0.23
1:A:41:GLU:OE1	1:A:78:LYS:CD[1_554]	1.97	0.23
4:A:160:HOH:O	4:A:388:HOH:O[1_554]	1.97	0.23
1:A:123:PHE:N	4:A:439:HOH:O[2_646]	1.98	0.22
4:A:350:HOH:O	4:A:473:HOH:O[2_646]	1.98	0.22
1:A:47:LYS:CB	4:A:391:HOH:O[1_554]	1.98	0.22
1:A:36:HIS:CG	4:A:295:HOH:O[1_554]	1.99	0.21
1:A:41:GLU:OE1	1:A:78:LYS:CG[1_554]	2.00	0.20
1:A:63:LYS:CB	4:A:493:HOH:O[2_655]	2.00	0.20
4:A:192:HOH:O	4:A:487:HOH:O[1_554]	2.00	0.20
1:A:54:GLU:OE1	4:A:433:HOH:O[1_554]	2.00	0.20
1:A:8:GLN:O	4:A:292:HOH:O[1_556]	2.00	0.20
4:A:441:HOH:O	4:A:530:HOH:O[2_646]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:CA	4:A:238:HOH:O[1_554]	2.01	0.19
1:A:38:GLU:CD	4:A:467:HOH:O[1_554]	2.01	0.19
1:A:9:LEU:CA	4:A:251:HOH:O[1_556]	2.01	0.19
4:A:270:HOH:O	4:A:475:HOH:O[2_655]	2.02	0.18
1:A:60:ASP:OD1	4:A:486:HOH:O[2_655]	2.02	0.18
1:A:50:LYS:CD	1:A:77:LYS:NZ[1_554]	2.02	0.18
1:A:106:PHE:CG	4:A:359:HOH:O[1_554]	2.03	0.17
4:A:232:HOH:O	4:A:471:HOH:O[1_554]	2.03	0.17
1:A:8:GLN:N	4:A:187:HOH:O[1_556]	2.03	0.17
1:A:38:GLU:CG	4:A:526:HOH:O[1_554]	2.03	0.17
1:A:37:PRO:C	1:A:79:LYS:CB[1_554]	2.03	0.17
1:A:38:GLU:OE2	4:A:526:HOH:O[1_554]	2.03	0.17
1:A:101:ILE:CB	4:A:437:HOH:O[1_554]	2.04	0.16
1:A:8:GLN:CB	4:A:186:HOH:O[1_556]	2.04	0.16
1:A:122:ASP:OD2	4:A:428:HOH:O[2_646]	2.04	0.16
1:A:103:TYR:CE1	4:A:430:HOH:O[1_554]	2.04	0.16
1:A:36:HIS:C	1:A:79:LYS:NZ[1_554]	2.04	0.16
1:A:4:GLU:CB	4:A:285:HOH:O[1_556]	2.05	0.15
1:A:47:LYS:CA	4:A:406:HOH:O[1_554]	2.05	0.15
1:A:136:GLU:CD	4:A:539:HOH:O[2_545]	2.05	0.15
4:A:193:HOH:O	4:A:371:HOH:O[2_645]	2.05	0.15
1:A:38:GLU:CG	4:A:461:HOH:O[1_554]	2.06	0.14
4:A:344:HOH:O	4:A:370:HOH:O[1_545]	2.06	0.14
1:A:4:GLU:OE1	1:A:36:HIS:C[1_556]	2.06	0.14
1:A:48:HIS:CE1	4:A:203:HOH:O[2_655]	2.07	0.13
4:A:189:HOH:O	4:A:488:HOH:O[1_554]	2.07	0.13
1:A:4:GLU:N	4:A:259:HOH:O[1_556]	2.07	0.13
1:A:38:GLU:OE2	4:A:336:HOH:O[1_554]	2.07	0.13
4:A:279:HOH:O	4:A:413:HOH:O[1_554]	2.07	0.13
4:A:211:HOH:O	4:A:286:HOH:O[1_556]	2.08	0.12
1:A:102:LYS:CD	4:A:484:HOH:O[1_554]	2.08	0.12
4:A:463:HOH:O	4:A:505:HOH:O[2_656]	2.08	0.12
1:A:8:GLN:CD	4:A:186:HOH:O[1_556]	2.08	0.12
1:A:45:ARG:CA	4:A:367:HOH:O[1_554]	2.08	0.12
1:A:26:GLN:CA	4:A:269:HOH:O[2_645]	2.09	0.11
1:A:47:LYS:CG	4:A:391:HOH:O[1_554]	2.09	0.11
1:A:41:GLU:CA	4:A:174:HOH:O[1_554]	2.09	0.11
1:A:122:ASP:C	4:A:462:HOH:O[2_646]	2.09	0.11
1:A:26:GLN:CG	4:A:269:HOH:O[2_645]	2.09	0.11
1:A:136:GLU:OE1	4:A:539:HOH:O[2_545]	2.09	0.11
1:A:41:GLU:OE2	1:A:78:LYS:CB[1_554]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:N	4:A:367:HOH:O[1_554]	2.10	0.10
1:A:12:HIS:NE2	4:A:417:HOH:O[2_646]	2.10	0.10
1:A:51:THR:CB	4:A:466:HOH:O[1_554]	2.10	0.10
1:A:40:LEU:CD2	4:A:420:HOH:O[1_554]	2.10	0.10
1:A:12:HIS:O	4:A:377:HOH:O[2_646]	2.11	0.09
4:A:170:HOH:O	4:A:470:HOH:O[2_556]	2.11	0.09
1:A:106:PHE:CZ	4:A:485:HOH:O[1_554]	2.12	0.08
4:A:159:HOH:O	4:A:530:HOH:O[1_545]	2.12	0.08
2:A:154:SO4:S	4:A:357:HOH:O[2_655]	2.12	0.08
1:A:102:LYS:CB	4:A:484:HOH:O[1_554]	2.13	0.07
1:A:48:HIS:CE1	4:A:368:HOH:O[1_554]	2.13	0.07
1:A:36:HIS:ND1	4:A:295:HOH:O[1_554]	2.13	0.07
4:A:183:HOH:O	4:A:505:HOH:O[2_656]	2.13	0.07
1:A:122:ASP:CG	4:A:428:HOH:O[2_646]	2.13	0.07
1:A:16:LYS:N	4:A:377:HOH:O[2_646]	2.14	0.06
1:A:41:GLU:CA	4:A:400:HOH:O[1_554]	2.14	0.06
1:A:48:HIS:N	4:A:388:HOH:O[1_554]	2.14	0.06
1:A:12:HIS:CD2	4:A:428:HOH:O[2_646]	2.15	0.05
1:A:54:GLU:OE2	4:A:362:HOH:O[1_554]	2.15	0.05
1:A:15:ALA:CB	1:A:51:THR:CG2[1_556]	2.15	0.05
1:A:40:LEU:CB	4:A:312:HOH:O[1_554]	2.16	0.04
1:A:39:THR:N	4:A:467:HOH:O[1_554]	2.16	0.04
1:A:153:GLY:C	4:A:540:HOH:O[2_555]	2.17	0.03
1:A:103:TYR:C	4:A:457:HOH:O[1_554]	2.17	0.03
1:A:96:LYS:NZ	4:A:338:HOH:O[1_565]	2.17	0.03
4:A:318:HOH:O	4:A:350:HOH:O[2_656]	2.17	0.03
1:A:46:PHE:N	4:A:367:HOH:O[1_554]	2.17	0.03
1:A:45:ARG:CB	4:A:520:HOH:O[1_564]	2.17	0.03
4:A:198:HOH:O	4:A:452:HOH:O[1_554]	2.17	0.03
1:A:18:GLU:CD	4:A:529:HOH:O[1_556]	2.18	0.02
4:A:268:HOH:O	4:A:477:HOH:O[1_554]	2.19	0.01
1:A:7:TRP:CG	1:A:37:PRO:CG[1_556]	2.19	0.01
1:A:48:HIS:N	4:A:391:HOH:O[1_554]	2.19	0.01
1:A:50:LYS:CD	1:A:77:LYS:CD[1_554]	2.19	0.01

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	155/153 (101%)	150 (97%)	4 (3%)	1 (1%)	25 7

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN

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	129/125 (103%)	123 (95%)	6 (5%)	26 4

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86[A]	LEU
1	A	86[B]	LEU
1	A	87	LYS
1	A	89[A]	LEU
1	A	89[B]	LEU
1	A	145	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	116	HIS
1	A	128	GLN

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 ⓘ

2 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	HEM	A	155	1	27,50,50	1.88	8 (29%)	17,82,82	3.45	9 (52%)
2	SO4	A	154	-	4,4,4	0.65	0	6,6,6	0.85	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	HEM	A	155	1	-	0/6/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C1A-NA	5.53	1.47	1.36
3	A	155	HEM	C4A-NA	4.23	1.44	1.36
3	A	155	HEM	CAA-C2A	-2.25	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C3C-C2C	2.17	1.43	1.40
3	A	155	HEM	C3C-CAC	2.16	1.52	1.47
3	A	155	HEM	CMB-C2B	2.09	1.56	1.51
3	A	155	HEM	C1B-C2B	2.03	1.47	1.42
3	A	155	HEM	C1D-ND	-2.02	1.32	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	155	HEM	C4C-C3C-C2C	-8.64	100.86	106.90
3	A	155	HEM	C1D-C2D-C3D	-7.43	101.83	107.00
3	A	155	HEM	CMB-C2B-C3B	3.89	131.96	124.68
3	A	155	HEM	CMD-C2D-C3D	3.39	131.32	124.94
3	A	155	HEM	CMA-C3A-C4A	-3.22	123.51	128.46
3	A	155	HEM	CMA-C3A-C2A	2.86	130.34	124.94
3	A	155	HEM	C3B-C4B-NB	2.66	112.65	109.21
3	A	155	HEM	CBD-CAD-C3D	-2.22	108.38	112.48
3	A	155	HEM	CMC-C2C-C3C	2.16	128.72	124.68

There are no chirality outliers.

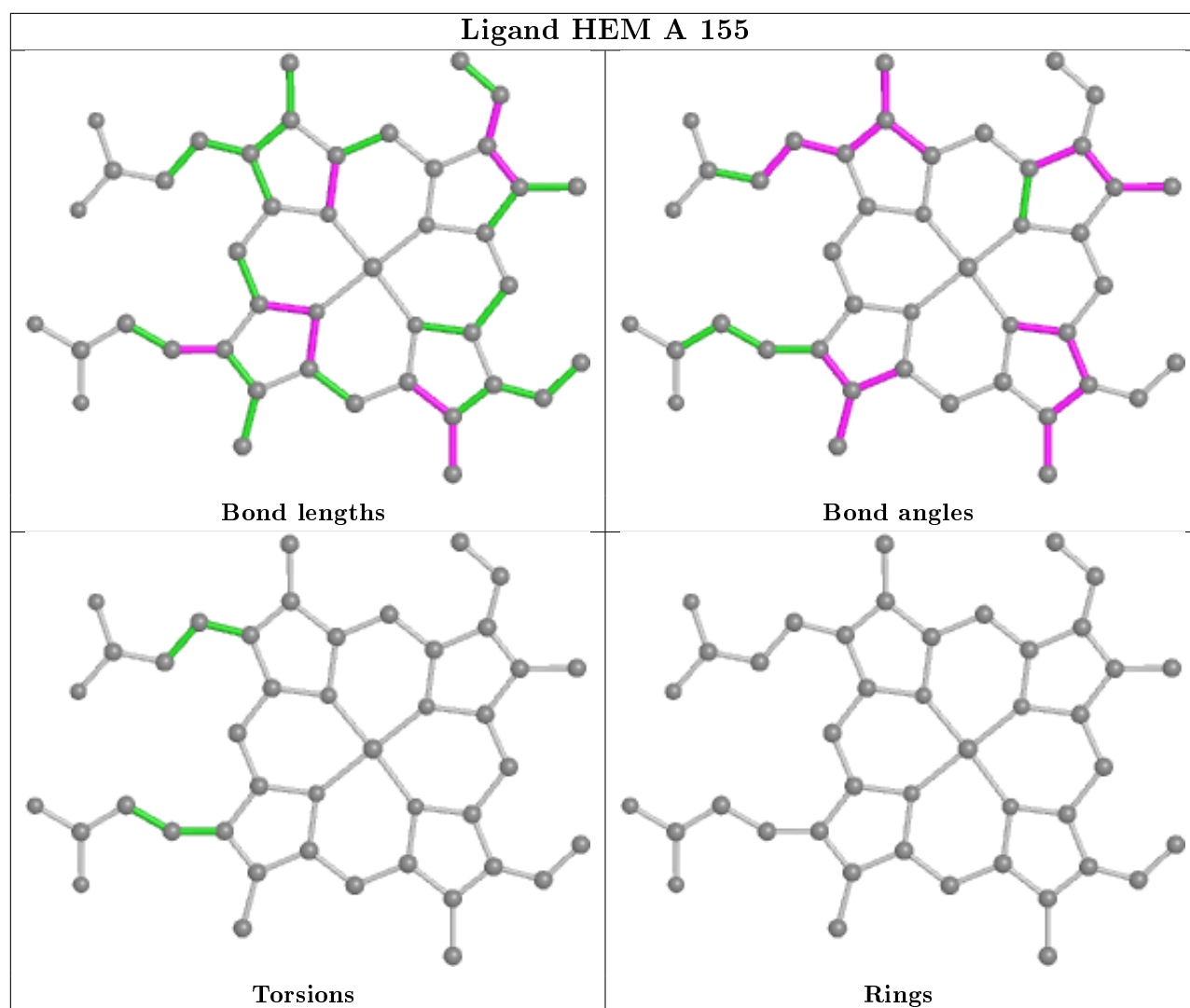
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	HEM	1	0
2	A	154	SO4	0	2

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.