



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:38 am BST

PDB ID : 2E75
Title : Crystal Structure of the Cytochrome b6f Complex with 2-nonyl-4-hydroxyquinoline N-oxide (NQNO) from *M.laminosus*
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.
Deposited on : 2007-01-05
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

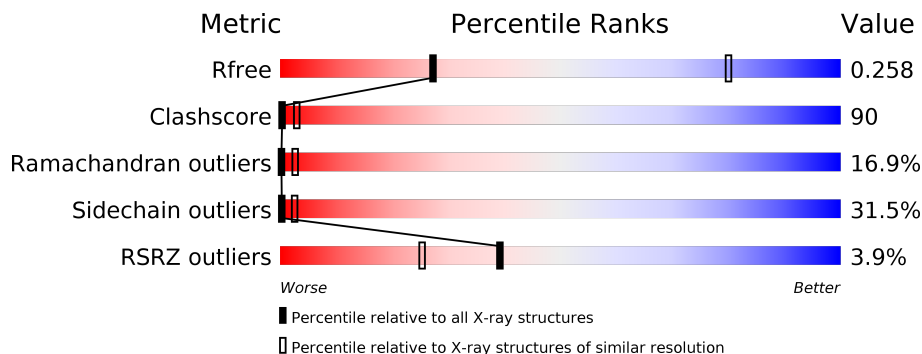
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	215	
2	B	160	
3	C	289	
4	D	179	
5	E	32	
6	F	35	

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Mol	Chain	Length	Quality of chain
7	G	37	
8	H	29	

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
10	HEM	A	301	-	-	X	-
10	HEM	A	302	-	-	X	-
10	HEM	C	301	-	-	X	-
11	OPC	A	1002	-	-	X	-
12	UMQ	A	1102	X	-	-	-
12	UMQ	A	1103	X	-	-	-
12	UMQ	A	1104	X	-	-	-
12	UMQ	C	1101	X	-	-	-
13	QNO	A	501	X	-	-	-
14	CLA	B	201	X	-	-	-
15	FES	D	200	-	-	X	-
16	SQD	D	201	X	X	-	-
17	BCR	G	101	-	X	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 8046 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 b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1711	1140	272	288	11	0	0	0

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	160	1249	841	193	209	6	0	0	0

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	288	2216	1415	369	424	8	0	0	0

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	166	1260	805	218	230	7	0	0	0

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	32	248	179	34	34	1	0	0	0

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	32	242	165	35	40	2	0	0	0

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	37	Total 283	C 188	N 44	O 50	S 1	0	0	0

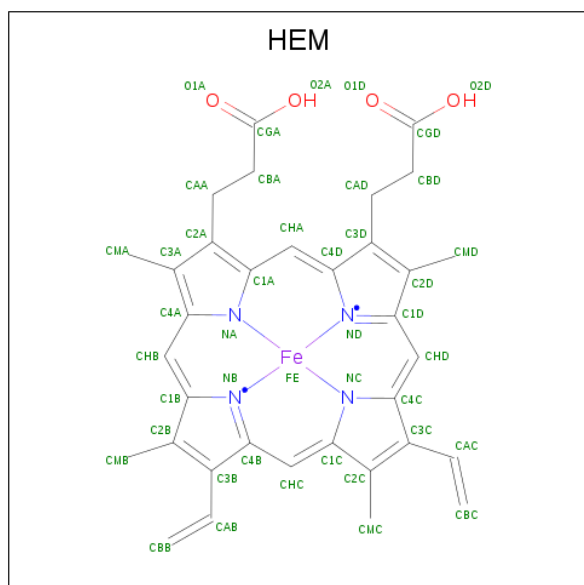
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	29	Total 230	C 156	N 36	O 36	S 2	0	0	0

- Molecule 9 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Cd 1	0	0
9	A	1	Total 1	Cd 1	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



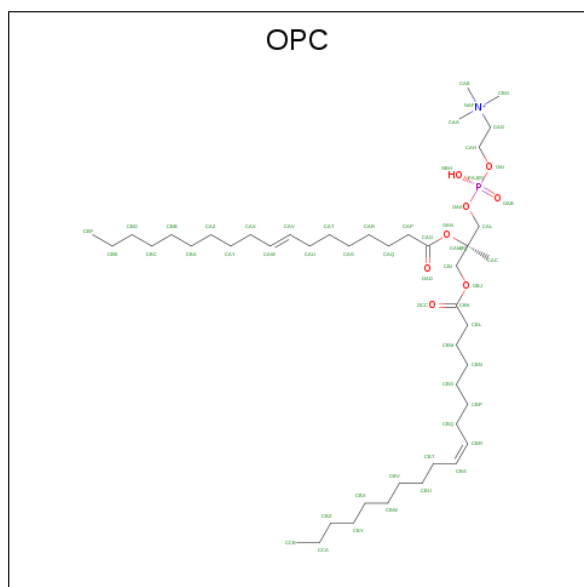
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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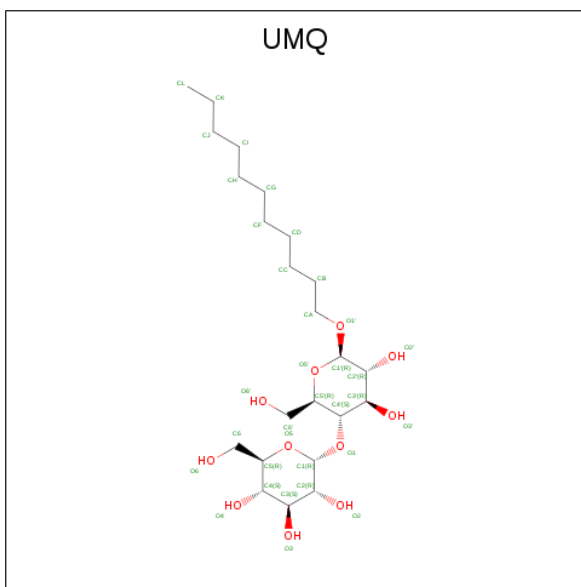
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
10	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: C₄₅H₈₇NO₈P).



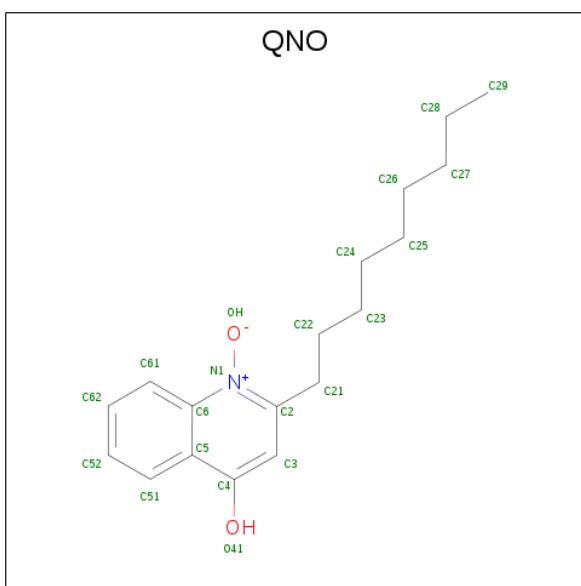
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
11	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
11	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).



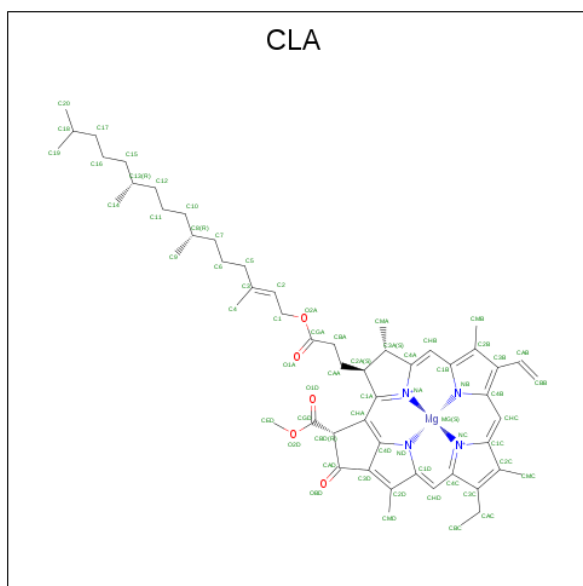
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		
12	C	1	Total	C	O	0	0
			34	23	11		

- Molecule 13 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (three-letter code: QNO) (formula: C₁₈H₂₅NO₂).



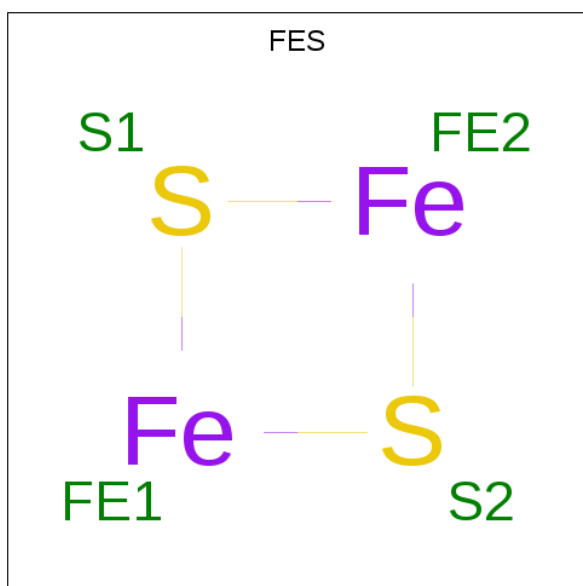
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



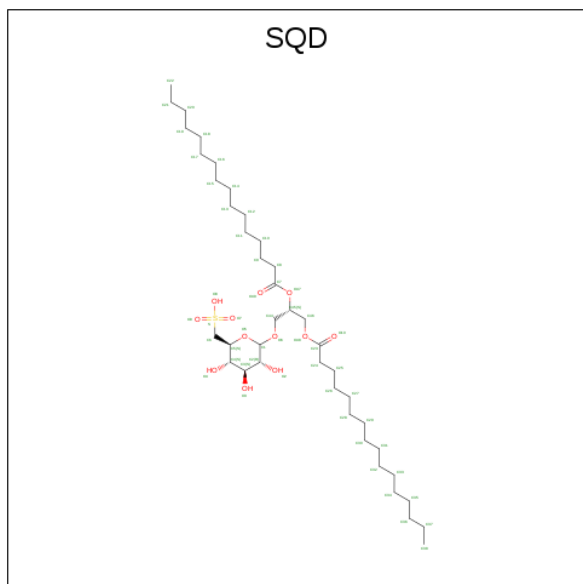
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



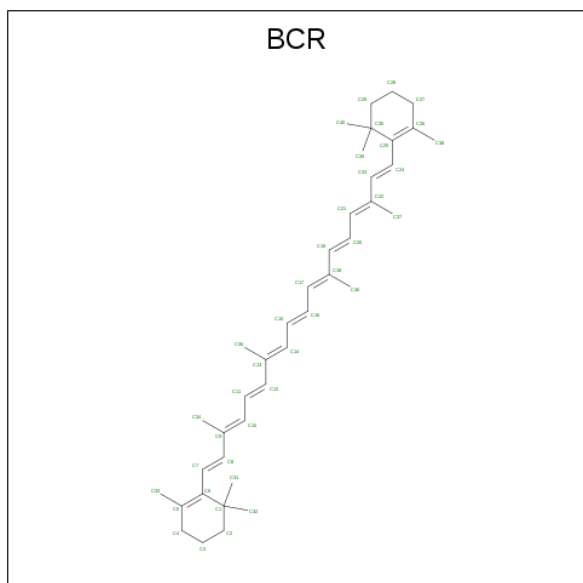
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total C 40 40	0	0

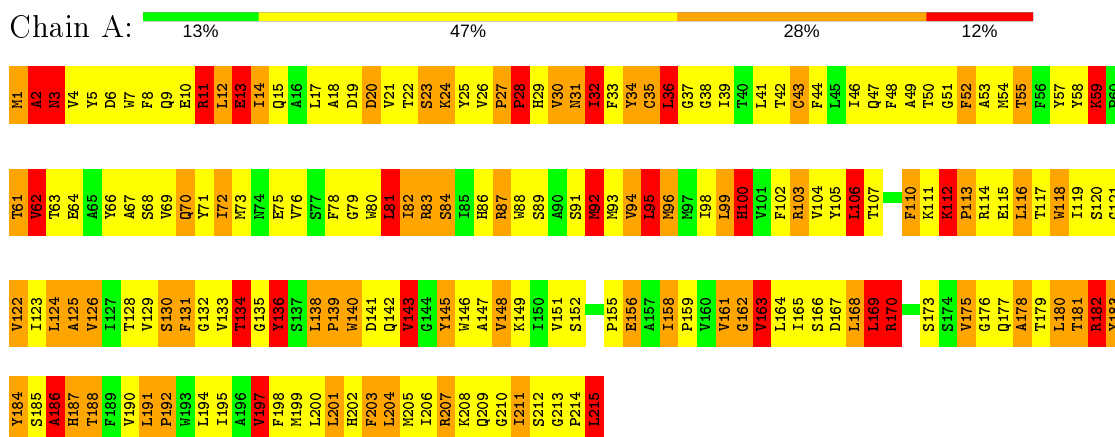
- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	3	Total O 3 3	0	0
18	B	2	Total O 2 2	0	0

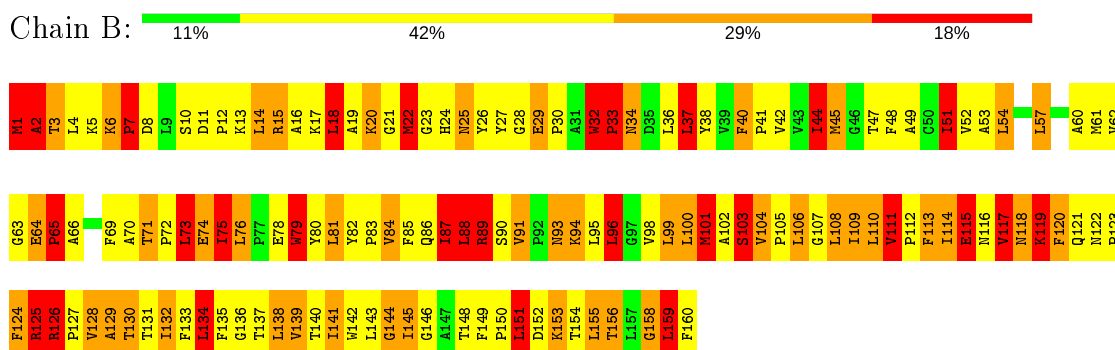
3 Residue-property plots

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

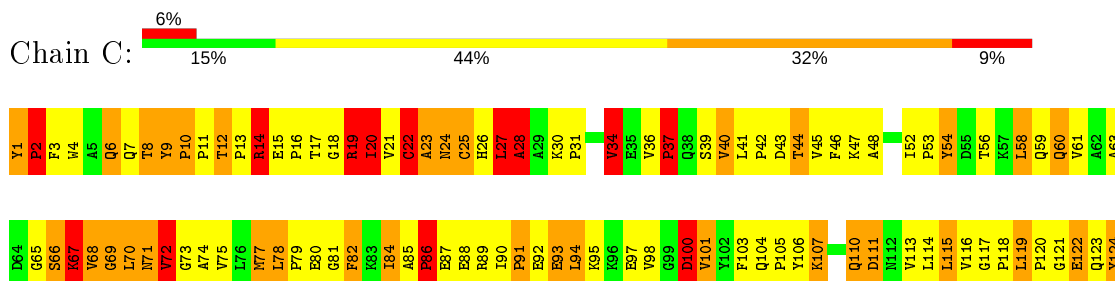
- Molecule 1: Cytochrome b6

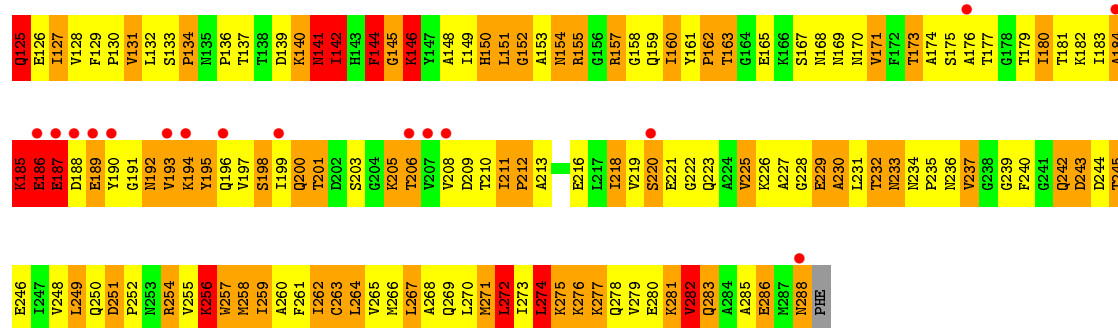


- Molecule 2: Cytochrome b6-f complex subunit 4

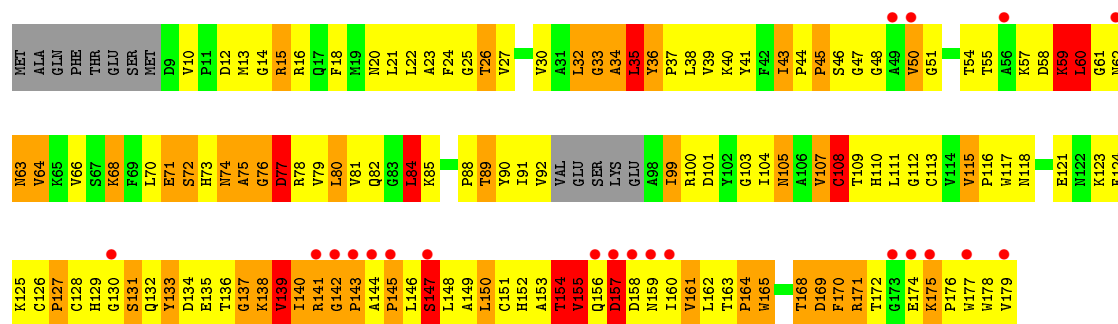
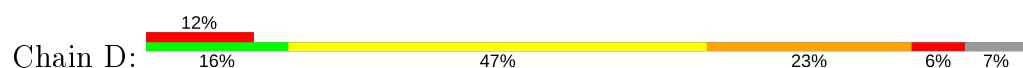


- Molecule 3: Apocytochrome f





• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



• Molecule 5: Cytochrome b6-f complex subunit 6



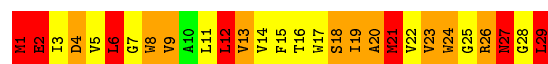
• Molecule 6: Cytochrome b6-f complex subunit 7



• Molecule 7: Cytochrome b6-f complex subunit 5



• Molecule 8: Cytochrome b6-f complex subunit 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	159.16Å 159.16Å 362.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.94 – 3.55 49.94 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.94-3.55) 99.7 (49.94-3.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.89 (at 3.57Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.267 0.198 , 0.258	Depositor DCC
R_{free} test set	1703 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	94.2	Xtrriage
Anisotropy	0.189	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 85.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8046	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: UMQ, CLA, CD, FES, OPC, HEM, QNO, BCR, SQD

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	1.99	39/1763 (2.2%)	2.01	64/2405 (2.7%)
2	B	1.88	24/1288 (1.9%)	2.04	46/1765 (2.6%)
3	C	1.53	29/2264 (1.3%)	1.52	25/3082 (0.8%)
4	D	1.26	3/1292 (0.2%)	1.37	14/1760 (0.8%)
5	E	1.79	3/253 (1.2%)	1.95	8/340 (2.4%)
6	F	2.27	10/246 (4.1%)	2.19	12/331 (3.6%)
7	G	1.78	3/289 (1.0%)	1.87	7/391 (1.8%)
8	H	1.97	6/236 (2.5%)	2.11	12/323 (3.7%)
All	All	1.73	117/7631 (1.5%)	1.78	188/10397 (1.8%)

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	6
2	B	0	7
3	C	0	8
5	E	0	4
6	F	0	1
7	G	0	4
8	H	0	2
All	All	0	32

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	ARG	CZ-NH1	11.16	1.47	1.33
2	B	115	GLU	CG-CD	11.14	1.68	1.51
1	A	122	VAL	CA-CB	-10.27	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	87	GLU	CG-CD	9.96	1.66	1.51
3	C	72	VAL	CB-CG1	-9.56	1.32	1.52
1	A	59	LYS	CD-CE	9.50	1.75	1.51
3	C	256	LYS	CD-CE	9.10	1.74	1.51
6	F	17	PHE	CE1-CZ	8.68	1.53	1.37
2	B	29	GLU	CG-CD	8.29	1.64	1.51
2	B	29	GLU	CB-CG	8.28	1.67	1.52
6	F	17	PHE	CD2-CE2	8.24	1.55	1.39
1	A	61	THR	CB-CG2	8.18	1.79	1.52
1	A	49	ALA	CA-CB	-8.16	1.35	1.52
3	C	87	GLU	CB-CG	8.02	1.67	1.52
1	A	10	GLU	CG-CD	7.74	1.63	1.51
1	A	67	ALA	CA-CB	-7.71	1.36	1.52
2	B	115	GLU	CD-OE1	7.58	1.33	1.25
6	F	17	PHE	CD1-CE1	7.58	1.54	1.39
2	B	84	VAL	CA-CB	-7.53	1.39	1.54
1	A	197	VAL	CB-CG2	-7.50	1.37	1.52
1	A	24	LYS	CB-CG	7.39	1.72	1.52
3	C	148	ALA	CA-CB	-7.37	1.36	1.52
3	C	22	CYS	CB-SG	-7.35	1.69	1.82
4	D	34	ALA	CA-CB	-7.30	1.37	1.52
3	C	256	LYS	CG-CD	7.29	1.77	1.52
1	A	156	GLU	CG-CD	7.20	1.62	1.51
1	A	52	PHE	CB-CG	-7.20	1.39	1.51
1	A	59	LYS	CE-NZ	7.17	1.67	1.49
8	H	29	LEU	CG-CD2	7.09	1.78	1.51
7	G	22	PHE	CD2-CE2	7.09	1.53	1.39
3	C	257	TRP	CB-CG	-7.08	1.37	1.50
3	C	280	GLU	CG-CD	6.99	1.62	1.51
8	H	8	TRP	CB-CG	-6.85	1.38	1.50
8	H	26	ARG	CZ-NH1	6.84	1.42	1.33
7	G	14	VAL	CB-CG2	-6.84	1.38	1.52
1	A	35	CYS	CB-SG	-6.83	1.70	1.82
2	B	79	TRP	CB-CG	-6.77	1.38	1.50
2	B	119	LYS	CB-CG	6.68	1.70	1.52
1	A	184	TYR	CZ-OH	6.66	1.49	1.37
3	C	145	GLY	N-CA	6.66	1.56	1.46
1	A	184	TYR	CG-CD2	-6.61	1.30	1.39
6	F	17	PHE	CE2-CZ	6.61	1.50	1.37
1	A	145	TYR	CA-CB	-6.51	1.39	1.53
1	A	20	ASP	CB-CG	6.51	1.65	1.51
1	A	134	THR	C-O	6.51	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	50	VAL	CA-CB	6.51	1.68	1.54
3	C	145	GLY	CA-C	6.50	1.62	1.51
1	A	207	ARG	CZ-NH2	6.50	1.41	1.33
2	B	71	THR	CA-CB	-6.48	1.36	1.53
6	F	6	LEU	CG-CD2	6.48	1.75	1.51
2	B	88	LEU	CG-CD1	6.42	1.75	1.51
6	F	9	ALA	CA-CB	-6.40	1.39	1.52
1	A	71	TYR	CE2-CZ	-6.38	1.30	1.38
1	A	118	TRP	CG-CD1	6.37	1.45	1.36
2	B	128	VAL	CB-CG1	6.32	1.66	1.52
3	C	146	LYS	CE-NZ	6.30	1.64	1.49
1	A	64	GLU	CD-OE1	6.22	1.32	1.25
1	A	156	GLU	CD-OE2	6.17	1.32	1.25
8	H	1	MET	CB-CG	6.17	1.71	1.51
8	H	13	VAL	CB-CG1	6.16	1.65	1.52
1	A	75	GLU	CD-OE2	6.12	1.32	1.25
2	B	117	VAL	CB-CG2	6.07	1.65	1.52
3	C	146	LYS	CD-CE	6.05	1.66	1.51
1	A	24	LYS	CD-CE	5.95	1.66	1.51
3	C	111	ASP	CB-CG	5.95	1.64	1.51
2	B	111	VAL	CB-CG2	5.91	1.65	1.52
1	A	62	VAL	CA-CB	-5.90	1.42	1.54
1	A	131	PHE	C-O	5.88	1.34	1.23
1	A	125	ALA	CA-CB	-5.84	1.40	1.52
3	C	113	VAL	CB-CG2	-5.83	1.40	1.52
3	C	25	CYS	CB-SG	-5.82	1.72	1.81
2	B	119	LYS	CD-CE	5.79	1.65	1.51
2	B	79	TRP	CZ3-CH2	5.78	1.49	1.40
1	A	34	TYR	CB-CG	5.76	1.60	1.51
3	C	82	PHE	CE2-CZ	5.72	1.48	1.37
3	C	16	PRO	C-O	5.69	1.34	1.23
2	B	120	PHE	CE1-CZ	5.68	1.48	1.37
4	D	36	TYR	CZ-OH	5.68	1.47	1.37
6	F	8	ALA	CA-CB	-5.67	1.40	1.52
2	B	88	LEU	CG-CD2	5.67	1.72	1.51
1	A	203	PHE	CE2-CZ	-5.66	1.26	1.37
1	A	110	PHE	CE2-CZ	5.65	1.48	1.37
1	A	34	TYR	CD2-CE2	5.64	1.47	1.39
7	G	22	PHE	CD1-CE1	5.64	1.50	1.39
3	C	142	ILE	C-O	5.63	1.34	1.23
6	F	20	TRP	C-O	5.54	1.33	1.23
2	B	40	PHE	CE2-CZ	5.53	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	32	TRP	CB-CG	5.53	1.60	1.50
3	C	82	PHE	CD1-CE1	5.52	1.50	1.39
3	C	142	ILE	CA-CB	-5.51	1.42	1.54
5	E	11	PHE	C-O	5.49	1.33	1.23
1	A	24	LYS	CG-CD	5.46	1.71	1.52
6	F	20	TRP	CG-CD1	5.45	1.44	1.36
2	B	40	PHE	CD1-CE1	5.43	1.50	1.39
8	H	1	MET	CG-SD	5.38	1.95	1.81
2	B	141	ILE	CA-CB	-5.38	1.42	1.54
5	E	20	VAL	CA-CB	-5.34	1.43	1.54
6	F	7	TYR	CE1-CZ	5.33	1.45	1.38
3	C	80	GLU	CG-CD	5.31	1.59	1.51
3	C	87	GLU	CD-OE1	5.30	1.31	1.25
3	C	144	PHE	N-CA	5.30	1.56	1.46
3	C	84	ILE	CA-CB	-5.29	1.42	1.54
2	B	40	PHE	CD2-CE2	5.25	1.49	1.39
3	C	256	LYS	CB-CG	5.25	1.66	1.52
1	A	112	LYS	CB-CG	5.25	1.66	1.52
1	A	58	TYR	CD1-CE1	-5.23	1.31	1.39
1	A	185	SER	CB-OG	5.21	1.49	1.42
3	C	87	GLU	N-CA	5.21	1.56	1.46
2	B	20	LYS	CD-CE	5.14	1.64	1.51
3	C	40	VAL	CA-CB	-5.13	1.44	1.54
1	A	140	TRP	C-O	5.12	1.33	1.23
1	A	181	THR	C-O	5.11	1.33	1.23
2	B	111	VAL	CB-CG1	5.08	1.63	1.52
5	E	32	ILE	CB-CG2	5.08	1.68	1.52
1	A	161	VAL	CB-CG2	-5.06	1.42	1.52
3	C	87	GLU	CA-CB	5.05	1.65	1.53
1	A	118	TRP	CD2-CE2	5.02	1.47	1.41

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	ARG	NE-CZ-NH2	-24.30	108.15	120.30
1	A	106	LEU	CB-CG-CD1	-12.98	88.93	111.00
1	A	83	ARG	NE-CZ-NH1	-12.94	113.83	120.30
2	B	125	ARG	NE-CZ-NH1	-12.28	114.16	120.30
2	B	15	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	59	LYS	CD-CE-NZ	10.79	136.51	111.70
6	F	11	LEU	CA-CB-CG	-10.64	90.82	115.30
8	H	26	ARG	NE-CZ-NH2	-10.56	115.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	159	LEU	CA-CB-CG	10.51	139.47	115.30
7	G	18	LEU	CB-CG-CD2	-10.35	93.41	111.00
1	A	138	LEU	CB-CG-CD2	-9.67	94.56	111.00
4	D	22	LEU	CA-CB-CG	-9.57	93.29	115.30
6	F	10	LEU	CB-CG-CD1	-9.55	94.76	111.00
1	A	112	LYS	C-N-CD	9.49	148.32	128.40
1	A	122	VAL	CA-CB-CG2	-9.33	96.91	110.90
2	B	134	LEU	CA-CB-CG	-9.06	94.46	115.30
2	B	57	LEU	CB-CG-CD1	-8.98	95.73	111.00
1	A	61	THR	CA-CB-CG2	8.98	124.97	112.40
2	B	134	LEU	CB-CG-CD1	-8.91	95.85	111.00
5	E	31	LEU	CA-CB-CG	-8.90	94.83	115.30
8	H	26	ARG	NE-CZ-NH1	8.88	124.74	120.30
6	F	15	LEU	CA-CB-CG	-8.88	94.88	115.30
1	A	81	LEU	CB-CG-CD2	-8.83	95.98	111.00
2	B	126	ARG	NE-CZ-NH1	8.73	124.67	120.30
6	F	5	MET	CG-SD-CE	8.67	114.08	100.20
2	B	99	LEU	CA-CB-CG	-8.57	95.60	115.30
1	A	169	LEU	CA-CB-CG	8.56	134.98	115.30
2	B	126	ARG	NE-CZ-NH2	-8.51	116.05	120.30
4	D	35	LEU	CA-CB-CG	-8.46	95.83	115.30
2	B	134	LEU	CB-CG-CD2	8.41	125.30	111.00
1	A	191	LEU	CB-CG-CD1	-8.40	96.72	111.00
3	C	254	ARG	NE-CZ-NH1	-8.37	116.12	120.30
7	G	9	LEU	CA-CB-CG	-8.27	96.28	115.30
4	D	108	CYS	CA-CB-SG	8.25	128.84	114.00
8	H	1	MET	CB-CG-SD	8.20	137.01	112.40
8	H	21	MET	CG-SD-CE	-7.94	87.49	100.20
5	E	14	LEU	CB-CG-CD2	-7.85	97.66	111.00
6	F	10	LEU	CA-CB-CG	-7.74	97.50	115.30
8	H	29	LEU	CB-CG-CD2	7.70	124.09	111.00
2	B	18	LEU	CA-CB-CG	-7.64	97.72	115.30
6	F	11	LEU	CB-CG-CD2	-7.52	98.22	111.00
4	D	60	LEU	CA-CB-CG	7.45	132.43	115.30
3	C	78	LEU	CB-CG-CD1	-7.37	98.48	111.00
1	A	168	LEU	CA-CB-CG	-7.36	98.36	115.30
1	A	201	LEU	CA-CB-CG	-7.33	98.45	115.30
7	G	18	LEU	CA-CB-CG	-7.33	98.45	115.30
8	H	23	VAL	CA-CB-CG1	-7.17	100.15	110.90
3	C	89	ARG	NE-CZ-NH1	-7.09	116.75	120.30
2	B	101	MET	CB-CG-SD	-7.08	91.17	112.40
6	F	26	LEU	CB-CG-CD2	-7.07	98.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	107	VAL	CB-CA-C	-7.03	98.04	111.40
2	B	22	MET	N-CA-C	6.98	129.85	111.00
2	B	106	LEU	CA-CB-CG	-6.95	99.33	115.30
2	B	151	LEU	CA-CB-CG	-6.95	99.33	115.30
1	A	182	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	A	215	LEU	N-CA-C	6.93	129.72	111.00
2	B	111	VAL	C-N-CD	6.93	142.96	128.40
1	A	92	MET	CG-SD-CE	-6.91	89.14	100.20
3	C	34	VAL	CB-CA-C	-6.85	98.39	111.40
1	A	100	HIS	CB-CA-C	6.81	124.01	110.40
8	H	12	LEU	CB-CG-CD2	6.80	122.56	111.00
1	A	201	LEU	CB-CG-CD1	6.79	122.55	111.00
1	A	24	LYS	N-CA-C	-6.73	92.82	111.00
1	A	20	ASP	CB-CG-OD1	6.69	124.32	118.30
2	B	22	MET	CB-CA-C	-6.68	97.05	110.40
3	C	244	ASP	CB-CG-OD1	6.65	124.28	118.30
3	C	115	LEU	CA-CB-CG	-6.64	100.03	115.30
2	B	18	LEU	CB-CG-CD2	-6.62	99.74	111.00
1	A	20	ASP	N-CA-CB	6.59	122.47	110.60
1	A	207	ARG	NE-CZ-NH2	6.59	123.59	120.30
2	B	44	ILE	CG1-CB-CG2	-6.55	96.98	111.40
8	H	1	MET	CG-SD-CE	6.52	110.63	100.20
4	D	84	LEU	CA-CB-CG	-6.51	100.34	115.30
2	B	14	LEU	CB-CG-CD1	-6.46	100.02	111.00
1	A	161	VAL	CG1-CB-CG2	-6.46	100.57	110.90
1	A	186	ALA	N-CA-CB	-6.41	101.12	110.10
2	B	45	MET	CB-CG-SD	-6.40	93.20	112.40
1	A	112	LYS	C-N-CA	-6.40	95.13	122.00
2	B	96	LEU	CA-CB-CG	-6.38	100.62	115.30
2	B	106	LEU	CB-CG-CD1	6.37	121.82	111.00
6	F	7	TYR	CB-CG-CD2	-6.31	117.22	121.00
2	B	125	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	180	LEU	CB-CG-CD1	-6.28	100.33	111.00
3	C	160	ILE	CB-CA-C	-6.27	99.06	111.60
1	A	94	VAL	CG1-CB-CG2	-6.25	100.90	110.90
1	A	36	LEU	CB-CG-CD2	6.16	121.48	111.00
2	B	89	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	B	138	LEU	CB-CG-CD2	-6.12	100.60	111.00
2	B	15	ARG	NH1-CZ-NH2	6.11	126.12	119.40
1	A	3	ASN	N-CA-C	6.08	127.42	111.00
3	C	201	THR	N-CA-C	6.03	127.27	111.00
1	A	116	LEU	CA-CB-CG	-6.02	101.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	12	ILE	CG1-CB-CG2	-6.02	98.16	111.40
5	E	26	ILE	CB-CA-C	6.01	123.63	111.60
1	A	24	LYS	CD-CE-NZ	5.98	125.45	111.70
6	F	22	LEU	CA-CB-CG	-5.98	101.55	115.30
3	C	263	CYS	CA-CB-SG	-5.98	103.24	114.00
2	B	1	MET	CB-CG-SD	-5.95	94.56	112.40
3	C	111	ASP	CB-CG-OD2	5.92	123.62	118.30
5	E	20	VAL	CA-CB-CG1	-5.92	102.03	110.90
7	G	23	TYR	C-N-CA	-5.91	106.92	121.70
7	G	2	VAL	CB-CA-C	-5.91	100.18	111.40
4	D	64	VAL	CB-CA-C	-5.89	100.20	111.40
2	B	84	VAL	CG1-CB-CG2	5.87	120.29	110.90
1	A	55	THR	CA-CB-CG2	-5.83	104.24	112.40
6	F	6	LEU	CB-CG-CD2	5.82	120.90	111.00
2	B	119	LYS	CD-CE-NZ	5.82	125.08	111.70
2	B	84	VAL	CB-CA-C	-5.81	100.36	111.40
2	B	70	ALA	C-N-CA	-5.81	107.18	121.70
3	C	282	VAL	CB-CA-C	-5.79	100.39	111.40
1	A	184	TYR	CB-CA-C	5.78	121.96	110.40
1	A	24	LYS	CB-CA-C	5.76	121.93	110.40
8	H	12	LEU	CB-CG-CD1	-5.76	101.21	111.00
4	D	137	GLY	N-CA-C	-5.75	98.72	113.10
2	B	125	ARG	CA-CB-CG	-5.72	100.81	113.40
2	B	37	LEU	CB-CG-CD1	-5.71	101.29	111.00
2	B	73	LEU	N-CA-C	-5.69	95.63	111.00
3	C	27	LEU	N-CA-C	5.69	126.36	111.00
2	B	99	LEU	CB-CG-CD1	5.67	120.64	111.00
2	B	104	VAL	CA-CB-CG2	-5.67	102.40	110.90
1	A	204	LEU	CA-CB-CG	-5.64	102.33	115.30
2	B	76	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	A	186	ALA	CB-CA-C	-5.62	101.67	110.10
8	H	9	VAL	CA-CB-CG2	-5.62	102.47	110.90
4	D	77	ASP	N-CA-C	5.62	126.17	111.00
3	C	1	TYR	CB-CA-C	-5.60	99.19	110.40
4	D	43	ILE	CB-CA-C	-5.59	100.42	111.60
1	A	187	HIS	C-N-CA	-5.59	107.73	121.70
3	C	256	LYS	CD-CE-NZ	5.56	124.49	111.70
2	B	57	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	184	TYR	CZ-CE2-CD2	5.54	124.79	119.80
8	H	23	VAL	CB-CA-C	-5.54	100.88	111.40
1	A	119	ILE	CG1-CB-CG2	-5.53	99.23	111.40
5	E	1	MET	CG-SD-CE	5.49	108.98	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	THR	N-CA-C	-5.46	96.24	111.00
1	A	134	THR	CA-CB-CG2	-5.46	104.76	112.40
1	A	112	LYS	N-CA-C	5.46	125.73	111.00
4	D	80	LEU	CA-CB-CG	-5.45	102.78	115.30
1	A	59	LYS	CB-CG-CD	5.41	125.66	111.60
1	A	126	VAL	CA-CB-CG2	-5.41	102.79	110.90
2	B	57	LEU	CB-CG-CD2	5.41	120.19	111.00
7	G	29	TYR	CB-CA-C	-5.39	99.62	110.40
3	C	68	VAL	CB-CA-C	-5.38	101.18	111.40
1	A	83	ARG	CA-CB-CG	-5.37	101.59	113.40
3	C	14	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	A	28	PRO	CA-N-CD	-5.36	104.00	111.50
1	A	61	THR	CA-CB-OG1	-5.36	97.75	109.00
1	A	11	ARG	CG-CD-NE	-5.35	100.57	111.80
1	A	188	THR	N-CA-CB	5.33	120.42	110.30
1	A	146	TRP	C-N-CA	-5.29	108.47	121.70
2	B	71	THR	CA-CB-CG2	-5.28	105.01	112.40
3	C	280	GLU	N-CA-C	-5.27	96.78	111.00
3	C	100	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	A	143	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	A	64	GLU	OE1-CD-OE2	5.25	129.59	123.30
4	D	32	LEU	CB-CG-CD1	-5.25	102.08	111.00
4	D	108	CYS	CB-CA-C	5.24	120.89	110.40
1	A	129	VAL	CA-CB-CG1	-5.22	103.07	110.90
1	A	199	MET	CG-SD-CE	-5.22	91.85	100.20
1	A	92	MET	CA-CB-CG	-5.21	104.44	113.30
1	A	136	TYR	C-N-CA	-5.21	108.66	121.70
6	F	24	VAL	CB-CA-C	-5.21	101.50	111.40
8	H	1	MET	CA-CB-CG	5.21	122.15	113.30
3	C	127	ILE	CB-CA-C	-5.20	101.20	111.60
6	F	10	LEU	N-CA-CB	5.20	120.80	110.40
1	A	138	LEU	CB-CG-CD1	-5.19	102.18	111.00
2	B	117	VAL	C-N-CA	-5.17	108.77	121.70
1	A	95	LEU	CB-CG-CD2	-5.16	102.22	111.00
3	C	256	LYS	CB-CA-C	5.16	120.71	110.40
2	B	51	ILE	CG1-CB-CG2	-5.13	100.12	111.40
3	C	146	LYS	CA-CB-CG	5.13	124.68	113.40
4	D	80	LEU	CB-CG-CD1	5.12	119.71	111.00
1	A	170	ARG	NE-CZ-NH1	5.11	122.86	120.30
5	E	1	MET	CB-CG-SD	5.11	127.74	112.40
2	B	2	ALA	C-N-CA	-5.10	108.94	121.70
3	C	125	GLN	N-CA-C	-5.08	97.29	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ALA	N-CA-CB	5.07	117.19	110.10
2	B	132	ILE	CG1-CB-CG2	-5.06	100.27	111.40
3	C	272	LEU	CA-CB-CG	-5.05	103.69	115.30
1	A	183	TYR	CB-CG-CD2	5.04	124.02	121.00
3	C	20	ILE	CG1-CB-CG2	-5.03	100.33	111.40
5	E	23	ILE	CB-CA-C	-5.03	101.54	111.60
1	A	122	VAL	C-N-CA	-5.03	109.14	121.70
1	A	190	VAL	CA-CB-CG1	-5.02	103.37	110.90
1	A	148	VAL	CB-CA-C	5.02	120.93	111.40
3	C	22	CYS	CA-CB-SG	-5.02	104.97	114.00
1	A	124	LEU	CA-CB-CG	-5.01	103.77	115.30
7	G	14	VAL	CA-CB-CG2	-5.01	103.39	110.90

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	PRO	Peptide
1	A	135	GLY	Peptide
1	A	158	ILE	Peptide
1	A	163	VAL	Peptide
1	A	2	ALA	Peptide
1	A	27	PRO	Peptide
2	B	1	MET	Peptide
2	B	2	ALA	Peptide
2	B	21	GLY	Peptide
2	B	32	TRP	Peptide
2	B	33	PRO	Peptide
2	B	64	GLU	Peptide
2	B	91	VAL	Peptide
3	C	100	ASP	Peptide
3	C	124	TYR	Peptide
3	C	125	GLN	Peptide
3	C	141	ASN	Peptide
3	C	150	HIS	Peptide
3	C	20	ILE	Peptide
3	C	22	CYS	Peptide
3	C	28	ALA	Peptide
5	E	12	ILE	Peptide
5	E	24	PHE	Peptide
5	E	28	SER	Peptide
5	E	31	LEU	Peptide

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Mol	Chain	Res	Type	Group
6	F	6	LEU	Peptide
7	G	1	MET	Peptide
7	G	17	THR	Peptide
7	G	29	TYR	Peptide
7	G	33	ASN	Peptide
8	H	2	GLU	Peptide
8	H	27	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1711	0	1736	339	0
2	B	1249	0	1308	324	0
3	C	2216	0	2232	414	0
4	D	1260	0	1243	185	0
5	E	248	0	284	77	0
6	F	242	0	260	69	0
7	G	283	0	289	61	0
8	H	230	0	239	82	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	129	0	90	56	0
10	C	43	0	30	22	0
11	A	54	0	79	27	0
11	B	54	0	83	11	0
12	A	102	0	123	11	0
12	C	34	0	42	10	0
13	A	21	0	24	7	0
14	B	65	0	72	16	0
15	D	4	0	0	3	0
16	D	54	0	53	11	0
17	G	40	0	52	12	0
18	A	3	0	0	0	0
18	B	2	0	0	0	0
All	All	8046	0	8239	1456	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 90.

All (1456) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:CE	1:A:59:LYS:CD	1.75	1.60
2:B:88:LEU:CG	2:B:88:LEU:CD1	1.75	1.59
6:F:6:LEU:CD2	6:F:6:LEU:CG	1.75	1.59
8:H:29:LEU:CD2	8:H:29:LEU:CG	1.78	1.58
5:E:12:ILE:CD1	5:E:12:ILE:CG1	1.79	1.58
3:C:256:LYS:CG	3:C:256:LYS:CD	1.77	1.57
3:C:225:VAL:CG1	3:C:229:GLU:HG2	1.13	1.57
1:A:61:THR:CB	1:A:61:THR:CG2	1.79	1.54
1:A:92:MET:HG3	11:A:1002:OPC:CCB	1.37	1.50
1:A:54:MET:CE	10:A:301:HEM:HBD1	1.48	1.40
3:C:233:ASN:ND2	3:C:234:ASN:N	1.69	1.39
3:C:225:VAL:HG11	3:C:229:GLU:CG	1.49	1.38
3:C:225:VAL:CG1	3:C:229:GLU:CG	2.03	1.37
3:C:233:ASN:ND2	3:C:234:ASN:H	1.19	1.36
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	1.46	1.34
1:A:92:MET:CG	11:A:1002:OPC:HCB1	1.58	1.30
4:D:123:LYS:HE3	4:D:132:GLN:NE2	1.50	1.26
2:B:128:VAL:O	2:B:132:ILE:HD12	1.35	1.24
2:B:101:MET:O	2:B:104:VAL:HG23	1.36	1.24
3:C:119:LEU:HD23	3:C:124:TYR:CD1	1.72	1.24
2:B:95:LEU:CD2	2:B:99:LEU:HD12	1.66	1.23
6:F:7:TYR:O	6:F:11:LEU:HD12	1.35	1.21
3:C:199:ILE:O	3:C:200:GLN:HG3	1.06	1.21
7:G:31:ARG:CG	7:G:31:ARG:HH11	1.56	1.18
3:C:151:LEU:CD1	3:C:152:GLY:H	1.55	1.17
1:A:96:MET:HA	1:A:96:MET:HE2	1.17	1.17
3:C:119:LEU:CD2	3:C:124:TYR:CD1	2.27	1.16
1:A:47:GLN:NE2	1:A:89:SER:HB3	1.60	1.14
3:C:285:ALA:O	3:C:286:GLU:OE1	1.64	1.14
1:A:92:MET:HE3	11:A:1002:OPC:HCB2	1.15	1.14
2:B:151:LEU:C	2:B:151:LEU:HD12	1.55	1.13
7:G:31:ARG:NH1	7:G:31:ARG:HG2	1.47	1.13
3:C:107:LYS:CD	3:C:110:GLN:NE2	2.12	1.13
4:D:62:ASN:O	4:D:63:ASN:ND2	1.82	1.12
7:G:30:LYS:HE2	7:G:30:LYS:O	1.48	1.12
4:D:78:ARG:HG3	4:D:117:TRP:CD1	1.82	1.12
4:D:105:ASN:HB3	4:D:149:ALA:HB3	1.29	1.12
2:B:134:LEU:HD13	2:B:134:LEU:N	1.43	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:LEU:HD12	3:C:152:GLY:N	1.63	1.11
3:C:25:CYS:SG	10:C:301:HEM:CAC	2.39	1.11
3:C:262:ILE:HG23	8:H:14:VAL:HG13	1.27	1.11
3:C:60:GLN:HE22	3:C:157:ARG:HG3	1.01	1.11
1:A:7:TRP:CE2	1:A:11:ARG:NH2	2.19	1.10
8:H:23:VAL:CG1	8:H:28:GLY:H	1.64	1.10
3:C:107:LYS:HD3	3:C:110:GLN:NE2	1.64	1.10
3:C:176:ALA:HB3	3:C:199:ILE:HD12	1.11	1.10
1:A:12:LEU:O	1:A:13:GLU:HB2	1.51	1.09
4:D:105:ASN:CB	4:D:149:ALA:HB3	1.81	1.09
3:C:199:ILE:O	3:C:200:GLN:CG	1.99	1.08
1:A:100:HIS:HE1	10:A:302:HEM:C1A	1.70	1.08
1:A:87:ARG:HG3	1:A:87:ARG:HH11	1.00	1.08
1:A:207:ARG:HH12	13:A:501:QNO:C3	1.65	1.08
6:F:29:ILE:CD1	6:F:29:ILE:O	1.99	1.08
2:B:95:LEU:HD21	2:B:99:LEU:HD12	1.24	1.08
3:C:22:CYS:HB2	10:C:301:HEM:CBB	1.83	1.08
4:D:152:HIS:CE1	4:D:165:TRP:CD1	2.41	1.08
2:B:158:GLY:O	2:B:159:LEU:HD23	1.54	1.07
1:A:7:TRP:NE1	1:A:11:ARG:NH2	2.03	1.07
10:A:302:HEM:HMC2	10:A:302:HEM:HBC2	1.28	1.07
1:A:54:MET:HE3	10:A:301:HEM:CBD	1.84	1.06
4:D:25:GLY:HA3	16:D:201:SQD:H341	1.29	1.06
10:A:301:HEM:CBB	10:A:301:HEM:HMB2	1.85	1.06
3:C:194:LYS:O	3:C:195:TYR:C	1.92	1.05
2:B:134:LEU:CD1	2:B:134:LEU:N	2.07	1.05
8:H:3:ILE:HG23	8:H:4:ASP:N	1.67	1.05
2:B:128:VAL:O	2:B:132:ILE:CD1	2.04	1.04
2:B:42:VAL:HG13	3:C:269:GLN:HG2	1.35	1.04
3:C:84:ILE:HD11	3:C:114:LEU:HD13	1.36	1.04
4:D:138:LYS:HA	4:D:147:SER:OG	1.55	1.04
1:A:100:HIS:HE1	10:A:302:HEM:NA	1.56	1.04
6:F:13:PHE:CE2	6:F:17:PHE:HE1	1.76	1.03
1:A:92:MET:CE	11:A:1002:OPC:CCB	2.36	1.02
2:B:109:ILE:HG22	2:B:110:LEU:N	1.74	1.02
1:A:96:MET:HA	1:A:96:MET:CE	1.89	1.01
3:C:233:ASN:HD22	3:C:234:ASN:N	1.39	1.01
2:B:151:LEU:C	2:B:151:LEU:CD1	2.26	1.01
2:B:118:ASN:ND2	2:B:120:PHE:H	1.57	1.01
8:H:3:ILE:CG2	8:H:4:ASP:H	1.72	1.01
1:A:31:ASN:HD22	1:A:31:ASN:C	1.64	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:O	2:B:151:LEU:HD12	1.60	1.01
10:A:301:HEM:HBB2	10:A:301:HEM:HMB2	1.03	1.00
3:C:225:VAL:HG12	3:C:229:GLU:HG2	1.05	1.00
1:A:207:ARG:HH12	13:A:501:QNO:H3	1.25	1.00
2:B:32:TRP:O	2:B:34:ASN:HB2	1.60	1.00
5:E:22:ILE:HG22	5:E:22:ILE:O	1.59	1.00
3:C:60:GLN:HE22	3:C:157:ARG:CG	1.75	0.99
1:A:95:LEU:HB2	2:B:79:TRP:HH2	1.26	0.99
3:C:225:VAL:HG11	3:C:229:GLU:HG2	0.99	0.99
3:C:71:ASN:HB2	10:C:301:HEM:O2A	1.63	0.99
2:B:151:LEU:O	2:B:154:THR:HG22	1.63	0.99
1:A:175:VAL:CG1	1:A:176:GLY:N	2.26	0.99
6:F:20:TRP:O	6:F:24:VAL:HG23	1.63	0.99
1:A:96:MET:N	1:A:96:MET:HE3	1.76	0.98
1:A:66:TYR:CZ	2:B:65:PRO:HD3	1.97	0.98
1:A:92:MET:CE	11:A:1002:OPC:HCB2	1.91	0.98
3:C:151:LEU:HD12	3:C:152:GLY:H	0.84	0.98
1:A:183:TYR:O	1:A:186:ALA:HB3	1.63	0.98
4:D:134:ASP:HB2	4:D:137:GLY:O	1.64	0.98
8:H:23:VAL:HG13	8:H:28:GLY:H	1.25	0.98
6:F:25:LEU:HD23	6:F:29:ILE:HG22	1.43	0.97
6:F:29:ILE:HD13	6:F:29:ILE:O	1.63	0.97
1:A:92:MET:HE3	11:A:1002:OPC:CCB	1.92	0.97
1:A:92:MET:CG	11:A:1002:OPC:CCB	2.30	0.97
1:A:96:MET:CA	1:A:96:MET:CE	2.42	0.97
2:B:118:ASN:ND2	2:B:120:PHE:N	2.12	0.97
11:A:1002:OPC:HAY1	11:A:1002:OPC:HBC2	1.47	0.97
3:C:173:THR:O	3:C:231:LEU:HG	1.63	0.97
3:C:60:GLN:NE2	3:C:157:ARG:HG3	1.80	0.96
3:C:225:VAL:HG11	3:C:229:GLU:HG3	1.44	0.96
1:A:96:MET:CA	1:A:96:MET:HE2	1.94	0.96
4:D:129:HIS:HB2	15:D:200:FES:S1	2.06	0.96
10:A:301:HEM:CMB	10:A:301:HEM:CBB	2.38	0.96
6:F:29:ILE:HD12	6:F:29:ILE:O	1.66	0.96
3:C:285:ALA:C	3:C:286:GLU:OE1	2.04	0.95
1:A:54:MET:CE	10:A:301:HEM:CBD	2.42	0.95
4:D:59:LYS:HG3	4:D:60:LEU:N	1.81	0.95
2:B:134:LEU:H	2:B:134:LEU:HD13	1.07	0.95
1:A:110:PHE:HD1	2:B:112:PRO:HB3	1.28	0.95
3:C:41:LEU:HD22	3:C:252:PRO:HG3	1.48	0.95
3:C:58:LEU:HD12	3:C:59:GLN:N	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ALA:O	1:A:191:LEU:HD12	1.66	0.95
6:F:4:GLU:O	6:F:6:LEU:N	1.99	0.95
5:E:10:VAL:O	5:E:13:ALA:CB	2.15	0.95
2:B:139:VAL:O	2:B:143:LEU:HD12	1.66	0.95
3:C:107:LYS:HD3	3:C:110:GLN:HE21	1.26	0.95
3:C:12:THR:HG23	3:C:14:ARG:H	1.28	0.94
4:D:109:THR:HG22	4:D:144:ALA:HB1	1.45	0.94
2:B:17:LYS:HE3	2:B:26:TYR:OH	1.65	0.94
3:C:70:LEU:HD23	3:C:70:LEU:H	1.31	0.94
1:A:92:MET:HG3	11:A:1002:OPC:HCB3	1.49	0.94
8:H:23:VAL:HG13	8:H:28:GLY:N	1.81	0.94
1:A:87:ARG:HH11	1:A:87:ARG:CG	1.81	0.93
1:A:111:LYS:O	1:A:113:PRO:HD2	1.68	0.93
3:C:71:ASN:OD1	3:C:120:PRO:HA	1.67	0.93
2:B:4:LEU:HD23	2:B:4:LEU:C	1.89	0.92
3:C:187:GLU:HG3	3:C:187:GLU:O	1.68	0.92
1:A:212:SER:HB3	10:A:302:HEM:O2D	1.69	0.92
3:C:144:PHE:CZ	3:C:251:ASP:HB2	2.05	0.92
5:E:10:VAL:O	5:E:13:ALA:HB3	1.70	0.92
1:A:39:ILE:HG22	1:A:96:MET:HG3	1.52	0.92
1:A:151:VAL:HG22	1:A:152:SER:N	1.84	0.92
8:H:3:ILE:CG2	8:H:4:ASP:N	2.29	0.92
1:A:161:VAL:HG23	1:A:162:GLY:H	1.33	0.91
6:F:27:LEU:HD11	8:H:27:ASN:HA	1.52	0.91
1:A:54:MET:HE3	10:A:301:HEM:HBD1	0.91	0.91
1:A:87:ARG:NH1	1:A:87:ARG:HG3	1.67	0.91
7:G:26:TYR:O	7:G:28:GLN:N	2.03	0.91
3:C:41:LEU:CD2	3:C:252:PRO:HG3	2.00	0.91
4:D:123:LYS:HE3	4:D:132:GLN:HE21	1.33	0.91
6:F:11:LEU:HB3	6:F:15:LEU:CD1	2.00	0.91
3:C:272:LEU:O	3:C:275:LYS:HB3	1.71	0.90
1:A:54:MET:HE1	10:A:301:HEM:HBD1	1.52	0.90
3:C:119:LEU:HD23	3:C:124:TYR:HD1	1.34	0.90
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.06	0.90
7:G:20:GLY:N	17:G:101:BCR:H363	1.87	0.90
2:B:124:PHE:O	2:B:126:ARG:N	2.06	0.89
5:E:10:VAL:O	5:E:14:LEU:HD12	1.73	0.89
6:F:13:PHE:HE2	6:F:17:PHE:CE1	1.91	0.89
2:B:109:ILE:O	2:B:112:PRO:CD	2.21	0.89
2:B:57:LEU:HD11	8:H:8:TRP:HA	1.54	0.88
4:D:169:ASP:O	4:D:171:ARG:N	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD21	2:B:133:PHE:CE1	2.08	0.88
2:B:74:GLU:O	2:B:74:GLU:HG3	1.72	0.88
1:A:215:LEU:HB2	7:G:28:GLN:OE1	1.73	0.88
1:A:156:GLU:HG2	1:A:163:VAL:HG22	1.53	0.88
2:B:79:TRP:C	2:B:79:TRP:CD1	2.48	0.88
1:A:103:ARG:HH12	1:A:104:VAL:HG23	1.38	0.87
1:A:103:ARG:NH1	1:A:104:VAL:HA	1.89	0.87
1:A:103:ARG:O	1:A:107:THR:HG22	1.73	0.87
1:A:95:LEU:HB2	2:B:79:TRP:CH2	2.08	0.87
10:C:301:HEM:HBB2	10:C:301:HEM:HHC	1.55	0.87
1:A:103:ARG:HH12	1:A:104:VAL:CG2	1.87	0.87
2:B:61:MET:HB2	3:C:146:LYS:HG2	1.55	0.87
3:C:262:ILE:HG23	8:H:14:VAL:CG1	2.04	0.87
3:C:276:LYS:HE2	8:H:25:GLY:O	1.74	0.87
1:A:96:MET:N	1:A:96:MET:CE	2.37	0.86
7:G:23:TYR:CE2	7:G:27:GLN:NE2	2.44	0.86
1:A:207:ARG:NH1	13:A:501:QNO:H3	1.89	0.86
3:C:125:GLN:HE21	3:C:125:GLN:HA	1.40	0.86
10:A:302:HEM:CMC	10:A:302:HEM:HBC2	2.01	0.85
4:D:152:HIS:CE1	4:D:165:TRP:NE1	2.44	0.85
1:A:175:VAL:HG12	1:A:176:GLY:N	1.90	0.85
2:B:101:MET:HE3	14:B:201:CLA:C9	2.06	0.85
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.56	0.85
1:A:175:VAL:HG13	1:A:176:GLY:H	1.39	0.85
4:D:78:ARG:HG3	4:D:117:TRP:NE1	1.91	0.85
2:B:115:GLU:OE2	2:B:126:ARG:NH1	2.10	0.85
1:A:24:LYS:NZ	12:A:1102:UMQ:HO31	1.73	0.85
3:C:54:TYR:HE1	3:C:70:LEU:HD21	1.41	0.84
3:C:19:ARG:HH11	3:C:19:ARG:HG2	1.43	0.84
1:A:156:GLU:HG2	1:A:163:VAL:CG2	2.07	0.84
2:B:95:LEU:HD21	2:B:99:LEU:CD1	2.07	0.84
3:C:98:VAL:HG11	3:C:130:PRO:HD3	1.57	0.84
3:C:94:LEU:O	3:C:98:VAL:HG23	1.76	0.84
3:C:66:SER:O	3:C:67:LYS:HB2	1.77	0.84
6:F:6:LEU:HG	6:F:6:LEU:CD2	2.04	0.84
6:F:7:TYR:O	6:F:11:LEU:CD1	2.23	0.84
8:H:3:ILE:HG23	8:H:4:ASP:H	1.27	0.84
1:A:207:ARG:HH12	13:A:501:QNO:C4	1.90	0.83
3:C:194:LYS:O	3:C:195:TYR:O	1.96	0.83
2:B:57:LEU:CD1	8:H:8:TRP:CD2	2.60	0.83
4:D:118:ASN:ND2	4:D:121:GLU:HB2	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:THR:O	4:D:57:LYS:HE3	1.79	0.83
1:A:93:MET:HE1	1:A:128:THR:HG23	1.61	0.83
2:B:118:ASN:HD21	2:B:120:PHE:H	1.24	0.83
3:C:70:LEU:N	3:C:70:LEU:HD23	1.91	0.83
3:C:184:ALA:O	3:C:185:LYS:HB3	1.79	0.83
1:A:141:ASP:C	2:B:66:ALA:HB2	1.97	0.83
4:D:25:GLY:CA	16:D:201:SQD:H341	2.07	0.83
2:B:113:PHE:O	2:B:115:GLU:N	2.13	0.82
3:C:47:LYS:NZ	3:C:97:GLU:OE2	2.12	0.82
5:E:9:ILE:O	5:E:13:ALA:HB2	1.79	0.82
4:D:109:THR:CG2	4:D:144:ALA:HB1	2.08	0.82
2:B:95:LEU:HD23	2:B:99:LEU:HD12	1.59	0.82
3:C:81:GLY:CA	3:C:142:ILE:HD11	2.08	0.82
2:B:88:LEU:CD1	2:B:101:MET:SD	2.68	0.82
3:C:19:ARG:O	3:C:20:ILE:HB	1.78	0.82
1:A:110:PHE:CD1	2:B:112:PRO:HB3	2.14	0.82
3:C:211:ILE:O	3:C:211:ILE:HG13	1.80	0.81
4:D:131:SER:HA	4:D:142:GLY:HA3	1.60	0.81
1:A:211:ILE:HD12	1:A:212:SER:H	1.45	0.81
1:A:104:VAL:O	1:A:107:THR:HG22	1.80	0.81
3:C:21:VAL:O	3:C:24:ASN:HB2	1.80	0.81
3:C:259:ILE:HD12	8:H:6:LEU:HD13	1.60	0.81
2:B:109:ILE:O	2:B:112:PRO:HD3	1.80	0.81
1:A:145:TYR:CD1	1:A:145:TYR:O	2.33	0.81
3:C:107:LYS:CD	3:C:110:GLN:HE22	1.91	0.81
6:F:13:PHE:CE2	6:F:17:PHE:CE1	2.64	0.81
1:A:103:ARG:HA	7:G:21:LEU:HD21	1.61	0.81
4:D:59:LYS:O	4:D:61:GLY:N	2.13	0.81
1:A:161:VAL:HG23	1:A:162:GLY:N	1.96	0.81
3:C:54:TYR:CE1	3:C:70:LEU:HD21	2.16	0.81
3:C:2:PRO:HD3	10:C:301:HEM:CHB	2.11	0.80
3:C:281:LYS:HG2	3:C:282:VAL:N	1.96	0.80
3:C:22:CYS:HB2	10:C:301:HEM:CAB	2.10	0.80
1:A:100:HIS:CE1	10:A:302:HEM:C1A	2.63	0.80
2:B:57:LEU:HD12	8:H:8:TRP:CD2	2.16	0.80
1:A:151:VAL:CG2	1:A:152:SER:N	2.44	0.80
4:D:116:PRO:HD2	4:D:125:LYS:O	1.81	0.80
2:B:75:ILE:HG12	2:B:75:ILE:O	1.82	0.80
3:C:159:GLN:NE2	3:C:169:ASN:HB3	1.96	0.80
4:D:78:ARG:CG	4:D:117:TRP:CD1	2.64	0.80
7:G:29:TYR:O	7:G:29:TYR:CG	2.34	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.17	0.80
6:F:11:LEU:O	6:F:15:LEU:HD12	1.82	0.80
3:C:159:GLN:HE21	3:C:169:ASN:HB3	1.46	0.79
3:C:196:GLN:O	3:C:197:VAL:CG2	2.31	0.79
1:A:29:HIS:CD2	1:A:214:PRO:HA	2.16	0.79
6:F:25:LEU:HD23	6:F:29:ILE:CG2	2.12	0.79
1:A:134:THR:HG22	1:A:183:TYR:CD2	2.17	0.79
2:B:79:TRP:CD1	2:B:80:TYR:N	2.51	0.79
2:B:11:ASP:OD1	2:B:13:LYS:HB2	1.82	0.78
3:C:107:LYS:HD2	3:C:110:GLN:HE22	1.46	0.78
1:A:103:ARG:HD2	1:A:107:THR:HG21	1.63	0.78
1:A:39:ILE:CG2	1:A:96:MET:HG3	2.13	0.78
11:A:1002:OPC:HAS1	5:E:4:GLY:HA3	1.66	0.78
1:A:211:ILE:CD1	1:A:212:SER:H	1.96	0.78
2:B:88:LEU:HD12	2:B:101:MET:SD	2.23	0.78
3:C:19:ARG:O	3:C:242:GLN:OE1	2.02	0.78
2:B:57:LEU:HD12	8:H:8:TRP:CE3	2.19	0.77
3:C:58:LEU:CD1	3:C:59:GLN:N	2.47	0.77
3:C:261:PHE:O	3:C:265:VAL:HG23	1.84	0.77
1:A:92:MET:HG3	11:A:1002:OPC:HCB1	0.77	0.77
3:C:180:ILE:HG13	3:C:198:SER:O	1.84	0.77
4:D:140:ILE:O	4:D:140:ILE:HG13	1.83	0.77
6:F:13:PHE:HE2	6:F:17:PHE:HE1	1.21	0.77
3:C:44:THR:HG22	3:C:45:VAL:N	2.00	0.77
7:G:15:PHE:O	7:G:17:THR:N	2.18	0.77
7:G:26:TYR:C	7:G:28:GLN:H	1.85	0.77
7:G:34:GLU:O	7:G:35:LEU:HD12	1.83	0.77
2:B:10:SER:O	2:B:12:PRO:HD3	1.83	0.77
3:C:125:GLN:NE2	3:C:125:GLN:HA	2.00	0.77
1:A:207:ARG:NH1	13:A:501:QNO:C3	2.46	0.77
2:B:142:TRP:CZ2	2:B:155:LEU:O	2.37	0.77
1:A:103:ARG:O	1:A:107:THR:CG2	2.33	0.76
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.49	0.76
2:B:88:LEU:CD1	2:B:88:LEU:HG	2.10	0.76
1:A:7:TRP:CD1	1:A:11:ARG:NH2	2.52	0.76
2:B:33:PRO:HG2	2:B:34:ASN:HD22	1.51	0.76
5:E:16:PHE:CD2	6:F:22:LEU:HD21	2.21	0.76
1:A:161:VAL:O	1:A:163:VAL:N	2.17	0.76
3:C:44:THR:HG22	3:C:45:VAL:H	1.48	0.76
2:B:96:LEU:O	2:B:100:LEU:HB2	1.85	0.76
4:D:77:ASP:OD2	4:D:92:VAL:O	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:MET:HG2	2:B:62:VAL:N	1.99	0.76
4:D:118:ASN:HD22	4:D:121:GLU:HB2	1.47	0.76
4:D:134:ASP:HB3	4:D:136:THR:H	1.51	0.75
3:C:262:ILE:CG2	8:H:14:VAL:HG13	2.14	0.75
1:A:175:VAL:HG13	1:A:176:GLY:N	1.96	0.75
1:A:31:ASN:C	1:A:31:ASN:ND2	2.38	0.75
2:B:149:PHE:HB3	2:B:150:PRO:CD	2.17	0.75
7:G:30:LYS:CE	7:G:30:LYS:O	2.32	0.75
3:C:173:THR:O	3:C:231:LEU:CG	2.33	0.75
4:D:89:THR:HG22	4:D:105:ASN:HA	1.68	0.75
11:A:1002:OPC:HBU2	8:H:15:PHE:CD1	2.21	0.75
6:F:4:GLU:O	6:F:5:MET:C	2.25	0.75
3:C:176:ALA:HB3	3:C:199:ILE:CD1	2.05	0.75
3:C:146:LYS:HB2	3:C:248:VAL:HG22	1.68	0.75
4:D:132:GLN:C	4:D:133:TYR:CD1	2.59	0.75
8:H:23:VAL:HG13	8:H:28:GLY:CA	2.16	0.75
2:B:142:TRP:HZ2	2:B:155:LEU:O	1.70	0.74
4:D:152:HIS:ND1	4:D:165:TRP:NE1	2.33	0.74
5:E:16:PHE:HD2	6:F:22:LEU:HD21	1.52	0.74
1:A:25:TYR:CD2	2:B:30:PRO:HA	2.22	0.74
3:C:188:ASP:O	3:C:190:TYR:N	2.19	0.74
1:A:103:ARG:HH11	1:A:104:VAL:HA	1.49	0.74
10:A:301:HEM:HBB2	10:A:301:HEM:HMB3	1.66	0.74
3:C:225:VAL:HG12	3:C:229:GLU:CG	1.88	0.74
6:F:24:VAL:O	6:F:27:LEU:HB2	1.87	0.74
2:B:109:ILE:O	2:B:112:PRO:HD2	1.87	0.74
2:B:82:TYR:N	2:B:83:PRO:HD2	2.02	0.74
3:C:107:LYS:HD2	3:C:110:GLN:NE2	1.99	0.74
5:E:6:VAL:O	5:E:10:VAL:HG23	1.86	0.74
3:C:71:ASN:CB	10:C:301:HEM:O2A	2.36	0.74
2:B:113:PHE:O	2:B:116:ASN:HB2	1.87	0.74
4:D:123:LYS:HE3	4:D:132:GLN:HE22	1.45	0.74
1:A:36:LEU:HB3	1:A:100:HIS:HB2	1.70	0.73
3:C:15:GLU:HB2	3:C:19:ARG:HB3	1.68	0.73
12:A:1102:UMQ:H3'1	12:A:1102:UMQ:O5	1.88	0.73
1:A:163:VAL:O	1:A:166:SER:N	2.21	0.73
1:A:80:TRP:O	1:A:84:SER:HB2	1.87	0.73
3:C:70:LEU:CD2	3:C:70:LEU:N	2.52	0.73
2:B:113:PHE:O	2:B:114:ILE:C	2.27	0.73
1:A:111:LYS:HE2	2:B:115:GLU:O	1.87	0.73
3:C:79:PRO:HD2	3:C:82:PHE:CD1	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:A:1:MET:HA	2.19	0.73
1:A:81:LEU:HD23	1:A:81:LEU:C	2.09	0.73
2:B:158:GLY:O	2:B:159:LEU:CD2	2.36	0.73
5:E:2:ILE:H	5:E:2:ILE:HD12	1.53	0.73
7:G:31:ARG:HG2	7:G:31:ARG:HH11	0.66	0.73
2:B:118:ASN:HD21	2:B:120:PHE:N	1.79	0.72
3:C:233:ASN:C	3:C:233:ASN:ND2	2.42	0.72
1:A:145:TYR:CG	1:A:145:TYR:O	2.43	0.72
4:D:59:LYS:C	4:D:61:GLY:H	1.92	0.72
4:D:81:VAL:O	4:D:88:PRO:HA	1.88	0.72
1:A:111:LYS:O	1:A:113:PRO:CD	2.38	0.72
4:D:105:ASN:HB3	4:D:149:ALA:CB	2.15	0.72
6:F:29:ILE:HD12	6:F:29:ILE:C	2.09	0.72
14:B:201:CLA:HBA1	14:B:201:CLA:HED3	1.70	0.72
6:F:11:LEU:HD23	6:F:15:LEU:HD11	1.71	0.72
3:C:12:THR:HG23	3:C:14:ARG:N	2.04	0.72
2:B:151:LEU:O	2:B:154:THR:CG2	2.38	0.72
1:A:31:ASN:H	1:A:34:TYR:HD2	1.36	0.72
3:C:279:VAL:O	3:C:283:GLN:HB2	1.90	0.72
4:D:115:VAL:HG13	4:D:125:LYS:O	1.88	0.72
4:D:25:GLY:HA3	16:D:201:SQD:C34	2.13	0.72
1:A:93:MET:HE2	1:A:128:THR:HG21	1.70	0.71
3:C:193:VAL:HG12	3:C:194:LYS:H	1.54	0.71
2:B:101:MET:O	2:B:104:VAL:CG2	2.29	0.71
1:A:61:THR:HB	1:A:61:THR:CG2	2.09	0.71
2:B:45:MET:HE1	4:D:27:VAL:HG13	1.72	0.71
5:E:12:ILE:CD1	5:E:12:ILE:CB	2.68	0.71
3:C:94:LEU:HD22	3:C:98:VAL:CG2	2.20	0.71
5:E:12:ILE:HG21	5:E:12:ILE:HD13	1.72	0.71
3:C:275:LYS:HE2	4:D:20:ASN:OD1	1.91	0.71
3:C:9:TYR:N	3:C:9:TYR:CD1	2.59	0.71
5:E:14:LEU:O	5:E:18:ILE:HG13	1.91	0.71
1:A:103:ARG:NH1	1:A:104:VAL:HG23	2.05	0.71
4:D:15:ARG:CD	5:E:31:LEU:HD21	2.21	0.71
8:H:9:VAL:HA	8:H:12:LEU:HD12	1.73	0.70
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.73	0.70
4:D:152:HIS:ND1	4:D:165:TRP:CD1	2.58	0.70
2:B:126:ARG:O	2:B:129:ALA:HB3	1.91	0.70
2:B:151:LEU:CD1	2:B:154:THR:HG21	2.21	0.70
1:A:104:VAL:HG12	1:A:105:TYR:N	2.05	0.70
1:A:29:HIS:CG	1:A:214:PRO:HA	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:LEU:CD2	3:C:124:TYR:CG	2.75	0.70
3:C:98:VAL:CG1	3:C:130:PRO:HD3	2.21	0.70
2:B:151:LEU:CD1	2:B:154:THR:CG2	2.69	0.70
3:C:151:LEU:CD1	3:C:152:GLY:N	2.38	0.70
4:D:138:LYS:O	4:D:139:VAL:O	2.07	0.70
4:D:59:LYS:HG3	4:D:60:LEU:H	1.54	0.70
1:A:207:ARG:NH1	13:A:501:QNO:O41	2.24	0.70
2:B:37:LEU:O	2:B:37:LEU:HG	1.90	0.70
3:C:81:GLY:HA2	3:C:142:ILE:HD11	1.72	0.70
3:C:288:ASN:C	3:C:288:ASN:HD22	1.95	0.69
1:A:43:CYS:HB3	1:A:93:MET:HB2	1.72	0.69
1:A:9:GLN:NE2	1:A:13:GLU:HA	2.07	0.69
6:F:29:ILE:CD1	6:F:29:ILE:C	2.60	0.69
3:C:128:VAL:CG1	3:C:129:PHE:N	2.55	0.69
3:C:176:ALA:CB	3:C:199:ILE:HD12	2.06	0.69
3:C:25:CYS:SG	10:C:301:HEM:HBC2	2.28	0.69
1:A:44:PHE:HB2	1:A:93:MET:SD	2.33	0.69
1:A:92:MET:HE2	11:A:1002:OPC:HCB3	1.75	0.69
3:C:54:TYR:HE1	3:C:70:LEU:CD2	2.03	0.69
7:G:17:THR:O	7:G:21:LEU:HB2	1.93	0.69
2:B:88:LEU:CD1	2:B:88:LEU:CB	2.70	0.69
1:A:72:ILE:HA	1:A:76:VAL:HG23	1.74	0.69
3:C:173:THR:O	3:C:231:LEU:CD2	2.40	0.69
1:A:12:LEU:O	1:A:13:GLU:CB	2.32	0.69
1:A:3:ASN:HB3	1:A:6:ASP:OD2	1.93	0.69
3:C:273:ILE:CD1	8:H:25:GLY:HA3	2.23	0.69
5:E:2:ILE:O	5:E:5:ALA:HB3	1.91	0.69
1:A:92:MET:HE2	11:A:1002:OPC:CCB	2.22	0.69
4:D:132:GLN:C	4:D:133:TYR:HD1	1.95	0.69
3:C:85:ALA:HB2	3:C:132:LEU:HB2	1.74	0.69
3:C:186:GLU:O	3:C:187:GLU:HB3	1.92	0.69
3:C:4:TRP:CD2	3:C:162:PRO:HG3	2.28	0.69
11:B:1001:OPC:OAI	11:B:1001:OPC:HBC2	1.92	0.68
3:C:273:ILE:CD1	8:H:25:GLY:CA	2.71	0.68
5:E:22:ILE:O	5:E:22:ILE:CG2	2.35	0.68
1:A:145:TYR:CD1	1:A:145:TYR:C	2.67	0.68
1:A:61:THR:HA	1:A:177:GLN:OE1	1.93	0.68
1:A:39:ILE:HD11	17:G:101:BCR:C31	2.24	0.68
7:G:15:PHE:O	7:G:16:ALA:C	2.32	0.68
11:A:1002:OPC:HBC2	11:A:1002:OPC:CAY	2.23	0.68
1:A:30:VAL:HG22	1:A:34:TYR:CG	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:PHE:CE1	3:C:251:ASP:HB2	2.28	0.68
8:H:24:TRP:CD1	8:H:24:TRP:O	2.47	0.68
3:C:1:TYR:HA	10:C:301:HEM:NA	2.08	0.68
3:C:251:ASP:OD2	3:C:252:PRO:HD2	1.93	0.68
3:C:2:PRO:HD3	10:C:301:HEM:C1B	2.29	0.68
3:C:40:VAL:HG11	3:C:46:PHE:CD2	2.28	0.68
5:E:23:ILE:O	5:E:27:LYS:N	2.25	0.68
2:B:151:LEU:HD12	2:B:154:THR:HG22	1.74	0.68
4:D:109:THR:HG21	4:D:146:LEU:O	1.95	0.67
3:C:266:MET:HE3	8:H:13:VAL:HG12	1.75	0.67
11:A:1002:OPC:HAY1	11:A:1002:OPC:CBC	2.21	0.67
3:C:82:PHE:HZ	3:C:249:LEU:HD23	1.60	0.67
4:D:153:ALA:O	4:D:154:THR:O	2.12	0.67
2:B:99:LEU:O	2:B:103:SER:OG	2.12	0.67
4:D:118:ASN:HD22	4:D:121:GLU:CB	2.08	0.67
2:B:118:ASN:HD22	2:B:119:LYS:N	1.93	0.67
2:B:124:PHE:CZ	7:G:26:TYR:HD1	2.13	0.67
2:B:129:ALA:O	2:B:131:THR:N	2.27	0.66
3:C:60:GLN:OE1	3:C:70:LEU:CB	2.43	0.66
3:C:46:PHE:CZ	3:C:131:VAL:HG22	2.30	0.66
11:A:1002:OPC:HAW	5:E:8:TYR:HD2	1.61	0.66
1:A:7:TRP:O	1:A:11:ARG:HG3	1.95	0.66
1:A:32:ILE:HG23	1:A:33:PHE:N	2.08	0.66
3:C:151:LEU:CG	3:C:152:GLY:N	2.59	0.66
4:D:82:GLN:O	4:D:82:GLN:CG	2.38	0.66
3:C:4:TRP:CG	3:C:162:PRO:HG3	2.31	0.66
3:C:180:ILE:HG12	3:C:181:THR:N	2.11	0.66
3:C:1:TYR:HA	10:C:301:HEM:C4A	2.31	0.66
6:F:31:GLY:O	6:F:32:ALA:HB2	1.96	0.66
3:C:174:ALA:HB3	3:C:228:GLY:N	2.10	0.66
6:F:25:LEU:O	6:F:26:LEU:C	2.33	0.66
3:C:52:ILE:O	3:C:52:ILE:HG22	1.96	0.66
8:H:3:ILE:HG22	8:H:4:ASP:H	1.57	0.66
8:H:23:VAL:O	8:H:24:TRP:C	2.32	0.66
2:B:126:ARG:N	2:B:127:PRO:HD3	2.10	0.65
3:C:279:VAL:HA	3:C:282:VAL:HG23	1.78	0.65
1:A:20:ASP:OD1	1:A:24:LYS:NZ	2.28	0.65
1:A:68:SER:O	1:A:72:ILE:HG13	1.94	0.65
1:A:93:MET:CE	1:A:128:THR:CG2	2.74	0.65
2:B:123:PRO:CD	7:G:25:ALA:HB1	2.25	0.65
1:A:62:VAL:HG22	1:A:177:GLN:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:ARG:NH1	7:G:31:ARG:CG	2.27	0.65
1:A:47:GLN:NE2	1:A:89:SER:CB	2.51	0.65
3:C:196:GLN:O	3:C:197:VAL:HG23	1.96	0.65
4:D:130:GLY:O	4:D:141:ARG:NH2	2.28	0.65
4:D:34:ALA:O	4:D:37:PRO:HD2	1.97	0.65
1:A:44:PHE:O	1:A:47:GLN:HB2	1.96	0.65
2:B:132:ILE:HD12	2:B:132:ILE:H	1.62	0.65
10:A:302:HEM:CHA	10:A:302:HEM:HBA1	2.27	0.65
11:A:1002:OPC:HBN1	7:G:5:LEU:CD1	2.27	0.65
3:C:233:ASN:HD22	3:C:234:ASN:H	0.68	0.65
7:G:1:MET:HG2	7:G:2:VAL:N	2.11	0.65
3:C:92:GLU:O	3:C:95:LYS:N	2.29	0.65
5:E:10:VAL:C	5:E:13:ALA:CB	2.65	0.65
5:E:23:ILE:O	5:E:26:ILE:N	2.30	0.65
3:C:270:LEU:HG	8:H:21:MET:CE	2.26	0.65
3:C:257:TRP:O	3:C:260:ALA:HB3	1.97	0.65
4:D:138:LYS:CA	4:D:147:SER:OG	2.40	0.64
3:C:277:LYS:HE2	8:H:24:TRP:NE1	2.13	0.64
11:A:1002:OPC:CBC	11:A:1002:OPC:CAY	2.74	0.64
3:C:151:LEU:CG	3:C:152:GLY:H	2.09	0.64
3:C:229:GLU:OE2	3:C:230:ALA:N	2.29	0.64
4:D:75:ALA:O	4:D:76:GLY:C	2.35	0.64
1:A:66:TYR:OH	2:B:65:PRO:HD3	1.96	0.64
10:C:301:HEM:HBC2	10:C:301:HEM:CMC	2.27	0.64
1:A:95:LEU:HD23	1:A:95:LEU:O	1.98	0.64
2:B:151:LEU:HD11	2:B:154:THR:HG21	1.79	0.64
4:D:59:LYS:CG	4:D:60:LEU:N	2.58	0.64
1:A:21:VAL:HA	1:A:207:ARG:HH21	1.63	0.64
1:A:32:ILE:CG2	1:A:33:PHE:N	2.60	0.64
2:B:118:ASN:HD22	2:B:120:PHE:N	1.95	0.64
3:C:263:CYS:O	3:C:264:LEU:C	2.34	0.64
5:E:14:LEU:O	5:E:18:ILE:CG1	2.46	0.64
6:F:25:LEU:CD2	6:F:29:ILE:HG22	2.25	0.64
1:A:103:ARG:HH22	10:A:302:HEM:CBD	2.10	0.64
1:A:211:ILE:HG12	10:A:303:HEM:HAA1	1.79	0.64
2:B:84:VAL:HG13	2:B:101:MET:CG	2.28	0.64
3:C:151:LEU:HD11	3:C:153:ALA:HB2	1.80	0.64
1:A:29:HIS:CD2	1:A:213:GLY:O	2.51	0.64
10:A:302:HEM:HBA1	10:A:302:HEM:HHA	1.80	0.64
1:A:212:SER:CB	10:A:302:HEM:O2D	2.43	0.64
1:A:72:ILE:HA	1:A:76:VAL:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:MET:CE	1:A:128:THR:HG23	2.27	0.64
1:A:211:ILE:HG23	1:A:212:SER:O	1.98	0.64
4:D:115:VAL:HG22	4:D:126:CYS:HA	1.80	0.64
4:D:177:TRP:NE1	4:D:178:TRP:CE3	2.66	0.64
2:B:139:VAL:HG12	2:B:143:LEU:HD11	1.78	0.63
4:D:25:GLY:HA2	16:D:201:SQD:C33	2.29	0.63
6:F:16:ILE:HG22	6:F:17:PHE:N	2.13	0.63
2:B:122:ASN:OD1	2:B:123:PRO:CD	2.46	0.63
6:F:11:LEU:HB3	6:F:15:LEU:HD12	1.81	0.63
1:A:14:ILE:N	1:A:14:ILE:HD13	2.13	0.63
1:A:212:SER:HB3	10:A:302:HEM:CGD	2.28	0.63
4:D:127:PRO:O	4:D:129:HIS:N	2.32	0.63
1:A:103:ARG:CA	7:G:21:LEU:HD21	2.27	0.63
1:A:111:LYS:HZ1	2:B:126:ARG:HD3	1.63	0.63
3:C:134:PRO:HB3	3:C:142:ILE:HD12	1.80	0.63
2:B:53:ALA:HA	3:C:258:MET:HE2	1.78	0.63
4:D:15:ARG:HD2	5:E:31:LEU:HD21	1.80	0.63
1:A:36:LEU:HD23	1:A:99:LEU:HB3	1.81	0.63
4:D:105:ASN:HB2	4:D:149:ALA:HB3	1.77	0.63
3:C:119:LEU:HD21	3:C:124:TYR:CD1	2.32	0.63
3:C:223:GLN:HB3	3:C:225:VAL:HG23	1.80	0.63
5:E:24:PHE:O	5:E:27:LYS:N	2.32	0.63
3:C:266:MET:CE	8:H:13:VAL:CG1	2.77	0.63
2:B:118:ASN:HD21	2:B:120:PHE:HB2	1.64	0.63
3:C:175:SER:HB2	3:C:209:ASP:OD1	1.99	0.63
5:E:10:VAL:C	5:E:13:ALA:HB2	2.19	0.63
3:C:196:GLN:O	3:C:197:VAL:HG22	1.98	0.62
4:D:99:ILE:HG13	4:D:100:ARG:H	1.63	0.62
2:B:110:LEU:O	2:B:111:VAL:C	2.32	0.62
8:H:16:THR:C	8:H:18:SER:H	1.99	0.62
1:A:93:MET:HE2	1:A:128:THR:CG2	2.29	0.62
5:E:12:ILE:CD1	5:E:12:ILE:HG21	2.28	0.62
1:A:211:ILE:HB	10:A:303:HEM:HBA2	1.80	0.62
2:B:87:ILE:HG12	2:B:143:LEU:HD22	1.82	0.62
3:C:25:CYS:SG	10:C:301:HEM:HBC1	2.29	0.62
3:C:158:GLY:H	10:C:301:HEM:CAD	2.11	0.62
1:A:35:CYS:O	1:A:39:ILE:HD12	2.00	0.62
1:A:95:LEU:HD23	1:A:95:LEU:C	2.20	0.62
3:C:84:ILE:CD1	3:C:114:LEU:HD13	2.20	0.62
3:C:270:LEU:HA	8:H:21:MET:CE	2.30	0.62
3:C:279:VAL:HA	3:C:282:VAL:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.35	0.62
2:B:79:TRP:CG	2:B:80:TYR:N	2.68	0.62
3:C:81:GLY:HA3	3:C:142:ILE:HD11	1.80	0.62
3:C:20:ILE:O	3:C:20:ILE:HG22	2.00	0.62
3:C:173:THR:OG1	3:C:174:ALA:N	2.32	0.62
3:C:278:GLN:O	3:C:278:GLN:HG2	2.00	0.62
3:C:44:THR:O	3:C:132:LEU:HD12	1.99	0.62
6:F:11:LEU:C	6:F:15:LEU:HD12	2.20	0.62
2:B:106:LEU:O	2:B:109:ILE:HB	2.00	0.61
2:B:4:LEU:HD23	2:B:4:LEU:O	1.99	0.61
11:A:1002:OPC:HAW	5:E:8:TYR:CD2	2.34	0.61
8:H:5:VAL:O	8:H:6:LEU:C	2.37	0.61
3:C:78:LEU:H	3:C:78:LEU:HD12	1.65	0.61
1:A:34:TYR:CE1	1:A:103:ARG:NE	2.67	0.61
1:A:39:ILE:CD1	17:G:101:BCR:C31	2.77	0.61
2:B:113:PHE:O	2:B:116:ASN:N	2.33	0.61
2:B:95:LEU:CD2	2:B:99:LEU:CD1	2.61	0.61
3:C:187:GLU:CG	3:C:187:GLU:O	2.45	0.61
3:C:84:ILE:HD12	3:C:103:PHE:CD1	2.36	0.61
3:C:237:VAL:CG2	3:C:237:VAL:O	2.48	0.61
2:B:118:ASN:HD21	2:B:120:PHE:CB	2.14	0.61
3:C:52:ILE:HG12	3:C:153:ALA:HB1	1.82	0.61
3:C:248:VAL:O	3:C:248:VAL:HG12	2.01	0.61
3:C:266:MET:CE	8:H:13:VAL:HG12	2.30	0.61
1:A:121:GLY:HA3	10:A:302:HEM:C3C	2.36	0.61
14:B:201:CLA:HBB1	11:B:1001:OPC:HBP1	1.83	0.61
3:C:17:THR:OG1	3:C:18:GLY:N	2.34	0.61
1:A:39:ILE:HD11	17:G:101:BCR:H313	1.80	0.61
2:B:37:LEU:HD21	2:B:38:TYR:CZ	2.36	0.61
3:C:175:SER:HB2	3:C:209:ASP:CG	2.21	0.60
5:E:28:SER:O	5:E:29:ILE:HG12	2.01	0.60
1:A:111:LYS:NZ	2:B:120:PHE:O	2.33	0.60
4:D:59:LYS:C	4:D:61:GLY:N	2.50	0.60
3:C:185:LYS:O	3:C:186:GLU:O	2.20	0.60
3:C:191:GLY:O	3:C:192:ASN:O	2.19	0.60
5:E:22:ILE:HA	5:E:25:ALA:HB3	1.84	0.60
1:A:95:LEU:CD2	1:A:95:LEU:C	2.69	0.60
2:B:150:PRO:O	2:B:151:LEU:O	2.20	0.60
2:B:89:ARG:HG3	2:B:90:SER:N	2.15	0.60
3:C:90:ILE:HG22	3:C:91:PRO:O	2.01	0.60
4:D:59:LYS:CG	4:D:60:LEU:H	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:CB	11:A:1002:OPC:HCB1	2.28	0.60
1:A:62:VAL:HG12	1:A:140:TRP:NE1	2.17	0.60
2:B:82:TYR:O	2:B:85:PHE:HB3	2.01	0.60
3:C:20:ILE:HD12	3:C:152:GLY:HA3	1.83	0.60
3:C:174:ALA:HB2	3:C:231:LEU:HD23	1.83	0.60
2:B:96:LEU:HD13	2:B:100:LEU:HD12	1.82	0.60
2:B:57:LEU:HD11	8:H:8:TRP:CA	2.30	0.60
3:C:71:ASN:OD1	3:C:120:PRO:CA	2.47	0.60
3:C:78:LEU:HB3	3:C:79:PRO:HD3	1.84	0.60
5:E:26:ILE:CG2	5:E:31:LEU:HB3	2.31	0.60
8:H:23:VAL:CG1	8:H:28:GLY:N	2.43	0.60
1:A:103:ARG:NH1	1:A:104:VAL:CG2	2.63	0.59
1:A:142:GLN:HA	1:A:142:GLN:OE1	2.02	0.59
4:D:90:TYR:N	4:D:104:ILE:O	2.35	0.59
5:E:8:TYR:OH	5:E:12:ILE:HD11	2.00	0.59
5:E:22:ILE:CG2	5:E:26:ILE:HG12	2.32	0.59
6:F:4:GLU:C	6:F:6:LEU:N	2.54	0.59
1:A:96:MET:H	1:A:96:MET:HE3	1.61	0.59
2:B:159:LEU:O	2:B:160:PHE:HB3	2.02	0.59
3:C:98:VAL:HG22	3:C:128:VAL:HG11	1.84	0.59
4:D:78:ARG:HD3	4:D:92:VAL:CG2	2.32	0.59
7:G:6:LEU:O	7:G:9:LEU:CB	2.50	0.59
1:A:47:GLN:HE21	1:A:89:SER:HB3	1.61	0.59
3:C:277:LYS:HE3	6:F:30:GLN:OE1	2.02	0.59
2:B:71:THR:CG2	2:B:72:PRO:HD2	2.33	0.59
3:C:60:GLN:OE1	3:C:70:LEU:HB3	2.02	0.59
4:D:110:HIS:CD2	4:D:143:PRO:HB2	2.37	0.59
3:C:273:ILE:HG13	8:H:21:MET:HG3	1.83	0.59
8:H:23:VAL:O	8:H:25:GLY:N	2.36	0.59
2:B:141:ILE:O	2:B:145:ILE:HG13	2.02	0.59
2:B:159:LEU:O	2:B:160:PHE:CD2	2.55	0.59
3:C:200:GLN:HG2	3:C:206:THR:HA	1.83	0.59
3:C:22:CYS:SG	3:C:23:ALA:N	2.75	0.59
3:C:68:VAL:O	3:C:68:VAL:HG13	2.03	0.59
8:H:29:LEU:CD2	8:H:29:LEU:CD1	2.79	0.59
1:A:103:ARG:HH11	1:A:104:VAL:CA	2.16	0.59
1:A:36:LEU:CB	1:A:100:HIS:HB2	2.32	0.59
1:A:79:GLY:O	1:A:83:ARG:N	2.30	0.59
3:C:232:THR:O	3:C:233:ASN:HB3	2.03	0.59
3:C:268:ALA:O	3:C:269:GLN:C	2.41	0.59
4:D:123:LYS:CE	4:D:132:GLN:HE21	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:HZ3	12:A:1102:UMQ:HO31	1.51	0.59
1:A:111:LYS:CE	2:B:115:GLU:O	2.51	0.59
2:B:57:LEU:CD1	8:H:8:TRP:CE2	2.85	0.59
1:A:117:THR:HG22	10:A:302:HEM:C2D	2.38	0.58
7:G:29:TYR:CD2	7:G:29:TYR:O	2.56	0.58
3:C:128:VAL:HG12	3:C:129:PHE:N	2.18	0.58
6:F:20:TRP:CZ3	17:G:101:BCR:H19C	2.38	0.58
3:C:266:MET:HE3	8:H:13:VAL:CG1	2.33	0.58
5:E:11:PHE:CD1	8:H:13:VAL:HG21	2.39	0.58
1:A:8:PHE:HB3	1:A:14:ILE:HG12	1.86	0.58
1:A:36:LEU:CD2	1:A:99:LEU:HB3	2.32	0.58
1:A:104:VAL:HG21	10:A:302:HEM:C2D	2.37	0.58
2:B:23:GLY:O	2:B:26:TYR:HD1	1.86	0.58
2:B:61:MET:CG	2:B:62:VAL:N	2.66	0.58
3:C:58:LEU:HG	3:C:237:VAL:HG21	1.85	0.58
4:D:177:TRP:NE1	4:D:178:TRP:CZ3	2.71	0.58
3:C:134:PRO:HB3	3:C:142:ILE:CD1	2.34	0.58
3:C:196:GLN:NE2	3:C:210:THR:HG22	2.19	0.58
6:F:25:LEU:CD2	6:F:29:ILE:CG2	2.81	0.58
12:A:1103:UMQ:H6'2	12:A:1103:UMQ:O5	2.03	0.58
4:D:134:ASP:CB	4:D:136:THR:H	2.16	0.58
3:C:278:GLN:O	3:C:282:VAL:HG22	2.04	0.58
1:A:39:ILE:HD13	17:G:101:BCR:H311	1.86	0.58
4:D:84:LEU:O	4:D:85:LYS:HB3	2.02	0.58
1:A:33:PHE:CD1	7:G:21:LEU:HD13	2.39	0.58
2:B:109:ILE:HG22	2:B:110:LEU:H	1.66	0.57
2:B:41:PRO:O	2:B:45:MET:HB2	2.04	0.57
3:C:78:LEU:HB3	3:C:79:PRO:CD	2.33	0.57
1:A:68:SER:OG	1:A:69:VAL:N	2.37	0.57
2:B:96:LEU:HD13	2:B:100:LEU:CD1	2.33	0.57
3:C:58:LEU:CD1	3:C:59:GLN:H	2.16	0.57
4:D:82:GLN:O	4:D:82:GLN:HG2	2.04	0.57
1:A:191:LEU:N	1:A:192:PRO:CD	2.68	0.57
3:C:237:VAL:O	3:C:237:VAL:HG23	2.04	0.57
3:C:273:ILE:O	3:C:276:LYS:N	2.38	0.57
7:G:26:TYR:C	7:G:28:GLN:N	2.48	0.57
1:A:138:LEU:N	1:A:139:PRO:CD	2.68	0.57
1:A:72:ILE:O	1:A:79:GLY:HA3	2.04	0.57
2:B:83:PRO:O	2:B:87:ILE:HG13	2.05	0.57
12:C:1101:UMQ:HL3	4:D:37:PRO:CG	2.33	0.57
6:F:11:LEU:CA	6:F:15:LEU:HD12	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:ILE:CG2	5:E:12:ILE:CD1	2.83	0.57
1:A:9:GLN:OE1	1:A:15:GLN:HB2	2.05	0.57
2:B:151:LEU:O	2:B:151:LEU:CD1	2.42	0.57
2:B:3:THR:O	2:B:29:GLU:CB	2.53	0.57
3:C:20:ILE:HG21	3:C:240:PHE:HZ	1.69	0.57
3:C:94:LEU:HD22	3:C:98:VAL:HG23	1.85	0.57
1:A:94:VAL:HG21	2:B:80:TYR:CE2	2.40	0.57
2:B:115:GLU:HG3	11:B:1001:OPC:OCC	2.05	0.57
2:B:134:LEU:HD21	7:G:22:PHE:CZ	2.40	0.57
3:C:81:GLY:HA3	3:C:142:ILE:CD1	2.35	0.57
3:C:30:LYS:HB3	3:C:31:PRO:HD2	1.87	0.57
6:F:10:LEU:N	6:F:10:LEU:HD13	1.91	0.57
6:F:20:TRP:HZ3	17:G:101:BCR:H19C	1.69	0.57
1:A:36:LEU:HB3	1:A:100:HIS:CB	2.33	0.57
1:A:113:PRO:HG2	1:A:114:ARG:HE	1.70	0.57
2:B:74:GLU:C	2:B:75:ILE:HG22	2.25	0.57
3:C:85:ALA:CB	3:C:132:LEU:HB2	2.34	0.57
3:C:34:VAL:HG22	3:C:151:LEU:HB2	1.87	0.57
12:C:1101:UMQ:HL3	4:D:37:PRO:HG3	1.86	0.57
4:D:90:TYR:OH	4:D:116:PRO:HA	2.04	0.57
5:E:5:ALA:O	5:E:6:VAL:C	2.41	0.57
1:A:158:ILE:O	1:A:162:GLY:HA3	2.05	0.57
2:B:101:MET:CE	14:B:201:CLA:C9	2.82	0.57
8:H:9:VAL:O	8:H:13:VAL:HG23	2.05	0.57
1:A:54:MET:HE1	10:A:301:HEM:CGD	2.35	0.56
3:C:28:ALA:HB2	3:C:236:ASN:ND2	2.19	0.56
6:F:13:PHE:CD2	6:F:17:PHE:HE1	2.22	0.56
1:A:54:MET:HE1	10:A:301:HEM:CBD	2.21	0.56
11:B:1001:OPC:OAI	11:B:1001:OPC:CBG	2.53	0.56
1:A:88:TRP:CE3	2:B:54:LEU:CD1	2.88	0.56
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.39	0.56
3:C:162:PRO:HD3	10:C:301:HEM:HAC	1.85	0.56
3:C:199:ILE:C	3:C:200:GLN:HG3	2.10	0.56
3:C:21:VAL:O	3:C:22:CYS:O	2.23	0.56
3:C:233:ASN:CG	3:C:234:ASN:N	2.55	0.56
1:A:143:VAL:O	1:A:143:VAL:HG13	2.03	0.56
1:A:168:LEU:O	1:A:182:ARG:NH1	2.38	0.56
1:A:1:MET:HA	1:A:1:MET:HE3	1.88	0.56
1:A:88:TRP:CZ3	2:B:54:LEU:CD1	2.89	0.56
2:B:80:TYR:CD1	2:B:81:LEU:HD23	2.40	0.56
3:C:288:ASN:C	3:C:288:ASN:ND2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:ARG:CG	5:E:31:LEU:HD21	2.35	0.56
2:B:45:MET:HG2	4:D:30:VAL:HG11	1.87	0.56
1:A:14:ILE:HG23	12:A:1103:UMQ:HF2	1.88	0.56
1:A:83:ARG:NH1	10:A:301:HEM:O2A	2.38	0.56
2:B:44:ILE:HG22	2:B:45:MET:N	2.21	0.56
3:C:77:MET:HG2	3:C:150:HIS:O	2.05	0.56
11:A:1002:OPC:HBC1	11:A:1002:OPC:HAX1	1.85	0.56
1:A:19:ASP:O	1:A:20:ASP:C	2.39	0.56
3:C:226:LYS:O	3:C:229:GLU:HB3	2.05	0.56
2:B:10:SER:O	2:B:12:PRO:CD	2.53	0.56
2:B:32:TRP:CG	2:B:33:PRO:N	2.74	0.56
3:C:146:LYS:HE2	3:C:246:GLU:HG2	1.87	0.56
3:C:9:TYR:O	3:C:106:TYR:OH	2.21	0.56
7:G:1:MET:HG2	7:G:2:VAL:H	1.69	0.56
4:D:177:TRP:CD1	4:D:178:TRP:CE3	2.94	0.56
2:B:17:LYS:O	2:B:20:LYS:N	2.39	0.56
3:C:119:LEU:CD2	3:C:124:TYR:CE1	2.85	0.56
3:C:98:VAL:HG11	3:C:130:PRO:CD	2.33	0.56
2:B:6:LYS:O	2:B:7:PRO:O	2.24	0.56
2:B:124:PHE:C	2:B:126:ARG:H	2.08	0.56
4:D:127:PRO:O	4:D:128:CYS:C	2.42	0.56
1:A:41:LEU:HD23	10:A:303:HEM:CBC	2.37	0.55
8:H:8:TRP:O	8:H:9:VAL:C	2.45	0.55
4:D:13:MET:O	4:D:15:ARG:N	2.29	0.55
1:A:186:ALA:C	1:A:191:LEU:HD12	2.27	0.55
2:B:151:LEU:HD12	2:B:154:THR:CG2	2.36	0.55
3:C:19:ARG:NH1	3:C:19:ARG:HG2	2.18	0.55
1:A:32:ILE:HG22	1:A:33:PHE:CD2	2.42	0.55
2:B:139:VAL:HG12	2:B:143:LEU:CD1	2.36	0.55
2:B:93:ASN:OD1	2:B:96:LEU:HB2	2.05	0.55
3:C:28:ALA:HB3	3:C:239:GLY:HA3	1.87	0.55
4:D:25:GLY:CA	16:D:201:SQD:C34	2.81	0.55
6:F:11:LEU:CB	6:F:15:LEU:HD12	2.37	0.55
3:C:266:MET:HE1	8:H:13:VAL:CG1	2.36	0.55
2:B:84:VAL:O	2:B:84:VAL:HG12	2.06	0.55
3:C:174:ALA:HB3	3:C:229:GLU:H	1.71	0.55
3:C:26:HIS:ND1	3:C:154:ASN:ND2	2.54	0.55
5:E:22:ILE:O	5:E:23:ILE:O	2.25	0.55
2:B:57:LEU:HD12	8:H:8:TRP:CE2	2.41	0.55
3:C:81:GLY:CA	3:C:142:ILE:CD1	2.82	0.55
2:B:25:ASN:C	2:B:25:ASN:HD22	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:O	2:B:40:PHE:HB2	2.06	0.55
3:C:71:ASN:CG	3:C:120:PRO:HA	2.27	0.55
3:C:193:VAL:HB	3:C:213:ALA:HB2	1.89	0.55
2:B:54:LEU:HD23	8:H:11:LEU:HD22	1.88	0.55
2:B:37:LEU:CD2	2:B:38:TYR:CE1	2.89	0.55
3:C:36:VAL:HG12	3:C:48:ALA:HB1	1.89	0.55
1:A:178:ALA:O	1:A:179:THR:C	2.45	0.54
1:A:83:ARG:HD2	10:A:301:HEM:O1D	2.08	0.54
2:B:136:GLY:HA2	14:B:201:CLA:HBC2	1.88	0.54
3:C:22:CYS:O	3:C:23:ALA:C	2.45	0.54
1:A:102:PHE:CD2	1:A:102:PHE:N	2.74	0.54
1:A:39:ILE:CD1	17:G:101:BCR:H311	2.37	0.54
3:C:139:ASP:O	3:C:141:ASN:N	2.40	0.54
3:C:180:ILE:CG2	3:C:223:GLN:N	2.70	0.54
3:C:225:VAL:HG12	3:C:229:GLU:CB	2.38	0.54
4:D:163:THR:O	4:D:164:PRO:O	2.24	0.54
4:D:25:GLY:HA2	16:D:201:SQD:C32	2.37	0.54
1:A:81:LEU:C	1:A:81:LEU:CD2	2.75	0.54
1:A:84:SER:HA	2:B:60:ALA:HB2	1.90	0.54
2:B:74:GLU:CG	2:B:74:GLU:O	2.50	0.54
6:F:20:TRP:C	6:F:20:TRP:CD1	2.80	0.54
3:C:60:GLN:OE1	3:C:70:LEU:HB2	2.07	0.54
4:D:116:PRO:CD	4:D:125:LYS:O	2.52	0.54
4:D:127:PRO:C	4:D:129:HIS:N	2.59	0.54
2:B:82:TYR:N	2:B:83:PRO:CD	2.70	0.54
3:C:20:ILE:O	3:C:23:ALA:HB3	2.07	0.54
3:C:66:SER:O	3:C:67:LYS:CB	2.52	0.54
5:E:2:ILE:O	5:E:6:VAL:HG23	2.06	0.54
6:F:20:TRP:O	6:F:20:TRP:HD1	1.91	0.54
7:G:22:PHE:O	7:G:23:TYR:C	2.44	0.54
1:A:47:GLN:O	1:A:51:GLY:N	2.39	0.54
1:A:88:TRP:CZ2	2:B:54:LEU:HD13	2.42	0.54
3:C:270:LEU:HG	8:H:21:MET:HE1	1.90	0.54
1:A:99:LEU:O	1:A:102:PHE:HB2	2.08	0.54
1:A:103:ARG:CD	1:A:107:THR:HG21	2.37	0.54
4:D:108:CYS:HB3	4:D:115:VAL:HG23	1.90	0.54
4:D:142:GLY:O	4:D:144:ALA:N	2.40	0.54
5:E:26:ILE:HG22	5:E:32:ILE:HD12	1.90	0.54
1:A:103:ARG:O	1:A:104:VAL:C	2.44	0.54
1:A:111:LYS:NZ	2:B:126:ARG:HD3	2.23	0.54
1:A:183:TYR:O	1:A:186:ALA:CB	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE2	1:A:1:MET:HA	1.88	0.54
2:B:100:LEU:CD2	11:B:1001:OPC:CBX	2.86	0.54
2:B:159:LEU:O	2:B:160:PHE:CB	2.56	0.54
7:G:33:ASN:O	7:G:34:GLU:O	2.26	0.53
3:C:270:LEU:HA	8:H:21:MET:HE3	1.89	0.53
1:A:94:VAL:HG11	2:B:80:TYR:CD2	2.43	0.53
1:A:95:LEU:HD22	1:A:96:MET:CE	2.39	0.53
2:B:4:LEU:CD2	2:B:4:LEU:C	2.65	0.53
3:C:61:VAL:HG11	3:C:168:ASN:ND2	2.23	0.53
3:C:171:VAL:HB	3:C:233:ASN:O	2.07	0.53
3:C:276:LYS:O	3:C:279:VAL:N	2.38	0.53
6:F:12:SER:OG	7:G:12:GLY:HA3	2.08	0.53
1:A:103:ARG:HH22	10:A:302:HEM:HBD1	1.72	0.53
2:B:37:LEU:CD2	2:B:38:TYR:CZ	2.92	0.53
3:C:79:PRO:HD2	3:C:82:PHE:CG	2.43	0.53
6:F:18:VAL:O	6:F:22:LEU:HB2	2.09	0.53
2:B:100:LEU:CD2	11:B:1001:OPC:HBX2	2.39	0.53
5:E:22:ILE:O	5:E:23:ILE:C	2.43	0.53
11:A:1002:OPC:HBU2	8:H:15:PHE:CG	2.43	0.53
3:C:154:ASN:HB2	3:C:240:PHE:HD1	1.74	0.53
4:D:139:VAL:O	4:D:140:ILE:HG22	2.09	0.53
1:A:211:ILE:HD13	10:A:302:HEM:O1D	2.09	0.53
1:A:26:VAL:O	2:B:28:GLY:HA3	2.09	0.53
2:B:145:ILE:O	2:B:148:THR:N	2.40	0.53
2:B:25:ASN:O	2:B:25:ASN:ND2	2.39	0.53
3:C:120:PRO:HD2	3:C:124:TYR:HD1	1.72	0.53
1:A:110:PHE:HE1	2:B:112:PRO:HA	1.73	0.53
2:B:69:PHE:N	2:B:69:PHE:CD2	2.76	0.53
7:G:20:GLY:H	17:G:101:BCR:H363	1.70	0.53
2:B:82:TYR:O	2:B:85:PHE:N	2.42	0.53
2:B:123:PRO:HD2	7:G:25:ALA:CB	2.33	0.53
4:D:107:VAL:HG12	4:D:112:GLY:HA2	1.91	0.53
1:A:19:ASP:N	1:A:19:ASP:OD1	2.41	0.52
1:A:30:VAL:HA	1:A:34:TYR:CD2	2.43	0.52
3:C:119:LEU:HD22	3:C:124:TYR:CG	2.43	0.52
4:D:70:LEU:O	4:D:72:SER:N	2.42	0.52
8:H:16:THR:C	8:H:18:SER:N	2.60	0.52
2:B:57:LEU:HD12	8:H:8:TRP:CZ3	2.44	0.52
2:B:71:THR:HG22	2:B:72:PRO:O	2.10	0.52
3:C:254:ARG:O	3:C:255:VAL:C	2.47	0.52
4:D:132:GLN:O	4:D:133:TYR:CD1	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:TYR:N	4:D:133:TYR:CD1	2.78	0.52
4:D:25:GLY:CA	16:D:201:SQD:C33	2.87	0.52
7:G:7:ASP:O	7:G:8:GLY:C	2.47	0.52
10:A:303:HEM:C1C	2:B:40:PHE:CE2	2.97	0.52
2:B:118:ASN:ND2	2:B:120:PHE:CB	2.72	0.52
2:B:84:VAL:HG13	2:B:101:MET:HG3	1.92	0.52
3:C:21:VAL:HG23	3:C:22:CYS:N	2.23	0.52
12:A:1104:UMQ:HL2	16:D:201:SQD:C13	2.39	0.52
2:B:137:THR:O	2:B:140:THR:HB	2.10	0.52
2:B:45:MET:HE1	4:D:27:VAL:HG22	1.91	0.52
3:C:103:PHE:CE1	3:C:130:PRO:HD2	2.44	0.52
1:A:4:VAL:O	1:A:5:TYR:C	2.47	0.52
3:C:61:VAL:CG1	3:C:168:ASN:ND2	2.73	0.52
2:B:104:VAL:O	2:B:108:LEU:HB2	2.09	0.52
3:C:174:ALA:HB3	3:C:228:GLY:H	1.75	0.52
3:C:28:ALA:HB3	3:C:239:GLY:CA	2.40	0.52
4:D:25:GLY:HA2	16:D:201:SQD:H332	1.90	0.52
2:B:102:ALA:O	2:B:105:PRO:HD2	2.10	0.52
2:B:156:THR:C	2:B:158:GLY:N	2.63	0.52
2:B:53:ALA:HB1	3:C:258:MET:HE1	1.92	0.52
2:B:71:THR:HG22	2:B:72:PRO:HD2	1.92	0.52
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.92	0.52
3:C:251:ASP:OD2	3:C:252:PRO:CD	2.58	0.52
4:D:15:ARG:HD2	5:E:31:LEU:CD2	2.40	0.52
5:E:3:LEU:O	5:E:7:PHE:HB2	2.09	0.52
3:C:276:LYS:CE	8:H:25:GLY:O	2.54	0.52
3:C:184:ALA:O	3:C:185:LYS:CB	2.54	0.52
3:C:281:LYS:C	3:C:283:GLN:N	2.63	0.52
2:B:121:GLN:O	2:B:126:ARG:NH2	2.43	0.52
5:E:24:PHE:O	5:E:25:ALA:C	2.48	0.52
1:A:133:VAL:O	1:A:136:TYR:HB3	2.10	0.52
1:A:86:HIS:CD2	10:A:301:HEM:NA	2.77	0.52
2:B:40:PHE:N	2:B:41:PRO:CD	2.72	0.52
1:A:88:TRP:CE2	2:B:54:LEU:HD13	2.45	0.52
4:D:70:LEU:C	4:D:72:SER:H	2.11	0.52
6:F:31:GLY:O	6:F:32:ALA:CB	2.58	0.52
2:B:150:PRO:O	2:B:151:LEU:C	2.46	0.51
2:B:40:PHE:HB2	2:B:41:PRO:HD3	1.93	0.51
3:C:43:ASP:HA	3:C:133:SER:O	2.10	0.51
3:C:13:PRO:HB3	3:C:106:TYR:HE1	1.72	0.51
3:C:70:LEU:CD2	3:C:70:LEU:H	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:NH1	1:A:104:VAL:CA	2.68	0.51
1:A:29:HIS:NE2	1:A:213:GLY:O	2.43	0.51
1:A:51:GLY:O	1:A:55:THR:HG23	2.09	0.51
1:A:70:GLN:HA	1:A:73:MET:HB2	1.91	0.51
3:C:161:TYR:O	3:C:163:THR:N	2.43	0.51
3:C:193:VAL:O	3:C:194:LYS:HG3	2.11	0.51
3:C:8:THR:C	3:C:10:PRO:HD3	2.29	0.51
4:D:58:ASP:OD1	4:D:62:ASN:HB2	2.09	0.51
5:E:21:GLY:O	5:E:25:ALA:HB2	2.10	0.51
2:B:136:GLY:HA2	14:B:201:CLA:CBC	2.40	0.51
2:B:3:THR:O	2:B:29:GLU:HA	2.10	0.51
3:C:159:GLN:HB3	3:C:170:ASN:HD22	1.75	0.51
8:H:1:MET:C	8:H:2:GLU:HG3	2.31	0.51
8:H:26:ARG:C	8:H:27:ASN:ND2	2.63	0.51
1:A:147:ALA:O	1:A:151:VAL:HG13	2.11	0.51
1:A:88:TRP:CH2	2:B:54:LEU:HD13	2.44	0.51
2:B:142:TRP:O	2:B:143:LEU:C	2.48	0.51
2:B:142:TRP:C	2:B:144:GLY:N	2.60	0.51
3:C:20:ILE:CD1	3:C:152:GLY:HA3	2.40	0.51
3:C:54:TYR:HE1	3:C:70:LEU:CG	2.23	0.51
1:A:110:PHE:CE1	2:B:112:PRO:HA	2.45	0.51
2:B:118:ASN:C	2:B:118:ASN:ND2	2.64	0.51
3:C:177:THR:HG23	3:C:226:LYS:HG2	1.91	0.51
4:D:70:LEU:C	4:D:72:SER:N	2.63	0.51
2:B:54:LEU:HD23	8:H:11:LEU:CD2	2.40	0.51
1:A:110:PHE:H	1:A:110:PHE:HD2	1.58	0.51
12:A:1102:UMQ:HB2	12:A:1102:UMQ:O2'	2.10	0.51
2:B:124:PHE:C	2:B:126:ARG:N	2.64	0.51
3:C:36:VAL:HG23	3:C:37:PRO:O	2.11	0.51
3:C:53:PRO:O	3:C:54:TYR:HB3	2.10	0.51
7:G:7:ASP:N	7:G:7:ASP:OD2	2.40	0.51
1:A:213:GLY:HA2	2:B:24:HIS:CD2	2.46	0.51
3:C:3:PHE:O	3:C:6:GLN:HB3	2.10	0.51
3:C:92:GLU:O	3:C:93:GLU:C	2.49	0.51
12:A:1102:UMQ:O5	12:A:1102:UMQ:C3'	2.58	0.51
1:A:122:VAL:O	1:A:123:ILE:C	2.47	0.51
1:A:9:GLN:OE1	1:A:15:GLN:CB	2.59	0.51
3:C:274:LEU:O	3:C:277:LYS:HB2	2.11	0.51
10:C:301:HEM:HBC2	10:C:301:HEM:HMC1	1.93	0.51
10:A:302:HEM:HMB1	10:A:302:HEM:HBB2	1.92	0.51
2:B:124:PHE:CE1	7:G:26:TYR:HD1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:196:GLN:C	3:C:197:VAL:HG23	2.31	0.50
1:A:215:LEU:CB	7:G:28:GLN:OE1	2.54	0.50
2:B:121:GLN:O	2:B:126:ARG:NE	2.41	0.50
2:B:149:PHE:HB3	2:B:150:PRO:HD2	1.93	0.50
2:B:80:TYR:CD1	2:B:80:TYR:C	2.85	0.50
3:C:208:VAL:HG12	3:C:209:ASP:N	2.25	0.50
3:C:263:CYS:O	3:C:265:VAL:N	2.44	0.50
2:B:122:ASN:OD1	2:B:123:PRO:HD2	2.11	0.50
2:B:32:TRP:CB	2:B:33:PRO:CD	2.89	0.50
3:C:61:VAL:HG11	3:C:168:ASN:HD22	1.74	0.50
3:C:22:CYS:SG	3:C:240:PHE:CE1	3.00	0.50
3:C:265:VAL:O	3:C:266:MET:C	2.49	0.50
4:D:68:LYS:O	4:D:68:LYS:HD3	2.12	0.50
14:B:201:CLA:HBB1	14:B:201:CLA:CHC	2.41	0.50
6:F:11:LEU:H	6:F:11:LEU:HD12	1.76	0.50
3:C:23:ALA:O	3:C:25:CYS:N	2.45	0.50
3:C:46:PHE:CZ	3:C:131:VAL:CG2	2.94	0.50
5:E:21:GLY:O	5:E:25:ALA:CB	2.59	0.50
2:B:129:ALA:O	2:B:132:ILE:N	2.45	0.50
2:B:32:TRP:HB3	2:B:33:PRO:CD	2.42	0.50
3:C:119:LEU:HD21	3:C:124:TYR:CE1	2.47	0.50
3:C:65:GLY:O	3:C:66:SER:O	2.29	0.50
1:A:59:LYS:HE2	1:A:59:LYS:CD	2.18	0.50
2:B:129:ALA:O	2:B:130:THR:C	2.50	0.50
3:C:101:VAL:HG11	3:C:103:PHE:CE2	2.47	0.50
7:G:26:TYR:O	7:G:27:GLN:C	2.46	0.50
12:C:1101:UMQ:C5'	12:C:1101:UMQ:HA1	2.42	0.50
3:C:144:PHE:CD2	3:C:251:ASP:N	2.79	0.50
3:C:47:LYS:NZ	3:C:97:GLU:CD	2.64	0.50
1:A:110:PHE:CD2	1:A:110:PHE:N	2.80	0.50
2:B:138:LEU:O	2:B:139:VAL:C	2.48	0.50
2:B:57:LEU:CD2	3:C:258:MET:HE3	2.42	0.50
1:A:93:MET:O	1:A:94:VAL:C	2.49	0.49
14:B:201:CLA:CBB	14:B:201:CLA:HHC	2.42	0.49
2:B:71:THR:HG22	2:B:72:PRO:N	2.26	0.49
2:B:87:ILE:O	2:B:88:LEU:C	2.49	0.49
3:C:117:GLY:HA2	3:C:118:PRO:C	2.33	0.49
2:B:149:PHE:CB	2:B:150:PRO:CD	2.82	0.49
1:A:25:TYR:CE2	2:B:30:PRO:HA	2.46	0.49
3:C:229:GLU:O	3:C:231:LEU:N	2.45	0.49
3:C:245:THR:OG1	3:C:246:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:TYR:N	4:D:133:TYR:HD1	2.09	0.49
2:B:45:MET:CG	4:D:30:VAL:HG11	2.42	0.49
4:D:74:ASN:O	4:D:75:ALA:O	2.30	0.49
4:D:77:ASP:CG	4:D:92:VAL:O	2.50	0.49
6:F:13:PHE:CD2	6:F:13:PHE:C	2.85	0.49
3:C:159:GLN:CG	3:C:170:ASN:HD22	2.25	0.49
3:C:262:ILE:N	3:C:262:ILE:HD13	2.26	0.49
6:F:11:LEU:CB	6:F:15:LEU:CD1	2.82	0.49
6:F:4:GLU:C	6:F:6:LEU:H	2.16	0.49
1:A:53:ALA:HB1	4:D:41:TYR:CE2	2.47	0.49
5:E:26:ILE:HG23	5:E:31:LEU:HB3	1.94	0.49
3:C:107:LYS:CG	3:C:110:GLN:NE2	2.76	0.49
3:C:206:THR:O	3:C:206:THR:CG2	2.60	0.49
4:D:178:TRP:O	4:D:179:VAL:HG12	2.12	0.49
3:C:268:ALA:HB2	4:D:26:THR:HB	1.93	0.49
2:B:101:MET:HE3	14:B:201:CLA:H92	1.92	0.49
4:D:152:HIS:CE1	4:D:165:TRP:HD1	2.18	0.49
3:C:273:ILE:CD1	8:H:25:GLY:HA2	2.42	0.49
3:C:60:GLN:HG2	3:C:70:LEU:HB3	1.95	0.49
4:D:123:LYS:CE	4:D:132:GLN:NE2	2.46	0.49
4:D:71:GLU:HG2	4:D:71:GLU:O	2.12	0.49
10:A:301:HEM:HHA	10:A:301:HEM:O2D	2.13	0.49
2:B:74:GLU:N	2:B:75:ILE:HG22	2.27	0.49
3:C:270:LEU:HG	8:H:21:MET:HE2	1.94	0.49
1:A:48:PHE:HA	10:A:301:HEM:HMC3	1.95	0.49
2:B:17:LYS:C	2:B:19:ALA:N	2.64	0.49
3:C:149:ILE:O	3:C:149:ILE:HG22	2.13	0.49
3:C:155:ARG:NH1	3:C:239:GLY:O	2.39	0.49
10:C:301:HEM:CBC	10:C:301:HEM:HMC1	2.43	0.49
1:A:18:ALA:HB1	12:A:1104:UMQ:HB1	1.95	0.48
1:A:32:ILE:CD1	8:H:22:VAL:HG11	2.43	0.48
2:B:118:ASN:HD21	2:B:120:PHE:CA	2.26	0.48
3:C:26:HIS:HD1	3:C:154:ASN:HD21	1.60	0.48
3:C:273:ILE:HD11	8:H:25:GLY:HA3	1.95	0.48
5:E:16:PHE:HE1	5:E:20:VAL:HG21	1.78	0.48
6:F:28:LYS:O	6:F:30:GLN:N	2.46	0.48
7:G:34:GLU:O	7:G:36:GLY:N	2.41	0.48
1:A:134:THR:HA	1:A:183:TYR:HD2	1.78	0.48
1:A:1:MET:O	1:A:2:ALA:CB	2.61	0.48
1:A:88:TRP:CZ3	2:B:54:LEU:HD13	2.48	0.48
2:B:32:TRP:HB3	2:B:33:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:ASN:O	4:D:148:LEU:HD22	2.13	0.48
2:B:45:MET:CE	4:D:27:VAL:HG13	2.42	0.48
2:B:57:LEU:CD1	8:H:8:TRP:CE3	2.92	0.48
1:A:59:LYS:HE3	1:A:59:LYS:CD	2.18	0.48
2:B:115:GLU:CG	11:B:1001:OPC:OCC	2.61	0.48
2:B:118:ASN:ND2	2:B:120:PHE:CD1	2.81	0.48
3:C:58:LEU:HD13	3:C:59:GLN:H	1.78	0.48
4:D:103:GLY:N	4:D:151:CYS:O	2.45	0.48
3:C:271:MET:HB3	4:D:23:ALA:HA	1.95	0.48
5:E:22:ILE:HG23	5:E:26:ILE:HG12	1.95	0.48
1:A:91:SER:O	1:A:92:MET:C	2.50	0.48
2:B:100:LEU:CD2	11:B:1001:OPC:HBX1	2.44	0.48
4:D:103:GLY:O	4:D:150:LEU:HA	2.12	0.48
4:D:44:PRO:HA	4:D:45:PRO:HD2	1.57	0.48
1:A:22:THR:O	1:A:23:SER:HB3	2.12	0.48
10:A:301:HEM:HHA	10:A:301:HEM:CGD	2.43	0.48
2:B:141:ILE:HG22	2:B:141:ILE:O	2.12	0.48
2:B:71:THR:HG22	2:B:72:PRO:CD	2.43	0.48
1:A:57:TYR:CE1	1:A:76:VAL:HG11	2.49	0.48
2:B:32:TRP:CD1	2:B:33:PRO:CD	2.92	0.48
3:C:82:PHE:CZ	3:C:249:LEU:HD23	2.43	0.48
4:D:81:VAL:HG21	4:D:91:ILE:HG13	1.96	0.48
3:C:36:VAL:HG11	3:C:149:ILE:HD13	1.95	0.48
4:D:78:ARG:HD3	4:D:92:VAL:HG21	1.94	0.48
6:F:6:LEU:O	6:F:7:TYR:C	2.52	0.48
2:B:129:ALA:C	2:B:131:THR:N	2.65	0.48
3:C:128:VAL:HG13	3:C:129:PHE:N	2.27	0.48
3:C:262:ILE:O	3:C:266:MET:HG2	2.13	0.48
2:B:40:PHE:CB	2:B:41:PRO:HD3	2.44	0.48
2:B:90:SER:O	2:B:91:VAL:HG23	2.13	0.48
1:A:134:THR:HA	1:A:183:TYR:CD2	2.49	0.48
1:A:78:PHE:O	1:A:79:GLY:C	2.51	0.48
3:C:133:SER:HA	3:C:134:PRO:HD2	1.62	0.48
2:B:57:LEU:HD21	3:C:258:MET:HE3	1.96	0.48
14:B:201:CLA:O2A	14:B:201:CLA:C4	2.62	0.47
2:B:1:MET:HB3	2:B:2:ALA:H	1.32	0.47
3:C:104:GLN:HA	3:C:105:PRO:HD3	1.41	0.47
2:B:37:LEU:HD21	2:B:38:TYR:CE2	2.50	0.47
6:F:17:PHE:O	6:F:20:TRP:HB3	2.14	0.47
2:B:37:LEU:O	2:B:37:LEU:CG	2.60	0.47
2:B:51:ILE:O	2:B:52:VAL:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:ILE:HG22	5:E:31:LEU:HB3	1.96	0.47
1:A:206:ILE:O	1:A:207:ARG:C	2.53	0.47
3:C:194:LYS:O	3:C:196:GLN:N	2.44	0.47
4:D:43:ILE:HG23	4:D:44:PRO:HD2	1.95	0.47
4:D:89:THR:HG23	4:D:105:ASN:OD1	2.15	0.47
2:B:100:LEU:HD22	11:B:1001:OPC:HBX1	1.95	0.47
1:A:215:LEU:CD2	2:B:121:GLN:HB2	2.44	0.47
2:B:123:PRO:O	2:B:130:THR:OG1	2.30	0.47
1:A:66:TYR:OH	2:B:63:GLY:O	2.24	0.47
3:C:144:PHE:CE2	3:C:251:ASP:CA	2.98	0.47
4:D:81:VAL:HB	4:D:89:THR:O	2.15	0.47
5:E:24:PHE:O	5:E:28:SER:N	2.46	0.47
2:B:123:PRO:CD	7:G:25:ALA:CB	2.91	0.47
2:B:14:LEU:HD12	2:B:14:LEU:HA	1.30	0.47
2:B:51:ILE:HG21	2:B:51:ILE:HD12	1.60	0.47
3:C:211:ILE:O	3:C:211:ILE:CG1	2.58	0.47
8:H:16:THR:O	8:H:18:SER:N	2.48	0.47
1:A:120:SER:O	1:A:124:LEU:N	2.46	0.47
1:A:142:GLN:N	2:B:66:ALA:HA	2.30	0.47
1:A:86:HIS:HE1	10:A:301:HEM:C1C	2.32	0.47
2:B:17:LYS:O	2:B:19:ALA:N	2.48	0.47
3:C:203:SER:HB2	3:C:205:LYS:HD2	1.97	0.47
3:C:144:PHE:CE2	3:C:251:ASP:HB2	2.50	0.47
4:D:35:LEU:O	4:D:39:VAL:HG23	2.15	0.47
4:D:78:ARG:CB	4:D:117:TRP:CD1	2.97	0.47
5:E:3:LEU:HD11	5:E:7:PHE:CE1	2.49	0.47
1:A:194:LEU:O	1:A:195:ILE:C	2.52	0.47
10:A:302:HEM:CMC	10:A:302:HEM:CBC	2.83	0.47
2:B:159:LEU:O	2:B:160:PHE:HD2	1.97	0.47
3:C:157:ARG:HB3	10:C:301:HEM:HAD2	1.94	0.47
3:C:20:ILE:HG21	3:C:240:PHE:CZ	2.50	0.47
3:C:232:THR:HG22	3:C:232:THR:O	2.14	0.47
6:F:17:PHE:O	6:F:18:VAL:C	2.53	0.47
1:A:202:HIS:HE1	10:A:302:HEM:C4C	2.32	0.47
2:B:15:ARG:O	2:B:18:LEU:HB2	2.14	0.47
2:B:94:LYS:O	2:B:98:VAL:HG23	2.15	0.47
3:C:161:TYR:C	3:C:163:THR:N	2.68	0.47
3:C:169:ASN:O	3:C:235:PRO:HB2	2.15	0.47
1:A:114:ARG:CZ	1:A:212:SER:HA	2.44	0.47
2:B:8:ASP:H	2:B:14:LEU:HD23	1.80	0.47
2:B:151:LEU:HD13	2:B:151:LEU:HA	1.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:SER:HB2	3:C:209:ASP:OD2	2.15	0.47
3:C:94:LEU:O	3:C:94:LEU:HD22	2.15	0.47
4:D:58:ASP:O	4:D:61:GLY:N	2.45	0.47
5:E:4:GLY:O	5:E:7:PHE:HB2	2.15	0.47
1:A:176:GLY:O	1:A:179:THR:N	2.48	0.47
1:A:34:TYR:O	10:A:303:HEM:C1B	2.69	0.47
2:B:82:TYR:H	2:B:83:PRO:HD2	1.78	0.47
3:C:234:ASN:HA	3:C:235:PRO:HD3	1.71	0.47
4:D:109:THR:HG23	4:D:145:PRO:HD2	1.97	0.47
5:E:3:LEU:O	5:E:4:GLY:C	2.53	0.47
8:H:6:LEU:O	8:H:9:VAL:HB	2.15	0.47
2:B:57:LEU:HD13	8:H:8:TRP:CE2	2.50	0.47
1:A:188:THR:HG22	10:A:301:HEM:CAC	2.45	0.46
2:B:156:THR:C	2:B:158:GLY:H	2.17	0.46
3:C:14:ARG:HA	3:C:20:ILE:HA	1.96	0.46
3:C:78:LEU:CB	3:C:79:PRO:CD	2.93	0.46
1:A:134:THR:HG21	1:A:186:ALA:HB1	1.96	0.46
1:A:27:PRO:HA	1:A:28:PRO:HD2	1.75	0.46
2:B:27:TYR:CD2	2:B:27:TYR:N	2.83	0.46
5:E:6:VAL:HG12	5:E:10:VAL:CG2	2.45	0.46
6:F:11:LEU:HB3	6:F:15:LEU:HD11	1.90	0.46
3:C:257:TRP:CD1	12:C:1101:UMQ:HB1	2.51	0.46
4:D:177:TRP:NE1	4:D:178:TRP:HE3	2.14	0.46
4:D:59:LYS:O	4:D:60:LEU:C	2.54	0.46
8:H:12:LEU:O	8:H:13:VAL:C	2.52	0.46
2:B:83:PRO:O	2:B:84:VAL:C	2.52	0.46
4:D:154:THR:O	4:D:155:VAL:HG22	2.15	0.46
5:E:9:ILE:H	5:E:9:ILE:HG12	1.51	0.46
1:A:103:ARG:HH11	1:A:104:VAL:N	2.14	0.46
2:B:125:ARG:C	2:B:127:PRO:HD3	2.36	0.46
2:B:44:ILE:O	2:B:47:THR:N	2.49	0.46
3:C:231:LEU:O	3:C:231:LEU:HD12	2.15	0.46
10:C:301:HEM:CHC	10:C:301:HEM:HBB2	2.14	0.46
5:E:1:MET:O	5:E:2:ILE:C	2.52	0.46
10:A:301:HEM:HMC2	10:A:301:HEM:HBC2	1.98	0.46
1:A:34:TYR:CD1	1:A:103:ARG:NE	2.66	0.46
3:C:81:GLY:HA2	3:C:142:ILE:CD1	2.43	0.46
11:A:1002:OPC:CAX	11:A:1002:OPC:HBC1	2.46	0.46
1:A:120:SER:O	1:A:123:ILE:N	2.49	0.46
1:A:180:LEU:O	1:A:181:THR:C	2.54	0.46
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HD2	1:A:208:LYS:C	2.35	0.46
2:B:17:LYS:C	2:B:19:ALA:H	2.17	0.46
2:B:32:TRP:CG	2:B:33:PRO:CD	2.99	0.46
3:C:278:GLN:O	3:C:282:VAL:CG2	2.64	0.46
4:D:117:TRP:CE3	4:D:117:TRP:HA	2.51	0.46
8:H:3:ILE:HD12	8:H:3:ILE:HA	1.73	0.46
2:B:71:THR:CG2	2:B:72:PRO:CD	2.94	0.46
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.46	0.46
4:D:133:TYR:CD2	4:D:148:LEU:HG	2.51	0.46
1:A:110:PHE:CD1	1:A:110:PHE:O	2.69	0.46
1:A:148:VAL:HG11	1:A:179:THR:HG21	1.97	0.46
1:A:208:LYS:HD2	1:A:208:LYS:O	2.16	0.46
1:A:141:ASP:CA	2:B:66:ALA:HB2	2.45	0.46
3:C:21:VAL:O	3:C:22:CYS:C	2.54	0.46
1:A:54:MET:HA	4:D:41:TYR:OH	2.16	0.46
4:D:79:VAL:CG1	4:D:80:LEU:N	2.79	0.46
1:A:155:PRO:HB2	1:A:166:SER:OG	2.16	0.45
1:A:186:ALA:HB3	1:A:187:HIS:H	1.12	0.45
8:H:29:LEU:CD2	8:H:29:LEU:HG	2.20	0.45
1:A:103:ARG:HH12	1:A:104:VAL:HG22	1.75	0.45
1:A:94:VAL:HG21	2:B:80:TYR:CD2	2.51	0.45
3:C:151:LEU:HG	3:C:152:GLY:N	2.30	0.45
4:D:79:VAL:HG12	4:D:80:LEU:N	2.30	0.45
3:C:273:ILE:HD13	8:H:25:GLY:CA	2.46	0.45
1:A:103:ARG:HH21	1:A:211:ILE:HD11	1.80	0.45
1:A:116:LEU:HB3	1:A:205:MET:SD	2.56	0.45
1:A:9:GLN:HE22	1:A:13:GLU:HA	1.81	0.45
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.72	0.45
1:A:41:LEU:HD23	10:A:303:HEM:HBC2	1.98	0.45
1:A:88:TRP:CD2	2:B:54:LEU:HD13	2.51	0.45
2:B:38:TYR:CE2	3:C:275:LYS:CG	2.99	0.45
3:C:146:LYS:HB2	3:C:248:VAL:CG2	2.43	0.45
3:C:180:ILE:CG1	3:C:198:SER:O	2.62	0.45
4:D:25:GLY:CA	16:D:201:SQD:H332	2.46	0.45
5:E:16:PHE:CD1	5:E:16:PHE:C	2.90	0.45
17:G:101:BCR:HC42	17:G:101:BCR:H312	1.98	0.45
11:A:1002:OPC:HBS	6:F:12:SER:HA	1.98	0.45
1:A:44:PHE:CD2	1:A:44:PHE:C	2.89	0.45
2:B:134:LEU:CD2	7:G:22:PHE:CZ	2.99	0.45
2:B:80:TYR:CE1	2:B:81:LEU:HD23	2.51	0.45
3:C:136:PRO:HA	3:C:142:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ILE:HG22	3:C:223:GLN:N	2.31	0.45
3:C:251:ASP:HA	3:C:252:PRO:HD3	1.64	0.45
4:D:177:TRP:CD1	4:D:178:TRP:HE3	2.32	0.45
1:A:4:VAL:HG12	1:A:5:TYR:N	2.31	0.45
3:C:159:GLN:HG3	3:C:170:ASN:ND2	2.32	0.45
7:G:31:ARG:CG	7:G:31:ARG:O	2.62	0.45
1:A:88:TRP:CE3	2:B:54:LEU:HD13	2.51	0.45
12:C:1101:UMQ:C5'	12:C:1101:UMQ:CA	2.94	0.45
3:C:254:ARG:HA	12:C:1101:UMQ:HB2	1.98	0.45
3:C:266:MET:CE	8:H:13:VAL:HG11	2.46	0.45
4:D:172:THR:HG22	4:D:174:GLU:H	1.82	0.45
2:B:124:PHE:O	2:B:127:PRO:HD3	2.17	0.45
2:B:37:LEU:HD23	2:B:38:TYR:CD1	2.52	0.45
2:B:61:MET:HG2	2:B:62:VAL:H	1.78	0.45
3:C:281:LYS:C	3:C:283:GLN:H	2.20	0.45
3:C:77:MET:H	3:C:77:MET:HG2	1.63	0.45
3:C:79:PRO:O	3:C:82:PHE:HD1	2.00	0.45
4:D:170:PHE:O	4:D:171:ARG:HB2	2.17	0.45
12:C:1101:UMQ:CL	4:D:37:PRO:CG	2.94	0.45
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.99	0.45
5:E:15:PHE:HA	5:E:18:ILE:HG13	1.98	0.45
7:G:6:LEU:O	7:G:9:LEU:HB2	2.17	0.45
8:H:23:VAL:HG13	8:H:28:GLY:HA3	1.98	0.45
3:C:161:TYR:HA	3:C:162:PRO:HD2	1.61	0.45
3:C:159:GLN:HA	3:C:167:SER:OG	2.17	0.45
8:H:22:VAL:HG12	8:H:23:VAL:N	2.31	0.45
8:H:24:TRP:CD1	8:H:24:TRP:C	2.85	0.45
1:A:126:VAL:O	1:A:130:SER:OG	2.35	0.45
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.34	0.45
1:A:138:LEU:N	1:A:139:PRO:HD3	2.31	0.45
1:A:113:PRO:HB2	2:B:22:MET:HE2	1.97	0.45
2:B:71:THR:C	2:B:72:PRO:O	2.54	0.45
2:B:73:LEU:H	2:B:73:LEU:HG	1.74	0.45
3:C:158:GLY:H	10:C:301:HEM:HAD2	1.82	0.45
3:C:221:GLU:OE1	3:C:222:GLY:N	2.48	0.45
5:E:22:ILE:HA	5:E:25:ALA:CB	2.47	0.45
7:G:16:ALA:O	17:G:101:BCR:H16C	2.17	0.45
1:A:33:PHE:CG	7:G:21:LEU:CD1	3.00	0.45
8:H:19:ILE:O	8:H:20:ALA:C	2.55	0.45
1:A:12:LEU:HD12	1:A:12:LEU:HA	1.51	0.45
1:A:215:LEU:HD21	2:B:121:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:GLN:NE2	3:C:157:ARG:CG	2.59	0.45
3:C:180:ILE:HG22	3:C:223:GLN:O	2.17	0.45
3:C:26:HIS:HD1	3:C:154:ASN:ND2	2.13	0.45
3:C:59:GLN:HB3	3:C:68:VAL:O	2.17	0.45
5:E:22:ILE:CG2	5:E:26:ILE:CG1	2.94	0.45
1:A:148:VAL:O	1:A:149:LYS:C	2.55	0.44
1:A:202:HIS:CE1	10:A:302:HEM:C4C	3.04	0.44
1:A:31:ASN:HD21	1:A:33:PHE:HD2	1.64	0.44
2:B:158:GLY:O	2:B:159:LEU:CB	2.65	0.44
2:B:32:TRP:HD1	2:B:33:PRO:HD3	1.75	0.44
2:B:95:LEU:HD23	2:B:95:LEU:C	2.37	0.44
3:C:6:GLN:OE1	3:C:106:TYR:O	2.36	0.44
3:C:257:TRP:CB	12:C:1101:UMQ:HD1	2.47	0.44
3:C:278:GLN:NE2	4:D:16:ARG:HA	2.33	0.44
5:E:14:LEU:O	5:E:18:ILE:HG12	2.17	0.44
5:E:3:LEU:O	5:E:4:GLY:O	2.34	0.44
2:B:118:ASN:ND2	2:B:119:LYS:N	2.63	0.44
2:B:82:TYR:O	2:B:83:PRO:C	2.56	0.44
3:C:159:GLN:CB	3:C:170:ASN:HD22	2.31	0.44
4:D:177:TRP:CD1	4:D:178:TRP:CZ3	3.05	0.44
1:A:30:VAL:HG22	1:A:34:TYR:CD1	2.52	0.44
3:C:12:THR:O	3:C:12:THR:HG22	2.17	0.44
3:C:15:GLU:HB2	3:C:19:ARG:CB	2.42	0.44
4:D:154:THR:C	4:D:155:VAL:HG22	2.38	0.44
2:B:69:PHE:HD2	2:B:69:PHE:N	2.13	0.44
3:C:74:ALA:CB	3:C:153:ALA:HA	2.48	0.44
4:D:58:ASP:O	4:D:61:GLY:HA2	2.17	0.44
6:F:13:PHE:HD2	6:F:13:PHE:C	2.20	0.44
3:C:101:VAL:CG1	3:C:103:PHE:CE2	3.01	0.44
5:E:16:PHE:O	5:E:19:ALA:HB3	2.18	0.44
1:A:209:GLN:HG2	2:B:22:MET:HE2	1.98	0.44
2:B:4:LEU:HD23	2:B:5:LYS:N	2.31	0.44
3:C:54:TYR:OH	3:C:121:GLY:HA3	2.17	0.44
3:C:58:LEU:HD12	3:C:59:GLN:CA	2.46	0.44
3:C:82:PHE:N	3:C:82:PHE:CD1	2.84	0.44
5:E:20:VAL:O	5:E:21:GLY:C	2.55	0.44
6:F:21:GLY:O	6:F:22:LEU:C	2.55	0.44
7:G:28:GLN:C	7:G:30:LYS:N	2.70	0.44
8:H:6:LEU:HA	8:H:6:LEU:HD23	1.50	0.44
2:B:118:ASN:ND2	2:B:120:PHE:HB2	2.29	0.44
14:B:201:CLA:CBB	14:B:201:CLA:CHC	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:THR:O	2:B:29:GLU:HB3	2.16	0.44
3:C:4:TRP:CD2	3:C:162:PRO:CG	2.99	0.44
3:C:34:VAL:CG2	3:C:243:ASP:HB3	2.48	0.44
3:C:278:GLN:HE22	4:D:16:ARG:HA	1.82	0.44
4:D:46:SER:O	4:D:48:GLY:N	2.51	0.44
1:A:81:LEU:O	1:A:82:ILE:C	2.55	0.44
1:A:99:LEU:HD13	7:G:17:THR:OG1	2.18	0.44
3:C:115:LEU:O	3:C:116:VAL:HG23	2.18	0.44
3:C:208:VAL:HG12	3:C:209:ASP:H	1.83	0.44
3:C:231:LEU:C	3:C:232:THR:OG1	2.56	0.44
3:C:27:LEU:H	3:C:27:LEU:CD2	2.31	0.44
4:D:89:THR:HG22	4:D:105:ASN:CA	2.42	0.44
5:E:3:LEU:CD1	5:E:7:PHE:CE1	3.00	0.44
7:G:17:THR:O	7:G:18:LEU:C	2.55	0.44
2:B:105:PRO:HG2	14:B:201:CLA:H102	2.00	0.44
3:C:101:VAL:HG11	3:C:103:PHE:CZ	2.52	0.44
3:C:15:GLU:H	3:C:20:ILE:H	1.66	0.44
4:D:60:LEU:HD12	4:D:62:ASN:HD21	1.83	0.44
1:A:131:PHE:HE1	1:A:195:ILE:HD12	1.83	0.43
1:A:125:ALA:HB2	10:A:302:HEM:HMC1	2.01	0.43
1:A:207:ARG:NH1	13:A:501:QNO:C4	2.71	0.43
3:C:139:ASP:O	3:C:140:LYS:C	2.56	0.43
3:C:272:LEU:HD23	3:C:272:LEU:HA	1.86	0.43
6:F:3:GLU:O	6:F:7:TYR:HB2	2.18	0.43
8:H:23:VAL:C	8:H:25:GLY:N	2.71	0.43
1:A:11:ARG:HB2	1:A:12:LEU:H	1.52	0.43
1:A:165:ILE:O	1:A:169:LEU:HG	2.18	0.43
14:B:201:CLA:H2	14:B:201:CLA:H61	1.39	0.43
14:B:201:CLA:HBB1	14:B:201:CLA:HHC	2.00	0.43
2:B:80:TYR:HD1	2:B:81:LEU:HD23	1.82	0.43
3:C:211:ILE:HA	3:C:212:PRO:HD2	1.94	0.43
4:D:160:ILE:HG22	4:D:161:VAL:N	2.33	0.43
16:D:201:SQD:H241	16:D:201:SQD:O49	2.18	0.43
2:B:124:PHE:HE1	7:G:26:TYR:N	2.15	0.43
1:A:102:PHE:O	1:A:103:ARG:C	2.55	0.43
2:B:38:TYR:CE2	3:C:275:LYS:HG3	2.53	0.43
3:C:263:CYS:C	3:C:265:VAL:N	2.72	0.43
6:F:24:VAL:O	6:F:27:LEU:CB	2.60	0.43
7:G:29:TYR:HB3	7:G:30:LYS:HB2	2.00	0.43
1:A:92:MET:SD	11:A:1002:OPC:CCB	3.06	0.43
2:B:101:MET:HE3	14:B:201:CLA:H91	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:HG23	2:B:44:ILE:HG12	2.00	0.43
1:A:142:GLN:N	2:B:66:ALA:CA	2.81	0.43
2:B:90:SER:OG	2:B:90:SER:O	2.35	0.43
4:D:115:VAL:HG22	4:D:126:CYS:CA	2.47	0.43
4:D:156:GLN:O	4:D:157:ASP:C	2.56	0.43
5:E:13:ALA:O	5:E:16:PHE:HB3	2.19	0.43
3:C:270:LEU:HD12	8:H:17:TRP:HZ2	1.82	0.43
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.78	0.43
3:C:72:VAL:HG13	3:C:72:VAL:H	1.56	0.43
4:D:80:LEU:HG	4:D:90:TYR:CE2	2.54	0.43
6:F:20:TRP:CD1	6:F:20:TRP:O	2.71	0.43
7:G:28:GLN:C	7:G:30:LYS:H	2.22	0.43
1:A:215:LEU:HD13	2:B:122:ASN:HA	2.01	0.43
2:B:149:PHE:CB	2:B:150:PRO:HD3	2.48	0.43
2:B:71:THR:HG23	2:B:72:PRO:HD2	2.00	0.43
3:C:61:VAL:HG13	3:C:65:GLY:HA2	2.00	0.43
2:B:95:LEU:O	2:B:95:LEU:HD23	2.18	0.43
3:C:262:ILE:HA	3:C:262:ILE:HD12	1.57	0.43
3:C:270:LEU:HD23	3:C:274:LEU:HG	2.01	0.43
4:D:115:VAL:CG1	4:D:124:PHE:HB3	2.49	0.43
4:D:36:TYR:CD2	4:D:36:TYR:C	2.91	0.43
1:A:177:GLN:O	1:A:178:ALA:C	2.56	0.43
1:A:197:VAL:HG12	1:A:198:PHE:N	2.32	0.43
1:A:38:GLY:HA3	10:A:303:HEM:C1C	2.54	0.43
1:A:80:TRP:CZ3	1:A:81:LEU:HG	2.54	0.43
1:A:86:HIS:HE1	10:A:301:HEM:NC	2.08	0.43
1:A:96:MET:CA	1:A:96:MET:HE3	2.31	0.43
2:B:151:LEU:O	2:B:154:THR:CB	2.66	0.43
2:B:6:LYS:C	2:B:7:PRO:O	2.57	0.43
3:C:12:THR:HG23	3:C:13:PRO:N	2.27	0.43
3:C:180:ILE:HA	3:C:199:ILE:HA	2.00	0.43
3:C:271:MET:O	3:C:272:LEU:C	2.57	0.43
3:C:84:ILE:HD12	3:C:103:PHE:CG	2.54	0.43
4:D:149:ALA:C	4:D:150:LEU:HD23	2.38	0.43
5:E:16:PHE:HD1	5:E:16:PHE:C	2.22	0.43
8:H:8:TRP:O	8:H:11:LEU:N	2.52	0.43
1:A:30:VAL:HG21	10:A:303:HEM:CMA	2.49	0.43
3:C:257:TRP:HB2	12:C:1101:UMQ:HD1	2.00	0.43
3:C:278:GLN:OE1	4:D:16:ARG:HA	2.19	0.43
4:D:59:LYS:HB2	4:D:59:LYS:NZ	2.34	0.43
2:B:48:PHE:HB3	2:B:49:ALA:H	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:TYR:CG	3:C:21:VAL:HG11	2.54	0.43
3:C:267:LEU:HD23	5:E:15:PHE:HE2	1.84	0.43
5:E:8:TYR:O	5:E:11:PHE:N	2.52	0.43
4:D:126:CYS:HA	4:D:127:PRO:HD3	1.74	0.42
4:D:169:ASP:OD1	4:D:176:PRO:HB3	2.19	0.42
1:A:158:ILE:HG23	1:A:159:PRO:HD3	2.00	0.42
1:A:88:TRP:CE3	2:B:54:LEU:HD12	2.53	0.42
3:C:44:THR:CG2	3:C:45:VAL:N	2.71	0.42
4:D:127:PRO:C	4:D:129:HIS:H	2.21	0.42
4:D:139:VAL:HG12	4:D:140:ILE:H	1.84	0.42
12:C:1101:UMQ:CL	4:D:37:PRO:HG3	2.49	0.42
7:G:31:ARG:HG2	7:G:31:ARG:O	2.18	0.42
1:A:207:ARG:HG2	12:A:1102:UMQ:H41	2.01	0.42
1:A:106:LEU:CD2	2:B:133:PHE:CE1	2.91	0.42
2:B:61:MET:CG	2:B:62:VAL:H	2.31	0.42
3:C:68:VAL:HG22	3:C:69:GLY:N	2.33	0.42
4:D:81:VAL:CG1	4:D:82:GLN:N	2.80	0.42
6:F:20:TRP:CD1	6:F:24:VAL:CG2	3.02	0.42
2:B:124:PHE:HE1	7:G:26:TYR:CA	2.32	0.42
7:G:3:GLU:HA	7:G:4:PRO:HD2	1.70	0.42
10:A:302:HEM:HBB2	10:A:302:HEM:CMB	2.49	0.42
2:B:126:ARG:HB3	11:B:1001:OPC:OBH	2.19	0.42
3:C:161:TYR:C	3:C:163:THR:H	2.22	0.42
3:C:250:GLN:HG3	3:C:251:ASP:O	2.19	0.42
5:E:10:VAL:O	5:E:14:LEU:CD1	2.56	0.42
6:F:8:ALA:O	6:F:11:LEU:N	2.53	0.42
1:A:80:TRP:CG	1:A:81:LEU:N	2.88	0.42
4:D:15:ARG:CD	5:E:31:LEU:CD2	2.96	0.42
4:D:168:THR:HG22	4:D:175:LYS:HA	2.01	0.42
1:A:204:LEU:O	1:A:205:MET:C	2.57	0.42
1:A:43:CYS:O	1:A:46:ILE:HB	2.20	0.42
2:B:106:LEU:O	2:B:107:GLY:C	2.58	0.42
3:C:275:LYS:O	3:C:276:LYS:C	2.57	0.42
3:C:281:LYS:O	3:C:283:GLN:N	2.52	0.42
4:D:66:VAL:HG21	4:D:155:VAL:CG1	2.49	0.42
6:F:17:PHE:HA	6:F:20:TRP:HB3	2.01	0.42
3:C:146:LYS:NZ	7:G:3:GLU:OE1	2.34	0.42
8:H:14:VAL:O	8:H:18:SER:HB2	2.20	0.42
1:A:104:VAL:HG22	10:A:302:HEM:HBD2	2.00	0.42
2:B:110:LEU:HB3	2:B:114:ILE:HD12	2.01	0.42
2:B:135:PHE:O	2:B:139:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:PRO:HB2	2:B:38:TYR:HE1	1.85	0.42
3:C:266:MET:HE1	8:H:13:VAL:HG11	2.02	0.42
2:B:38:TYR:CE2	3:C:275:LYS:HG2	2.55	0.42
4:D:46:SER:OG	4:D:46:SER:O	2.32	0.42
4:D:62:ASN:O	4:D:63:ASN:CG	2.50	0.42
6:F:30:GLN:HG3	6:F:31:GLY:N	2.34	0.42
1:A:130:SER:HB2	1:A:191:LEU:CD2	2.50	0.42
1:A:14:ILE:HD12	1:A:14:ILE:HA	1.26	0.42
1:A:20:ASP:OD1	12:A:1102:UMQ:C3	2.65	0.42
2:B:124:PHE:CE1	7:G:26:TYR:CD1	3.08	0.42
3:C:104:GLN:HG3	3:C:115:LEU:HB2	2.02	0.42
3:C:115:LEU:HA	3:C:115:LEU:HD23	1.17	0.42
3:C:85:ALA:HA	3:C:86:PRO:HD2	1.51	0.42
4:D:153:ALA:C	4:D:154:THR:O	2.57	0.42
11:A:1002:OPC:HAS1	5:E:4:GLY:CA	2.44	0.42
1:A:47:GLN:NE2	1:A:47:GLN:HA	2.33	0.42
1:A:80:TRP:CD2	1:A:81:LEU:N	2.88	0.42
2:B:100:LEU:HD21	11:B:1001:OPC:HBX2	2.01	0.42
2:B:106:LEU:HA	2:B:106:LEU:HD23	1.63	0.42
2:B:13:LYS:O	2:B:16:ALA:N	2.53	0.42
2:B:76:LEU:HA	2:B:76:LEU:HD12	1.71	0.42
3:C:255:VAL:HG23	3:C:255:VAL:H	1.49	0.42
3:C:85:ALA:HB2	3:C:132:LEU:CB	2.45	0.42
5:E:16:PHE:CD2	6:F:22:LEU:CD2	2.97	0.42
4:D:144:ALA:HA	4:D:145:PRO:HD3	1.89	0.42
4:D:111:LEU:N	15:D:200:FES:S2	2.93	0.42
1:A:78:PHE:CE1	4:D:37:PRO:HA	2.55	0.42
6:F:26:LEU:HA	6:F:26:LEU:HD13	1.65	0.42
1:A:50:THR:HG23	1:A:50:THR:H	1.62	0.41
2:B:104:VAL:CB	2:B:105:PRO:CD	2.98	0.41
3:C:192:ASN:HB3	3:C:193:VAL:H	1.67	0.41
3:C:41:LEU:O	3:C:42:PRO:C	2.57	0.41
4:D:131:SER:CA	4:D:142:GLY:HA3	2.43	0.41
2:B:122:ASN:HA	2:B:123:PRO:HD3	1.92	0.41
2:B:37:LEU:HD23	2:B:37:LEU:C	2.41	0.41
3:C:73:GLY:C	10:C:301:HEM:HMB2	2.40	0.41
1:A:29:HIS:CD2	1:A:214:PRO:CA	2.95	0.41
2:B:106:LEU:O	2:B:109:ILE:N	2.53	0.41
4:D:117:TRP:HE3	4:D:117:TRP:HA	1.85	0.41
6:F:25:LEU:C	6:F:27:LEU:N	2.73	0.41
1:A:37:GLY:HA3	10:A:302:HEM:C3A	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:GLN:HG3	3:C:170:ASN:HD22	1.85	0.41
4:D:43:ILE:HG22	4:D:44:PRO:O	2.20	0.41
6:F:25:LEU:O	6:F:27:LEU:N	2.53	0.41
2:B:153:LYS:HE3	2:B:153:LYS:HB3	1.71	0.41
3:C:273:ILE:HD13	8:H:25:GLY:HA2	2.02	0.41
7:G:34:GLU:HB3	7:G:35:LEU:H	1.64	0.41
2:B:79:TRP:CE3	7:G:6:LEU:HD11	2.56	0.41
3:C:21:VAL:CG2	3:C:22:CYS:N	2.83	0.41
3:C:77:MET:CG	3:C:150:HIS:O	2.67	0.41
4:D:60:LEU:HD12	4:D:62:ASN:ND2	2.35	0.41
1:A:111:LYS:O	1:A:113:PRO:N	2.53	0.41
1:A:133:VAL:O	1:A:134:THR:C	2.59	0.41
1:A:184:TYR:O	1:A:188:THR:N	2.48	0.41
2:B:3:THR:O	2:B:29:GLU:CA	2.68	0.41
7:G:20:GLY:HA2	7:G:23:TYR:HB3	2.02	0.41
1:A:107:THR:O	2:B:121:GLN:HB3	2.19	0.41
3:C:98:VAL:HA	3:C:128:VAL:HB	2.01	0.41
4:D:89:THR:CG2	4:D:105:ASN:OD1	2.69	0.41
1:A:62:VAL:HG12	1:A:140:TRP:CD1	2.55	0.41
5:E:18:ILE:O	5:E:22:ILE:HG13	2.21	0.41
5:E:2:ILE:H	5:E:2:ILE:CD1	2.28	0.41
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.04	0.41
7:G:11:LEU:O	7:G:12:GLY:C	2.59	0.41
1:A:112:LYS:O	1:A:113:PRO:C	2.50	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.43	0.41
1:A:98:ILE:HG22	1:A:99:LEU:N	2.34	0.41
2:B:84:VAL:CG1	2:B:101:MET:CG	2.97	0.41
3:C:139:ASP:OD1	3:C:141:ASN:ND2	2.54	0.41
3:C:2:PRO:O	3:C:3:PHE:C	2.59	0.41
3:C:45:VAL:HG22	3:C:85:ALA:CB	2.51	0.41
4:D:137:GLY:HA2	4:D:148:LEU:HB2	2.02	0.41
4:D:139:VAL:HG22	4:D:147:SER:N	2.36	0.41
4:D:23:ALA:O	4:D:24:PHE:C	2.55	0.41
6:F:23:GLY:O	6:F:26:LEU:HB2	2.20	0.41
2:B:17:LYS:HE3	2:B:26:TYR:HH	1.80	0.41
3:C:144:PHE:HB3	3:C:145:GLY:H	1.71	0.41
3:C:159:GLN:CD	3:C:159:GLN:N	2.74	0.41
3:C:218:ILE:CG2	3:C:233:ASN:HB2	2.51	0.41
3:C:25:CYS:SG	10:C:301:HEM:C3C	3.10	0.41
3:C:78:LEU:HD12	3:C:78:LEU:N	2.33	0.41
4:D:32:LEU:O	4:D:33:GLY:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HD2	1:A:107:THR:CG2	2.44	0.40
2:B:76:LEU:HG	2:B:82:TYR:CE2	2.56	0.40
2:B:11:ASP:HA	2:B:12:PRO:HD3	1.69	0.40
3:C:176:ALA:O	3:C:227:ALA:HA	2.21	0.40
3:C:27:LEU:H	3:C:27:LEU:HD23	1.86	0.40
4:D:38:LEU:HA	4:D:38:LEU:HD12	1.82	0.40
4:D:80:LEU:HA	4:D:80:LEU:HD23	1.40	0.40
17:G:101:BCR:H361	17:G:101:BCR:H20C	1.11	0.40
1:A:32:ILE:HD12	8:H:22:VAL:HG11	2.04	0.40
1:A:142:GLN:HG3	2:B:72:PRO:HG3	2.03	0.40
10:A:303:HEM:HAD2	10:A:303:HEM:HMD2	1.79	0.40
1:A:95:LEU:HD22	1:A:96:MET:HE1	2.03	0.40
14:B:201:CLA:HAB	14:B:201:CLA:HMB1	1.86	0.40
3:C:273:ILE:HD12	8:H:25:GLY:CA	2.51	0.40
3:C:121:GLY:O	3:C:122:GLU:C	2.57	0.40
4:D:152:HIS:O	4:D:162:LEU:HD23	2.21	0.40
4:D:68:LYS:O	4:D:68:LYS:CD	2.69	0.40
1:A:7:TRP:CZ2	1:A:11:ARG:NH2	2.84	0.40
1:A:100:HIS:CE1	10:A:302:HEM:C4A	2.97	0.40
2:B:128:VAL:HG23	2:B:128:VAL:H	1.42	0.40
3:C:183:ILE:HD11	3:C:220:SER:O	2.22	0.40
3:C:254:ARG:HH11	3:C:254:ARG:HD2	1.60	0.40
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.64	0.40
4:D:129:HIS:CB	15:D:200:FES:S1	2.95	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	213/215 (99%)	142 (67%)	53 (25%)	18 (8%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	158/160 (99%)	91 (58%)	36 (23%)	31 (20%)	0	2
3	C	286/289 (99%)	195 (68%)	50 (18%)	41 (14%)	0	4
4	D	162/179 (90%)	93 (57%)	39 (24%)	30 (18%)	0	2
5	E	30/32 (94%)	9 (30%)	10 (33%)	11 (37%)	0	0
6	F	30/35 (86%)	14 (47%)	8 (27%)	8 (27%)	0	0
7	G	35/37 (95%)	13 (37%)	9 (26%)	13 (37%)	0	0
8	H	27/29 (93%)	14 (52%)	6 (22%)	7 (26%)	0	0
All	All	941/976 (96%)	571 (61%)	211 (22%)	159 (17%)	0	3

All (159) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	23	SER
1	A	28	PRO
1	A	112	LYS
1	A	136	TYR
1	A	162	GLY
1	A	164	LEU
1	A	186	ALA
2	B	7	PRO
2	B	22	MET
2	B	33	PRO
2	B	34	ASN
2	B	75	ILE
2	B	87	ILE
2	B	109	ILE
2	B	110	LEU
2	B	114	ILE
2	B	117	VAL
2	B	125	ARG
2	B	129	ALA
2	B	130	THR
2	B	151	LEU
2	B	159	LEU
3	C	22	CYS
3	C	23	ALA
3	C	24	ASN
3	C	27	LEU
3	C	63	ALA

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Mol	Chain	Res	Type
3	C	66	SER
3	C	67	LYS
3	C	144	PHE
3	C	185	LYS
3	C	186	GLU
3	C	187	GLU
3	C	189	GLU
3	C	192	ASN
3	C	201	THR
3	C	205	LYS
3	C	212	PRO
3	C	230	ALA
4	D	47	GLY
4	D	59	LYS
4	D	60	LEU
4	D	63	ASN
4	D	75	ALA
4	D	77	ASP
4	D	139	VAL
4	D	140	ILE
4	D	147	SER
4	D	154	THR
4	D	157	ASP
4	D	164	PRO
4	D	170	PHE
4	D	171	ARG
5	E	8	TYR
5	E	9	ILE
5	E	25	ALA
6	F	5	MET
6	F	7	TYR
6	F	8	ALA
6	F	9	ALA
7	G	16	ALA
7	G	30	LYS
7	G	34	GLU
7	G	35	LEU
1	A	3	ASN
1	A	13	GLU
1	A	32	ILE
1	A	43	CYS
1	A	132	GLY

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Mol	Chain	Res	Type
1	A	134	THR
1	A	170	ARG
2	B	2	ALA
2	B	18	LEU
2	B	65	PRO
2	B	103	SER
2	B	113	PHE
2	B	124	PHE
2	B	158	GLY
3	C	134	PRO
3	C	162	PRO
3	C	193	VAL
3	C	194	LYS
3	C	195	TYR
3	C	200	GLN
3	C	232	THR
3	C	274	LEU
3	C	282	VAL
4	D	51	GLY
4	D	72	SER
4	D	76	GLY
4	D	101	ASP
4	D	138	LYS
4	D	155	VAL
5	E	13	ALA
5	E	21	GLY
7	G	15	PHE
7	G	18	LEU
7	G	19	GLY
7	G	27	GLN
7	G	29	TYR
8	H	2	GLU
8	H	6	LEU
8	H	20	ALA
8	H	24	TRP
2	B	44	ILE
2	B	108	LEU
3	C	184	ALA
4	D	33	GLY
4	D	50	VAL
5	E	24	PHE
6	F	13	PHE

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Mol	Chain	Res	Type
6	F	24	VAL
7	G	4	PRO
7	G	20	GLY
8	H	4	ASP
8	H	19	ILE
2	B	32	TRP
2	B	86	GLN
2	B	111	VAL
2	B	146	GLY
3	C	19	ARG
3	C	20	ILE
3	C	28	ALA
3	C	110	GLN
3	C	272	LEU
3	C	275	LYS
4	D	71	GLU
4	D	143	PRO
2	B	134	LEU
3	C	86	PRO
3	C	100	ASP
4	D	18	PHE
4	D	74	ASN
4	D	127	PRO
5	E	14	LEU
5	E	19	ALA
2	B	144	GLY
3	C	2	PRO
3	C	37	PRO
3	C	91	PRO
3	C	152	GLY
4	D	14	GLY
5	E	4	GLY
5	E	6	VAL
5	E	20	VAL
6	F	26	LEU
6	F	29	ILE
3	C	69	GLY
8	H	7	GLY
1	A	82	ILE
1	A	197	VAL
2	B	139	VAL
3	C	11	PRO

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Mol	Chain	Res	Type
4	D	142	GLY
4	D	145	PRO
7	G	12	GLY
1	A	210	GLY
7	G	36	GLY

5.3.2 Protein sidechains [i](#)

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	184/184 (100%)	138 (75%)	46 (25%)	0	4
2	B	137/137 (100%)	98 (72%)	39 (28%)	0	3
3	C	242/243 (100%)	151 (62%)	91 (38%)	0	1
4	D	134/146 (92%)	96 (72%)	38 (28%)	0	3
5	E	25/25 (100%)	17 (68%)	8 (32%)	0	2
6	F	24/27 (89%)	11 (46%)	13 (54%)	0	0
7	G	28/28 (100%)	20 (71%)	8 (29%)	0	3
8	H	24/24 (100%)	16 (67%)	8 (33%)	0	2
All	All	798/814 (98%)	547 (68%)	251 (32%)	0	2

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ARG
1	A	12	LEU
1	A	13	GLU
1	A	14	ILE
1	A	17	LEU
1	A	28	PRO
1	A	30	VAL
1	A	31	ASN
1	A	32	ILE

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	52	PHE
1	A	59	LYS
1	A	62	VAL
1	A	63	THR
1	A	70	GLN
1	A	72	ILE
1	A	81	LEU
1	A	84	SER
1	A	87	ARG
1	A	92	MET
1	A	95	LEU
1	A	96	MET
1	A	99	LEU
1	A	100	HIS
1	A	103	ARG
1	A	106	LEU
1	A	112	LYS
1	A	115	GLU
1	A	118	TRP
1	A	130	SER
1	A	136	TYR
1	A	139	PRO
1	A	143	VAL
1	A	163	VAL
1	A	167	ASP
1	A	169	LEU
1	A	170	ARG
1	A	173	SER
1	A	175	VAL
1	A	182	ARG
1	A	192	PRO
1	A	200	LEU
1	A	203	PHE
1	A	211	ILE
1	A	215	LEU
2	B	1	MET
2	B	3	THR
2	B	6	LYS
2	B	7	PRO
2	B	25	ASN
2	B	37	LEU

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Mol	Chain	Res	Type
2	B	44	ILE
2	B	51	ILE
2	B	54	LEU
2	B	64	GLU
2	B	65	PRO
2	B	73	LEU
2	B	74	GLU
2	B	75	ILE
2	B	78	GLU
2	B	79	TRP
2	B	81	LEU
2	B	87	ILE
2	B	88	LEU
2	B	89	ARG
2	B	93	ASN
2	B	94	LYS
2	B	96	LEU
2	B	100	LEU
2	B	101	MET
2	B	103	SER
2	B	115	GLU
2	B	117	VAL
2	B	118	ASN
2	B	119	LYS
2	B	126	ARG
2	B	134	LEU
2	B	145	ILE
2	B	151	LEU
2	B	152	ASP
2	B	153	LYS
2	B	155	LEU
2	B	156	THR
2	B	159	LEU
3	C	2	PRO
3	C	6	GLN
3	C	7	GLN
3	C	8	THR
3	C	9	TYR
3	C	10	PRO
3	C	12	THR
3	C	14	ARG
3	C	19	ARG

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Mol	Chain	Res	Type
3	C	20	ILE
3	C	27	LEU
3	C	34	VAL
3	C	37	PRO
3	C	39	SER
3	C	44	THR
3	C	54	TYR
3	C	56	THR
3	C	58	LEU
3	C	60	GLN
3	C	67	LYS
3	C	70	LEU
3	C	71	ASN
3	C	72	VAL
3	C	75	VAL
3	C	77	MET
3	C	86	PRO
3	C	88	GLU
3	C	93	GLU
3	C	94	LEU
3	C	101	VAL
3	C	107	LYS
3	C	111	ASP
3	C	119	LEU
3	C	122	GLU
3	C	123	GLN
3	C	125	GLN
3	C	126	GLU
3	C	127	ILE
3	C	131	VAL
3	C	137	THR
3	C	140	LYS
3	C	141	ASN
3	C	142	ILE
3	C	146	LYS
3	C	151	LEU
3	C	154	ASN
3	C	155	ARG
3	C	157	ARG
3	C	160	ILE
3	C	163	THR
3	C	165	GLU

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Mol	Chain	Res	Type
3	C	171	VAL
3	C	173	THR
3	C	179	THR
3	C	180	ILE
3	C	182	LYS
3	C	185	LYS
3	C	186	GLU
3	C	187	GLU
3	C	189	GLU
3	C	198	SER
3	C	206	THR
3	C	211	ILE
3	C	216	GLU
3	C	218	ILE
3	C	219	VAL
3	C	220	SER
3	C	225	VAL
3	C	229	GLU
3	C	233	ASN
3	C	237	VAL
3	C	242	GLN
3	C	243	ASP
3	C	245	THR
3	C	249	LEU
3	C	251	ASP
3	C	256	LYS
3	C	258	MET
3	C	259	ILE
3	C	262	ILE
3	C	264	LEU
3	C	267	LEU
3	C	271	MET
3	C	274	LEU
3	C	276	LYS
3	C	277	LYS
3	C	281	LYS
3	C	282	VAL
3	C	283	GLN
3	C	286	GLU
3	C	288	ASN
4	D	10	VAL
4	D	12	ASP

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Mol	Chain	Res	Type
4	D	15	ARG
4	D	21	LEU
4	D	26	THR
4	D	35	LEU
4	D	40	LYS
4	D	45	PRO
4	D	54	THR
4	D	59	LYS
4	D	64	VAL
4	D	68	LYS
4	D	73	HIS
4	D	77	ASP
4	D	84	LEU
4	D	89	THR
4	D	99	ILE
4	D	105	ASN
4	D	108	CYS
4	D	113	CYS
4	D	115	VAL
4	D	131	SER
4	D	133	TYR
4	D	135	GLU
4	D	139	VAL
4	D	141	ARG
4	D	147	SER
4	D	150	LEU
4	D	154	THR
4	D	155	VAL
4	D	157	ASP
4	D	158	ASP
4	D	159	ASN
4	D	161	VAL
4	D	165	TRP
4	D	168	THR
4	D	169	ASP
4	D	175	LYS
5	E	3	LEU
5	E	9	ILE
5	E	11	PHE
5	E	14	LEU
5	E	16	PHE
5	E	18	ILE

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Mol	Chain	Res	Type
5	E	23	ILE
5	E	29	ILE
6	F	1	MET
6	F	3	GLU
6	F	5	MET
6	F	6	LEU
6	F	7	TYR
6	F	10	LEU
6	F	13	PHE
6	F	15	LEU
6	F	16	ILE
6	F	22	LEU
6	F	26	LEU
6	F	29	ILE
6	F	30	GLN
7	G	1	MET
7	G	6	LEU
7	G	7	ASP
7	G	9	LEU
7	G	21	LEU
7	G	30	LYS
7	G	31	ARG
7	G	35	LEU
8	H	1	MET
8	H	2	GLU
8	H	6	LEU
8	H	12	LEU
8	H	18	SER
8	H	21	MET
8	H	27	ASN
8	H	29	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
2	B	34	ASN
2	B	118	ASN
3	C	6	GLN
3	C	110	GLN
3	C	125	GLN

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Mol	Chain	Res	Type
3	C	141	ASN
3	C	154	ASN
3	C	159	GLN
3	C	168	ASN
3	C	170	ASN
3	C	233	ASN
3	C	234	ASN
3	C	242	GLN
3	C	250	GLN
3	C	283	GLN
3	C	288	ASN
4	D	62	ASN
4	D	110	HIS
4	D	118	ASN
4	D	132	GLN
8	H	27	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	G	101	-	41,41,41	3.66	22 (53%)	56,56,56	6.75	35 (62%)
11	OPC	A	1002	-	53,53,54	2.10	13 (24%)	59,61,64	2.85	27 (45%)
10	HEM	A	302	1	27,50,50	2.57	12 (44%)	17,82,82	3.52	7 (41%)
12	UMQ	A	1104	-	35,35,35	1.60	3 (8%)	46,46,46	2.77	12 (26%)
13	QNO	A	501	10	22,22,22	2.61	5 (22%)	20,28,28	2.56	5 (25%)
15	FES	D	200	4	0,4,4	0.00	-	-	-	-
10	HEM	A	303	1,18,13	27,50,50	2.99	8 (29%)	17,82,82	3.81	10 (58%)
12	UMQ	A	1103	-	35,35,35	1.73	5 (14%)	46,46,46	2.94	16 (34%)
10	HEM	A	301	1	27,50,50	2.31	10 (37%)	17,82,82	2.98	8 (47%)
12	UMQ	A	1102	1	35,35,35	2.03	7 (20%)	46,46,46	3.06	20 (43%)
16	SQD	D	201	-	53,54,54	2.52	24 (45%)	62,65,65	4.84	35 (56%)
14	CLA	B	201	18	59,73,73	2.07	13 (22%)	67,113,113	3.56	39 (58%)
10	HEM	C	301	3	27,50,50	2.50	15 (55%)	17,82,82	2.29	5 (29%)
12	UMQ	C	1101	-	35,35,35	1.85	8 (22%)	46,46,46	3.38	20 (43%)
11	OPC	B	1001	-	53,53,54	2.12	16 (30%)	59,61,64	2.52	26 (44%)

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
17	BCR	G	101	-	-	10/29/63/63	0/2/2/2
11	OPC	A	1002	-	-	23/57/57/60	-
10	HEM	A	302	1	-	1/6/54/54	-
12	UMQ	A	1104	-	2/2/10/10	16/20/60/60	0/2/2/2
13	QNO	A	501	10	1/1/0/0	3/9/9/9	0/2/2/2
15	FES	D	200	4	-	-	0/1/1/1
10	HEM	A	303	1,18,13	-	2/6/54/54	-
12	UMQ	A	1103	-	2/2/10/10	12/20/60/60	0/2/2/2
10	HEM	A	301	1	-	0/6/54/54	-
10	HEM	C	301	3	-	0/6/54/54	-
16	SQD	D	201	-	3/3/9/9	24/49/69/69	0/1/1/1
14	CLA	B	201	18	4/4/20/25	12/37/135/135	-
12	UMQ	A	1102	1	2/2/10/10	12/20/60/60	0/2/2/2
12	UMQ	C	1101	-	2/2/10/10	9/20/60/60	0/2/2/2
11	OPC	B	1001	-	-	25/57/57/60	-

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	101	BCR	C8-C9	-11.19	1.21	1.45
10	A	303	HEM	C3C-C2C	-9.38	1.27	1.40
13	A	501	QNO	C2-N1	8.91	1.51	1.36
10	A	303	HEM	C3B-C2B	-8.81	1.28	1.40
14	B	201	CLA	OBD-CAD	8.13	1.33	1.22
17	G	101	BCR	C21-C22	7.50	1.45	1.35
17	G	101	BCR	C23-C22	-6.52	1.31	1.45
12	A	1102	UMQ	O1'-C1'	6.42	1.51	1.40
17	G	101	BCR	C8-C7	-6.16	1.14	1.33
12	A	1103	UMQ	C1'-C2'	-5.98	1.35	1.52
17	G	101	BCR	C26-C25	5.95	1.44	1.34
11	A	1002	OPC	OAN-CAO	5.92	1.51	1.34
10	C	301	HEM	C3C-C2C	-5.69	1.32	1.40
10	A	302	HEM	C3B-C2B	-5.59	1.32	1.40
16	D	201	SQD	C17-C16	-5.48	1.20	1.51
12	C	1101	UMQ	C4'-C5'	5.43	1.67	1.52
12	A	1103	UMQ	O1'-C1'	5.25	1.49	1.40
11	A	1002	OPC	CBP-CBQ	-5.22	1.31	1.52
10	A	302	HEM	C3C-C2C	-5.20	1.33	1.40
12	A	1104	UMQ	O1'-C1'	5.20	1.49	1.40
17	G	101	BCR	C7-C6	-5.19	1.26	1.45
17	G	101	BCR	C19-C18	-5.15	1.34	1.45
10	A	301	HEM	C3B-C2B	-5.14	1.33	1.40
12	A	1102	UMQ	C1'-C2'	-5.14	1.37	1.52
11	A	1002	OPC	OBJ-CBK	5.06	1.48	1.33
16	D	201	SQD	C6-S	-4.98	1.59	1.77
10	C	301	HEM	C3B-C2B	-4.93	1.33	1.40
17	G	101	BCR	C12-C13	-4.92	1.35	1.45
16	D	201	SQD	O47-C7	4.90	1.48	1.34
12	C	1101	UMQ	C1'-C2'	-4.89	1.38	1.52
11	B	1001	OPC	CAG-CAH	-4.88	1.35	1.51
14	B	201	CLA	O2A-CGA	4.87	1.47	1.33
14	B	201	CLA	C3C-C2C	4.83	1.47	1.36
11	A	1002	OPC	CAG-CAH	-4.80	1.36	1.51
10	A	301	HEM	CMC-C2C	4.74	1.62	1.51
12	A	1104	UMQ	C1'-C2'	-4.73	1.38	1.52
16	D	201	SQD	O48-C23	4.67	1.47	1.33
16	D	201	SQD	C12-C11	-4.62	1.25	1.51
14	B	201	CLA	C3D-C2D	4.62	1.47	1.39
16	D	201	SQD	O6-C1	4.61	1.48	1.40
11	B	1001	OPC	OBJ-CBK	4.61	1.46	1.33
13	A	501	QNO	O41-C4	-4.53	1.23	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	101	BCR	C24-C23	-4.52	1.19	1.33
11	B	1001	OPC	CAV-CAW	4.36	1.57	1.31
17	G	101	BCR	C38-C26	4.35	1.58	1.50
16	D	201	SQD	C16-C15	-4.25	1.27	1.51
14	B	201	CLA	O2D-CGD	4.22	1.43	1.33
17	G	101	BCR	C30-C25	4.21	1.59	1.53
11	B	1001	OPC	CAQ-CAP	-4.18	1.36	1.52
11	B	1001	OPC	CAG-NAF	-4.15	1.37	1.51
17	G	101	BCR	C24-C25	-4.15	1.30	1.45
11	A	1002	OPC	CAQ-CAP	-4.14	1.37	1.52
10	A	302	HEM	C3B-CAB	4.13	1.56	1.47
16	D	201	SQD	C18-C17	-4.13	1.28	1.51
14	B	201	CLA	CHC-C1C	4.04	1.45	1.35
10	C	301	HEM	C3D-C2D	4.02	1.49	1.37
11	A	1002	OPC	CAV-CAW	3.95	1.54	1.31
16	D	201	SQD	C11-C10	-3.91	1.29	1.51
10	A	303	HEM	C3D-C2D	3.90	1.49	1.37
16	D	201	SQD	C13-C12	-3.85	1.30	1.51
11	A	1002	OPC	CBP-CBO	-3.78	1.30	1.51
10	A	303	HEM	CAD-C3D	3.76	1.58	1.52
10	A	302	HEM	C3D-C2D	3.71	1.48	1.37
12	C	1101	UMQ	C3'-C4'	3.66	1.62	1.52
17	G	101	BCR	C1-C6	-3.64	1.48	1.53
11	B	1001	OPC	OAN-CAO	3.63	1.44	1.34
12	A	1103	UMQ	O2'-C2'	-3.58	1.34	1.43
10	A	301	HEM	C1C-C2C	3.51	1.50	1.42
13	A	501	QNO	C21-C2	3.49	1.60	1.50
10	A	301	HEM	CMB-C2B	3.47	1.59	1.51
10	A	303	HEM	CAA-C2A	3.46	1.57	1.52
10	A	301	HEM	C3C-CAC	3.45	1.54	1.47
10	A	302	HEM	C1D-CHD	-3.43	1.31	1.41
10	C	301	HEM	C1D-CHD	-3.39	1.31	1.41
12	C	1101	UMQ	O5'-C1'	3.38	1.50	1.41
10	C	301	HEM	CAA-C2A	3.28	1.56	1.52
10	A	301	HEM	C3D-C2D	3.24	1.47	1.37
11	B	1001	OPC	CBP-CBQ	-3.22	1.39	1.52
12	A	1104	UMQ	O2'-C2'	-3.22	1.35	1.43
16	D	201	SQD	C21-C20	-3.21	1.28	1.51
12	A	1102	UMQ	O2'-C2'	-3.21	1.35	1.43
12	A	1102	UMQ	O5'-C1'	3.17	1.49	1.41
11	B	1001	OPC	CAE-NAF	-3.17	1.40	1.50
11	B	1001	OPC	CBL-CBK	3.16	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	302	HEM	C1B-C2B	3.14	1.49	1.42
16	D	201	SQD	C36-C35	-3.13	1.34	1.51
17	G	101	BCR	C37-C22	3.11	1.57	1.50
10	A	302	HEM	C4B-CHC	-3.08	1.32	1.41
14	B	201	CLA	C1D-C2D	3.07	1.49	1.42
10	A	301	HEM	C4A-CHB	-3.02	1.32	1.41
10	C	301	HEM	C1C-C2C	3.00	1.49	1.42
10	A	301	HEM	C3C-C2C	-3.00	1.36	1.40
11	A	1002	OPC	CBT-CBS	-2.98	1.33	1.50
14	B	201	CLA	MG-NA	-2.97	1.99	2.06
16	D	201	SQD	C15-C14	-2.94	1.35	1.51
10	A	302	HEM	C4D-C3D	2.93	1.49	1.42
10	C	301	HEM	C3B-CAB	2.93	1.53	1.47
12	C	1101	UMQ	O1'-C1'	2.90	1.45	1.40
10	A	302	HEM	C4A-CHB	-2.87	1.33	1.41
17	G	101	BCR	C14-C13	2.85	1.39	1.35
10	A	302	HEM	CAA-C2A	2.83	1.56	1.52
10	C	301	HEM	C3C-CAC	2.81	1.53	1.47
10	C	301	HEM	C4A-CHB	-2.80	1.33	1.41
11	A	1002	OPC	CAQ-CAR	-2.80	1.35	1.51
11	A	1002	OPC	CAR-CAS	-2.74	1.36	1.51
10	A	303	HEM	C3B-CAB	2.74	1.53	1.47
16	D	201	SQD	C22-C21	-2.74	1.27	1.49
17	G	101	BCR	C27-C26	2.71	1.56	1.51
16	D	201	SQD	C20-C19	-2.71	1.36	1.51
16	D	201	SQD	C14-C13	-2.71	1.36	1.51
16	D	201	SQD	C19-C18	-2.69	1.36	1.51
10	A	302	HEM	C3C-CAC	2.61	1.53	1.47
11	A	1002	OPC	CBQ-CBR	-2.60	1.35	1.50
16	D	201	SQD	C37-C36	-2.54	1.33	1.51
16	D	201	SQD	C4-C3	-2.53	1.45	1.52
10	C	301	HEM	CMA-C3A	2.51	1.56	1.51
17	G	101	BCR	C11-C10	-2.51	1.35	1.43
17	G	101	BCR	C40-C30	2.49	1.58	1.53
11	B	1001	OPC	CBB-CBC	-2.49	1.37	1.51
13	A	501	QNO	C5-C6	-2.48	1.38	1.42
10	A	301	HEM	C1A-CHA	-2.48	1.34	1.41
16	D	201	SQD	C35-C34	-2.47	1.37	1.51
11	B	1001	OPC	OCC-CBK	2.46	1.29	1.22
11	B	1001	OPC	CAQ-CAR	-2.45	1.37	1.51
14	B	201	CLA	CAA-C2A	-2.44	1.49	1.54
13	A	501	QNO	OH-N1	2.44	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1001	OPC	CAR-CAS	-2.41	1.38	1.51
16	D	201	SQD	C1-C2	2.41	1.59	1.52
11	A	1002	OPC	CAG-NAF	-2.39	1.43	1.51
12	A	1103	UMQ	O5'-C1'	2.37	1.47	1.41
11	B	1001	OPC	CBQ-CBR	-2.37	1.36	1.50
11	B	1001	OPC	CBC-CBD	-2.36	1.38	1.51
14	B	201	CLA	C3D-CAD	2.34	1.52	1.46
14	B	201	CLA	C1B-NB	2.33	1.37	1.35
17	G	101	BCR	C15-C14	-2.32	1.36	1.43
12	A	1102	UMQ	C3-C4	2.30	1.58	1.52
10	C	301	HEM	C4D-C3D	2.28	1.47	1.42
10	A	301	HEM	C2A-C3A	-2.25	1.31	1.37
17	G	101	BCR	C35-C13	2.25	1.55	1.50
11	B	1001	OPC	CBT-CBS	-2.24	1.37	1.50
16	D	201	SQD	C32-C31	-2.21	1.39	1.51
16	D	201	SQD	C34-C33	-2.21	1.39	1.51
12	A	1103	UMQ	O5-C1	2.21	1.47	1.41
17	G	101	BCR	C17-C18	2.19	1.38	1.35
10	C	301	HEM	CMB-C2B	2.19	1.56	1.51
10	A	303	HEM	C4A-CHB	-2.18	1.34	1.41
11	A	1002	OPC	CBC-CBD	-2.17	1.39	1.51
10	C	301	HEM	C2A-C3A	-2.17	1.31	1.37
14	B	201	CLA	C1B-CHB	2.16	1.47	1.41
12	C	1101	UMQ	O5-C1	2.15	1.47	1.41
12	A	1102	UMQ	C4-C5	2.14	1.57	1.53
10	A	302	HEM	CMC-C2C	2.14	1.56	1.51
12	A	1102	UMQ	C4'-C5'	2.12	1.58	1.52
10	C	301	HEM	C4B-NB	2.11	1.40	1.36
12	C	1101	UMQ	O3'-C3'	2.10	1.47	1.43
12	C	1101	UMQ	C6'-C5'	2.10	1.58	1.51
14	B	201	CLA	C1C-NC	-2.08	1.34	1.37
17	G	101	BCR	C10-C9	-2.05	1.33	1.35
16	D	201	SQD	C38-C37	-2.04	1.33	1.49
10	A	303	HEM	C3C-CAC	2.03	1.52	1.47
10	C	301	HEM	C1A-CHA	-2.03	1.35	1.41

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C7-C8-C9	28.81	169.77	126.23
17	G	101	BCR	C24-C23-C22	25.52	164.79	126.23
17	G	101	BCR	C8-C7-C6	16.10	172.42	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C23-C24-C25	14.56	168.11	127.20
16	D	201	SQD	O4-C4-C3	13.41	141.36	110.35
16	D	201	SQD	O3-C3-C4	-12.40	81.67	110.35
12	A	1104	UMQ	O1'-C1'-C2'	12.10	127.19	108.30
16	D	201	SQD	C18-C17-C16	12.06	175.67	114.42
16	D	201	SQD	O7-S-C6	11.35	120.43	106.94
14	B	201	CLA	CMB-C2B-C1B	11.25	145.75	128.46
14	B	201	CLA	C4A-NA-C1A	11.20	111.74	106.71
16	D	201	SQD	C17-C16-C15	11.11	170.85	114.42
10	A	303	HEM	CBD-CAD-C3D	10.96	132.67	112.48
12	A	1102	UMQ	CA-O1'-C1'	10.44	131.15	113.84
16	D	201	SQD	C12-C11-C10	9.83	164.35	114.42
17	G	101	BCR	C33-C5-C6	-9.76	113.57	124.53
12	A	1103	UMQ	CA-O1'-C1'	9.54	129.66	113.84
12	C	1101	UMQ	C1'-O5'-C5'	-9.39	95.27	113.69
11	A	1002	OPC	CAA-NAF-CAE	-9.20	85.31	108.97
16	D	201	SQD	C13-C12-C11	8.68	158.51	114.42
12	C	1101	UMQ	O1'-C1'-C2'	8.67	121.84	108.30
12	A	1102	UMQ	O1'-C1'-C2'	8.51	121.59	108.30
10	A	302	HEM	CAA-CBA-CGA	8.39	126.74	112.67
16	D	201	SQD	C22-C21-C20	8.24	175.99	113.42
10	A	301	HEM	C4C-C3C-C2C	7.97	112.47	106.90
11	A	1002	OPC	CAA-NAF-CBG	-7.89	88.70	108.97
16	D	201	SQD	O47-C7-C8	7.40	127.44	111.50
16	D	201	SQD	O6-C1-C2	7.34	119.76	108.30
16	D	201	SQD	O9-S-C6	7.24	115.55	106.94
13	A	501	QNO	O41-C4-C5	7.19	125.29	116.31
17	G	101	BCR	C3-C4-C5	-7.04	101.50	114.08
12	A	1104	UMQ	O2'-C2'-C1'	7.03	127.13	110.05
10	A	302	HEM	CBA-CAA-C2A	-6.98	99.62	112.49
10	A	302	HEM	C4C-C3C-C2C	6.81	111.65	106.90
12	C	1101	UMQ	O5'-C1'-C2'	6.73	124.59	110.35
12	A	1102	UMQ	C1'-C2'-C3'	6.71	123.98	110.00
12	C	1101	UMQ	O2'-C2'-C1'	6.69	126.31	110.05
12	A	1103	UMQ	O1-C4'-C3'	-6.68	89.51	107.28
17	G	101	BCR	C15-C14-C13	-6.46	118.09	127.31
17	G	101	BCR	C32-C1-C6	-6.45	99.84	110.30
14	B	201	CLA	CED-O2D-CGD	-6.36	101.54	115.94
12	A	1103	UMQ	O1'-C1'-C2'	6.24	118.05	108.30
13	A	501	QNO	C21-C2-C3	-6.24	110.04	120.74
14	B	201	CLA	CBC-CAC-C3C	-6.12	95.55	112.43
12	C	1101	UMQ	O2'-C2'-C3'	6.11	124.48	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1104	UMQ	C1'-C2'-C3'	6.05	122.60	110.00
17	G	101	BCR	C1-C6-C5	-6.01	114.15	122.61
10	C	301	HEM	C1D-C2D-C3D	-5.91	102.89	107.00
14	B	201	CLA	CMB-C2B-C3B	-5.81	113.80	124.68
14	B	201	CLA	O2D-CGD-CBD	5.76	121.51	111.27
14	B	201	CLA	CHB-C4A-NA	5.74	132.45	124.51
11	A	1002	OPC	CAA-NAF-CAG	-5.73	86.46	109.92
11	B	1001	OPC	OAN-CAO-CAP	5.70	123.79	111.50
12	A	1104	UMQ	CA-O1'-C1'	5.63	123.18	113.84
14	B	201	CLA	CAA-CBA-CGA	-5.58	96.95	113.25
14	B	201	CLA	C4-C3-C5	5.54	124.60	115.27
14	B	201	CLA	C2C-C1C-NC	5.49	115.11	109.97
12	A	1103	UMQ	C1-O5-C5	5.45	124.39	113.69
14	B	201	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
11	B	1001	OPC	CAA-NAF-CBG	5.32	122.65	108.97
12	C	1101	UMQ	C6'-C5'-C4'	5.31	128.78	113.33
17	G	101	BCR	C16-C15-C14	5.24	134.21	123.47
10	A	303	HEM	CMA-C3A-C4A	-5.18	120.51	128.46
17	G	101	BCR	C20-C19-C18	-5.13	112.01	126.42
14	B	201	CLA	C3C-C4C-NC	5.10	116.29	110.57
11	B	1001	OPC	OAN-CAO-OAD	-5.06	111.48	123.70
17	G	101	BCR	C37-C22-C23	5.04	126.02	118.08
11	B	1001	OPC	CBU-CBT-CBS	4.98	140.96	112.43
12	A	1103	UMQ	O5'-C1'-O1'	4.97	121.75	109.97
12	C	1101	UMQ	C4-C3-C2	-4.93	102.21	110.82
11	A	1002	OPC	OAN-CAO-CAP	4.89	122.03	111.50
11	A	1002	OPC	CBI-CAM-CAL	-4.87	100.28	111.79
11	A	1002	OPC	CAQ-CAR-CAS	4.86	139.10	114.42
10	A	303	HEM	CAD-CBD-CGD	4.71	120.58	112.67
10	A	301	HEM	CBA-CAA-C2A	-4.70	103.82	112.49
12	C	1101	UMQ	O2-C2-C3	4.69	121.20	110.35
17	G	101	BCR	C33-C5-C4	4.67	122.59	113.62
12	A	1103	UMQ	O5'-C1'-C2'	4.65	120.19	110.35
12	A	1103	UMQ	C1'-C2'-C3'	4.60	119.58	110.00
16	D	201	SQD	O5-C5-C4	4.60	118.05	109.69
12	C	1101	UMQ	C2'-C3'-C4'	-4.60	99.18	109.68
17	G	101	BCR	C31-C1-C6	-4.59	102.86	110.30
16	D	201	SQD	O2-C2-C1	4.58	121.17	110.05
16	D	201	SQD	O47-C7-O49	-4.52	112.77	123.70
16	D	201	SQD	O5-C1-O6	4.50	120.63	109.97
11	B	1001	OPC	CAA-NAF-CAE	-4.47	97.49	108.97
16	D	201	SQD	C14-C13-C12	4.46	137.08	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C11-C10-C9	4.44	133.64	127.31
16	D	201	SQD	O8-S-C6	-4.39	98.75	105.74
14	B	201	CLA	O2A-CGA-CBA	4.39	125.68	111.91
12	A	1102	UMQ	O1-C1-C2	4.35	119.36	108.10
14	B	201	CLA	O2A-C1-C2	4.28	119.89	108.64
12	C	1101	UMQ	C3'-C4'-C5'	4.24	120.65	110.93
12	A	1102	UMQ	O5'-C1'-O1'	4.23	120.00	109.97
12	A	1103	UMQ	O2'-C2'-C1'	4.22	120.31	110.05
12	A	1103	UMQ	O2'-C2'-C3'	4.21	120.09	110.35
11	B	1001	OPC	CAQ-CAP-CAO	4.21	128.93	113.62
16	D	201	SQD	C15-C14-C13	4.12	135.36	114.42
12	A	1103	UMQ	O1-C4'-C5'	4.12	120.73	109.45
11	A	1002	OPC	CBG-NAF-CAE	4.10	119.52	108.97
12	A	1104	UMQ	O5'-C1'-C2'	4.09	119.01	110.35
11	B	1001	OPC	CBO-CBP-CBQ	4.06	131.47	113.79
11	B	1001	OPC	CBM-CBL-CBK	4.02	128.25	113.62
17	G	101	BCR	C20-C21-C22	4.01	133.03	127.31
11	A	1002	OPC	CAR-CAS-CAT	3.99	134.68	114.42
14	B	201	CLA	C4D-C3D-CAD	3.95	110.67	108.47
11	A	1002	OPC	CAQ-CAP-CAO	3.95	127.98	113.62
12	A	1102	UMQ	O2'-C2'-C1'	3.93	119.59	110.05
17	G	101	BCR	C34-C9-C10	-3.91	117.45	122.92
10	A	301	HEM	CBD-CAD-C3D	-3.90	105.28	112.48
10	C	301	HEM	CBD-CAD-C3D	-3.83	105.42	112.48
11	B	1001	OPC	CAM-OAN-CAO	3.82	127.20	117.79
11	A	1002	OPC	OAI-CAH-CAG	3.82	129.26	109.16
12	C	1101	UMQ	C1-O5-C5	3.82	121.18	113.69
16	D	201	SQD	C44-O6-C1	-3.82	106.28	113.74
10	A	301	HEM	CMA-C3A-C4A	-3.81	122.61	128.46
12	A	1102	UMQ	O5'-C1'-C2'	3.75	118.29	110.35
10	C	301	HEM	CAD-CBD-CGD	3.74	118.95	112.67
16	D	201	SQD	O8-S-O9	-3.73	102.15	111.27
11	B	1001	OPC	CAE-NAF-CAG	3.71	125.11	109.92
12	A	1102	UMQ	O3-C3-C4	3.71	118.93	110.35
17	G	101	BCR	C12-C13-C14	-3.68	113.30	118.94
12	A	1103	UMQ	O3'-C3'-C2'	3.67	118.84	110.35
12	C	1101	UMQ	C3-C4-C5	-3.67	103.69	110.24
10	A	302	HEM	CAD-C3D-C2D	-3.66	116.74	127.25
16	D	201	SQD	O6-C44-C45	3.64	119.68	110.90
11	A	1002	OPC	CAH-CAG-NAF	3.56	127.66	115.78
14	B	201	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
11	A	1002	OPC	OAN-CAM-CBI	3.55	121.25	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	501	QNO	C61-C6-C5	3.53	123.81	119.41
10	A	303	HEM	C4A-C3A-C2A	3.52	109.45	107.00
12	A	1102	UMQ	O3-C3-C2	-3.52	102.20	110.35
11	B	1001	OPC	OBJ-CBK-OCC	-3.50	114.75	123.59
10	A	303	HEM	C1D-C2D-C3D	3.49	109.43	107.00
10	A	302	HEM	CBD-CAD-C3D	-3.49	106.05	112.48
16	D	201	SQD	C35-C34-C33	3.47	132.03	114.42
11	A	1002	OPC	CBV-CBU-CBT	-3.42	98.89	113.79
16	D	201	SQD	C16-C15-C14	3.41	131.75	114.42
10	A	303	HEM	CAD-C3D-C2D	-3.40	117.46	127.25
17	G	101	BCR	C27-C26-C25	-3.40	117.80	122.73
11	B	1001	OPC	CBA-CBB-CBC	3.39	131.62	114.42
14	B	201	CLA	OBD-CAD-C3D	3.38	133.60	127.98
11	A	1002	OPC	CBA-CBB-CBC	3.38	131.59	114.42
11	B	1001	OPC	CBP-CBO-CBN	3.35	131.45	114.42
12	A	1102	UMQ	C3-C4-C5	3.35	116.22	110.24
14	B	201	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
12	C	1101	UMQ	O3-C3-C2	3.34	118.06	110.35
16	D	201	SQD	C33-C32-C31	3.33	131.34	114.42
14	B	201	CLA	C16-C15-C13	-3.33	105.16	115.92
14	B	201	CLA	C3B-C4B-NB	3.30	113.47	109.21
14	B	201	CLA	C1-O2A-CGA	-3.29	107.80	116.44
11	A	1002	OPC	CBP-CBQ-CBR	3.28	131.25	112.43
12	A	1102	UMQ	C1-C2-C3	3.21	116.68	110.00
16	D	201	SQD	C34-C33-C32	3.21	130.72	114.42
14	B	201	CLA	CAA-C2A-C3A	-3.21	104.00	112.78
10	A	303	HEM	CMD-C2D-C3D	-3.19	118.93	124.94
11	B	1001	OPC	CAQ-CAR-CAS	3.14	130.36	114.42
16	D	201	SQD	C32-C31-C30	3.14	130.35	114.42
12	A	1102	UMQ	O1-C4'-C5'	3.13	118.04	109.45
12	C	1101	UMQ	O3'-C3'-C4'	3.10	118.15	109.94
16	D	201	SQD	C1-O5-C5	-3.08	107.65	113.69
12	C	1101	UMQ	O3-C3-C4	3.05	117.40	110.35
14	B	201	CLA	CAC-C3C-C2C	3.04	132.73	127.53
10	A	302	HEM	C3B-C4B-NB	3.03	113.13	109.21
12	A	1102	UMQ	O5-C5-C4	3.02	115.18	109.69
12	A	1102	UMQ	O1'-CA-CB	3.02	120.13	109.56
10	A	301	HEM	C4A-C3A-C2A	3.02	109.09	107.00
10	A	303	HEM	C4C-C3C-C2C	3.01	109.00	106.90
17	G	101	BCR	C39-C30-C25	3.01	115.18	110.30
13	A	501	QNO	O41-C4-C3	-2.99	112.40	121.17
17	G	101	BCR	C21-C20-C19	2.99	132.55	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C36-C18-C17	2.99	127.11	122.92
14	B	201	CLA	C3D-CAD-CBD	-2.99	103.67	107.61
12	A	1102	UMQ	CI-CH-CG	2.98	129.58	114.42
11	B	1001	OPC	CAR-CAQ-CAP	2.98	123.90	113.19
11	B	1001	OPC	CBO-CBN-CBM	2.98	129.55	114.42
11	A	1002	OPC	CBN-CBM-CBL	-2.97	102.51	113.19
14	B	201	CLA	O1A-CGA-CBA	-2.97	112.16	123.73
16	D	201	SQD	C4-C3-C2	-2.95	105.67	110.82
17	G	101	BCR	C37-C22-C21	-2.93	118.81	122.92
12	C	1101	UMQ	C1-C2-C3	-2.92	103.92	110.00
12	A	1103	UMQ	O5-C5-C4	2.90	114.96	109.69
11	A	1002	OPC	CAM-OAN-CAO	2.89	124.91	117.79
11	B	1001	OPC	CBI-CAM-CAL	-2.89	104.96	111.79
11	A	1002	OPC	CBY-CBX-CBW	-2.88	99.80	114.42
12	A	1104	UMQ	O1'-CA-CB	2.86	119.59	109.56
11	B	1001	OPC	CAA-NAF-CAG	-2.86	98.22	109.92
11	A	1002	OPC	CAZ-CAY-CAX	2.82	126.09	113.79
11	B	1001	OPC	CAH-CAG-NAF	2.78	125.07	115.78
17	G	101	BCR	C36-C18-C19	-2.77	113.71	118.08
17	G	101	BCR	C34-C9-C8	2.74	122.39	118.08
17	G	101	BCR	C32-C1-C2	2.72	119.77	108.91
14	B	201	CLA	CBA-CAA-C2A	-2.71	105.87	113.86
10	A	303	HEM	CMA-C3A-C2A	2.71	130.04	124.94
16	D	201	SQD	O48-C23-C24	2.69	120.33	111.91
12	C	1101	UMQ	O1-C4'-C5'	2.68	116.78	109.45
11	B	1001	OPC	OAI-CAH-CAG	2.68	123.23	109.16
17	G	101	BCR	C2-C1-C6	2.65	114.56	110.48
10	C	301	HEM	CMD-C2D-C1D	2.64	132.52	128.46
14	B	201	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
11	B	1001	OPC	CBG-NAF-CAE	-2.61	102.27	108.97
12	A	1102	UMQ	O2-C2-C1	2.60	116.37	110.05
12	A	1102	UMQ	O2'-C2'-C3'	2.60	116.35	110.35
14	B	201	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
12	A	1102	UMQ	C2'-C3'-C4'	2.58	115.57	109.68
14	B	201	CLA	CMA-C3A-C4A	-2.56	104.89	111.77
17	G	101	BCR	C16-C17-C18	-2.56	123.66	127.31
14	B	201	CLA	C14-C13-C12	2.54	120.48	111.29
17	G	101	BCR	C29-C30-C25	-2.54	106.58	110.48
16	D	201	SQD	C46-O48-C23	2.53	126.47	117.12
17	G	101	BCR	C10-C11-C12	-2.52	115.36	123.22
12	A	1104	UMQ	C1-O1-C4'	2.48	124.11	117.96
14	B	201	CLA	O2D-CGD-O1D	-2.47	119.01	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	201	CLA	C1D-CHD-C4C	2.46	125.81	122.56
17	G	101	BCR	C23-C22-C21	-2.46	115.17	118.94
12	A	1103	UMQ	O5-C1-C2	2.44	115.52	110.35
14	B	201	CLA	CGD-CBD-CAD	-2.44	102.83	110.73
11	A	1002	OPC	CBG-NAF-CAG	2.42	119.83	109.92
14	B	201	CLA	C12-C11-C10	2.42	124.35	113.24
12	A	1103	UMQ	O2-C2-C1	2.42	115.91	110.05
12	A	1103	UMQ	O4-C4-C3	2.41	115.92	110.35
10	C	301	HEM	CBA-CAA-C2A	2.40	116.92	112.49
11	A	1002	OPC	CAE-NAF-CAG	2.40	119.74	109.92
14	B	201	CLA	OBD-CAD-CBD	-2.39	122.48	125.89
11	B	1001	OPC	CBP-CBQ-CBR	2.39	126.14	112.43
10	A	301	HEM	CAA-CBA-CGA	2.38	116.66	112.67
11	B	1001	OPC	CBZ-CBY-CBX	2.36	126.42	114.42
11	A	1002	OPC	CBB-CBC-CBD	2.33	126.26	114.42
16	D	201	SQD	O48-C23-O10	-2.33	117.71	123.59
17	G	101	BCR	C2-C3-C4	2.32	116.55	111.38
12	C	1101	UMQ	O5-C5-C6	2.30	112.17	106.44
12	A	1103	UMQ	O3'-C3'-C4'	-2.30	103.85	109.94
11	B	1001	OPC	OBJ-CBI-CAM	2.29	115.11	108.43
10	A	301	HEM	CMC-C2C-C3C	2.28	128.94	124.68
10	A	301	HEM	CMD-C2D-C1D	2.26	131.93	128.46
10	A	303	HEM	C3B-C4B-NB	2.25	112.12	109.21
12	A	1102	UMQ	O5'-C5'-C4'	2.25	114.50	109.75
11	A	1002	OPC	OAD-CAO-CAP	-2.25	114.96	123.73
17	G	101	BCR	C35-C13-C12	2.24	121.61	118.08
12	A	1104	UMQ	C1-O5-C5	2.24	118.09	113.69
11	B	1001	OPC	CBW-CBV-CBU	2.23	125.74	114.42
17	G	101	BCR	C24-C25-C26	-2.21	116.12	121.46
17	G	101	BCR	C11-C12-C13	2.19	132.56	126.42
11	A	1002	OPC	OBJ-CBK-CBL	2.19	118.77	111.91
14	B	201	CLA	C5-C3-C2	-2.19	116.69	121.12
12	A	1104	UMQ	O3'-C3'-C4'	2.16	115.67	109.94
12	C	1101	UMQ	O1-C1-C2	2.15	113.67	108.10
16	D	201	SQD	C36-C35-C34	2.15	125.32	114.42
16	D	201	SQD	C45-O47-C7	2.15	123.07	117.79
14	B	201	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
12	A	1104	UMQ	C1-C2-C3	2.09	114.34	110.00
11	A	1002	OPC	CBQ-CBR-CBS	-2.09	108.72	124.73
13	A	501	QNO	C3-C2-N1	-2.08	116.66	118.94
11	A	1002	OPC	CBM-CBL-CBK	-2.08	106.06	113.62
12	C	1101	UMQ	O4-C4-C3	2.07	115.14	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	201	SQD	C19-C18-C17	2.07	124.91	114.42
14	B	201	CLA	C3A-C2A-C1A	2.06	104.42	101.34
14	B	201	CLA	C7-C6-C5	2.05	118.93	113.36
16	D	201	SQD	O9-S-O7	-2.05	106.86	113.95
11	B	1001	OPC	CAT-CAU-CAV	2.04	124.15	112.43
10	A	302	HEM	CMC-C2C-C3C	2.04	128.49	124.68
12	A	1102	UMQ	O5'-C5'-C6'	2.02	111.45	106.44
11	A	1002	OPC	OBJ-CBI-CAM	2.02	114.30	108.43
12	A	1104	UMQ	O4-C4-C5	2.01	114.28	109.30
12	A	1104	UMQ	O5-C5-C4	2.00	113.33	109.69

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1104	UMQ	C2'
12	A	1104	UMQ	C1'
16	D	201	SQD	C3
16	D	201	SQD	C5
16	D	201	SQD	C4
13	A	501	QNO	C2
12	A	1103	UMQ	C2'
12	A	1103	UMQ	C1'
12	A	1102	UMQ	C2'
12	A	1102	UMQ	C1'
14	B	201	CLA	C8
14	B	201	CLA	NC
14	B	201	CLA	ND
14	B	201	CLA	NA
12	C	1101	UMQ	C2'
12	C	1101	UMQ	C1'

All (149) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	G	101	BCR	C7-C8-C9-C34
17	G	101	BCR	C21-C22-C23-C24
17	G	101	BCR	C37-C22-C23-C24
11	A	1002	OPC	NAF-CAG-CAH-OAI
11	A	1002	OPC	CBO-CBP-CBQ-CBR
12	A	1104	UMQ	O5'-C1'-O1'-CA
12	A	1104	UMQ	CB-CA-O1'-C1'
16	D	201	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
16	D	201	SQD	O49-C7-O47-C45
16	D	201	SQD	C8-C7-O47-C45
16	D	201	SQD	O5-C5-C6-S
10	A	303	HEM	C2A-CAA-CBA-CGA
10	A	303	HEM	C2D-C3D-CAD-CBD
12	A	1103	UMQ	O5'-C1'-O1'-CA
12	A	1103	UMQ	CB-CA-O1'-C1'
12	A	1102	UMQ	C3'-C4'-O1-C1
12	A	1102	UMQ	O5'-C1'-O1'-CA
14	B	201	CLA	C1A-C2A-CAA-CBA
14	B	201	CLA	C3A-C2A-CAA-CBA
14	B	201	CLA	O2A-C1-C2-C3
11	B	1001	OPC	CAH-OAI-PAJ-OAK
11	B	1001	OPC	CAH-OAI-PAJ-OBH
11	B	1001	OPC	CAH-OAI-PAJ-OAB
11	B	1001	OPC	NAF-CAG-CAH-OAI
11	B	1001	OPC	CBO-CBP-CBQ-CBR
12	C	1101	UMQ	O5'-C1'-O1'-CA
12	C	1101	UMQ	CB-CA-O1'-C1'
14	B	201	CLA	CBD-CGD-O2D-CED
14	B	201	CLA	O1D-CGD-O2D-CED
12	A	1104	UMQ	O5-C1-O1-C4'
11	B	1001	OPC	OAD-CAO-OAN-CAM
16	D	201	SQD	C24-C23-O48-C46
11	B	1001	OPC	CAP-CAO-OAN-CAM
16	D	201	SQD	C31-C32-C33-C34
16	D	201	SQD	C33-C34-C35-C36
12	A	1103	UMQ	O5-C5-C6-O6
11	B	1001	OPC	CAU-CAV-CAW-CAX
16	D	201	SQD	C13-C14-C15-C16
16	D	201	SQD	C12-C13-C14-C15
12	A	1104	UMQ	O5'-C5'-C6'-O6'
16	D	201	SQD	O10-C23-O48-C46
11	A	1002	OPC	CAQ-CAR-CAS-CAT
11	A	1002	OPC	CAZ-CBA-CBB-CBC
11	A	1002	OPC	CAY-CAZ-CBA-CBB
12	A	1104	UMQ	CH-CI-CJ-CK
14	B	201	CLA	C3-C5-C6-C7
12	A	1102	UMQ	O5'-C5'-C6'-O6'
12	A	1104	UMQ	O5-C5-C6-O6
12	C	1101	UMQ	O5'-C5'-C6'-O6'
12	A	1104	UMQ	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
12	A	1103	UMQ	C4-C5-C6-O6
13	A	501	QNO	C2-C21-C22-C23
11	B	1001	OPC	CAH-CAG-NAF-CBG
12	A	1104	UMQ	C4-C5-C6-O6
16	D	201	SQD	C2-C1-O6-C44
12	A	1102	UMQ	C2'-C1'-O1'-CA
17	G	101	BCR	C7-C8-C9-C10
14	B	201	CLA	C13-C15-C16-C17
11	B	1001	OPC	CBK-CBL-CBM-CBN
12	C	1101	UMQ	C4'-C5'-C6'-O6'
11	A	1002	OPC	CAH-CAG-NAF-CAA
12	A	1103	UMQ	CH-CI-CJ-CK
14	B	201	CLA	C16-C17-C18-C20
12	A	1104	UMQ	CB-CC-CD-CF
16	D	201	SQD	C44-C45-O47-C7
16	D	201	SQD	C29-C30-C31-C32
12	A	1102	UMQ	C4'-C5'-C6'-O6'
11	B	1001	OPC	CBM-CBN-CBO-CBP
12	A	1103	UMQ	CF-CG-CH-CI
11	A	1002	OPC	CBL-CBM-CBN-CBO
16	D	201	SQD	C15-C16-C17-C18
12	A	1104	UMQ	CG-CH-CI-CJ
11	A	1002	OPC	CBK-CBL-CBM-CBN
12	A	1102	UMQ	CB-CC-CD-CF
11	B	1001	OPC	CAH-CAG-NAF-CAA
12	A	1102	UMQ	CA-CB-CC-CD
12	C	1101	UMQ	CD-CF-CG-CH
16	D	201	SQD	C16-C17-C18-C19
16	D	201	SQD	C10-C11-C12-C13
11	B	1001	OPC	CAZ-CBA-CBB-CBC
12	C	1101	UMQ	CH-CI-CJ-CK
16	D	201	SQD	C27-C28-C29-C30
12	A	1103	UMQ	C3'-C4'-O1-C1
17	G	101	BCR	C1-C6-C7-C8
17	G	101	BCR	C5-C6-C7-C8
17	G	101	BCR	C23-C24-C25-C26
11	A	1002	OPC	CAX-CAY-CAZ-CBA
11	A	1002	OPC	CBY-CBZ-CCA-CCB
12	A	1104	UMQ	CC-CD-CF-CG
16	D	201	SQD	C23-C24-C25-C26
11	B	1001	OPC	CAR-CAS-CAT-CAU
12	A	1104	UMQ	C2'-C1'-O1'-CA

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Mol	Chain	Res	Type	Atoms
11	B	1001	OPC	CAH-CAG-NAF-CAE
13	A	501	QNO	C22-C23-C24-C25
14	B	201	CLA	C16-C17-C18-C19
11	A	1002	OPC	CBV-CBW-CBX-CBY
16	D	201	SQD	C28-C29-C30-C31
12	A	1104	UMQ	CI-CJ-CK-CL
12	A	1102	UMQ	CI-CJ-CK-CL
11	B	1001	OPC	CBT-CBU-CBV-CBW
12	A	1102	UMQ	O5-C5-C6-O6
13	A	501	QNO	C21-C22-C23-C24
14	B	201	CLA	C11-C10-C8-C7
14	B	201	CLA	C8-C10-C11-C12
16	D	201	SQD	C19-C20-C21-C22
12	C	1101	UMQ	CC-CD-CF-CG
12	A	1102	UMQ	CB-CA-O1'-C1'
11	A	1002	OPC	CAL-CAM-CBI-OBJ
12	A	1104	UMQ	CD-CF-CG-CH
16	D	201	SQD	O6-C44-C45-O47
14	B	201	CLA	C5-C6-C7-C8
12	A	1103	UMQ	O5-C1-O1-C4'
12	A	1103	UMQ	CB-CC-CD-CF
17	G	101	BCR	C23-C24-C25-C30
11	B	1001	OPC	CBU-CBV-CBW-CBX
12	A	1103	UMQ	CI-CJ-CK-CL
11	B	1001	OPC	OAK-CAL-CAM-OAN
11	A	1002	OPC	OAN-CAM-CBI-OBJ
12	A	1104	UMQ	CF-CG-CH-CI
12	A	1103	UMQ	C5'-C4'-O1-C1
11	B	1001	OPC	OAK-CAL-CAM-CBI
12	A	1104	UMQ	O1'-CA-CB-CC
11	A	1002	OPC	OAK-CAL-CAM-OAN
10	A	302	HEM	C1A-C2A-CAA-CBA
16	D	201	SQD	O6-C44-C45-C46
11	A	1002	OPC	CAH-CAG-NAF-CAE
11	A	1002	OPC	CAM-CAL-OAK-PAJ
11	A	1002	OPC	CBP-CBQ-CBR-CBS
11	B	1001	OPC	CBP-CBQ-CBR-CBS
12	C	1101	UMQ	CF-CG-CH-CI
16	D	201	SQD	C25-C26-C27-C28
11	A	1002	OPC	OAN-CAO-CAP-CAQ
11	B	1001	OPC	CAS-CAT-CAU-CAV
17	G	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
17	G	101	BCR	C11-C10-C9-C8
16	D	201	SQD	C24-C25-C26-C27
12	A	1102	UMQ	CC-CD-CF-CG
11	B	1001	OPC	CBL-CBK-OBJ-CBI
12	C	1101	UMQ	CG-CH-CI-CJ
11	A	1002	OPC	OAK-CAL-CAM-CBI
11	A	1002	OPC	OCC-CBK-OBJ-CBI
11	A	1002	OPC	CAT-CAU-CAV-CAW
11	A	1002	OPC	CBL-CBK-OBJ-CBI
12	A	1103	UMQ	O1'-CA-CB-CC
12	A	1102	UMQ	CH-CI-CJ-CK
11	A	1002	OPC	CBU-CBV-CBW-CBX
11	B	1001	OPC	CBR-CBS-CBT-CBU
11	B	1001	OPC	OCC-CBK-CBL-CBM
11	B	1001	OPC	OBJ-CBK-CBL-CBM

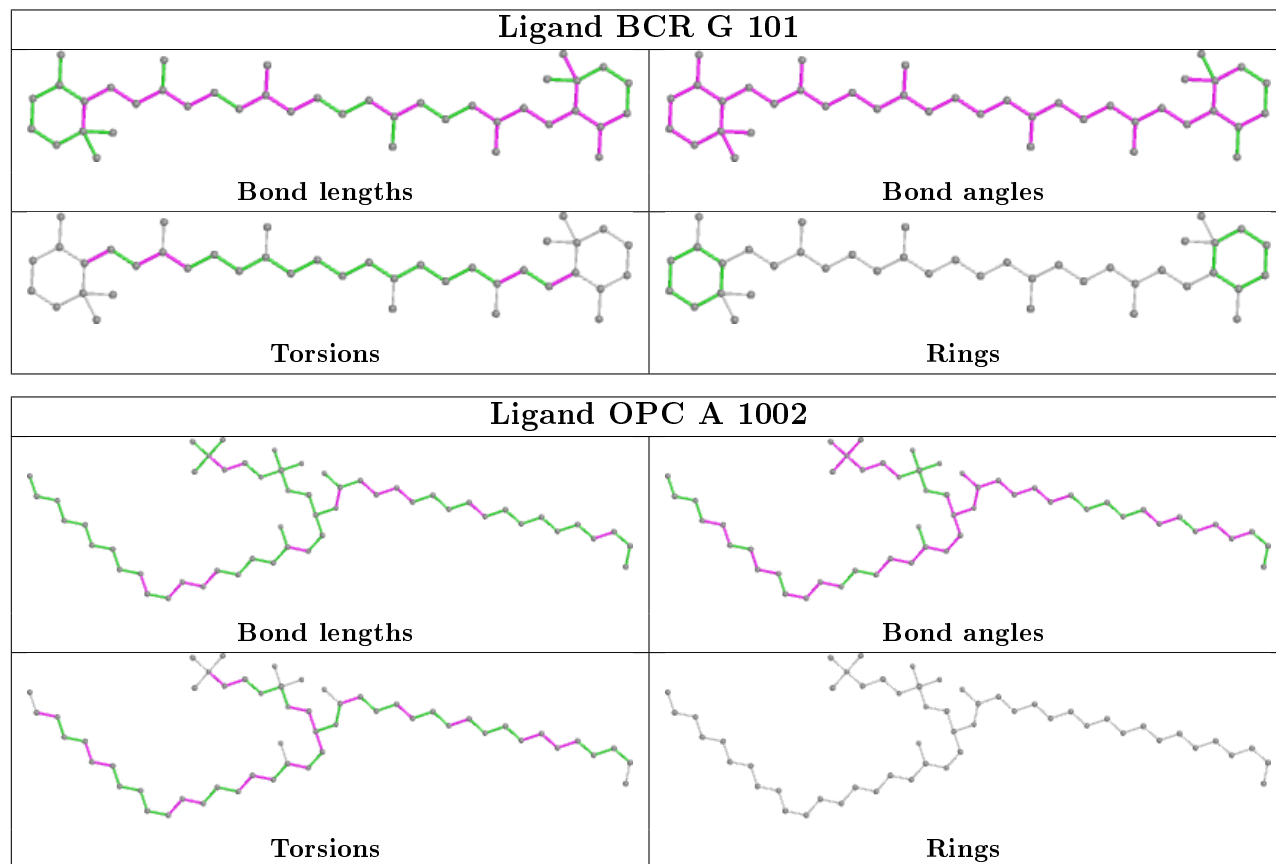
There are no ring outliers.

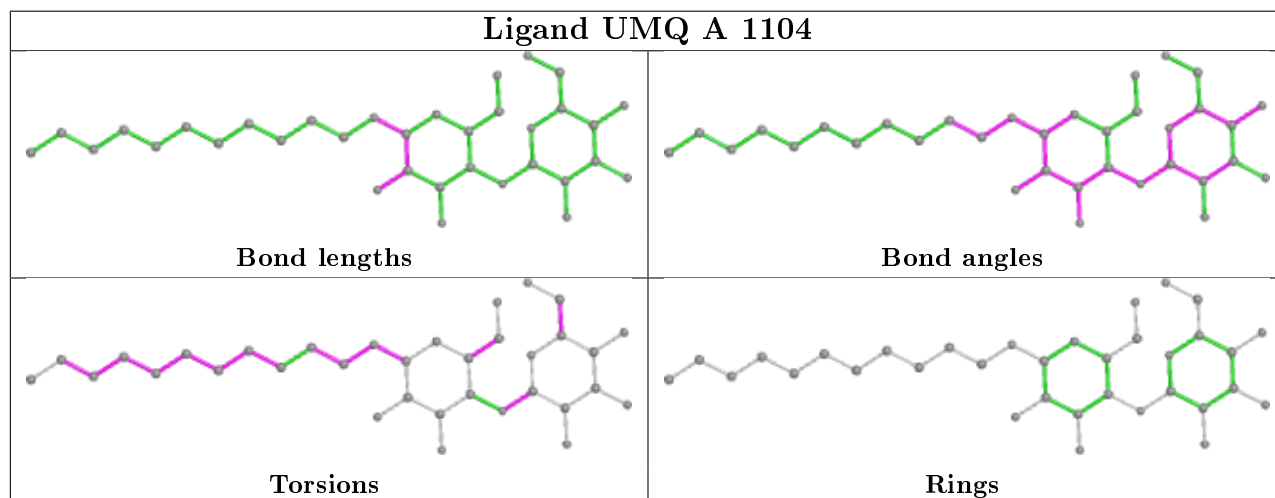
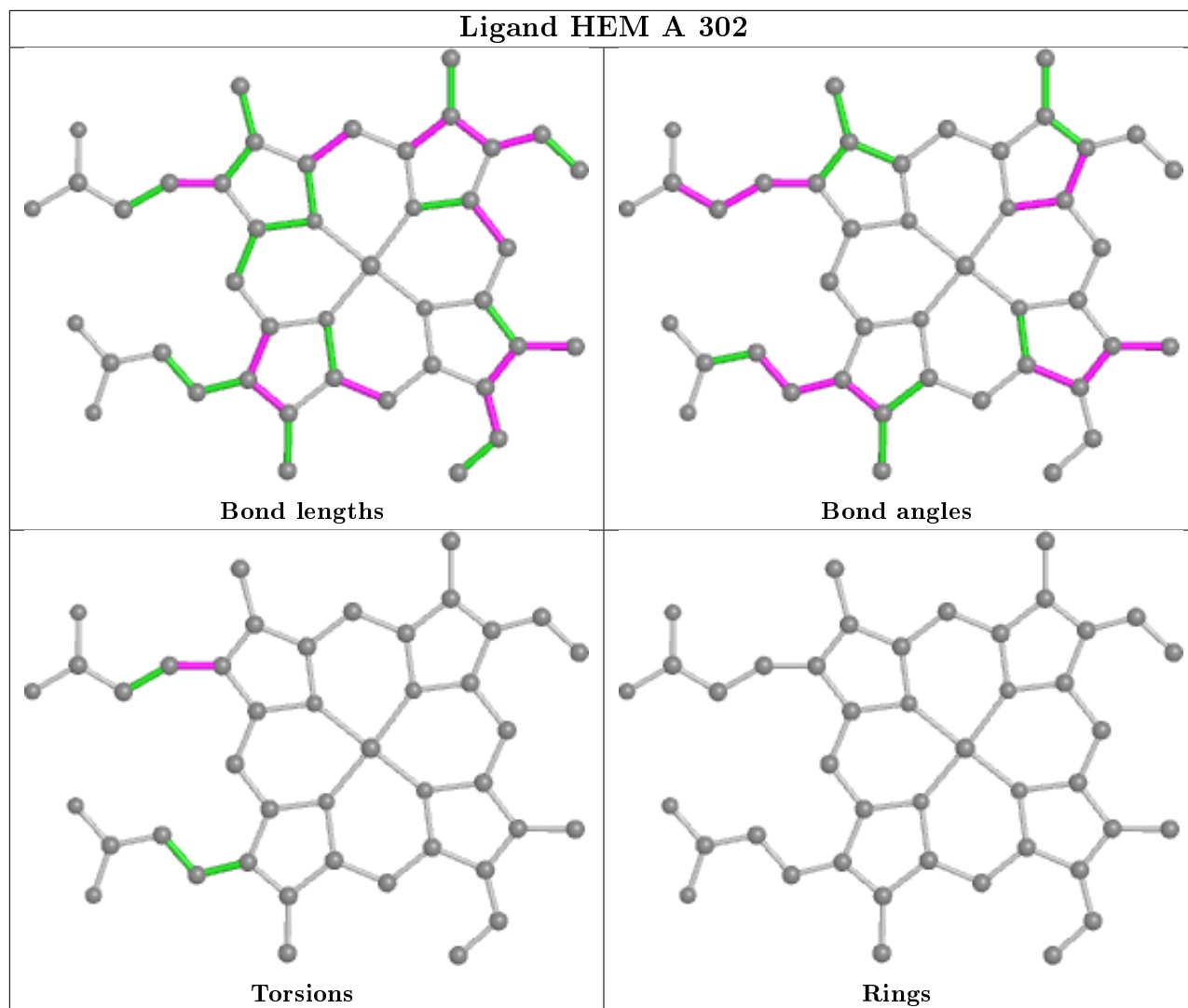
15 monomers are involved in 184 short contacts:

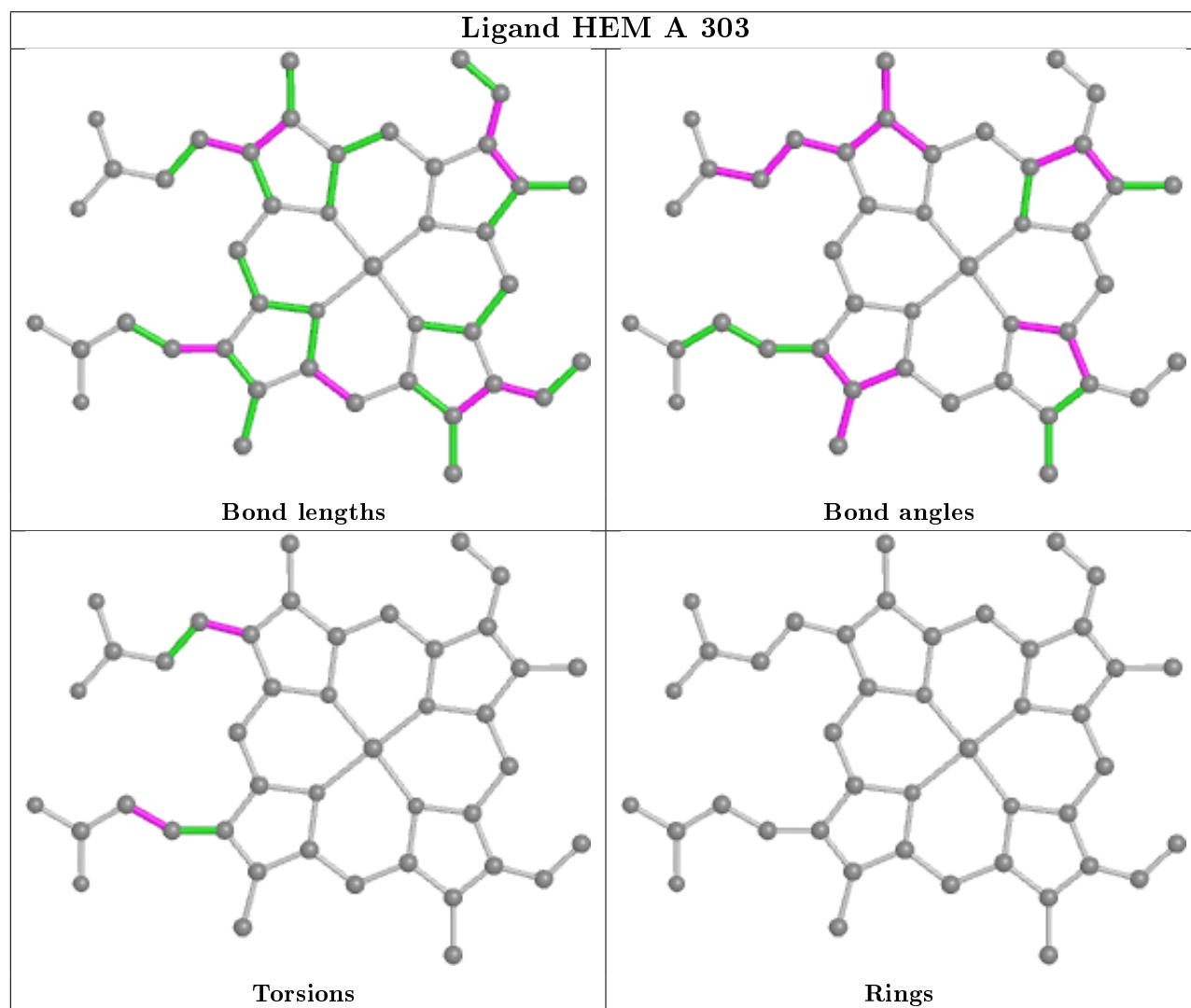
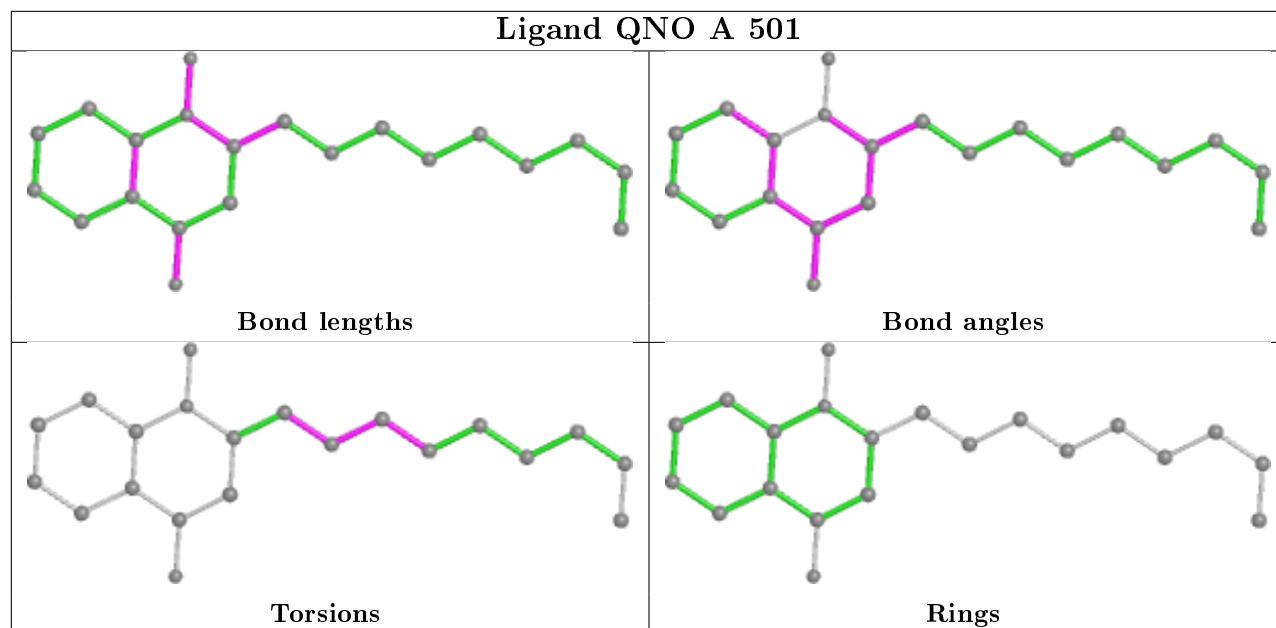
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	101	BCR	12	0
11	A	1002	OPC	27	0
10	A	302	HEM	25	0
12	A	1104	UMQ	2	0
13	A	501	QNO	7	0
15	D	200	FES	3	0
10	A	303	HEM	9	0
12	A	1103	UMQ	2	0
10	A	301	HEM	22	0
12	A	1102	UMQ	7	0
16	D	201	SQD	11	0
14	B	201	CLA	16	0
10	C	301	HEM	22	0
12	C	1101	UMQ	10	0
11	B	1001	OPC	11	0

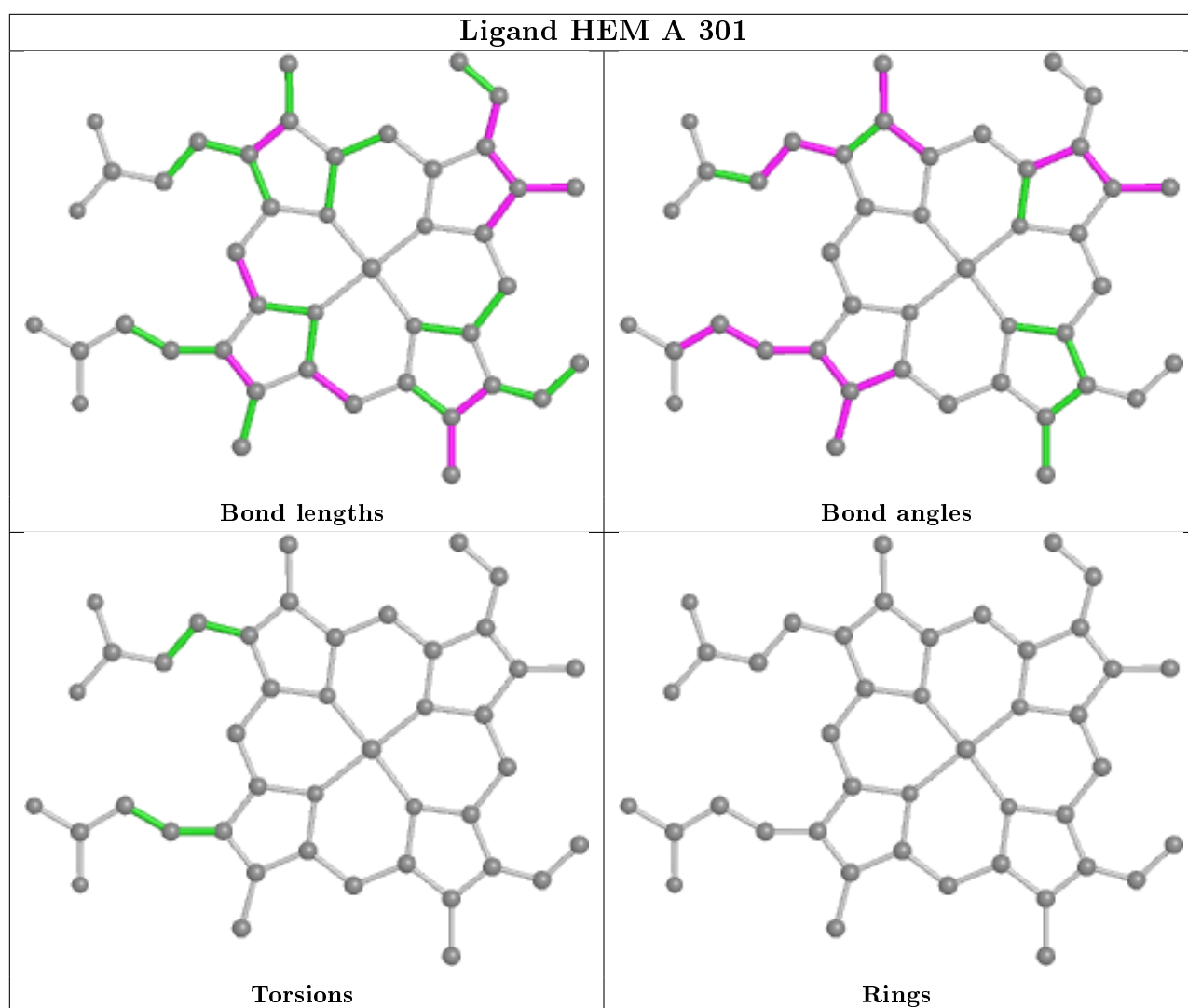
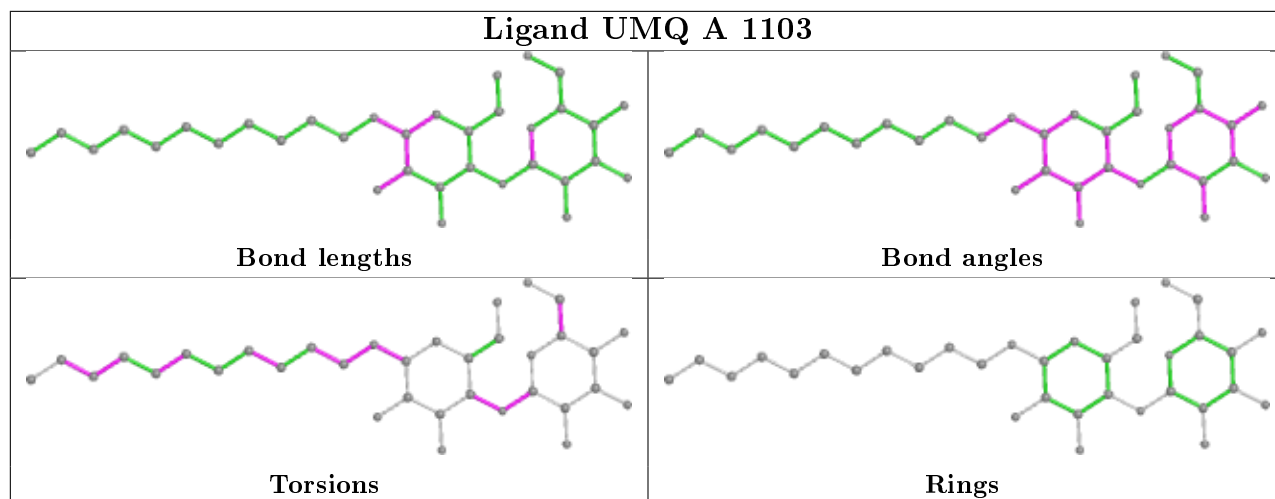
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

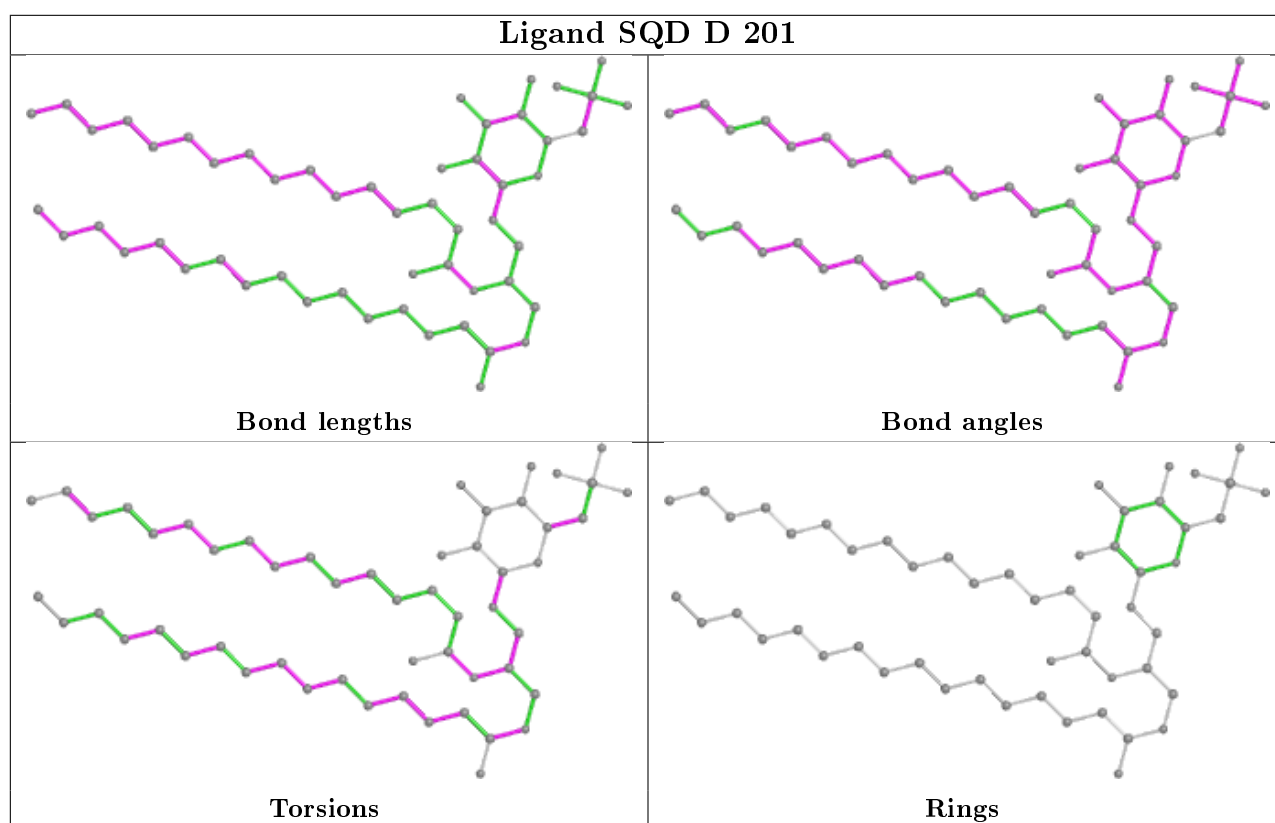
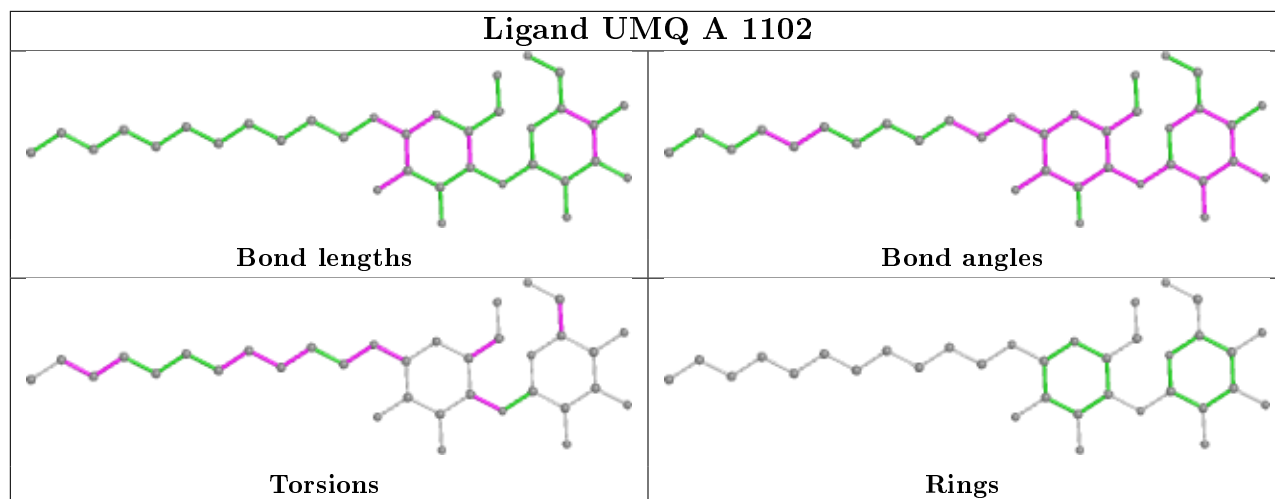
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

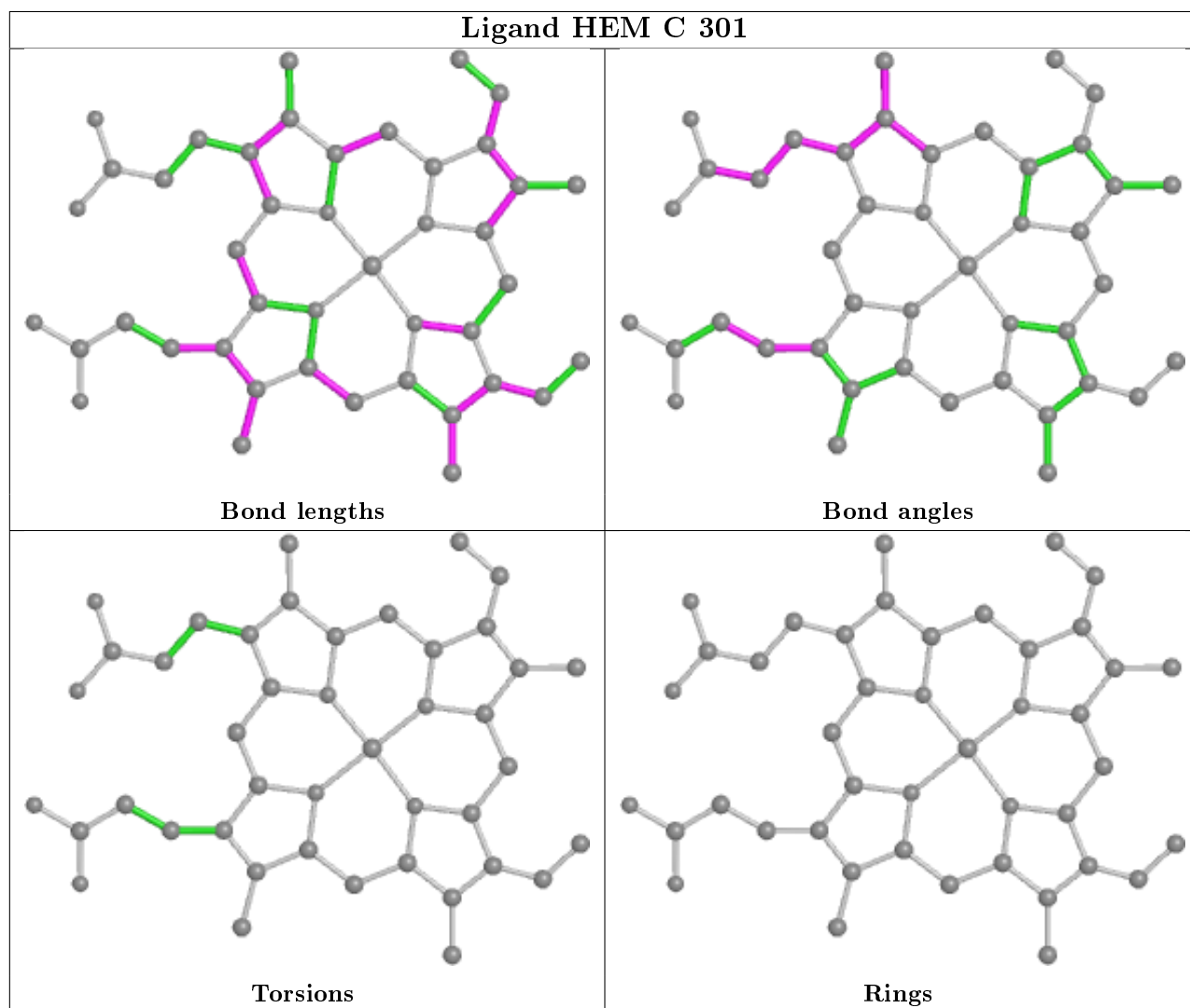
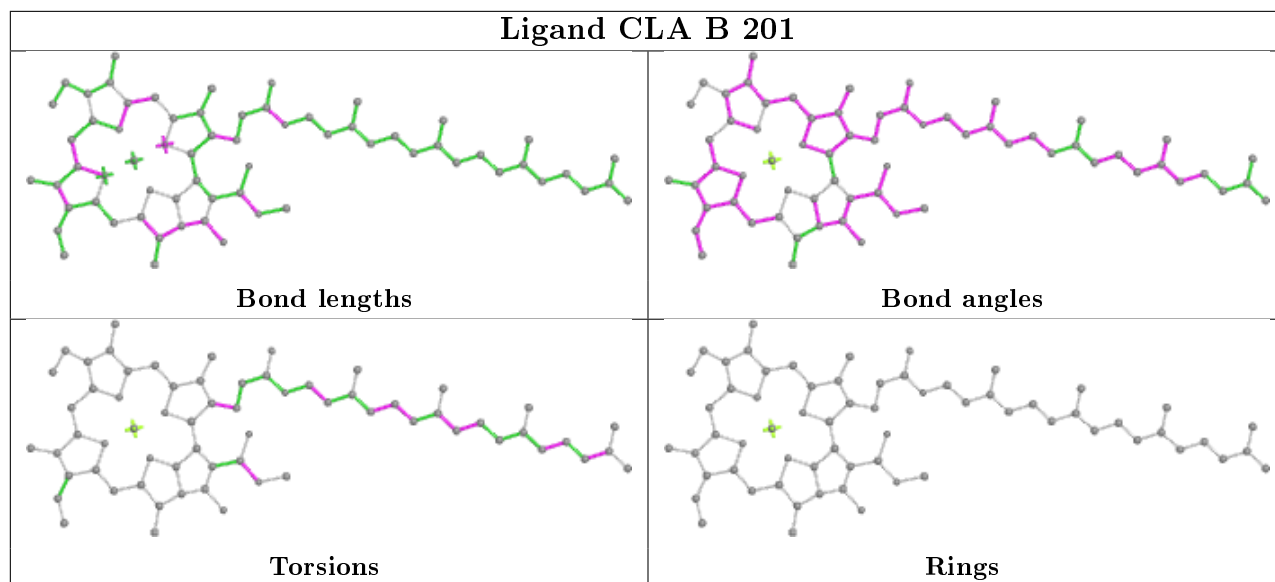


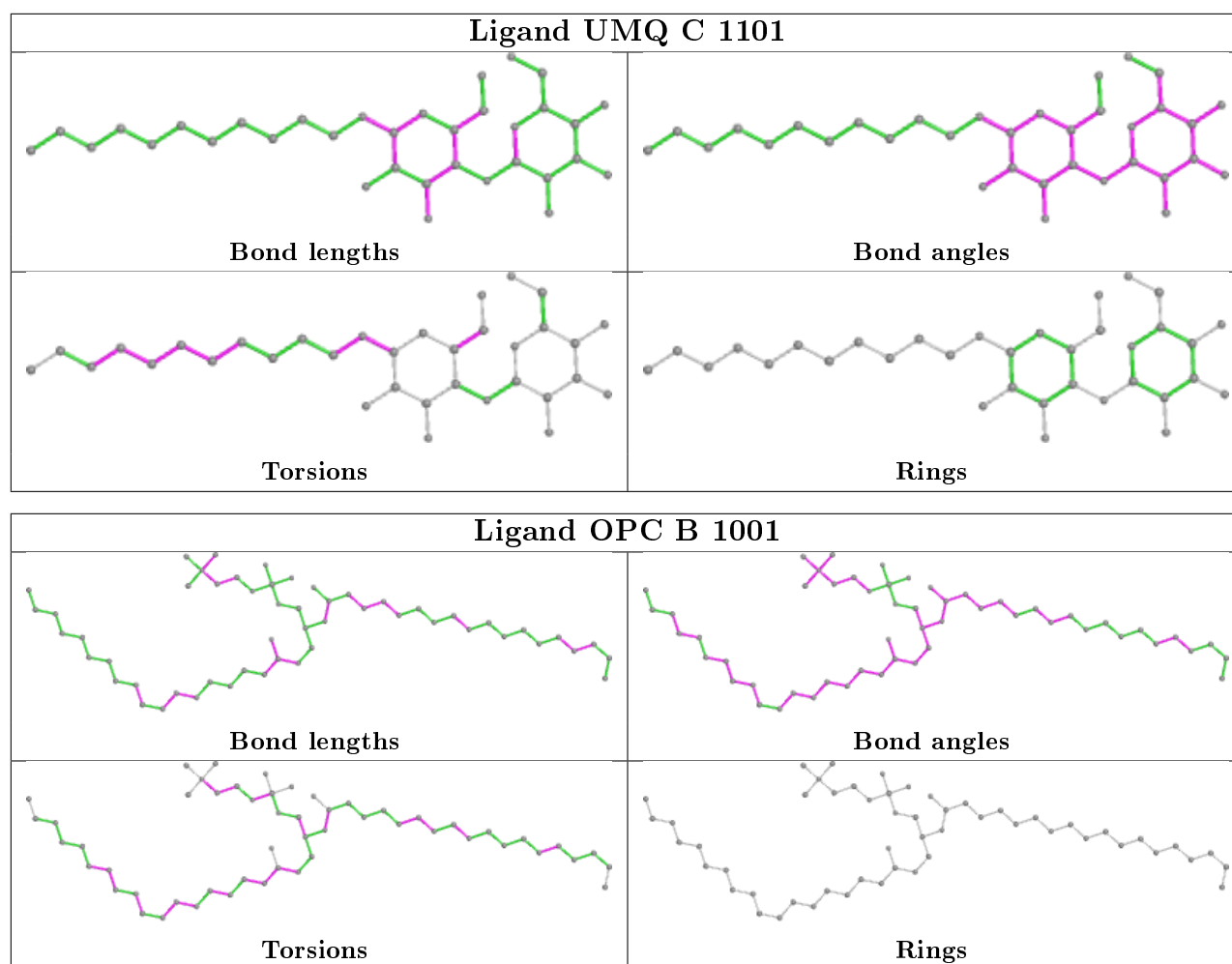












5.7 Other polymers [i](#)

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	215/215 (100%)	-0.89	0 100 100	4, 22, 60, 162	0
2	B	160/160 (100%)	-0.84	0 100 100	9, 41, 93, 133	0
3	C	288/289 (99%)	-0.13	16 (5%) 24 15	5, 47, 145, 170	1 (0%)
4	D	166/179 (92%)	0.20	21 (12%) 3 3	8, 101, 150, 182	0
5	E	32/32 (100%)	-0.71	0 100 100	22, 52, 98, 119	0
6	F	32/35 (91%)	-0.64	0 100 100	10, 41, 112, 123	0
7	G	37/37 (100%)	-0.79	0 100 100	13, 33, 115, 123	0
8	H	29/29 (100%)	-0.84	0 100 100	15, 28, 51, 97	0
All	All	959/976 (98%)	-0.44	37 (3%) 39 25	4, 42, 139, 182	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	179	VAL	6.9
4	D	144	ALA	4.1
4	D	49	ALA	4.1
4	D	175	LYS	4.0
4	D	145	PRO	4.0
3	C	189	GLU	3.9
3	C	190	TYR	3.7
4	D	157	ASP	3.6
3	C	196	GLN	3.5
3	C	184	ALA	3.2
4	D	143	PRO	3.1
4	D	173	GLY	2.9
3	C	207	VAL	2.8
4	D	159	ASN	2.8
4	D	158	ASP	2.7
4	D	56	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	199	ILE	2.6
4	D	50	VAL	2.6
3	C	206	THR	2.6
3	C	194	LYS	2.5
4	D	156	GLN	2.5
3	C	288	ASN	2.4
4	D	142	GLY	2.4
3	C	176	ALA	2.3
3	C	186	GLU	2.3
3	C	188	ASP	2.3
4	D	174	GLU	2.2
4	D	147	SER	2.2
4	D	62	ASN	2.2
4	D	160	ILE	2.2
4	D	141	ARG	2.2
4	D	130	GLY	2.1
3	C	193	VAL	2.1
3	C	220	SER	2.1
3	C	187	GLU	2.1
3	C	208	VAL	2.0
4	D	177	TRP	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 carbohydrates 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.

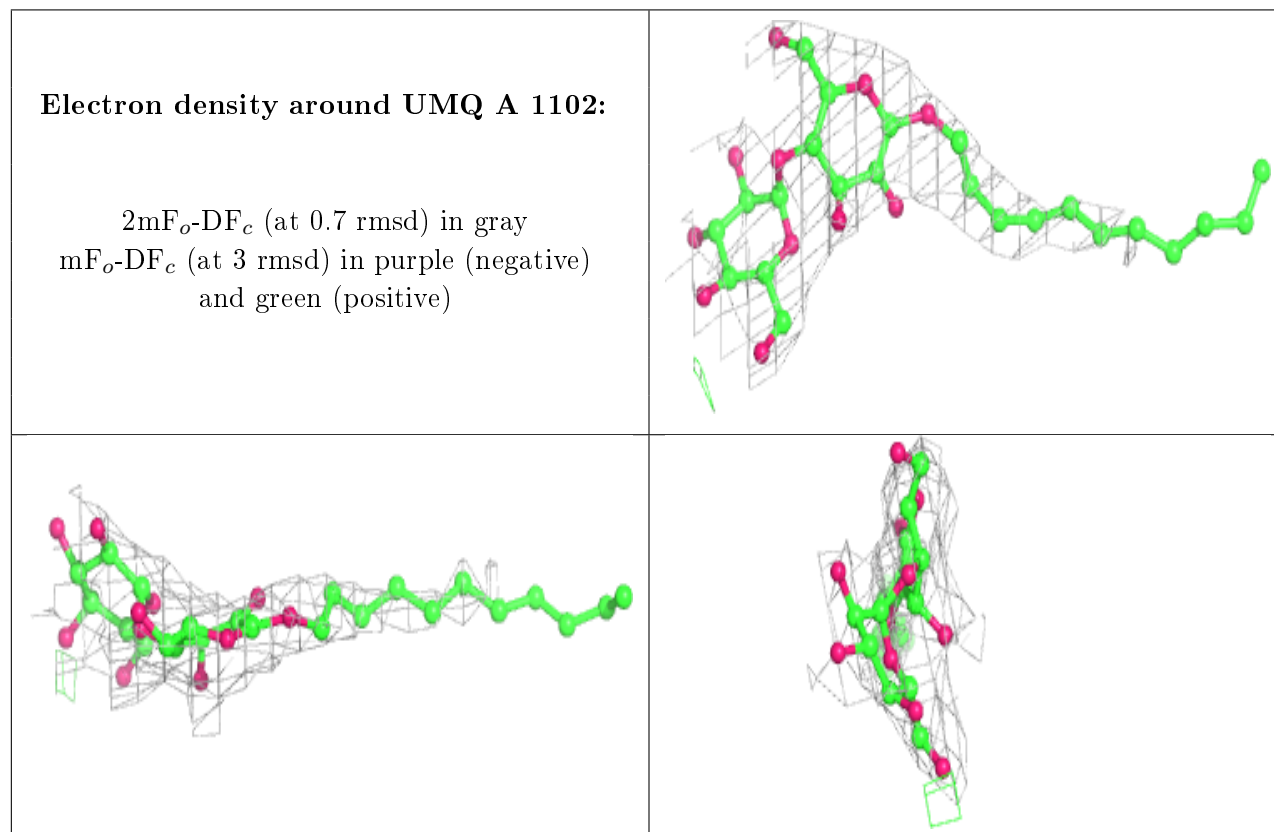
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	UMQ	A	1102	34/34	0.83	0.32	31,112,145,149	0
12	UMQ	A	1104	34/34	0.85	0.28	23,131,208,216	0

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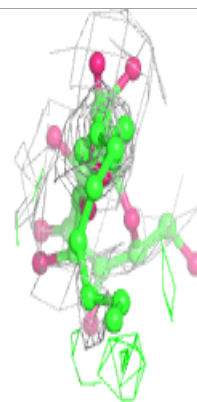
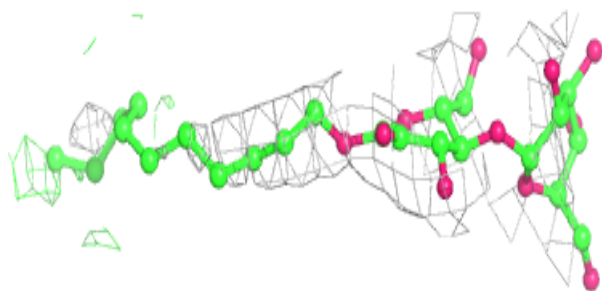
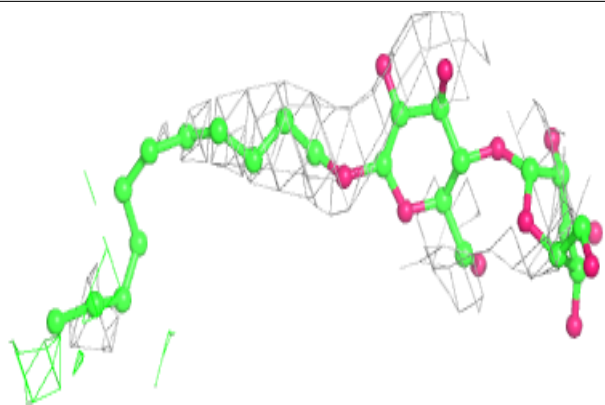
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	UMQ	C	1101	34/34	0.86	0.23	4,86,151,160	0
16	SQD	D	201	54/54	0.87	0.41	39,165,201,204	0
11	OPC	A	1002	54/55	0.90	0.40	2,64,206,220	0
17	BCR	G	101	40/40	0.93	0.36	2,49,145,149	0
12	UMQ	A	1103	34/34	0.93	0.30	40,101,144,155	0
11	OPC	B	1001	54/55	0.94	0.38	8,70,138,157	0
13	QNO	A	501	21/21	0.95	0.20	45,63,95,120	0
14	CLA	B	201	65/65	0.97	0.20	12,42,72,111	0
9	CD	B	161	1/1	0.98	0.08	161,161,161,161	0
10	HEM	C	301	43/43	0.98	0.21	2,33,74,95	0
15	FES	D	200	4/4	0.98	0.11	89,90,95,104	0
10	HEM	A	303	43/43	0.99	0.15	2,35,56,61	0
10	HEM	A	302	43/43	0.99	0.15	2,8,43,49	0
10	HEM	A	301	43/43	0.99	0.16	2,13,37,60	0
9	CD	A	216	1/1	1.00	0.12	47,47,47,47	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.

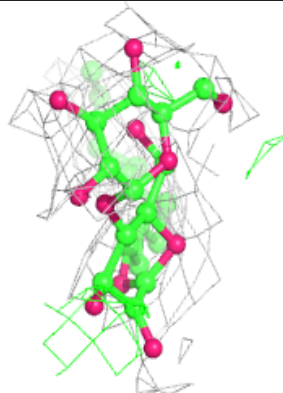
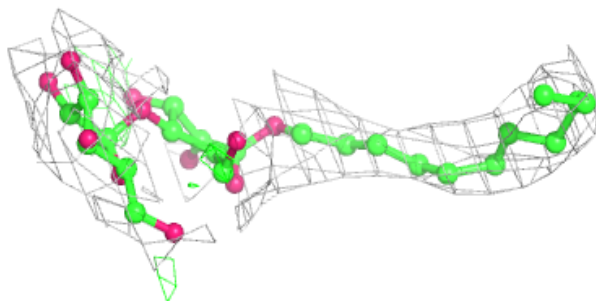
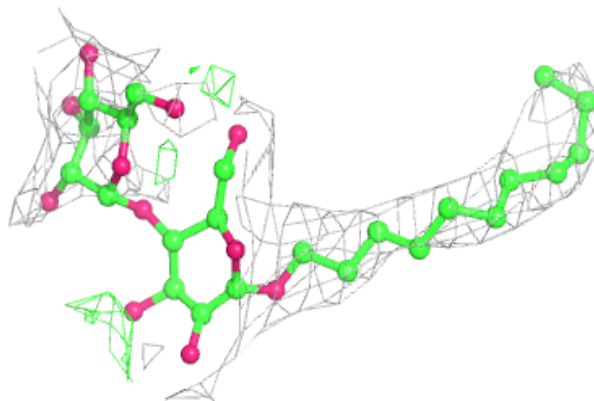


Electron density around UMQ A 1104:

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

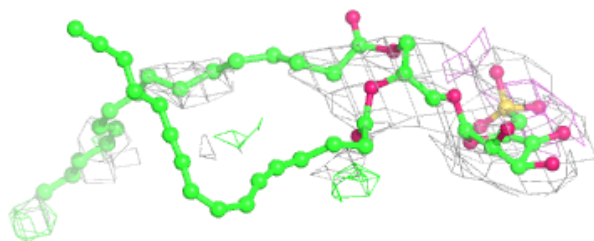
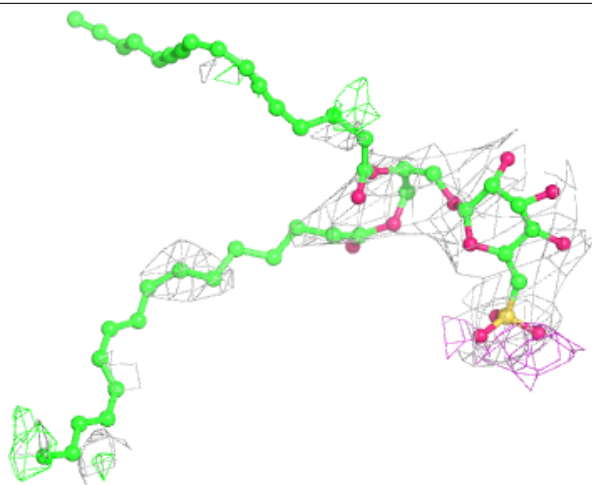
**Electron density around UMQ C 1101:**

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



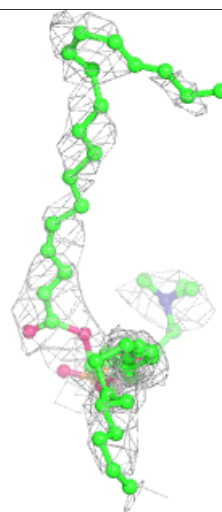
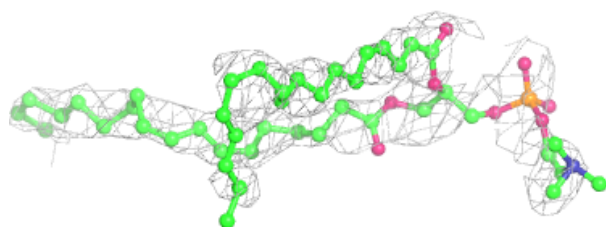
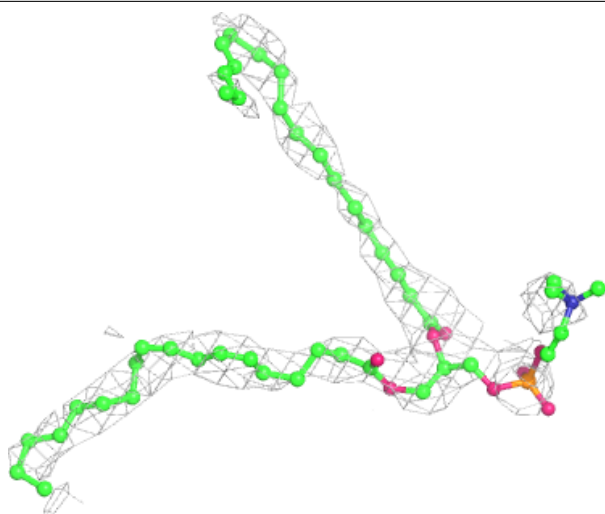
Electron density around SQD D 201:

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



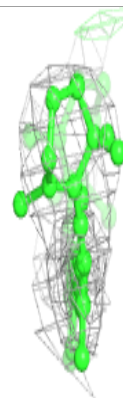
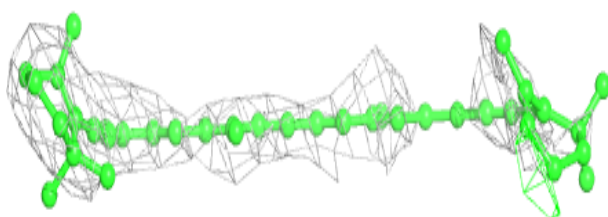
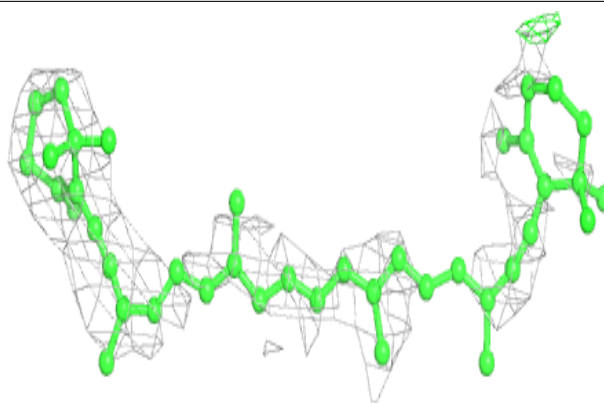
Electron density around OPC A 1002:

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

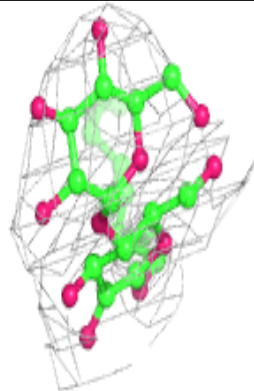
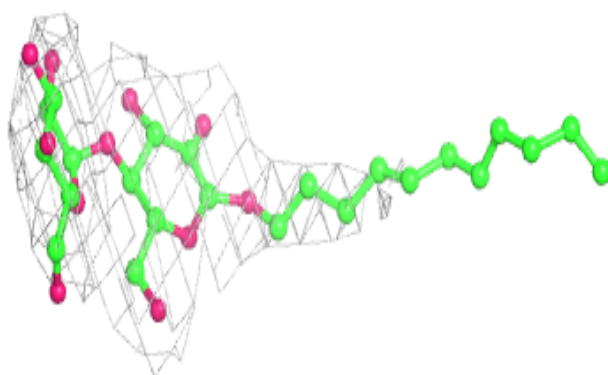
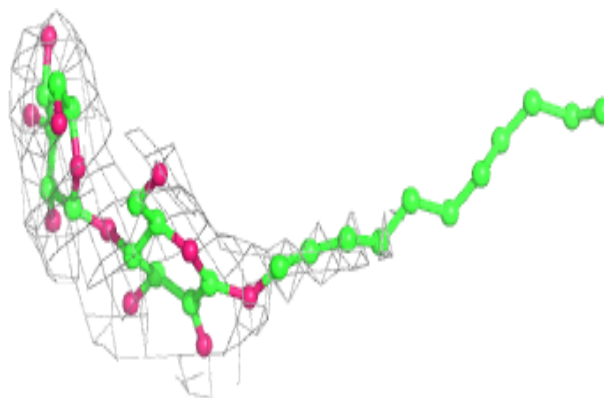


Electron density around BCR G 101:

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

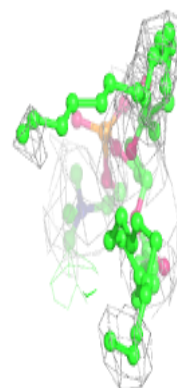
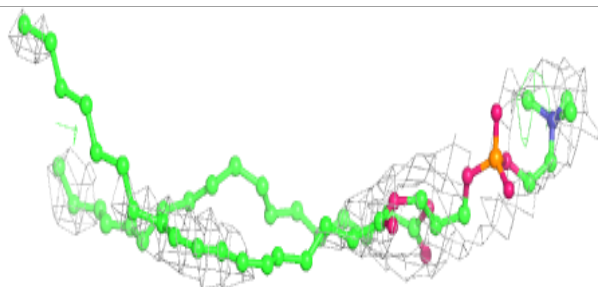
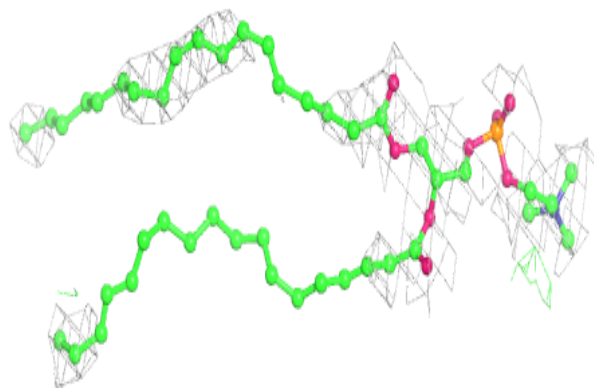
**Electron density around UMQ A 1103:**

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

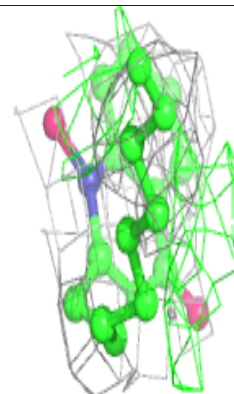
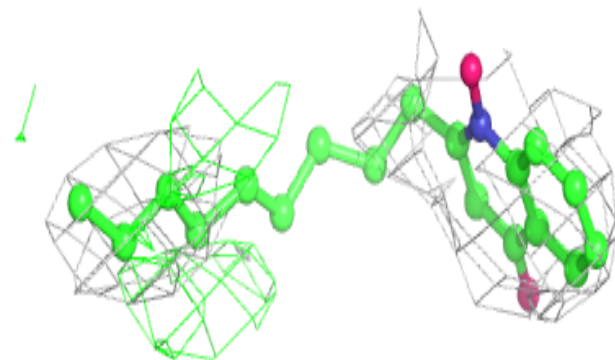
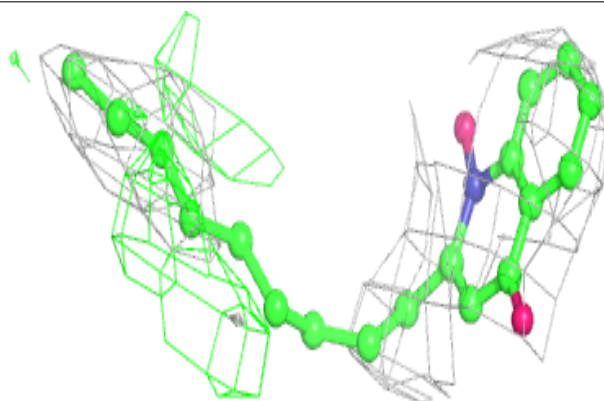


Electron density around OPC B 1001:

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

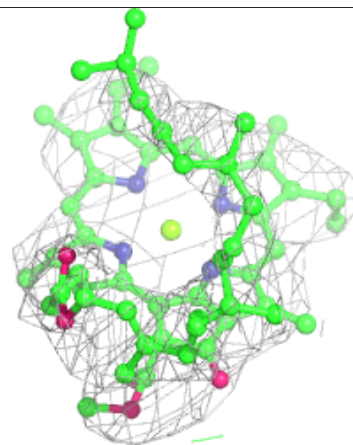
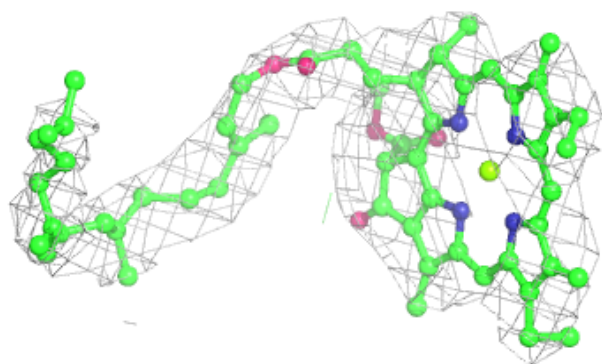
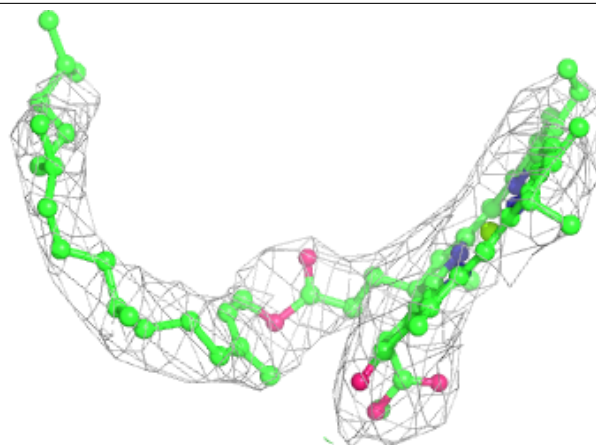
**Electron density around QNO A 501:**

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



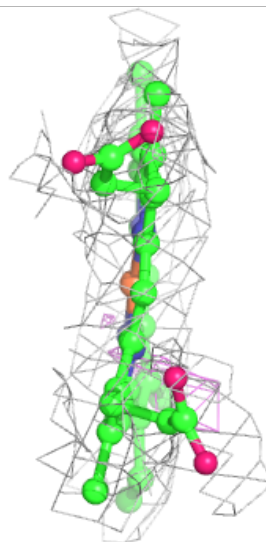
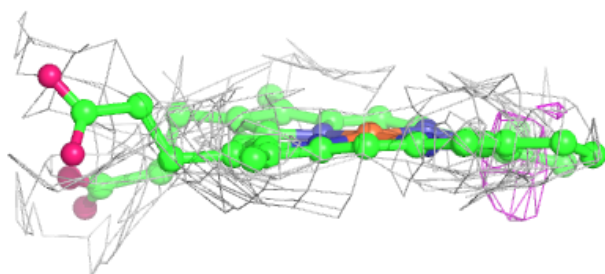
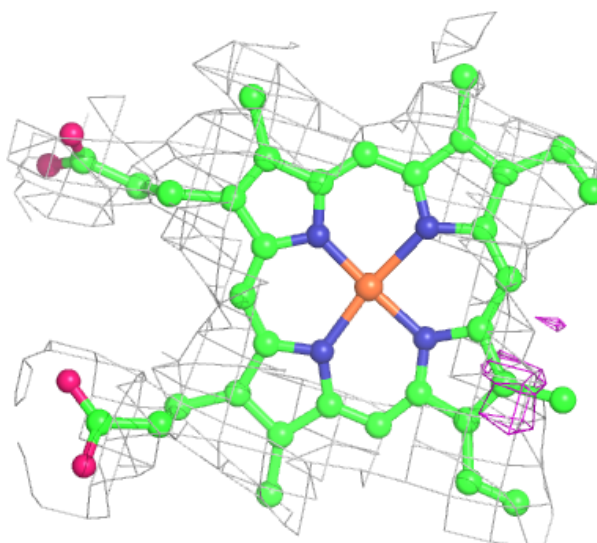
Electron density around CLA B 201:

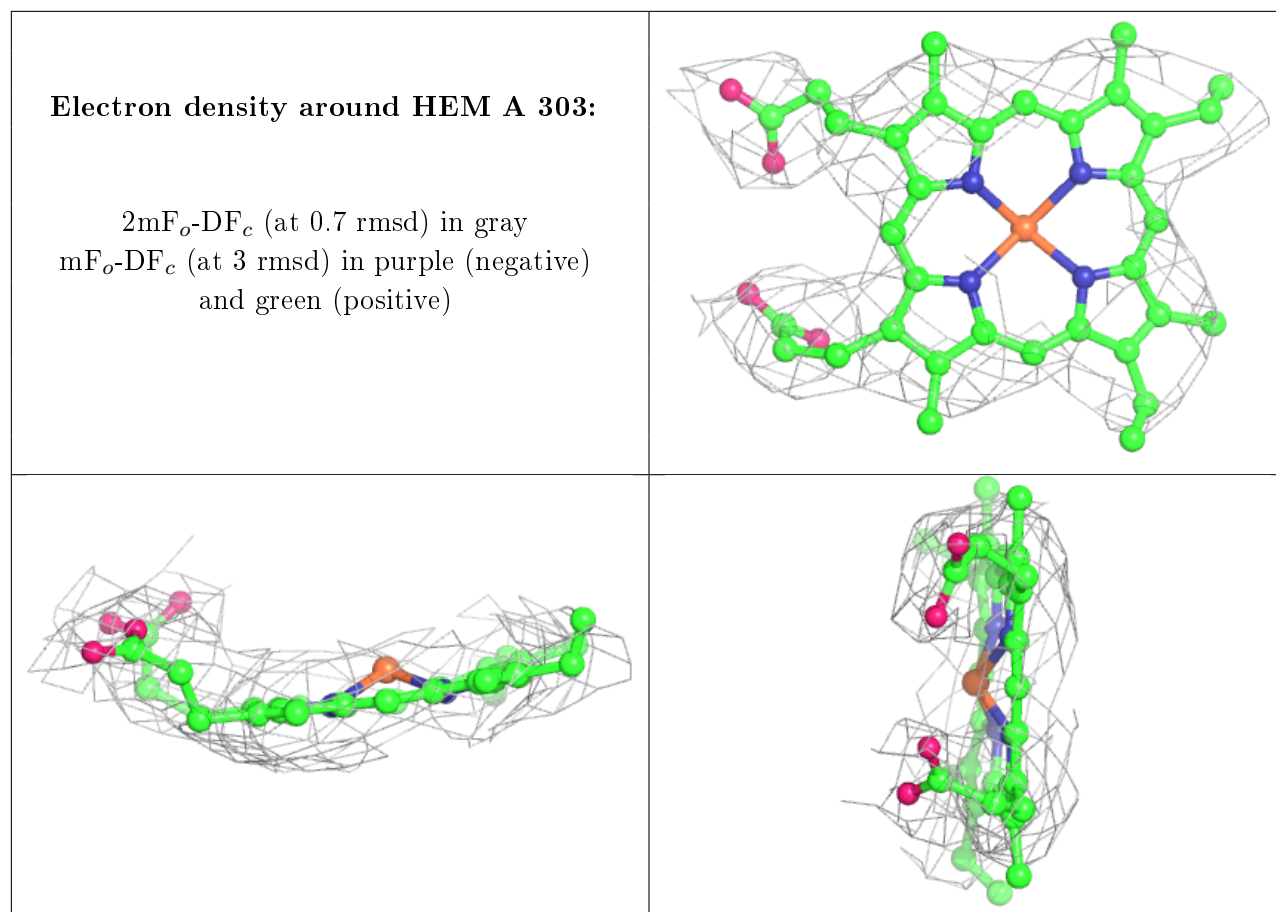
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 301:

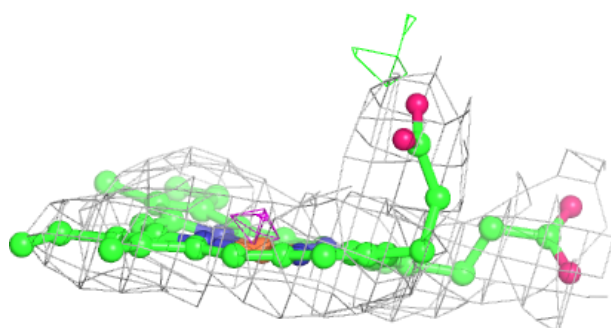
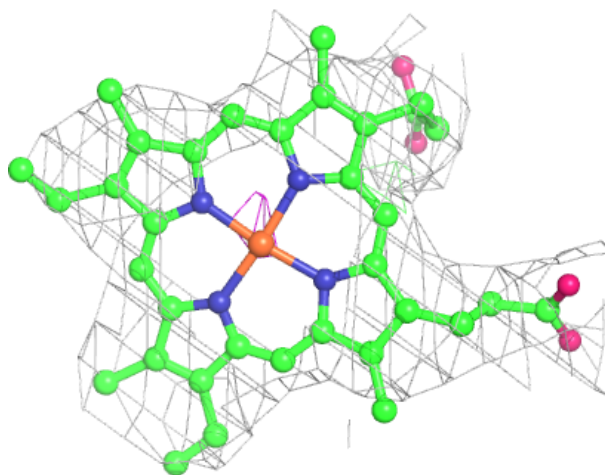
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

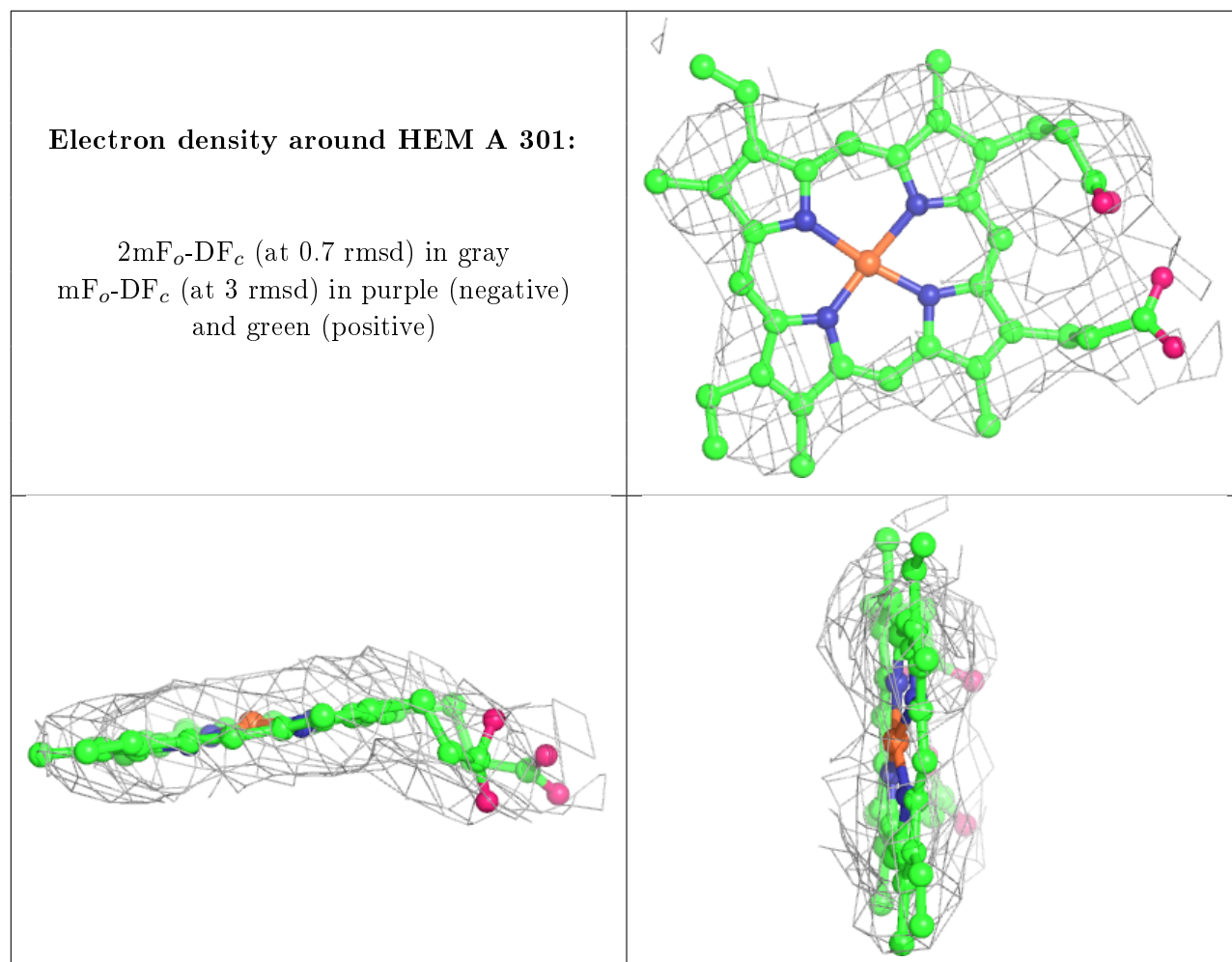




Electron density around HEM A 302:

$2mF_o-DF_c$ (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.