



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 3MZS / pdb_00003mzs
Title : Crystal Structure of Cytochrome P450 CYP11A1 in complex with 22-hydroxy-cholesterol
Authors : Stout, C.D.; Annalora, A.; Mast, N.; Pikuleva, I.
Deposited on : 2010-05-12
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

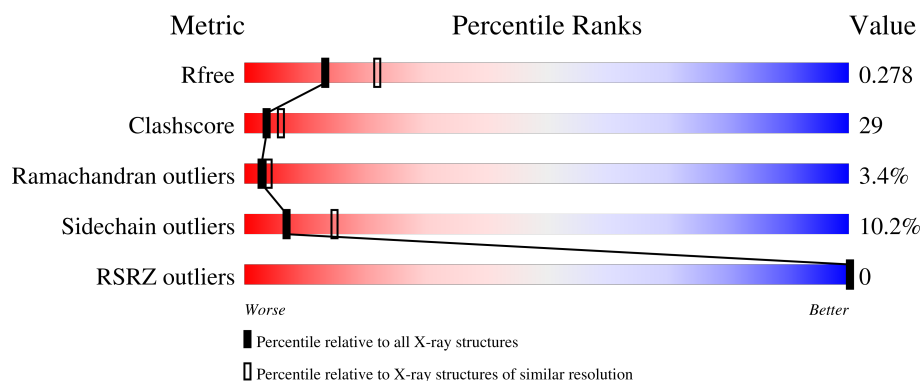
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

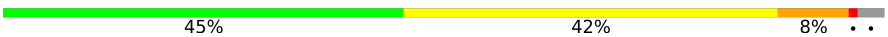
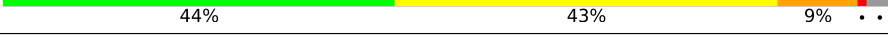
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	486	
1	B	486	
1	C	486	
1	D	486	

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
4	IPA	B	502	-	-	X	-
4	IPA	C	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16012 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 Cholesterol side-chain cleavage enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3904	2541	664	683	16			
1	B	470	Total	C	N	O	S	0	0	0
			3904	2541	664	683	16			
1	C	470	Total	C	N	O	S	0	0	0
			3904	2541	664	683	16			
1	D	470	Total	C	N	O	S	0	0	0
			3904	2541	664	683	16			

There are 24 discrepancies between the modelled and reference sequences:

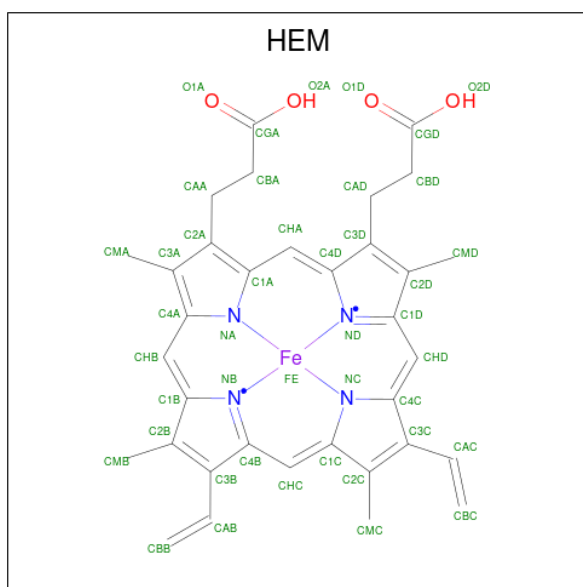
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P00189
A	2	ALA	-	expression tag	UNP P00189
A	483	HIS	-	expression tag	UNP P00189
A	484	HIS	-	expression tag	UNP P00189
A	485	HIS	-	expression tag	UNP P00189
A	486	HIS	-	expression tag	UNP P00189
B	1	MET	-	expression tag	UNP P00189
B	2	ALA	-	expression tag	UNP P00189
B	483	HIS	-	expression tag	UNP P00189
B	484	HIS	-	expression tag	UNP P00189
B	485	HIS	-	expression tag	UNP P00189
B	486	HIS	-	expression tag	UNP P00189
C	1	MET	-	expression tag	UNP P00189
C	2	ALA	-	expression tag	UNP P00189
C	483	HIS	-	expression tag	UNP P00189
C	484	HIS	-	expression tag	UNP P00189
C	485	HIS	-	expression tag	UNP P00189
C	486	HIS	-	expression tag	UNP P00189
D	1	MET	-	expression tag	UNP P00189
D	2	ALA	-	expression tag	UNP P00189
D	483	HIS	-	expression tag	UNP P00189

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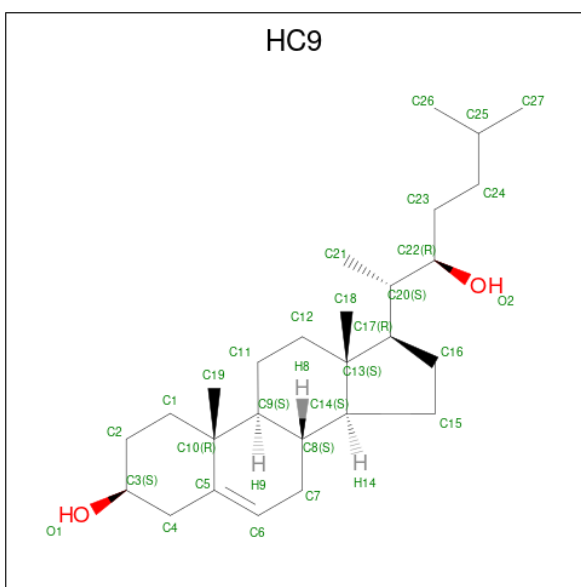
Chain	Residue	Modelled	Actual	Comment	Reference
D	484	HIS	-	expression tag	UNP P00189
D	485	HIS	-	expression tag	UNP P00189
D	486	HIS	-	expression tag	UNP P00189

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



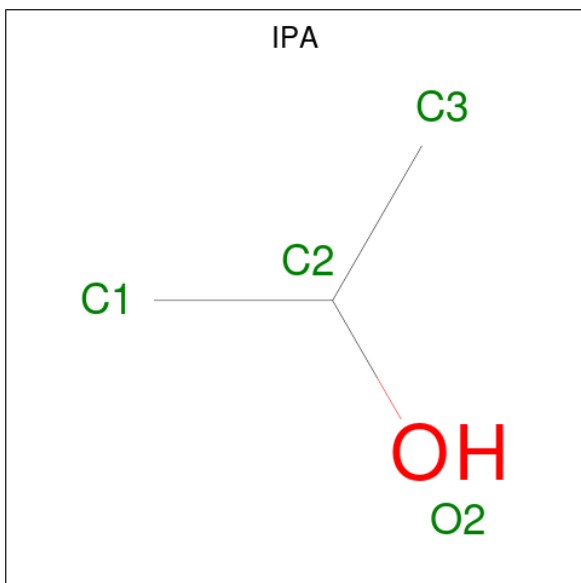
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (3alpha,8alpha,22R)-cholest-5-ene-3,22-diol (CCD ID: HC9) (formula: $C_{27}H_{46}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			29	27	2		
3	B	1	Total	C	O	0	0
			29	27	2		
3	C	1	Total	C	O	0	0
			29	27	2		
3	D	1	Total	C	O	0	0
			29	27	2		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 3 1	0	0
4	B	1	Total C O 4 3 1	0	0
4	C	1	Total C O 4 3 1	0	0
4	D	1	Total C O 4 3 1	0	0

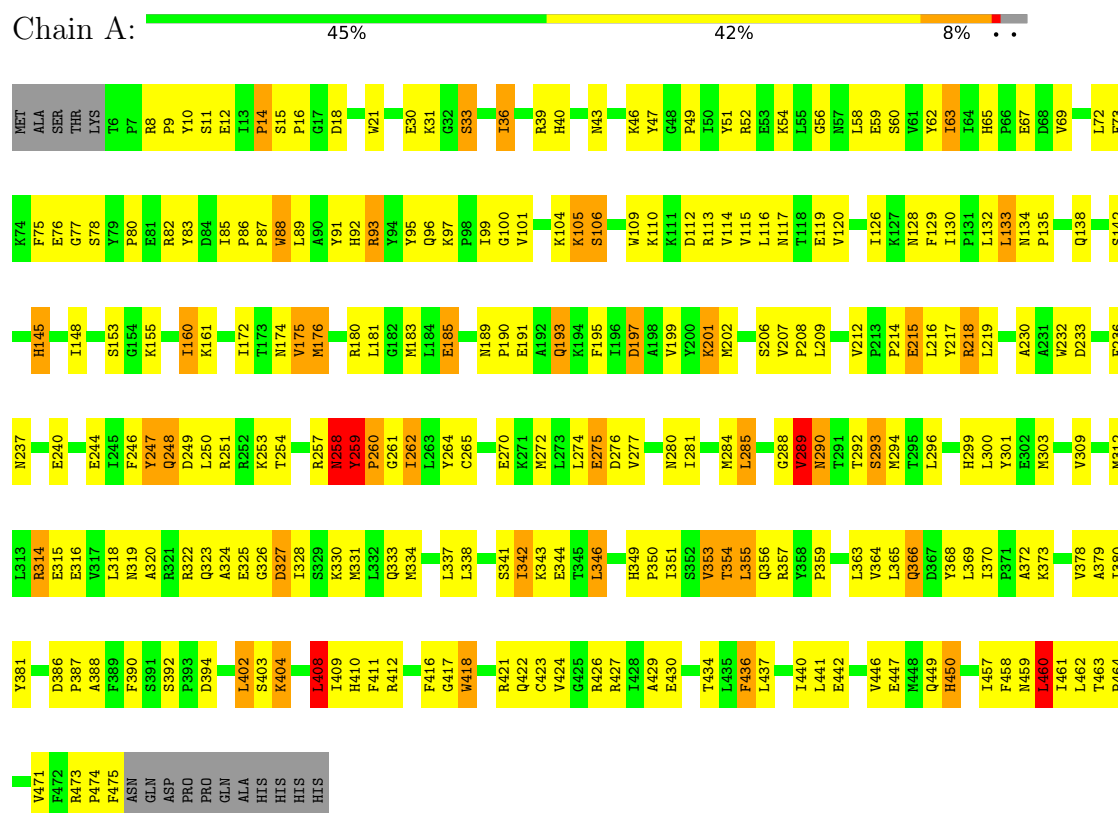
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	B	15	Total O 15 15	0	0
5	C	27	Total O 27 27	0	0
5	D	25	Total O 25 25	0	0

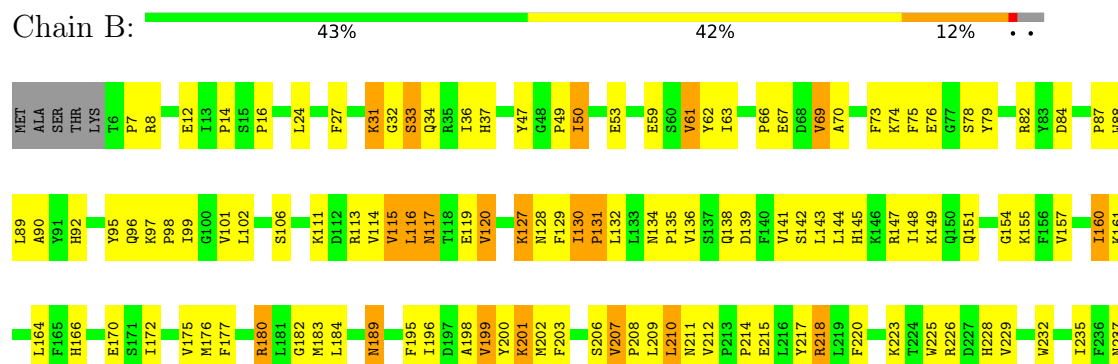
3 Residue-property plots

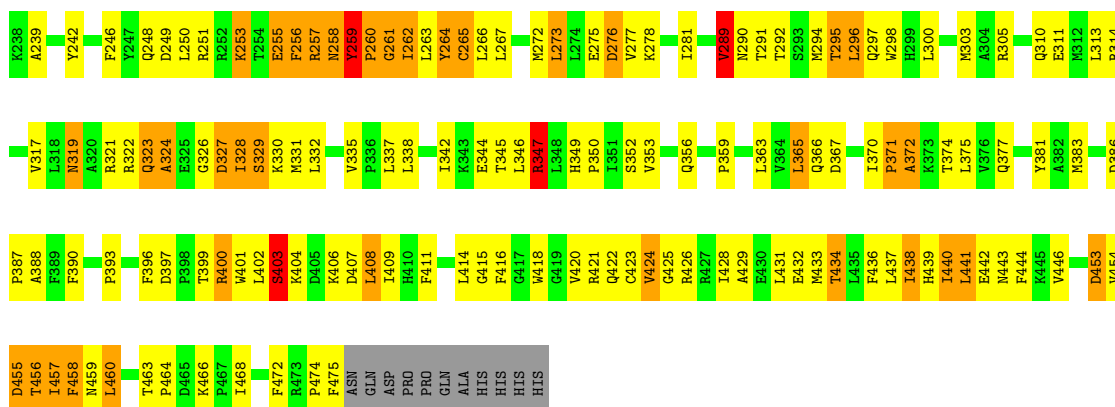
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cholesterol side-chain cleavage enzyme



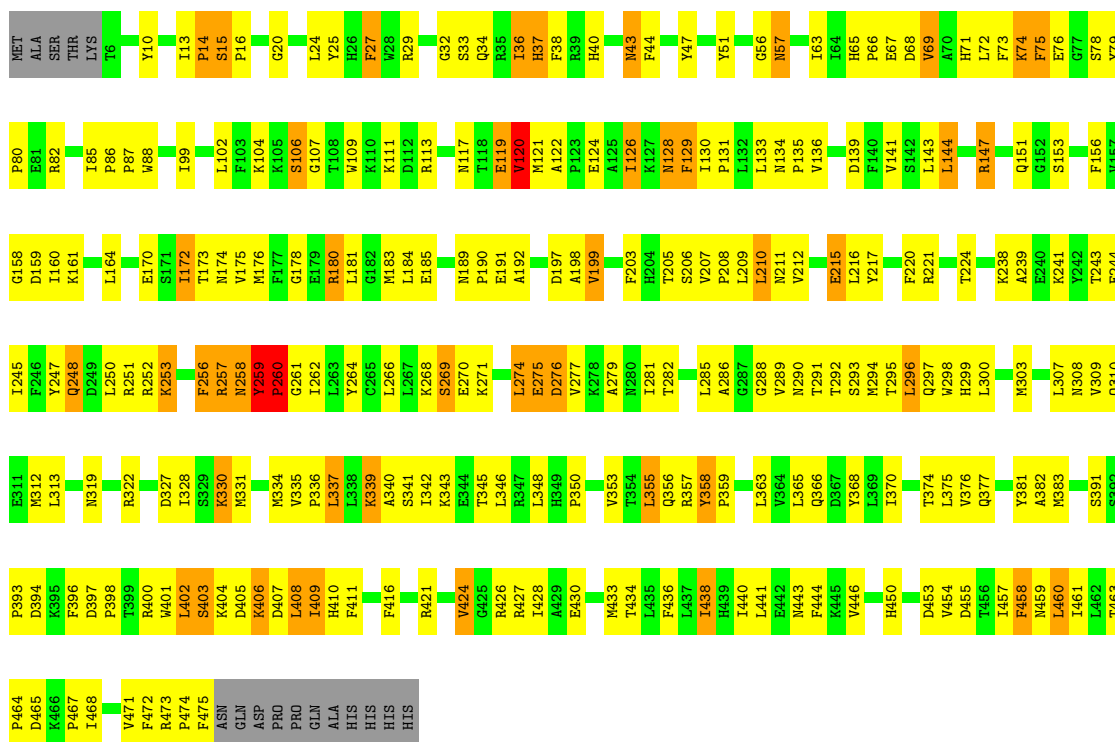
• Molecule 1: Cholesterol side-chain cleavage enzyme





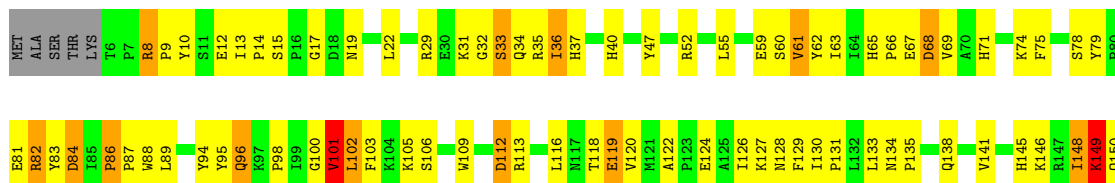
• Molecule 1: Cholesterol side-chain cleavage enzyme

Chain C: 44% 43% 9% ..



• Molecule 1: Cholesterol side-chain cleavage enzyme

Chain D: 41% 44% 9% ..





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.45Å 94.63Å 113.50Å 90.00° 89.96° 90.00°	Depositor
Resolution (Å)	60.01 – 2.50 60.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (60.01-2.50) 99.3 (60.01-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.266 , 0.281 0.260 , 0.278	Depositor DCC
R_{free} test set	4004 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 96.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -l,k,h 0.276 for h,-k,-l 0.000 for -l,-k,-h	Xtriage
Reported twinning fraction	0.546 for H, K, L 0.454 for -h,-k,l	Depositor
Outliers	1 of 80275 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16012	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, IPA, HC9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.28	23/4014 (0.6%)	1.16	19/5435 (0.3%)
1	B	1.13	12/4014 (0.3%)	1.14	25/5435 (0.5%)
1	C	1.24	15/4014 (0.4%)	1.18	24/5435 (0.4%)
1	D	1.19	18/4014 (0.4%)	1.17	28/5435 (0.5%)
All	All	1.21	68/16056 (0.4%)	1.16	96/21740 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	VAL	CA-CB	-17.47	1.35	1.54
1	D	156	PHE	C-N	12.01	1.50	1.33
1	C	260	PRO	N-CA	9.87	1.59	1.47
1	C	259	TYR	CA-C	8.99	1.61	1.52
1	D	212	VAL	CA-CB	8.43	1.65	1.54
1	A	289	VAL	N-CA	8.26	1.56	1.46
1	C	350	PRO	CA-C	-8.21	1.43	1.52
1	C	212	VAL	CA-CB	7.49	1.63	1.54
1	A	351	ILE	CA-CB	-7.44	1.45	1.54
1	A	260	PRO	N-CA	7.25	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	VAL	N-CA	7.16	1.54	1.46
1	A	342	ILE	CA-CB	-7.01	1.44	1.54
1	A	350	PRO	N-CA	-6.91	1.39	1.47
1	A	460	LEU	C-O	6.77	1.32	1.24
1	B	349	HIS	CA-CB	6.77	1.62	1.53
1	A	88	TRP	CA-C	-6.72	1.44	1.52
1	B	350	PRO	CA-C	-6.59	1.44	1.52
1	B	438	ILE	CA-CB	6.54	1.62	1.54
1	D	349	HIS	CA-CB	6.45	1.60	1.53
1	B	207	VAL	CA-CB	-6.43	1.45	1.54
1	B	260	PRO	N-CA	6.36	1.55	1.47
1	D	438	ILE	CA-CB	6.30	1.61	1.54
1	A	349	HIS	CA-CB	6.27	1.61	1.53
1	C	463	THR	CA-CB	-6.09	1.46	1.53
1	B	352	SER	CA-C	-6.05	1.45	1.52
1	C	69	VAL	CA-CB	6.04	1.61	1.54
1	C	382	ALA	N-CA	5.95	1.53	1.46
1	D	84	ASP	CA-C	5.92	1.60	1.52
1	D	354	THR	CA-C	5.86	1.59	1.52
1	D	350	PRO	C-O	-5.77	1.17	1.23
1	A	346	LEU	CA-C	5.67	1.60	1.52
1	C	458	PHE	CA-C	-5.66	1.45	1.52
1	D	292	THR	C-O	5.65	1.30	1.24
1	C	350	PRO	N-CA	-5.59	1.40	1.47
1	C	458	PHE	CA-CB	5.56	1.60	1.53
1	B	458	PHE	CA-CB	5.56	1.61	1.53
1	D	86	PRO	CA-C	5.54	1.57	1.52
1	D	375	LEU	CA-C	-5.51	1.46	1.52
1	A	288	GLY	N-CA	5.49	1.52	1.45
1	C	335	VAL	CA-C	5.49	1.58	1.52
1	A	458	PHE	CA-CB	5.47	1.60	1.53
1	D	259	TYR	CA-C	5.46	1.59	1.52
1	A	353	VAL	CA-CB	5.36	1.60	1.54
1	A	172	ILE	CA-CB	5.36	1.61	1.54
1	D	89	LEU	CA-C	-5.35	1.45	1.52
1	A	462	LEU	C-O	5.35	1.30	1.24
1	D	418	TRP	CA-C	-5.35	1.46	1.52
1	B	61	VAL	C-O	-5.34	1.17	1.24
1	D	460	LEU	C-O	5.29	1.30	1.24
1	A	418	TRP	CA-C	-5.28	1.46	1.52
1	A	355	LEU	N-CA	5.26	1.52	1.46
1	B	264	TYR	C-O	5.26	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	LEU	CA-C	5.24	1.59	1.52
1	A	292	THR	C-O	5.21	1.30	1.24
1	B	377	GLN	CA-C	-5.21	1.46	1.52
1	B	212	VAL	CA-CB	5.20	1.60	1.54
1	B	260	PRO	CA-C	-5.20	1.46	1.52
1	C	38	PHE	CA-C	5.19	1.59	1.52
1	D	418	TRP	N-CA	5.18	1.52	1.46
1	C	358	TYR	CA-C	5.18	1.59	1.52
1	C	345	THR	CA-CB	5.16	1.61	1.53
1	D	350	PRO	CA-C	-5.14	1.45	1.52
1	D	352	SER	CA-C	-5.09	1.46	1.52
1	D	350	PRO	N-CA	-5.08	1.41	1.47
1	C	172	ILE	CA-CB	5.07	1.60	1.54
1	A	429	ALA	CA-C	-5.05	1.46	1.52
1	A	290	ASN	N-CA	5.05	1.52	1.46
1	A	212	VAL	CA-CB	5.03	1.60	1.54

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	PHE	CA-C-O	17.09	142.28	121.60
1	C	289	VAL	N-CA-C	14.87	125.24	110.82
1	D	156	PHE	O-C-N	-11.34	106.71	122.81
1	A	69	VAL	N-CA-C	-11.10	100.10	110.53
1	A	289	VAL	N-CA-C	11.05	121.96	110.36
1	D	289	VAL	N-CA-C	10.17	120.16	110.30
1	B	228	HIS	N-CA-C	-9.29	100.27	111.69
1	A	260	PRO	N-CA-C	8.66	130.32	112.47
1	C	69	VAL	N-CA-C	-8.66	102.86	110.74
1	A	258	ASN	N-CA-C	8.54	128.99	110.80
1	C	158	GLY	N-CA-C	8.39	120.94	110.96
1	C	260	PRO	N-CA-C	8.16	129.27	112.47
1	A	206	SER	N-CA-C	-8.00	104.05	113.88
1	D	269	SER	N-CA-C	-8.00	105.50	114.62
1	B	258	ASN	N-CA-C	7.79	125.35	113.51
1	D	345	THR	N-CA-C	-7.60	102.35	111.69
1	D	261	GLY	N-CA-C	-7.58	95.23	113.18
1	C	424	VAL	CB-CA-C	-7.42	102.32	112.04
1	A	197	ASP	N-CA-C	-7.40	104.25	113.28
1	A	343	LYS	N-CA-C	-7.38	102.19	112.45
1	B	403	SER	N-CA-C	7.35	126.46	110.80
1	D	260	PRO	N-CA-C	7.26	126.00	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	VAL	N-CA-C	7.23	124.38	109.34
1	C	319	ASN	N-CA-C	-7.17	104.66	113.41
1	D	388	ALA	N-CA-C	-6.89	104.69	113.23
1	D	258	ASN	N-CA-C	6.79	125.27	110.80
1	B	434	THR	N-CA-C	-6.71	103.43	111.69
1	B	420	VAL	N-CA-C	6.61	119.35	111.09
1	A	247	TYR	N-CA-C	-6.55	104.06	111.07
1	B	436	PHE	N-CA-C	-6.54	105.46	113.50
1	D	149	LYS	N-CA-C	-6.53	104.56	113.30
1	D	325	GLU	N-CA-C	6.51	119.16	111.02
1	D	82	ARG	N-CA-C	-6.47	100.63	109.95
1	D	304	ALA	N-CA-C	6.41	118.34	111.36
1	D	434	THR	N-CA-C	-6.40	104.23	111.14
1	C	269	SER	CB-CA-C	6.32	119.64	109.27
1	C	37	HIS	N-CA-C	6.25	117.75	111.07
1	C	106	SER	N-CA-C	6.16	117.67	108.31
1	B	347	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	B	455	ASP	N-CA-C	-6.10	101.17	110.14
1	A	353	VAL	N-CA-C	-6.07	104.82	110.53
1	D	55	LEU	N-CA-C	-6.07	99.50	109.40
1	D	438	ILE	N-CA-C	-6.02	104.76	110.42
1	B	260	PRO	N-CA-C	6.02	119.89	110.80
1	C	197	ASP	N-CA-C	-6.01	104.10	112.45
1	B	249	ASP	N-CA-C	-5.96	106.61	114.31
1	D	141	VAL	CB-CA-C	-5.96	104.33	111.97
1	D	61	VAL	CB-CA-C	-5.96	101.36	110.95
1	C	106	SER	CB-CA-C	-5.95	109.70	116.54
1	C	206	SER	N-CA-C	-5.93	103.50	112.04
1	B	406	LYS	N-CA-C	-5.85	103.94	113.19
1	B	441	LEU	N-CA-C	-5.81	106.15	113.18
1	A	277	VAL	N-CA-C	-5.80	105.08	110.53
1	C	297	GLN	N-CA-C	5.69	117.48	111.28
1	C	129	PHE	N-CA-C	-5.69	106.21	114.12
1	B	69	VAL	N-CA-C	-5.67	104.82	111.00
1	D	406	LYS	N-CA-C	-5.66	105.96	112.92
1	A	450	HIS	N-CA-C	5.62	115.53	108.45
1	C	424	VAL	N-CA-C	5.62	117.02	110.62
1	D	195	PHE	N-CA-C	-5.61	106.56	113.41
1	B	388	ALA	N-CA-C	-5.59	106.22	113.16
1	C	382	ALA	N-CA-C	5.54	117.32	111.28
1	A	333	GLN	N-CA-C	-5.51	105.34	113.61
1	C	27	PHE	N-CA-C	-5.49	104.13	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	ASP	N-CA-C	-5.45	106.76	113.41
1	D	69	VAL	N-CA-C	-5.45	105.41	110.53
1	C	421	ARG	N-CA-C	-5.43	103.93	110.88
1	A	388	ALA	N-CA-C	-5.39	106.71	113.28
1	B	261	GLY	N-CA-C	-5.39	100.41	113.18
1	D	348	LEU	N-CA-C	5.37	118.62	111.75
1	A	138	GLN	N-CA-C	-5.36	104.86	111.40
1	A	183	MET	N-CA-C	-5.35	106.71	113.18
1	B	256	PHE	N-CA-C	5.34	116.11	108.74
1	B	220	PHE	N-CA-C	5.32	119.46	112.92
1	C	438	ILE	N-CA-C	-5.29	105.34	110.42
1	B	324	ALA	N-CA-C	-5.28	108.10	114.75
1	A	408	LEU	N-CA-C	-5.27	107.02	113.50
1	B	420	VAL	CB-CA-C	-5.27	103.73	112.26
1	D	84	ASP	N-CA-C	5.25	117.88	108.17
1	C	126	ILE	CB-CA-C	-5.22	105.13	111.87
1	C	343	LYS	N-CA-C	-5.22	105.03	111.40
1	C	455	ASP	N-CA-C	-5.21	101.74	109.96
1	A	314	ARG	N-CA-C	-5.20	105.69	111.36
1	C	43	ASN	N-CA-C	5.20	117.69	111.71
1	D	156	PHE	CA-C-N	-5.19	112.62	121.97
1	D	156	PHE	C-N-CA	-5.19	112.62	121.97
1	B	371	PRO	N-CA-C	5.11	118.87	110.55
1	C	247	TYR	N-CA-C	-5.10	104.80	111.02
1	D	119	GLU	N-CA-C	5.09	118.75	112.54
1	A	366	GLN	N-CA-C	-5.09	99.97	110.80
1	B	438	ILE	N-CA-C	-5.09	105.75	110.53
1	B	425	GLY	N-CA-C	-5.08	106.93	115.62
1	B	239	ALA	N-CA-C	-5.05	106.46	113.18
1	D	457	ILE	N-CA-C	-5.05	100.64	108.81
1	B	418	TRP	N-CA-C	5.04	116.19	108.52
1	A	354	THR	N-CA-C	5.00	116.59	109.14

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	TYR	Peptide
1	B	259	TYR	Peptide
1	C	259	TYR	Peptide
1	D	259	TYR	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	3904	0	3910	201	0
1	B	3904	0	3910	279	0
1	C	3904	0	3910	222	0
1	D	3904	0	3910	245	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	5	0
3	A	29	0	46	2	0
3	B	29	0	46	2	0
3	C	29	0	45	5	0
3	D	29	0	45	1	0
4	A	4	0	8	1	0
4	B	4	0	8	7	0
4	C	4	0	8	5	0
4	D	4	0	8	3	0
5	A	25	0	0	1	0
5	B	15	0	0	1	0
5	C	27	0	0	2	0
5	D	25	0	0	3	0
All	All	16012	0	15974	932	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 29.

All (932) 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:128:ASN:HB3	1:B:260:PRO:CG	1.22	1.61
1:B:128:ASN:HB3	1:B:260:PRO:CD	1.31	1.60
1:B:128:ASN:CB	1:B:260:PRO:CG	1.83	1.55
1:B:128:ASN:CB	1:B:260:PRO:HG2	1.42	1.45
1:D:156:PHE:O	1:D:157:VAL:HG23	1.47	1.12
1:B:128:ASN:HB2	1:B:260:PRO:HG2	1.14	1.10
1:A:128:ASN:HB3	1:A:260:PRO:CD	1.82	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:HG3	1:C:253:LYS:O	1.50	1.08
1:D:79:TYR:CD1	1:D:106:SER:HA	1.91	1.04
1:B:313:LEU:O	1:B:317:VAL:HG23	1.59	1.03
1:B:128:ASN:CB	1:B:260:PRO:HG3	1.88	1.02
1:B:120:VAL:HG12	1:B:262:ILE:HD13	1.41	1.02
1:B:128:ASN:CB	1:B:260:PRO:CD	2.27	1.02
1:A:326:GLY:HA3	1:A:330:LYS:HD2	1.43	1.00
1:C:65:HIS:HB2	1:C:68:ASP:OD2	1.61	1.00
1:B:128:ASN:HB3	1:B:260:PRO:HD3	1.42	0.99
1:D:156:PHE:O	1:D:157:VAL:CG2	2.09	0.99
1:B:88:TRP:CH2	1:B:460:LEU:HD11	1.98	0.98
1:D:262:ILE:HD12	1:D:262:ILE:H	1.28	0.98
1:B:141:VAL:HG11	1:B:443:ASN:ND2	1.78	0.98
1:C:67:GLU:HG2	1:D:67:GLU:OE1	1.61	0.98
1:B:180:ARG:HB3	1:B:180:ARG:HH21	1.25	0.97
1:B:305:ARG:NH1	5:B:572:HOH:O	1.95	0.97
1:B:116:LEU:HD13	1:B:272:MET:HE1	1.47	0.96
1:C:383:MET:HE2	4:C:502:IPA:H13	1.48	0.95
1:B:166:HIS:CD2	1:B:183:MET:HE3	2.01	0.94
1:D:128:ASN:OD1	1:D:260:PRO:CG	2.17	0.93
1:B:257:ARG:HG2	1:B:257:ARG:HH11	1.30	0.93
1:D:257:ARG:O	1:D:258:ASN:HB3	1.67	0.93
1:A:411:PHE:CE2	1:B:408:LEU:HD22	2.04	0.92
1:B:253:LYS:HD2	1:B:256:PHE:HE2	1.34	0.90
1:C:128:ASN:HB3	1:C:260:PRO:HG2	1.54	0.89
1:C:248:GLN:HE21	1:C:251:ARG:HG2	1.38	0.88
1:C:342:ILE:O	1:C:346:LEU:HD23	1.74	0.88
1:A:113:ARG:O	1:A:117:ASN:ND2	2.05	0.88
1:B:386:ASP:OD1	1:B:387:PRO:HD2	1.74	0.88
1:C:129:PHE:CZ	1:C:262:ILE:HD11	2.08	0.87
1:D:259:TYR:OH	1:D:264:TYR:HB2	1.74	0.87
1:A:128:ASN:HB3	1:A:260:PRO:HD2	1.56	0.87
1:C:209:LEU:HD11	1:C:224:THR:HG22	1.57	0.86
1:A:189:ASN:HD22	1:A:190:PRO:HD2	1.40	0.86
1:C:205:THR:O	1:C:209:LEU:HD12	1.76	0.86
1:B:128:ASN:HB2	1:B:260:PRO:CG	1.77	0.86
1:D:353:VAL:HG13	1:D:462:LEU:HD21	1.59	0.85
1:A:365:LEU:HD23	1:A:370:ILE:HG13	1.55	0.85
1:B:259:TYR:CE1	1:B:261:GLY:HA3	2.12	0.84
1:C:303:MET:HE1	1:C:441:LEU:HD21	1.57	0.84
1:D:383:MET:HE2	4:D:502:IPA:H33	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:GLU:HG3	1:D:105:LYS:HE2	1.60	0.83
1:C:436:PHE:CE2	1:C:440:ILE:HG13	2.13	0.83
1:C:474:PRO:O	1:C:475:PHE:HB2	1.76	0.83
1:B:88:TRP:CH2	1:B:460:LEU:CD1	2.61	0.83
1:D:128:ASN:CB	1:D:260:PRO:HG2	2.09	0.83
1:D:289:VAL:O	1:D:293:SER:OG	1.96	0.82
1:C:248:GLN:HA	1:C:251:ARG:HB3	1.59	0.82
1:D:128:ASN:HB3	1:D:260:PRO:HD2	1.62	0.82
1:D:175:VAL:O	1:D:261:GLY:HA2	1.80	0.82
1:C:356:GLN:HG3	1:C:377:GLN:HE21	1.46	0.80
1:B:453:ASP:OD2	1:B:466:LYS:HE2	1.80	0.80
1:A:324:ALA:O	1:A:326:GLY:N	2.14	0.80
1:B:383:MET:HE2	4:B:502:IPA:C1	2.12	0.80
1:B:88:TRP:CZ2	1:B:460:LEU:HD11	2.16	0.80
1:A:88:TRP:CZ2	1:A:460:LEU:CD1	2.66	0.79
1:B:383:MET:HE2	4:B:502:IPA:H13	1.65	0.78
1:C:128:ASN:OD1	1:C:260:PRO:HD2	1.84	0.78
1:D:408:LEU:O	5:D:570:HOH:O	2.02	0.77
1:D:426:ARG:O	1:D:430:GLU:HG3	1.84	0.77
1:D:170:GLU:OE1	1:D:180:ARG:NH2	2.18	0.77
1:D:313:LEU:O	1:D:317:VAL:HG23	1.84	0.77
1:A:436:PHE:CE2	1:A:440:ILE:HG13	2.20	0.76
1:B:200:TYR:HB2	1:B:290:ASN:HD21	1.48	0.76
1:B:253:LYS:HD2	1:B:256:PHE:CE2	2.20	0.76
1:B:119:GLU:HG3	1:B:266:LEU:HD23	1.68	0.76
1:A:88:TRP:CZ2	1:A:460:LEU:HD11	2.21	0.76
1:A:148:ILE:HG23	1:A:155:LYS:N	2.01	0.76
1:C:129:PHE:HZ	1:C:262:ILE:HD11	1.49	0.76
1:C:121:MET:SD	1:C:427:ARG:HD3	2.26	0.75
1:A:261:GLY:O	1:A:264:TYR:N	2.17	0.75
1:B:257:ARG:HG2	1:B:257:ARG:NH1	1.91	0.75
1:A:408:LEU:HD11	1:B:70:ALA:HA	1.69	0.75
1:C:73:PHE:O	1:C:76:GLU:HG2	1.87	0.75
1:D:84:ASP:HB2	5:D:529:HOH:O	1.86	0.75
1:A:257:ARG:O	1:A:258:ASN:HB2	1.87	0.74
1:A:128:ASN:CB	1:A:260:PRO:HG2	2.17	0.74
1:B:291:THR:O	1:B:295:THR:OG1	2.03	0.74
1:B:314:ARG:HH21	1:B:314:ARG:HG3	1.51	0.74
1:A:324:ALA:C	1:A:326:GLY:H	1.94	0.74
1:D:148:ILE:HD11	1:D:155:LYS:HA	1.69	0.74
1:A:128:ASN:HB3	1:A:260:PRO:CG	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:VAL:CG1	1:B:443:ASN:ND2	2.51	0.74
1:B:127:LYS:O	1:B:130:ILE:HD12	1.87	0.74
1:C:220:PHE:O	1:C:221:ARG:HG2	1.87	0.74
1:C:409:ILE:HD13	1:C:410:HIS:H	1.52	0.74
1:A:342:ILE:HG22	1:A:342:ILE:O	1.86	0.73
1:D:79:TYR:CD1	1:D:106:SER:CA	2.71	0.73
1:D:434:THR:O	1:D:438:ILE:HG12	1.89	0.73
1:B:365:LEU:HD23	1:B:370:ILE:HG13	1.70	0.73
1:A:309:VAL:HA	1:A:312:MET:HE2	1.71	0.73
1:D:128:ASN:HB3	1:D:260:PRO:CD	2.18	0.73
1:C:65:HIS:CB	1:C:68:ASP:OD2	2.36	0.73
1:A:390:PHE:HZ	4:A:502:IPA:H13	1.52	0.72
1:B:202:MET:HE1	1:B:203:PHE:CE2	2.24	0.72
1:A:474:PRO:O	1:A:475:PHE:HB2	1.89	0.72
1:C:15:SER:O	1:C:47:TYR:CE1	2.43	0.72
1:B:166:HIS:CD2	1:B:183:MET:CE	2.72	0.72
1:B:328:ILE:HD12	1:B:328:ILE:H	1.53	0.72
1:D:306:SER:O	1:D:309:VAL:HG12	1.88	0.72
1:C:71:HIS:CD2	1:C:75:PHE:CE1	2.78	0.71
1:C:327:ASP:HB3	1:C:330:LYS:CD	2.21	0.71
1:A:319:ASN:O	1:A:323:GLN:HB3	1.91	0.71
1:C:66:PRO:HD2	1:D:67:GLU:OE2	1.90	0.71
1:A:33:SER:HB2	5:A:533:HOH:O	1.91	0.71
1:B:328:ILE:HA	1:B:331:MET:HG2	1.71	0.70
1:B:50:ILE:HD11	1:B:61:VAL:HG11	1.73	0.70
1:C:430:GLU:O	1:C:434:THR:OG1	2.04	0.70
1:A:411:PHE:HE2	1:B:408:LEU:HD22	1.56	0.70
1:C:207:VAL:HA	1:C:210:LEU:HD22	1.72	0.70
1:C:426:ARG:O	1:C:430:GLU:HG3	1.90	0.70
1:B:200:TYR:CD1	1:B:200:TYR:O	2.44	0.70
1:B:88:TRP:CZ2	1:B:460:LEU:CD1	2.74	0.70
1:D:348:LEU:H	1:D:348:LEU:HD12	1.57	0.70
1:A:133:LEU:HD21	1:A:175:VAL:HG21	1.72	0.69
1:A:218:ARG:C	1:A:219:LEU:HD12	2.17	0.69
1:B:319:ASN:O	1:B:323:GLN:HG2	1.93	0.69
1:C:239:ALA:HB1	1:C:282:THR:HG22	1.74	0.69
1:D:207:VAL:HB	1:D:208:PRO:HD3	1.75	0.69
1:C:208:PRO:HG2	1:C:224:THR:HG21	1.73	0.69
1:C:303:MET:HE2	1:C:310:GLN:HA	1.74	0.69
1:A:259:TYR:CZ	1:A:261:GLY:HA3	2.28	0.68
1:A:354:THR:HG22	1:A:379:ALA:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ASN:N	1:C:57:ASN:OD1	2.27	0.68
1:C:383:MET:HE2	4:C:502:IPA:C1	2.23	0.68
1:A:323:GLN:HE21	1:A:334:MET:HE1	1.58	0.68
1:B:129:PHE:CZ	1:B:262:ILE:HD11	2.27	0.68
1:D:128:ASN:OD1	1:D:260:PRO:CD	2.42	0.68
1:B:170:GLU:HG2	1:B:183:MET:HB2	1.75	0.68
1:D:19:ASN:HB3	1:D:22:LEU:CB	2.23	0.68
1:C:391:SER:O	1:C:400:ARG:NH2	2.27	0.68
1:D:119:GLU:OE2	1:D:265:CYS:HB3	1.94	0.68
1:A:176:MET:HA	1:A:262:ILE:HB	1.76	0.67
1:C:253:LYS:O	1:C:253:LYS:CG	2.33	0.67
1:B:134:ASN:N	1:B:135:PRO:HD2	2.08	0.67
1:B:327:ASP:HB3	1:B:330:LYS:NZ	2.10	0.67
1:D:216:LEU:HD13	1:D:220:PHE:HE1	1.60	0.67
1:C:120:VAL:CG2	1:C:428:ILE:HD11	2.25	0.67
1:A:315:GLU:O	1:A:319:ASN:HB2	1.95	0.67
1:A:342:ILE:O	1:A:342:ILE:CG2	2.43	0.67
1:A:75:PHE:CD1	1:A:363:LEU:HD13	2.30	0.67
1:A:88:TRP:CZ2	1:A:460:LEU:HD12	2.30	0.67
1:D:32:GLY:O	1:D:33:SER:C	2.38	0.67
1:D:437:LEU:O	1:D:441:LEU:HD12	1.95	0.67
1:D:36:ILE:O	1:D:40:HIS:CD2	2.48	0.67
1:B:423:CYS:HB2	2:B:500:HEM:NA	2.09	0.66
1:A:430:GLU:O	1:A:434:THR:OG1	2.13	0.66
1:C:180:ARG:HH21	1:C:180:ARG:HB3	1.60	0.66
1:C:82:ARG:HH21	2:C:500:HEM:CGA	2.09	0.66
1:B:411:PHE:CE1	1:B:414:LEU:HD11	2.31	0.66
1:C:457:ILE:HG23	1:C:459:ASN:ND2	2.11	0.66
1:D:128:ASN:OD1	1:D:260:PRO:HG2	1.93	0.66
1:D:220:PHE:O	1:D:221:ARG:HD2	1.96	0.66
1:C:409:ILE:HD13	1:C:410:HIS:N	2.10	0.65
1:A:175:VAL:HG12	1:A:262:ILE:HD12	1.79	0.65
1:A:60:SER:OG	1:A:62:TYR:CE2	2.50	0.65
1:C:71:HIS:CD2	1:C:75:PHE:HE1	2.13	0.65
1:B:248:GLN:OE1	1:B:251:ARG:HD2	1.96	0.65
1:B:82:ARG:NH2	1:B:421:ARG:HG2	2.12	0.65
1:B:322:ARG:C	1:B:324:ALA:H	2.04	0.65
1:B:172:ILE:O	1:B:176:MET:HB2	1.97	0.65
1:D:262:ILE:H	1:D:262:ILE:CD1	2.04	0.65
1:B:253:LYS:CD	1:B:256:PHE:HE2	2.08	0.64
1:D:150:GLN:O	1:D:150:GLN:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ASP:OD2	1:D:161:LYS:HB2	1.96	0.64
1:C:471:VAL:HG11	1:C:473:ARG:HH12	1.61	0.64
1:C:147:ARG:HB3	1:C:156:PHE:CD2	2.33	0.64
1:C:215:GLU:CD	1:C:215:GLU:H	2.04	0.64
1:D:418:TRP:CD1	1:D:419:GLY:N	2.66	0.64
1:A:318:LEU:HD23	1:A:442:GLU:HG2	1.79	0.64
1:B:189:ASN:N	1:B:189:ASN:HD22	1.93	0.64
1:B:314:ARG:HH22	1:B:441:LEU:HA	1.63	0.64
1:C:85:ILE:HG22	1:C:87:PRO:HD2	1.79	0.64
1:C:296:LEU:HD22	1:C:433:MET:HG2	1.78	0.64
1:C:248:GLN:NE2	1:C:251:ARG:HG2	2.12	0.64
1:B:294:MET:SD	1:B:463:THR:HG22	2.37	0.63
1:B:290:ASN:O	1:B:294:MET:HG2	1.99	0.63
1:C:102:LEU:HD22	3:C:501:HC9:H27A	1.80	0.63
1:C:327:ASP:HB3	1:C:330:LYS:HD3	1.80	0.63
1:C:259:TYR:H	1:C:259:TYR:HD2	1.45	0.63
1:C:259:TYR:CE1	1:C:261:GLY:HA3	2.34	0.63
1:B:314:ARG:HG3	1:B:441:LEU:O	1.99	0.63
1:D:100:GLY:O	1:D:102:LEU:N	2.32	0.63
1:B:36:ILE:HG23	1:B:37:HIS:N	2.12	0.63
1:D:397:ASP:O	1:D:400:ARG:HG2	1.98	0.63
1:A:110:LYS:O	1:A:114:VAL:HG23	1.99	0.63
1:A:176:MET:HG3	1:A:262:ILE:HB	1.81	0.63
1:B:310:GLN:HE22	1:B:446:VAL:H	1.46	0.63
1:C:120:VAL:HG22	1:C:428:ILE:HD11	1.79	0.63
1:C:239:ALA:O	1:C:243:THR:HG22	1.98	0.63
1:D:347:ARG:O	1:D:350:PRO:HD3	1.99	0.63
1:D:403:SER:O	1:D:405:ASP:OD2	2.17	0.63
1:D:430:GLU:O	1:D:434:THR:OG1	2.09	0.63
1:C:36:ILE:HG22	1:C:37:HIS:N	2.14	0.63
1:C:290:ASN:O	1:C:294:MET:HB2	1.99	0.62
1:A:126:ILE:HD11	1:A:427:ARG:HB3	1.81	0.62
1:D:354:THR:HG21	1:D:377:GLN:HE21	1.64	0.62
1:B:144:LEU:O	1:B:148:ILE:HG23	1.99	0.62
1:B:257:ARG:HH11	1:B:257:ARG:CG	2.07	0.62
1:A:128:ASN:HB2	1:A:260:PRO:HG2	1.81	0.62
1:A:423:CYS:HB3	1:A:426:ARG:HB2	1.80	0.62
1:A:446:VAL:HA	1:A:471:VAL:O	1.99	0.62
1:D:292:THR:O	1:D:296:LEU:HB2	1.99	0.62
1:A:88:TRP:HZ2	1:A:460:LEU:HD12	1.62	0.62
1:B:346:LEU:HD23	1:B:415:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:LEU:HB2	1:C:370:ILE:CD1	2.30	0.62
1:C:383:MET:CE	4:C:502:IPA:H32	2.29	0.62
1:D:216:LEU:HD13	1:D:220:PHE:CE1	2.34	0.62
1:B:180:ARG:HB3	1:B:180:ARG:NH2	2.07	0.62
1:C:85:ILE:HD11	3:C:501:HC9:H7	1.82	0.62
1:B:189:ASN:HD22	1:B:189:ASN:H	1.46	0.62
1:B:347:ARG:HA	4:B:502:IPA:H31	1.81	0.62
1:B:88:TRP:HH2	1:B:460:LEU:CD1	2.10	0.62
1:A:426:ARG:O	1:A:430:GLU:HG3	1.99	0.62
1:D:196:ILE:HG23	1:D:289:VAL:HG11	1.82	0.62
1:A:128:ASN:CB	1:A:260:PRO:CG	2.78	0.61
1:A:386:ASP:OD2	1:A:387:PRO:HD2	2.00	0.61
1:C:119:GLU:HG2	1:C:266:LEU:HG	1.81	0.61
1:C:160:ILE:HG12	1:C:164:LEU:HG	1.82	0.61
1:D:423:CYS:HB3	1:D:426:ARG:HB2	1.82	0.61
1:A:402:LEU:HA	1:A:404:LYS:HE3	1.82	0.61
1:B:8:ARG:HH21	1:B:367:ASP:HB3	1.65	0.61
1:C:76:GLU:OE1	1:C:80:PRO:CG	2.48	0.61
1:A:233:ASP:O	1:A:237:ASN:ND2	2.33	0.61
1:B:383:MET:CE	4:B:502:IPA:C1	2.79	0.61
1:D:19:ASN:HB3	1:D:22:LEU:HB3	1.81	0.61
1:D:212:VAL:HG11	1:D:221:ARG:HE	1.66	0.61
1:C:208:PRO:HB2	1:C:221:ARG:HH21	1.64	0.61
1:C:113:ARG:O	1:C:113:ARG:HG3	2.00	0.61
1:D:79:TYR:CG	1:D:106:SER:HA	2.34	0.61
1:A:119:GLU:OE2	1:A:265:CYS:HB3	1.99	0.61
1:B:141:VAL:HG11	1:B:443:ASN:HD22	1.64	0.61
1:C:208:PRO:O	1:C:221:ARG:HD2	2.00	0.61
1:D:128:ASN:CG	1:D:260:PRO:HG2	2.26	0.61
1:B:263:LEU:HD13	1:B:281:ILE:HD11	1.82	0.61
1:C:259:TYR:O	1:C:259:TYR:CD2	2.54	0.61
1:B:438:ILE:O	1:B:442:GLU:HB2	2.01	0.61
1:B:160:ILE:HG13	1:B:164:LEU:HG	1.83	0.60
1:C:342:ILE:O	1:C:346:LEU:CD2	2.49	0.60
1:D:180:ARG:HB3	1:D:180:ARG:HH21	1.65	0.60
1:D:353:VAL:CG1	1:D:462:LEU:HD21	2.30	0.60
1:B:8:ARG:HE	1:B:367:ASP:HB3	1.65	0.60
1:D:176:MET:HE1	1:D:281:ILE:HA	1.82	0.60
1:D:435:LEU:O	1:D:438:ILE:N	2.25	0.60
1:D:349:HIS:N	1:D:350:PRO:HD3	2.17	0.60
1:B:344:GLU:OE1	1:B:347:ARG:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:THR:O	1:C:295:THR:OG1	2.10	0.60
1:D:153:SER:O	1:D:154:GLY:C	2.44	0.60
1:A:261:GLY:O	1:A:262:ILE:C	2.44	0.60
1:A:270:GLU:O	1:A:270:GLU:HG2	2.02	0.60
1:C:143:LEU:O	1:C:147:ARG:HG2	2.02	0.60
1:B:32:GLY:O	1:B:34:GLN:N	2.35	0.60
1:B:113:ARG:NH1	1:B:424:VAL:HG22	2.16	0.60
1:D:250:LEU:O	1:D:254:THR:HB	2.01	0.60
1:B:128:ASN:CB	1:B:260:PRO:HD3	2.14	0.59
1:B:259:TYR:OH	1:B:264:TYR:HB2	2.02	0.59
1:B:345:THR:OG1	1:B:396:PHE:HE2	1.85	0.59
1:D:172:ILE:HA	1:D:175:VAL:HG12	1.83	0.59
1:D:199:VAL:HA	1:D:235:ILE:HD11	1.84	0.59
1:D:298:TRP:CZ3	1:D:349:HIS:CE1	2.90	0.59
1:B:383:MET:CE	4:B:502:IPA:H11	2.32	0.59
1:B:386:ASP:OD1	1:B:387:PRO:CD	2.49	0.59
1:D:134:ASN:N	1:D:135:PRO:HD2	2.18	0.59
1:A:422:GLN:NE2	1:A:426:ARG:HH21	2.00	0.59
1:B:262:ILE:O	1:B:266:LEU:HG	2.02	0.59
1:C:241:LYS:O	1:C:244:GLU:HB3	2.02	0.59
1:D:60:SER:HB2	1:D:375:LEU:HD23	1.85	0.59
1:B:147:ARG:O	1:B:151:GLN:HG2	2.03	0.58
1:C:160:ILE:O	1:C:161:LYS:C	2.46	0.58
1:D:327:ASP:OD1	1:D:327:ASP:C	2.46	0.58
1:A:8:ARG:NH2	1:A:12:GLU:OE1	2.36	0.58
1:D:298:TRP:CE3	1:D:349:HIS:CE1	2.91	0.58
1:B:141:VAL:CG1	1:B:443:ASN:HD22	2.16	0.58
1:B:429:ALA:O	1:B:433:MET:HG3	2.02	0.58
1:C:134:ASN:N	1:C:135:PRO:HD2	2.18	0.58
1:D:81:GLU:CG	1:D:105:LYS:HE2	2.32	0.58
1:A:113:ARG:HG3	1:A:117:ASN:HD21	1.68	0.58
1:D:88:TRP:CZ2	1:D:460:LEU:HD12	2.39	0.58
1:D:96:GLN:H	1:D:96:GLN:HE21	1.52	0.58
1:C:348:LEU:HD21	1:C:393:PRO:O	2.04	0.58
1:D:128:ASN:HB3	1:D:260:PRO:CG	2.34	0.58
1:B:328:ILE:O	1:B:329:SER:C	2.47	0.58
1:B:454:VAL:HA	1:B:466:LYS:NZ	2.19	0.58
1:D:383:MET:HE2	4:D:502:IPA:C3	2.33	0.57
1:A:21:TRP:CE3	1:A:56:GLY:HA2	2.40	0.57
1:A:128:ASN:CB	1:A:260:PRO:CD	2.72	0.57
1:B:144:LEU:HD12	1:B:444:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ARG:O	1:C:359:PRO:HD3	2.04	0.57
1:D:19:ASN:HB3	1:D:22:LEU:HB2	1.85	0.57
1:D:81:GLU:HG3	1:D:105:LYS:CE	2.34	0.57
1:D:135:PRO:HA	1:D:138:GLN:NE2	2.19	0.57
1:C:239:ALA:CB	1:C:282:THR:HG22	2.34	0.57
1:B:321:ARG:HD2	1:B:442:GLU:OE2	2.04	0.57
1:B:154:GLY:O	1:B:155:LYS:HG3	2.04	0.57
1:B:207:VAL:HA	1:B:210:LEU:HD22	1.87	0.57
1:A:189:ASN:ND2	1:A:190:PRO:HD2	2.17	0.57
1:B:328:ILE:HD12	1:B:328:ILE:N	2.20	0.57
1:D:78:SER:O	1:D:79:TYR:HD2	1.87	0.57
1:D:319:ASN:HB3	1:D:323:GLN:OE1	2.05	0.57
1:D:424:VAL:C	1:D:426:ARG:H	2.13	0.57
1:A:215:GLU:CD	1:A:215:GLU:H	2.13	0.56
2:A:500:HEM:HMB1	2:A:500:HEM:HBB2	1.86	0.56
1:D:119:GLU:HA	1:D:119:GLU:OE1	2.04	0.56
1:B:170:GLU:OE1	1:B:180:ARG:NH2	2.38	0.56
1:D:156:PHE:CG	1:D:157:VAL:N	2.73	0.56
1:B:128:ASN:CG	1:B:260:PRO:HG3	2.31	0.56
1:A:337:LEU:HD22	1:A:402:LEU:HD21	1.86	0.56
1:B:119:GLU:OE2	1:B:265:CYS:HB3	2.04	0.56
1:A:15:SER:HB3	1:A:52:ARG:HB2	1.86	0.56
1:A:197:ASP:O	1:A:201:LYS:HB2	2.06	0.56
1:D:296:LEU:HD22	1:D:433:MET:HG2	1.87	0.56
1:D:366:GLN:O	1:D:367:ASP:HB2	2.06	0.56
1:A:318:LEU:O	1:A:322:ARG:HG2	2.06	0.56
1:D:32:GLY:O	1:D:34:GLN:N	2.39	0.56
1:A:230:ALA:O	1:A:233:ASP:HB2	2.05	0.56
1:C:408:LEU:HD22	1:D:411:PHE:CE2	2.41	0.56
1:A:113:ARG:CZ	1:A:424:VAL:HG22	2.35	0.56
1:B:141:VAL:CG2	1:B:439:HIS:HB3	2.36	0.56
1:B:314:ARG:HG3	1:B:314:ARG:NH2	2.18	0.56
1:B:314:ARG:NH2	1:B:441:LEU:HA	2.20	0.56
1:C:250:LEU:HD22	1:C:264:TYR:HD1	1.71	0.56
1:C:457:ILE:HB	1:C:465:ASP:HB3	1.86	0.56
1:D:128:ASN:OD1	1:D:260:PRO:HD3	2.05	0.56
1:B:141:VAL:HG21	1:B:439:HIS:HB3	1.87	0.56
1:B:328:ILE:O	1:B:331:MET:N	2.39	0.56
1:C:292:THR:O	1:C:296:LEU:HB2	2.05	0.56
1:C:454:VAL:HG21	1:C:468:ILE:HD13	1.87	0.56
1:D:118:THR:HA	1:D:122:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:TRP:CD1	1:D:419:GLY:H	2.23	0.56
1:A:463:THR:HB	1:A:464:PRO:HD2	1.86	0.55
1:B:202:MET:HE1	1:B:203:PHE:CD2	2.41	0.55
1:B:202:MET:HG2	1:B:232:TRP:NE1	2.20	0.55
1:B:259:TYR:H	1:B:259:TYR:HD2	1.52	0.55
1:C:129:PHE:CE1	1:C:262:ILE:HD11	2.40	0.55
1:C:461:ILE:HG13	1:C:461:ILE:O	2.05	0.55
1:A:60:SER:OG	1:A:62:TYR:HE2	1.88	0.55
1:A:104:LYS:HE3	1:A:112:ASP:OD1	2.07	0.55
1:A:176:MET:SD	1:A:281:ILE:HG23	2.47	0.55
1:A:324:ALA:C	1:A:326:GLY:N	2.61	0.55
1:B:273:LEU:HB2	1:B:276:ASP:HB2	1.89	0.55
1:D:219:LEU:O	1:D:219:LEU:HD23	2.06	0.55
1:B:319:ASN:N	1:B:319:ASN:HD22	2.04	0.55
1:B:399:THR:O	1:B:401:TRP:N	2.38	0.55
1:A:85:ILE:HG22	1:A:87:PRO:HG2	1.89	0.55
1:C:337:LEU:CD2	1:C:398:PRO:HB2	2.36	0.55
1:D:96:GLN:HE21	1:D:96:GLN:N	2.03	0.55
1:A:67:GLU:HG2	1:B:67:GLU:OE1	2.07	0.55
1:B:95:TYR:O	1:B:97:LYS:HG2	2.06	0.55
1:C:408:LEU:HA	1:D:418:TRP:CZ2	2.42	0.55
1:B:371:PRO:O	1:B:372:ALA:C	2.50	0.55
1:C:411:PHE:CE2	1:D:408:LEU:CD2	2.90	0.55
1:B:119:GLU:CD	1:B:265:CYS:HB3	2.32	0.55
1:D:128:ASN:OD1	1:D:260:PRO:HG3	2.03	0.55
1:D:146:LYS:HA	1:D:149:LYS:NZ	2.22	0.55
1:A:113:ARG:NH1	1:A:424:VAL:HG22	2.22	0.55
1:B:327:ASP:HB3	1:B:330:LYS:HZ1	1.71	0.55
1:B:263:LEU:HD13	1:B:281:ILE:CD1	2.37	0.54
1:B:328:ILE:H	1:B:328:ILE:CD1	2.20	0.54
1:A:110:LYS:HZ3	1:A:114:VAL:HG22	1.72	0.54
1:D:324:ALA:HB1	1:D:330:LYS:HG2	1.89	0.54
1:D:459:ASN:O	1:D:460:LEU:HB2	2.08	0.54
1:B:324:ALA:HB3	1:B:331:MET:HE2	1.89	0.54
1:C:203:PHE:CE2	1:C:460:LEU:HD12	2.43	0.54
1:D:379:ALA:HB1	1:D:382:ALA:HB3	1.90	0.54
1:C:119:GLU:OE1	1:C:119:GLU:HA	2.07	0.54
1:C:356:GLN:N	1:C:356:GLN:CD	2.66	0.54
1:A:148:ILE:HA	1:A:155:LYS:O	2.07	0.54
1:A:284:MET:HA	2:A:500:HEM:HAC	1.90	0.54
1:B:198:ALA:O	1:B:201:LYS:N	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:LEU:HB2	1:C:370:ILE:HD12	1.89	0.54
1:B:166:HIS:HD2	1:B:183:MET:CE	2.18	0.54
1:C:313:LEU:HD21	1:C:341:SER:HB3	1.90	0.54
1:D:8:ARG:HB3	1:D:9:PRO:HD2	1.90	0.54
1:D:96:GLN:N	1:D:96:GLN:NE2	2.56	0.54
1:A:30:GLU:O	1:A:31:LYS:HB2	2.07	0.54
1:C:277:VAL:O	1:C:281:ILE:HG12	2.08	0.54
1:B:145:HIS:O	1:B:149:LYS:HG2	2.08	0.53
1:C:43:ASN:HB3	1:C:51:TYR:CZ	2.43	0.53
1:A:10:TYR:O	1:A:12:GLU:N	2.41	0.53
1:C:102:LEU:CD2	3:C:501:HC9:H27A	2.38	0.53
1:C:406:LYS:HE3	1:C:406:LYS:C	2.33	0.53
1:B:88:TRP:CH2	1:B:460:LEU:HD12	2.43	0.53
1:A:259:TYR:CE2	1:A:261:GLY:HA3	2.44	0.53
1:A:133:LEU:HD21	1:A:175:VAL:CG2	2.38	0.53
1:B:195:PHE:O	1:B:196:ILE:C	2.51	0.53
1:C:299:HIS:CE1	1:C:303:MET:SD	3.02	0.53
1:D:86:PRO:N	1:D:87:PRO:HD2	2.23	0.53
1:B:75:PHE:CD1	1:B:363:LEU:HD13	2.44	0.53
1:B:428:ILE:O	1:B:432:GLU:HB2	2.09	0.53
1:A:128:ASN:HB3	1:A:260:PRO:HD3	1.86	0.53
1:C:151:GLN:HG3	1:C:156:PHE:HA	1.89	0.53
1:C:356:GLN:HG3	1:C:377:GLN:NE2	2.21	0.53
1:B:277:VAL:O	1:B:281:ILE:HD12	2.08	0.53
1:D:32:GLY:O	1:D:35:ARG:N	2.22	0.53
1:D:257:ARG:O	1:D:258:ASN:CB	2.50	0.53
1:D:128:ASN:CB	1:D:260:PRO:CG	2.83	0.53
1:B:8:ARG:NH2	1:B:367:ASP:HB3	2.24	0.52
1:B:335:VAL:HB	1:B:338:LEU:HB3	1.90	0.52
1:A:46:LYS:HD2	1:A:47:TYR:CZ	2.44	0.52
1:B:381:TYR:CE1	1:B:456:THR:HG21	2.44	0.52
1:C:25:TYR:HE2	1:C:29:ARG:HH21	1.56	0.52
1:D:314:ARG:NH1	1:D:445:LYS:HG2	2.24	0.52
1:A:193:GLN:O	1:A:197:ASP:OD2	2.27	0.52
1:A:424:VAL:HG23	2:A:500:HEM:HBD2	1.90	0.52
1:A:100:GLY:O	1:A:101:VAL:C	2.51	0.52
1:B:130:ILE:C	1:B:132:LEU:H	2.16	0.52
1:D:327:ASP:OD1	1:D:330:LYS:HB3	2.09	0.52
1:D:386:ASP:HB3	1:D:389:PHE:CD2	2.44	0.52
1:B:73:PHE:O	1:B:76:GLU:HG2	2.09	0.52
1:B:78:SER:O	1:B:79:TYR:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ARG:NH1	2:C:500:HEM:O2D	2.43	0.52
1:C:328:ILE:HA	1:C:331:MET:HG2	1.91	0.52
1:C:374:THR:O	1:C:376:VAL:HG23	2.09	0.52
1:B:8:ARG:NE	1:B:367:ASP:HB3	2.25	0.52
1:D:364:VAL:HA	1:D:368:TYR:O	2.09	0.52
1:D:471:VAL:HG12	1:D:472:PHE:N	2.23	0.52
1:B:198:ALA:O	1:B:199:VAL:C	2.51	0.52
1:A:73:PHE:O	1:A:76:GLU:HG2	2.09	0.52
1:B:129:PHE:CE1	1:B:175:VAL:HG13	2.45	0.52
1:B:356:GLN:HB3	1:B:375:LEU:HD11	1.91	0.52
1:C:365:LEU:CB	1:C:370:ILE:HD11	2.39	0.52
1:D:414:LEU:HB2	4:D:502:IPA:O2	2.10	0.52
1:D:436:PHE:CE2	1:D:440:ILE:HG13	2.45	0.52
1:A:63:ILE:HD11	1:A:72:LEU:HD22	1.91	0.52
1:B:128:ASN:O	1:B:260:PRO:HD2	2.10	0.52
1:C:207:VAL:HG22	1:C:458:PHE:CE2	2.44	0.52
1:C:416:PHE:CG	1:C:426:ARG:HG3	2.45	0.52
1:B:82:ARG:NE	2:B:500:HEM:O1A	2.33	0.52
1:B:246:PHE:O	1:B:250:LEU:HB2	2.10	0.51
1:C:209:LEU:CD1	1:C:224:THR:HG22	2.37	0.51
1:B:303:MET:HB3	1:B:310:GLN:HG3	1.93	0.51
1:B:411:PHE:CZ	1:B:414:LEU:HD11	2.44	0.51
1:B:423:CYS:HB2	2:B:500:HEM:C4A	2.45	0.51
1:C:365:LEU:HB3	1:C:370:ILE:HD11	1.92	0.51
1:A:289:VAL:O	1:A:293:SER:OG	2.28	0.51
1:B:134:ASN:O	1:B:138:GLN:HG3	2.11	0.51
1:B:214:PRO:HA	1:B:217:TYR:CE2	2.46	0.51
1:C:174:ASN:O	1:C:178:GLY:N	2.35	0.51
1:D:102:LEU:HD12	3:D:501:HC9:H27A	1.93	0.51
1:D:128:ASN:HB3	1:D:260:PRO:HG2	1.84	0.51
1:D:148:ILE:HD11	1:D:155:LYS:CA	2.40	0.51
1:D:302:GLU:OE2	1:D:302:GLU:HA	2.09	0.51
1:D:344:GLU:OE1	1:D:401:TRP:NE1	2.40	0.51
1:B:36:ILE:CG2	1:B:37:HIS:N	2.74	0.51
1:D:259:TYR:OH	1:D:264:TYR:CB	2.55	0.51
1:A:134:ASN:N	1:A:135:PRO:HD2	2.25	0.51
1:A:195:PHE:CD1	1:A:195:PHE:C	2.89	0.51
1:B:53:GLU:O	1:B:59:GLU:HG3	2.11	0.51
1:B:97:LYS:HE2	1:B:98:PRO:HD2	1.92	0.51
1:C:25:TYR:CE2	1:C:29:ARG:HD2	2.46	0.51
1:C:368:TYR:O	1:C:370:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:HIS:HE2	1:D:341:SER:HB3	1.76	0.51
1:A:9:PRO:HD2	1:A:12:GLU:OE2	2.10	0.51
1:A:116:LEU:O	1:A:120:VAL:HG22	2.10	0.51
1:C:32:GLY:O	1:C:34:GLN:N	2.44	0.51
1:C:173:THR:HG21	1:C:181:LEU:HD12	1.92	0.51
1:A:254:THR:O	1:A:254:THR:HG23	2.11	0.51
1:B:115:VAL:HG22	1:B:116:LEU:N	2.26	0.51
1:C:275:GLU:O	1:C:275:GLU:HG2	2.11	0.51
1:D:94:TYR:CD1	1:D:94:TYR:O	2.64	0.51
1:D:36:ILE:O	1:D:40:HIS:HD2	1.94	0.51
1:D:192:ALA:O	1:D:196:ILE:HG13	2.11	0.51
1:B:128:ASN:CG	1:B:260:PRO:CG	2.79	0.51
1:B:296:LEU:HD21	1:B:433:MET:HG2	1.92	0.51
1:D:359:PRO:HD2	1:D:374:THR:O	2.10	0.51
1:A:54:LYS:HG3	1:A:59:GLU:HB2	1.92	0.50
1:A:176:MET:HE1	1:A:284:MET:HB3	1.92	0.50
1:B:27:PHE:CE1	1:B:211:ASN:ND2	2.79	0.50
1:B:344:GLU:CD	1:B:400:ARG:HD2	2.36	0.50
1:B:422:GLN:OE1	1:B:426:ARG:NH2	2.36	0.50
1:B:102:LEU:HD22	3:B:501:HC9:H27A	1.93	0.50
1:B:434:THR:O	1:B:438:ILE:HG12	2.11	0.50
1:C:220:PHE:C	1:C:221:ARG:HG2	2.35	0.50
1:D:68:ASP:OD1	1:D:366:GLN:HG2	2.11	0.50
1:A:113:ARG:HG3	1:A:117:ASN:ND2	2.27	0.50
1:D:160:ILE:HG23	1:D:164:LEU:HG	1.93	0.50
1:D:290:ASN:O	1:D:294:MET:HG2	2.10	0.50
1:A:320:ALA:O	1:A:331:MET:HB3	2.11	0.50
1:C:10:TYR:CD1	1:C:13:ILE:HD12	2.47	0.50
1:C:136:VAL:HG22	1:C:180:ARG:CZ	2.42	0.50
1:D:15:SER:HB3	1:D:17:GLY:H	1.76	0.50
1:A:132:LEU:O	1:A:174:ASN:ND2	2.45	0.50
1:A:318:LEU:CD2	1:A:442:GLU:HG2	2.41	0.50
1:C:252:ARG:O	1:C:253:LYS:CB	2.58	0.50
1:D:238:LYS:HE2	1:D:238:LYS:N	2.27	0.50
1:A:357:ARG:O	1:A:359:PRO:HD3	2.12	0.50
1:C:71:HIS:O	1:C:74:LYS:HB3	2.11	0.50
1:B:264:TYR:O	1:B:266:LEU:N	2.45	0.49
1:B:322:ARG:C	1:B:324:ALA:N	2.70	0.49
1:B:381:TYR:HE1	1:B:456:THR:HG21	1.76	0.49
1:C:257:ARG:O	1:C:258:ASN:HB3	2.11	0.49
1:C:313:LEU:HD21	1:C:341:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:GLU:OE1	1:C:80:PRO:HG3	2.11	0.49
1:C:340:ALA:HB1	1:C:401:TRP:HB2	1.93	0.49
1:A:110:LYS:HZ3	1:A:114:VAL:CG2	2.25	0.49
1:B:474:PRO:O	1:B:475:PHE:CB	2.60	0.49
1:C:252:ARG:O	1:C:253:LYS:HB2	2.13	0.49
1:D:120:VAL:HG22	1:D:262:ILE:HG12	1.94	0.49
1:D:120:VAL:HG13	1:D:428:ILE:HD11	1.95	0.49
1:D:316:GLU:HG2	1:D:335:VAL:HG12	1.94	0.49
1:B:128:ASN:HB2	1:B:260:PRO:HG3	1.74	0.49
1:C:299:HIS:HE1	1:C:303:MET:SD	2.36	0.49
1:C:300:LEU:HD22	1:C:446:VAL:HG21	1.94	0.49
1:D:113:ARG:NH1	1:D:424:VAL:HG22	2.28	0.49
1:D:133:LEU:HD22	1:D:171:SER:HB3	1.94	0.49
1:D:160:ILE:O	1:D:161:LYS:C	2.55	0.49
1:B:128:ASN:OD1	1:B:260:PRO:HG3	2.13	0.49
1:B:200:TYR:HB2	1:B:290:ASN:ND2	2.24	0.49
1:B:390:PHE:HB3	1:B:400:ARG:NH1	2.27	0.49
1:B:437:LEU:O	1:B:441:LEU:HD12	2.13	0.49
1:C:303:MET:CE	1:C:310:GLN:HA	2.43	0.49
1:D:349:HIS:N	1:D:350:PRO:CD	2.76	0.49
1:D:435:LEU:O	1:D:436:PHE:C	2.56	0.49
1:B:454:VAL:HA	1:B:466:LYS:HZ2	1.77	0.49
1:C:355:LEU:HA	5:C:513:HOH:O	2.13	0.49
1:D:68:ASP:N	1:D:68:ASP:OD2	2.45	0.49
1:A:10:TYR:C	1:A:12:GLU:H	2.19	0.49
1:A:457:ILE:HG23	1:A:459:ASN:ND2	2.27	0.49
1:B:209:LEU:O	1:B:217:TYR:OH	2.20	0.49
1:B:439:HIS:O	1:B:440:ILE:HG12	2.13	0.49
1:D:82:ARG:NE	2:D:500:HEM:O1A	2.39	0.49
1:D:116:LEU:O	1:D:120:VAL:N	2.46	0.49
1:B:84:ASP:HB3	1:B:89:LEU:HD11	1.95	0.48
1:B:143:LEU:O	1:B:147:ARG:HB2	2.13	0.48
1:D:71:HIS:CE1	1:D:75:PHE:HE1	2.30	0.48
1:D:82:ARG:NH1	2:D:500:HEM:O1D	2.37	0.48
1:A:76:GLU:HG3	1:A:77:GLY:N	2.27	0.48
1:A:246:PHE:HA	1:A:249:ASP:HB2	1.95	0.48
1:A:408:LEU:CD1	1:B:70:ALA:HA	2.41	0.48
1:B:264:TYR:O	1:B:267:LEU:N	2.38	0.48
1:C:36:ILE:HG23	1:C:40:HIS:CE1	2.47	0.48
1:C:65:HIS:O	1:C:69:VAL:HG23	2.13	0.48
1:B:78:SER:C	1:B:79:TYR:CD2	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HB3	1:B:444:PHE:CZ	2.48	0.48
1:B:200:TYR:O	1:B:200:TYR:CG	2.66	0.48
1:C:309:VAL:HG11	1:C:396:PHE:CD1	2.48	0.48
1:A:88:TRP:HZ2	1:A:460:LEU:CD1	2.16	0.48
1:B:411:PHE:HE1	1:B:414:LEU:HD11	1.78	0.48
1:C:337:LEU:HD22	1:C:398:PRO:HB2	1.95	0.48
1:B:88:TRP:HH2	1:B:460:LEU:HD12	1.79	0.48
1:D:95:TYR:O	1:D:96:GLN:C	2.55	0.48
1:B:27:PHE:HE1	1:B:211:ASN:ND2	2.12	0.48
1:B:206:SER:O	1:B:207:VAL:C	2.56	0.48
1:C:88:TRP:CZ3	3:C:501:HC9:H26B	2.49	0.48
1:D:129:PHE:CD1	1:D:175:VAL:HG23	2.49	0.48
1:B:88:TRP:N	1:B:88:TRP:CD1	2.80	0.48
1:B:120:VAL:HG12	1:B:262:ILE:CD1	2.27	0.48
1:B:383:MET:HE1	4:B:502:IPA:H11	1.95	0.48
1:A:180:ARG:C	1:A:181:LEU:HD12	2.39	0.47
1:A:299:HIS:ND1	1:A:303:MET:HE2	2.29	0.47
1:B:67:GLU:O	1:B:70:ALA:HB3	2.14	0.47
1:B:79:TYR:HD1	1:B:106:SER:HA	1.79	0.47
1:B:139:ASP:OD2	1:B:180:ARG:NH1	2.47	0.47
1:C:269:SER:C	1:C:271:LYS:H	2.22	0.47
1:B:332:LEU:HD21	1:B:431:LEU:CD1	2.44	0.47
1:C:71:HIS:NE2	1:C:75:PHE:CE1	2.82	0.47
1:C:128:ASN:HB3	1:C:260:PRO:CG	2.35	0.47
1:C:128:ASN:CB	1:C:260:PRO:HG2	2.33	0.47
1:C:191:GLU:HG3	1:C:238:LYS:HD2	1.95	0.47
1:D:465:ASP:OD2	1:D:466:LYS:N	2.47	0.47
1:A:8:ARG:NE	1:A:12:GLU:OE1	2.43	0.47
1:B:79:TYR:CD1	1:B:106:SER:HA	2.49	0.47
1:D:254:THR:HG23	1:D:254:THR:O	2.15	0.47
1:D:259:TYR:CD2	1:D:260:PRO:C	2.92	0.47
1:A:365:LEU:O	1:A:366:GLN:CB	2.62	0.47
1:B:160:ILE:O	1:B:161:LYS:C	2.57	0.47
1:C:141:VAL:HG11	1:C:443:ASN:ND2	2.30	0.47
1:C:274:LEU:C	1:C:276:ASP:H	2.22	0.47
1:B:78:SER:O	1:B:79:TYR:CD2	2.67	0.47
1:D:130:ILE:N	1:D:131:PRO:HD2	2.30	0.47
1:D:176:MET:HE1	1:D:281:ILE:HG13	1.96	0.47
1:A:115:VAL:HG11	1:A:272:MET:HE3	1.97	0.47
1:B:324:ALA:O	1:B:326:GLY:N	2.42	0.47
1:C:257:ARG:HD3	1:C:257:ARG:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PHE:CG	1:A:426:ARG:HG3	2.50	0.47
1:A:447:GLU:OE1	1:A:473:ARG:NH2	2.47	0.47
1:B:207:VAL:HG22	1:B:458:PHE:CE2	2.50	0.47
1:B:411:PHE:HE1	1:B:414:LEU:CD1	2.27	0.47
1:D:118:THR:O	1:D:122:ALA:CB	2.62	0.47
1:D:128:ASN:CB	1:D:260:PRO:CD	2.91	0.47
1:D:354:THR:HG21	1:D:377:GLN:NE2	2.27	0.47
1:A:95:TYR:O	1:A:96:GLN:HB2	2.14	0.47
1:A:248:GLN:NE2	1:A:251:ARG:HG2	2.30	0.47
1:C:68:ASP:OD1	1:C:366:GLN:HG2	2.14	0.47
1:C:365:LEU:CB	1:C:370:ILE:CD1	2.93	0.47
1:C:172:ILE:O	1:C:176:MET:HB2	2.15	0.47
1:A:128:ASN:HB3	1:A:260:PRO:HG2	1.82	0.47
1:A:250:LEU:O	1:A:254:THR:HB	2.15	0.47
1:B:189:ASN:H	1:B:189:ASN:ND2	2.12	0.47
1:C:130:ILE:N	1:C:131:PRO:HD2	2.30	0.47
1:C:337:LEU:HA	1:C:337:LEU:HD23	1.57	0.47
1:D:206:SER:O	1:D:207:VAL:C	2.57	0.47
1:A:409:ILE:HG13	1:B:409:ILE:HD11	1.97	0.46
1:B:92:HIS:CD2	1:B:99:ILE:HG22	2.50	0.46
1:B:200:TYR:CD1	1:B:200:TYR:C	2.93	0.46
1:B:291:THR:HG21	3:B:501:HC9:H21	1.96	0.46
1:C:309:VAL:HA	1:C:312:MET:HE3	1.96	0.46
1:C:397:ASP:OD1	1:C:397:ASP:C	2.56	0.46
1:D:78:SER:C	1:D:79:TYR:HD2	2.24	0.46
1:A:202:MET:HE2	1:A:232:TRP:CZ2	2.50	0.46
1:A:299:HIS:HE1	1:A:303:MET:SD	2.38	0.46
1:A:409:ILE:CG1	1:B:409:ILE:HD11	2.46	0.46
1:A:436:PHE:C	1:A:436:PHE:CD2	2.92	0.46
1:B:381:TYR:C	1:B:381:TYR:CD2	2.92	0.46
1:D:79:TYR:HD1	1:D:106:SER:HA	1.69	0.46
1:B:12:GLU:O	1:B:12:GLU:HG2	2.16	0.46
1:C:67:GLU:OE2	1:D:65:HIS:HD2	1.97	0.46
1:C:474:PRO:O	1:C:475:PHE:CB	2.57	0.46
1:D:425:GLY:HA3	2:D:500:HEM:HBC2	1.97	0.46
1:B:16:PRO:HG2	1:B:53:GLU:HG3	1.98	0.46
1:B:321:ARG:HE	1:B:331:MET:HE1	1.80	0.46
1:D:10:TYR:OH	1:D:59:GLU:HG2	2.15	0.46
1:D:213:PRO:HA	1:D:214:PRO:HD2	1.79	0.46
1:A:89:LEU:HG	1:A:93:ARG:HD3	1.96	0.46
1:D:61:VAL:HG12	1:D:62:TYR:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:TYR:HA	1:D:448:MET:HE1	1.98	0.46
1:A:82:ARG:NE	2:A:500:HEM:O1A	2.44	0.46
1:B:202:MET:CG	1:B:232:TRP:NE1	2.79	0.46
1:C:82:ARG:NH2	2:C:500:HEM:O1A	2.39	0.46
1:C:106:SER:OG	1:C:107:GLY:N	2.47	0.46
1:C:139:ASP:OD1	1:C:180:ARG:NH1	2.48	0.46
1:C:144:LEU:HD21	1:C:472:PHE:CD1	2.50	0.46
1:D:145:HIS:O	1:D:148:ILE:HG22	2.15	0.46
1:B:129:PHE:HZ	1:B:262:ILE:HD11	1.76	0.46
1:D:318:LEU:O	1:D:319:ASN:C	2.59	0.46
1:D:470:LEU:HD12	1:D:470:LEU:H	1.81	0.46
1:A:214:PRO:HA	1:A:217:TYR:CE2	2.51	0.46
1:A:408:LEU:HD12	1:A:409:ILE:HG22	1.98	0.46
1:B:202:MET:CE	1:B:203:PHE:CD2	2.98	0.46
1:A:43:ASN:HB3	1:A:51:TYR:CZ	2.50	0.46
1:B:298:TRP:CZ2	1:B:464:PRO:HB3	2.51	0.46
1:C:147:ARG:HB3	1:C:156:PHE:CE2	2.51	0.45
1:C:210:LEU:HD12	1:C:210:LEU:HA	1.71	0.45
1:C:411:PHE:CE2	1:D:408:LEU:HD22	2.51	0.45
1:D:429:ALA:HB1	1:D:433:MET:HE2	1.97	0.45
1:A:232:TRP:CE3	1:A:236:PHE:HE2	2.33	0.45
1:B:14:PRO:HB2	1:B:47:TYR:HB3	1.97	0.45
1:B:37:HIS:HB3	1:B:353:VAL:CG2	2.47	0.45
1:B:199:VAL:HA	1:B:235:ILE:HD11	1.98	0.45
1:C:128:ASN:CG	1:C:260:PRO:HD2	2.41	0.45
1:D:381:TYR:C	1:D:381:TYR:CD2	2.95	0.45
1:A:10:TYR:C	1:A:12:GLU:N	2.74	0.45
1:A:248:GLN:HA	1:A:251:ARG:HB3	1.99	0.45
1:C:71:HIS:HD2	1:C:75:PHE:CE1	2.29	0.45
1:C:120:VAL:HG21	1:C:428:ILE:HD11	1.94	0.45
1:C:159:ASP:OD2	1:C:467:PRO:HB3	2.16	0.45
1:D:19:ASN:CG	1:D:22:LEU:HB2	2.42	0.45
1:B:199:VAL:HG11	1:B:289:VAL:HB	1.98	0.45
1:C:78:SER:O	1:C:79:TYR:HD2	1.99	0.45
1:A:421:ARG:O	1:A:421:ARG:HG2	2.17	0.45
1:C:403:SER:O	1:C:405:ASP:N	2.49	0.45
1:D:266:LEU:HD11	1:D:272:MET:SD	2.56	0.45
1:A:355:LEU:HD13	1:A:417:GLY:HA2	1.98	0.45
1:B:397:ASP:OD2	1:B:397:ASP:C	2.59	0.45
1:C:383:MET:HE2	4:C:502:IPA:C2	2.47	0.45
1:D:277:VAL:HG13	1:D:281:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:ASP:OD2	1:D:397:ASP:C	2.58	0.45
1:A:207:VAL:HB	1:A:208:PRO:HD3	1.97	0.45
1:B:33:SER:O	1:B:207:VAL:CG1	2.65	0.45
1:B:295:THR:HG21	1:B:346:LEU:HD13	1.99	0.45
1:C:85:ILE:CG2	1:C:87:PRO:HD2	2.45	0.45
1:B:237:ASN:N	1:B:237:ASN:HD22	2.13	0.45
1:B:399:THR:C	1:B:401:TRP:N	2.75	0.45
1:C:209:LEU:O	1:C:217:TYR:OH	2.20	0.45
1:C:309:VAL:HA	1:C:312:MET:CE	2.46	0.45
1:C:402:LEU:HD12	1:C:402:LEU:C	2.42	0.45
1:D:128:ASN:CG	1:D:260:PRO:CG	2.83	0.45
1:B:142:SER:O	1:B:145:HIS:HB2	2.17	0.45
1:B:303:MET:SD	1:B:310:GLN:HG3	2.57	0.45
1:C:257:ARG:O	1:C:257:ARG:HD3	2.16	0.45
1:A:284:MET:O	1:A:285:LEU:C	2.58	0.44
3:A:501:HC9:H26A	3:A:501:HC9:H23A	1.68	0.44
1:B:344:GLU:OE2	1:B:400:ARG:HD2	2.16	0.44
1:D:279:ALA:O	1:D:282:THR:HB	2.17	0.44
1:A:31:LYS:HD3	1:A:31:LYS:HA	1.61	0.44
1:B:61:VAL:HG12	1:B:62:TYR:N	2.31	0.44
1:B:237:ASN:N	1:B:237:ASN:ND2	2.64	0.44
1:D:13:ILE:HB	1:D:52:ARG:HH11	1.83	0.44
1:A:21:TRP:CZ3	1:A:56:GLY:HA2	2.51	0.44
1:A:126:ILE:CD1	1:A:427:ARG:HB3	2.45	0.44
1:B:457:ILE:HG12	1:B:458:PHE:H	1.81	0.44
1:C:144:LEU:HD23	1:C:444:PHE:CE1	2.52	0.44
1:D:196:ILE:HG23	1:D:289:VAL:CG1	2.46	0.44
1:D:320:ALA:C	1:D:331:MET:HE3	2.42	0.44
1:A:129:PHE:O	1:A:130:ILE:C	2.60	0.44
1:A:133:LEU:CD2	1:A:175:VAL:CG2	2.95	0.44
1:A:257:ARG:O	1:A:258:ASN:CB	2.59	0.44
1:A:276:ASP:O	1:A:280:ASN:ND2	2.49	0.44
1:C:184:LEU:C	1:C:185:GLU:HG3	2.42	0.44
1:B:129:PHE:O	1:B:130:ILE:C	2.60	0.44
1:C:327:ASP:HB3	1:C:330:LYS:HD2	1.97	0.44
1:D:29:ARG:C	1:D:31:LYS:H	2.25	0.44
1:D:100:GLY:C	1:D:102:LEU:N	2.76	0.44
1:D:314:ARG:HG2	1:D:318:LEU:CD1	2.48	0.44
1:A:314:ARG:HG3	1:A:441:LEU:O	2.17	0.44
1:B:344:GLU:OE1	1:B:400:ARG:HD2	2.18	0.44
1:C:10:TYR:HD1	1:C:13:ILE:HD12	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:PRO:CD	1:D:87:PRO:HD2	2.48	0.44
1:D:314:ARG:HH21	1:D:314:ARG:HG3	1.83	0.44
1:A:290:ASN:O	1:A:294:MET:HG2	2.18	0.44
1:B:446:VAL:HG22	1:B:472:PHE:CE1	2.53	0.44
1:C:183:MET:HE1	1:C:192:ALA:HB3	2.00	0.44
1:C:307:LEU:H	1:C:307:LEU:HD12	1.83	0.44
1:D:262:ILE:HD12	1:D:262:ILE:N	2.12	0.44
1:A:437:LEU:O	1:A:441:LEU:HB2	2.18	0.44
1:B:111:LYS:O	1:B:114:VAL:HG12	2.16	0.44
1:C:40:HIS:O	1:C:44:PHE:HD1	2.00	0.44
1:C:86:PRO:N	1:C:87:PRO:HD2	2.33	0.44
1:A:106:SER:O	1:A:109:TRP:HB3	2.18	0.44
1:A:240:GLU:O	1:A:244:GLU:HG2	2.18	0.44
1:A:259:TYR:CE2	1:A:261:GLY:CA	3.01	0.44
1:A:365:LEU:CD2	1:A:370:ILE:HG13	2.37	0.44
1:A:412:ARG:HG2	1:B:408:LEU:O	2.18	0.44
1:B:259:TYR:N	1:B:259:TYR:CD2	2.86	0.44
1:C:43:ASN:HB3	1:C:51:TYR:CE2	2.53	0.44
1:C:259:TYR:CD2	1:C:259:TYR:N	2.86	0.44
1:B:383:MET:CE	4:B:502:IPA:H13	2.41	0.43
1:D:412:ARG:HB2	1:D:418:TRP:CH2	2.53	0.43
1:D:424:VAL:C	1:D:426:ARG:N	2.74	0.43
1:A:12:GLU:HG2	1:A:12:GLU:O	2.19	0.43
1:C:72:LEU:HD21	1:C:359:PRO:HG3	1.99	0.43
1:D:13:ILE:O	1:D:52:ARG:NH1	2.51	0.43
1:D:146:LYS:HA	1:D:149:LYS:HZ3	1.84	0.43
1:A:86:PRO:N	1:A:87:PRO:HD2	2.33	0.43
1:D:243:THR:OG1	1:D:281:ILE:HG21	2.17	0.43
1:A:109:TRP:CD1	1:A:421:ARG:CZ	3.01	0.43
1:B:36:ILE:HG21	1:B:458:PHE:CD1	2.53	0.43
1:C:471:VAL:HG11	1:C:473:ARG:NH1	2.31	0.43
1:D:242:TYR:O	1:D:246:PHE:HD2	2.01	0.43
1:B:346:LEU:CD2	1:B:416:PHE:CE2	3.01	0.43
1:D:88:TRP:CD1	1:D:88:TRP:N	2.86	0.43
1:D:164:LEU:O	1:D:165:PHE:C	2.58	0.43
1:D:261:GLY:O	1:D:262:ILE:C	2.62	0.43
1:A:253:LYS:O	1:A:253:LYS:HG3	2.19	0.43
1:A:328:ILE:HD12	1:A:328:ILE:HA	1.76	0.43
1:B:113:ARG:O	1:B:113:ARG:HG3	2.18	0.43
1:B:210:LEU:HD12	1:B:210:LEU:HA	1.60	0.43
1:D:425:GLY:CA	2:D:500:HEM:HBC2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HG3	1:A:83:TYR:O	2.19	0.43
1:A:92:HIS:CD2	1:A:99:ILE:HG22	2.54	0.43
1:B:128:ASN:HB3	1:B:260:PRO:HD2	1.68	0.43
1:B:134:ASN:N	1:B:135:PRO:CD	2.80	0.43
1:B:463:THR:HB	1:B:464:PRO:HD2	2.00	0.43
1:C:88:TRP:CZ2	1:C:460:LEU:HD11	2.53	0.43
1:C:277:VAL:C	1:C:279:ALA:H	2.27	0.43
1:A:176:MET:HG3	1:A:262:ILE:CG2	2.49	0.43
1:A:246:PHE:HA	1:A:249:ASP:CB	2.49	0.43
1:C:285:LEU:O	1:C:286:ALA:C	2.62	0.43
1:C:381:TYR:C	1:C:381:TYR:CD2	2.97	0.43
1:D:19:ASN:CB	1:D:22:LEU:HB2	2.47	0.43
1:D:100:GLY:C	1:D:102:LEU:H	2.27	0.43
1:D:102:LEU:HD13	1:D:103:PHE:CZ	2.54	0.43
1:D:118:THR:O	1:D:122:ALA:HB3	2.19	0.43
1:B:278:LYS:HE3	1:B:278:LYS:HB2	1.87	0.43
1:B:297:GLN:OE1	1:B:468:ILE:HB	2.19	0.43
1:C:250:LEU:HD22	1:C:264:TYR:CD1	2.53	0.43
1:D:78:SER:C	1:D:79:TYR:CD2	2.97	0.43
1:D:320:ALA:O	1:D:324:ALA:HB3	2.19	0.43
1:A:105:LYS:O	1:A:106:SER:HB2	2.17	0.43
1:A:327:ASP:CG	1:A:328:ILE:H	2.27	0.43
1:A:372:ALA:O	1:A:373:LYS:HB2	2.19	0.43
1:A:380:ILE:O	1:A:381:TYR:C	2.61	0.43
1:A:412:ARG:HG3	1:A:418:TRP:CH2	2.54	0.43
1:B:99:ILE:O	1:B:99:ILE:HG13	2.18	0.43
1:B:359:PRO:HD2	1:B:374:THR:O	2.19	0.43
1:C:67:GLU:OE1	1:D:66:PRO:HD2	2.19	0.43
1:C:175:VAL:O	1:C:262:ILE:HG12	2.19	0.43
1:C:434:THR:O	1:C:438:ILE:HG13	2.19	0.43
1:C:457:ILE:CG2	1:C:459:ASN:ND2	2.81	0.43
1:D:12:GLU:O	1:D:12:GLU:CG	2.67	0.43
1:A:76:GLU:OE1	1:A:80:PRO:CG	2.67	0.42
1:B:342:ILE:O	1:B:346:LEU:HB2	2.18	0.42
1:C:295:THR:HA	5:C:573:HOH:O	2.18	0.42
1:D:169:PHE:CE2	1:D:192:ALA:HB1	2.54	0.42
1:D:400:ARG:HH11	1:D:400:ARG:HB2	1.84	0.42
1:A:10:TYR:CE1	1:A:52:ARG:HD3	2.54	0.42
1:A:36:ILE:O	1:A:36:ILE:HG23	2.17	0.42
1:B:66:PRO:O	1:B:69:VAL:N	2.52	0.42
1:B:399:THR:O	1:B:400:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:PRO:CB	1:C:221:ARG:HH21	2.30	0.42
1:D:101:VAL:HG22	1:D:109:TRP:CD1	2.54	0.42
1:A:274:LEU:O	1:A:275:GLU:C	2.62	0.42
1:A:356:GLN:O	1:A:357:ARG:NH1	2.44	0.42
1:B:144:LEU:CB	1:B:444:PHE:CZ	3.02	0.42
1:B:172:ILE:O	1:B:176:MET:CB	2.64	0.42
1:B:182:GLY:C	1:B:184:LEU:N	2.76	0.42
1:B:459:ASN:O	1:B:460:LEU:CB	2.67	0.42
1:D:14:PRO:HB2	1:D:47:TYR:HB3	2.00	0.42
1:D:37:HIS:HA	1:D:40:HIS:HD2	1.84	0.42
1:D:291:THR:O	1:D:295:THR:OG1	2.30	0.42
1:C:346:LEU:N	1:C:346:LEU:HD22	2.35	0.42
1:D:122:ALA:C	1:D:124:GLU:H	2.27	0.42
1:D:298:TRP:O	1:D:301:TYR:HB3	2.20	0.42
1:A:355:LEU:O	1:A:378:VAL:N	2.50	0.42
1:B:130:ILE:C	1:B:132:LEU:N	2.78	0.42
1:C:288:GLY:HA2	2:C:500:HEM:HMC2	2.01	0.42
1:D:357:ARG:O	1:D:359:PRO:HD3	2.18	0.42
1:A:202:MET:HE1	3:A:501:HC9:H26	2.02	0.42
1:A:247:TYR:HD1	1:A:248:GLN:OE1	2.03	0.42
1:B:399:THR:C	1:B:401:TRP:H	2.28	0.42
1:C:99:ILE:O	1:C:104:LYS:HE2	2.18	0.42
1:C:126:ILE:C	1:C:128:ASN:H	2.27	0.42
1:C:383:MET:HE1	4:C:502:IPA:H32	2.01	0.42
1:D:128:ASN:CG	1:D:260:PRO:CD	2.92	0.42
1:D:465:ASP:OD2	1:D:466:LYS:HG3	2.19	0.42
1:B:53:GLU:C	1:B:59:GLU:HG3	2.44	0.42
1:B:130:ILE:N	1:B:131:PRO:HD2	2.34	0.42
1:C:170:GLU:O	1:C:173:THR:HG22	2.20	0.42
1:D:277:VAL:HG12	1:D:278:LYS:N	2.34	0.42
1:A:91:TYR:HE2	1:A:97:LYS:HG3	1.85	0.42
1:A:129:PHE:O	1:A:133:LEU:HD23	2.20	0.42
1:A:392:SER:C	1:A:394:ASP:H	2.27	0.42
1:B:225:TRP:O	1:B:229:VAL:HG23	2.19	0.42
1:C:117:ASN:O	1:C:122:ALA:N	2.49	0.42
1:D:8:ARG:HB3	1:D:9:PRO:CD	2.50	0.42
1:D:166:HIS:NE2	1:D:193:GLN:OE1	2.50	0.42
1:A:93:ARG:HE	1:A:93:ARG:HB2	1.61	0.42
1:A:364:VAL:HA	1:A:368:TYR:O	2.20	0.42
1:B:128:ASN:CG	1:B:260:PRO:HD3	2.43	0.42
1:D:212:VAL:HG11	1:D:221:ARG:NE	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:HG3	1:B:266:LEU:CD2	2.43	0.42
1:C:198:ALA:O	1:C:199:VAL:C	2.62	0.42
1:C:203:PHE:HE2	1:C:460:LEU:HD12	1.83	0.42
1:C:339:LYS:HD2	1:C:339:LYS:HA	1.85	0.42
1:A:338:LEU:O	1:A:341:SER:HB3	2.19	0.41
1:B:443:ASN:OD1	1:B:443:ASN:N	2.53	0.41
1:C:78:SER:C	1:C:79:TYR:HD2	2.28	0.41
1:C:298:TRP:CZ2	1:C:464:PRO:HB3	2.55	0.41
1:C:424:VAL:HG23	2:C:500:HEM:HBD2	2.01	0.41
1:D:305:ARG:NH1	5:D:536:HOH:O	2.53	0.41
1:A:160:ILE:O	1:A:161:LYS:C	2.62	0.41
1:A:461:ILE:O	1:A:461:ILE:HG13	2.18	0.41
1:B:8:ARG:HH21	1:B:367:ASP:CB	2.32	0.41
1:B:214:PRO:HA	1:B:217:TYR:CD2	2.55	0.41
1:C:460:LEU:HD22	1:C:460:LEU:HA	1.91	0.41
1:D:128:ASN:HB2	1:D:260:PRO:HG2	1.99	0.41
1:D:277:VAL:O	1:D:278:LYS:C	2.63	0.41
1:D:332:LEU:HD21	1:D:431:LEU:CD1	2.50	0.41
1:D:344:GLU:O	1:D:348:LEU:HD12	2.20	0.41
1:C:257:ARG:O	1:C:258:ASN:CB	2.68	0.41
1:D:390:PHE:O	1:D:391:SER:C	2.63	0.41
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.20	0.41
1:C:134:ASN:N	1:C:135:PRO:CD	2.83	0.41
1:D:371:PRO:O	1:D:372:ALA:C	2.63	0.41
1:D:443:ASN:O	1:D:474:PRO:HA	2.20	0.41
1:A:300:LEU:O	1:A:301:TYR:C	2.62	0.41
1:C:27:PHE:CE1	1:C:211:ASN:ND2	2.88	0.41
1:C:334:MET:C	1:C:336:PRO:HD3	2.45	0.41
1:D:259:TYR:HD2	1:D:260:PRO:C	2.28	0.41
1:A:250:LEU:HD11	1:A:259:TYR:OH	2.20	0.41
1:C:78:SER:C	1:C:79:TYR:CD2	2.99	0.41
1:C:109:TRP:CZ2	1:C:113:ARG:HG2	2.56	0.41
1:C:189:ASN:HA	1:C:190:PRO:HD3	1.85	0.41
1:C:363:LEU:HD23	1:C:370:ILE:HB	2.02	0.41
1:D:71:HIS:CE1	1:D:75:PHE:CE1	3.09	0.41
1:A:30:GLU:HG2	1:C:322:ARG:NH1	2.36	0.41
1:A:175:VAL:CG1	1:A:262:ILE:HD12	2.48	0.41
1:D:331:MET:C	1:D:333:GLN:H	2.28	0.41
1:A:410:HIS:O	1:B:409:ILE:HD12	2.20	0.41
1:B:37:HIS:HB3	1:B:353:VAL:HG21	2.03	0.41
1:B:87:PRO:O	1:B:88:TRP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LYS:O	1:B:226:ARG:HG2	2.21	0.41
1:C:20:GLY:HA3	1:C:56:GLY:O	2.21	0.41
1:D:218:ARG:HE	1:D:218:ARG:HB2	1.72	0.41
1:A:109:TRP:CE3	1:A:110:LYS:HA	2.56	0.41
1:A:176:MET:HG3	1:A:262:ILE:CB	2.49	0.41
1:A:185:GLU:OE1	1:A:185:GLU:HA	2.21	0.41
1:A:199:VAL:HG12	1:A:290:ASN:ND2	2.36	0.41
1:A:422:GLN:HE21	1:A:426:ARG:HD2	1.85	0.41
1:B:259:TYR:CD1	1:B:261:GLY:HA3	2.54	0.41
1:B:347:ARG:NH1	1:B:393:PRO:O	2.48	0.41
1:B:365:LEU:O	1:B:366:GLN:HB2	2.21	0.41
1:C:259:TYR:CD2	1:C:259:TYR:C	2.99	0.41
1:C:358:TYR:CE1	1:C:375:LEU:HD13	2.56	0.41
1:C:473:ARG:HH11	1:C:473:ARG:HG3	1.85	0.41
1:D:128:ASN:N	1:D:128:ASN:HD22	2.19	0.41
1:D:250:LEU:HD12	1:D:263:LEU:HD23	2.02	0.41
1:D:257:ARG:CZ	1:D:257:ARG:HB3	2.51	0.41
1:D:259:TYR:CD2	1:D:261:GLY:N	2.89	0.41
1:D:263:LEU:O	1:D:267:LEU:HD12	2.20	0.41
1:D:299:HIS:NE2	1:D:341:SER:HB3	2.35	0.41
1:D:348:LEU:O	1:D:385:ARG:NH2	2.54	0.41
1:D:350:PRO:O	1:D:462:LEU:HD12	2.21	0.41
1:D:355:LEU:HD11	1:D:417:GLY:HA2	2.03	0.41
1:A:39:ARG:O	1:A:40:HIS:C	2.64	0.41
1:A:142:SER:HA	1:A:145:HIS:HB2	2.03	0.41
1:A:176:MET:HE3	1:A:176:MET:HB2	1.92	0.41
1:B:97:LYS:HA	1:B:98:PRO:HD2	1.88	0.41
1:B:207:VAL:HB	1:B:208:PRO:HD3	2.03	0.41
1:B:363:LEU:HD11	1:B:365:LEU:HD21	2.02	0.41
1:C:85:ILE:CD1	3:C:501:HC9:H7	2.49	0.41
1:C:113:ARG:O	1:C:117:ASN:OD1	2.39	0.41
1:D:86:PRO:HD2	1:D:87:PRO:HD2	2.03	0.41
1:D:160:ILE:HD12	1:D:160:ILE:HA	1.89	0.41
1:A:209:LEU:HD22	1:A:217:TYR:CD1	2.56	0.40
1:B:102:LEU:HD13	2:B:500:HEM:HAD2	2.03	0.40
1:B:119:GLU:HA	1:B:119:GLU:OE1	2.21	0.40
1:B:202:MET:HE3	1:B:202:MET:HB3	2.01	0.40
1:C:36:ILE:HD13	1:C:36:ILE:HG21	1.69	0.40
1:D:321:ARG:NH2	1:D:326:GLY:O	2.52	0.40
1:A:86:PRO:HD2	1:A:87:PRO:HD2	2.03	0.40
1:B:117:ASN:HD22	1:B:117:ASN:HA	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PHE:CZ	1:B:242:TYR:O	2.75	0.40
1:B:218:ARG:NH1	1:B:218:ARG:HG2	2.36	0.40
1:B:311:GLU:OE2	1:B:311:GLU:HA	2.21	0.40
1:B:460:LEU:HA	1:B:460:LEU:HD22	1.61	0.40
2:D:500:HEM:CMA	2:D:500:HEM:CBA	3.00	0.40
1:B:202:MET:HG3	1:B:232:TRP:CE2	2.56	0.40
1:B:337:LEU:HA	1:B:337:LEU:HD12	1.67	0.40
1:B:347:ARG:NH1	1:B:393:PRO:HA	2.36	0.40
1:D:35:ARG:NH2	1:D:35:ARG:HB3	2.37	0.40
1:D:83:TYR:H	1:D:356:GLN:HB2	1.85	0.40
1:D:120:VAL:O	1:D:120:VAL:HG12	2.21	0.40
1:A:49:PRO:HB3	1:A:65:HIS:HD2	1.86	0.40
1:A:316:GLU:OE1	1:A:337:LEU:HD23	2.21	0.40
1:B:87:PRO:O	1:B:90:ALA:HB3	2.22	0.40
1:B:143:LEU:O	1:B:143:LEU:HD23	2.22	0.40
1:D:112:ASP:OD2	1:D:280:ASN:ND2	2.44	0.40
1:D:126:ILE:HG23	1:D:127:LYS:N	2.36	0.40
1:D:355:LEU:CD1	1:D:417:GLY:HA2	2.51	0.40
1:A:101:VAL:HG11	1:A:116:LEU:HD12	2.03	0.40
1:C:133:LEU:HD21	1:C:175:VAL:HG21	2.04	0.40
1:C:269:SER:C	1:C:271:LYS:N	2.79	0.40
1:D:88:TRP:CZ2	1:D:460:LEU:CD1	3.04	0.40
1:D:302:GLU:O	1:D:305:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	468/486 (96%)	390 (83%)	66 (14%)	12 (3%)	4 7
1	B	468/486 (96%)	391 (84%)	59 (13%)	18 (4%)	2 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	468/486 (96%)	391 (84%)	59 (13%)	18 (4%)	2	3
1	D	468/486 (96%)	376 (80%)	77 (16%)	15 (3%)	3	4
All	All	1872/1944 (96%)	1548 (83%)	261 (14%)	63 (3%)	3	4

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	404	LYS
1	B	33	SER
1	B	255	GLU
1	B	327	ASP
1	B	329	SER
1	B	403	SER
1	C	33	SER
1	C	120	VAL
1	C	253	LYS
1	C	258	ASN
1	C	404	LYS
1	D	33	SER
1	D	101	VAL
1	D	422	GLN
1	A	11	SER
1	A	14	PRO
1	A	33	SER
1	A	106	SER
1	A	218	ARG
1	A	262	ILE
1	A	325	GLU
1	B	96	GLN
1	B	265	CYS
1	B	372	ALA
1	B	400	ARG
1	C	74	LYS
1	C	256	PHE
1	D	258	ASN
1	D	404	LYS
1	D	435	LEU
1	D	436	PHE
1	A	275	GLU
1	A	327	ASP

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Mol	Chain	Res	Type
1	B	31	LYS
1	B	74	LYS
1	C	14	PRO
1	C	16	PRO
1	C	260	PRO
1	C	274	LEU
1	C	275	GLU
1	D	218	ARG
1	D	219	LEU
1	D	367	ASP
1	C	124	GLU
1	C	453	ASP
1	D	152	GLY
1	B	199	VAL
1	B	440	ILE
1	B	453	ASP
1	C	270	GLU
1	D	8	ARG
1	D	460	LEU
1	B	7	PRO
1	B	262	ILE
1	C	245	ILE
1	B	131	PRO
1	C	15	SER
1	C	199	VAL
1	D	182	GLY
1	A	16	PRO
1	B	120	VAL
1	D	425	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	426/440 (97%)	391 (92%)	35 (8%)	10	23
1	B	426/440 (97%)	378 (89%)	48 (11%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	426/440 (97%)	386 (91%)	40 (9%)	8	18
1	D	426/440 (97%)	375 (88%)	51 (12%)	5	10
All	All	1704/1760 (97%)	1530 (90%)	174 (10%)	7	15

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	18	ASP
1	A	36	ILE
1	A	58	LEU
1	A	63	ILE
1	A	78	SER
1	A	93	ARG
1	A	105	LYS
1	A	133	LEU
1	A	145	HIS
1	A	153	SER
1	A	160	ILE
1	A	175	VAL
1	A	176	MET
1	A	185	GLU
1	A	191	GLU
1	A	193	GLN
1	A	201	LYS
1	A	215	GLU
1	A	248	GLN
1	A	259	TYR
1	A	285	LEU
1	A	289	VAL
1	A	293	SER
1	A	296	LEU
1	A	346	LEU
1	A	353	VAL
1	A	369	LEU
1	A	402	LEU
1	A	403	SER
1	A	408	LEU
1	A	436	PHE
1	A	449	GLN
1	A	450	HIS

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Mol	Chain	Res	Type
1	A	460	LEU
1	B	24	LEU
1	B	31	LYS
1	B	49	PRO
1	B	50	ILE
1	B	63	ILE
1	B	101	VAL
1	B	115	VAL
1	B	116	LEU
1	B	117	ASN
1	B	127	LYS
1	B	130	ILE
1	B	136	VAL
1	B	157	VAL
1	B	160	ILE
1	B	180	ARG
1	B	189	ASN
1	B	201	LYS
1	B	210	LEU
1	B	215	GLU
1	B	218	ARG
1	B	253	LYS
1	B	255	GLU
1	B	257	ARG
1	B	258	ASN
1	B	259	TYR
1	B	273	LEU
1	B	275	GLU
1	B	276	ASP
1	B	289	VAL
1	B	292	THR
1	B	295	THR
1	B	296	LEU
1	B	300	LEU
1	B	319	ASN
1	B	323	GLN
1	B	328	ILE
1	B	347	ARG
1	B	365	LEU
1	B	402	LEU
1	B	403	SER
1	B	404	LYS

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Mol	Chain	Res	Type
1	B	407	ASP
1	B	408	LEU
1	B	424	VAL
1	B	455	ASP
1	B	456	THR
1	B	457	ILE
1	B	460	LEU
1	C	14	PRO
1	C	24	LEU
1	C	36	ILE
1	C	57	ASN
1	C	63	ILE
1	C	75	PHE
1	C	111	LYS
1	C	119	GLU
1	C	120	VAL
1	C	128	ASN
1	C	144	LEU
1	C	147	ARG
1	C	153	SER
1	C	180	ARG
1	C	210	LEU
1	C	215	GLU
1	C	216	LEU
1	C	248	GLN
1	C	256	PHE
1	C	257	ARG
1	C	259	TYR
1	C	268	LYS
1	C	276	ASP
1	C	293	SER
1	C	296	LEU
1	C	308	ASN
1	C	330	LYS
1	C	337	LEU
1	C	339	LYS
1	C	353	VAL
1	C	355	LEU
1	C	394	ASP
1	C	402	LEU
1	C	403	SER
1	C	406	LYS

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Mol	Chain	Res	Type
1	C	407	ASP
1	C	408	LEU
1	C	409	ILE
1	C	450	HIS
1	C	460	LEU
1	D	36	ILE
1	D	63	ILE
1	D	68	ASP
1	D	74	LYS
1	D	96	GLN
1	D	98	PRO
1	D	101	VAL
1	D	102	LEU
1	D	112	ASP
1	D	148	ILE
1	D	149	LYS
1	D	151	GLN
1	D	153	SER
1	D	160	ILE
1	D	180	ARG
1	D	187	THR
1	D	212	VAL
1	D	241	LYS
1	D	245	ILE
1	D	249	ASP
1	D	253	LYS
1	D	257	ARG
1	D	258	ASN
1	D	262	ILE
1	D	273	LEU
1	D	281	ILE
1	D	289	VAL
1	D	292	THR
1	D	293	SER
1	D	296	LEU
1	D	327	ASP
1	D	328	ILE
1	D	330	LYS
1	D	338	LEU
1	D	353	VAL
1	D	356	GLN
1	D	362	ASP

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Mol	Chain	Res	Type
1	D	363	LEU
1	D	391	SER
1	D	404	LYS
1	D	407	ASP
1	D	424	VAL
1	D	427	ARG
1	D	435	LEU
1	D	445	LYS
1	D	450	HIS
1	D	455	ASP
1	D	460	LEU
1	D	467	PRO
1	D	470	LEU
1	D	473	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	40	HIS
1	A	117	ASN
1	A	189	ASN
1	A	193	GLN
1	A	237	ASN
1	A	290	ASN
1	A	297	GLN
1	A	310	GLN
1	A	319	ASN
1	A	323	GLN
1	A	422	GLN
1	A	443	ASN
1	A	449	GLN
1	A	450	HIS
1	A	459	ASN
1	B	19	ASN
1	B	71	HIS
1	B	92	HIS
1	B	117	ASN
1	B	150	GLN
1	B	166	HIS
1	B	189	ASN
1	B	211	ASN

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Mol	Chain	Res	Type
1	B	237	ASN
1	B	290	ASN
1	B	308	ASN
1	B	310	GLN
1	B	319	ASN
1	B	333	GLN
1	B	366	GLN
1	C	19	ASN
1	C	40	HIS
1	C	45	GLN
1	C	65	HIS
1	C	92	HIS
1	C	138	GLN
1	C	237	ASN
1	C	248	GLN
1	C	297	GLN
1	C	377	GLN
1	C	459	ASN
1	D	40	HIS
1	D	65	HIS
1	D	96	GLN
1	D	117	ASN
1	D	138	GLN
1	D	145	HIS
1	D	237	ASN
1	D	297	GLN
1	D	319	ASN
1	D	366	GLN
1	D	377	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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
4	IPA	C	502	-	3,3,3	0.66	0	3,3,3	0.53	0
2	HEM	D	500	1,3	50,50,50	3.34	29 (58%)	67,82,82	2.34	17 (25%)
4	IPA	D	502	-	3,3,3	0.73	0	3,3,3	0.63	0
2	HEM	B	500	1,3	50,50,50	3.04	28 (56%)	67,82,82	2.38	20 (29%)
2	HEM	A	500	1,3	50,50,50	3.37	27 (54%)	67,82,82	2.26	17 (25%)
3	HC9	B	501	2	32,32,32	0.93	1 (3%)	50,50,50	1.69	8 (16%)
4	IPA	B	502	-	3,3,3	0.72	0	3,3,3	0.90	0
2	HEM	C	500	1,3	50,50,50	3.31	26 (52%)	67,82,82	2.16	18 (26%)
3	HC9	A	501	2	32,32,32	1.19	2 (6%)	50,50,50	1.79	12 (24%)
4	IPA	A	502	-	3,3,3	0.88	0	3,3,3	0.52	0
3	HC9	D	501	2	32,32,32	1.34	6 (18%)	50,50,50	2.35	17 (34%)
3	HC9	C	501	2	32,32,32	0.96	1 (3%)	50,50,50	1.74	13 (26%)

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	D	500	1,3	-	7/14/54/54	-
2	HEM	B	500	1,3	-	5/14/54/54	-
2	HEM	A	500	1,3	-	0/14/54/54	-
3	HC9	B	501	2	-	5/13/71/71	0/4/4/4
2	HEM	C	500	1,3	-	3/14/54/54	-
3	HC9	A	501	2	-	2/13/71/71	0/4/4/4
3	HC9	D	501	2	-	1/13/71/71	0/4/4/4
3	HC9	C	501	2	-	1/13/71/71	0/4/4/4

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-C4C	-7.84	1.32	1.46
2	D	500	HEM	C1C-C2C	-7.42	1.30	1.45
2	D	500	HEM	C3B-C2B	7.22	1.51	1.37
2	C	500	HEM	C1C-C2C	-7.03	1.31	1.45
2	D	500	HEM	C3C-C4C	-6.88	1.34	1.46
2	A	500	HEM	C1C-C2C	-6.70	1.32	1.45
2	D	500	HEM	C3C-C2C	6.53	1.50	1.37
2	B	500	HEM	C3B-C2B	6.48	1.50	1.37
2	A	500	HEM	C3B-C2B	6.46	1.50	1.37
2	C	500	HEM	CHD-C4C	6.39	1.50	1.38
2	C	500	HEM	C3C-C2C	6.09	1.49	1.37
2	C	500	HEM	C3C-C4C	-6.07	1.35	1.46
2	B	500	HEM	C1C-C2C	-5.88	1.33	1.45
2	D	500	HEM	CHD-C4C	5.66	1.49	1.38
2	B	500	HEM	C3C-C2C	5.62	1.48	1.37
2	A	500	HEM	CBB-CAB	5.58	1.57	1.30
2	A	500	HEM	CAB-C3B	-5.49	1.32	1.47
2	A	500	HEM	CHD-C4C	5.48	1.49	1.38
2	C	500	HEM	CBB-CAB	5.40	1.56	1.30
2	C	500	HEM	CAB-C3B	-5.38	1.33	1.47
2	D	500	HEM	CBB-CAB	5.37	1.56	1.30
2	C	500	HEM	C3B-C2B	5.23	1.47	1.37
2	A	500	HEM	C3C-C2C	5.22	1.47	1.37
2	C	500	HEM	CHA-C1A	5.15	1.51	1.39
2	B	500	HEM	CHD-C4C	5.12	1.48	1.38
2	C	500	HEM	C3B-C4B	4.99	1.54	1.44
2	A	500	HEM	C3B-C4B	4.87	1.54	1.44
2	A	500	HEM	FE-NC	4.84	2.11	1.95
2	C	500	HEM	C1B-C2B	-4.76	1.34	1.44
2	A	500	HEM	C4A-NA	-4.74	1.30	1.39
2	B	500	HEM	CBB-CAB	4.73	1.53	1.30
2	B	500	HEM	CHB-C4A	-4.72	1.28	1.39
2	A	500	HEM	C1D-ND	-4.72	1.29	1.38
2	D	500	HEM	C1D-ND	-4.71	1.29	1.38
2	D	500	HEM	C1B-C2B	-4.70	1.35	1.44
2	A	500	HEM	C1B-C2B	-4.70	1.35	1.44
2	B	500	HEM	C1B-C2B	-4.68	1.35	1.44
2	C	500	HEM	C4A-NA	-4.63	1.30	1.39
2	D	500	HEM	C3B-C4B	4.62	1.53	1.44
2	B	500	HEM	FE-NC	4.52	2.10	1.95
2	D	500	HEM	CHB-C4A	-4.50	1.29	1.39
2	B	500	HEM	CHB-C1B	4.45	1.47	1.38
2	B	500	HEM	CHA-C1A	4.45	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	CHB-C4A	-4.41	1.29	1.39
2	D	500	HEM	C1A-C2A	4.39	1.53	1.44
2	A	500	HEM	CHA-C1A	4.38	1.49	1.39
2	B	500	HEM	CAB-C3B	-4.38	1.35	1.47
2	C	500	HEM	CHB-C1B	4.32	1.47	1.38
2	C	500	HEM	FE-NC	4.31	2.09	1.95
2	A	500	HEM	CHB-C4A	-4.29	1.29	1.39
2	D	500	HEM	C1B-NB	-4.26	1.32	1.40
2	A	500	HEM	C4D-C3D	4.15	1.52	1.45
2	D	500	HEM	CHA-C1A	4.09	1.48	1.39
2	D	500	HEM	C4A-NA	-4.07	1.31	1.39
2	A	500	HEM	C1B-NB	-4.07	1.33	1.40
2	A	500	HEM	CHB-C1B	4.01	1.46	1.38
2	B	500	HEM	C4A-NA	-3.97	1.32	1.39
2	B	500	HEM	C3B-C4B	3.85	1.52	1.44
2	C	500	HEM	C1D-C2D	3.78	1.52	1.44
2	D	500	HEM	CHB-C1B	3.75	1.46	1.38
2	B	500	HEM	C1B-NB	-3.65	1.33	1.40
2	D	500	HEM	C1C-NC	-3.64	1.32	1.39
2	C	500	HEM	C4D-C3D	3.61	1.51	1.45
2	C	500	HEM	C1C-NC	-3.60	1.32	1.39
2	B	500	HEM	CHC-C4B	-3.53	1.31	1.39
2	D	500	HEM	FE-NC	3.53	2.06	1.95
2	B	500	HEM	CHC-C1C	3.50	1.45	1.38
2	B	500	HEM	C4D-C3D	3.47	1.50	1.45
2	D	500	HEM	CAB-C3B	-3.41	1.38	1.47
2	A	500	HEM	C1A-C2A	3.39	1.51	1.44
2	C	500	HEM	C1B-NB	-3.37	1.34	1.40
2	C	500	HEM	C1A-NA	3.36	1.45	1.39
2	B	500	HEM	C1D-ND	-3.34	1.32	1.38
2	A	500	HEM	C2A-C3A	-3.33	1.30	1.38
2	C	500	HEM	CHC-C1C	3.22	1.44	1.38
2	C	500	HEM	C2A-C3A	-3.21	1.30	1.38
3	D	501	HC9	C18-C13	-3.16	1.49	1.54
2	C	500	HEM	C1A-C2A	3.16	1.50	1.44
2	D	500	HEM	CHC-C4B	-3.06	1.32	1.39
2	D	500	HEM	C2A-C3A	-3.06	1.30	1.38
2	B	500	HEM	C1A-C2A	3.01	1.50	1.44
3	D	501	HC9	C4-C3	3.00	1.57	1.52
2	A	500	HEM	C1C-NC	-2.99	1.34	1.39
2	B	500	HEM	C3C-C4C	-2.99	1.40	1.46
2	C	500	HEM	FE-NA	2.96	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C2A-C3A	-2.95	1.31	1.38
2	A	500	HEM	FE-NA	2.89	2.04	1.95
3	A	501	HC9	C4-C3	2.87	1.57	1.52
2	D	500	HEM	FE-NA	2.85	2.04	1.95
2	A	500	HEM	CHC-C1C	2.81	1.43	1.38
2	D	500	HEM	CHA-C4D	-2.80	1.32	1.38
3	D	501	HC9	C7-C8	2.79	1.57	1.53
2	C	500	HEM	CHA-C4D	-2.77	1.32	1.38
2	D	500	HEM	CHC-C1C	2.62	1.43	1.38
2	A	500	HEM	C1D-C2D	2.60	1.49	1.44
2	D	500	HEM	C1A-NA	2.60	1.44	1.39
2	D	500	HEM	C4D-C3D	2.54	1.49	1.45
2	B	500	HEM	C1D-C2D	2.52	1.49	1.44
2	A	500	HEM	C4A-C3A	2.51	1.49	1.43
2	B	500	HEM	C4A-C3A	2.46	1.48	1.43
2	B	500	HEM	CHA-C4D	-2.45	1.33	1.38
2	A	500	HEM	C1A-NA	2.44	1.44	1.39
2	A	500	HEM	C4B-NB	2.44	1.43	1.38
2	B	500	HEM	C1A-NA	2.43	1.44	1.39
2	C	500	HEM	C1D-ND	-2.41	1.34	1.38
2	B	500	HEM	FE-NA	2.37	2.03	1.95
2	B	500	HEM	C1C-NC	-2.33	1.35	1.39
3	D	501	HC9	C12-C11	2.32	1.58	1.53
2	D	500	HEM	C1D-C2D	2.30	1.49	1.44
2	D	500	HEM	CHD-C1D	-2.26	1.34	1.39
2	B	500	HEM	CHD-C1D	-2.24	1.34	1.39
3	D	501	HC9	C6-C5	2.22	1.37	1.33
3	C	501	HC9	C4-C3	2.18	1.56	1.52
2	D	500	HEM	C4B-NB	2.16	1.43	1.38
2	C	500	HEM	C4A-C3A	2.13	1.48	1.43
2	A	500	HEM	CHD-C1D	-2.13	1.34	1.39
3	D	501	HC9	C7-C6	2.11	1.54	1.50
3	A	501	HC9	C18-C13	-2.11	1.50	1.54
3	B	501	HC9	C19-C10	-2.07	1.51	1.54
2	D	500	HEM	C4A-C3A	2.02	1.47	1.43

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	HEM	C4B-C3B-C2B	-8.50	99.47	107.28
2	B	500	HEM	C4B-C3B-C2B	-8.07	99.86	107.28
2	A	500	HEM	C4B-C3B-C2B	-7.97	99.96	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C4B-C3B-C2B	-7.40	100.48	107.28
2	D	500	HEM	CHC-C4B-C3B	-7.08	110.94	125.07
2	A	500	HEM	CHC-C4B-C3B	-7.04	111.02	125.07
2	A	500	HEM	C2B-C1B-NB	6.97	117.86	109.84
2	D	500	HEM	C2B-C1B-NB	6.97	117.85	109.84
3	D	501	HC9	C18-C13-C14	6.66	123.75	111.68
2	C	500	HEM	CHC-C4B-C3B	-6.27	112.57	125.07
2	B	500	HEM	CHC-C1C-NC	-5.91	118.02	124.45
3	D	501	HC9	C12-C13-C14	-5.90	98.42	107.25
3	B	501	HC9	C17-C20-C22	5.76	118.16	111.19
2	C	500	HEM	C2B-C1B-NB	5.62	116.30	109.84
2	B	500	HEM	CHC-C4B-C3B	-5.61	113.87	125.07
2	B	500	HEM	CHC-C4B-NB	5.58	130.43	124.42
3	C	501	HC9	C15-C14-C13	-5.42	97.47	103.84
2	B	500	HEM	C2B-C1B-NB	5.23	115.85	109.84
3	B	501	HC9	C4-C5-C6	-5.12	113.62	120.57
2	D	500	HEM	CHD-C1D-ND	4.96	129.76	124.42
3	D	501	HC9	C13-C14-C8	4.88	121.34	114.41
2	A	500	HEM	C2A-C1A-NA	-4.71	104.93	110.15
2	D	500	HEM	CHA-C4D-ND	4.51	129.95	124.37
3	C	501	HC9	C2-C3-C4	-4.45	104.03	110.29
2	B	500	HEM	CHA-C4D-ND	4.42	129.83	124.37
2	A	500	HEM	CHC-C1C-NC	-4.35	119.72	124.45
3	A	501	HC9	C13-C14-C8	4.35	120.58	114.41
2	B	500	HEM	CHD-C1D-C2D	-4.31	118.22	125.03
3	D	501	HC9	C21-C20-C22	-4.29	104.25	111.09
3	D	501	HC9	C2-C3-C4	-4.27	104.29	110.29
3	B	501	HC9	C2-C3-C4	-4.27	104.29	110.29
2	C	500	HEM	CHA-C4D-ND	4.19	129.55	124.37
2	C	500	HEM	CHB-C1B-C2B	-3.99	115.61	126.95
2	C	500	HEM	CHC-C4B-NB	3.95	128.67	124.42
2	B	500	HEM	C2A-C1A-NA	-3.93	105.79	110.15
2	B	500	HEM	CHD-C1D-ND	3.88	128.59	124.42
3	A	501	HC9	C17-C20-C22	3.62	115.57	111.19
2	D	500	HEM	C2A-C1A-NA	-3.60	106.16	110.15
2	C	500	HEM	C2A-C1A-NA	-3.60	106.16	110.15
3	D	501	HC9	C17-C20-C22	3.56	115.50	111.19
3	A	501	HC9	C4-C5-C6	-3.53	115.78	120.57
2	D	500	HEM	CHB-C1B-C2B	-3.53	116.93	126.95
2	B	500	HEM	C3C-C2C-C1C	-3.51	103.72	107.05
3	A	501	HC9	C10-C5-C6	-3.48	117.84	122.93
3	D	501	HC9	C4-C5-C6	-3.44	115.90	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HC9	C18-C13-C14	3.34	117.73	111.68
2	D	500	HEM	C4D-ND-C1D	3.31	109.12	105.21
2	A	500	HEM	CHD-C1D-C2D	-3.31	119.81	125.03
3	C	501	HC9	O2-C22-C23	3.28	116.58	109.14
2	B	500	HEM	CHD-C4C-C3C	-3.27	119.70	125.21
3	D	501	HC9	C13-C17-C20	3.26	123.68	118.99
3	A	501	HC9	C9-C10-C5	3.23	114.39	109.65
2	D	500	HEM	C3C-C2C-C1C	-3.23	103.99	107.05
2	A	500	HEM	C1C-CHC-C4B	-3.14	119.34	126.02
3	C	501	HC9	C4-C5-C6	-3.13	116.33	120.57
3	A	501	HC9	C12-C13-C14	-3.08	102.64	107.25
3	D	501	HC9	C16-C17-C13	3.08	107.46	103.84
2	A	500	HEM	CHB-C1B-C2B	-3.04	118.31	126.95
2	B	500	HEM	CHB-C1B-C2B	-3.02	118.37	126.95
3	D	501	HC9	C18-C13-C12	-2.97	106.22	110.61
2	D	500	HEM	CHD-C1D-C2D	-2.96	120.36	125.03
3	C	501	HC9	C9-C10-C5	2.92	113.93	109.65
2	A	500	HEM	CHD-C4C-C3C	-2.83	120.43	125.21
2	C	500	HEM	C1C-CHC-C4B	-2.83	120.02	126.02
3	D	501	HC9	C15-C14-C13	2.77	107.10	103.84
2	A	500	HEM	CHA-C4D-ND	2.77	127.79	124.37
2	A	500	HEM	C1A-CHA-C4D	-2.69	119.93	126.25
2	D	500	HEM	CHC-C1C-NC	-2.69	121.53	124.45
2	C	500	HEM	CHC-C1C-NC	-2.68	121.53	124.45
2	C	500	HEM	C3C-C2C-C1C	-2.67	104.52	107.05
2	C	500	HEM	CHD-C1D-C2D	-2.65	120.84	125.03
3	D	501	HC9	C11-C12-C13	-2.64	108.29	112.74
2	D	500	HEM	C1C-CHC-C4B	-2.62	120.45	126.02
3	D	501	HC9	C14-C8-C9	-2.60	105.69	109.09
3	B	501	HC9	C1-C2-C3	-2.58	107.06	110.48
3	D	501	HC9	C7-C6-C5	-2.57	120.69	125.02
3	C	501	HC9	C21-C20-C17	2.56	117.41	112.78
3	C	501	HC9	C14-C8-C9	2.55	112.42	109.09
2	C	500	HEM	CHD-C1D-ND	2.54	127.16	124.42
3	C	501	HC9	C17-C20-C22	2.53	114.26	111.19
3	B	501	HC9	O2-C22-C20	-2.48	104.69	110.09
2	D	500	HEM	CAC-C3C-C4C	2.44	130.65	124.82
2	B	500	HEM	CHA-C1A-NA	2.43	128.27	123.86
3	C	501	HC9	C1-C10-C9	-2.43	105.52	108.74
3	B	501	HC9	C19-C10-C9	-2.43	108.94	111.66
2	C	500	HEM	CHD-C4C-C3C	-2.39	121.19	125.21
2	B	500	HEM	C2C-C1C-NC	2.36	113.99	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	HC9	C4-C5-C10	-2.35	113.41	116.42
2	B	500	HEM	C3D-C4D-ND	-2.35	107.59	110.17
2	B	500	HEM	CHA-C4D-C3D	-2.34	120.91	125.23
2	C	500	HEM	C4A-CHB-C1B	-2.33	120.77	126.25
2	C	500	HEM	O2D-CGD-O1D	-2.28	117.46	123.33
3	B	501	HC9	C12-C13-C14	-2.28	103.83	107.25
3	C	501	HC9	C8-C7-C6	-2.27	109.61	112.76
2	A	500	HEM	C4D-ND-C1D	2.26	107.88	105.21
2	C	500	HEM	C3B-C4B-NB	-2.25	107.85	109.47
3	A	501	HC9	C13-C17-C20	2.25	122.22	118.99
2	B	500	HEM	C4A-CHB-C1B	-2.24	120.97	126.25
2	A	500	HEM	C3C-C2C-C1C	-2.24	104.93	107.05
2	A	500	HEM	C3D-C4D-ND	-2.23	107.73	110.17
2	C	500	HEM	C4C-NC-C1C	2.23	109.45	105.82
2	A	500	HEM	CBA-CAA-C2A	-2.21	106.41	112.53
2	B	500	HEM	C4D-C3D-C2D	-2.20	103.69	106.89
2	D	500	HEM	C4A-CHB-C1B	-2.18	121.12	126.25
3	B	501	HC9	C3-C4-C5	2.18	115.52	112.05
2	D	500	HEM	C3D-C4D-ND	-2.17	107.79	110.17
2	C	500	HEM	C3D-C4D-ND	-2.16	107.80	110.17
3	C	501	HC9	O2-C22-C20	-2.16	105.38	110.09
2	D	500	HEM	C3A-C4A-NA	2.15	113.58	110.14
3	D	501	HC9	C11-C9-C10	2.14	115.72	113.08
3	A	501	HC9	C24-C23-C22	2.12	116.75	113.43
3	C	501	HC9	C2-C1-C10	2.11	117.28	112.78
3	C	501	HC9	C7-C8-C14	2.11	113.92	110.93
3	A	501	HC9	C1-C10-C9	-2.10	105.96	108.74
2	D	500	HEM	CMB-C2B-C1B	-2.09	121.77	125.03
3	D	501	HC9	O1-C3-C2	-2.09	104.71	110.17
2	A	500	HEM	CHB-C4A-C3A	-2.04	121.50	127.43
3	A	501	HC9	C11-C12-C13	-2.04	109.30	112.74
2	A	500	HEM	C4C-CHD-C1D	-2.03	121.71	126.02
2	B	500	HEM	O2D-CGD-CBD	2.02	120.38	114.00
2	B	500	HEM	CMC-C2C-C3C	-2.02	123.54	128.43
3	A	501	HC9	C23-C24-C25	-2.02	107.05	113.91

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C2C-C3C-CAC-CBC
2	D	500	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	D	500	HEM	C4C-C3C-CAC-CBC
3	B	501	HC9	C20-C22-C23-C24
3	B	501	HC9	O2-C22-C23-C24
3	B	501	HC9	C23-C24-C25-C27
3	B	501	HC9	C23-C24-C25-C26
3	B	501	HC9	C22-C23-C24-C25
3	C	501	HC9	C17-C20-C22-O2
3	D	501	HC9	C23-C24-C25-C26
3	A	501	HC9	O2-C22-C23-C24
2	D	500	HEM	C3A-C2A-CAA-CBA
2	D	500	HEM	C2A-CAA-CBA-CGA
3	A	501	HC9	C20-C22-C23-C24
2	C	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	C1A-C2A-CAA-CBA
2	D	500	HEM	CAD-CBD-CGD-O1D
2	C	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	CAD-CBD-CGD-O2D

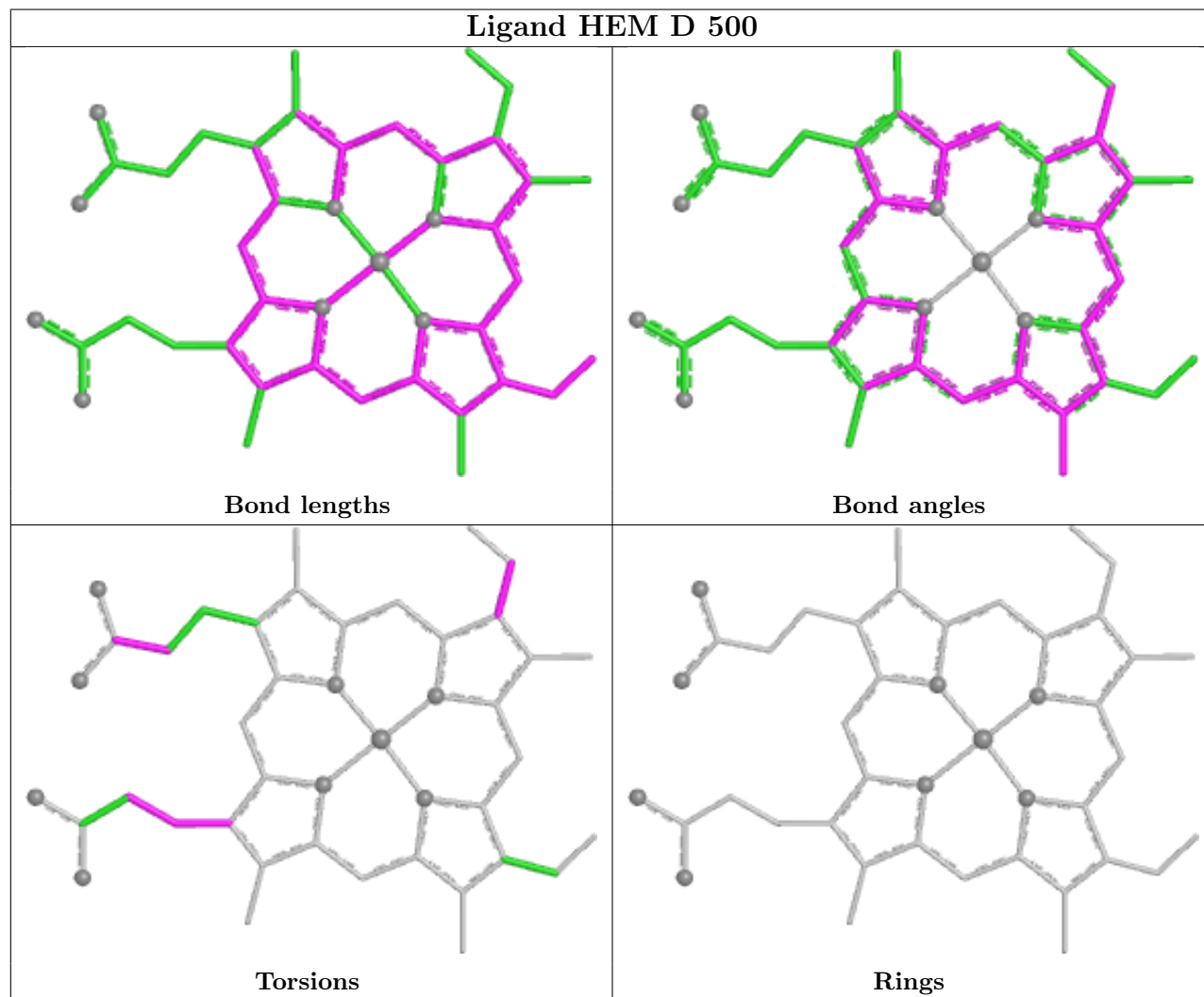
There are no ring outliers.

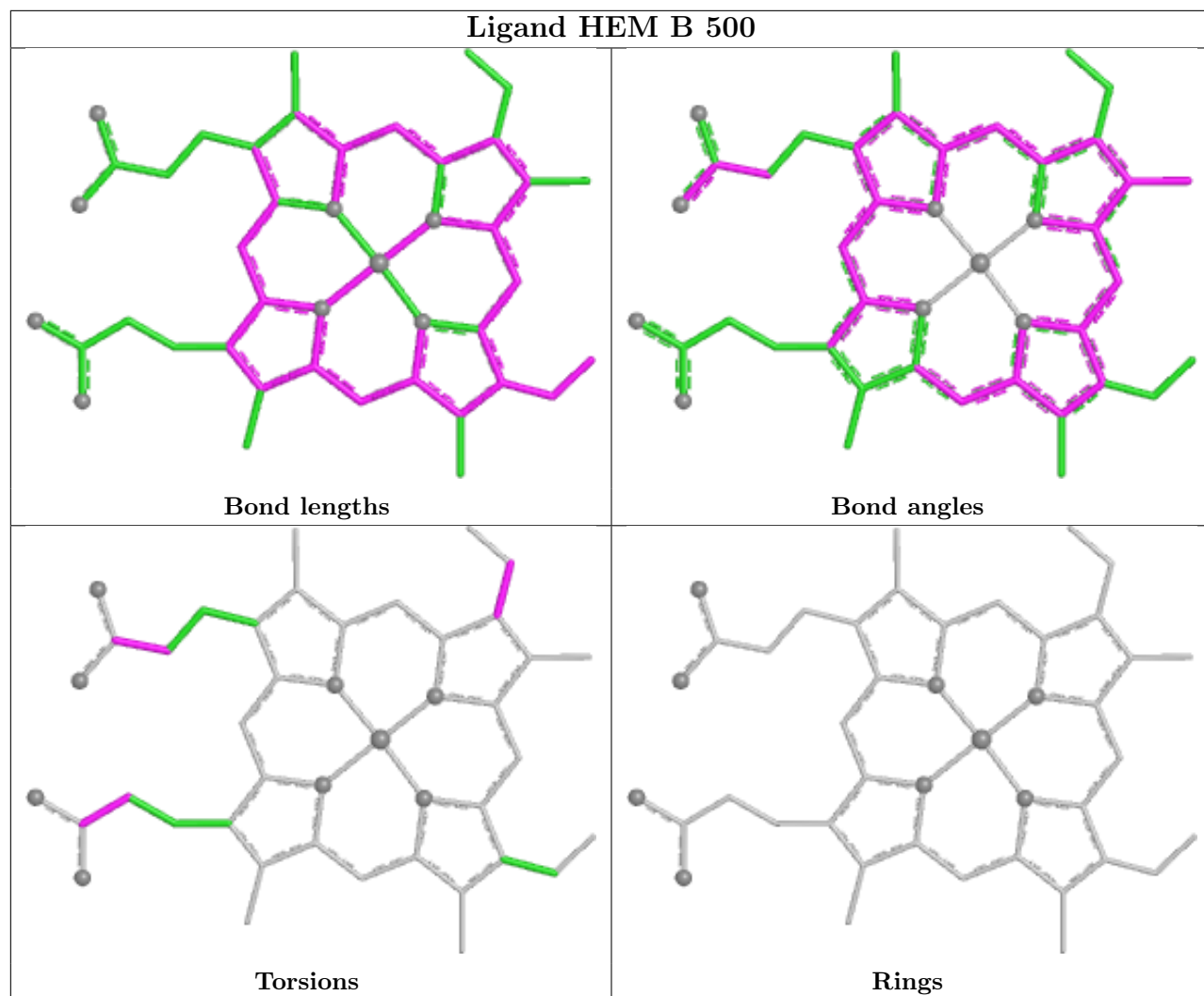
12 monomers are involved in 44 short contacts:

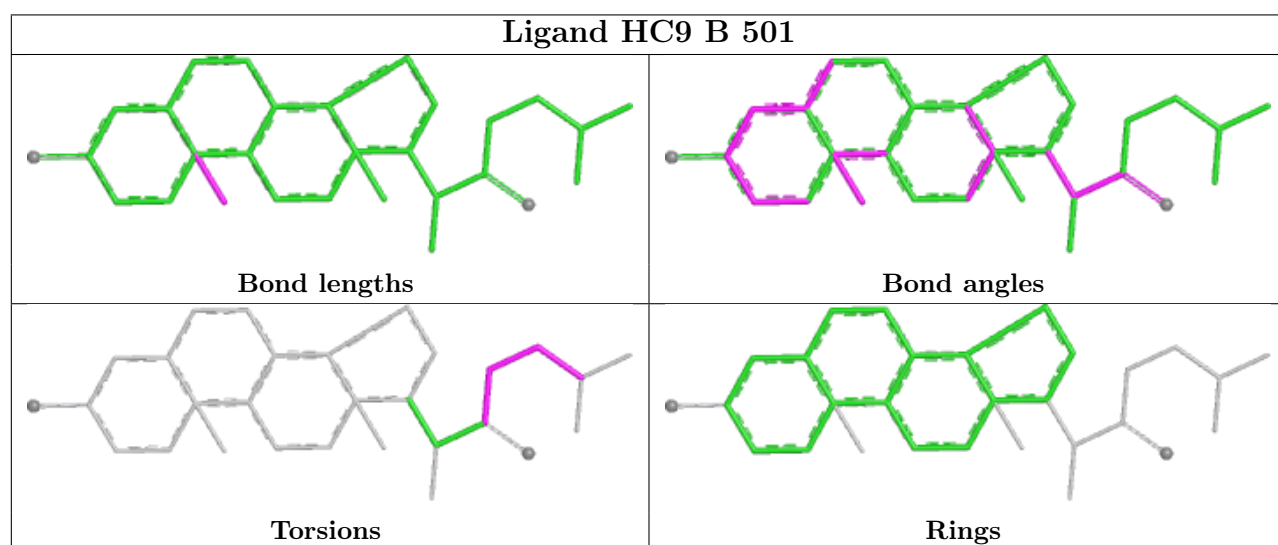
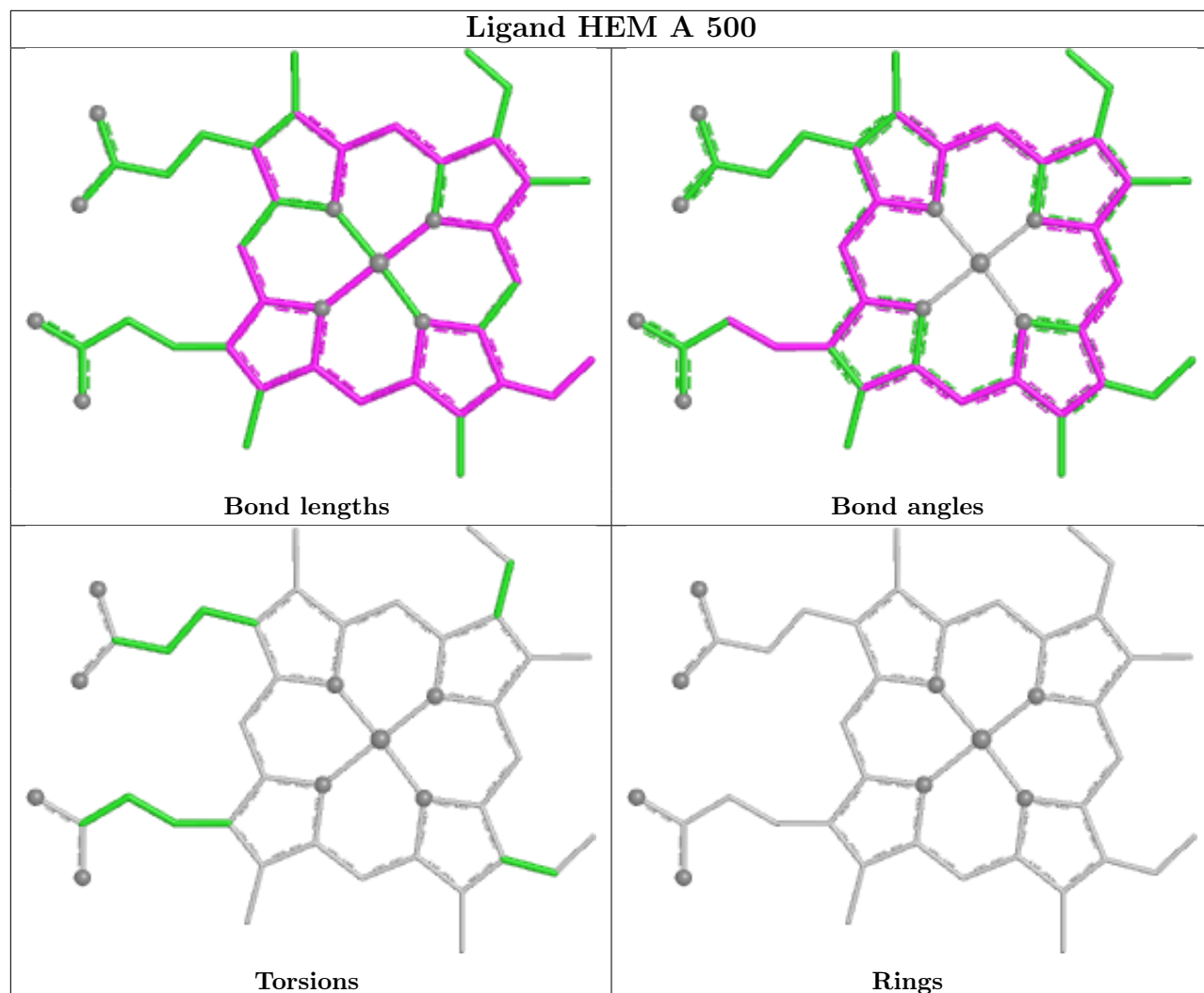
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	IPA	5	0
2	D	500	HEM	5	0
4	D	502	IPA	3	0
2	B	500	HEM	4	0
2	A	500	HEM	4	0
3	B	501	HC9	2	0
4	B	502	IPA	7	0
2	C	500	HEM	5	0
3	A	501	HC9	2	0
4	A	502	IPA	1	0
3	D	501	HC9	1	0
3	C	501	HC9	5	0

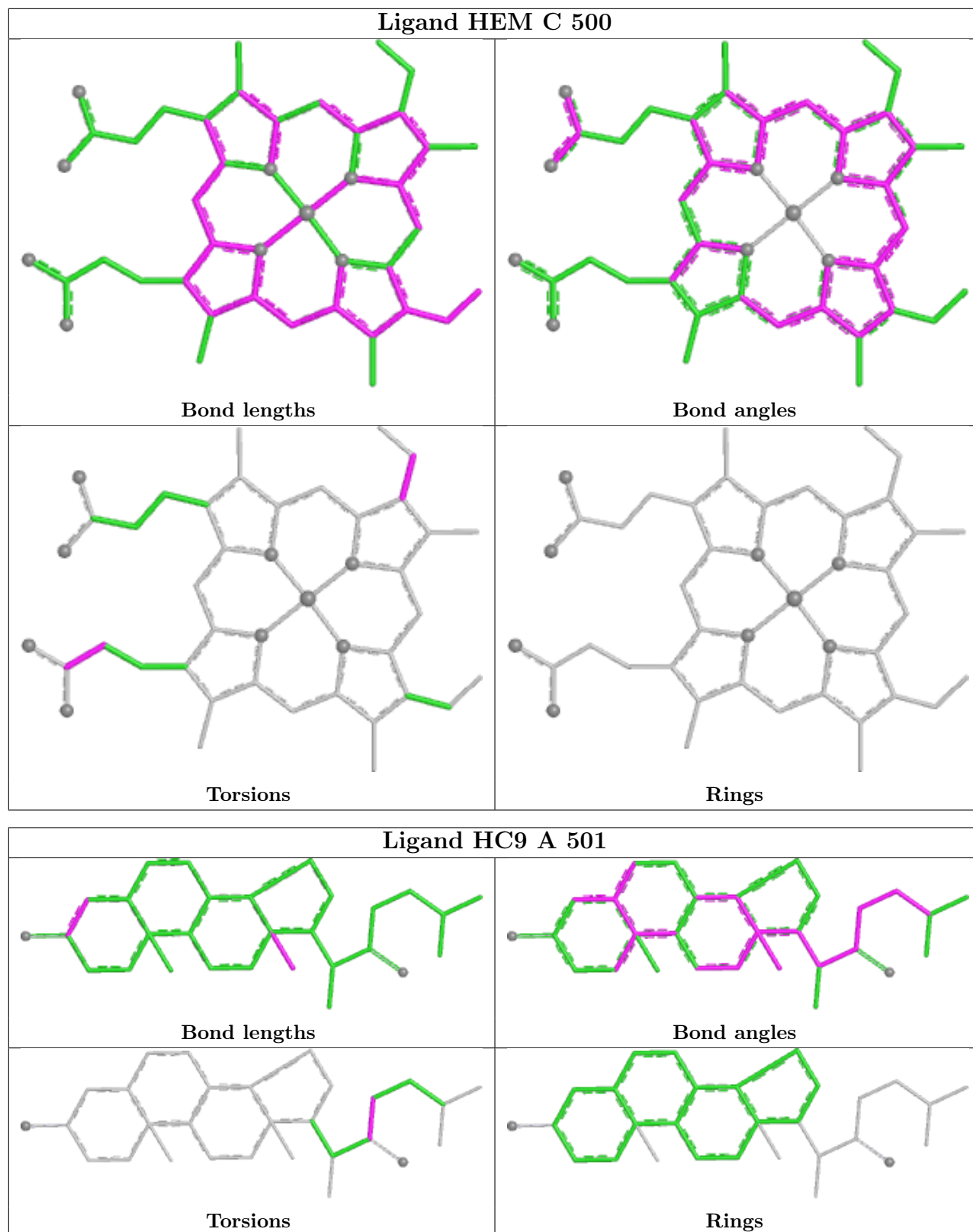
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

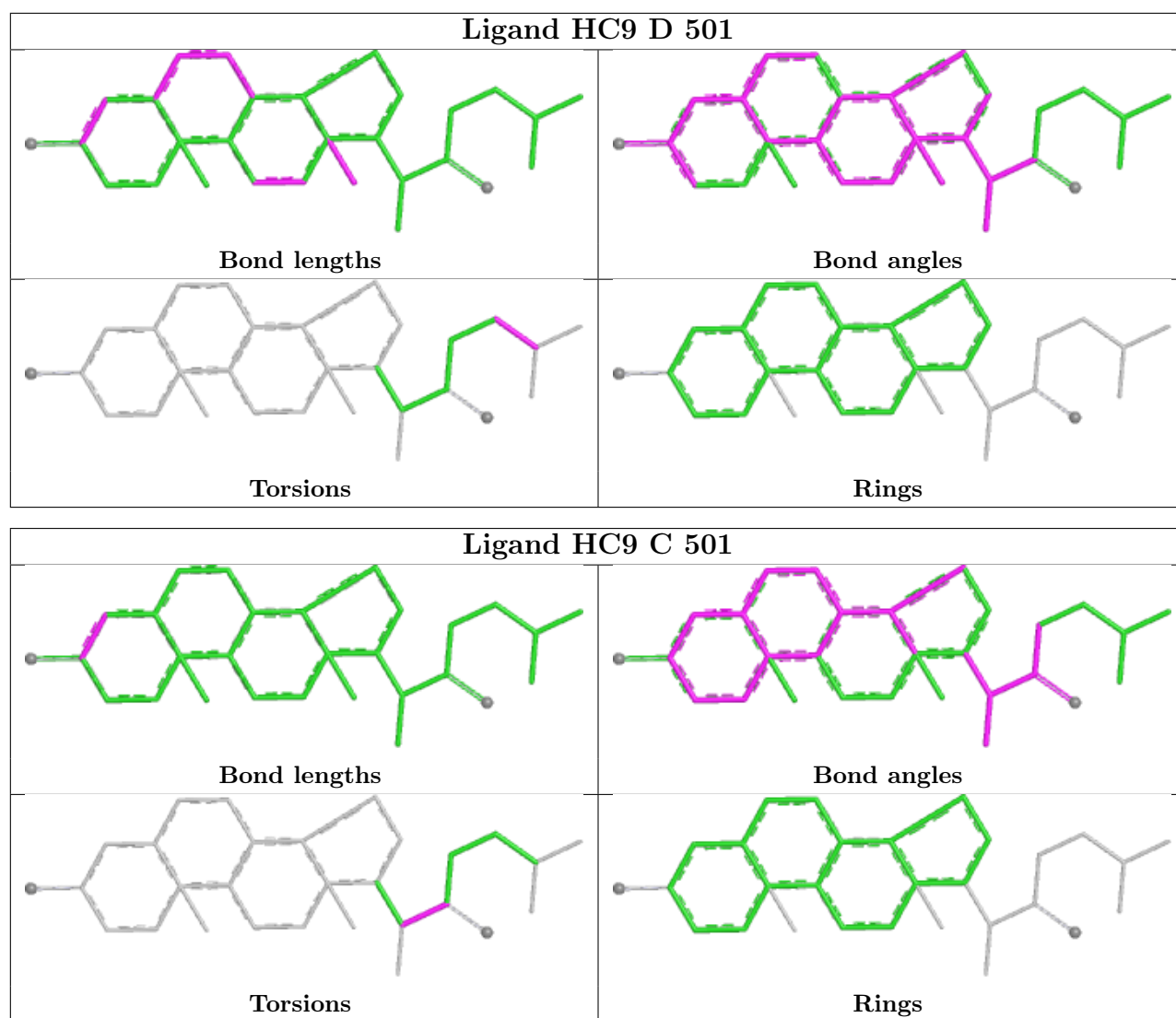
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/486 (96%)	-1.16	0 100 100	34, 65, 84, 96	0
1	B	470/486 (96%)	-1.14	0 100 100	39, 67, 87, 97	0
1	C	470/486 (96%)	-1.14	0 100 100	35, 65, 84, 93	0
1	D	470/486 (96%)	-1.17	0 100 100	32, 67, 86, 94	0
All	All	1880/1944 (96%)	-1.15	0 100 100	32, 66, 85, 97	0

There are no RSRZ outliers to report.

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.

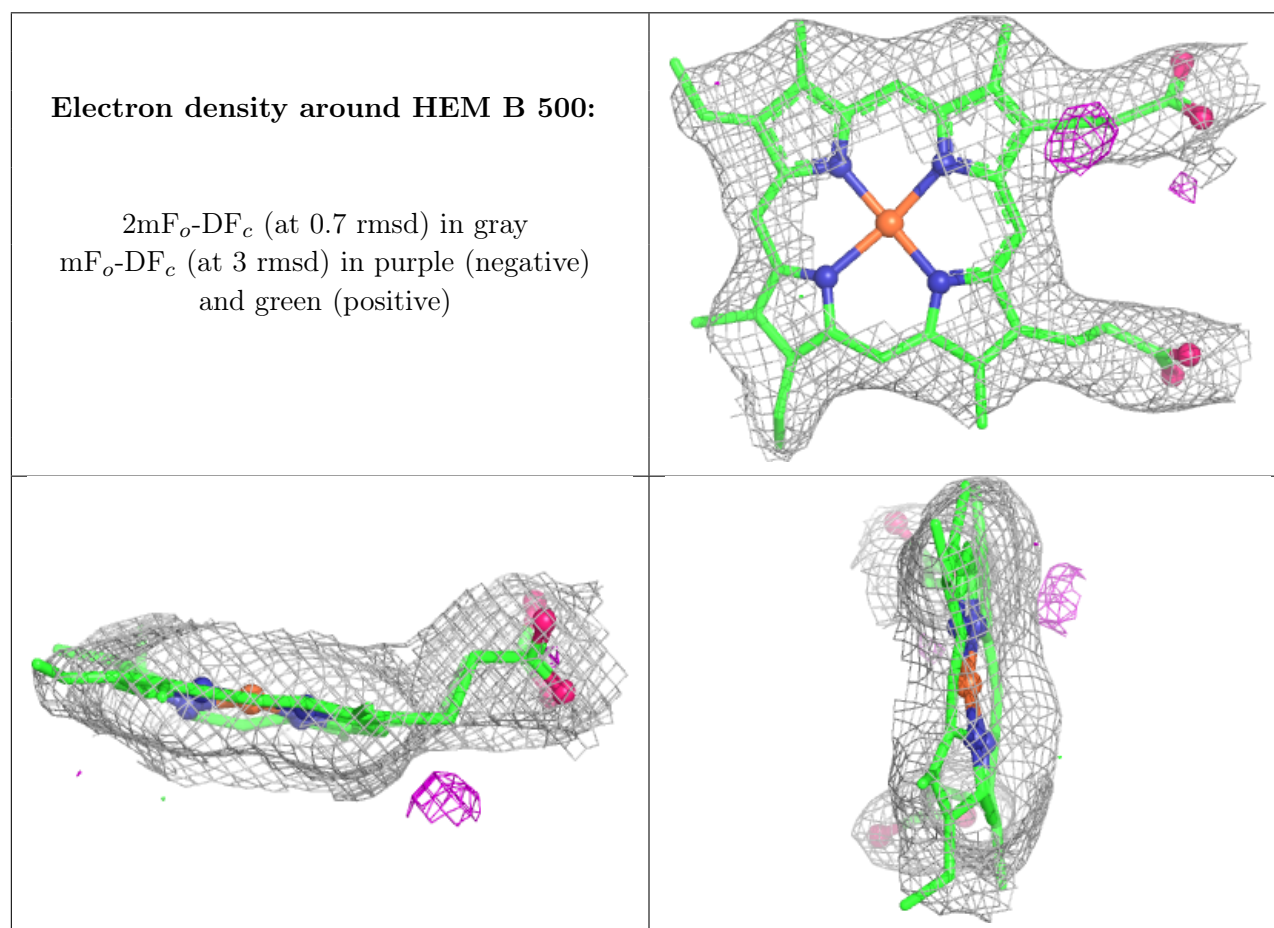
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	B	500	43/43	0.99	0.03	34,47,55,60	0
3	HC9	A	501	29/29	0.99	0.05	41,49,58,60	0
3	HC9	B	501	29/29	0.99	0.05	44,53,64,68	0
3	HC9	C	501	29/29	0.99	0.05	44,54,61,66	0

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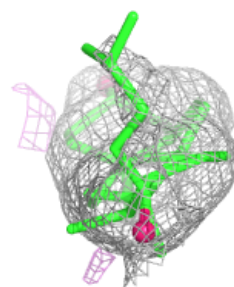
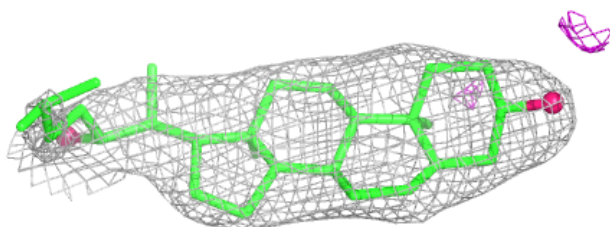
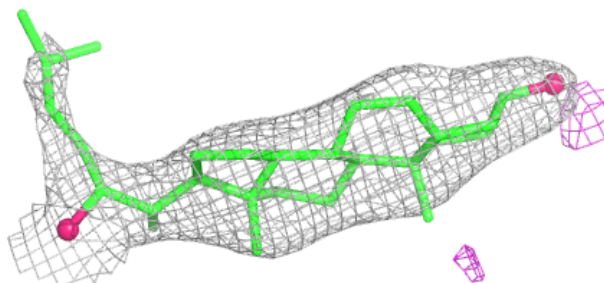
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HC9	D	501	29/29	0.99	0.05	39,48,56,61	0
4	IPA	A	502	4/4	0.99	0.14	49,49,50,51	0
4	IPA	B	502	4/4	0.99	0.08	60,61,62,63	0
4	IPA	C	502	4/4	0.99	0.08	60,61,61,63	0
4	IPA	D	502	4/4	0.99	0.07	59,59,61,65	0
2	HEM	D	500	43/43	1.00	0.03	18,41,56,62	0
2	HEM	A	500	43/43	1.00	0.03	25,43,54,57	0
2	HEM	C	500	43/43	1.00	0.04	37,50,56,59	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.

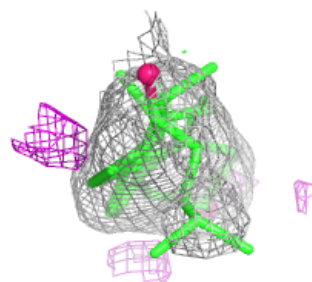
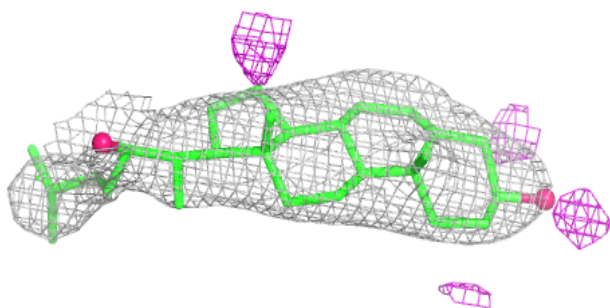
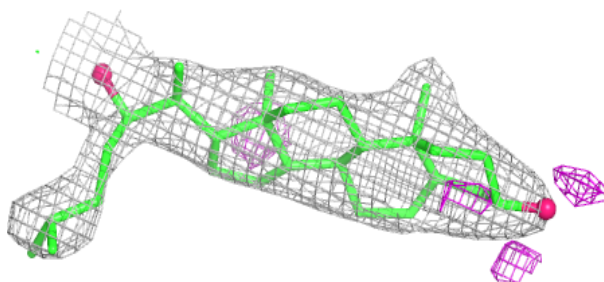


Electron density around HC9 A 501:

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

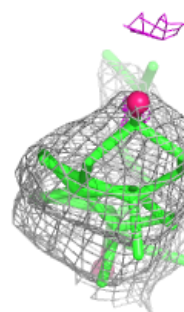
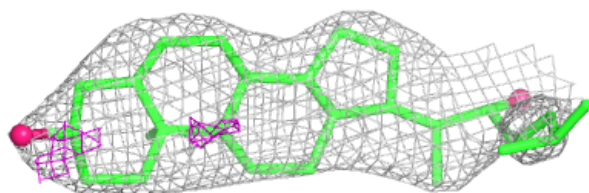
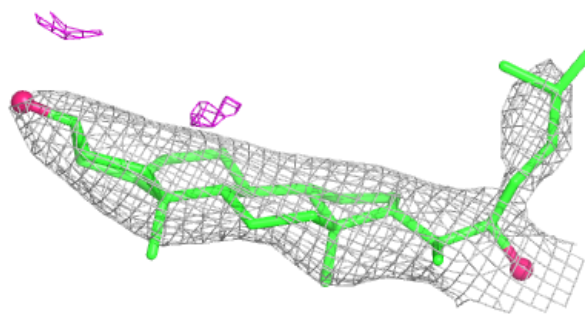
**Electron density around HC9 B 501:**

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

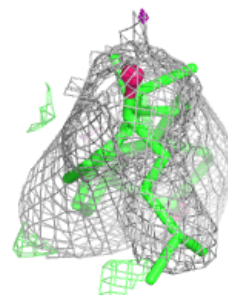
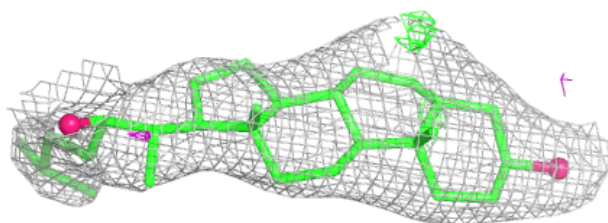
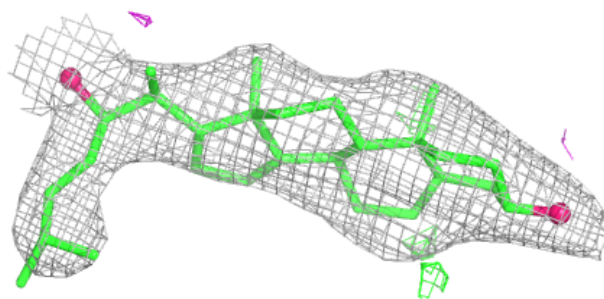


Electron density around HC9 C 501:

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

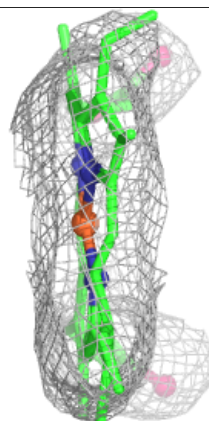
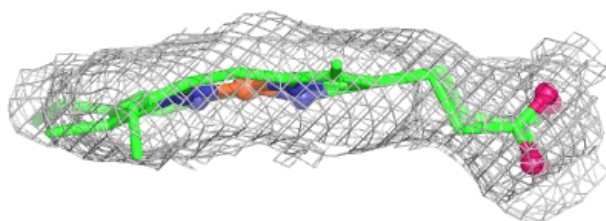
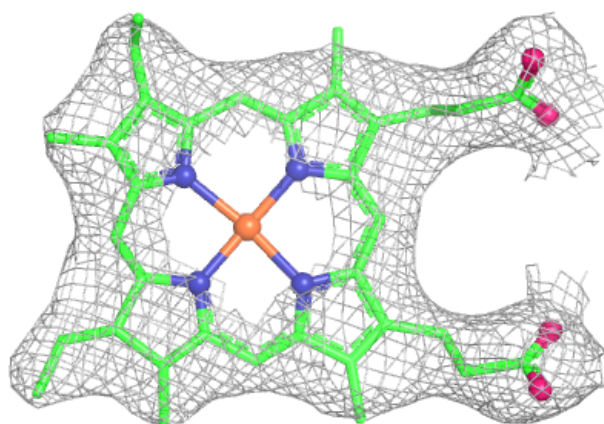
**Electron density around HC9 D 501:**

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



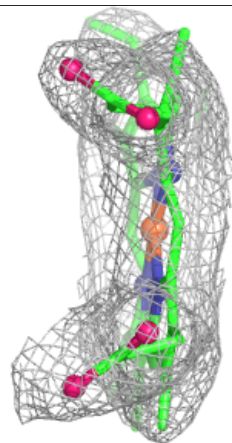
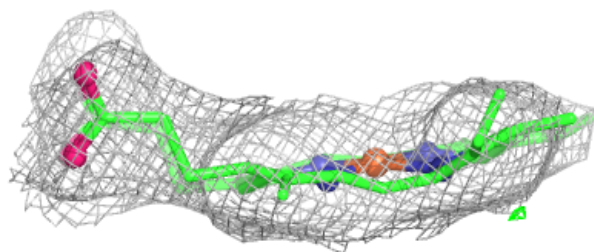
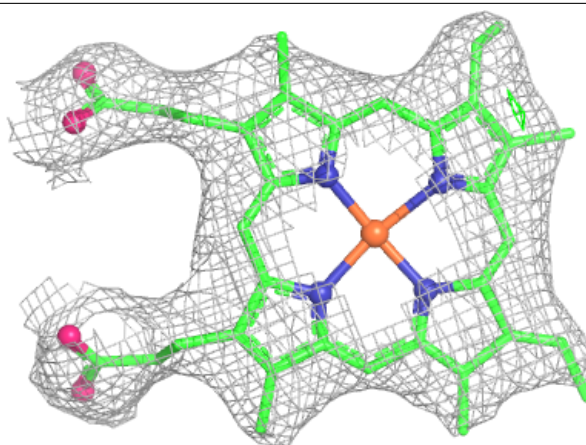
Electron density around HEM D 500:

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



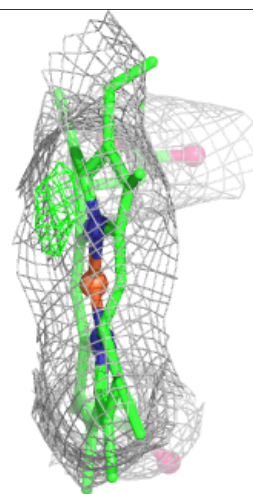
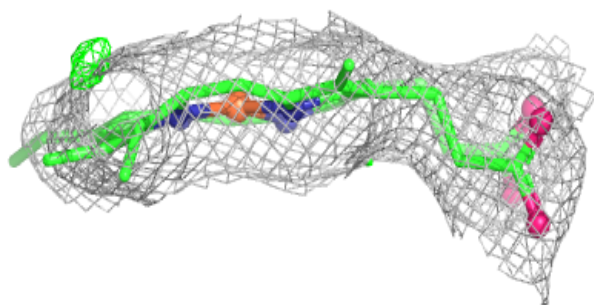
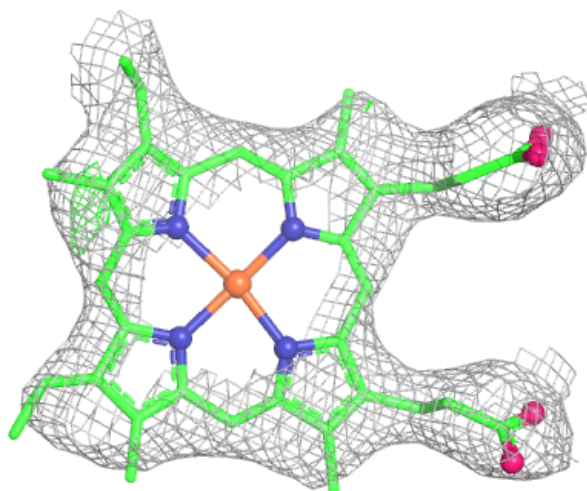
Electron density around HEM A 500:

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



Electron density around HEM C 500:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.