



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:43 AM UTC

PDB ID : 3RE8 / pdb_00003re8
Title : Structural and Kinetic Analysis of the Beef liver Catalase interacting with Nitric Oxide
Authors : Purwar, N.; Schmidt, M.
Deposited on : 2011-04-03
Resolution : 1.90 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

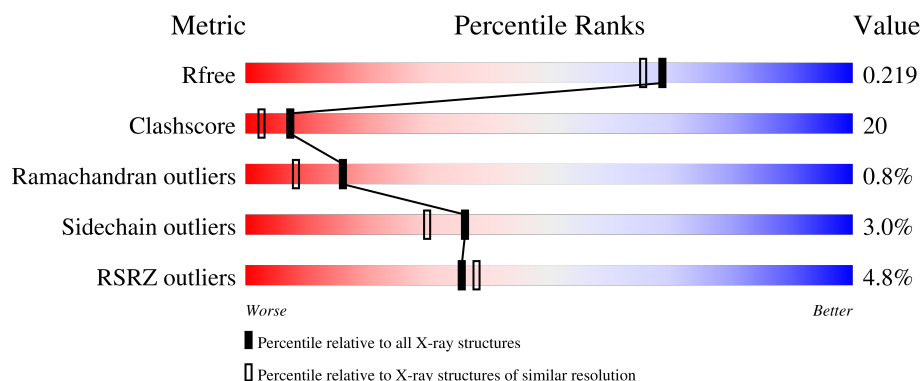
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	499	3% 69% 28% .
1	B	499	6% 60% 36% .
1	C	499	5% 67% 29% .
1	D	499	5% 65% 32% .

2 Entry composition [i](#)

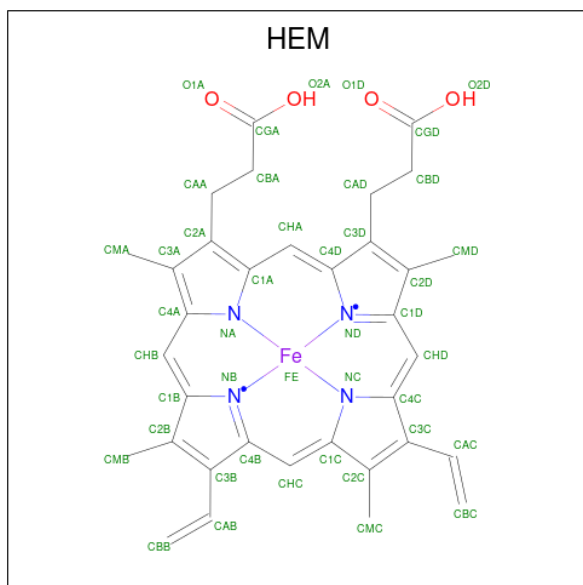
There are 3 unique types of molecules in this entry. The entry contains 17527 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	1	0
			4018	2548	717	738	15			
1	B	499	Total	C	N	O	S	0	1	0
			4018	2548	717	738	15			
1	C	499	Total	C	N	O	S	0	1	0
			4018	2548	717	738	15			
1	D	499	Total	C	N	O	S	0	1	0
			4018	2548	717	738	15			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

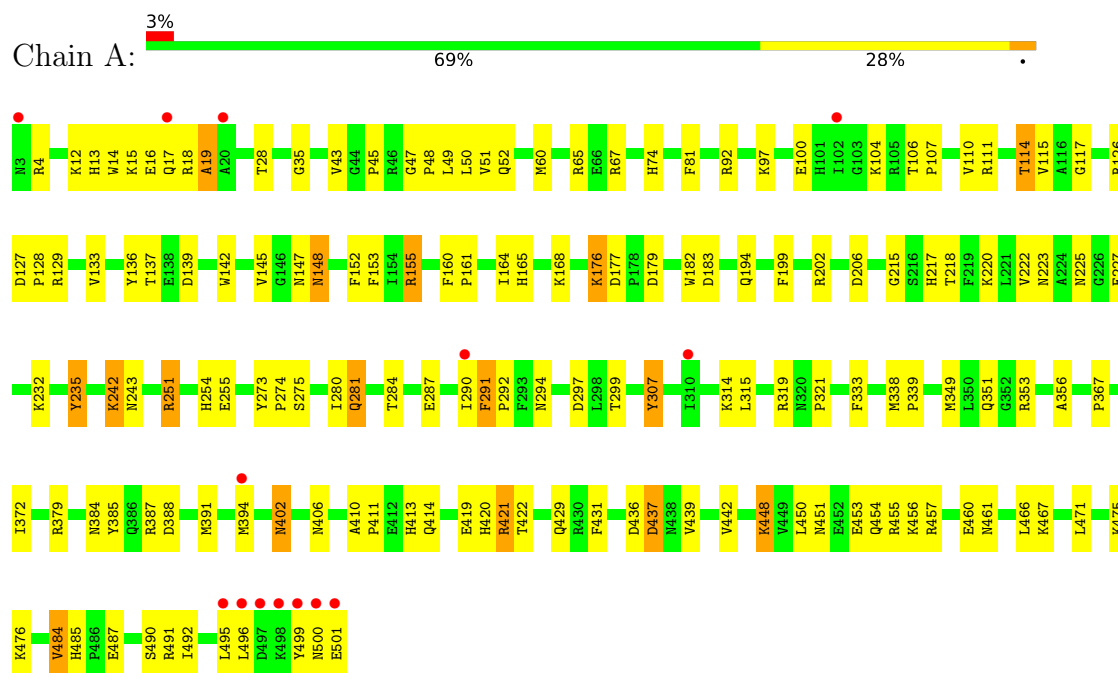
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	300	Total	O	0	0
			300	300		
3	B	319	Total	O	0	0
			319	319		
3	C	356	Total	O	0	0
			356	356		
3	D	308	Total	O	0	0
			308	308		

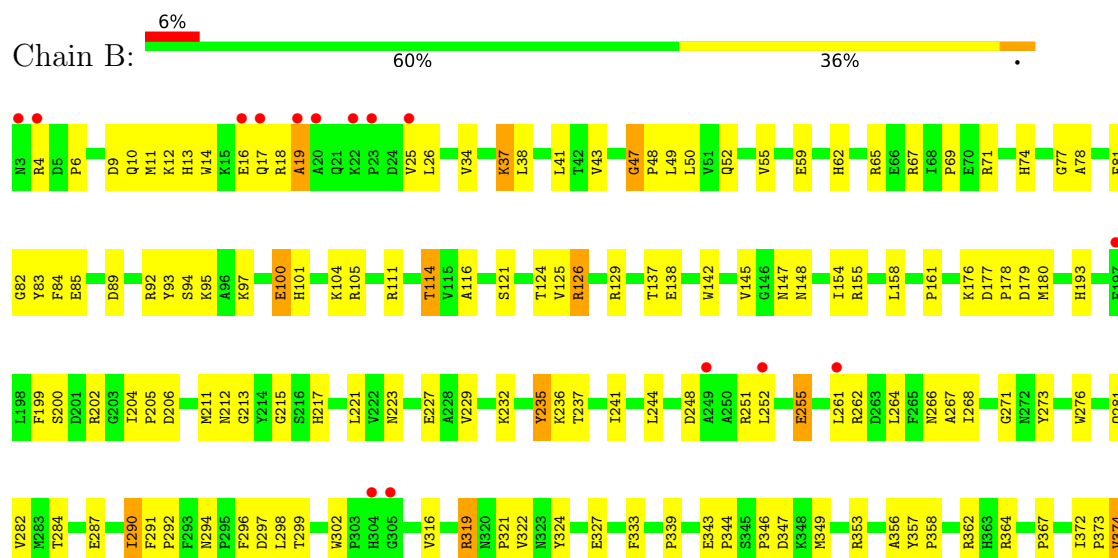
3 Residue-property plots

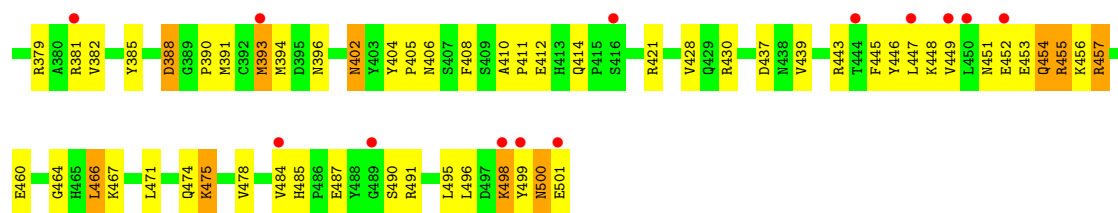
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Catalase

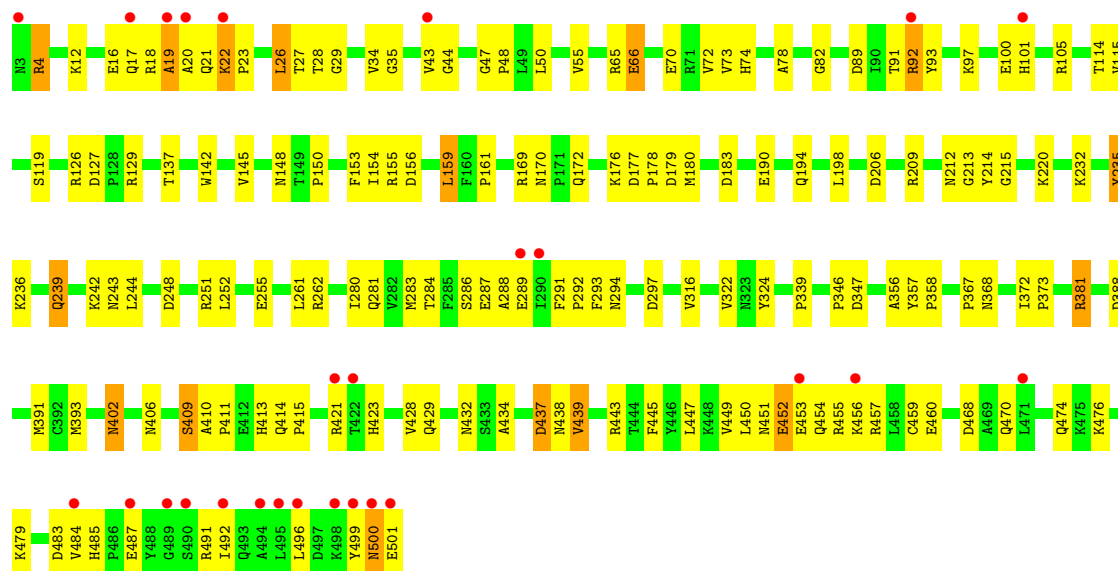


• Molecule 1: Catalase

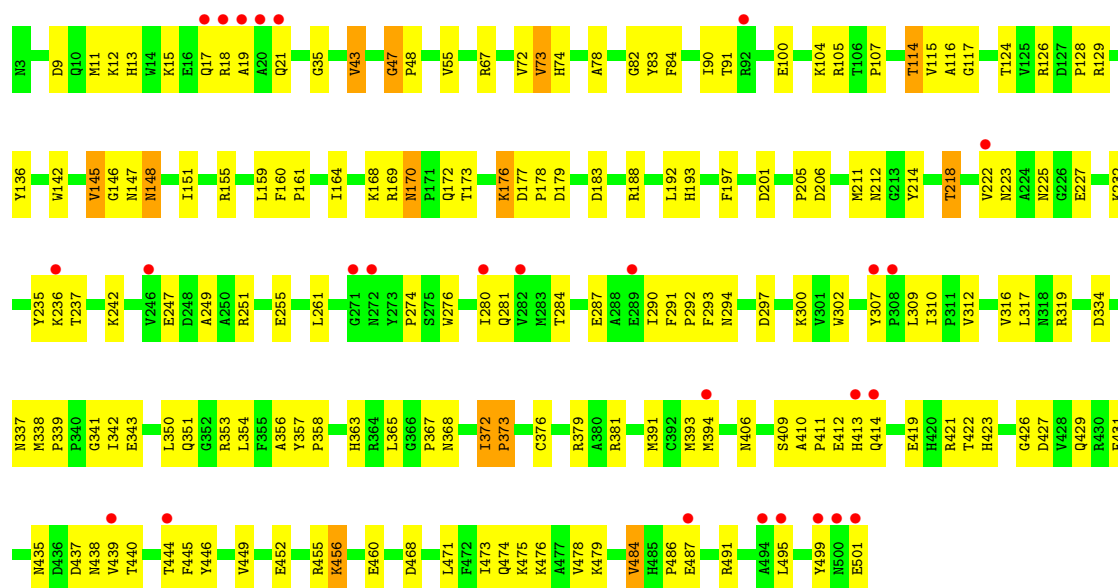




● Molecule 1: Catalase



● Molecule 1: Catalase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.22Å 140.92Å 229.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.40 – 1.90 38.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (38.40-1.90) 97.5 (38.40-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.259 0.220 , 0.219	Depositor DCC
R_{free} test set	10401 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17527	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/4143	0.95	22/5628 (0.4%)
1	B	0.41	0/4143	0.96	18/5628 (0.3%)
1	C	0.41	0/4143	0.98	23/5628 (0.4%)
1	D	0.39	0/4143	0.95	21/5628 (0.4%)
All	All	0.40	0/16572	0.96	84/22512 (0.4%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	VAL	N-CA-C	10.00	120.52	112.12
1	C	356	ALA	N-CA-C	9.18	122.44	111.33
1	B	356	ALA	N-CA-C	9.05	120.75	111.07
1	A	115	VAL	N-CA-C	8.84	118.61	111.62
1	D	47	GLY	CA-C-N	8.36	128.29	119.85
1	D	47	GLY	C-N-CA	8.36	128.29	119.85
1	D	116	ALA	N-CA-C	7.41	119.14	111.14
1	A	356	ALA	N-CA-C	7.27	120.12	111.33
1	C	281	GLN	N-CA-C	-7.07	98.21	109.59
1	D	356	ALA	N-CA-C	7.04	119.56	111.11
1	D	55	VAL	N-CA-C	-7.00	103.95	110.53
1	D	145	VAL	N-CA-C	7.00	113.70	106.21
1	A	176	LYS	N-CA-C	-6.91	100.96	110.35
1	D	183	ASP	N-CA-C	-6.90	103.69	111.14
1	C	439	VAL	N-CA-C	6.88	120.25	113.71
1	C	372	ILE	N-CA-C	-6.87	102.22	108.95
1	B	215	GLY	N-CA-C	-6.85	106.16	114.66
1	A	281	GLN	N-CA-C	-6.72	98.78	109.59
1	A	218	THR	N-CA-C	-6.61	98.48	109.46
1	C	215	GLY	N-CA-C	-6.55	106.74	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	THR	N-CA-C	-6.55	100.14	109.96
1	B	281	GLN	N-CA-C	-6.48	99.35	109.72
1	A	183	ASP	N-CA-C	-6.45	104.17	111.14
1	C	388	ASP	N-CA-C	6.31	119.62	109.02
1	D	439	VAL	N-CA-C	6.29	117.41	112.12
1	C	170	ASN	CA-C-N	6.27	126.74	119.47
1	C	170	ASN	C-N-CA	6.27	126.74	119.47
1	A	215	GLY	N-CA-C	-6.25	106.60	114.16
1	C	409	SER	N-CA-C	6.20	119.97	111.54
1	B	372	ILE	N-CA-C	-6.18	102.89	108.95
1	C	119	SER	N-CA-C	6.16	118.78	111.33
1	B	388	ASP	N-CA-C	6.09	117.02	108.00
1	B	484	VAL	N-CA-C	-5.96	104.92	110.53
1	C	55	VAL	N-CA-C	-5.95	104.52	111.00
1	A	307	TYR	CA-C-N	5.94	125.96	119.90
1	A	307	TYR	C-N-CA	5.94	125.96	119.90
1	D	176	LYS	N-CA-C	-5.92	102.30	110.35
1	D	128	PRO	N-CA-C	-5.89	102.97	111.22
1	A	28	THR	N-CA-C	-5.89	101.24	110.36
1	D	307	TYR	CA-C-N	5.88	125.89	119.89
1	D	307	TYR	C-N-CA	5.88	125.89	119.89
1	B	322	VAL	N-CA-C	-5.88	105.98	111.45
1	A	388	ASP	N-CA-C	5.81	116.60	108.00
1	B	55	VAL	N-CA-C	-5.68	105.19	110.53
1	B	47	GLY	CA-C-N	5.66	125.63	120.03
1	B	47	GLY	C-N-CA	5.66	125.63	120.03
1	C	44	GLY	CA-C-N	5.56	125.66	119.32
1	C	44	GLY	C-N-CA	5.56	125.66	119.32
1	D	114	THR	N-CA-C	-5.54	101.23	109.94
1	C	47	GLY	CA-C-N	5.53	125.44	119.85
1	C	47	GLY	C-N-CA	5.53	125.44	119.85
1	A	394	MET	CB-CA-C	-5.52	110.19	116.54
1	A	139	ASP	N-CA-C	-5.51	106.34	112.57
1	B	176	LYS	N-CA-C	-5.47	102.29	110.23
1	C	449	VAL	N-CA-C	5.46	115.66	110.53
1	B	121	SER	N-CA-C	5.44	117.10	110.41
1	B	394	MET	CB-CA-C	-5.43	108.73	116.34
1	D	117	GLY	N-CA-C	5.42	118.17	111.93
1	A	67	ARG	N-CA-C	5.38	118.70	110.20
1	A	128	PRO	N-CA-C	-5.37	103.70	111.22
1	B	116	ALA	N-CA-C	5.35	118.97	112.23
1	C	388	ASP	CB-CA-C	-5.35	108.83	115.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	THR	N-CA-C	-5.34	101.55	109.94
1	C	66	GLU	N-CA-C	5.33	117.84	111.71
1	C	183	ASP	N-CA-C	-5.33	105.38	111.14
1	D	67	ARG	N-CA-C	5.32	118.60	110.20
1	D	372	ILE	N-CA-C	-5.31	103.75	108.95
1	A	372	ILE	N-CA-C	-5.30	103.18	108.96
1	C	28	THR	N-CA-C	-5.28	103.72	110.53
1	C	169	ARG	N-CA-C	5.18	118.51	110.17
1	D	169	ARG	N-CA-C	5.17	118.54	110.32
1	A	117	GLY	N-CA-C	5.16	117.87	111.93
1	B	455	ARG	N-CA-C	-5.16	105.83	111.82
1	A	484	VAL	N-CA-C	-5.12	105.71	110.53
1	D	409	SER	N-CA-C	5.12	119.48	113.23
1	D	484	VAL	N-CA-C	-5.11	105.73	110.53
1	A	439	VAL	N-CA-C	5.10	119.95	109.34
1	B	324	TYR	N-CA-C	5.09	117.22	111.11
1	C	324	TYR	N-CA-C	5.08	116.51	111.07
1	D	170	ASN	N-CA-C	-5.03	103.26	109.64
1	A	291	PHE	CA-C-N	5.01	124.73	119.82
1	A	291	PHE	C-N-CA	5.01	124.73	119.82
1	A	114	THR	N-CA-C	-5.01	102.07	109.94
1	C	322	VAL	N-CA-C	-5.01	106.27	111.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4018	0	3844	144	0
1	B	4018	0	3844	230	0
1	C	4018	0	3844	163	0
1	D	4018	0	3844	159	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	1	0
3	A	300	0	0	37	0
3	B	319	0	0	40	1
3	C	356	0	0	41	1
3	D	308	0	0	42	0
All	All	17527	0	15496	650	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 20.

All (650) 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:D:350:LEU:HG	3:D:773:HOH:O	1.42	1.20
1:D:444:THR:HB	3:D:1074:HOH:O	1.50	1.09
1:C:91:THR:HB	3:C:1015:HOH:O	1.55	1.06
1:B:374:VAL:HG23	3:B:517:HOH:O	1.59	0.99
3:A:869:HOH:O	1:C:409:SER:HB3	1.63	0.99
1:B:319:ARG:HH11	1:B:319:ARG:HB3	1.32	0.94
1:C:92:ARG:HD2	3:C:572:HOH:O	1.65	0.94
1:A:429:GLN:HB3	1:B:421:ARG:HD2	1.49	0.94
1:B:327:GLU:HA	1:B:374:VAL:HG21	1.48	0.94
1:A:314:LYS:HG3	3:A:939:HOH:O	1.70	0.92
1:B:466:LEU:HD22	1:B:474:GLN:HG2	1.50	0.91
1:C:452:GLU:HG3	3:C:769:HOH:O	1.71	0.90
1:C:155:ARG:HH22	1:C:438:ASN:HD21	1.17	0.89
1:A:111:ARG:CZ	3:A:505:HOH:O	2.20	0.89
1:B:126:ARG:CZ	3:B:737:HOH:O	2.21	0.88
1:A:111:ARG:NE	3:A:505:HOH:O	2.07	0.87
1:A:126:ARG:NH2	3:A:846:HOH:O	2.07	0.87
1:B:155:ARG:HG3	3:B:833:HOH:O	1.74	0.86
1:B:62:HIS:HE1	1:D:368:ASN:HD21	1.25	0.85
1:B:4:ARG:CZ	3:B:655:HOH:O	2.24	0.84
1:C:126:ARG:NE	3:C:639:HOH:O	2.11	0.84
1:A:176:LYS:HE2	3:A:667:HOH:O	1.77	0.84
1:C:487:GLU:O	1:C:491:ARG:HG3	1.77	0.84
1:A:155:ARG:NH2	3:A:649:HOH:O	2.11	0.84
1:D:338:MET:HE2	1:D:342:ILE:HG22	1.58	0.82
1:A:307:TYR:HA	3:A:651:HOH:O	1.78	0.82
1:B:290:ILE:HD13	1:B:290:ILE:O	1.79	0.82
1:A:155:ARG:NE	3:A:649:HOH:O	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASP:HA	1:C:244:LEU:CD2	2.10	0.81
1:D:223:ASN:HD21	1:D:227:GLU:HB2	1.43	0.81
1:D:12:LYS:HG3	3:D:1056:HOH:O	1.81	0.81
1:B:37:LYS:O	1:B:37:LYS:HG3	1.80	0.81
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.44	0.81
1:B:25:VAL:HG13	1:D:414:GLN:HG3	1.63	0.80
1:C:155:ARG:NH2	1:C:438:ASN:HD21	1.79	0.80
1:C:89:ASP:OD1	1:C:91:THR:HG22	1.82	0.79
1:B:62:HIS:HD2	3:B:504:HOH:O	1.66	0.79
1:B:4:ARG:NE	3:B:655:HOH:O	2.15	0.79
1:A:126:ARG:CZ	3:A:899:HOH:O	2.32	0.78
1:A:155:ARG:HH11	1:A:155:ARG:HB3	1.49	0.77
1:C:161:PRO:HG2	3:C:644:HOH:O	1.85	0.77
1:B:319:ARG:HD3	3:B:612:HOH:O	1.84	0.77
1:C:126:ARG:CZ	3:C:639:HOH:O	2.30	0.77
1:B:491:ARG:O	1:B:495:LEU:HD23	1.83	0.77
1:A:111:ARG:NH2	3:A:505:HOH:O	2.19	0.76
1:D:376[A]:CYS:SG	3:D:659:HOH:O	2.44	0.76
1:A:155:ARG:CZ	3:A:649:HOH:O	2.34	0.75
1:D:338:MET:CE	1:D:342:ILE:HG22	2.15	0.75
1:B:126:ARG:HE	1:B:199:PHE:HA	1.51	0.75
1:B:138:GLU:HG2	3:B:974:HOH:O	1.86	0.75
1:C:21:GLN:HB3	3:C:662:HOH:O	1.85	0.75
1:D:452:GLU:HG3	3:D:1189:HOH:O	1.86	0.75
1:C:262:ARG:NH1	3:C:1073:HOH:O	2.19	0.75
1:B:452:GLU:HG3	3:B:796:HOH:O	1.86	0.75
1:A:251:ARG:HH11	1:A:251:ARG:HB3	1.51	0.75
1:C:451:ASN:HD21	1:C:453:GLU:HB2	1.51	0.75
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.51	0.74
1:D:354:LEU:HG	3:D:773:HOH:O	1.87	0.74
1:C:414:GLN:CD	3:C:1030:HOH:O	2.31	0.73
1:C:155:ARG:HH22	1:C:438:ASN:ND2	1.87	0.73
1:B:77:GLY:CA	1:B:111:ARG:HH12	2.02	0.73
1:B:487:GLU:O	1:B:491:ARG:HG3	1.89	0.73
1:B:37:LYS:H	1:D:413:HIS:CE1	2.07	0.72
1:C:284:THR:OG1	1:C:287:GLU:HG3	1.89	0.72
3:A:1188:HOH:O	1:D:176:LYS:HE2	1.88	0.72
1:C:381:ARG:HD3	3:C:810:HOH:O	1.90	0.72
1:C:78:ALA:HB2	1:C:261:LEU:HD22	1.70	0.71
1:B:202:ARG:HH21	1:B:241:ILE:HD13	1.53	0.71
1:A:126:ARG:HH12	1:A:461:ASN:HB3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:NH2	3:B:655:HOH:O	2.22	0.71
1:B:319:ARG:HH11	1:B:319:ARG:CB	2.02	0.71
1:A:12:LYS:O	1:A:16:GLU:HG3	1.90	0.71
1:D:284:THR:OG1	1:D:287:GLU:HG3	1.90	0.71
1:A:448:LYS:HA	1:A:448:LYS:HE3	1.71	0.71
1:D:471:LEU:O	1:D:475:LYS:HG3	1.91	0.71
1:B:13:HIS:HD2	3:B:726:HOH:O	1.73	0.71
1:B:138:GLU:H	1:B:138:GLU:CD	1.98	0.71
1:A:319:ARG:NH1	3:A:585:HOH:O	2.15	0.71
1:C:492:ILE:O	1:C:496:LEU:HD23	1.91	0.71
1:D:13:HIS:O	1:D:17:GLN:HG3	1.90	0.70
1:D:170:ASN:ND2	1:D:172:GLN:H	1.88	0.70
1:B:126:ARG:HH21	1:B:199:PHE:C	1.99	0.70
1:C:206:ASP:HA	1:C:244:LEU:HD21	1.71	0.70
1:B:111:ARG:CZ	3:B:615:HOH:O	2.39	0.70
1:C:476:LYS:NZ	1:C:476:LYS:HB3	2.07	0.70
1:B:178:PRO:HG2	3:B:1149:HOH:O	1.89	0.70
1:D:456:LYS:O	1:D:460:GLU:HG3	1.90	0.70
1:B:77:GLY:HA3	1:B:111:ARG:HH12	1.57	0.70
1:A:485:HIS:HD2	1:A:487:GLU:H	1.40	0.69
1:C:150:PRO:HG3	1:C:214:TYR:CE1	2.27	0.69
1:C:438:ASN:N	3:C:678:HOH:O	2.26	0.69
1:B:12:LYS:O	1:B:16:GLU:HG2	1.93	0.69
1:C:91:THR:CB	3:C:1015:HOH:O	2.24	0.69
3:A:632:HOH:O	1:C:18:ARG:HD2	1.93	0.68
1:B:454:GLN:NE2	3:B:905:HOH:O	2.18	0.68
1:C:206:ASP:HA	1:C:244:LEU:HD22	1.75	0.68
1:B:261:LEU:CD1	3:B:1281:HOH:O	2.41	0.68
1:B:105:ARG:HD2	3:B:1245:HOH:O	1.92	0.68
1:D:491:ARG:NH1	3:D:896:HOH:O	2.27	0.68
1:A:17:GLN:HG2	3:A:975:HOH:O	1.92	0.68
1:B:100:GLU:HB3	1:B:104:LYS:HD2	1.77	0.67
1:C:391:MET:HE3	1:C:393:MET:HE1	1.76	0.67
1:C:291:PHE:CD1	1:C:292:PRO:HD2	2.30	0.67
1:C:381:ARG:HH11	1:C:381:ARG:HB2	1.60	0.67
1:A:491:ARG:O	1:A:495:LEU:HD23	1.95	0.67
1:A:225:ASN:HB2	1:A:227:GLU:OE2	1.95	0.66
1:B:248:ASP:O	1:B:252:LEU:HD13	1.95	0.66
1:B:62:HIS:HE1	1:D:368:ASN:ND2	1.91	0.66
1:C:17:GLN:HG3	3:C:695:HOH:O	1.94	0.66
1:D:429:GLN:HB2	3:D:750:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLY:HA3	1:B:111:ARG:NH1	2.11	0.66
1:A:351:GLN:HG3	3:A:989:HOH:O	1.96	0.66
1:A:126:ARG:NH1	1:A:461:ASN:HB3	2.11	0.65
1:D:486:PRO:HA	3:D:948:HOH:O	1.94	0.65
1:C:432:ASN:ND2	1:C:434:ALA:H	1.95	0.65
1:B:447:LEU:HD12	1:B:448:LYS:N	2.11	0.65
1:A:421:ARG:HG2	3:A:878:HOH:O	1.97	0.65
1:B:161:PRO:HG2	3:B:543:HOH:O	1.96	0.65
1:A:422:THR:N	3:A:619:HOH:O	2.30	0.65
1:A:50:LEU:HD12	1:B:48:PRO:HB2	1.79	0.64
1:A:476:LYS:HE3	3:A:551:HOH:O	1.96	0.64
1:B:264:LEU:O	1:B:268:ILE:HD13	1.96	0.64
1:A:451:ASN:H	1:A:454:GLN:HE21	1.45	0.64
1:C:43:VAL:CG1	1:C:48:PRO:HD2	2.28	0.64
1:D:170:ASN:HD22	1:D:173:THR:H	1.45	0.64
1:D:456:LYS:HD2	1:D:460:GLU:OE1	1.98	0.64
1:C:474:GLN:NE2	1:C:496:LEU:HD12	2.12	0.63
1:B:148:ASN:CB	1:B:211:MET:HE2	2.28	0.63
1:B:267:ALA:HA	3:B:1117:HOH:O	1.99	0.63
1:D:124:THR:HA	3:D:1133:HOH:O	1.98	0.63
1:A:485:HIS:CD2	1:A:487:GLU:H	2.16	0.63
1:C:500:ASN:ND2	3:C:882:HOH:O	2.30	0.63
1:B:456:LYS:O	1:B:460:GLU:HG3	1.98	0.63
1:C:26:LEU:HG	1:C:34:VAL:HG21	1.81	0.63
1:B:205:PRO:HG3	1:B:211:MET:CE	2.28	0.63
1:C:261:LEU:CD2	3:C:1279:HOH:O	2.46	0.63
1:C:421:ARG:HG2	3:C:876:HOH:O	2.00	0.62
1:B:406:ASN:ND2	1:B:410:ALA:HB3	2.13	0.62
1:D:294:ASN:HB3	1:D:297:ASP:HB2	1.82	0.62
1:B:475:LYS:HD2	3:B:1120:HOH:O	1.99	0.62
1:C:209:ARG:O	1:C:239:GLN:HG2	1.99	0.62
1:B:10:GLN:HE21	1:C:172:GLN:NE2	1.98	0.62
1:B:202:ARG:HH21	1:B:241:ILE:CD1	2.11	0.62
1:D:338:MET:HE1	1:D:343:GLU:C	2.25	0.62
1:B:41:LEU:HD11	1:C:428:VAL:CG1	2.30	0.61
1:B:498:LYS:O	1:B:498:LYS:HD3	2.00	0.61
1:B:138:GLU:CD	1:B:138:GLU:N	2.58	0.61
1:C:236:LYS:HE2	3:C:1106:HOH:O	1.98	0.61
1:A:421:ARG:CG	3:A:878:HOH:O	2.48	0.61
1:B:10:GLN:HE21	1:C:172:GLN:HE21	1.48	0.61
1:C:445:PHE:O	1:C:450:LEU:HD13	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:PHE:HZ	1:D:440:THR:HG21	1.65	0.61
1:B:261:LEU:HD12	3:B:1281:HOH:O	2.00	0.61
1:B:111:ARG:NE	3:B:615:HOH:O	2.34	0.61
1:D:151:ILE:HD13	1:D:193:HIS:CD2	2.36	0.60
1:D:251:ARG:HD3	3:D:1228:HOH:O	2.01	0.60
1:C:12:LYS:O	1:C:16:GLU:HG3	2.01	0.60
1:C:155:ARG:HH12	1:C:438:ASN:ND2	1.99	0.60
1:D:473:ILE:HA	1:D:476:LYS:HE2	1.82	0.60
3:A:619:HOH:O	1:B:428:VAL:CG2	2.49	0.60
1:A:43:VAL:O	1:A:43:VAL:HG13	2.01	0.60
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.83	0.60
1:C:391:MET:HE3	1:C:393:MET:CE	2.32	0.60
1:A:453:GLU:HG2	1:A:457:ARG:HH12	1.67	0.60
1:B:382:VAL:HG13	3:B:669:HOH:O	2.01	0.60
1:C:499:TYR:CZ	3:C:1036:HOH:O	2.50	0.60
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.31	0.60
1:A:499:TYR:C	1:A:501:GLU:H	2.09	0.60
1:B:49:LEU:HD23	1:B:50:LEU:N	2.16	0.59
1:D:310:ILE:HD11	3:D:1200:HOH:O	2.02	0.59
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.85	0.59
1:C:451:ASN:ND2	1:C:453:GLU:HB2	2.17	0.59
1:D:146:GLY:HA3	1:D:214:TYR:O	2.03	0.59
1:A:126:ARG:NH2	3:A:899:HOH:O	2.35	0.59
1:A:126:ARG:HH12	1:A:461:ASN:CB	2.14	0.59
1:A:206:ASP:CB	1:A:242:LYS:HD2	2.33	0.58
1:D:393:MET:CA	3:D:753:HOH:O	2.51	0.58
1:B:147:ASN:CG	2:B:1:HEM:HAC	2.29	0.58
1:D:223:ASN:ND2	1:D:227:GLU:HB2	2.15	0.58
1:C:451:ASN:H	1:C:454:GLN:NE2	2.00	0.58
1:C:73:VAL:HG12	1:C:74:HIS:CD2	2.39	0.58
1:A:65:ARG:HD3	1:C:367:PRO:HG3	1.86	0.57
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.86	0.57
1:D:435:ASN:OD1	3:D:1026:HOH:O	2.17	0.57
1:A:164:ILE:O	1:A:168:LYS:HG2	2.05	0.57
1:B:402:ASN:C	1:B:402:ASN:HD22	2.11	0.57
1:B:298:LEU:HA	3:B:926:HOH:O	2.04	0.57
1:D:212:ASN:OD1	1:D:236:LYS:HA	2.05	0.57
1:B:388:ASP:H	1:B:396:ASN:HD21	1.52	0.57
1:D:280:ILE:O	1:D:280:ILE:HG13	2.04	0.57
1:C:156:ASP:HB3	1:C:159:LEU:HD23	1.87	0.57
1:B:205:PRO:HG3	1:B:211:MET:HE1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:HB3	1:B:104:LYS:CD	2.35	0.56
1:B:464:GLY:O	1:B:467:LYS:HE3	2.05	0.56
1:C:468:ASP:OD2	3:C:936:HOH:O	2.17	0.56
1:C:251:ARG:HG3	1:C:252:LEU:N	2.19	0.56
1:B:126:ARG:HH12	1:B:204:ILE:HG13	1.71	0.56
1:B:498:LYS:HD3	1:B:498:LYS:C	2.31	0.56
1:C:402:ASN:C	1:C:402:ASN:HD22	2.13	0.56
1:A:155:ARG:HH12	1:A:299:THR:CG2	2.18	0.56
1:A:314:LYS:HE2	3:A:939:HOH:O	2.04	0.56
3:A:619:HOH:O	1:B:428:VAL:HG23	2.04	0.56
1:B:379:ARG:NH2	3:B:907:HOH:O	2.35	0.56
1:D:90:ILE:HG21	1:D:312:VAL:HG22	1.87	0.56
1:D:170:ASN:HD22	1:D:172:GLN:H	1.52	0.56
1:C:150:PRO:HG3	1:C:214:TYR:CD1	2.41	0.56
3:C:570:HOH:O	1:D:363:HIS:HD2	1.88	0.56
1:B:138:GLU:CD	3:B:974:HOH:O	2.49	0.56
1:B:284:THR:OG1	1:B:287:GLU:HG3	2.06	0.56
1:C:26:LEU:HD12	1:C:27:THR:N	2.21	0.56
1:A:492:ILE:O	1:A:496:LEU:HD13	2.07	0.55
1:B:92:ARG:HD2	1:B:93:TYR:CZ	2.41	0.55
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.71	0.55
1:B:9:ASP:OD2	3:B:929:HOH:O	2.18	0.55
1:B:138:GLU:CG	3:B:974:HOH:O	2.51	0.55
1:C:92:ARG:HG3	1:C:92:ARG:HH11	1.70	0.55
1:B:296:PHE:CD2	1:B:346:PRO:HG2	2.42	0.55
1:D:91:THR:HG21	3:D:649:HOH:O	2.06	0.55
1:D:168:LYS:HB3	3:D:895:HOH:O	2.05	0.55
1:D:232:LYS:HB2	1:D:281:GLN:CG	2.36	0.55
1:C:50:LEU:HB3	3:C:508:HOH:O	2.05	0.55
1:B:447:LEU:HA	1:B:455:ARG:NH1	2.22	0.55
1:C:126:ARG:HD2	1:C:198:LEU:O	2.06	0.55
1:D:394:MET:N	3:D:753:HOH:O	2.21	0.55
1:B:37:LYS:H	1:D:413:HIS:HE1	1.53	0.54
1:D:82:GLY:HA3	1:D:316:VAL:O	2.07	0.54
1:D:393:MET:O	3:D:988:HOH:O	2.18	0.54
1:A:321:PRO:HG2	3:D:607:HOH:O	2.06	0.54
1:B:229:VAL:HG21	1:B:282:VAL:CG1	2.38	0.54
1:D:100:GLU:HB3	1:D:104:LYS:HD2	1.89	0.54
1:A:18:ARG:O	1:A:19:ALA:C	2.49	0.54
1:A:176:LYS:NZ	3:A:615:HOH:O	2.40	0.54
1:C:499:TYR:C	1:C:501:GLU:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:O	1:C:100:GLU:HB2	2.07	0.54
1:B:34:VAL:HG11	1:B:37:LYS:HB3	1.89	0.54
1:B:43:VAL:O	1:B:43:VAL:HG13	2.07	0.54
1:B:126:ARG:NH1	3:B:737:HOH:O	2.37	0.54
1:C:381:ARG:NH1	3:C:810:HOH:O	2.41	0.54
1:B:177:ASP:OD1	1:B:179:ASP:HB2	2.08	0.54
1:D:350:LEU:C	3:D:773:HOH:O	2.51	0.54
1:D:393:MET:HA	3:D:753:HOH:O	2.08	0.53
1:D:393:MET:HB3	3:D:753:HOH:O	2.07	0.53
1:D:446:TYR:O	1:D:455:ARG:HD3	2.08	0.53
1:B:129:ARG:HG2	1:B:211:MET:HE1	1.89	0.53
1:D:391:MET:HE3	1:D:393:MET:CE	2.38	0.53
1:C:73:VAL:HG12	1:C:74:HIS:HD2	1.73	0.53
1:C:248:ASP:CG	1:C:251:ARG:HH12	2.17	0.53
1:A:421:ARG:HD2	1:A:421:ARG:C	2.33	0.53
1:A:487:GLU:HA	1:A:490:SER:OG	2.09	0.53
1:B:125:VAL:HG22	3:B:643:HOH:O	2.08	0.53
1:B:126:ARG:NE	1:B:199:PHE:HA	2.22	0.53
1:C:92:ARG:CD	3:C:572:HOH:O	2.40	0.53
1:B:499:TYR:C	1:B:501:GLU:H	2.16	0.53
1:C:456:LYS:O	1:C:460:GLU:HG3	2.09	0.53
1:D:391:MET:HE3	1:D:393:MET:HE3	1.91	0.53
1:D:406:ASN:ND2	1:D:410:ALA:HB3	2.21	0.53
1:A:287:GLU:HA	1:A:290:ILE:HG12	1.91	0.53
1:A:485:HIS:CD2	1:A:487:GLU:HB3	2.44	0.53
1:B:147:ASN:ND2	2:B:1:HEM:HAC	2.24	0.53
1:A:13:HIS:HD2	3:A:594:HOH:O	1.91	0.53
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.74	0.53
1:B:154:ILE:HG13	1:B:349:MET:CE	2.39	0.53
1:B:428:VAL:HG23	1:B:428:VAL:O	2.09	0.52
1:C:476:LYS:HB3	1:C:476:LYS:HZ2	1.73	0.52
1:D:487:GLU:O	1:D:491:ARG:HG3	2.08	0.52
1:C:92:ARG:HG3	1:C:92:ARG:NH1	2.24	0.52
1:A:419:GLU:CD	1:A:419:GLU:H	2.17	0.52
1:C:19:ALA:O	1:C:20:ALA:HB3	2.08	0.52
3:A:869:HOH:O	1:C:409:SER:CB	2.39	0.52
1:B:4:ARG:HB2	1:B:4:ARG:NH1	2.25	0.52
1:C:43:VAL:O	1:C:43:VAL:HG13	2.08	0.52
1:C:176:LYS:HE3	3:C:525:HOH:O	2.09	0.52
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.92	0.52
1:B:11:MET:HE2	1:C:180:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:O	1:B:362:ARG:HG3	2.10	0.52
3:A:883:HOH:O	1:B:430:ARG:HG3	2.09	0.52
1:D:232:LYS:HB2	1:D:281:GLN:HG2	1.92	0.52
1:C:450:LEU:HA	1:C:454:GLN:NE2	2.25	0.52
1:D:74:HIS:CE1	1:D:115:VAL:HG22	2.44	0.52
1:A:155:ARG:HH11	1:A:155:ARG:CB	2.19	0.51
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.74	0.51
1:C:155:ARG:HH12	1:C:438:ASN:HD22	1.58	0.51
1:D:142:TRP:HB2	1:D:339:PRO:HD3	1.91	0.51
1:A:206:ASP:HB2	1:A:242:LYS:HD2	1.92	0.51
1:B:321:PRO:HG2	3:C:1280:HOH:O	2.08	0.51
1:C:92:ARG:NE	1:C:93:TYR:CE2	2.78	0.51
1:D:148:ASN:N	1:D:148:ASN:HD22	2.08	0.51
1:A:314:LYS:CG	3:A:939:HOH:O	2.41	0.51
1:D:43:VAL:CG1	1:D:48:PRO:HD2	2.40	0.51
1:A:495:LEU:CD2	3:A:978:HOH:O	2.58	0.51
1:D:357:TYR:HB2	1:D:358:PRO:HD3	1.93	0.51
1:A:387:ARG:O	1:C:66:GLU:HG2	2.10	0.51
1:B:421:ARG:HG3	3:B:1071:HOH:O	2.10	0.51
1:D:280:ILE:HG23	1:D:312:VAL:HG21	1.91	0.51
1:C:443:ARG:HG2	1:C:484:VAL:O	2.11	0.51
1:B:466:LEU:CD2	1:B:474:GLN:HG2	2.31	0.51
1:B:4:ARG:CB	1:B:4:ARG:HH11	2.23	0.51
1:B:490:SER:HA	3:B:1268:HOH:O	2.10	0.51
1:D:12:LYS:CG	3:D:1056:HOH:O	2.51	0.51
1:D:249:ALA:HB3	3:D:1062:HOH:O	2.10	0.51
1:D:456:LYS:N	3:D:896:HOH:O	2.44	0.51
1:B:321:PRO:CG	3:C:1280:HOH:O	2.59	0.51
1:B:454:GLN:CD	3:B:905:HOH:O	2.54	0.51
1:B:148:ASN:HD22	1:B:211:MET:HE2	1.76	0.50
1:C:92:ARG:HG3	3:C:809:HOH:O	2.11	0.50
1:D:9:ASP:CG	3:D:609:HOH:O	2.54	0.50
1:D:129:ARG:HG3	1:D:205:PRO:HG3	1.92	0.50
1:D:155:ARG:NH2	1:D:438:ASN:OD1	2.35	0.50
1:A:314:LYS:CE	3:A:939:HOH:O	2.58	0.50
1:D:148:ASN:HD22	1:D:148:ASN:H	1.59	0.50
1:A:74:HIS:HA	1:A:114:THR:O	2.11	0.50
1:A:501:GLU:OE1	1:A:501:GLU:HA	2.10	0.50
1:A:177:ASP:OD1	1:A:179:ASP:HB2	2.11	0.50
1:A:35:GLY:HA2	1:C:414:GLN:O	2.10	0.50
1:A:148:ASN:HD22	1:A:148:ASN:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ARG:O	1:B:255:GLU:HB2	2.11	0.50
1:A:43:VAL:O	1:A:47:GLY:HA3	2.12	0.50
1:B:453:GLU:OE2	1:B:457:ARG:NH1	2.45	0.50
1:B:475:LYS:NZ	1:B:475:LYS:HB3	2.26	0.50
1:D:479:LYS:HD3	1:D:479:LYS:C	2.37	0.50
1:A:155:ARG:NH1	1:A:297:ASP:OD1	2.44	0.50
1:B:466:LEU:HD13	1:B:496:LEU:HD11	1.94	0.50
1:C:445:PHE:CZ	1:C:450:LEU:HD11	2.46	0.50
1:B:10:GLN:NE2	1:C:172:GLN:HE21	2.10	0.50
1:B:391:MET:HE3	1:D:365:LEU:O	2.11	0.50
1:C:243:ASN:ND2	3:C:697:HOH:O	2.45	0.50
1:C:452:GLU:OE1	1:C:452:GLU:HA	2.12	0.50
1:B:404:TYR:HE1	1:B:412:GLU:OE2	1.95	0.49
1:A:147:ASN:CG	2:A:1:HEM:HAC	2.37	0.49
1:A:155:ARG:NH1	1:A:299:THR:OG1	2.40	0.49
1:A:456:LYS:O	1:A:460:GLU:HG3	2.13	0.49
1:B:193:HIS:HD2	1:B:299:THR:O	1.95	0.49
1:C:445:PHE:CE2	1:C:450:LEU:HD11	2.47	0.49
1:B:101:HIS:CE1	1:B:104:LYS:HB2	2.48	0.49
1:C:154:ILE:HD12	1:C:159:LEU:HB2	1.94	0.49
1:C:439:VAL:O	1:C:443:ARG:HG3	2.12	0.49
1:D:136:TYR:O	1:D:379:ARG:HG3	2.12	0.49
1:A:126:ARG:NH1	1:A:199:PHE:HA	2.26	0.49
1:B:262:ARG:HB3	3:B:1241:HOH:O	2.11	0.49
1:B:129:ARG:HB2	1:B:211:MET:HE1	1.95	0.49
1:D:309:LEU:C	1:D:310:ILE:HD12	2.38	0.49
1:A:453:GLU:CG	1:A:457:ARG:HH12	2.25	0.49
1:A:429:GLN:HB3	1:B:421:ARG:CD	2.31	0.49
1:D:18:ARG:HG3	1:D:21:GLN:HB2	1.94	0.49
1:C:206:ASP:OD2	1:C:242:LYS:NZ	2.45	0.49
1:C:286:SER:O	1:C:289:GLU:HB3	2.12	0.49
1:C:423:HIS:HA	1:D:427:ASP:HA	1.95	0.49
1:C:447:LEU:HD11	1:C:485:HIS:CD2	2.47	0.49
1:B:148:ASN:ND2	1:B:211:MET:HE2	2.28	0.49
1:C:437:ASP:C	3:C:678:HOH:O	2.56	0.49
1:B:443:ARG:O	1:B:447:LEU:HG	2.13	0.48
1:A:338:MET:HE3	3:A:608:HOH:O	2.13	0.48
1:B:125:VAL:HG22	1:B:126:ARG:N	2.28	0.48
1:D:84:PHE:O	1:D:105:ARG:HA	2.13	0.48
1:B:237:THR:HA	1:B:276:TRP:CD1	2.48	0.48
1:B:373:PRO:CG	3:D:753:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:TYR:CE2	1:B:404:TYR:HB2	2.48	0.48
1:C:22:LYS:HD3	1:C:23:PRO:HD2	1.95	0.48
1:D:74:HIS:HA	1:D:114:THR:O	2.14	0.48
1:C:451:ASN:H	1:C:454:GLN:HE21	1.62	0.48
1:C:452:GLU:CG	3:C:769:HOH:O	2.44	0.48
1:A:129:ARG:H	1:A:148:ASN:ND2	2.11	0.48
1:C:82:GLY:HA3	1:C:316:VAL:O	2.13	0.48
1:D:145:VAL:HB	1:D:353:ARG:NH2	2.29	0.48
1:A:429:GLN:CB	1:B:421:ARG:HD2	2.32	0.48
1:A:104:LYS:HG3	3:A:542:HOH:O	2.13	0.48
1:B:71:ARG:HD2	1:B:111:ARG:HH21	1.77	0.48
1:B:126:ARG:NH1	1:B:204:ILE:HG13	2.29	0.47
1:B:487:GLU:HG2	1:B:491:ARG:HD2	1.96	0.47
1:C:153:PHE:CZ	1:C:194:GLN:HG3	2.49	0.47
1:D:351:GLN:HG3	3:D:744:HOH:O	2.14	0.47
1:D:410:ALA:HB1	1:D:411:PRO:HD2	1.95	0.47
1:D:444:THR:CB	3:D:1074:HOH:O	2.32	0.47
1:C:293:PHE:HE2	1:C:437:ASP:OD2	1.97	0.47
1:A:15:LYS:NZ	3:A:869:HOH:O	2.46	0.47
1:B:357:TYR:HB2	1:B:358:PRO:HD3	1.96	0.47
1:B:381:ARG:HH11	1:B:381:ARG:HG2	1.79	0.47
1:A:148:ASN:HD22	1:A:148:ASN:N	2.12	0.47
1:B:62:HIS:CE1	1:D:368:ASN:HD21	2.17	0.47
1:B:111:ARG:NH2	3:B:615:HOH:O	2.44	0.47
1:D:232:LYS:O	1:D:280:ILE:HA	2.14	0.47
1:D:456:LYS:HG2	1:D:491:ARG:HH22	1.78	0.47
1:A:152:PHE:CD1	2:A:1:HEM:HMC3	2.49	0.47
1:C:101:HIS:CE1	3:C:770:HOH:O	2.67	0.47
1:A:391:MET:HE1	1:C:368:ASN:O	2.13	0.47
1:C:190:GLU:HA	1:C:438:ASN:ND2	2.29	0.47
1:C:429:GLN:OE1	1:D:421:ARG:HD2	2.15	0.47
1:D:145:VAL:HB	1:D:353:ARG:HH22	1.79	0.47
1:D:274:PRO:HD2	1:D:317:LEU:O	2.14	0.47
1:D:460:GLU:HA	1:D:495:LEU:HD13	1.95	0.47
1:A:92:ARG:HB3	3:A:597:HOH:O	2.15	0.47
1:A:220:LYS:HZ2	1:A:420:HIS:HB3	1.80	0.47
1:B:4:ARG:HB2	1:B:4:ARG:HH11	1.79	0.47
1:B:271:GLY:HA2	1:B:273:TYR:CZ	2.50	0.47
1:C:432:ASN:HD21	1:C:434:ALA:CB	2.28	0.47
1:B:78:ALA:HB2	1:B:261:LEU:HD12	1.96	0.47
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ARG:HH11	1:C:381:ARG:CB	2.26	0.47
1:D:72:VAL:HG13	1:D:73:VAL:HG22	1.96	0.47
1:A:97:LYS:NZ	3:A:1135:HOH:O	2.47	0.47
1:C:206:ASP:CA	1:C:244:LEU:HD22	2.45	0.47
1:A:242:LYS:HD3	1:A:243:ASN:N	2.31	0.46
1:B:232:LYS:HE2	1:B:302:TRP:CE2	2.50	0.46
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.45	0.46
1:D:159:LEU:HD21	1:D:188:ARG:CZ	2.45	0.46
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.80	0.46
1:A:499:TYR:C	1:A:501:GLU:N	2.74	0.46
1:B:82:GLY:HA3	1:B:316:VAL:O	2.15	0.46
1:B:447:LEU:CD1	1:B:448:LYS:HE2	2.45	0.46
1:A:14:TRP:CH2	1:A:18:ARG:HD2	2.51	0.46
1:A:153:PHE:CE1	1:A:194:GLN:HG3	2.50	0.46
1:A:402:ASN:C	1:A:402:ASN:HD22	2.23	0.46
1:A:385:TYR:HE1	1:C:26:LEU:HD22	1.80	0.46
1:B:26:LEU:HD21	1:B:37:LYS:HD3	1.98	0.46
1:C:251:ARG:O	1:C:255:GLU:HG3	2.16	0.46
1:A:50:LEU:CD1	1:B:48:PRO:HB2	2.44	0.46
1:C:177:ASP:OD1	1:C:179:ASP:HB2	2.16	0.46
1:D:43:VAL:HG13	1:D:48:PRO:HD2	1.98	0.46
1:D:393:MET:CB	3:D:753:HOH:O	2.64	0.46
1:D:446:TYR:CZ	1:D:455:ARG:HD2	2.51	0.46
1:A:275:SER:HA	1:A:315:LEU:O	2.15	0.46
1:B:445:PHE:HA	1:B:449:VAL:CG2	2.46	0.46
1:C:220:LYS:NZ	3:C:1236:HOH:O	2.48	0.46
1:A:51:VAL:HG21	1:B:49:LEU:HB3	1.97	0.46
1:A:451:ASN:H	1:A:454:GLN:NE2	2.12	0.46
1:C:402:ASN:C	1:C:402:ASN:ND2	2.73	0.46
1:B:18:ARG:O	1:B:19:ALA:C	2.58	0.46
1:B:193:HIS:HE1	3:B:650:HOH:O	1.98	0.46
1:B:229:VAL:HG23	1:B:284:THR:HA	1.97	0.46
1:B:471:LEU:HD21	1:B:500:ASN:ND2	2.31	0.46
1:C:437:ASP:N	3:C:678:HOH:O	2.48	0.46
1:C:500:ASN:O	1:C:501:GLU:C	2.59	0.46
1:D:126:ARG:NE	3:D:613:HOH:O	2.24	0.46
1:A:453:GLU:HG2	1:A:457:ARG:NH1	2.32	0.46
1:B:126:ARG:NH2	1:B:200:SER:O	2.49	0.46
1:C:476:LYS:HB3	1:C:476:LYS:HZ3	1.81	0.46
1:D:499:TYR:C	1:D:501:GLU:H	2.23	0.46
1:D:274:PRO:HG2	1:D:317:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TYR:CD1	1:A:235:TYR:N	2.84	0.45
1:A:485:HIS:HD2	1:A:487:GLU:N	2.09	0.45
1:B:14:TRP:O	1:B:17:GLN:HG2	2.17	0.45
1:C:26:LEU:HG	1:C:34:VAL:CG2	2.46	0.45
1:C:479:LYS:HD2	1:C:479:LYS:O	2.16	0.45
1:A:487:GLU:HA	1:A:490:SER:HG	1.80	0.45
1:B:349:MET:O	1:B:353:ARG:HG3	2.16	0.45
1:C:232:LYS:O	1:C:280:ILE:HA	2.15	0.45
1:C:248:ASP:HA	1:C:251:ARG:NH1	2.31	0.45
1:D:83:TYR:CD1	1:D:83:TYR:C	2.95	0.45
1:D:419:GLU:H	1:D:419:GLU:CD	2.23	0.45
1:D:479:LYS:HD3	1:D:479:LYS:O	2.16	0.45
1:B:25:VAL:CG1	1:D:414:GLN:HG3	2.40	0.45
1:B:402:ASN:C	1:B:402:ASN:ND2	2.74	0.45
1:D:222:VAL:HG22	1:D:341:GLY:HA2	1.99	0.45
1:B:217:HIS:CD2	1:B:353:ARG:HH11	2.35	0.45
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.98	0.45
1:A:217:HIS:CD2	1:A:353:ARG:HH11	2.34	0.45
1:A:232:LYS:HB2	1:A:281:GLN:HB2	1.97	0.45
1:B:37:LYS:HE2	1:B:59:GLU:OE1	2.16	0.45
1:B:49:LEU:HD23	1:B:50:LEU:H	1.82	0.45
1:B:408:PHE:HA	1:D:15:LYS:HD2	1.98	0.45
1:B:499:TYR:C	1:B:501:GLU:N	2.75	0.45
1:D:319:ARG:NH1	3:D:1137:HOH:O	2.37	0.45
1:B:81:PHE:HB2	1:B:319:ARG:NH1	2.31	0.45
1:B:125:VAL:CG2	3:B:643:HOH:O	2.64	0.45
1:C:452:GLU:N	1:C:455:ARG:NH2	2.64	0.45
1:D:107:PRO:HG2	1:D:136:TYR:HB2	1.99	0.45
1:A:51:VAL:HG22	1:B:49:LEU:O	2.17	0.45
1:B:69:PRO:HG2	1:B:364:ARG:HA	1.98	0.45
1:B:446:TYR:CZ	1:B:455:ARG:HD2	2.52	0.45
1:B:84:PHE:O	1:B:105:ARG:HA	2.17	0.45
1:B:213:GLY:HA3	1:B:235:TYR:CE2	2.52	0.45
1:C:72:VAL:HG13	1:C:73:VAL:HG23	1.99	0.45
1:C:452:GLU:CD	3:C:769:HOH:O	2.60	0.45
1:A:254:HIS:CE1	1:A:255:GLU:HG3	2.52	0.45
1:B:454:GLN:HE21	1:B:454:GLN:HB3	1.52	0.45
1:D:445:PHE:HA	1:D:449:VAL:CG2	2.47	0.45
1:D:445:PHE:CE1	1:D:449:VAL:HG11	2.51	0.45
1:B:6:PRO:HG2	1:B:266:ASN:OD1	2.17	0.44
1:B:12:LYS:HG3	3:C:1090:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:C	1:B:41:LEU:HD13	2.43	0.44
1:B:94:SER:HB2	1:B:221:LEU:HB3	1.99	0.44
1:B:129:ARG:CB	1:B:211:MET:HE1	2.47	0.44
1:B:268:ILE:N	1:B:268:ILE:HD12	2.32	0.44
1:C:450:LEU:HD12	1:C:450:LEU:N	2.32	0.44
1:B:52:GLN:HB2	3:D:503:HOH:O	2.16	0.44
1:D:43:VAL:O	1:D:47:GLY:HA3	2.17	0.44
1:D:193:HIS:HB2	3:D:511:HOH:O	2.16	0.44
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.99	0.44
1:C:89:ASP:OD1	1:C:91:THR:CG2	2.60	0.44
1:A:414:GLN:O	1:C:35:GLY:HA2	2.18	0.44
1:A:450:LEU:HA	1:A:454:GLN:NE2	2.33	0.44
1:D:78:ALA:HB2	1:D:261:LEU:HG	2.00	0.44
1:B:74:HIS:HA	1:B:114:THR:O	2.17	0.44
1:B:206:ASP:HA	1:B:244:LEU:HG	1.99	0.44
1:B:223:ASN:ND2	1:B:227:GLU:HB2	2.32	0.44
1:D:468:ASP:OD2	3:D:763:HOH:O	2.20	0.44
1:A:402:ASN:HD21	1:B:180:MET:HE3	1.83	0.44
1:B:343:GLU:HB3	1:B:344:PRO:HD2	1.99	0.44
1:B:373:PRO:CD	3:D:753:HOH:O	2.66	0.44
1:C:410:ALA:HB1	1:C:411:PRO:CD	2.48	0.44
1:C:451:ASN:O	1:C:454:GLN:N	2.51	0.44
1:A:222:VAL:HG21	1:A:420:HIS:HB2	1.99	0.44
1:B:148:ASN:HD22	1:B:211:MET:CE	2.31	0.44
1:D:475:LYS:HE3	3:D:1277:HOH:O	2.17	0.44
1:A:165:HIS:HB3	1:B:402:ASN:ND2	2.32	0.43
1:B:205:PRO:HG3	1:B:211:MET:HE3	1.97	0.43
1:C:126:ARG:HG2	1:C:126:ARG:HH11	1.83	0.43
1:D:206:ASP:OD2	1:D:242:LYS:HE2	2.18	0.43
1:A:51:VAL:CG2	1:B:49:LEU:HB3	2.48	0.43
1:B:124:THR:HG21	1:B:252:LEU:HD23	2.00	0.43
1:C:213:GLY:HA3	1:C:235:TYR:CE2	2.54	0.43
1:D:197:PHE:CD1	1:D:197:PHE:C	2.96	0.43
1:D:293:PHE:CG	1:D:300:LYS:HD3	2.54	0.43
1:D:474:GLN:O	1:D:478:VAL:HG23	2.19	0.43
1:B:393:MET:HE2	1:D:393:MET:HG3	2.00	0.43
1:A:251:ARG:HB3	1:A:251:ARG:NH1	2.27	0.43
1:B:41:LEU:HD12	1:B:50:LEU:HB2	2.00	0.43
1:C:432:ASN:HD21	1:C:434:ALA:HB3	1.83	0.43
1:D:310:ILE:HD12	1:D:310:ILE:N	2.33	0.43
1:C:126:ARG:O	1:C:127:ASP:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:LYS:HE2	3:C:884:HOH:O	2.19	0.43
1:D:17:GLN:NE2	3:D:852:HOH:O	2.51	0.43
1:D:381:ARG:HH11	1:D:381:ARG:HG2	1.84	0.43
1:A:284:THR:OG1	1:A:287:GLU:HG3	2.18	0.43
1:A:410:ALA:HB1	1:A:411:PRO:HD2	2.00	0.43
1:A:442:VAL:HG12	1:A:484:VAL:HG11	2.00	0.43
1:B:12:LYS:CE	3:B:1023:HOH:O	2.66	0.43
1:D:73:VAL:HG11	1:D:164:ILE:HD12	2.00	0.43
1:D:456:LYS:HE2	3:D:919:HOH:O	2.18	0.43
1:A:126:ARG:O	1:A:127:ASP:HB2	2.18	0.43
1:B:100:GLU:HG3	1:B:101:HIS:HD2	1.83	0.43
1:C:470:GLN:HE21	1:C:470:GLN:HB2	1.58	0.43
1:A:467:LYS:HD3	1:A:499:TYR:CD1	2.54	0.43
1:B:179:ASP:CG	1:C:4:ARG:HH22	2.26	0.43
1:A:384:ASN:HA	1:C:26:LEU:HD13	2.00	0.43
1:C:357:TYR:HB2	1:C:358:PRO:HD3	2.00	0.43
1:D:334:ASP:O	1:D:337:ASN:HB2	2.18	0.43
1:A:182:TRP:CD2	1:A:466:LEU:HD13	2.53	0.42
1:B:65:ARG:HD3	1:D:367:PRO:HG3	2.01	0.42
1:B:95:LYS:NZ	3:B:778:HOH:O	2.52	0.42
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.84	0.42
1:D:291:PHE:HA	1:D:292:PRO:HD3	1.91	0.42
1:B:100:GLU:HG3	1:B:101:HIS:CD2	2.54	0.42
1:B:404:TYR:CD1	1:B:405:PRO:HA	2.53	0.42
1:D:148:ASN:HA	1:D:212:ASN:O	2.18	0.42
1:B:41:LEU:HD11	1:C:428:VAL:HG13	2.01	0.42
1:B:97:LYS:O	1:B:100:GLU:HB2	2.20	0.42
1:B:319:ARG:CB	1:B:319:ARG:NH1	2.78	0.42
1:B:447:LEU:HD23	1:B:485:HIS:CD2	2.54	0.42
1:C:443:ARG:NE	1:C:484:VAL:O	2.52	0.42
1:D:251:ARG:O	1:D:255:GLU:HG3	2.18	0.42
1:A:436:ASP:O	1:A:437:ASP:C	2.61	0.42
1:D:177:ASP:OD1	1:D:179:ASP:HB2	2.20	0.42
1:B:262:ARG:HG2	1:B:266:ASN:ND2	2.35	0.42
1:D:176:LYS:NZ	3:D:725:HOH:O	2.53	0.42
1:D:410:ALA:HB1	1:D:411:PRO:CD	2.49	0.42
1:A:110:VAL:HG22	1:A:133:VAL:HG22	2.02	0.42
1:A:145:VAL:HG22	1:A:333:PHE:HB3	2.01	0.42
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.50	0.42
1:B:391:MET:HE3	1:D:365:LEU:C	2.45	0.42
1:B:43:VAL:CG1	1:B:48:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:HD3	1:C:23:PRO:CD	2.49	0.42
1:D:290:ILE:O	1:D:291:PHE:C	2.61	0.42
1:A:429:GLN:HG3	1:A:431:PHE:CE2	2.54	0.42
1:B:229:VAL:HG21	1:B:282:VAL:HG13	2.02	0.42
1:B:346:PRO:O	1:B:347:ASP:C	2.61	0.42
3:B:637:HOH:O	1:C:70:GLU:HG2	2.19	0.42
1:D:201:ASP:CG	3:D:634:HOH:O	2.62	0.42
1:D:237:THR:HA	1:D:276:TRP:CD1	2.55	0.42
1:D:445:PHE:O	1:D:449:VAL:HB	2.20	0.42
1:A:45:PRO:HD3	1:D:431:PHE:CE2	2.55	0.42
1:B:271:GLY:HA2	1:B:273:TYR:CE1	2.55	0.42
1:C:142:TRP:HB2	1:C:339:PRO:HD3	2.02	0.42
1:D:148:ASN:HB3	1:D:211:MET:HE3	2.02	0.42
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.80	0.42
1:A:448:LYS:HA	1:A:448:LYS:CE	2.45	0.42
1:B:367:PRO:HD2	1:B:390:PRO:HG2	2.01	0.42
1:A:136:TYR:O	1:A:379:ARG:HG3	2.19	0.41
1:A:451:ASN:O	1:A:455:ARG:HG3	2.20	0.41
1:B:85:GLU:OE2	1:B:105:ARG:NE	2.45	0.41
1:B:291:PHE:CD1	1:B:292:PRO:HD2	2.55	0.41
1:C:209:ARG:O	1:C:239:GLN:CG	2.65	0.41
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.85	0.41
1:B:385:TYR:CD2	1:B:404:TYR:HB2	2.55	0.41
1:D:473:ILE:HA	1:D:476:LYS:CE	2.50	0.41
1:A:60:MET:HE1	1:D:161:PRO:HD3	2.02	0.41
1:B:129:ARG:CG	1:B:211:MET:HE1	2.50	0.41
1:B:374:VAL:CG2	3:B:517:HOH:O	2.40	0.41
1:C:452:GLU:H	1:C:455:ARG:NH2	2.18	0.41
1:B:126:ARG:HH21	1:B:199:PHE:HA	1.85	0.41
1:B:212:ASN:OD1	1:B:236:LYS:HA	2.20	0.41
1:C:74:HIS:HA	1:C:114:THR:O	2.20	0.41
1:C:499:TYR:CE2	3:C:1036:HOH:O	2.71	0.41
1:D:147:ASN:ND2	2:D:1:HEM:HAC	2.35	0.41
1:B:83:TYR:CD1	1:B:83:TYR:C	2.99	0.41
1:A:81:PHE:HE1	1:A:321:PRO:HB3	1.85	0.41
1:B:38:LEU:HG	1:D:413:HIS:CE1	2.56	0.41
1:B:414:GLN:O	1:D:35:GLY:HA2	2.20	0.41
1:C:294:ASN:HB3	1:C:297:ASP:HB2	2.03	0.41
1:A:155:ARG:HH12	1:A:299:THR:CB	2.33	0.41
1:A:232:LYS:O	1:A:280:ILE:HA	2.20	0.41
1:A:367:PRO:HG3	1:C:65:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:HB2	1:B:211:MET:HE2	2.02	0.41
1:B:393:MET:HE3	1:D:372:ILE:HA	2.03	0.41
1:C:148:ASN:HA	1:C:212:ASN:O	2.21	0.41
1:D:218:THR:HG23	1:D:302:TRP:CZ2	2.56	0.41
1:B:158:LEU:HD11	1:B:430:ARG:HH21	1.84	0.41
1:B:467:LYS:HD3	1:B:499:TYR:CD1	2.56	0.41
1:D:476:LYS:HE3	1:D:476:LYS:HB2	1.83	0.41
1:D:499:TYR:C	1:D:501:GLU:N	2.78	0.41
1:A:471:LEU:O	1:A:475:LYS:HG3	2.21	0.41
1:B:43:VAL:O	1:B:47:GLY:HA3	2.21	0.41
1:B:89:ASP:OD1	1:B:89:ASP:C	2.63	0.41
1:B:451:ASN:OD1	1:B:454:GLN:HG2	2.20	0.41
1:B:456:LYS:O	1:B:456:LYS:HD3	2.21	0.41
1:C:155:ARG:CZ	1:C:438:ASN:HD21	2.31	0.41
1:C:177:ASP:HA	1:C:178:PRO:HD2	1.94	0.41
1:C:346:PRO:O	1:C:347:ASP:C	2.64	0.41
1:C:414:GLN:NE2	3:C:1030:HOH:O	2.48	0.41
1:C:451:ASN:O	1:C:452:GLU:C	2.64	0.41
1:D:11:MET:O	1:D:12:LYS:C	2.64	0.41
1:A:106:THR:HA	1:A:107:PRO:HD3	1.94	0.41
1:B:142:TRP:HB2	1:B:339:PRO:HD3	2.02	0.41
1:D:192:LEU:HD13	1:D:484:VAL:CG2	2.51	0.41
1:A:223:ASN:ND2	1:A:227:GLU:HB2	2.36	0.40
1:B:34:VAL:HG11	1:B:37:LYS:CB	2.51	0.40
1:B:474:GLN:O	1:B:478:VAL:HG23	2.20	0.40
1:C:74:HIS:CE1	1:C:115:VAL:HG22	2.56	0.40
1:C:414:GLN:OE1	1:C:414:GLN:HA	2.20	0.40
1:C:453:GLU:O	1:C:457:ARG:NH1	2.55	0.40
1:D:223:ASN:OD1	1:D:225:ASN:HB2	2.21	0.40
1:D:426:GLY:HA3	3:D:768:HOH:O	2.21	0.40
1:A:52:GLN:HB2	3:C:550:HOH:O	2.20	0.40
1:A:291:PHE:HA	1:A:292:PRO:HD3	1.90	0.40
1:B:71:ARG:CZ	1:B:111:ARG:HE	2.34	0.40
1:B:391:MET:CE	1:D:372:ILE:HD11	2.51	0.40
1:C:29:GLY:HA3	3:C:515:HOH:O	2.22	0.40
1:C:414:GLN:HA	1:C:415:PRO:HD2	1.92	0.40
1:D:319:ARG:HH11	1:D:319:ARG:HG2	1.86	0.40
1:D:422:THR:HG22	1:D:423:HIS:N	2.36	0.40
1:A:294:ASN:HB3	1:A:297:ASP:HB2	2.03	0.40
1:B:452:GLU:OE2	1:B:491:ARG:NH1	2.52	0.40
1:C:437:ASP:CA	3:C:678:HOH:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:CYS:HB3	1:C:492:ILE:HD13	2.02	0.40
1:D:129:ARG:H	1:D:148:ASN:ND2	2.20	0.40
1:D:177:ASP:HA	1:D:178:PRO:HD2	1.92	0.40
1:A:251:ARG:HH11	1:A:251:ARG:CB	2.28	0.40
1:A:349:MET:O	1:A:353:ARG:HG3	2.21	0.40
1:C:283:MET:SD	1:C:288:ALA:HA	2.61	0.40
1:D:337:ASN:HD22	1:D:337:ASN:HA	1.68	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)
3:B:943:HOH:O	3:C:823:HOH:O[3_555]	1.87	0.33

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	498/499 (100%)	475 (95%)	19 (4%)	4 (1%)	16	8
1	B	498/499 (100%)	470 (94%)	24 (5%)	4 (1%)	16	8
1	C	498/499 (100%)	469 (94%)	25 (5%)	4 (1%)	16	8
1	D	498/499 (100%)	468 (94%)	27 (5%)	3 (1%)	21	13
All	All	1992/1996 (100%)	1882 (94%)	95 (5%)	15 (1%)	16	8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	437	ASP
1	C	437	ASP

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Mol	Chain	Res	Type
1	B	437	ASP
1	C	19	ALA
1	D	19	ALA
1	D	437	ASP
1	A	500	ASN
1	B	500	ASN
1	C	452	GLU
1	C	500	ASN
1	A	100	GLU
1	B	19	ALA
1	B	100	GLU
1	D	373	PRO

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	432/431 (100%)	420 (97%)	12 (3%)	38	32
1	B	432/431 (100%)	416 (96%)	16 (4%)	30	22
1	C	432/431 (100%)	416 (96%)	16 (4%)	30	22
1	D	432/431 (100%)	424 (98%)	8 (2%)	50	47
All	All	1728/1724 (100%)	1676 (97%)	52 (3%)	36	30

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	49	LEU
1	A	137	THR
1	A	148	ASN
1	A	155	ARG
1	A	235	TYR
1	A	242	LYS
1	A	251	ARG
1	A	402	ASN

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Mol	Chain	Res	Type
1	A	413	HIS
1	A	421	ARG
1	A	448	LYS
1	B	37	LYS
1	B	67	ARG
1	B	126	ARG
1	B	137	THR
1	B	235	TYR
1	B	255	GLU
1	B	290	ILE
1	B	319	ARG
1	B	374	VAL
1	B	393	MET
1	B	402	ASN
1	B	454	GLN
1	B	457	ARG
1	B	466	LEU
1	B	475	LYS
1	B	498	LYS
1	C	4	ARG
1	C	22	LYS
1	C	26	LEU
1	C	92	ARG
1	C	105	ARG
1	C	129	ARG
1	C	137	THR
1	C	145	VAL
1	C	159	LEU
1	C	235	TYR
1	C	239	GLN
1	C	373	PRO
1	C	381	ARG
1	C	402	ASN
1	C	413	HIS
1	C	483	ASP
1	D	43	VAL
1	D	73	VAL
1	D	148	ASN
1	D	235	TYR
1	D	247	GLU
1	D	373	PRO
1	D	412	GLU

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Mol	Chain	Res	Type
1	D	456	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	17	GLN
1	A	148	ASN
1	A	167	GLN
1	A	210	HIS
1	A	320	ASN
1	A	337	ASN
1	A	402	ASN
1	A	420	HIS
1	A	429	GLN
1	A	454	GLN
1	A	465	HIS
1	A	470	GLN
1	A	485	HIS
1	A	500	ASN
1	B	13	HIS
1	B	17	GLN
1	B	32	ASN
1	B	62	HIS
1	B	167	GLN
1	B	193	HIS
1	B	210	HIS
1	B	254	HIS
1	B	272	ASN
1	B	396	ASN
1	B	402	ASN
1	B	454	GLN
1	B	461	ASN
1	B	500	ASN
1	C	3	ASN
1	C	21	GLN
1	C	88	HIS
1	C	172	GLN
1	C	210	HIS
1	C	243	ASN
1	C	272	ASN
1	C	337	ASN

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Mol	Chain	Res	Type
1	C	386	GLN
1	C	402	ASN
1	C	432	ASN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	470	GLN
1	C	474	GLN
1	C	480	ASN
1	C	500	ASN
1	D	17	GLN
1	D	21	GLN
1	D	148	ASN
1	D	167	GLN
1	D	170	ASN
1	D	193	HIS
1	D	337	ASN
1	D	363	HIS
1	D	368	ASN
1	D	413	HIS
1	D	420	HIS
1	D	470	GLN
1	D	500	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HEM	B	1	1	50,50,50	1.19	4 (8%)	67,82,82	0.86	1 (1%)
2	HEM	C	1	1	50,50,50	1.16	4 (8%)	67,82,82	1.00	1 (1%)
2	HEM	A	1	1	50,50,50	1.15	4 (8%)	67,82,82	1.03	4 (5%)
2	HEM	D	1	1	50,50,50	1.17	4 (8%)	67,82,82	0.98	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	1	1	-	4/14/54/54	-
2	HEM	C	1	1	-	2/14/54/54	-
2	HEM	A	1	1	-	4/14/54/54	-
2	HEM	D	1	1	-	4/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	HEM	CBC-CAC	3.43	1.46	1.30
2	D	1	HEM	CBB-CAB	3.25	1.46	1.30
2	C	1	HEM	CBC-CAC	3.21	1.45	1.30
2	C	1	HEM	CBB-CAB	3.16	1.45	1.30
2	B	1	HEM	CBB-CAB	3.12	1.45	1.30
2	B	1	HEM	CBC-CAC	3.07	1.45	1.30
2	A	1	HEM	CBC-CAC	3.07	1.45	1.30
2	A	1	HEM	CBB-CAB	2.99	1.44	1.30
2	D	1	HEM	CAB-C3B	-2.82	1.39	1.47
2	D	1	HEM	CAC-C3C	-2.43	1.40	1.47
2	C	1	HEM	CAC-C3C	-2.39	1.41	1.47
2	A	1	HEM	CAC-C3C	-2.36	1.41	1.47
2	B	1	HEM	CAB-C3B	-2.35	1.41	1.47
2	B	1	HEM	CAC-C3C	-2.24	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	CAB-C3B	-2.22	1.41	1.47
2	C	1	HEM	CAB-C3B	-2.09	1.41	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	HEM	CAD-C3D-C2D	-2.78	122.65	127.87
2	C	1	HEM	C3B-C4B-NB	2.64	111.36	109.47
2	A	1	HEM	CMD-C2D-C1D	2.59	129.08	125.03
2	D	1	HEM	CAD-C3D-C4D	2.58	129.20	124.70
2	D	1	HEM	CAD-C3D-C2D	-2.35	123.47	127.87
2	A	1	HEM	C4C-C3C-C2C	-2.23	104.88	106.81
2	A	1	HEM	CAD-C3D-C4D	2.09	128.34	124.70
2	B	1	HEM	CAD-C3D-C4D	2.02	128.22	124.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

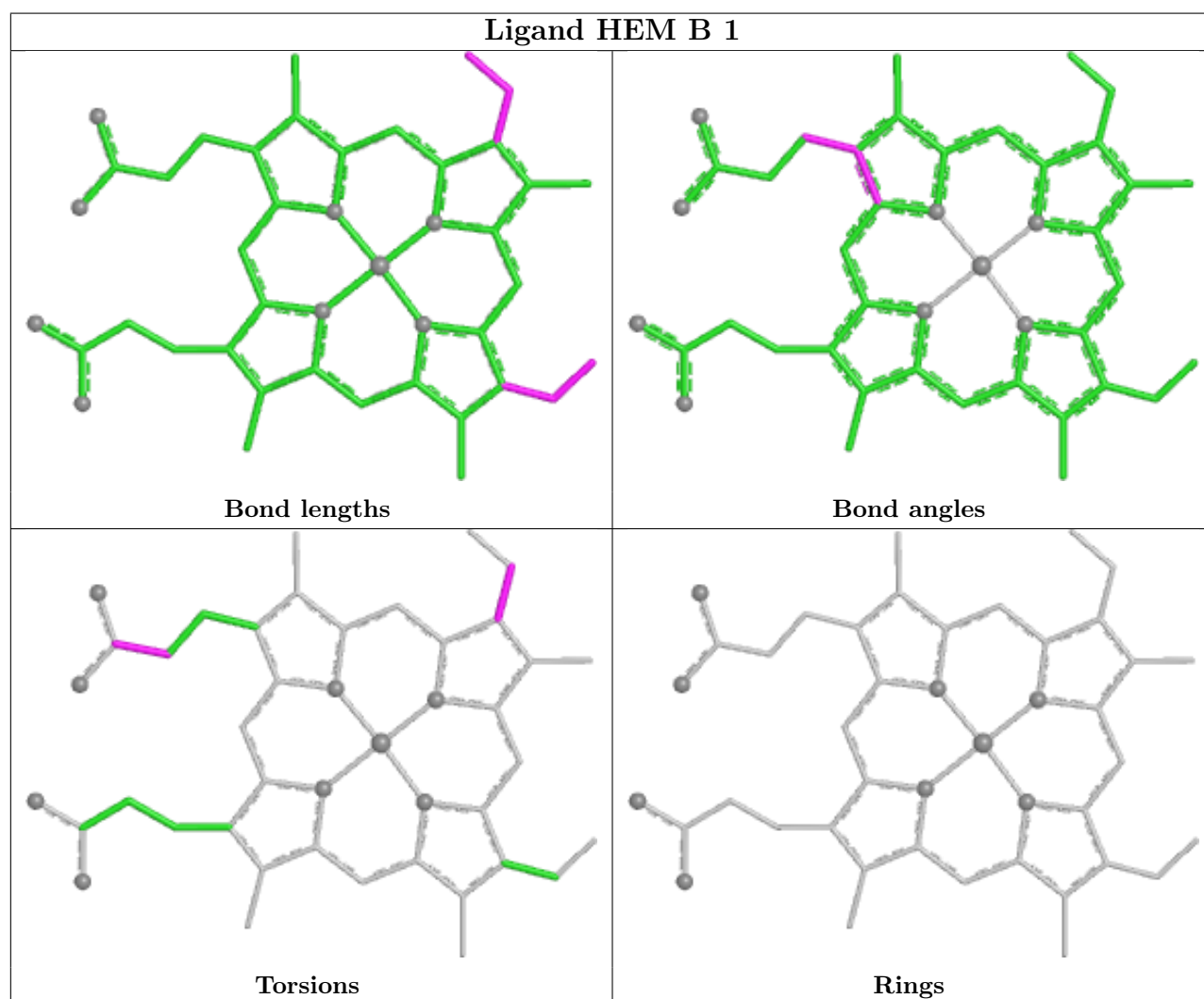
Mol	Chain	Res	Type	Atoms
2	A	1	HEM	C2C-C3C-CAC-CBC
2	B	1	HEM	C2C-C3C-CAC-CBC
2	B	1	HEM	CAD-CBD-CGD-O2D
2	B	1	HEM	CAD-CBD-CGD-O1D
2	A	1	HEM	CAD-CBD-CGD-O2D
2	D	1	HEM	CAD-CBD-CGD-O2D
2	C	1	HEM	CAD-CBD-CGD-O2D
2	A	1	HEM	CAD-CBD-CGD-O1D
2	A	1	HEM	C4C-C3C-CAC-CBC
2	B	1	HEM	C4C-C3C-CAC-CBC
2	D	1	HEM	C4C-C3C-CAC-CBC
2	C	1	HEM	CAD-CBD-CGD-O1D
2	D	1	HEM	CAD-CBD-CGD-O1D
2	D	1	HEM	C2C-C3C-CAC-CBC

There are no ring outliers.

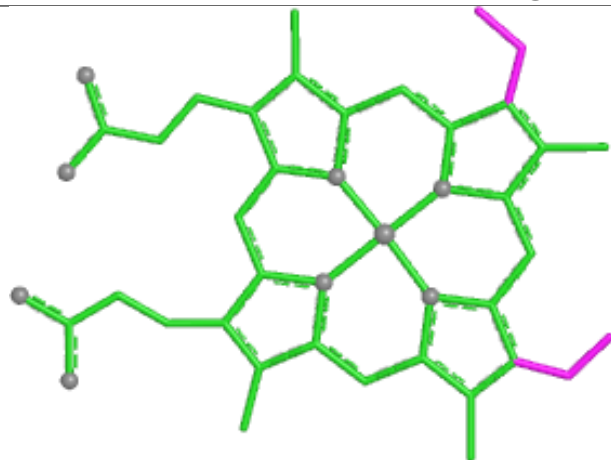
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	HEM	2	0
2	A	1	HEM	2	0
2	D	1	HEM	1	0

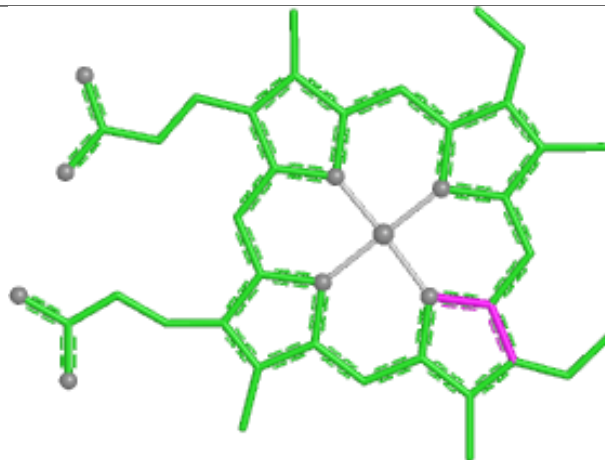
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



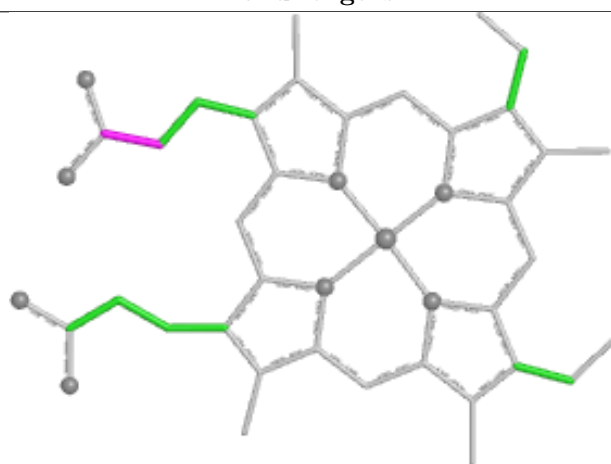
Ligand HEM C 1



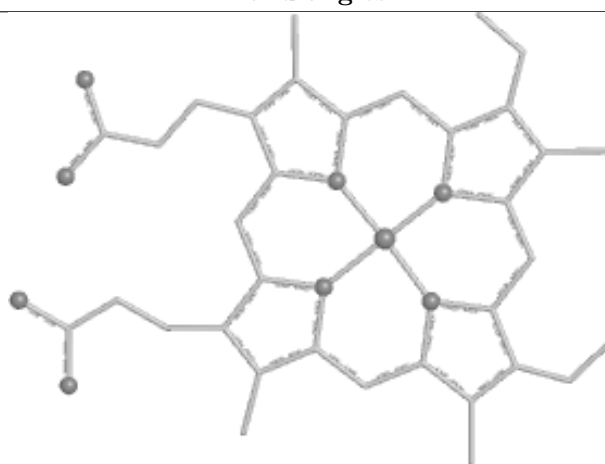
Bond lengths



Bond angles

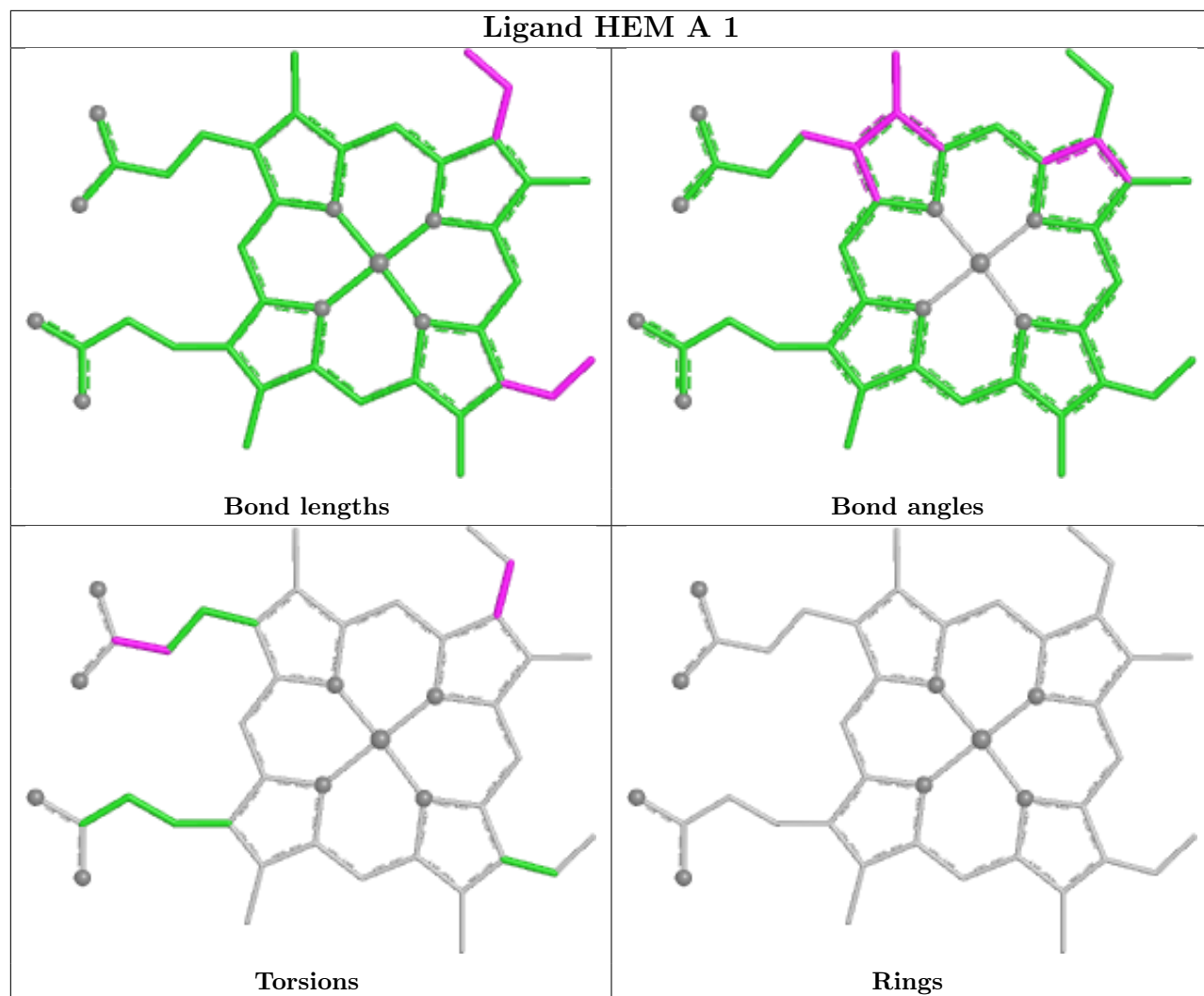


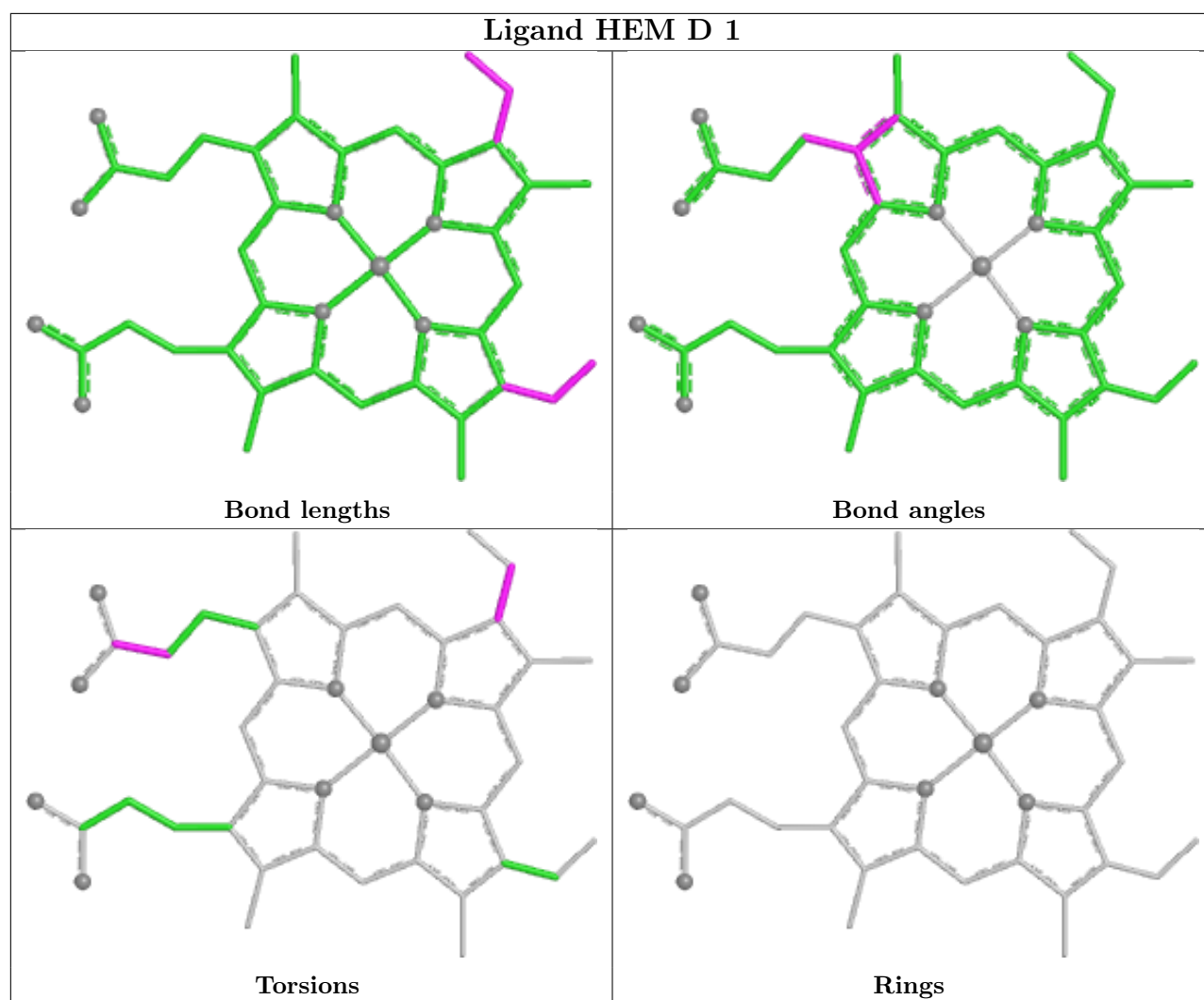
Torsions



Rings

Ligand HEM A 1





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	499/499 (100%)	0.24	14 (2%) 55 59	12, 24, 39, 61	1 (0%)
1	B	499/499 (100%)	0.37	28 (5%) 30 32	12, 25, 42, 60	1 (0%)
1	C	499/499 (100%)	0.26	27 (5%) 31 33	12, 23, 43, 78	1 (0%)
1	D	499/499 (100%)	0.54	27 (5%) 31 33	11, 28, 43, 73	1 (0%)
All	All	1996/1996 (100%)	0.35	96 (4%) 35 38	11, 25, 42, 78	4 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	4.5
1	B	19	ALA	4.3
1	C	489	GLY	4.0
1	D	19	ALA	4.0
1	D	18	ARG	3.9
1	C	499	TYR	3.8
1	C	20	ALA	3.8
1	D	499	TYR	3.8
1	B	416	SER	3.7
1	B	501	GLU	3.6
1	B	17	GLN	3.5
1	A	499	TYR	3.4
1	B	449	VAL	3.3
1	B	447	LEU	3.3
1	D	20	ALA	3.2
1	C	500	ASN	3.1
1	A	17	GLN	3.1
1	C	471	LEU	3.0
1	C	19	ALA	3.0
1	A	498	LYS	3.0
1	D	394	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	496	LEU	2.9
1	D	444	THR	2.8
1	B	197	PHE	2.8
1	C	3	ASN	2.8
1	C	17	GLN	2.8
1	B	304	HIS	2.8
1	B	452	GLU	2.8
1	D	17	GLN	2.7
1	B	252	LEU	2.7
1	B	450	LEU	2.7
1	D	414	GLN	2.7
1	C	289	GLU	2.7
1	D	246	VAL	2.7
1	A	3	ASN	2.7
1	B	499	TYR	2.6
1	B	16	GLU	2.6
1	C	498	LYS	2.6
1	B	25	VAL	2.6
1	C	43	VAL	2.6
1	B	444	THR	2.6
1	D	413	HIS	2.5
1	D	307	TYR	2.5
1	D	236	LYS	2.5
1	B	489	GLY	2.5
1	A	394	MET	2.5
1	C	456	LYS	2.5
1	C	92	ARG	2.5
1	A	310	ILE	2.5
1	C	501	GLU	2.5
1	C	22	LYS	2.5
1	D	500	ASN	2.4
1	A	500	ASN	2.4
1	D	289	GLU	2.4
1	D	92	ARG	2.4
1	D	282	VAL	2.4
1	B	3	ASN	2.4
1	C	495	LEU	2.4
1	D	272	ASN	2.4
1	A	495	LEU	2.3
1	B	20	ALA	2.3
1	C	453	GLU	2.3
1	A	496	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	484	VAL	2.3
1	D	487	GLU	2.3
1	B	249	ALA	2.3
1	D	21	GLN	2.3
1	D	439	VAL	2.3
1	B	498	LYS	2.3
1	D	494	ALA	2.2
1	A	290	ILE	2.2
1	D	222	VAL	2.2
1	B	22	LYS	2.2
1	C	494	ALA	2.2
1	C	290	ILE	2.2
1	D	280	ILE	2.2
1	D	495	LEU	2.2
1	B	261	LEU	2.2
1	B	23	PRO	2.2
1	B	4	ARG	2.2
1	D	501	GLU	2.1
1	A	102	ILE	2.1
1	C	421	ARG	2.1
1	B	305	GLY	2.1
1	C	487	GLU	2.1
1	B	393	MET	2.1
1	C	101	HIS	2.1
1	C	492	ILE	2.1
1	D	271	GLY	2.1
1	B	484	VAL	2.1
1	A	501	GLU	2.0
1	A	497	ASP	2.0
1	B	381	ARG	2.0
1	C	490	SER	2.0
1	C	422	THR	2.0
1	D	308	PRO	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 oligosaccharides in this entry.

6.4 Ligands

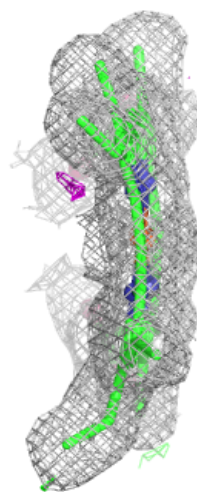
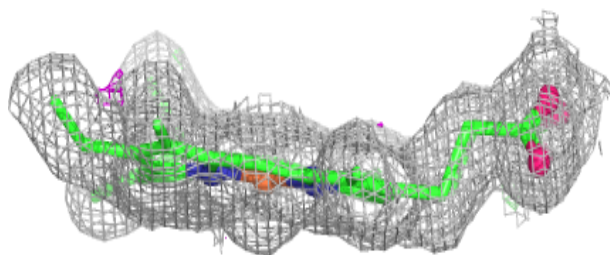
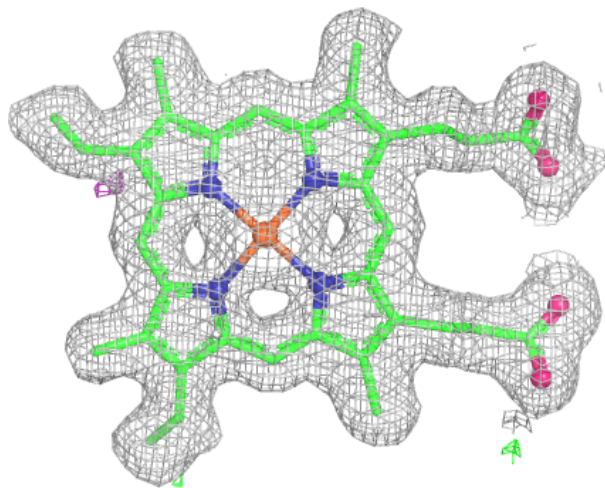
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	1	43/43	0.98	0.07	15,19,23,25	0
2	HEM	B	1	43/43	0.98	0.06	13,19,23,26	0
2	HEM	C	1	43/43	0.98	0.06	12,18,23,24	0
2	HEM	D	1	43/43	0.98	0.06	13,21,25,26	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.

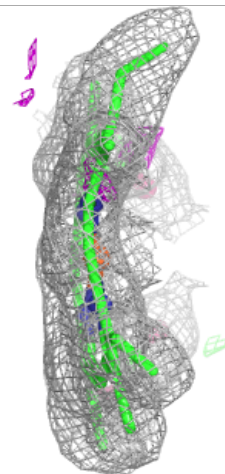
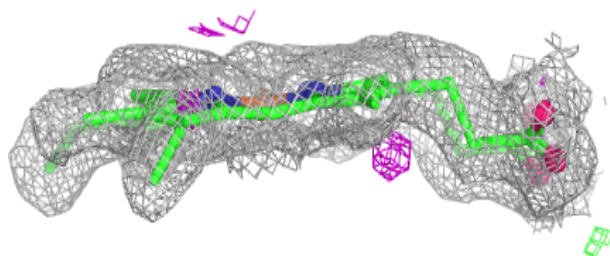
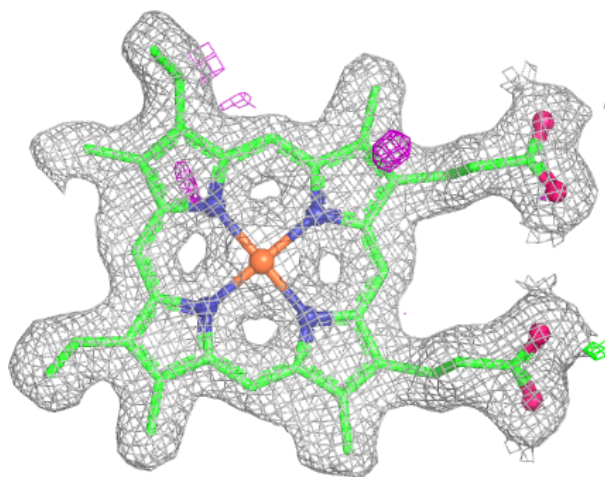
Electron density around HEM A 1:

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



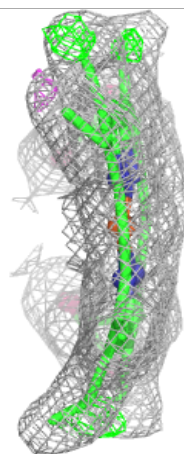
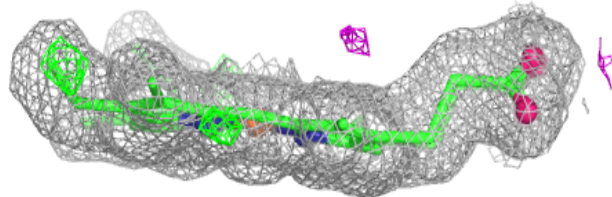
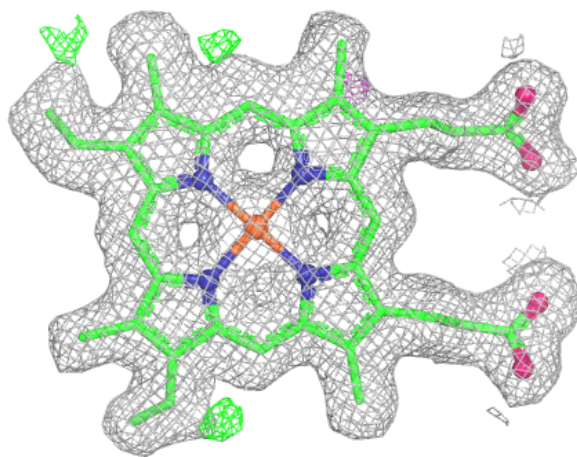
Electron density around HEM B 1:

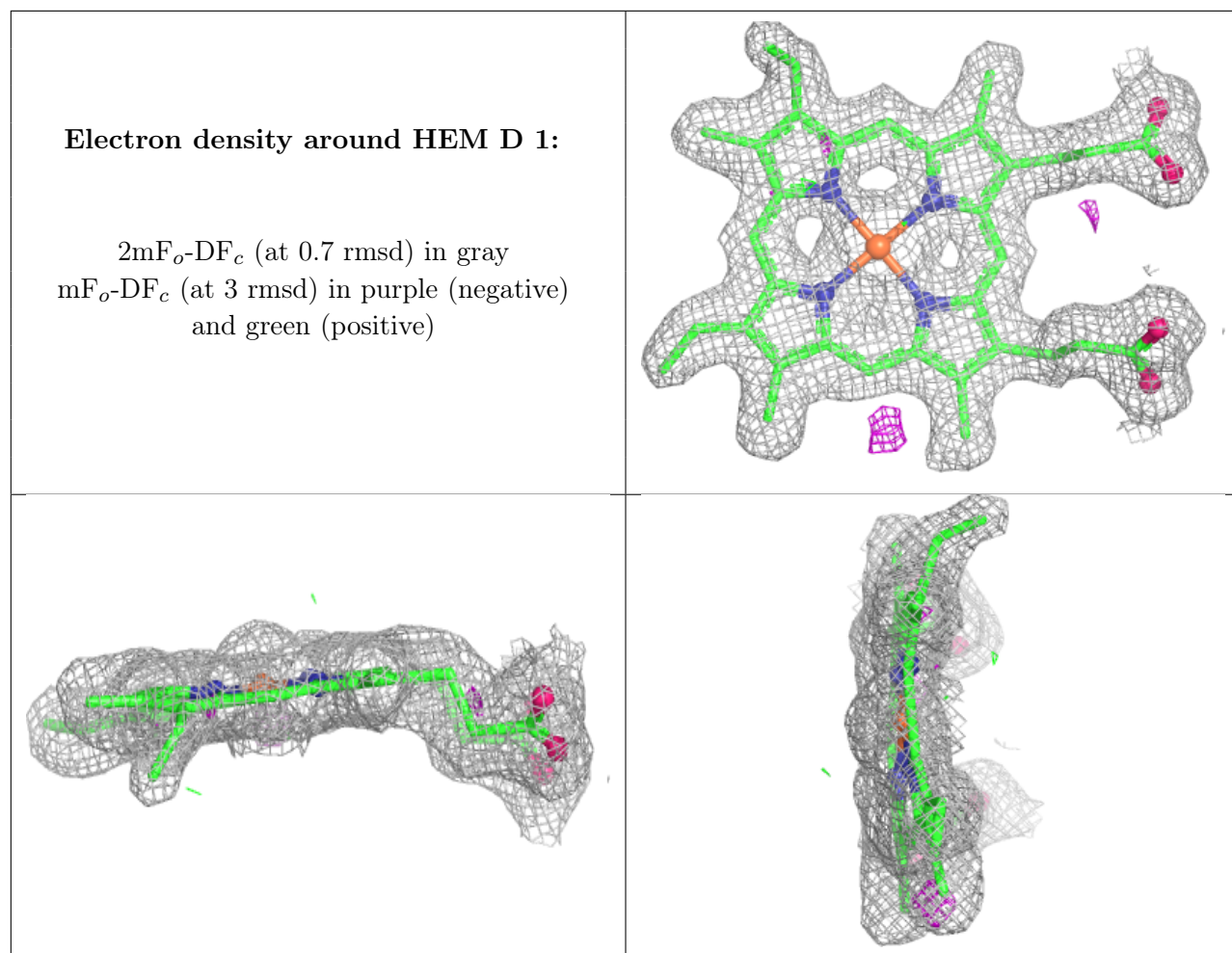
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 1:

$2mF_o-DF_c$ (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.