



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:13 PM UTC

PDB ID : 2F9Q / pdb_00002f9q
Title : Crystal Structure of Human Cytochrome P450 2D6
Authors : Rowland, P.
Deposited on : 2005-12-06
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

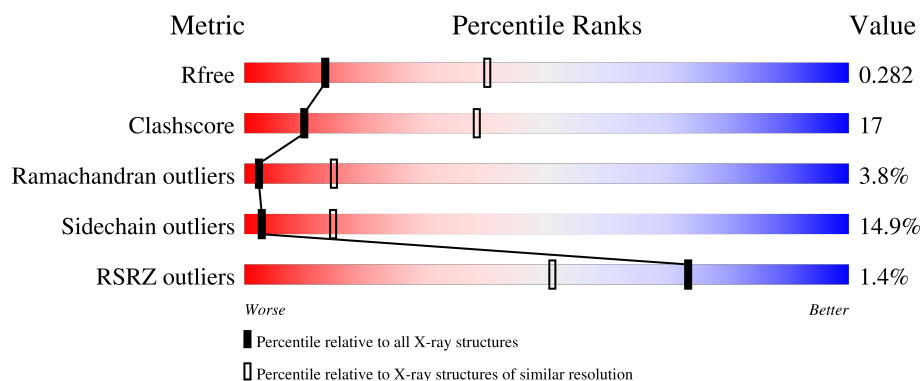
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	479	2% 58% 28% 8% 5%
1	B	479	2% 58% 27% 8% 6%
1	C	479	2% 55% 30% 8% 5%
1	D	479	2% 58% 27% 9% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	2000	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome P450 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3569	2281	634	639	15			
1	B	451	Total	C	N	O	S	0	0	0
			3545	2265	630	635	15			
1	C	454	Total	C	N	O	S	0	0	0
			3569	2281	634	639	15			
1	D	451	Total	C	N	O	S	0	0	0
			3545	2265	630	635	15			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	HIS	cloning artifact	UNP P10635
A	25	LYS	ARG	cloning artifact	UNP P10635
A	26	LYS	ARG	cloning artifact	UNP P10635
A	27	THR	GLN	cloning artifact	UNP P10635
A	28	SER	ARG	cloning artifact	UNP P10635
A	29	SER	TRP	cloning artifact	UNP P10635
A	30	LYS	ALA	cloning artifact	UNP P10635
A	31	GLY	ALA	cloning artifact	UNP P10635
A	32	LYS	ARG	cloning artifact	UNP P10635
A	33	LEU	TYR	cloning artifact	UNP P10635
A	230	ASP	LEU	engineered mutation	UNP P10635
A	231	ARG	LEU	engineered mutation	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	24	ALA	HIS	cloning artifact	UNP P10635
B	25	LYS	ARG	cloning artifact	UNP P10635
B	26	LYS	ARG	cloning artifact	UNP P10635
B	27	THR	GLN	cloning artifact	UNP P10635
B	28	SER	ARG	cloning artifact	UNP P10635

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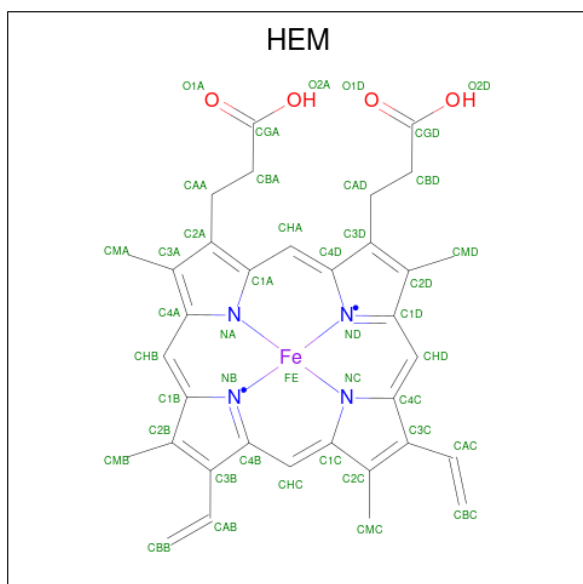
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	TRP	cloning artifact	UNP P10635
B	30	LYS	ALA	cloning artifact	UNP P10635
B	31	GLY	ALA	cloning artifact	UNP P10635
B	32	LYS	ARG	cloning artifact	UNP P10635
B	33	LEU	TYR	cloning artifact	UNP P10635
B	230	ASP	LEU	engineered mutation	UNP P10635
B	231	ARG	LEU	engineered mutation	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635
C	24	ALA	HIS	cloning artifact	UNP P10635
C	25	LYS	ARG	cloning artifact	UNP P10635
C	26	LYS	ARG	cloning artifact	UNP P10635
C	27	THR	GLN	cloning artifact	UNP P10635
C	28	SER	ARG	cloning artifact	UNP P10635
C	29	SER	TRP	cloning artifact	UNP P10635
C	30	LYS	ALA	cloning artifact	UNP P10635
C	31	GLY	ALA	cloning artifact	UNP P10635
C	32	LYS	ARG	cloning artifact	UNP P10635
C	33	LEU	TYR	cloning artifact	UNP P10635
C	230	ASP	LEU	engineered mutation	UNP P10635
C	231	ARG	LEU	engineered mutation	UNP P10635
C	498	HIS	-	expression tag	UNP P10635
C	499	HIS	-	expression tag	UNP P10635
C	500	HIS	-	expression tag	UNP P10635
C	501	HIS	-	expression tag	UNP P10635
D	24	ALA	HIS	cloning artifact	UNP P10635
D	25	LYS	ARG	cloning artifact	UNP P10635
D	26	LYS	ARG	cloning artifact	UNP P10635
D	27	THR	GLN	cloning artifact	UNP P10635
D	28	SER	ARG	cloning artifact	UNP P10635
D	29	SER	TRP	cloning artifact	UNP P10635
D	30	LYS	ALA	cloning artifact	UNP P10635
D	31	GLY	ALA	cloning artifact	UNP P10635
D	32	LYS	ARG	cloning artifact	UNP P10635
D	33	LEU	TYR	cloning artifact	UNP P10635
D	230	ASP	LEU	engineered mutation	UNP P10635
D	231	ARG	LEU	engineered mutation	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635

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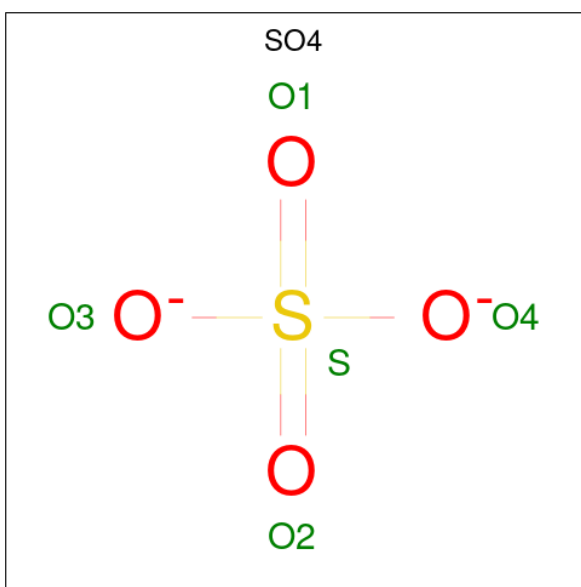
Chain	Residue	Modelled	Actual	Comment	Reference
D	501	HIS	-	expression tag	UNP P10635

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

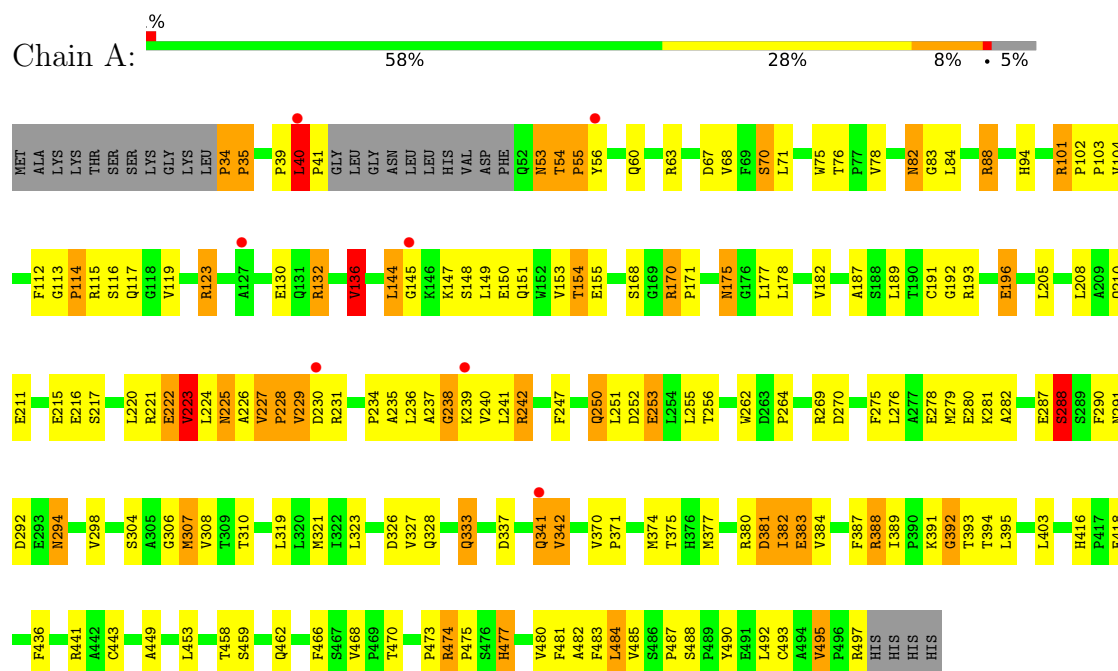
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	3	Total	O	0	0
			3	3		
4	C	2	Total	O	0	0
			2	2		
4	D	2	Total	O	0	0
			2	2		

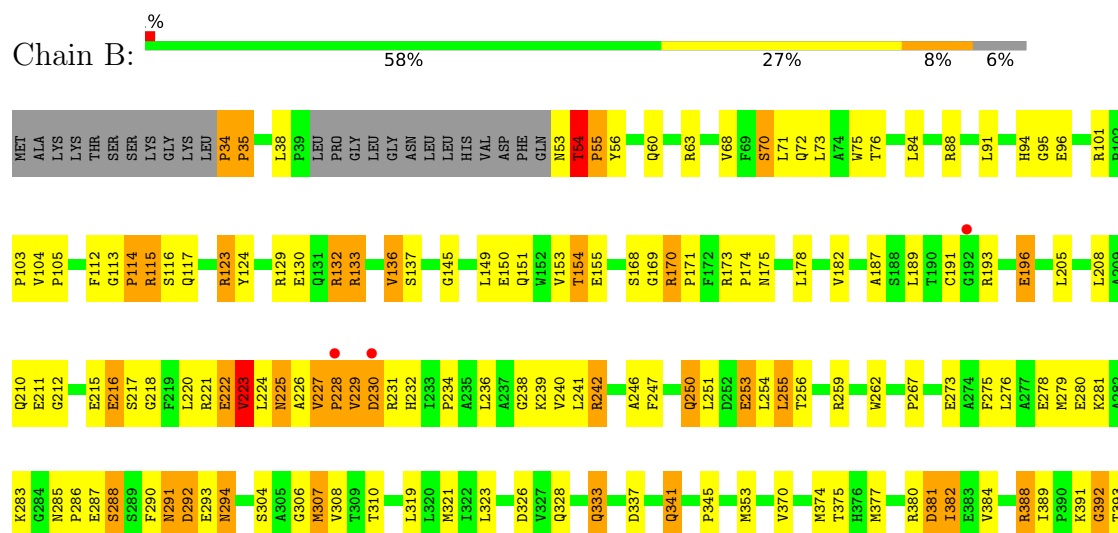
3 Residue-property plots

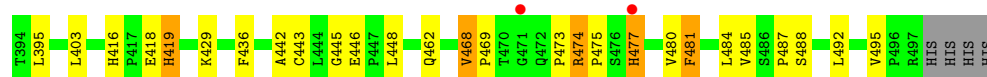
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome P450 2D6

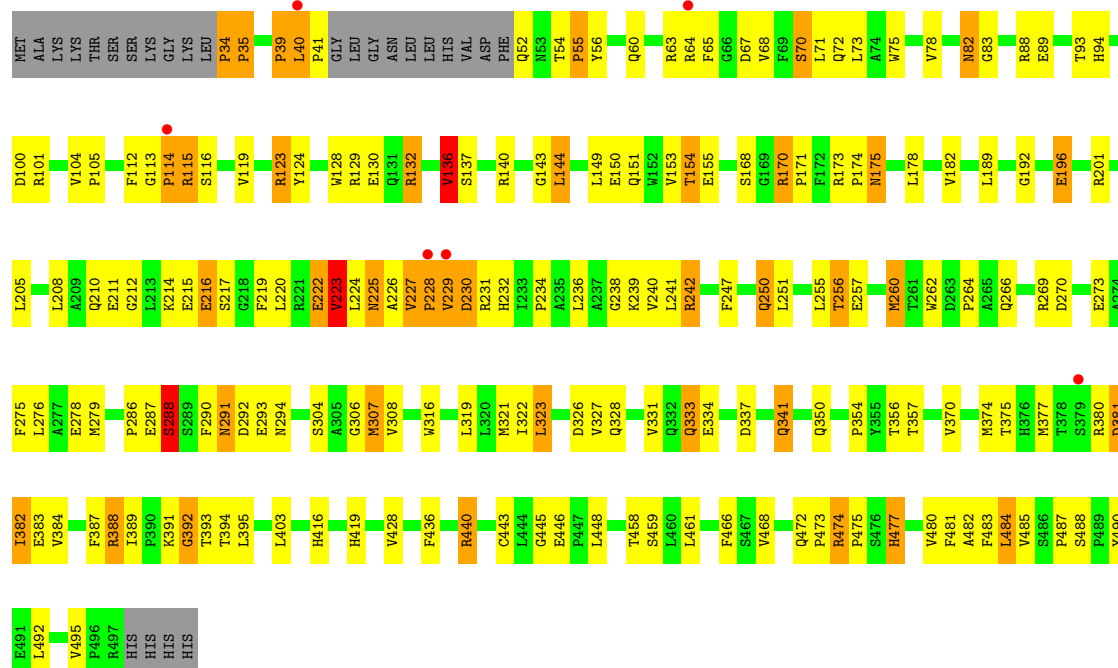


• Molecule 1: Cytochrome P450 2D6

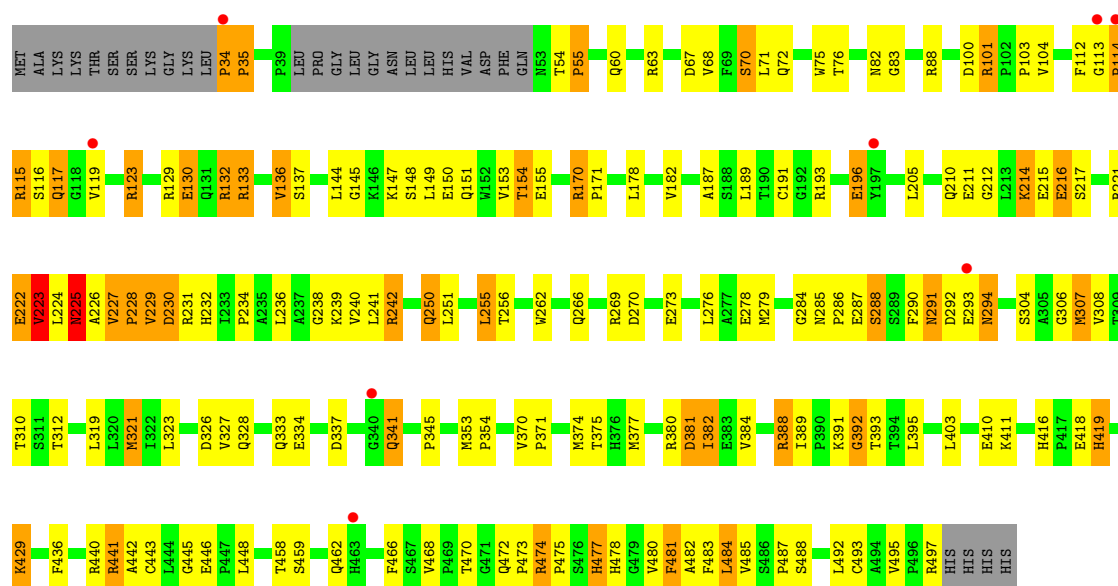




• Molecule 1: Cytochrome P450 2D6



• Molecule 1: Cytochrome P450 2D6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.07Å 155.50Å 95.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.00 – 3.00 106.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (106.00-3.00) 89.6 (106.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.230 , 0.286 0.230 , 0.282	Depositor DCC
R_{free} test set	1601 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14421	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.96	0/3664	1.19	18/4982 (0.4%)
1	B	0.87	0/3639	1.14	17/4947 (0.3%)
1	C	0.97	0/3664	1.20	16/4982 (0.3%)
1	D	0.90	3/3639 (0.1%)	1.15	21/4947 (0.4%)
All	All	0.93	3/14606 (0.0%)	1.17	72/19858 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	269	ARG	CZ-NH1	14.60	1.53	1.32
1	D	226	ALA	N-CA	5.25	1.52	1.45
1	D	269	ARG	CZ-NH2	5.20	1.40	1.33

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	PRO	CA-C-N	9.75	132.03	119.84
1	A	34	PRO	C-N-CA	9.75	132.03	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	34	PRO	CA-C-N	9.62	131.87	119.84
1	D	34	PRO	C-N-CA	9.62	131.87	119.84
1	C	34	PRO	CA-C-N	9.56	131.79	119.84
1	C	34	PRO	C-N-CA	9.56	131.79	119.84
1	B	34	PRO	CA-C-N	9.54	131.76	119.84
1	B	34	PRO	C-N-CA	9.54	131.76	119.84
1	A	389	ILE	CA-C-N	8.90	128.96	119.89
1	A	389	ILE	C-N-CA	8.90	128.96	119.89
1	D	227	VAL	CA-C-N	8.48	130.44	119.84
1	D	227	VAL	C-N-CA	8.48	130.44	119.84
1	D	227	VAL	N-CA-C	8.27	116.71	109.02
1	D	234	PRO	N-CA-CB	8.03	111.15	103.52
1	A	342	VAL	N-CA-C	7.95	119.22	111.67
1	A	227	VAL	CA-C-N	7.94	129.76	119.84
1	A	227	VAL	C-N-CA	7.94	129.76	119.84
1	C	119	VAL	N-CA-C	-7.76	105.49	111.62
1	C	234	PRO	N-CA-CB	7.73	110.86	103.52
1	B	234	PRO	N-CA-CB	7.55	111.03	103.48
1	C	82	ASN	N-CA-C	7.49	122.30	112.72
1	A	234	PRO	N-CA-CB	7.40	110.55	103.52
1	C	389	ILE	CA-C-N	7.27	127.30	119.89
1	C	389	ILE	C-N-CA	7.27	127.30	119.89
1	A	119	VAL	N-CA-C	-7.26	105.89	111.62
1	C	226	ALA	N-CA-C	7.23	119.90	110.43
1	A	236	LEU	N-CA-C	-7.21	103.42	111.71
1	B	84	LEU	N-CA-C	-7.09	103.63	111.36
1	D	472	GLN	N-CA-C	6.99	118.71	109.83
1	B	389	ILE	CA-C-N	6.80	126.83	119.89
1	B	389	ILE	C-N-CA	6.80	126.83	119.89
1	A	470	THR	N-CA-C	6.60	119.30	111.71
1	C	236	LEU	N-CA-C	-6.56	104.16	111.71
1	D	269	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	D	226	ALA	N-CA-C	6.44	118.86	110.43
1	B	227	VAL	CA-C-N	6.34	127.77	119.84
1	B	227	VAL	C-N-CA	6.34	127.77	119.84
1	C	227	VAL	CA-C-N	6.27	127.68	119.84
1	C	227	VAL	C-N-CA	6.27	127.68	119.84
1	A	483	PHE	N-CA-C	-6.11	105.92	113.19
1	D	119	VAL	N-CA-C	-6.07	106.83	111.62
1	A	226	ALA	N-CA-C	6.03	118.33	110.43
1	C	214	LYS	N-CA-C	-5.99	104.44	110.97
1	A	82	ASN	N-CA-C	5.97	120.37	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	PRO	CA-C-N	5.97	127.30	119.84
1	B	267	PRO	C-N-CA	5.97	127.30	119.84
1	A	84	LEU	N-CA-C	-5.96	104.78	111.28
1	C	483	PHE	N-CA-C	-5.96	105.86	113.01
1	D	353	MET	CA-C-N	5.92	125.13	118.97
1	D	353	MET	C-N-CA	5.92	125.13	118.97
1	B	226	ALA	N-CA-C	5.82	118.06	110.43
1	B	175	ASN	N-CA-C	5.78	117.26	111.07
1	D	389	ILE	CA-C-N	5.75	125.75	119.89
1	D	389	ILE	C-N-CA	5.75	125.75	119.89
1	A	175	ASN	N-CA-C	5.74	117.99	111.11
1	D	236	LEU	N-CA-C	-5.72	105.13	111.71
1	B	236	LEU	N-CA-C	-5.66	105.20	111.71
1	B	353	MET	CA-C-N	5.59	125.05	119.24
1	B	353	MET	C-N-CA	5.59	125.05	119.24
1	B	54	THR	N-CA-C	5.58	122.14	109.81
1	A	495	VAL	N-CA-C	5.50	113.89	107.89
1	D	481	PHE	N-CA-C	5.46	118.13	108.24
1	D	483	PHE	N-CA-C	-5.43	106.49	113.01
1	A	136	VAL	N-CA-CB	5.35	116.81	110.55
1	C	472	GLN	N-CA-C	5.22	116.41	109.93
1	D	214	LYS	N-CA-C	-5.21	105.52	111.14
1	C	136	VAL	N-CA-CB	5.17	117.58	110.54
1	C	175	ASN	N-CA-C	5.17	116.60	111.07
1	D	470	THR	N-CA-C	5.15	118.66	112.38
1	D	429	LYS	CA-C-N	5.09	125.08	119.89
1	D	429	LYS	C-N-CA	5.09	125.08	119.89
1	B	481	PHE	N-CA-C	5.07	117.39	108.56

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	GLY	Peptide
1	A	40	LEU	Peptide
1	A	53	ASN	Peptide
1	A	83	GLY	Peptide
1	B	113	GLY	Peptide
1	C	113	GLY	Peptide
1	C	83	GLY	Peptide
1	D	113	GLY	Peptide
1	D	83	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3569	0	3513	133	0
1	B	3545	0	3487	124	0
1	C	3569	0	3513	148	0
1	D	3545	0	3487	132	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
2	C	43	0	30	5	0
2	D	43	0	30	8	0
3	B	10	0	0	2	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	14421	0	14120	499	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (499) 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:B:227:VAL:HB	1:C:227:VAL:CB	1.75	1.16
1:B:227:VAL:CB	1:C:227:VAL:HB	1.75	1.15
1:A:60:GLN:NE2	1:B:60:GLN:HE21	1.49	1.11
1:C:60:GLN:HE21	1:D:60:GLN:NE2	1.53	1.05
1:A:60:GLN:NE2	1:B:60:GLN:NE2	2.06	1.03
1:A:60:GLN:HE21	1:B:60:GLN:NE2	1.58	1.00
1:A:287:GLU:O	1:A:288:SER:HB3	1.60	0.98
1:C:287:GLU:O	1:C:288:SER:HB3	1.61	0.97
1:C:40:LEU:H	1:C:41:PRO:HD3	1.29	0.97
1:C:115:ARG:NH2	1:C:286:PRO:O	2.01	0.94
1:A:229:VAL:HA	1:D:75:TRP:O	1.69	0.93
2:D:600:HEM:HBC2	2:D:600:HEM:HMC2	1.50	0.91
1:B:287:GLU:O	1:B:288:SER:HB3	1.70	0.90
1:A:227:VAL:CG2	1:A:228:PRO:HD2	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:VAL:CG2	1:D:228:PRO:HD2	2.04	0.88
1:D:34:PRO:HD3	1:D:388:ARG:NH1	1.90	0.87
1:A:227:VAL:HG13	1:D:76:THR:HG23	1.56	0.87
1:B:227:VAL:CG2	1:B:228:PRO:HD2	2.04	0.86
1:D:287:GLU:O	1:D:288:SER:HB3	1.74	0.85
1:C:227:VAL:CG2	1:C:228:PRO:HD2	2.06	0.85
1:A:60:GLN:HE21	1:B:60:GLN:HE21	0.85	0.84
1:A:227:VAL:CG1	1:D:76:THR:HG23	2.07	0.84
1:C:473:PRO:O	1:C:474:ARG:HB3	1.78	0.84
1:A:227:VAL:HG23	1:A:228:PRO:HD2	1.60	0.84
1:D:321:MET:HE3	1:D:328:GLN:HA	1.61	0.82
1:C:227:VAL:HG23	1:C:228:PRO:HD2	1.59	0.82
1:B:227:VAL:HG23	1:B:228:PRO:HD2	1.59	0.82
1:C:39:PRO:HB2	1:C:41:PRO:HD3	1.62	0.81
1:D:211:GLU:O	1:D:215:GLU:HG3	1.79	0.81
1:B:321:MET:HE3	1:B:328:GLN:HA	1.62	0.81
1:C:34:PRO:HD3	1:C:388:ARG:NH1	1.97	0.80
1:C:40:LEU:H	1:C:41:PRO:CD	1.94	0.80
1:A:76:THR:HG23	1:D:227:VAL:CG1	2.12	0.80
1:D:473:PRO:O	1:D:474:ARG:HB3	1.81	0.80
1:D:227:VAL:HG23	1:D:228:PRO:HD2	1.62	0.79
1:A:39:PRO:HB2	1:A:41:PRO:HD3	1.63	0.79
1:C:321:MET:HE3	1:C:328:GLN:HA	1.64	0.79
1:A:76:THR:HG23	1:D:227:VAL:HG13	1.66	0.78
2:D:600:HEM:HBC2	2:D:600:HEM:CMC	2.13	0.78
1:A:34:PRO:HD3	1:A:388:ARG:NH1	2.00	0.77
1:B:221:ARG:NH2	1:C:41:PRO:O	2.18	0.77
1:C:137:SER:HA	1:C:140:ARG:NH2	2.00	0.76
1:A:75:TRP:O	1:D:229:VAL:HA	1.86	0.75
1:B:211:GLU:O	1:B:215:GLU:HG3	1.86	0.75
2:B:600:HEM:HBC2	2:B:600:HEM:HMC2	1.68	0.74
2:B:600:HEM:HBC2	2:B:600:HEM:CMC	2.18	0.74
1:B:34:PRO:HD3	1:B:388:ARG:NH1	2.02	0.74
1:C:211:GLU:O	1:C:215:GLU:HG3	1.85	0.74
1:A:473:PRO:O	1:A:474:ARG:HB3	1.86	0.73
1:B:321:MET:CE	1:B:328:GLN:HA	2.17	0.73
1:D:229:VAL:O	1:D:231:ARG:N	2.17	0.73
1:B:473:PRO:O	1:B:474:ARG:HB3	1.90	0.72
1:C:40:LEU:N	1:C:41:PRO:HD3	2.04	0.71
1:B:129:ARG:NH1	3:B:2000:SO4:O3	2.23	0.71
1:C:56:TYR:O	1:D:60:GLN:NE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:GLU:HA	1:D:196:GLU:OE2	1.88	0.71
1:B:133:ARG:NH2	3:B:2000:SO4:O2	2.23	0.71
1:A:278:GLU:HG2	1:A:290:PHE:CZ	2.25	0.71
1:C:115:ARG:HE	1:C:287:GLU:HA	1.55	0.71
1:C:143:GLY:C	1:C:144:LEU:HG	2.14	0.71
2:A:600:HEM:HMC2	2:A:600:HEM:HBC2	1.73	0.71
1:A:306:GLY:HA2	2:A:600:HEM:C2C	2.25	0.70
1:D:133:ARG:HG2	1:D:133:ARG:HH11	1.57	0.70
1:D:388:ARG:HH11	1:D:388:ARG:HG2	1.55	0.70
1:A:321:MET:HE3	1:A:328:GLN:HA	1.71	0.70
1:A:388:ARG:HH11	1:A:388:ARG:HG2	1.57	0.70
2:C:600:HEM:HBC2	2:C:600:HEM:HMC2	1.73	0.70
1:A:211:GLU:O	1:A:215:GLU:HG3	1.91	0.69
1:B:278:GLU:HG2	1:B:290:PHE:CZ	2.27	0.69
1:D:117:GLN:O	1:D:294:ASN:ND2	2.20	0.69
1:C:278:GLU:HG2	1:C:290:PHE:CZ	2.28	0.69
1:B:388:ARG:HG2	1:B:388:ARG:HH11	1.57	0.68
1:D:34:PRO:HD3	1:D:388:ARG:HH12	1.57	0.68
1:A:151:GLN:O	1:A:155:GLU:HG2	1.92	0.68
1:D:321:MET:CE	1:D:328:GLN:HA	2.23	0.68
1:C:229:VAL:O	1:C:231:ARG:N	2.21	0.68
1:A:196:GLU:OE2	1:A:196:GLU:HA	1.93	0.68
1:A:227:VAL:CG1	1:D:76:THR:CG2	2.72	0.68
1:C:229:VAL:C	1:C:231:ARG:H	2.02	0.68
1:C:388:ARG:HG2	1:C:388:ARG:HH11	1.58	0.67
1:D:104:VAL:HG12	1:D:223:VAL:HG21	1.77	0.67
1:A:56:TYR:HB3	1:B:60:GLN:HG3	1.76	0.66
1:A:229:VAL:C	1:A:231:ARG:H	2.03	0.66
1:C:151:GLN:O	1:C:155:GLU:HG2	1.95	0.66
1:C:205:LEU:HD12	1:C:250:GLN:NE2	2.10	0.66
1:A:54:THR:H	1:A:55:PRO:HD3	1.61	0.66
1:A:76:THR:CG2	1:D:227:VAL:HG11	2.25	0.66
1:D:381:ASP:O	1:D:382:ILE:HD13	1.96	0.66
1:B:306:GLY:HA2	2:B:600:HEM:C2C	2.29	0.66
1:D:217:SER:O	1:D:221:ARG:HG2	1.94	0.66
1:B:170:ARG:HD2	1:B:171:PRO:HD2	1.76	0.66
1:C:321:MET:CE	1:C:328:GLN:HA	2.26	0.65
1:D:34:PRO:CD	1:D:388:ARG:HH12	2.09	0.65
1:B:104:VAL:HG12	1:B:223:VAL:HG21	1.78	0.65
1:A:227:VAL:HG11	1:D:76:THR:CG2	2.26	0.65
1:B:205:LEU:HD12	1:B:250:GLN:NE2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:HA	1:B:279:MET:HE3	1.79	0.65
1:C:39:PRO:CB	1:C:41:PRO:HD3	2.27	0.64
1:C:34:PRO:HD3	1:C:388:ARG:HH12	1.59	0.64
1:C:64:ARG:CZ	1:D:478:HIS:CE1	2.81	0.64
1:B:178:LEU:O	1:B:182:VAL:HG23	1.98	0.64
1:A:34:PRO:HD3	1:A:388:ARG:HH12	1.61	0.64
1:B:96:GLU:HG3	1:B:124:TYR:OH	1.98	0.64
1:D:278:GLU:HG2	1:D:290:PHE:CZ	2.35	0.62
1:A:76:THR:CG2	1:D:227:VAL:CG1	2.77	0.62
1:A:436:PHE:HB3	1:A:443:CYS:HB3	1.80	0.62
1:D:306:GLY:HA2	2:D:600:HEM:C2C	2.33	0.62
1:A:229:VAL:O	1:A:231:ARG:N	2.25	0.62
1:C:477:HIS:H	1:C:477:HIS:CD2	2.16	0.62
1:D:149:LEU:O	1:D:153:VAL:HG23	2.00	0.62
1:B:114:PRO:HB2	1:B:115:ARG:CZ	2.30	0.62
1:B:278:GLU:OE1	1:B:281:LYS:NZ	2.24	0.62
1:C:276:LEU:HA	1:C:279:MET:HE3	1.80	0.62
1:A:222:GLU:HB3	1:D:75:TRP:CZ2	2.34	0.61
1:B:34:PRO:HD3	1:B:388:ARG:HH12	1.65	0.61
1:D:477:HIS:CD2	1:D:477:HIS:H	2.16	0.61
1:A:104:VAL:HG12	1:A:223:VAL:HG21	1.81	0.61
1:B:227:VAL:CG2	1:B:228:PRO:CD	2.76	0.61
1:C:377:MET:HA	1:C:393:THR:O	2.00	0.61
1:C:306:GLY:HA2	2:C:600:HEM:C2C	2.35	0.61
1:A:60:GLN:HG3	1:B:56:TYR:HB3	1.82	0.61
1:C:64:ARG:HH22	1:D:478:HIS:CG	2.19	0.61
1:C:60:GLN:NE2	1:D:60:GLN:NE2	2.38	0.61
1:C:60:GLN:HE21	1:D:60:GLN:HE21	1.47	0.61
1:C:64:ARG:NH2	1:D:478:HIS:CG	2.69	0.61
1:C:104:VAL:HG12	1:C:223:VAL:HG21	1.83	0.61
1:C:256:THR:O	1:C:260:MET:HE3	2.00	0.61
1:A:189:LEU:O	1:A:270:ASP:HB2	2.01	0.60
1:A:276:LEU:HA	1:A:279:MET:HE3	1.82	0.60
2:A:600:HEM:HBC2	2:A:600:HEM:CMC	2.31	0.60
1:B:279:MET:HG3	1:B:290:PHE:O	2.02	0.60
1:B:229:VAL:C	1:B:231:ARG:H	2.10	0.59
1:C:223:VAL:O	1:C:223:VAL:HG13	2.02	0.59
1:A:321:MET:CE	1:A:328:GLN:HA	2.33	0.59
1:C:39:PRO:HB2	1:C:41:PRO:CD	2.32	0.59
1:C:227:VAL:CG2	1:C:228:PRO:CD	2.79	0.59
1:C:149:LEU:O	1:C:153:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:PRO:CD	1:D:388:ARG:NH1	2.64	0.58
1:A:192:GLY:CA	1:A:269:ARG:HH22	2.17	0.57
1:D:205:LEU:HD12	1:D:250:GLN:NE2	2.18	0.57
1:B:227:VAL:HG22	1:B:228:PRO:CD	2.34	0.57
1:C:380:ARG:HA	1:C:391:LYS:HG3	1.86	0.57
1:B:208:LEU:HB3	1:B:247:PHE:HB2	1.86	0.57
1:C:56:TYR:HB3	1:D:60:GLN:CD	2.29	0.57
1:A:205:LEU:HD12	1:A:250:GLN:NE2	2.20	0.57
1:B:132:ARG:O	1:B:136:VAL:HG13	2.05	0.57
2:C:600:HEM:HBC2	2:C:600:HEM:CMC	2.35	0.57
1:D:380:ARG:HG2	1:D:380:ARG:HH11	1.71	0.56
1:C:436:PHE:HB3	1:C:443:CYS:HB3	1.87	0.56
1:D:229:VAL:C	1:D:231:ARG:H	2.09	0.56
1:A:223:VAL:HG13	1:A:223:VAL:O	2.04	0.56
1:C:178:LEU:O	1:C:182:VAL:HG23	2.05	0.56
1:D:279:MET:HG3	1:D:290:PHE:O	2.06	0.56
1:B:436:PHE:HB3	1:B:443:CYS:HB3	1.88	0.56
1:A:374:MET:SD	1:A:375:THR:HG22	2.45	0.56
1:A:443:CYS:HB2	2:A:600:HEM:NA	2.21	0.56
1:A:238:GLY:O	1:A:240:VAL:N	2.39	0.56
1:C:60:GLN:HE21	1:D:60:GLN:HE22	1.46	0.56
1:B:477:HIS:CD2	1:B:477:HIS:H	2.23	0.55
1:D:276:LEU:HA	1:D:279:MET:HE3	1.88	0.55
1:B:377:MET:HE3	1:B:392:GLY:HA2	1.89	0.55
1:B:151:GLN:O	1:B:155:GLU:HG2	2.07	0.55
1:C:64:ARG:NH1	1:D:478:HIS:ND1	2.55	0.55
1:A:477:HIS:H	1:A:477:HIS:CD2	2.24	0.55
1:C:196:GLU:OE2	1:C:196:GLU:HA	2.07	0.55
1:B:321:MET:HE3	1:B:328:GLN:CA	2.34	0.55
1:A:103:PRO:HD3	1:A:123:ARG:HH21	1.70	0.54
1:B:377:MET:HA	1:B:393:THR:O	2.07	0.54
1:C:227:VAL:HG22	1:C:228:PRO:CD	2.37	0.54
1:C:443:CYS:HB2	2:C:600:HEM:NA	2.21	0.54
1:A:377:MET:HA	1:A:393:THR:O	2.07	0.54
1:B:229:VAL:O	1:B:231:ARG:N	2.28	0.54
1:A:170:ARG:HD2	1:A:171:PRO:HD2	1.89	0.54
1:C:251:LEU:O	1:C:255:LEU:HG	2.07	0.54
1:D:223:VAL:HG13	1:D:223:VAL:O	2.08	0.54
1:B:103:PRO:HD3	1:B:123:ARG:HH21	1.72	0.54
1:D:251:LEU:O	1:D:255:LEU:HG	2.08	0.54
1:B:381:ASP:O	1:B:382:ILE:HD13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ARG:HD2	1:C:171:PRO:HD2	1.90	0.53
1:D:227:VAL:HG22	1:D:228:PRO:HD2	1.88	0.53
1:A:227:VAL:HG22	1:A:228:PRO:HD2	1.88	0.53
1:B:196:GLU:OE2	1:B:196:GLU:HA	2.07	0.53
1:D:212:GLY:O	1:D:216:GLU:HG2	2.07	0.53
1:B:212:GLY:O	1:B:216:GLU:HG2	2.09	0.53
1:D:132:ARG:NH1	1:D:441:ARG:HA	2.23	0.53
1:C:212:GLY:O	1:C:216:GLU:HG2	2.08	0.53
1:D:377:MET:HA	1:D:393:THR:O	2.08	0.53
1:D:133:ARG:HG2	1:D:133:ARG:NH1	2.24	0.53
1:B:149:LEU:O	1:B:153:VAL:HG23	2.08	0.53
1:B:381:ASP:OD2	1:B:381:ASP:N	2.41	0.53
1:D:170:ARG:HD2	1:D:171:PRO:HD2	1.90	0.53
1:A:279:MET:HG3	1:A:290:PHE:O	2.10	0.52
1:B:35:PRO:O	1:B:70:SER:HB2	2.09	0.52
1:D:319:LEU:HD22	1:D:487:PRO:HB3	1.91	0.52
1:A:462:GLN:O	1:A:497:ARG:NH1	2.42	0.52
1:C:381:ASP:O	1:C:382:ILE:HD13	2.08	0.52
1:D:436:PHE:HB3	1:D:443:CYS:HB3	1.90	0.52
1:B:223:VAL:HG13	1:B:223:VAL:O	2.09	0.52
1:A:383:GLU:HA	1:A:387:PHE:O	2.09	0.52
1:D:388:ARG:NH1	1:D:388:ARG:HG2	2.24	0.52
1:A:40:LEU:N	1:A:41:PRO:HD3	2.25	0.52
1:D:114:PRO:HB2	1:D:115:ARG:HG2	1.90	0.52
1:D:151:GLN:O	1:D:155:GLU:HG2	2.10	0.52
1:D:170:ARG:CD	1:D:171:PRO:HD2	2.40	0.52
1:A:380:ARG:HA	1:A:391:LYS:HG3	1.92	0.51
1:A:381:ASP:O	1:A:382:ILE:HD13	2.10	0.51
2:D:600:HEM:CMB	2:D:600:HEM:HBB2	2.41	0.51
1:A:377:MET:HE3	1:A:392:GLY:HA2	1.91	0.51
1:D:481:PHE:CG	1:D:481:PHE:O	2.62	0.51
1:A:178:LEU:O	1:A:182:VAL:HG23	2.10	0.51
1:B:168:SER:C	1:B:170:ARG:H	2.19	0.51
1:D:443:CYS:HB2	2:D:600:HEM:NA	2.26	0.51
1:A:227:VAL:HG22	1:A:228:PRO:CD	2.39	0.51
1:C:64:ARG:NH2	1:D:478:HIS:CD2	2.78	0.51
1:A:227:VAL:HG11	1:D:76:THR:HG21	1.92	0.51
1:D:35:PRO:O	1:D:70:SER:HB2	2.10	0.51
1:D:129:ARG:O	1:D:133:ARG:HB2	2.10	0.51
1:A:41:PRO:C	1:D:221:ARG:HH21	2.18	0.50
1:C:64:ARG:CZ	1:D:478:HIS:ND1	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:PRO:HD3	1:D:462:GLN:HE22	1.77	0.50
1:A:319:LEU:HD22	1:A:487:PRO:HB3	1.93	0.50
1:A:341:GLN:HE21	1:A:341:GLN:HA	1.77	0.50
1:B:227:VAL:CG2	1:C:227:VAL:CG2	2.89	0.50
1:C:377:MET:HE3	1:C:392:GLY:HA2	1.93	0.50
1:A:307:MET:HG2	1:A:308:VAL:N	2.27	0.50
1:D:308:VAL:O	1:D:312:THR:OG1	2.27	0.50
1:A:388:ARG:NH1	1:A:388:ARG:HG2	2.25	0.50
1:D:307:MET:HG2	1:D:308:VAL:N	2.25	0.50
1:A:34:PRO:CD	1:A:388:ARG:HH12	2.25	0.50
1:D:238:GLY:O	1:D:240:VAL:N	2.45	0.50
1:A:227:VAL:CG2	1:A:228:PRO:CD	2.82	0.50
1:B:416:HIS:HB3	1:B:419:HIS:CE1	2.47	0.49
1:C:35:PRO:O	1:C:70:SER:HB2	2.12	0.49
1:D:189:LEU:O	1:D:270:ASP:HB2	2.11	0.49
1:A:208:LEU:HB3	1:A:247:PHE:HB2	1.94	0.49
1:D:230:ASP:C	1:D:232:HIS:H	2.21	0.49
1:C:341:GLN:HA	1:C:341:GLN:HE21	1.77	0.49
1:C:388:ARG:NH1	1:C:388:ARG:HG2	2.26	0.49
1:B:374:MET:SD	1:B:375:THR:HG22	2.52	0.49
1:C:189:LEU:O	1:C:270:ASP:HB2	2.13	0.49
1:C:241:LEU:O	1:C:242:ARG:C	2.56	0.49
1:C:279:MET:HG3	1:C:290:PHE:O	2.13	0.49
1:D:381:ASP:OD2	1:D:381:ASP:N	2.46	0.49
1:A:40:LEU:H	1:A:41:PRO:CD	2.25	0.49
1:B:253:GLU:HG2	1:B:254:LEU:N	2.27	0.49
1:C:275:PHE:CD2	1:C:279:MET:HE2	2.48	0.49
1:C:333:GLN:HA	1:C:333:GLN:NE2	2.28	0.49
1:D:227:VAL:HG22	1:D:228:PRO:CD	2.42	0.49
1:C:114:PRO:HB2	1:C:115:ARG:HD3	1.94	0.49
1:B:319:LEU:HD22	1:B:487:PRO:HB3	1.94	0.48
1:C:56:TYR:HB3	1:D:60:GLN:CG	2.43	0.48
1:D:149:LEU:HD13	1:D:448:LEU:HD13	1.94	0.48
1:A:76:THR:HG21	1:D:227:VAL:HG11	1.95	0.48
1:A:371:PRO:HG2	1:A:481:PHE:HE1	1.78	0.48
1:C:56:TYR:HB3	1:D:60:GLN:HG3	1.95	0.48
1:C:334:GLU:OE1	1:C:354:PRO:HD2	2.13	0.48
1:C:78:VAL:HG22	1:C:394:THR:HB	1.94	0.48
1:C:137:SER:HA	1:C:140:ARG:HH21	1.77	0.48
1:C:383:GLU:HA	1:C:387:PHE:O	2.12	0.48
1:D:334:GLU:OE1	1:D:354:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:O	1:B:323:LEU:HB2	2.13	0.48
1:B:94:HIS:ND1	1:B:382:ILE:HD12	2.29	0.48
1:B:208:LEU:HD22	1:B:246:ALA:HB3	1.96	0.48
1:C:374:MET:SD	1:C:375:THR:HG22	2.53	0.48
1:C:481:PHE:CG	1:C:481:PHE:O	2.64	0.48
1:A:333:GLN:NE2	1:A:333:GLN:HA	2.28	0.48
1:B:443:CYS:HB2	2:B:600:HEM:NA	2.28	0.48
1:C:192:GLY:HA2	1:C:269:ARG:HH12	1.79	0.48
1:D:55:PRO:HD3	1:D:481:PHE:CE2	2.49	0.48
1:A:319:LEU:O	1:A:323:LEU:HB2	2.14	0.48
1:B:76:THR:HG22	1:C:230:ASP:N	2.28	0.48
1:C:140:ARG:HB3	1:C:140:ARG:CZ	2.44	0.48
1:A:75:TRP:CZ2	1:D:222:GLU:HB3	2.49	0.47
1:B:445:GLY:O	1:B:446:GLU:C	2.57	0.47
1:C:238:GLY:O	1:C:240:VAL:N	2.47	0.47
1:C:123:ARG:HH11	1:C:123:ARG:HB3	1.79	0.47
1:C:132:ARG:O	1:C:136:VAL:HG13	2.13	0.47
1:C:238:GLY:C	1:C:240:VAL:H	2.22	0.47
1:D:374:MET:SD	1:D:375:THR:HG22	2.54	0.47
1:A:123:ARG:HB3	1:A:123:ARG:HH11	1.79	0.47
1:A:381:ASP:OD2	1:A:381:ASP:N	2.46	0.47
1:C:229:VAL:C	1:C:231:ARG:N	2.70	0.47
1:D:72:GLN:HE22	1:D:225:ASN:HB3	1.80	0.47
1:D:123:ARG:HH11	1:D:123:ARG:HB3	1.78	0.47
1:A:321:MET:HE1	1:A:327:VAL:HG12	1.95	0.47
1:B:54:THR:H	1:B:55:PRO:HD3	1.80	0.47
1:C:341:GLN:HE21	1:C:341:GLN:CA	2.25	0.47
1:A:482:ALA:C	1:A:484:LEU:N	2.73	0.47
1:B:217:SER:HA	1:B:220:LEU:HB2	1.97	0.47
1:C:262:TRP:HD1	1:C:273:GLU:OE2	1.97	0.47
1:C:319:LEU:HD22	1:C:487:PRO:HB3	1.97	0.47
1:D:443:CYS:HB2	2:D:600:HEM:C4A	2.50	0.47
1:A:94:HIS:ND1	1:A:382:ILE:HD12	2.29	0.47
1:B:218:GLY:HA2	1:B:221:ARG:CZ	2.45	0.47
1:B:345:PRO:HD3	1:B:462:GLN:HE22	1.80	0.47
1:C:319:LEU:HB2	1:C:490:TYR:CE2	2.50	0.46
1:C:350:GLN:NE2	1:C:357:THR:OG1	2.48	0.46
1:A:115:ARG:H	1:A:115:ARG:HG2	1.57	0.46
1:B:291:ASN:HD22	1:B:293:GLU:HB2	1.80	0.46
1:D:103:PRO:HD3	1:D:123:ARG:HH21	1.80	0.46
1:D:114:PRO:HB2	1:D:115:ARG:CZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ARG:CD	1:C:171:PRO:HD2	2.45	0.46
1:C:291:ASN:HD22	1:C:293:GLU:HB2	1.80	0.46
1:D:445:GLY:O	1:D:446:GLU:C	2.58	0.46
1:B:280:GLU:O	1:B:281:LYS:C	2.59	0.46
1:C:94:HIS:ND1	1:C:382:ILE:HD12	2.30	0.46
1:C:321:MET:HE1	1:C:327:VAL:HG12	1.98	0.46
1:D:380:ARG:HA	1:D:391:LYS:HG3	1.96	0.46
1:A:238:GLY:C	1:A:240:VAL:H	2.23	0.46
1:C:208:LEU:HB3	1:C:247:PHE:HB2	1.96	0.46
1:D:321:MET:HE3	1:D:328:GLN:CA	2.38	0.46
1:A:35:PRO:O	1:A:70:SER:HB2	2.16	0.46
1:A:333:GLN:HA	1:A:333:GLN:HE21	1.80	0.46
1:B:149:LEU:HD13	1:B:448:LEU:HD13	1.98	0.46
1:B:388:ARG:NH1	1:B:388:ARG:HG2	2.26	0.46
1:C:150:GLU:O	1:C:154:THR:OG1	2.32	0.46
1:C:316:TRP:CD2	1:C:487:PRO:HG3	2.50	0.46
1:C:482:ALA:C	1:C:484:LEU:N	2.72	0.46
1:D:341:GLN:HE21	1:D:341:GLN:HA	1.81	0.46
1:B:227:VAL:CG2	1:C:227:VAL:HG21	2.46	0.46
1:C:149:LEU:HD13	1:C:448:LEU:HD13	1.97	0.46
1:C:482:ALA:C	1:C:484:LEU:H	2.24	0.46
1:A:458:THR:O	1:A:459:SER:C	2.58	0.45
1:B:129:ARG:O	1:B:133:ARG:HB2	2.15	0.45
1:A:229:VAL:C	1:A:231:ARG:N	2.72	0.45
1:C:89:GLU:O	1:C:93:THR:HB	2.16	0.45
1:C:319:LEU:O	1:C:323:LEU:HB2	2.16	0.45
1:B:250:GLN:HE21	1:B:250:GLN:HB3	1.59	0.45
1:A:175:ASN:ND2	1:A:175:ASN:H	2.15	0.45
1:A:262:TRP:CZ2	1:A:264:PRO:HA	2.51	0.45
1:A:416:HIS:NE2	1:A:418:GLU:HB2	2.31	0.45
1:C:34:PRO:CD	1:C:388:ARG:HH12	2.26	0.45
1:A:251:LEU:O	1:A:253:GLU:N	2.49	0.45
2:C:600:HEM:HBB2	2:C:600:HEM:HMB2	1.97	0.45
1:D:100:ASP:OD1	1:D:377:MET:HE2	2.16	0.45
1:D:291:ASN:HD22	1:D:293:GLU:HB2	1.82	0.45
1:B:230:ASP:C	1:B:232:HIS:H	2.25	0.45
1:D:474:ARG:HA	1:D:475:PRO:HD3	1.81	0.45
1:A:40:LEU:HD23	1:A:40:LEU:O	2.16	0.45
1:A:132:ARG:O	1:A:136:VAL:HG13	2.17	0.45
1:A:416:HIS:CD2	1:A:418:GLU:HB2	2.52	0.45
1:C:381:ASP:OD2	1:C:381:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:GLY:C	1:D:240:VAL:H	2.24	0.45
1:B:259:ARG:HE	1:B:276:LEU:HD22	1.82	0.45
1:C:458:THR:O	1:C:459:SER:C	2.60	0.45
1:D:150:GLU:O	1:D:154:THR:OG1	2.34	0.45
1:B:227:VAL:HG21	1:C:227:VAL:CG2	2.47	0.45
1:B:333:GLN:HA	1:B:333:GLN:NE2	2.32	0.45
1:B:443:CYS:HB2	2:B:600:HEM:C4A	2.52	0.45
1:C:54:THR:N	1:C:55:PRO:HD3	2.32	0.45
1:C:220:LEU:HD23	1:C:220:LEU:HA	1.85	0.45
1:B:218:GLY:HA2	1:B:221:ARG:NH1	2.32	0.44
1:B:251:LEU:O	1:B:255:LEU:HG	2.16	0.44
1:C:307:MET:HG2	1:C:308:VAL:N	2.32	0.44
1:A:88:ARG:HB3	1:A:88:ARG:HH11	1.81	0.44
1:A:55:PRO:HD3	1:A:481:PHE:CE2	2.52	0.44
1:B:75:TRP:HH2	1:C:219:PHE:O	2.00	0.44
1:C:222:GLU:C	1:C:224:LEU:H	2.25	0.44
1:C:217:SER:HA	1:C:220:LEU:HB2	1.99	0.44
1:D:321:MET:HE1	1:D:327:VAL:HG12	1.99	0.44
1:A:187:ALA:O	1:A:191:CYS:HB2	2.17	0.44
1:B:34:PRO:CD	1:B:388:ARG:HH12	2.30	0.44
1:B:72:GLN:O	1:B:73:LEU:C	2.61	0.44
1:C:474:ARG:HA	1:C:475:PRO:HD3	1.88	0.44
1:B:187:ALA:O	1:B:191:CYS:N	2.48	0.44
1:B:287:GLU:O	1:B:288:SER:CB	2.50	0.44
1:D:67:ASP:O	1:D:82:ASN:HB2	2.18	0.44
1:D:178:LEU:O	1:D:182:VAL:HG23	2.17	0.44
1:D:416:HIS:HB3	1:D:419:HIS:CE1	2.52	0.44
1:C:257:GLU:HA	1:C:260:MET:HG2	2.00	0.44
1:A:150:GLU:O	1:A:154:THR:OG1	2.36	0.44
1:B:123:ARG:HH11	1:B:123:ARG:HB3	1.83	0.44
1:B:221:ARG:O	1:B:224:LEU:HG	2.18	0.44
1:B:262:TRP:HD1	1:B:273:GLU:CD	2.26	0.44
1:D:114:PRO:HB2	1:D:115:ARG:NH1	2.32	0.44
1:A:474:ARG:HA	1:A:475:PRO:HD3	1.91	0.43
1:B:105:PRO:HD3	1:C:75:TRP:CZ3	2.53	0.43
1:B:418:GLU:O	1:B:419:HIS:C	2.60	0.43
1:C:72:GLN:O	1:C:73:LEU:C	2.61	0.43
1:D:101:ARG:NH2	1:D:374:MET:HG3	2.33	0.43
1:A:241:LEU:O	1:A:242:ARG:C	2.60	0.43
1:A:251:LEU:O	1:A:255:LEU:HG	2.17	0.43
1:A:294:ASN:O	1:A:298:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:PHE:HA	1:D:493:CYS:O	2.18	0.43
1:A:114:PRO:HB2	1:A:115:ARG:NH1	2.33	0.43
1:B:114:PRO:HB2	1:B:115:ARG:NH2	2.32	0.43
1:C:333:GLN:HA	1:C:333:GLN:HE21	1.83	0.43
1:A:101:ARG:HA	1:A:102:PRO:HD3	1.91	0.43
1:B:380:ARG:HA	1:B:391:LYS:HG3	2.00	0.43
1:D:482:ALA:C	1:D:484:LEU:H	2.27	0.43
1:A:482:ALA:C	1:A:484:LEU:H	2.25	0.43
1:A:251:LEU:C	1:A:253:GLU:N	2.76	0.43
1:B:241:LEU:O	1:B:242:ARG:C	2.60	0.43
1:D:380:ARG:O	1:D:382:ILE:HG12	2.19	0.43
1:A:149:LEU:HD21	1:A:189:LEU:HD13	2.01	0.43
1:B:150:GLU:O	1:B:154:THR:OG1	2.36	0.43
1:D:132:ARG:NH2	1:D:442:ALA:O	2.27	0.43
1:B:132:ARG:NH2	1:B:442:ALA:O	2.36	0.43
1:B:149:LEU:HD21	1:B:189:LEU:HD13	2.01	0.43
1:B:323:LEU:HD13	1:B:475:PRO:HD2	2.01	0.43
1:C:461:LEU:HD23	1:C:466:PHE:CE1	2.54	0.43
2:B:600:HEM:CMB	2:B:600:HEM:HBB2	2.48	0.43
1:D:345:PRO:HD3	1:D:462:GLN:NE2	2.34	0.43
1:D:227:VAL:CG2	1:D:228:PRO:CD	2.85	0.43
1:D:377:MET:HE3	1:D:392:GLY:HA2	1.99	0.43
1:B:170:ARG:CD	1:B:171:PRO:HD2	2.46	0.42
1:B:227:VAL:HB	1:C:227:VAL:HB	0.79	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.94	0.42
1:B:182:VAL:HG11	1:B:310:THR:HB	2.01	0.42
1:B:280:GLU:O	1:B:283:LYS:HG3	2.19	0.42
1:D:323:LEU:HD12	1:D:323:LEU:HA	1.86	0.42
1:A:221:ARG:O	1:A:224:LEU:HG	2.19	0.42
1:A:275:PHE:CD2	1:A:279:MET:HE2	2.54	0.42
1:C:149:LEU:HD21	1:C:189:LEU:HD13	2.01	0.42
1:C:321:MET:HE3	1:C:328:GLN:CA	2.43	0.42
1:A:40:LEU:N	1:A:41:PRO:CD	2.81	0.42
1:A:371:PRO:HG2	1:A:481:PHE:CE1	2.54	0.42
1:C:173:ARG:HA	1:C:174:PRO:HD3	1.86	0.42
1:D:241:LEU:O	1:D:242:ARG:C	2.62	0.42
1:B:294:ASN:HD22	1:B:294:ASN:HA	1.54	0.42
1:C:230:ASP:C	1:C:232:HIS:H	2.27	0.42
1:C:445:GLY:O	1:C:446:GLU:C	2.61	0.42
1:A:67:ASP:O	1:A:82:ASN:HB2	2.19	0.42
1:A:78:VAL:HG22	1:A:394:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PRO:CD	1:C:75:TRP:CZ3	3.03	0.42
1:B:238:GLY:C	1:B:240:VAL:H	2.28	0.42
1:A:117:GLN:O	1:A:294:ASN:ND2	2.33	0.42
1:A:235:ALA:C	1:A:237:ALA:N	2.76	0.42
1:B:75:TRP:HZ2	1:C:219:PHE:HA	1.84	0.42
1:C:175:ASN:H	1:C:175:ASN:ND2	2.18	0.42
1:D:182:VAL:HG11	1:D:310:THR:HB	2.01	0.42
1:D:319:LEU:O	1:D:323:LEU:HB2	2.19	0.42
1:B:114:PRO:CB	1:B:115:ARG:NH2	2.83	0.42
1:C:262:TRP:HD1	1:C:273:GLU:CD	2.27	0.42
1:A:149:LEU:O	1:A:153:VAL:HG23	2.19	0.42
1:C:129:ARG:HD3	1:C:440:ARG:HH22	1.85	0.42
1:D:285:ASN:HA	1:D:286:PRO:HD2	1.95	0.42
1:A:147:LYS:O	1:A:151:GLN:HB2	2.20	0.42
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.80	0.42
1:A:481:PHE:O	1:A:481:PHE:CG	2.72	0.42
1:D:187:ALA:O	1:D:191:CYS:N	2.51	0.42
1:A:280:GLU:O	1:A:282:ALA:N	2.53	0.41
1:A:319:LEU:HB2	1:A:490:TYR:CE2	2.55	0.41
1:B:307:MET:HG2	1:B:308:VAL:N	2.34	0.41
1:B:481:PHE:O	1:B:481:PHE:CG	2.72	0.41
1:D:130:GLU:OE2	1:D:290:PHE:CE1	2.73	0.41
1:D:132:ARG:O	1:D:136:VAL:HG13	2.20	0.41
1:D:262:TRP:HD1	1:D:273:GLU:OE2	2.03	0.41
1:D:371:PRO:HG2	1:D:481:PHE:HE1	1.84	0.41
1:A:170:ARG:NH2	1:C:201:ARG:HH11	2.19	0.41
1:C:67:ASP:O	1:C:82:ASN:HB2	2.20	0.41
1:C:223:VAL:CG1	1:C:375:THR:HG21	2.50	0.41
1:C:416:HIS:HB3	1:C:419:HIS:CE1	2.56	0.41
1:A:54:THR:N	1:A:55:PRO:HD3	2.31	0.41
1:B:275:PHE:CD2	1:B:279:MET:HE2	2.56	0.41
1:A:473:PRO:O	1:A:474:ARG:CB	2.61	0.41
1:B:222:GLU:C	1:B:224:LEU:H	2.29	0.41
1:A:132:ARG:NH1	1:A:441:ARG:HA	2.36	0.41
1:A:449:ALA:O	1:A:453:LEU:HG	2.21	0.41
1:B:217:SER:C	1:B:221:ARG:NH1	2.79	0.41
1:C:143:GLY:O	1:C:144:LEU:HG	2.21	0.41
2:D:600:HEM:HBB2	2:D:600:HEM:HMB2	2.02	0.41
1:B:238:GLY:O	1:B:240:VAL:N	2.54	0.41
1:C:100:ASP:HA	1:C:124:TYR:HB2	2.03	0.41
1:D:410:GLU:O	1:D:411:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:ALA:C	1:D:484:LEU:N	2.76	0.41
1:A:168:SER:C	1:A:170:ARG:H	2.28	0.41
1:B:285:ASN:HA	1:B:286:PRO:HD2	1.92	0.41
1:B:341:GLN:HE21	1:B:341:GLN:CA	2.33	0.41
1:C:262:TRP:CZ2	1:C:264:PRO:HA	2.55	0.41
1:D:222:GLU:C	1:D:224:LEU:H	2.29	0.41
1:A:217:SER:HA	1:A:220:LEU:HB2	2.03	0.41
1:A:443:CYS:HB2	2:A:600:HEM:C4A	2.56	0.41
1:A:466:PHE:HA	1:A:493:CYS:O	2.21	0.41
1:C:128:TRP:CZ2	1:C:132:ARG:HD2	2.56	0.41
1:C:168:SER:C	1:C:170:ARG:H	2.29	0.41
1:A:192:GLY:HA2	1:A:269:ARG:HH22	1.86	0.40
1:B:75:TRP:CZ2	1:C:219:PHE:HA	2.55	0.40
1:B:468:VAL:HA	1:B:469:PRO:HD3	1.97	0.40
1:C:323:LEU:HD13	1:C:475:PRO:HD2	2.03	0.40
1:B:173:ARG:HA	1:B:174:PRO:HD3	1.85	0.40
1:B:416:HIS:CD2	1:B:418:GLU:HB2	2.57	0.40
1:C:149:LEU:HD23	1:C:149:LEU:HA	1.92	0.40
1:C:331:VAL:HG13	1:C:356:THR:OG1	2.20	0.40
1:D:458:THR:O	1:D:459:SER:C	2.63	0.40
1:D:462:GLN:O	1:D:497:ARG:NH1	2.53	0.40
1:A:182:VAL:HG11	1:A:310:THR:HB	2.04	0.40
1:A:323:LEU:HD13	1:A:475:PRO:HD2	2.03	0.40
1:B:75:TRP:CZ3	1:C:105:PRO:HD3	2.57	0.40
1:C:64:ARG:HG2	1:C:65:PHE:CD1	2.56	0.40
1:C:323:LEU:HD12	1:C:323:LEU:HA	1.85	0.40
1:B:292:ASP:OD2	1:B:292:ASP:N	2.50	0.40
1:D:144:LEU:O	1:D:147:LYS:N	2.48	0.40
1:D:418:GLU:O	1:D:419:HIS:C	2.63	0.40
1:A:40:LEU:H	1:A:41:PRO:HD3	1.83	0.40
1:B:38:LEU:HD22	1:C:240:VAL:CG2	2.52	0.40
1:B:91:LEU:O	1:B:95:GLY:CA	2.70	0.40
1:D:294:ASN:HD22	1:D:294:ASN:HA	1.55	0.40
2:D:600:HEM:CMC	2:D:600:HEM:CBC	2.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/479 (94%)	396 (88%)	34 (8%)	20 (4%)	2	12
1	B	447/479 (93%)	397 (89%)	33 (7%)	17 (4%)	2	15
1	C	450/479 (94%)	397 (88%)	38 (8%)	15 (3%)	3	17
1	D	447/479 (93%)	395 (88%)	36 (8%)	16 (4%)	2	16
All	All	1794/1916 (94%)	1585 (88%)	141 (8%)	68 (4%)	2	15

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	A	40	LEU
1	A	114	PRO
1	A	145	GLY
1	A	229	VAL
1	A	230	ASP
1	A	239	LYS
1	B	35	PRO
1	B	229	VAL
1	B	230	ASP
1	C	35	PRO
1	C	40	LEU
1	C	112	PHE
1	C	229	VAL
1	C	230	ASP
1	C	239	LYS
1	D	35	PRO
1	D	145	GLY
1	D	229	VAL
1	D	230	ASP
1	A	112	PHE
1	A	252	ASP

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Mol	Chain	Res	Type
1	B	145	GLY
1	B	239	LYS
1	B	392	GLY
1	D	112	PHE
1	D	239	LYS
1	A	225	ASN
1	A	228	PRO
1	A	281	LYS
1	B	114	PRO
1	B	225	ASN
1	B	228	PRO
1	C	39	PRO
1	C	114	PRO
1	C	225	ASN
1	C	228	PRO
1	D	225	ASN
1	D	228	PRO
1	D	419	HIS
1	A	55	PRO
1	A	144	LEU
1	A	474	ARG
1	B	55	PRO
1	B	112	PHE
1	B	474	ARG
1	C	55	PRO
1	C	288	SER
1	C	392	GLY
1	C	474	ARG
1	D	55	PRO
1	D	288	SER
1	D	474	ARG
1	A	54	THR
1	A	288	SER
1	B	54	THR
1	B	288	SER
1	D	114	PRO
1	A	392	GLY
1	B	419	HIS
1	D	223	VAL
1	D	392	GLY
1	A	223	VAL
1	B	169	GLY

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Mol	Chain	Res	Type
1	B	223	VAL
1	C	223	VAL
1	D	284	GLY
1	A	238	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/409 (93%)	326 (86%)	54 (14%)	3	16
1	B	377/409 (92%)	321 (85%)	56 (15%)	3	15
1	C	380/409 (93%)	324 (85%)	56 (15%)	3	15
1	D	377/409 (92%)	317 (84%)	60 (16%)	2	13
All	All	1514/1636 (92%)	1288 (85%)	226 (15%)	3	15

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	63	ARG
1	A	68	VAL
1	A	70	SER
1	A	71	LEU
1	A	88	ARG
1	A	101	ARG
1	A	116	SER
1	A	123	ARG
1	A	130	GLU
1	A	132	ARG
1	A	136	VAL
1	A	144	LEU
1	A	148	SER
1	A	154	THR
1	A	170	ARG
1	A	193	ARG

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Mol	Chain	Res	Type
1	A	196	GLU
1	A	210	GLN
1	A	216	GLU
1	A	222	GLU
1	A	223	VAL
1	A	225	ASN
1	A	242	ARG
1	A	250	GLN
1	A	253	GLU
1	A	256	THR
1	A	288	SER
1	A	291	ASN
1	A	292	ASP
1	A	294	ASN
1	A	304	SER
1	A	307	MET
1	A	326	ASP
1	A	333	GLN
1	A	337	ASP
1	A	341	GLN
1	A	342	VAL
1	A	370	VAL
1	A	381	ASP
1	A	382	ILE
1	A	383	GLU
1	A	384	VAL
1	A	388	ARG
1	A	395	LEU
1	A	403	LEU
1	A	468	VAL
1	A	477	HIS
1	A	480	VAL
1	A	484	LEU
1	A	485	VAL
1	A	488	SER
1	A	492	LEU
1	A	495	VAL
1	B	53	ASN
1	B	54	THR
1	B	63	ARG
1	B	68	VAL
1	B	70	SER

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Mol	Chain	Res	Type
1	B	71	LEU
1	B	88	ARG
1	B	101	ARG
1	B	115	ARG
1	B	116	SER
1	B	117	GLN
1	B	123	ARG
1	B	130	GLU
1	B	132	ARG
1	B	133	ARG
1	B	136	VAL
1	B	137	SER
1	B	154	THR
1	B	170	ARG
1	B	193	ARG
1	B	196	GLU
1	B	210	GLN
1	B	216	GLU
1	B	222	GLU
1	B	223	VAL
1	B	225	ASN
1	B	242	ARG
1	B	250	GLN
1	B	253	GLU
1	B	255	LEU
1	B	256	THR
1	B	291	ASN
1	B	292	ASP
1	B	294	ASN
1	B	304	SER
1	B	307	MET
1	B	326	ASP
1	B	333	GLN
1	B	337	ASP
1	B	341	GLN
1	B	370	VAL
1	B	381	ASP
1	B	382	ILE
1	B	384	VAL
1	B	388	ARG
1	B	395	LEU
1	B	403	LEU

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Mol	Chain	Res	Type
1	B	429	LYS
1	B	468	VAL
1	B	477	HIS
1	B	480	VAL
1	B	484	LEU
1	B	485	VAL
1	B	488	SER
1	B	492	LEU
1	B	495	VAL
1	C	52	GLN
1	C	63	ARG
1	C	68	VAL
1	C	70	SER
1	C	71	LEU
1	C	88	ARG
1	C	101	ARG
1	C	115	ARG
1	C	116	SER
1	C	123	ARG
1	C	130	GLU
1	C	132	ARG
1	C	136	VAL
1	C	144	LEU
1	C	154	THR
1	C	170	ARG
1	C	196	GLU
1	C	210	GLN
1	C	216	GLU
1	C	222	GLU
1	C	223	VAL
1	C	225	ASN
1	C	242	ARG
1	C	250	GLN
1	C	256	THR
1	C	260	MET
1	C	266	GLN
1	C	288	SER
1	C	291	ASN
1	C	292	ASP
1	C	294	ASN
1	C	304	SER
1	C	307	MET

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Mol	Chain	Res	Type
1	C	322	ILE
1	C	323	LEU
1	C	326	ASP
1	C	333	GLN
1	C	337	ASP
1	C	341	GLN
1	C	370	VAL
1	C	381	ASP
1	C	382	ILE
1	C	384	VAL
1	C	388	ARG
1	C	395	LEU
1	C	403	LEU
1	C	428	VAL
1	C	440	ARG
1	C	468	VAL
1	C	477	HIS
1	C	480	VAL
1	C	484	LEU
1	C	485	VAL
1	C	488	SER
1	C	492	LEU
1	C	495	VAL
1	D	54	THR
1	D	63	ARG
1	D	68	VAL
1	D	70	SER
1	D	71	LEU
1	D	88	ARG
1	D	101	ARG
1	D	115	ARG
1	D	116	SER
1	D	117	GLN
1	D	123	ARG
1	D	130	GLU
1	D	132	ARG
1	D	133	ARG
1	D	136	VAL
1	D	137	SER
1	D	148	SER
1	D	154	THR
1	D	170	ARG

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Mol	Chain	Res	Type
1	D	193	ARG
1	D	196	GLU
1	D	210	GLN
1	D	214	LYS
1	D	216	GLU
1	D	222	GLU
1	D	223	VAL
1	D	225	ASN
1	D	242	ARG
1	D	250	GLN
1	D	255	LEU
1	D	256	THR
1	D	266	GLN
1	D	291	ASN
1	D	292	ASP
1	D	294	ASN
1	D	304	SER
1	D	307	MET
1	D	321	MET
1	D	326	ASP
1	D	333	GLN
1	D	337	ASP
1	D	341	GLN
1	D	370	VAL
1	D	381	ASP
1	D	382	ILE
1	D	384	VAL
1	D	388	ARG
1	D	395	LEU
1	D	403	LEU
1	D	429	LYS
1	D	440	ARG
1	D	441	ARG
1	D	468	VAL
1	D	477	HIS
1	D	480	VAL
1	D	484	LEU
1	D	485	VAL
1	D	488	SER
1	D	492	LEU
1	D	495	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	60	GLN
1	A	72	GLN
1	A	166	ASN
1	A	175	ASN
1	A	250	GLN
1	A	291	ASN
1	A	324	HIS
1	A	332	GLN
1	A	333	GLN
1	A	341	GLN
1	A	350	GLN
1	A	477	HIS
1	B	53	ASN
1	B	72	GLN
1	B	166	ASN
1	B	244	GLN
1	B	250	GLN
1	B	285	ASN
1	B	291	ASN
1	B	333	GLN
1	B	341	GLN
1	B	350	GLN
1	B	424	GLN
1	B	477	HIS
1	C	52	GLN
1	C	72	GLN
1	C	166	ASN
1	C	175	ASN
1	C	210	GLN
1	C	250	GLN
1	C	291	ASN
1	C	294	ASN
1	C	324	HIS
1	C	333	GLN
1	C	341	GLN
1	C	350	GLN
1	C	385	GLN
1	C	462	GLN
1	C	477	HIS
1	C	478	HIS
1	D	60	GLN

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Mol	Chain	Res	Type
1	D	72	GLN
1	D	166	ASN
1	D	175	ASN
1	D	250	GLN
1	D	291	ASN
1	D	333	GLN
1	D	341	GLN
1	D	350	GLN
1	D	424	GLN
1	D	477	HIS

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 ⓘ

6 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	SO4	B	2000	-	4,4,4	0.42	0	6,6,6	0.93	0
3	SO4	B	2001	-	4,4,4	0.38	0	6,6,6	0.82	0
2	HEM	D	600	1	50,50,50	2.11	11 (22%)	67,82,82	1.23	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	600	1	50,50,50	2.18	9 (18%)	67,82,82	1.56	13 (19%)
2	HEM	C	600	1	50,50,50	1.96	10 (20%)	67,82,82	1.33	9 (13%)
2	HEM	B	600	1	50,50,50	2.26	9 (18%)	67,82,82	1.34	7 (10%)

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	A	600	1	-	4/14/54/54	-
2	HEM	B	600	1	-	2/14/54/54	-
2	HEM	D	600	1	-	2/14/54/54	-
2	HEM	C	600	1	-	2/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	C3D-C2D	7.83	1.53	1.36
2	A	600	HEM	C3D-C2D	7.61	1.53	1.36
2	B	600	HEM	FE-ND	7.15	2.16	1.94
2	D	600	HEM	C3D-C2D	7.13	1.52	1.36
2	C	600	HEM	C3D-C2D	6.53	1.50	1.36
2	A	600	HEM	FE-ND	6.19	2.13	1.94
2	D	600	HEM	FE-ND	5.98	2.13	1.94
2	A	600	HEM	CBC-CAC	5.16	1.55	1.30
2	C	600	HEM	CBC-CAC	5.04	1.54	1.30
2	D	600	HEM	CBC-CAC	4.90	1.53	1.30
2	C	600	HEM	CBB-CAB	4.88	1.53	1.30
2	B	600	HEM	CBC-CAC	4.85	1.53	1.30
2	A	600	HEM	CBB-CAB	4.85	1.53	1.30
2	D	600	HEM	CBB-CAB	4.79	1.53	1.30
2	B	600	HEM	CBB-CAB	4.71	1.53	1.30
2	A	600	HEM	FE-NC	4.57	2.10	1.95
2	B	600	HEM	FE-NC	3.95	2.08	1.95
2	C	600	HEM	FE-ND	3.77	2.06	1.94
2	C	600	HEM	CAB-C3B	3.68	1.57	1.47
2	B	600	HEM	CAB-C3B	3.57	1.56	1.47
2	D	600	HEM	CAB-C3B	3.30	1.56	1.47
2	D	600	HEM	CAC-C3C	3.26	1.56	1.47
2	C	600	HEM	CAC-C3C	3.23	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	CMC-C2C	3.00	1.56	1.50
2	A	600	HEM	CAC-C3C	2.94	1.55	1.47
2	C	600	HEM	FE-NA	2.89	2.04	1.95
2	B	600	HEM	CAC-C3C	2.88	1.55	1.47
2	A	600	HEM	CMC-C2C	2.77	1.56	1.50
2	A	600	HEM	CAB-C3B	2.65	1.54	1.47
2	D	600	HEM	CMB-C2B	2.64	1.56	1.50
2	B	600	HEM	CMC-C2C	2.53	1.56	1.50
2	C	600	HEM	FE-NB	2.35	2.02	1.94
2	D	600	HEM	FE-NA	2.34	2.02	1.95
2	B	600	HEM	C1B-NB	-2.29	1.36	1.40
2	C	600	HEM	CMB-C2B	2.21	1.55	1.50
2	C	600	HEM	CMC-C2C	2.14	1.55	1.50
2	D	600	HEM	CMD-C2D	2.13	1.55	1.50
2	A	600	HEM	CMA-C3A	2.11	1.55	1.50
2	D	600	HEM	C2A-C3A	-2.09	1.33	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	C4D-ND-C1D	5.06	111.20	105.21
2	B	600	HEM	C4D-ND-C1D	4.60	110.65	105.21
2	C	600	HEM	C4D-ND-C1D	3.54	109.40	105.21
2	D	600	HEM	C4D-ND-C1D	3.52	109.37	105.21
2	D	600	HEM	CBC-CAC-C3C	-3.26	111.24	127.53
2	A	600	HEM	CBB-CAB-C3B	-3.03	112.37	127.53
2	B	600	HEM	CBC-CAC-C3C	-2.99	112.59	127.53
2	A	600	HEM	C4C-C3C-C2C	2.90	109.33	106.81
2	A	600	HEM	C3C-C2C-C1C	-2.84	104.36	107.05
2	B	600	HEM	CBB-CAB-C3B	-2.83	113.39	127.53
2	D	600	HEM	CBB-CAB-C3B	-2.77	113.70	127.53
2	C	600	HEM	CBC-CAC-C3C	-2.72	113.94	127.53
2	A	600	HEM	CBC-CAC-C3C	-2.71	113.99	127.53
2	D	600	HEM	CAD-C3D-C4D	2.69	129.39	124.70
2	D	600	HEM	CMD-C2D-C1D	2.64	129.16	125.03
2	D	600	HEM	CHD-C4C-NC	2.58	127.27	124.45
2	C	600	HEM	CMD-C2D-C1D	2.55	129.02	125.03
2	A	600	HEM	C1B-NB-C4B	2.53	108.20	105.21
2	C	600	HEM	C3B-C4B-NB	2.52	111.28	109.47
2	A	600	HEM	C3B-C2B-C1B	2.51	108.29	106.41
2	C	600	HEM	CMC-C2C-C1C	-2.49	120.34	124.73
2	A	600	HEM	CMC-C2C-C1C	-2.42	120.46	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	HEM	C3B-C2B-C1B	2.40	108.21	106.41
2	A	600	HEM	CHD-C4C-NC	2.39	127.06	124.45
2	A	600	HEM	O2D-CGD-CBD	2.31	121.30	114.00
2	B	600	HEM	CHD-C4C-NC	2.22	126.87	124.45
2	A	600	HEM	CHC-C4B-NB	2.21	126.80	124.42
2	A	600	HEM	CMB-C2B-C1B	-2.14	121.69	125.03
2	B	600	HEM	C2A-C1A-NA	-2.14	107.78	110.15
2	A	600	HEM	C2A-C1A-NA	-2.13	107.79	110.15
2	C	600	HEM	CBB-CAB-C3B	-2.12	116.94	127.53
2	B	600	HEM	CAA-CBA-CGA	-2.11	108.06	113.67
2	D	600	HEM	C4D-C3D-C2D	-2.07	103.88	106.89
2	C	600	HEM	C3B-C2B-C1B	2.04	107.95	106.41
2	C	600	HEM	C4A-C3A-C2A	2.01	109.12	106.82
2	C	600	HEM	CHC-C4B-NB	2.01	126.58	124.42

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAA-CBA-CGA-O2A
2	C	600	HEM	CAA-CBA-CGA-O2A
2	C	600	HEM	CAA-CBA-CGA-O1A
2	D	600	HEM	CAA-CBA-CGA-O1A
2	D	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAD-CBD-CGD-O1D
2	A	600	HEM	CAD-CBD-CGD-O2D

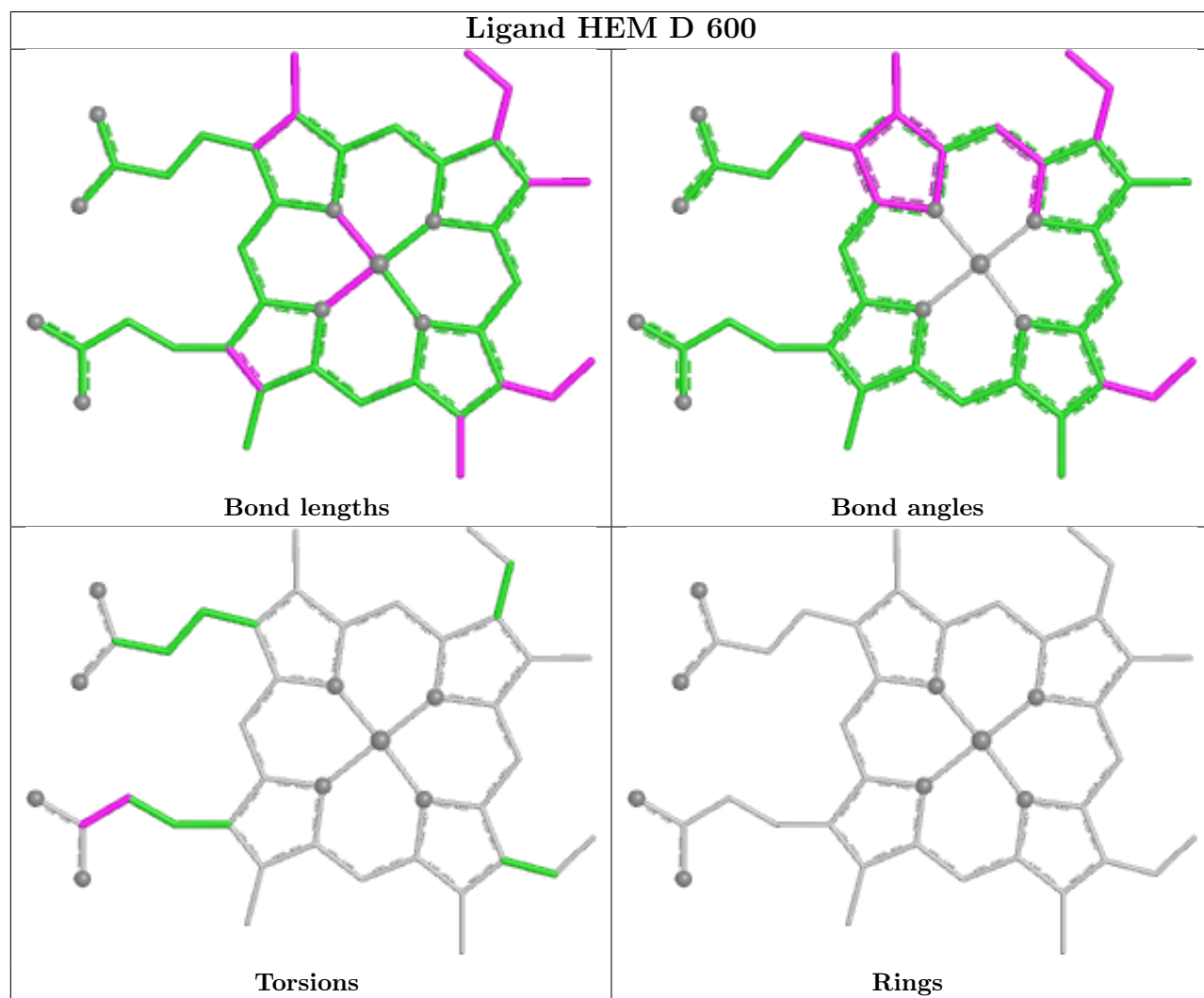
There are no ring outliers.

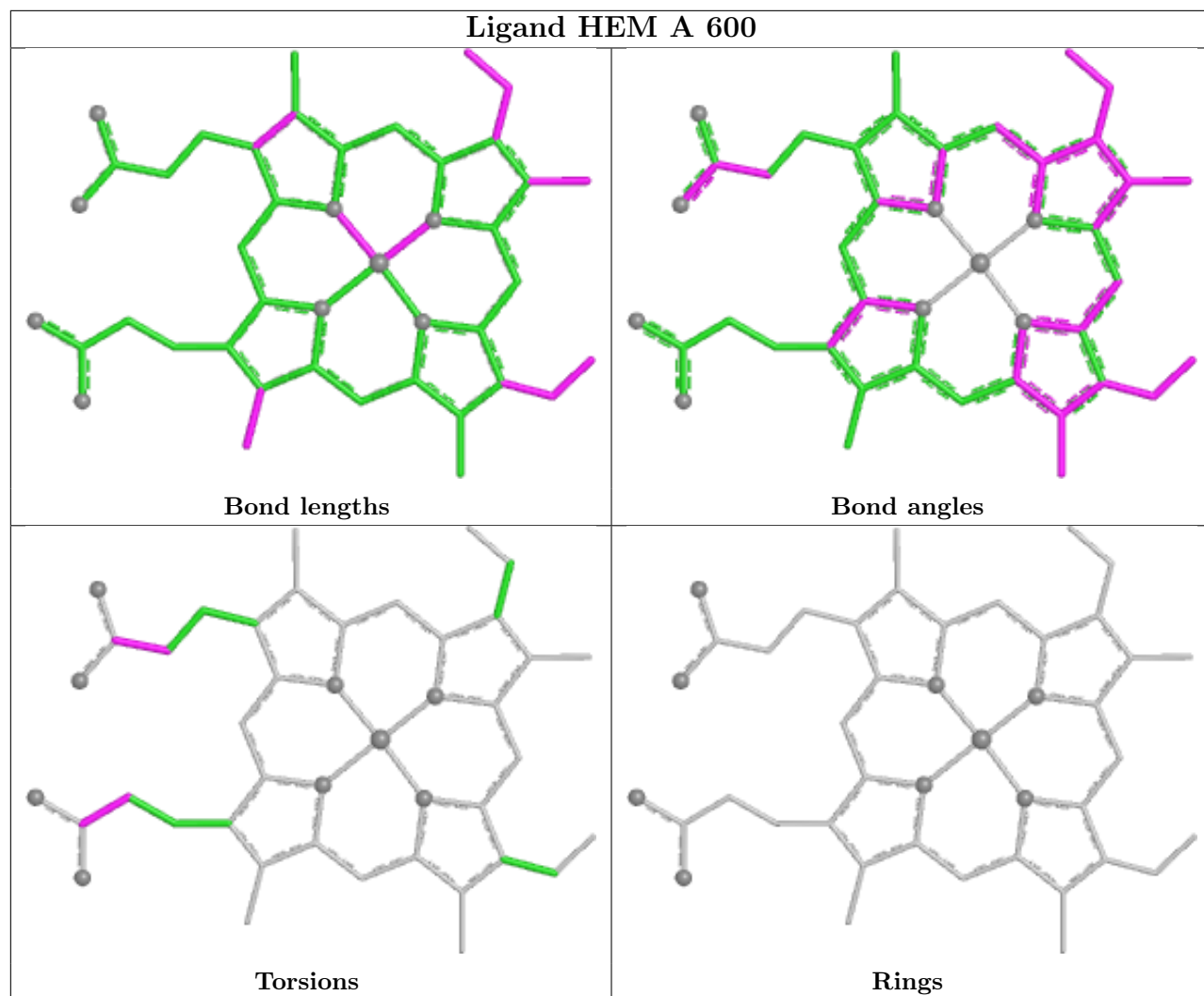
5 monomers are involved in 26 short contacts:

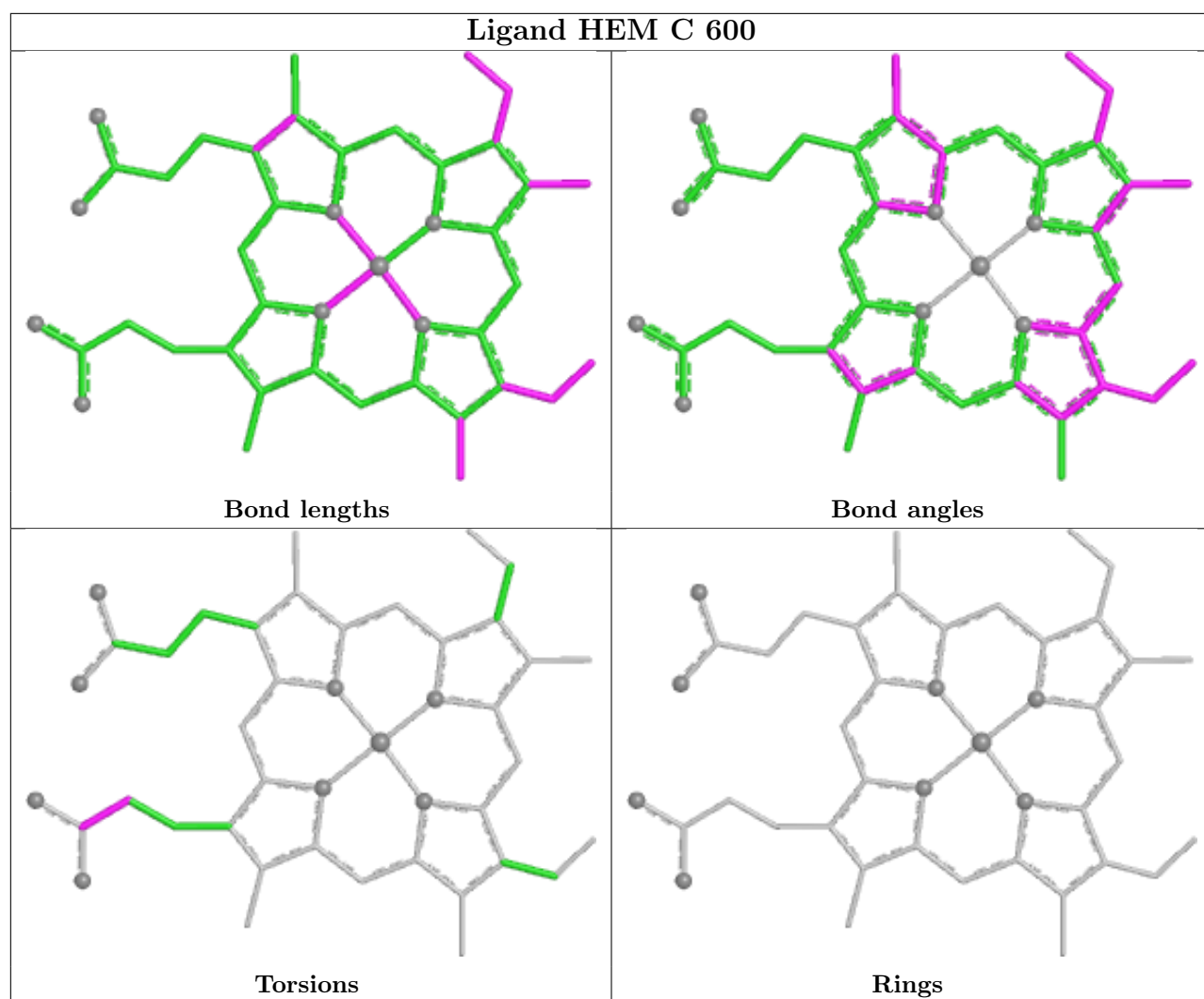
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2000	SO4	2	0
2	D	600	HEM	8	0
2	A	600	HEM	5	0
2	C	600	HEM	5	0
2	B	600	HEM	6	0

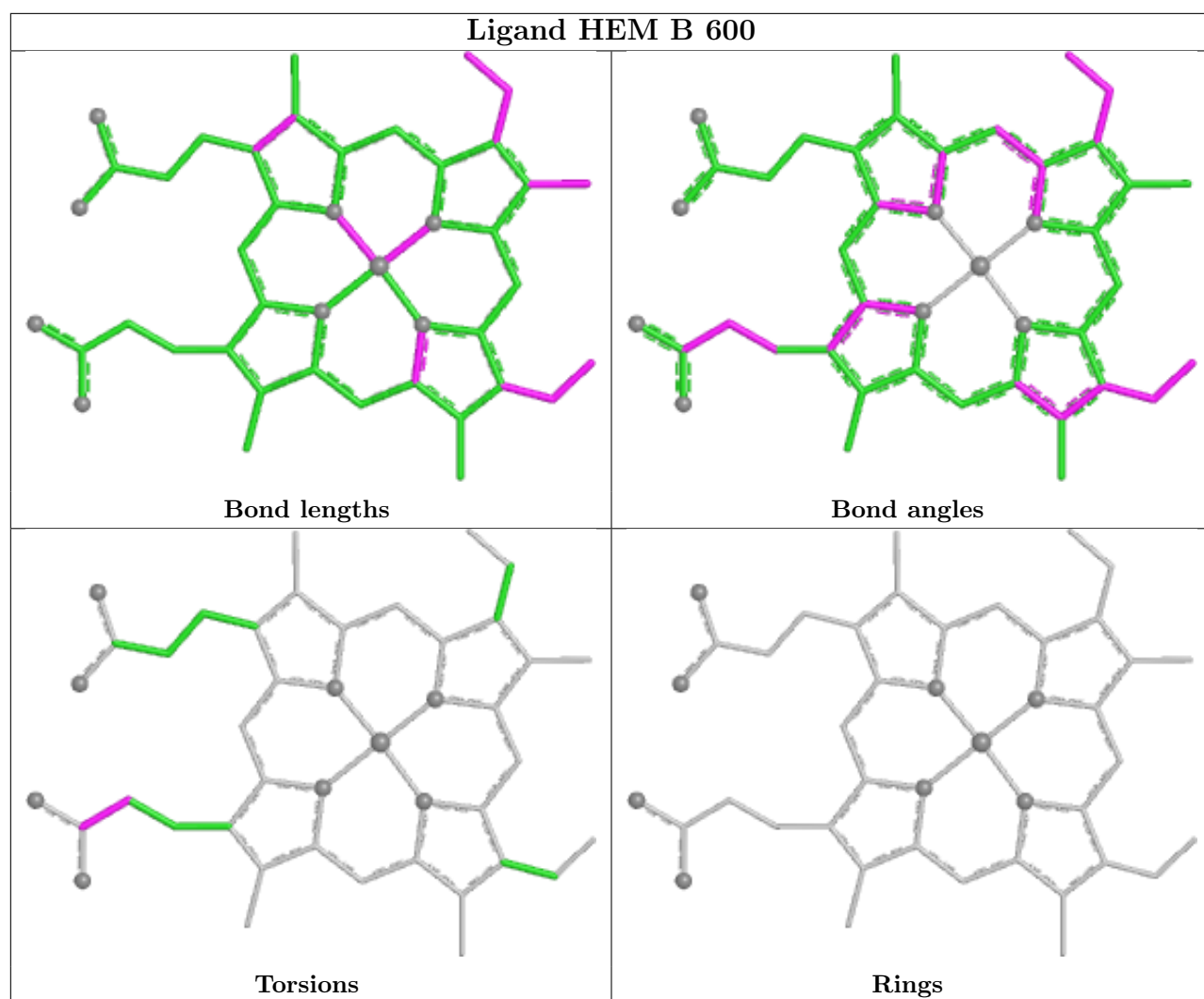
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	454/479 (94%)	0.17	7 (1%)	72 49	50, 57, 63, 77	0
1	B	451/479 (94%)	0.14	5 (1%)	78 57	46, 57, 63, 71	0
1	C	454/479 (94%)	0.27	6 (1%)	75 53	49, 57, 63, 75	0
1	D	451/479 (94%)	0.37	8 (1%)	67 44	48, 57, 63, 72	0
All	All	1810/1916 (94%)	0.24	26 (1%)	73 51	46, 57, 63, 77	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	GLY	4.3
1	A	40	LEU	3.7
1	B	230	ASP	2.9
1	C	40	LEU	2.9
1	D	197	TYR	2.8
1	C	229	VAL	2.7
1	A	341	GLN	2.7
1	C	228	PRO	2.6
1	A	230	ASP	2.6
1	D	34	PRO	2.5
1	D	293	GLU	2.5
1	B	228	PRO	2.4
1	D	113	GLY	2.4
1	A	56	TYR	2.3
1	D	114	PRO	2.3
1	D	340	GLY	2.3
1	B	192	GLY	2.2
1	C	379	SER	2.2
1	D	463	HIS	2.2
1	B	477	HIS	2.1
1	A	239	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	127	ALA	2.1
1	C	64	ARG	2.0
1	B	471	GLY	2.0
1	C	114	PRO	2.0
1	D	119	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

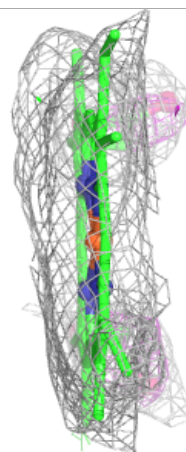
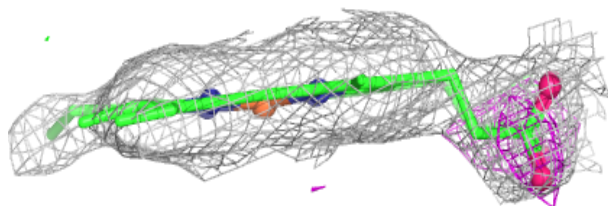
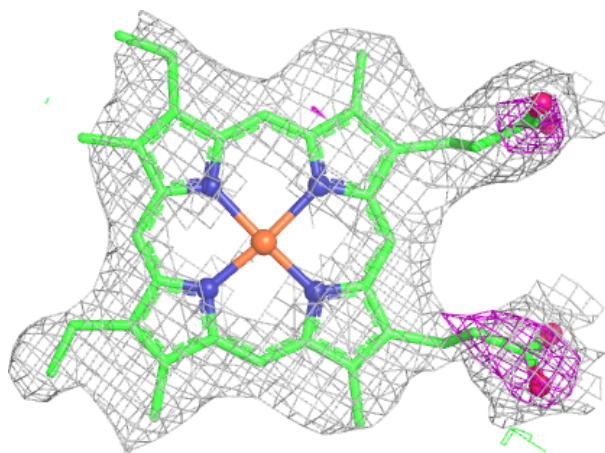
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	2001	5/5	0.89	0.16	52,54,57,58	0
2	HEM	B	600	43/43	0.95	0.10	48,52,55,56	0
2	HEM	D	600	43/43	0.96	0.11	48,52,55,56	0
2	HEM	A	600	43/43	0.97	0.09	48,52,55,56	0
3	SO4	B	2000	5/5	0.97	0.11	46,51,54,54	0
2	HEM	C	600	43/43	0.97	0.09	48,52,55,56	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.

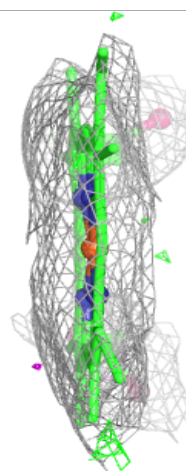
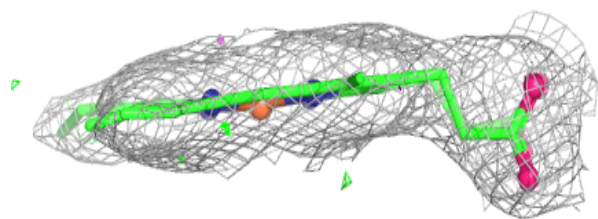
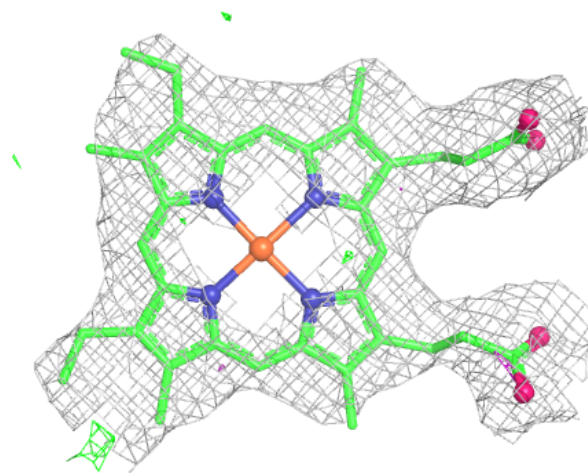
Electron density around HEM B 600:

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



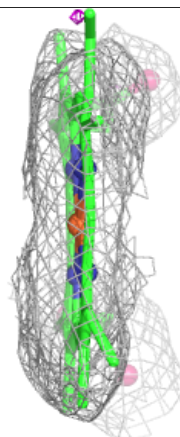
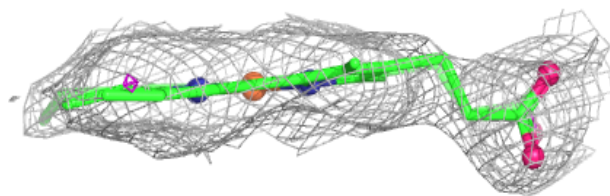
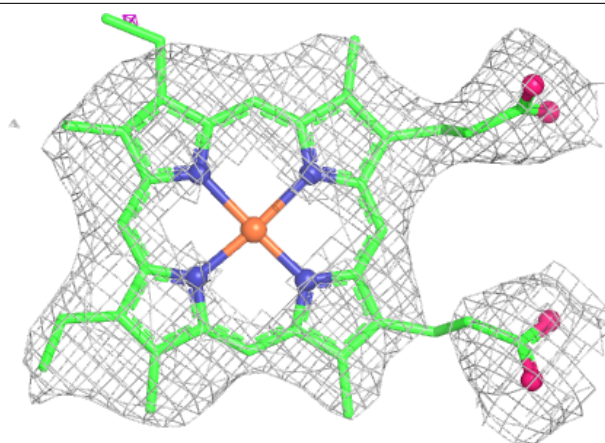
Electron density around HEM D 600:

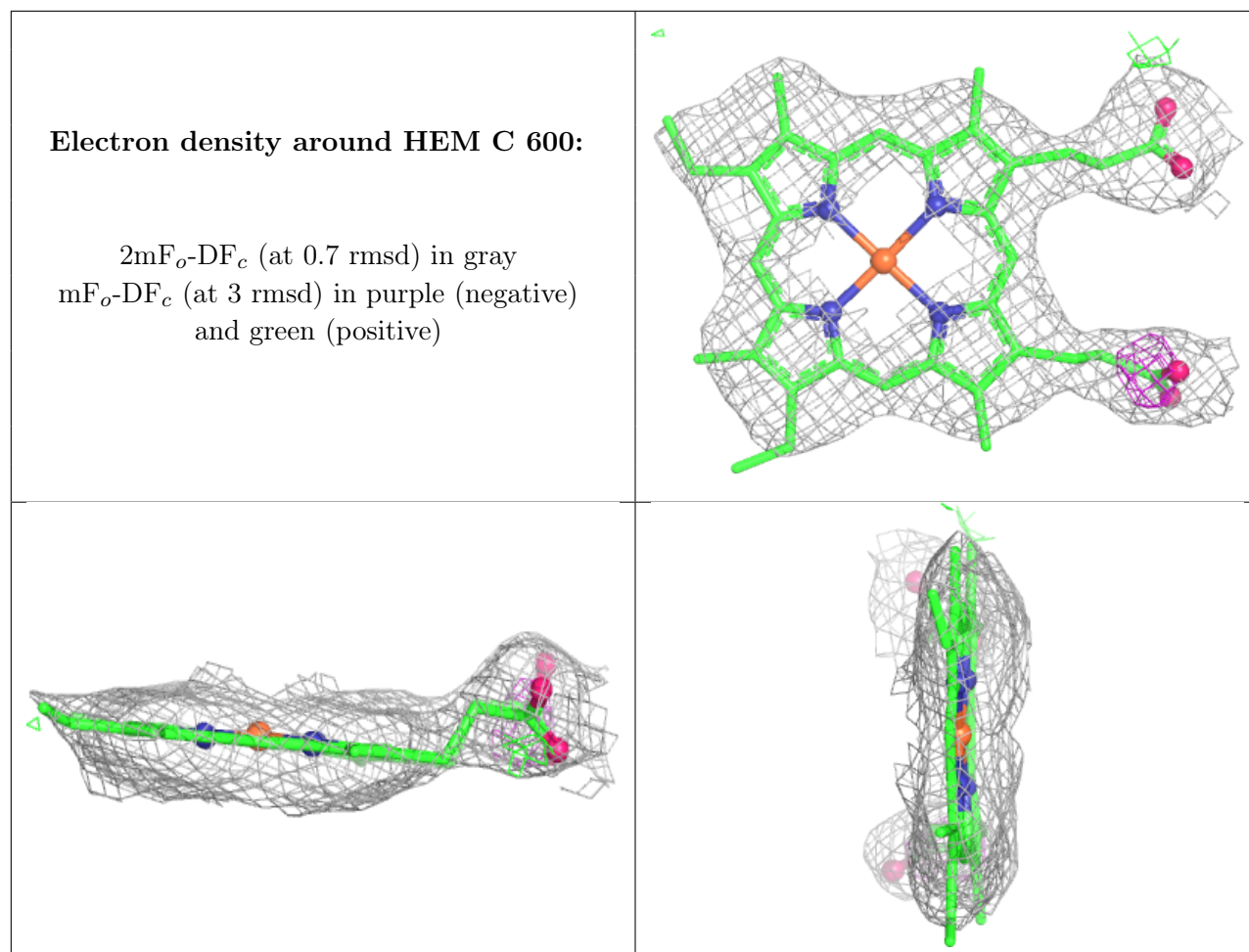
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 600:

$2mF_o-DF_c$ (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.