



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:17 PM UTC

PDB ID : 1BCC / pdb_00001bcc
Title : CYTOCHROME BC1 COMPLEX FROM CHICKEN
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.;
Crofts, A.R.; Berry, E.A.; Kim, S.-H.
Deposited on : 1998-03-23
Resolution : 3.16 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

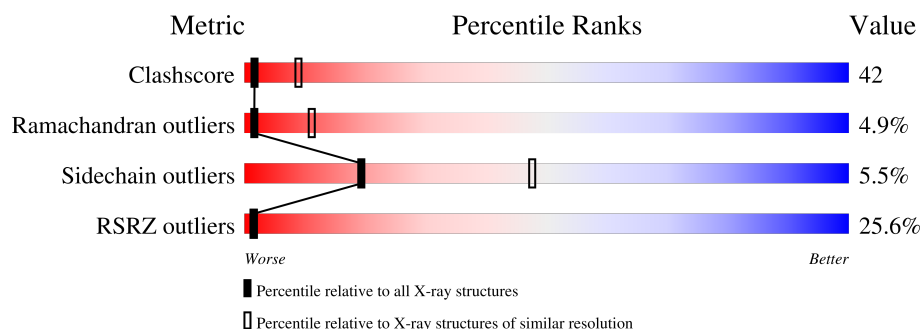
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	25% 38% 52% 9% .
2	B	422	27% 37% 49% 10% .
3	C	380	12% 39% 51% 9% .
4	D	241	16% 40% 52% 8%
5	E	196	58% 33% 53% 13% .
6	F	109	15% 49% 38% 5% 8% .
7	G	81	22% 38% 48% 9% .

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Mol	Chain	Length	Quality of chain
8	H	78	
9	I	33	
10	J	62	

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
13	PEE	C	384	X	-	-	-
13	PEE	E	198	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15719 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 UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3423	2147	601	657	18			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	TYR	THR	conflict	UNP P13272
A	23	VAL	LEU	conflict	UNP P13272
A	59	LEU	VAL	conflict	UNP P13272
A	72	GLN	GLY	conflict	UNP P13272
A	91	SER	THR	conflict	UNP P13272
A	106	VAL	LEU	conflict	UNP P13272
A	135	VAL	LEU	conflict	UNP P13272
A	136	ARG	GLN	conflict	UNP P13272
A	147	GLU	ASP	conflict	UNP P13272
A	162	GLY	PRO	conflict	UNP P13272
A	174	ILE	VAL	conflict	UNP P13272
A	188	THR	ARG	conflict	UNP P13272
A	191	THR	LYS	conflict	UNP P13272
A	203	VAL	LEU	conflict	UNP P13272
A	206	GLN	ARG	conflict	UNP P13272
A	210	GLU	ASP	conflict	UNP P13272
A	217	GLY	SER	conflict	UNP P13272
A	219	VAL	LEU	conflict	UNP P13272
A	220	PRO	SER	conflict	UNP P13272
A	221	PHE	GLY	conflict	UNP P13272
A	225	ASP	GLU	conflict	UNP P13272
A	233	LYS	PRO	conflict	UNP P13272
A	242	ARG	CYS	conflict	UNP P13272
A	267	LEU	ASN	conflict	UNP P13272
A	282	ARG	CYS	conflict	UNP P13272
A	288	LEU	ALA	conflict	UNP P13272
A	290	SER	LEU	conflict	UNP P13272

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Chain	Residue	Modelled	Actual	Comment	Reference
A	299	VAL	ALA	conflict	UNP P13272
A	311	SER	ASN	conflict	UNP P13272
A	315	SER	ALA	conflict	UNP P13272
A	316	GLU	ASP	conflict	UNP P13272
A	320	PHE	LEU	conflict	UNP P13272
A	322	PHE	ALA	conflict	UNP P13272
A	323	TYR	HIS	conflict	UNP P13272
A	328	ARG	HIS	conflict	UNP P13272
A	349	ILE	ALA	conflict	UNP P13272
A	350	SER	THR	conflict	UNP P13272
A	360	PHE	LEU	conflict	UNP P13272
A	382	GLU	SER	conflict	UNP P13272
A	393	GLU	ALA	conflict	UNP P13272
A	397	GLU	SER	conflict	UNP P13272
A	399	LEU	ILE	conflict	UNP P13272
A	406	MET	VAL	conflict	UNP P13272
A	415	ILE	PHE	conflict	UNP P13272
A	425	PRO	PHE	conflict	UNP P13272

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	0	0
			2994	1878	518	591	7			

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ILE	PHE	conflict	UNP P23004
B	28	LYS	ARG	conflict	UNP P23004
B	42	SER	ALA	conflict	UNP P23004
B	44	GLY	ALA	conflict	UNP P23004
B	46	THR	ARG	conflict	UNP P23004
B	49	VAL	LEU	conflict	UNP P23004
B	61	SER	ASN	conflict	UNP P23004
B	99	GLU	THR	conflict	UNP P23004
B	117	GLU	ASP	conflict	UNP P23004
B	134	PRO	ARG	conflict	UNP P23004
B	139	ASP	ALA	conflict	UNP P23004
B	145	LYS	ARG	conflict	UNP P23004
B	152	PHE	LEU	conflict	UNP P23004
B	157	THR	ALA	conflict	UNP P23004

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Chain	Residue	Modelled	Actual	Comment	Reference
B	174	ASP	ASN	conflict	UNP P23004
B	188	SER	PRO	conflict	UNP P23004
B	194	PHE	TYR	conflict	UNP P23004
B	207	VAL	ILE	conflict	UNP P23004
B	218	ASN	GLN	conflict	UNP P23004
B	223	LEU	PHE	conflict	UNP P23004
B	240	ARG	HIS	conflict	UNP P23004
B	257	ILE	LEU	conflict	UNP P23004
B	266	GLY	SER	conflict	UNP P23004
B	282	ASN	GLY	conflict	UNP P23004
B	321	LEU	SER	conflict	UNP P23004
B	332	TYR	SER	conflict	UNP P23004
B	335	GLN	ASP	conflict	UNP P23004
B	352	VAL	LEU	conflict	UNP P23004
B	355	GLU	PRO	conflict	UNP P23004
B	356	ASN	ASP	conflict	UNP P23004
B	367	LYS	GLY	conflict	UNP P23004
B	380	GLU	ASP	conflict	UNP P23004
B	393	ASN	THR	conflict	UNP P23004
B	412	LYS	ASN	conflict	UNP P23004
B	420	ARG	GLY	conflict	UNP P23004
B	421	GLN	ARG	conflict	UNP P23004
B	436	VAL	ILE	conflict	UNP P23004

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3002	2013	473	504	12			

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1899	1214	326	345	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	17	PRO	LEU	conflict	UNP P00125
D	143	VAL	LEU	conflict	UNP P00125
D	167	ASP	GLU	conflict	UNP P00125

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Chain	Residue	Modelled	Actual	Comment	Reference
D	216	VAL	LEU	conflict	UNP P00125
D	221	TYR	ALA	conflict	UNP P00125

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1512	953	266	285	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ASN	ASP	conflict	UNP P13272
E	17	PRO	GLU	conflict	UNP P13272
E	18	ASP	VAL	conflict	UNP P13272
E	19	ASP	LEU	conflict	UNP P13272
E	20	TYR	ASP	conflict	UNP P13272
E	26	ARG	LYS	conflict	UNP P13272
E	29	ASP	SER	conflict	UNP P13272
E	30	PRO	GLU	conflict	UNP P13272
E	31	SER	ALA	conflict	UNP P13272
E	42	VAL	THR	conflict	UNP P13272
E	45	LEU	VAL	conflict	UNP P13272
E	56	THR	SER	conflict	UNP P13272

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			875	557	153	162	3			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	29	TYR	LEU	conflict	UNP P00129
F	38	TYR	HIS	conflict	UNP P00129
F	59	MET	VAL	conflict	UNP P00129
F	69	ASN	SER	conflict	UNP P00129
F	87	VAL	LYS	conflict	UNP P00129
F	88	PRO	SER	conflict	UNP P00129
F	108	ASP	ALA	conflict	UNP P00129

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	78	Total	C	N	O	S	0	0	0
			626	411	114	100	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	LEU	VAL	conflict	UNP P13271
G	25	PRO	ALA	conflict	UNP P13271
G	34	VAL	ILE	conflict	UNP P13271
G	38	TRP	LEU	conflict	UNP P13271
G	41	LEU	THR	conflict	UNP P13271
G	53	LEU	VAL	conflict	UNP P13271
G	58	LEU	VAL	conflict	UNP P13271
G	78	VAL	GLU	conflict	UNP P13271

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			490	301	88	96	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	59	PHE	LEU	conflict	UNP P00126

- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	0	0	0
			159	92	33	34			

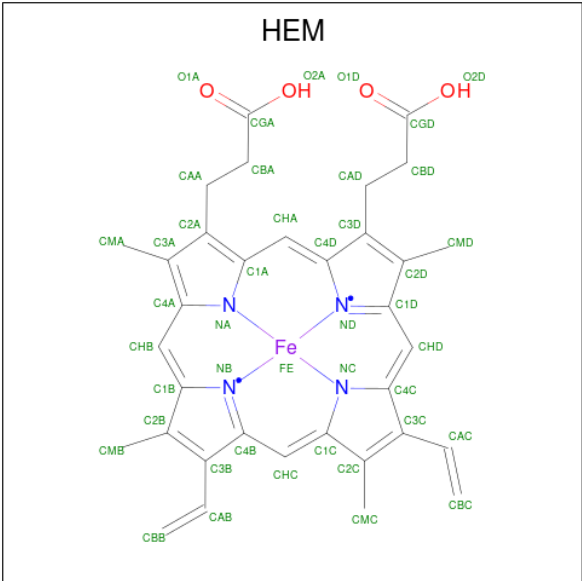
- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			459	299	78	82			

There is a discrepancy between the modelled and reference sequences:

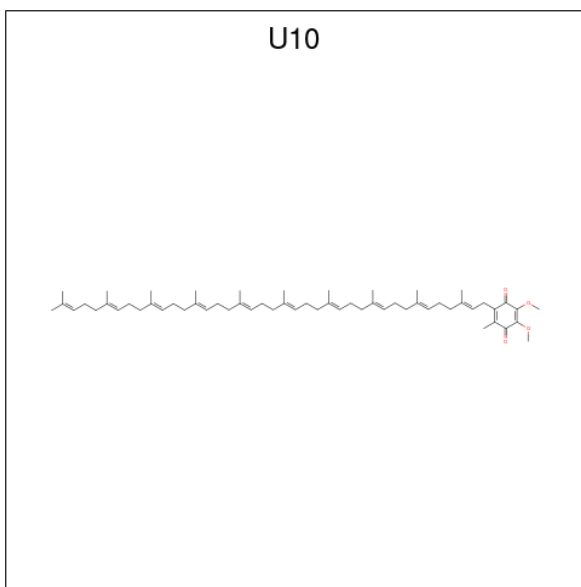
Chain	Residue	Modelled	Actual	Comment	Reference
J	30	LEU	PHE	conflict	UNP P00130

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



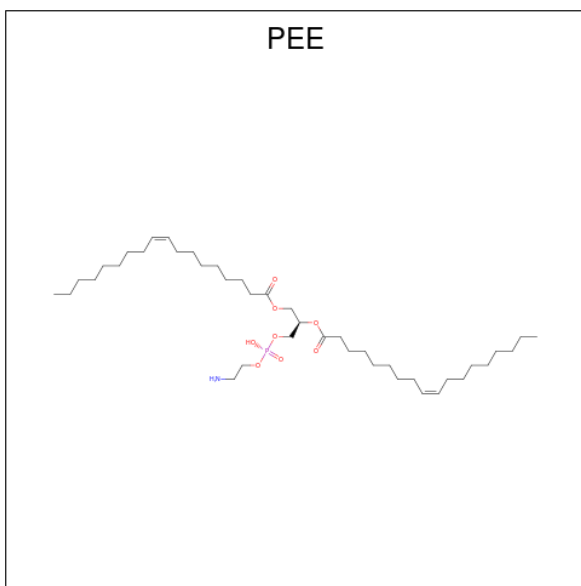
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



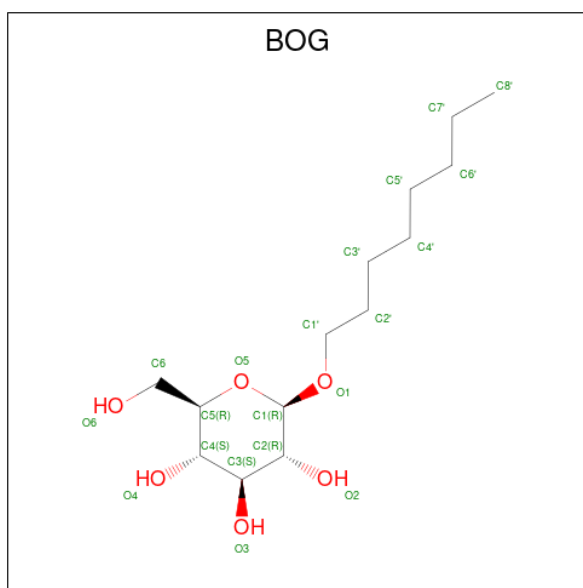
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			29	25	4		

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



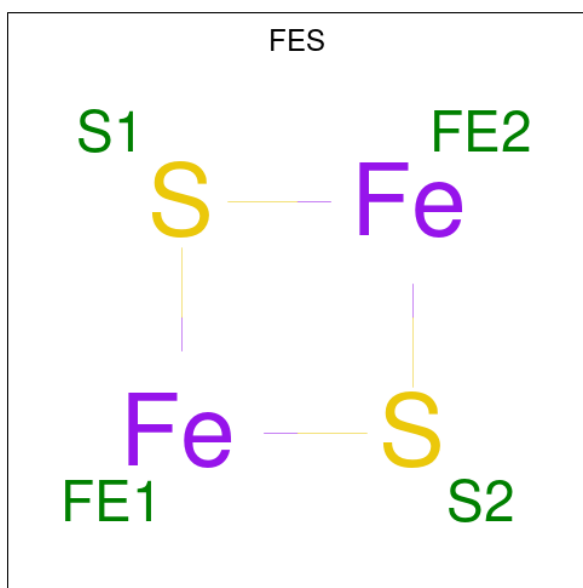
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 14 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

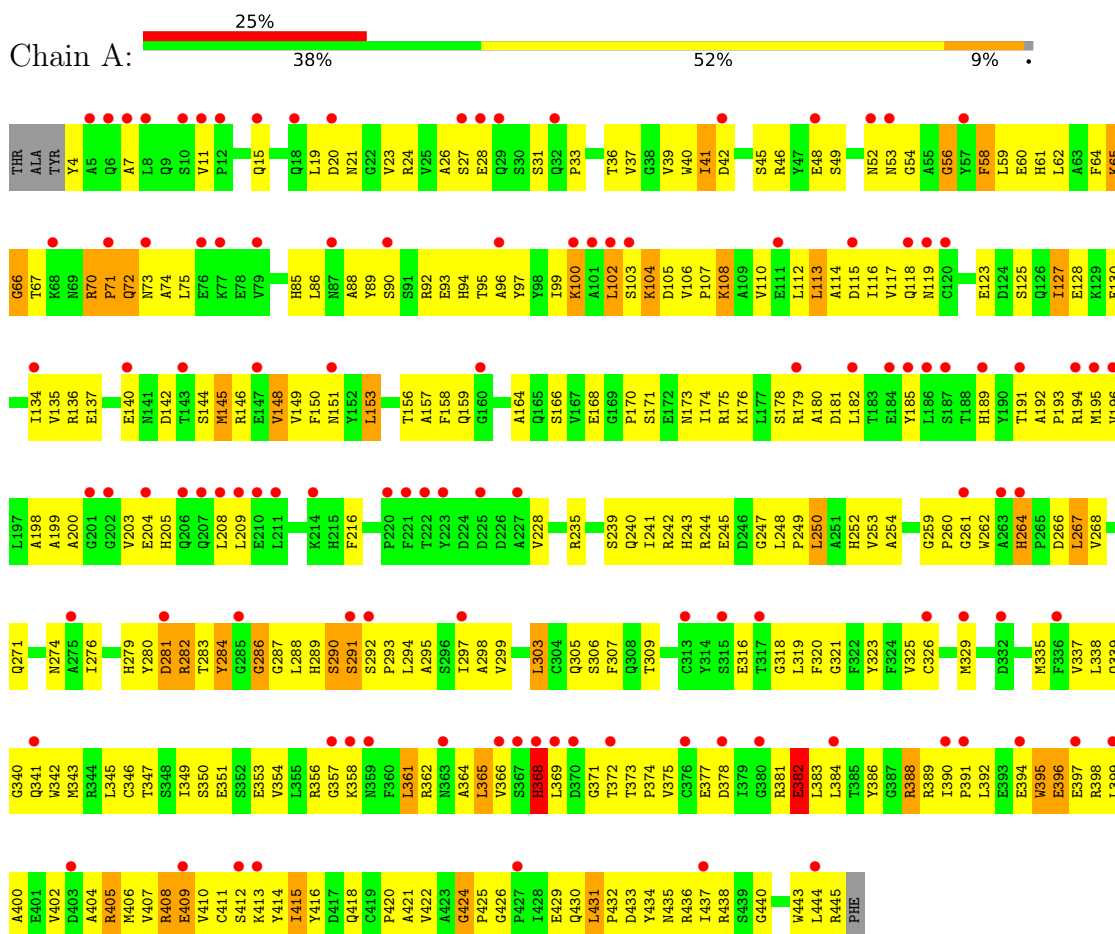


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	E	1	Total	Fe	S	0	0
			4	2	2		

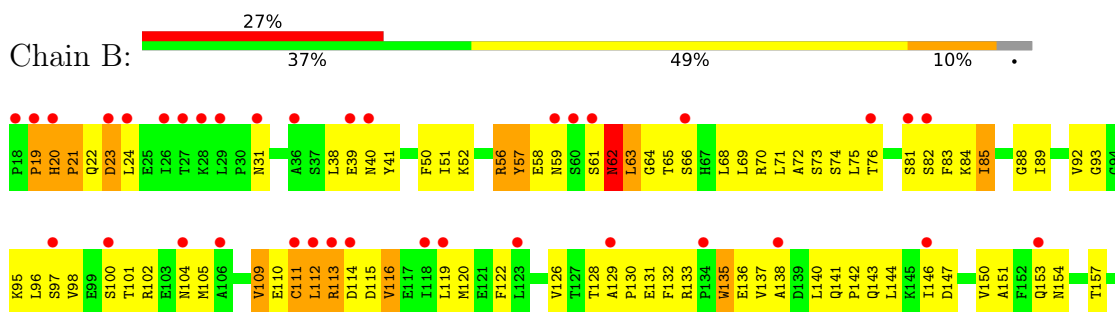
3 Residue-property plots

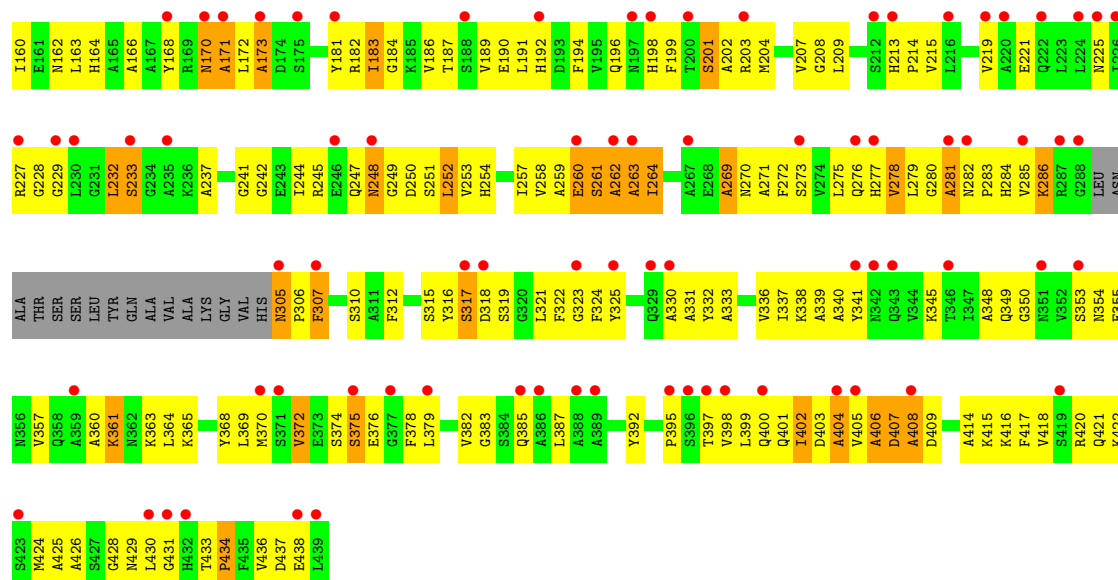
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

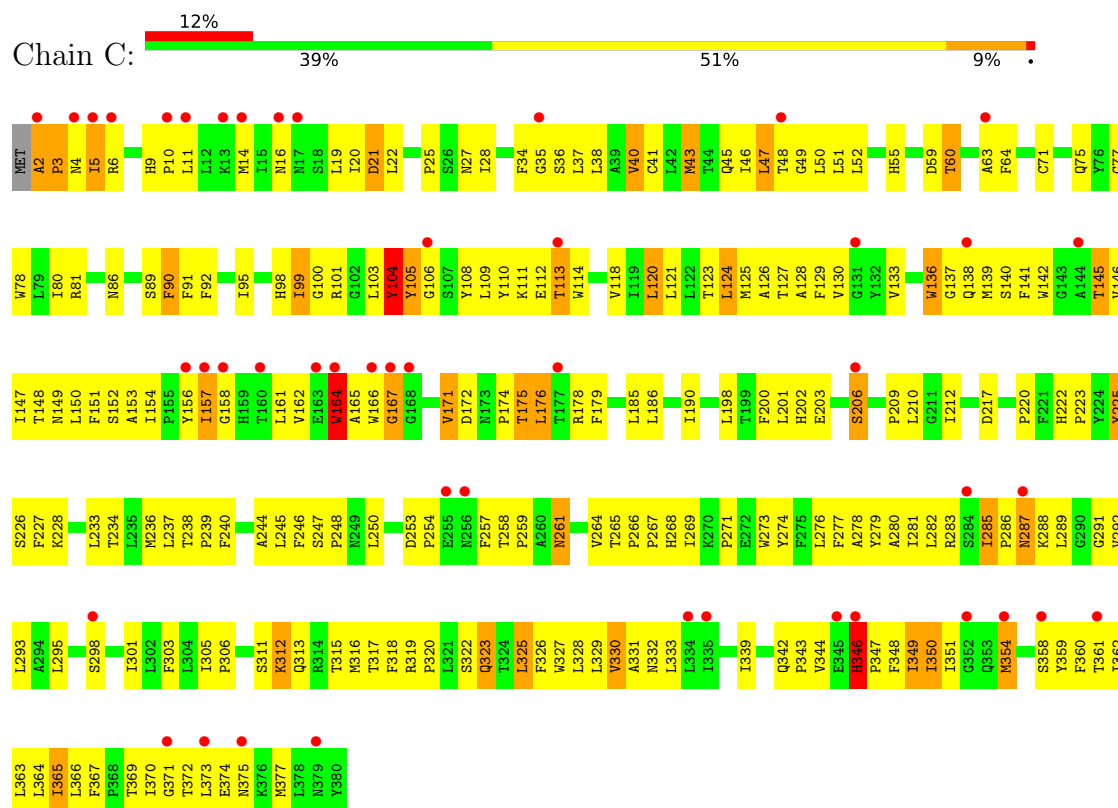


• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

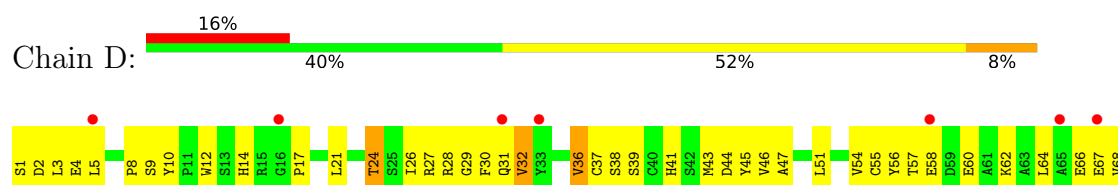


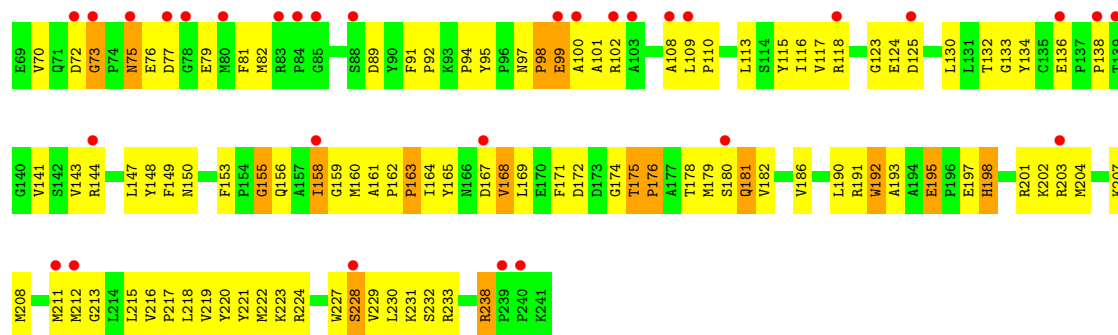


• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

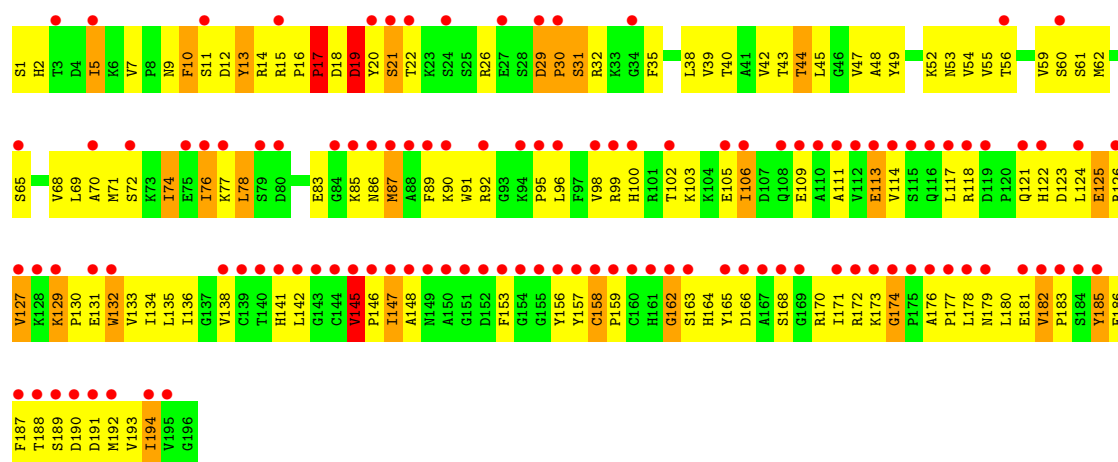


• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

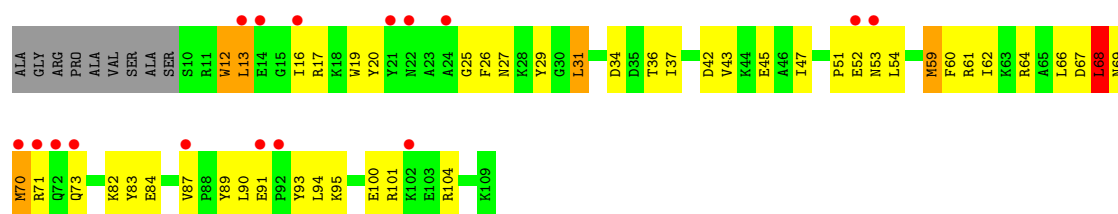




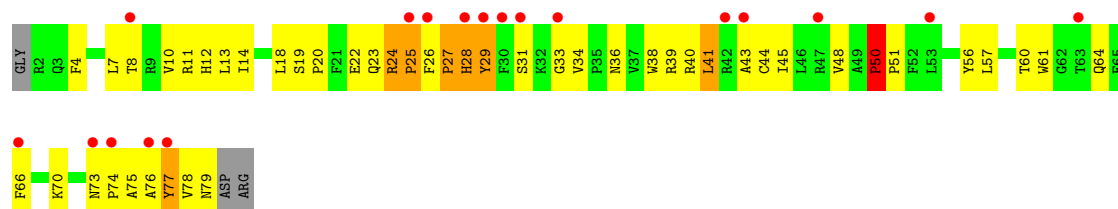
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

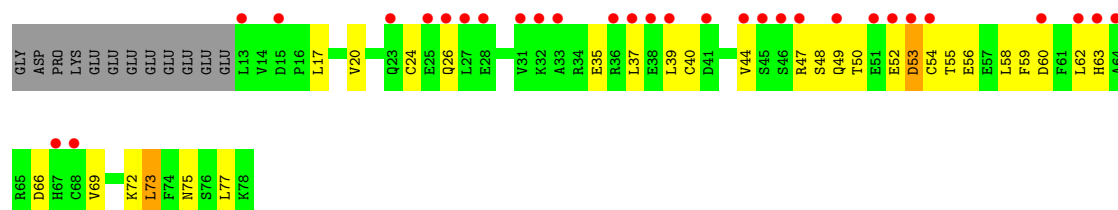


• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



● Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain H: 



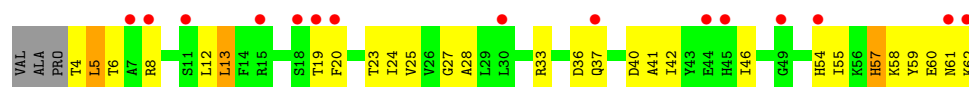
● Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain I: 



● Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	169.59Å 182.52Å 240.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.16 12.00 – 3.16	Depositor EDS
% Data completeness (in resolution range)	85.5 (12.00-3.16) 89.4 (12.00-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 3.17Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.270 , 0.310 0.285 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	15719	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, BOG, FES, PEE, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	0/3495	1.14	29/4742 (0.6%)
2	B	0.54	0/3046	1.03	9/4132 (0.2%)
3	C	0.69	0/3104	1.13	25/4252 (0.6%)
4	D	0.65	0/1960	1.17	15/2665 (0.6%)
5	E	0.72	0/1548	1.30	31/2095 (1.5%)
6	F	0.62	0/896	1.10	5/1206 (0.4%)
7	G	0.62	0/648	1.15	8/882 (0.9%)
8	H	0.54	0/495	0.93	1/669 (0.1%)
10	J	0.57	0/470	1.04	4/635 (0.6%)
All	All	0.63	0/15662	1.13	127/21278 (0.6%)

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
3	C	0	1

There are no bond length outliers.

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	76	GLU	N-CA-C	-12.69	97.77	113.38
3	C	365	ILE	N-CA-C	10.05	120.04	111.90
1	A	287	GLY	N-CA-C	-9.82	98.83	115.62
6	F	13	LEU	N-CA-C	-9.27	101.05	111.71
1	A	104	LYS	N-CA-C	-9.16	101.63	113.17
1	A	248	LEU	CA-C-N	8.81	128.83	119.05
1	A	248	LEU	C-N-CA	8.81	128.83	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ASP	N-CA-C	-8.44	102.88	113.01
5	E	158	CYS	CA-C-N	8.32	127.97	119.82
5	E	158	CYS	C-N-CA	8.32	127.97	119.82
1	A	424	GLY	CA-C-N	8.31	130.23	119.84
1	A	424	GLY	C-N-CA	8.31	130.23	119.84
3	C	105	TYR	N-CA-C	-8.12	100.10	113.50
7	G	78	VAL	N-CA-C	-8.01	103.44	111.77
10	J	60	GLU	N-CA-C	-8.01	98.42	109.71
1	A	58	PHE	N-CA-C	-7.88	102.69	111.28
3	C	285	ILE	CA-C-N	7.83	127.38	119.24
3	C	285	ILE	C-N-CA	7.83	127.38	119.24
5	E	30	PRO	N-CA-C	-7.73	104.19	113.86
5	E	185	TYR	N-CA-C	7.47	117.75	107.73
1	A	259	GLY	CA-C-N	7.46	126.73	118.97
1	A	259	GLY	C-N-CA	7.46	126.73	118.97
1	A	66	GLY	N-CA-C	7.45	121.47	111.72
5	E	132	TRP	N-CA-C	7.21	120.16	108.41
5	E	129	LYS	CA-C-N	7.17	127.01	119.05
5	E	129	LYS	C-N-CA	7.17	127.01	119.05
7	G	24	ARG	CA-C-N	7.16	128.79	119.84
7	G	24	ARG	C-N-CA	7.16	128.79	119.84
5	E	111	ALA	N-CA-C	7.14	121.22	112.23
3	C	226	SER	N-CA-C	-7.06	103.27	110.97
6	F	87	VAL	N-CA-C	6.98	114.46	107.55
4	D	175	THR	CA-C-N	6.98	128.56	119.84
4	D	175	THR	C-N-CA	6.98	128.56	119.84
3	C	346	HIS	N-CA-C	6.94	125.15	109.81
3	C	176	LEU	N-CA-C	-6.93	103.73	111.28
2	B	253	VAL	N-CA-C	6.82	118.49	109.21
5	E	26	ARG	N-CA-C	6.82	119.73	111.82
1	A	140	GLU	N-CA-C	-6.77	104.65	113.12
3	C	129	PHE	N-CA-C	-6.77	102.51	111.24
5	E	125	GLU	N-CA-C	-6.59	104.47	113.30
4	D	195	GLU	CA-C-N	6.48	127.94	119.84
4	D	195	GLU	C-N-CA	6.48	127.94	119.84
1	A	119	ASN	N-CA-C	6.43	119.25	110.06
6	F	68	LEU	N-CA-C	-6.35	104.05	110.97
4	D	44	ASP	N-CA-C	6.32	119.84	111.75
5	E	10	PHE	N-CA-C	-6.29	104.87	113.30
5	E	5	ILE	N-CA-C	6.25	117.11	108.12
3	C	206	SER	N-CA-C	-6.24	99.54	109.59
5	E	113	GLU	N-CA-C	6.15	119.18	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	90	PHE	N-CA-C	-6.14	103.89	111.33
1	A	415	ILE	N-CA-C	6.14	116.84	111.56
4	D	159	GLY	N-CA-C	-6.10	107.96	114.67
1	A	329	MET	N-CA-C	6.08	120.77	113.23
3	C	104	TYR	N-CA-C	6.04	121.11	111.81
4	D	203	ARG	N-CA-C	-6.02	104.78	111.71
2	B	281	ALA	N-CA-C	-5.95	104.13	111.33
3	C	164	TRP	N-CA-C	-5.95	105.94	113.43
1	A	364	ALA	N-CA-C	-5.92	104.46	111.03
3	C	99	ILE	N-CA-C	-5.90	104.57	110.30
5	E	162	GLY	N-CA-C	5.89	124.26	114.48
3	C	6	ARG	N-CA-C	-5.86	105.89	114.39
8	H	53	ASP	N-CA-C	-5.85	100.60	109.85
10	J	13	LEU	N-CA-C	5.85	120.92	113.55
5	E	114	VAL	N-CA-C	5.83	116.57	110.62
5	E	19	ASP	N-CA-C	5.81	120.03	107.49
7	G	19	SER	CA-C-N	5.80	125.48	119.56
7	G	19	SER	C-N-CA	5.80	125.48	119.56
2	B	74	SER	N-CA-C	5.80	120.35	113.16
10	J	57	HIS	N-CA-C	5.77	118.31	111.33
3	C	35	GLY	N-CA-C	-5.74	105.84	112.50
7	G	50	PRO	N-CA-C	5.71	117.67	110.70
1	A	45	SER	N-CA-C	-5.69	105.06	112.23
5	E	182	VAL	CA-C-N	5.67	125.62	119.78
5	E	182	VAL	C-N-CA	5.67	125.62	119.78
5	E	44	THR	N-CA-C	-5.66	105.11	111.28
5	E	127	VAL	N-CA-C	5.64	118.06	108.86
5	E	147	ILE	N-CA-C	5.62	117.09	108.71
3	C	185	LEU	N-CA-C	5.62	117.26	111.03
3	C	2	ALA	CA-C-N	5.60	126.84	119.84
3	C	2	ALA	C-N-CA	5.60	126.84	119.84
1	A	368	HIS	N-CA-C	-5.58	105.73	112.54
3	C	267	PRO	N-CA-C	-5.58	101.74	112.01
3	C	279	TYR	N-CA-C	-5.58	105.30	111.71
2	B	438	GLU	N-CA-C	-5.53	105.89	113.30
6	F	100	GLU	N-CA-C	-5.51	105.27	111.28
5	E	145	VAL	N-CA-C	5.50	114.01	107.73
6	F	45	GLU	N-CA-C	-5.49	105.19	111.07
1	A	284	TYR	N-CA-C	5.49	120.48	113.18
1	A	176	LYS	N-CA-C	5.46	122.51	113.89
4	D	155	GLY	N-CA-C	-5.45	108.20	114.69
5	E	174	GLY	CA-C-N	5.40	125.12	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	174	GLY	C-N-CA	5.40	125.12	119.82
5	E	29	ASP	CA-C-N	-5.38	114.13	119.56
5	E	29	ASP	C-N-CA	-5.38	114.13	119.56
1	A	290	SER	N-CA-C	-5.37	102.67	110.24
5	E	31	SER	N-CA-C	-5.37	105.08	111.69
4	D	238	ARG	N-CA-C	5.36	118.37	109.79
2	B	116	VAL	N-CA-C	-5.34	105.64	110.82
4	D	110	PRO	CA-C-N	5.32	125.61	119.92
4	D	110	PRO	C-N-CA	5.32	125.61	119.92
2	B	93	GLY	N-CA-C	-5.27	106.43	115.08
1	A	426	GLY	CA-C-N	5.25	126.40	119.84
1	A	426	GLY	C-N-CA	5.25	126.40	119.84
2	B	278	VAL	N-CA-C	-5.24	104.50	111.05
2	B	98	VAL	N-CA-C	5.23	116.03	107.24
10	J	8	ARG	N-CA-C	-5.21	105.50	111.07
1	A	416	TYR	N-CA-C	5.18	117.86	110.24
1	A	70	ARG	CA-C-N	5.18	126.31	119.84
1	A	70	ARG	C-N-CA	5.18	126.31	119.84
7	G	8	THR	N-CA-C	5.17	116.70	108.79
5	E	65	SER	N-CA-C	5.16	117.51	110.55
1	A	264	HIS	N-CA-C	5.13	116.16	109.64
3	C	312	LYS	N-CA-C	-5.13	107.09	113.19
5	E	76	ILE	N-CA-C	5.12	115.28	108.11
3	C	111	LYS	N-CA-C	5.12	119.77	111.37
5	E	29	ASP	N-CA-C	5.12	121.12	109.81
4	D	45	TYR	N-CA-C	5.11	119.51	113.28
7	G	76	ALA	N-CA-C	-5.11	106.74	112.87
1	A	41	ILE	N-CA-C	5.08	117.15	109.12
4	D	158	ILE	CB-CA-C	-5.08	103.81	110.98
5	E	74	ILE	N-CA-C	5.06	115.41	108.12
3	C	317	THR	N-CA-C	-5.04	105.69	111.14
4	D	24	THR	N-CA-C	-5.03	105.80	111.28
3	C	261	ASN	CA-C-N	5.03	126.12	119.84
3	C	261	ASN	C-N-CA	5.03	126.12	119.84
1	A	303	LEU	N-CA-C	5.02	119.12	112.89
2	B	173	ALA	N-CA-C	-5.01	106.94	113.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	225	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3423	0	3286	308	0
2	B	2994	0	2906	297	0
3	C	3002	0	3036	273	0
4	D	1899	0	1822	166	0
5	E	1512	0	1485	164	0
6	F	875	0	839	55	0
7	G	626	0	591	54	0
8	H	490	0	445	39	0
9	I	159	0	42	19	0
10	J	459	0	424	23	0
11	C	86	0	60	12	0
11	D	43	0	30	0	0
12	C	29	0	33	2	0
13	C	49	0	70	2	0
13	E	49	0	70	1	0
14	D	20	0	28	3	0
15	E	4	0	0	1	0
All	All	15719	0	15167	1283	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 42.

All (1283) 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)
4:D:158:ILE:HG22	4:D:160:MET:H	1.07	1.15
1:A:282:ARG:NH1	9:I:202:UNK:H	1.47	1.11
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.33	1.10
3:C:27:ASN:HD22	6:F:69:ASN:ND2	1.56	1.02
2:B:76:THR:HG22	2:B:82:SER:H	1.23	1.01
1:A:88:ALA:HB1	1:A:96:ALA:O	1.62	1.00
2:B:241:GLY:HA3	2:B:421:GLN:HE21	1.26	0.99
2:B:280:GLY:H	2:B:283:PRO:HD2	1.30	0.96
5:E:62:MET:HE3	5:E:62:MET:HA	1.46	0.96
3:C:99:ILE:HD13	11:C:382:HEM:HBC2	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:HB3	1:A:194:ARG:HB3	1.48	0.93
3:C:167:GLY:H	3:C:175:THR:HG22	1.34	0.93
1:A:49:SER:H	1:A:52:ASN:HB3	1.35	0.91
3:C:139:MET:HE1	3:C:269:ILE:HA	1.49	0.91
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.53	0.89
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.54	0.89
2:B:20:HIS:N	2:B:21:PRO:HD3	1.85	0.89
2:B:162:ASN:HB3	2:B:244:ILE:HD11	1.54	0.88
8:H:47:ARG:HD3	8:H:48:SER:H	1.38	0.88
2:B:120:MET:HE2	2:B:219:VAL:HG11	1.56	0.88
4:D:32:VAL:O	4:D:36:VAL:HG13	1.73	0.87
4:D:130:LEU:HD11	4:D:158:ILE:HD11	1.57	0.87
6:F:59:MET:HE3	6:F:59:MET:HA	1.57	0.86
3:C:238:THR:HG23	3:C:239:PRO:HD3	1.57	0.86
4:D:164:ILE:HD11	4:D:182:VAL:HG13	1.57	0.85
2:B:199:PHE:C	2:B:204:MET:HE3	2.01	0.85
3:C:104:TYR:CE2	3:C:316:MET:HB2	2.11	0.85
4:D:158:ILE:HG22	4:D:160:MET:N	1.92	0.85
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.40	0.85
1:A:88:ALA:HB2	1:A:97:TYR:HA	1.59	0.83
1:A:282:ARG:NH1	9:I:202:UNK:N	2.26	0.83
1:A:36:THR:HG22	1:A:100:LYS:HB3	1.58	0.83
1:A:286:GLY:HA3	1:A:289:HIS:CD2	2.13	0.83
5:E:14:ARG:HG2	5:E:14:ARG:HH11	1.42	0.83
1:A:291:SER:HB2	1:A:356:ARG:NH2	1.94	0.83
2:B:128:THR:C	2:B:130:PRO:HD3	2.04	0.83
5:E:121:GLN:HB3	5:E:126:ARG:HD2	1.59	0.82
6:F:43:VAL:O	6:F:47:ILE:HG13	1.80	0.81
1:A:361:LEU:HD13	1:A:399:LEU:HD22	1.61	0.81
2:B:129:ALA:N	2:B:130:PRO:HD3	1.93	0.81
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.80	0.80
3:C:99:ILE:CD1	11:C:382:HEM:HBC2	2.10	0.80
5:E:11:SER:HA	5:E:15:ARG:HD2	1.62	0.80
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.61	0.80
3:C:27:ASN:HB2	6:F:69:ASN:ND2	1.97	0.80
1:A:94:HIS:NE2	1:A:381:ARG:HG2	1.97	0.80
4:D:98:PRO:HG2	4:D:99:GLU:OE2	1.81	0.80
1:A:433:ASP:OD2	1:A:435:ASN:HB2	1.82	0.80
5:E:45:LEU:HD21	10:J:27:GLY:C	2.07	0.79
4:D:54:VAL:HG21	4:D:192:TRP:CZ3	2.18	0.79
2:B:232:LEU:HG	2:B:233:SER:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:325:LEU:HD11	3:C:366:LEU:HB3	1.66	0.78
1:A:281:ASP:O	1:A:283:THR:N	2.17	0.78
3:C:27:ASN:HD22	6:F:69:ASN:HD22	1.32	0.78
3:C:123:THR:O	3:C:127:THR:HG23	1.84	0.77
5:E:157:TYR:HE1	5:E:162:GLY:HA2	1.48	0.77
3:C:238:THR:OG1	4:D:212:MET:HG3	1.84	0.77
4:D:167:ASP:C	4:D:169:LEU:H	1.92	0.77
8:H:50:THR:HG22	8:H:52:GLU:H	1.50	0.77
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.65	0.76
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.16	0.76
1:A:145:MET:HA	1:A:148:VAL:CG1	2.16	0.76
2:B:227:ARG:O	2:B:229:GLY:N	2.18	0.76
1:A:282:ARG:HH12	9:I:202:UNK:H	1.32	0.76
5:E:136:ILE:HG13	5:E:181:GLU:HG2	1.67	0.76
2:B:69:LEU:HD12	2:B:105:MET:HE1	1.68	0.75
5:E:45:LEU:HD21	10:J:28:ALA:N	2.00	0.75
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.67	0.75
3:C:325:LEU:HD22	3:C:362:ILE:HG23	1.66	0.75
1:A:362:ARG:HG3	1:A:399:LEU:HD11	1.68	0.75
3:C:172:ASP:O	3:C:175:THR:HG23	1.85	0.75
5:E:60:SER:C	5:E:62:MET:H	1.93	0.75
1:A:85:HIS:HB2	1:A:100:LYS:CG	2.17	0.75
10:J:42:ILE:O	10:J:46:ILE:HG13	1.87	0.75
5:E:11:SER:O	5:E:13:TYR:N	2.19	0.75
5:E:83:GLU:HA	5:E:100:HIS:HB3	1.68	0.75
5:E:122:HIS:O	5:E:125:GLU:HG2	1.87	0.75
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.20	0.75
5:E:123:ASP:HB2	5:E:170:ARG:NH2	2.02	0.75
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.68	0.74
4:D:211:MET:HG3	14:D:242:BOG:H5'1	1.69	0.74
3:C:43:MET:HE2	3:C:43:MET:HA	1.68	0.74
2:B:399:LEU:HA	2:B:402:ILE:HG22	1.69	0.74
3:C:127:THR:HG22	3:C:186:LEU:HB3	1.69	0.74
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.67	0.74
7:G:36:ASN:O	7:G:40:ARG:HG3	1.87	0.74
1:A:85:HIS:HB2	1:A:100:LYS:HG3	1.69	0.74
1:A:23:VAL:HG23	1:A:192:ALA:HB1	1.70	0.73
1:A:178:SER:HB2	1:A:181:ASP:OD1	1.87	0.73
1:A:291:SER:HB2	1:A:356:ARG:HH22	1.52	0.73
4:D:167:ASP:O	4:D:169:LEU:N	2.21	0.73
3:C:360:PHE:O	3:C:364:LEU:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.24	0.72
2:B:241:GLY:HA3	2:B:421:GLN:NE2	2.04	0.72
1:A:106:VAL:HG21	1:A:203:VAL:HG13	1.70	0.72
2:B:405:VAL:HG12	2:B:406:ALA:H	1.54	0.72
2:B:257:ILE:HD11	2:B:424:MET:HE2	1.71	0.72
3:C:52:LEU:HD13	3:C:80:ILE:HG22	1.70	0.72
3:C:167:GLY:H	3:C:175:THR:CG2	2.00	0.72
10:J:12:LEU:O	10:J:19:THR:HG21	1.89	0.72
1:A:102:LEU:HD12	1:A:102:LEU:N	2.05	0.72
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.71	0.72
2:B:111:CYS:SG	2:B:119:LEU:HD22	2.30	0.72
2:B:280:GLY:N	2:B:283:PRO:HD2	2.03	0.71
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.70	0.71
3:C:148:THR:HG22	3:C:162:VAL:HG13	1.72	0.71
1:A:295:ALA:O	1:A:299:VAL:HG23	1.90	0.71
1:A:354:VAL:O	1:A:358:LYS:HG3	1.90	0.71
3:C:238:THR:CG2	3:C:239:PRO:HD3	2.20	0.71
2:B:280:GLY:H	2:B:283:PRO:CD	2.02	0.71
4:D:21:LEU:HD13	4:D:26:ILE:HD11	1.73	0.71
5:E:47:VAL:HG21	13:E:198:PEE:H24	1.73	0.71
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.55	0.71
1:A:243:HIS:O	1:A:425:PRO:HA	1.91	0.71
1:A:282:ARG:HH11	9:I:202:UNK:H	1.39	0.71
2:B:407:ASP:C	2:B:409:ASP:H	1.98	0.71
4:D:212:MET:O	4:D:216:VAL:HG22	1.90	0.71
1:A:267:LEU:O	1:A:271:GLN:HB2	1.91	0.71
1:A:382:GLU:HG2	1:A:389:ARG:HA	1.73	0.71
2:B:81:SER:O	2:B:85:ILE:HG22	1.90	0.71
2:B:264:ILE:HG12	2:B:316:TYR:O	1.91	0.70
1:A:37:VAL:HG12	1:A:199:ALA:HB2	1.73	0.70
4:D:116:ILE:HG23	4:D:117:VAL:N	2.07	0.70
7:G:50:PRO:HG2	7:G:51:PRO:HD2	1.73	0.70
1:A:4:TYR:HB2	2:B:113:ARG:HB3	1.73	0.70
2:B:92:VAL:CG1	2:B:115:ASP:HB3	2.20	0.70
3:C:320:PRO:HA	3:C:323:GLN:HE21	1.55	0.70
1:A:106:VAL:O	1:A:110:VAL:HG23	1.90	0.70
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.57	0.70
3:C:370:ILE:O	3:C:374:GLU:HB2	1.91	0.70
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.27	0.70
2:B:353:SER:C	2:B:355:GLU:H	1.99	0.70
2:B:248:ASN:C	2:B:248:ASN:HD22	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LYS:O	2:B:109:VAL:HA	1.92	0.69
4:D:224:ARG:HH21	7:G:26:PHE:HA	1.56	0.69
1:A:399:LEU:O	1:A:399:LEU:HD12	1.93	0.69
1:A:282:ARG:HB2	9:I:203:UNK:CB	2.23	0.69
2:B:132:PHE:CE2	2:B:191:LEU:HB3	2.28	0.69
2:B:109:VAL:HG22	2:B:119:LEU:HD21	1.73	0.69
3:C:142:TRP:CH2	3:C:265:THR:HG22	2.27	0.69
4:D:30:PHE:CE2	4:D:64:LEU:HD21	2.28	0.69
6:F:70:MET:HE2	6:F:70:MET:C	2.18	0.68
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.75	0.68
3:C:27:ASN:ND2	6:F:69:ASN:ND2	2.36	0.68
5:E:17:PRO:HD3	7:G:24:ARG:HE	1.59	0.68
1:A:64:PHE:O	1:A:75:LEU:HD23	1.93	0.68
2:B:76:THR:CG2	2:B:82:SER:H	2.04	0.68
2:B:132:PHE:CD2	2:B:191:LEU:HB3	2.28	0.68
2:B:209:LEU:HG	2:B:379:LEU:HD23	1.76	0.68
5:E:13:TYR:O	5:E:14:ARG:HD3	1.93	0.68
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.24	0.68
2:B:424:MET:HG2	2:B:425:ALA:N	2.08	0.68
1:A:40:TRP:CH2	1:A:377:GLU:HA	2.28	0.67
4:D:165:TYR:CE2	4:D:168:VAL:HG22	2.30	0.67
1:A:292:SER:N	1:A:293:PRO:HD3	2.07	0.67
3:C:316:MET:SD	3:C:319:ARG:NE	2.67	0.67
2:B:395:PRO:O	2:B:398:VAL:HG12	1.94	0.67
3:C:198:LEU:HD21	11:C:382:HEM:HMA1	1.75	0.67
3:C:332:ASN:C	3:C:332:ASN:HD22	2.03	0.67
1:A:58:PHE:HB3	1:A:182:LEU:HD11	1.77	0.67
2:B:258:VAL:HG12	2:B:259:ALA:N	2.09	0.67
3:C:110:TYR:HB3	3:C:113:THR:CG2	2.24	0.67
3:C:238:THR:CB	4:D:212:MET:HG3	2.25	0.67
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.29	0.67
1:A:23:VAL:HG23	1:A:192:ALA:CB	2.25	0.67
1:A:371:GLY:O	1:A:375:VAL:HG23	1.95	0.67
2:B:38:LEU:HD23	2:B:378:PHE:HZ	1.60	0.67
1:A:205:HIS:NE2	1:A:209:LEU:HD21	2.09	0.67
3:C:127:THR:HG22	3:C:186:LEU:CB	2.25	0.67
5:E:15:ARG:HH11	5:E:19:ASP:HB3	1.58	0.67
5:E:43:THR:O	5:E:47:VAL:HG23	1.95	0.67
3:C:354:MET:HE2	3:C:354:MET:HA	1.78	0.66
1:A:36:THR:HG22	1:A:100:LYS:CB	2.26	0.66
1:A:110:VAL:HA	1:A:113:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:ASN:HB3	2:B:244:ILE:CD1	2.23	0.66
2:B:333:ALA:O	2:B:337:ILE:HG13	1.95	0.66
5:E:86:ASN:HB3	5:E:148:ALA:HB1	1.77	0.66
6:F:13:LEU:O	6:F:17:ARG:HG3	1.95	0.66
4:D:132:THR:HA	4:D:179:MET:HE2	1.77	0.66
3:C:27:ASN:ND2	6:F:69:ASN:HD22	1.93	0.66
2:B:154:ASN:O	2:B:157:THR:HG22	1.96	0.66
2:B:405:VAL:HG12	2:B:406:ALA:N	2.11	0.66
3:C:28:ILE:HD12	3:C:225:TYR:CZ	2.30	0.66
3:C:167:GLY:HA3	3:C:174:PRO:HG2	1.77	0.66
3:C:222:HIS:O	3:C:223:PRO:C	2.38	0.66
7:G:60:THR:HG22	7:G:64:GLN:HE21	1.61	0.66
7:G:79:ASN:O	8:H:47:ARG:NH1	2.29	0.65
2:B:111:CYS:SG	2:B:116:VAL:HA	2.37	0.65
5:E:136:ILE:HG12	5:E:183:PRO:HD3	1.78	0.65
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.76	0.65
3:C:5:ILE:O	3:C:5:ILE:HG22	1.97	0.65
3:C:146:VAL:O	3:C:150:LEU:HD13	1.96	0.65
1:A:102:LEU:HD12	1:A:102:LEU:H	1.62	0.65
1:A:288:LEU:HD22	2:B:83:PHE:HD1	1.61	0.65
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.77	0.65
4:D:164:ILE:HD11	4:D:182:VAL:CG1	2.27	0.65
3:C:104:TYR:CE2	3:C:316:MET:CB	2.80	0.64
5:E:16:PRO:HD2	7:G:22:GLU:O	1.96	0.64
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.77	0.64
3:C:120:LEU:HG	11:C:382:HEM:HAB	1.79	0.64
5:E:171:ILE:HG22	5:E:179:ASN:OD1	1.96	0.64
2:B:100:SER:O	9:I:106:UNK:HA	1.97	0.64
4:D:192:TRP:CD1	4:D:193:ALA:N	2.65	0.64
1:A:362:ARG:HH22	2:B:113:ARG:NH1	1.95	0.64
5:E:62:MET:HA	5:E:62:MET:CE	2.22	0.64
3:C:198:LEU:HD21	11:C:382:HEM:CMA	2.27	0.64
13:C:384:PEE:O5	7:G:48:VAL:HG21	1.98	0.64
4:D:51:LEU:O	4:D:54:VAL:HG12	1.98	0.64
8:H:72:LYS:HA	8:H:75:ASN:ND2	2.12	0.64
2:B:357:VAL:HG11	2:B:406:ALA:HB1	1.80	0.64
3:C:104:TYR:CZ	3:C:316:MET:HG3	2.33	0.64
4:D:195:GLU:HG3	4:D:195:GLU:O	1.97	0.64
5:E:162:GLY:O	5:E:164:HIS:HD2	1.81	0.64
5:E:142:LEU:HB2	15:E:197:FES:S2	2.37	0.64
4:D:238:ARG:HD2	5:E:5:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:SER:O	2:B:324:PHE:HB2	1.99	0.63
2:B:96:LEU:HD23	2:B:97:SER:N	2.12	0.63
2:B:272:PHE:O	2:B:276:GLN:N	2.26	0.63
3:C:236:MET:O	3:C:239:PRO:HD2	1.99	0.63
5:E:109:GLU:OE1	5:E:166:ASP:HB2	1.98	0.63
2:B:39:GLU:HG3	2:B:41:TYR:CE1	2.34	0.63
3:C:103:LEU:O	3:C:103:LEU:HD13	1.99	0.63
4:D:216:VAL:HG23	4:D:217:PRO:HD3	1.81	0.63
1:A:53:ASN:HD22	1:A:54:GLY:N	1.97	0.63
1:A:378:ASP:O	1:A:382:GLU:HB2	1.98	0.63
1:A:429:GLU:OE2	7:G:7:LEU:HB2	1.99	0.63
2:B:70:ARG:HD3	2:B:100:SER:HB3	1.78	0.63
2:B:133:ARG:HD3	2:B:135:TRP:CH2	2.34	0.63
3:C:34:PHE:HD1	3:C:37:LEU:HD12	1.63	0.63
1:A:245:GLU:HG3	7:G:11:ARG:HG2	1.80	0.62
2:B:62:ASN:O	2:B:65:THR:HG22	1.99	0.62
5:E:122:HIS:CE1	5:E:124:LEU:HB2	2.34	0.62
5:E:45:LEU:C	5:E:45:LEU:HD13	2.24	0.62
1:A:108:LYS:HE3	1:A:108:LYS:HA	1.80	0.62
3:C:142:TRP:CD1	3:C:266:PRO:HD3	2.34	0.62
5:E:78:LEU:HG	5:E:191:ASP:C	2.23	0.62
1:A:343:MET:HE2	1:A:343:MET:HA	1.81	0.62
2:B:31:ASN:HB3	2:B:201:SER:HB2	1.81	0.62
2:B:202:ALA:HB3	2:B:229:GLY:O	2.00	0.62
5:E:44:THR:HB	10:J:24:ILE:HD12	1.80	0.62
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.80	0.62
4:D:149:PHE:HA	4:D:156:GLN:O	2.00	0.62
5:E:147:ILE:O	5:E:156:TYR:HA	2.00	0.62
1:A:245:GLU:HG2	1:A:247:GLY:H	1.64	0.62
4:D:155:GLY:C	4:D:156:GLN:NE2	2.58	0.62
4:D:218:LEU:HD11	5:E:42:VAL:HG12	1.82	0.62
5:E:16:PRO:HD3	7:G:23:GLN:HA	1.81	0.62
3:C:167:GLY:N	3:C:175:THR:HG22	2.12	0.62
1:A:284:TYR:CE1	9:I:112:UNK:O	2.53	0.62
2:B:163:LEU:HD21	2:B:258:VAL:HG21	1.80	0.61
3:C:247:SER:HB3	3:C:250:LEU:HB2	1.82	0.61
8:H:50:THR:HG22	8:H:52:GLU:N	2.15	0.61
3:C:25:PRO:HD2	3:C:28:ILE:HD11	1.82	0.61
5:E:123:ASP:HB2	5:E:170:ARG:CZ	2.30	0.61
1:A:342:TRP:O	1:A:345:LEU:HB3	1.99	0.61
2:B:92:VAL:HG11	2:B:115:ASP:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:LEU:O	3:C:124:LEU:HD22	2.00	0.61
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.82	0.61
2:B:207:VAL:HG12	2:B:208:GLY:N	2.15	0.61
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.30	0.61
5:E:183:PRO:O	5:E:185:TYR:HD1	1.84	0.61
1:A:56:GLY:HA2	1:A:185:TYR:CE2	2.35	0.61
2:B:360:ALA:O	2:B:363:LYS:N	2.31	0.61
3:C:104:TYR:OH	3:C:322:SER:HB2	1.99	0.61
5:E:14:ARG:O	7:G:24:ARG:HG3	2.00	0.61
1:A:250:LEU:C	1:A:250:LEU:HD22	2.25	0.61
3:C:166:TRP:HB2	3:C:175:THR:HG21	1.81	0.61
3:C:125:MET:O	3:C:128:ALA:N	2.33	0.61
3:C:238:THR:HG23	3:C:239:PRO:CD	2.31	0.61
1:A:102:LEU:C	1:A:104:LYS:H	2.09	0.61
5:E:102:THR:O	5:E:106:ILE:HG13	2.01	0.61
2:B:122:PHE:O	2:B:126:VAL:HG23	2.01	0.60
2:B:166:ALA:HB1	2:B:242:GLY:HA3	1.82	0.60
2:B:170:ASN:HD21	2:B:237:ALA:HA	1.66	0.60
3:C:142:TRP:O	3:C:146:VAL:HG22	2.01	0.60
3:C:209:PRO:O	3:C:315:THR:HG21	2.01	0.60
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.83	0.60
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.82	0.60
2:B:260:GLU:O	2:B:261:SER:HB3	2.01	0.60
3:C:112:GLU:N	3:C:112:GLU:OE1	2.34	0.60
5:E:59:VAL:HG12	5:E:59:VAL:O	2.01	0.60
5:E:99:ARG:H	5:E:133:VAL:HG12	1.65	0.60
3:C:49:GLY:C	11:C:381:HEM:HAC	2.27	0.60
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.31	0.60
4:D:167:ASP:C	4:D:169:LEU:N	2.59	0.60
5:E:78:LEU:HD12	5:E:190:ASP:O	2.02	0.60
1:A:252:HIS:CE1	1:A:325:VAL:HG22	2.37	0.59
2:B:52:LYS:O	2:B:203:ARG:NH2	2.27	0.59
2:B:101:THR:HG22	2:B:102:ARG:N	2.17	0.59
2:B:405:VAL:O	2:B:406:ALA:HB2	2.02	0.59
4:D:32:VAL:CG1	4:D:186:VAL:HG22	2.31	0.59
4:D:167:ASP:O	4:D:169:LEU:HD23	2.02	0.59
1:A:279:HIS:HA	1:A:307:PHE:CE1	2.36	0.59
2:B:24:LEU:H	2:B:24:LEU:HD23	1.67	0.59
2:B:258:VAL:CG1	2:B:321:LEU:HB3	2.29	0.59
3:C:110:TYR:HB3	3:C:113:THR:HG23	1.83	0.59
4:D:116:ILE:CG2	4:D:117:VAL:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.31	0.59
2:B:95:LYS:HB2	2:B:110:GLU:CG	2.32	0.59
3:C:27:ASN:HD22	6:F:69:ASN:HD21	1.43	0.59
3:C:136:TRP:CD1	3:C:176:LEU:HD13	2.37	0.59
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.37	0.59
1:A:102:LEU:O	1:A:104:LYS:N	2.35	0.59
1:A:381:ARG:O	1:A:382:GLU:C	2.46	0.59
1:A:61:HIS:CD2	1:A:134:ILE:HG12	2.37	0.59
2:B:101:THR:HB	2:B:104:ASN:OD1	2.02	0.59
2:B:207:VAL:HG11	2:B:382:VAL:HG23	1.83	0.59
3:C:45:GLN:CB	11:C:381:HEM:HAB	2.32	0.59
3:C:301:ILE:HD11	3:C:364:LEU:HD11	1.85	0.59
5:E:16:PRO:HD3	7:G:23:GLN:CA	2.33	0.59
2:B:406:ALA:O	2:B:408:ALA:N	2.35	0.59
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.38	0.59
1:A:252:HIS:ND1	1:A:325:VAL:HG22	2.18	0.59
3:C:120:LEU:CG	11:C:382:HEM:HAB	2.33	0.59
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.84	0.59
4:D:227:TRP:O	4:D:229:VAL:N	2.36	0.59
10:J:13:LEU:HA	10:J:19:THR:HG21	1.85	0.58
2:B:341:TYR:OH	2:B:422:LYS:HE3	2.02	0.58
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.85	0.58
4:D:182:VAL:O	4:D:186:VAL:HG23	2.03	0.58
2:B:353:SER:C	2:B:355:GLU:N	2.59	0.58
3:C:175:THR:HA	3:C:178:ARG:HG2	1.86	0.58
3:C:225:TYR:HA	3:C:228:LYS:HB3	1.86	0.58
3:C:346:HIS:O	3:C:350:ILE:HG12	2.02	0.58
5:E:96:LEU:HD12	5:E:135:LEU:O	2.04	0.58
2:B:171:ALA:C	2:B:173:ALA:H	2.10	0.58
3:C:45:GLN:HB3	11:C:381:HEM:HAB	1.86	0.58
5:E:12:ASP:O	5:E:13:TYR:C	2.46	0.58
1:A:151:ASN:ND2	5:E:2:HIS:NE2	2.51	0.58
2:B:95:LYS:HB2	2:B:110:GLU:HG2	1.85	0.58
3:C:347:PRO:HG3	7:G:66:PHE:HB2	1.86	0.58
2:B:357:VAL:HG12	2:B:361:LYS:CD	2.34	0.58
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.33	0.57
3:C:64:PHE:CD2	3:C:259:PRO:HG3	2.39	0.57
4:D:171:PHE:HE2	4:D:181:GLN:HE22	1.50	0.57
5:E:76:ILE:O	5:E:193:VAL:HG12	2.04	0.57
2:B:146:ILE:HG13	2:B:147:ASP:N	2.19	0.57
5:E:85:LYS:HD2	5:E:87:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ALA:O	1:A:11:VAL:HG23	2.04	0.57
3:C:220:PRO:HG2	3:C:223:PRO:HG2	1.86	0.57
2:B:112:LEU:HD23	2:B:112:LEU:N	2.19	0.57
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.36	0.57
4:D:2:ASP:OD2	7:G:70:LYS:HE2	2.04	0.57
1:A:88:ALA:CB	1:A:97:TYR:HA	2.32	0.57
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.57
2:B:258:VAL:HG13	2:B:322:PHE:H	1.68	0.57
1:A:356:ARG:O	1:A:357:GLY:C	2.47	0.57
3:C:89:SER:O	3:C:90:PHE:C	2.47	0.57
1:A:4:TYR:CB	2:B:113:ARG:HB3	2.35	0.57
1:A:130:GLU:O	1:A:134:ILE:HG13	2.04	0.57
2:B:19:PRO:C	2:B:21:PRO:HD3	2.29	0.57
4:D:3:LEU:HD23	4:D:4:GLU:N	2.20	0.57
4:D:165:TYR:O	4:D:168:VAL:HG23	2.05	0.57
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.87	0.57
3:C:245:LEU:O	4:D:201:ARG:HD3	2.04	0.57
3:C:330:VAL:CG2	3:C:331:ALA:N	2.68	0.57
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.87	0.57
4:D:232:SER:CB	7:G:23:GLN:HE22	2.17	0.57
7:G:77:TYR:CE1	8:H:52:GLU:HB2	2.39	0.57
1:A:297:ILE:HG21	1:A:337:VAL:HG11	1.85	0.56
4:D:30:PHE:HE2	4:D:64:LEU:HD21	1.68	0.56
5:E:17:PRO:HD3	7:G:24:ARG:NE	2.20	0.56
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.40	0.56
6:F:51:PRO:HD2	6:F:54:LEU:HD12	1.86	0.56
3:C:95:ILE:O	3:C:99:ILE:HG12	2.05	0.56
1:A:250:LEU:HD13	1:A:250:LEU:N	2.20	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.40	0.56
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.69	0.56
2:B:307:PHE:CD1	2:B:307:PHE:C	2.83	0.56
2:B:357:VAL:O	2:B:361:LYS:HG3	2.05	0.56
3:C:64:PHE:CE2	3:C:259:PRO:HG3	2.40	0.56
3:C:81:ARG:NH1	11:C:381:HEM:O1D	2.38	0.56
4:D:32:VAL:HG21	4:D:186:VAL:CG2	2.35	0.56
8:H:35:GLU:O	8:H:39:LEU:HD13	2.05	0.56
1:A:205:HIS:O	1:A:208:LEU:HB3	2.06	0.56
2:B:257:ILE:O	2:B:323:GLY:HA3	2.05	0.56
3:C:146:VAL:HG23	3:C:147:ILE:N	2.21	0.56
1:A:48:GLU:CD	1:A:53:ASN:HA	2.31	0.56
1:A:388:ARG:HG3	1:A:388:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:PRO:C	2:B:398:VAL:HG12	2.31	0.56
6:F:67:ASP:O	6:F:71:ARG:HG3	2.06	0.56
2:B:56:ARG:HB2	2:B:102:ARG:O	2.06	0.56
1:A:61:HIS:HD2	1:A:134:ILE:HG12	1.69	0.56
1:A:346:CYS:HB3	1:A:411:CYS:HB2	1.87	0.56
2:B:20:HIS:N	2:B:21:PRO:CD	2.64	0.56
2:B:101:THR:HG22	2:B:102:ARG:H	1.70	0.56
2:B:258:VAL:HA	2:B:322:PHE:O	2.06	0.56
3:C:156:TYR:C	3:C:158:GLY:H	2.13	0.56
3:C:293:LEU:N	3:C:293:LEU:HD22	2.21	0.56
3:C:373:LEU:HD23	3:C:373:LEU:O	2.05	0.56
6:F:12:TRP:HA	6:F:12:TRP:CE3	2.41	0.56
1:A:33:PRO:HG3	2:B:369:LEU:HD22	1.87	0.56
2:B:109:VAL:CG2	2:B:119:LEU:HD11	2.35	0.56
2:B:372:VAL:HG12	2:B:372:VAL:O	2.06	0.56
2:B:397:THR:O	2:B:401:GLN:HG2	2.05	0.56
3:C:20:ILE:C	3:C:22:LEU:H	2.14	0.55
3:C:157:ILE:HG12	3:C:157:ILE:O	2.06	0.55
2:B:140:LEU:C	2:B:142:PRO:HD2	2.30	0.55
2:B:250:ASP:O	2:B:251:SER:HB3	2.05	0.55
3:C:209:PRO:HG2	6:F:69:ASN:HD21	1.71	0.55
3:C:319:ARG:HH12	3:C:371:GLY:HA2	1.72	0.55
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.87	0.55
3:C:167:GLY:HA3	3:C:174:PRO:CG	2.36	0.55
4:D:207:LYS:O	4:D:211:MET:HG2	2.06	0.55
5:E:100:HIS:CD2	5:E:131:GLU:HB2	2.42	0.55
9:I:310:UNK:O	9:I:311:UNK:C	2.54	0.55
3:C:261:ASN:HD21	3:C:264:VAL:HG23	1.71	0.55
4:D:68:VAL:HG11	4:D:92:PRO:HG2	1.89	0.55
1:A:39:VAL:HA	1:A:196:VAL:O	2.06	0.55
1:A:108:LYS:O	1:A:112:LEU:HG	2.06	0.55
2:B:126:VAL:O	2:B:130:PRO:HG3	2.06	0.55
3:C:105:TYR:CD1	3:C:209:PRO:HA	2.41	0.55
3:C:246:PHE:C	3:C:248:PRO:HD3	2.32	0.55
5:E:98:VAL:HA	5:E:133:VAL:O	2.05	0.55
2:B:76:THR:HG22	2:B:82:SER:N	2.07	0.55
3:C:273:TRP:HA	3:C:276:LEU:HG	1.88	0.55
3:C:293:LEU:HD22	3:C:293:LEU:H	1.72	0.55
4:D:75:ASN:HB2	4:D:77:ASP:H	1.70	0.55
4:D:213:GLY:O	4:D:217:PRO:CD	2.54	0.55
4:D:215:LEU:O	4:D:219:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:ARG:O	7:G:12:HIS:HB2	2.07	0.55
1:A:291:SER:CB	1:A:356:ARG:HH22	2.17	0.55
1:A:307:PHE:CD1	1:A:307:PHE:C	2.84	0.55
2:B:248:ASN:HD22	2:B:249:GLY:N	2.05	0.55
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.07	0.55
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.16	0.55
4:D:130:LEU:HD11	4:D:158:ILE:CD1	2.35	0.55
6:F:12:TRP:HA	6:F:12:TRP:HE3	1.72	0.55
6:F:91:GLU:O	6:F:95:LYS:HG3	2.07	0.55
2:B:407:ASP:C	2:B:409:ASP:N	2.64	0.55
3:C:27:ASN:HB2	6:F:69:ASN:HD22	1.71	0.55
1:A:280:TYR:CG	1:A:281:ASP:N	2.75	0.55
1:A:291:SER:O	1:A:292:SER:C	2.48	0.55
3:C:3:PRO:HG2	3:C:4:ASN:H	1.71	0.55
5:E:77:LYS:HA	5:E:191:ASP:O	2.07	0.55
10:J:36:ASP:O	10:J:37:GLN:C	2.50	0.55
1:A:26:ALA:O	1:A:198:ALA:HA	2.07	0.54
1:A:346:CYS:HB3	1:A:411:CYS:CB	2.36	0.54
3:C:293:LEU:H	3:C:293:LEU:CD2	2.21	0.54
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.42	0.54
10:J:13:LEU:HA	10:J:19:THR:CG2	2.37	0.54
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.73	0.54
1:A:290:SER:O	1:A:291:SER:C	2.49	0.54
1:A:349:ILE:HD12	1:A:407:VAL:HG11	1.89	0.54
2:B:143:GLN:O	2:B:144:LEU:C	2.49	0.54
3:C:358:SER:O	3:C:362:ILE:HG13	2.06	0.54
4:D:181:GLN:CB	8:H:77:LEU:HD22	2.37	0.54
5:E:103:LYS:HA	5:E:106:ILE:HD12	1.89	0.54
1:A:58:PHE:CE1	1:A:127:ILE:HG23	2.42	0.54
1:A:85:HIS:O	1:A:99:ILE:HA	2.07	0.54
1:A:266:ASP:C	1:A:268:VAL:H	2.15	0.54
1:A:284:TYR:HE1	9:I:112:UNK:O	1.90	0.54
1:A:374:PRO:O	1:A:377:GLU:HB3	2.07	0.54
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.70	0.54
5:E:189:SER:OG	5:E:192:MET:HB2	2.08	0.54
3:C:166:TRP:HB2	3:C:175:THR:CG2	2.38	0.54
3:C:289:LEU:O	3:C:293:LEU:HD23	2.07	0.54
4:D:216:VAL:HG23	4:D:217:PRO:CD	2.37	0.54
5:E:48:ALA:O	5:E:49:TYR:C	2.51	0.54
2:B:414:ALA:O	2:B:417:PHE:HB3	2.08	0.54
2:B:109:VAL:HG22	2:B:119:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:LYS:O	4:D:66:GLU:HG2	2.07	0.54
3:C:133:VAL:HA	3:C:140:SER:HB3	1.90	0.54
5:E:52:LYS:C	5:E:52:LYS:HD3	2.33	0.54
2:B:400:GLN:O	2:B:404:ALA:HB2	2.06	0.54
4:D:165:TYR:CD2	4:D:168:VAL:HG22	2.43	0.54
7:G:60:THR:O	7:G:61:TRP:C	2.50	0.54
1:A:15:GLN:HB3	1:A:205:HIS:ND1	2.22	0.54
1:A:394:GLU:O	1:A:395:TRP:C	2.51	0.54
2:B:143:GLN:OE1	2:B:146:ILE:HD11	2.07	0.54
3:C:105:TYR:CE1	3:C:209:PRO:HA	2.43	0.54
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.89	0.54
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.38	0.54
5:E:164:HIS:CB	5:E:173:LYS:HB3	2.34	0.54
8:H:47:ARG:CD	8:H:48:SER:H	2.14	0.54
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.23	0.54
4:D:148:TYR:N	4:D:148:TYR:CD1	2.76	0.54
5:E:147:ILE:HD12	5:E:159:PRO:HD3	1.90	0.54
1:A:318:GLY:O	1:A:319:LEU:HD23	2.08	0.53
2:B:129:ALA:N	2:B:130:PRO:CD	2.69	0.53
3:C:34:PHE:CD1	3:C:37:LEU:HD12	2.42	0.53
4:D:117:VAL:O	4:D:123:GLY:HA2	2.08	0.53
6:F:59:MET:HA	6:F:59:MET:CE	2.34	0.53
1:A:40:TRP:CD1	1:A:40:TRP:N	2.77	0.53
2:B:59:ASN:C	2:B:61:SER:N	2.65	0.53
10:J:13:LEU:HG	10:J:23:THR:HG21	1.90	0.53
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.41	0.53
1:A:350:SER:HG	1:A:353:GLU:HG3	1.74	0.53
1:A:362:ARG:HH22	2:B:113:ARG:HH12	1.56	0.53
3:C:127:THR:CG2	3:C:186:LEU:HB3	2.37	0.53
2:B:213:HIS:N	2:B:214:PRO:HD2	2.24	0.53
2:B:305:ASN:CB	2:B:306:PRO:HD2	2.38	0.53
3:C:20:ILE:O	3:C:22:LEU:N	2.42	0.53
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.44	0.53
6:F:71:ARG:O	6:F:73:GLN:HG2	2.09	0.53
1:A:40:TRP:CZ3	1:A:377:GLU:CD	2.87	0.53
1:A:250:LEU:HD21	1:A:325:VAL:HG13	1.91	0.53
2:B:348:ALA:C	2:B:350:GLY:H	2.17	0.53
3:C:19:LEU:C	3:C:20:ILE:HG13	2.33	0.53
4:D:75:ASN:ND2	4:D:79:GLU:O	2.42	0.53
4:D:75:ASN:H	4:D:79:GLU:H	1.57	0.53
1:A:189:HIS:CD2	1:A:194:ARG:HH12	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:ILE:HD13	2:B:402:ILE:C	2.33	0.53
5:E:177:PRO:O	5:E:178:LEU:HD23	2.09	0.53
1:A:242:ARG:O	7:G:14:ILE:HA	2.09	0.52
2:B:109:VAL:HG13	2:B:119:LEU:HD21	1.91	0.52
2:B:353:SER:O	2:B:355:GLU:N	2.42	0.52
2:B:424:MET:HE3	2:B:436:VAL:HG13	1.90	0.52
4:D:32:VAL:HG21	4:D:186:VAL:HG22	1.91	0.52
6:F:16:ILE:O	6:F:19:TRP:HB3	2.09	0.52
6:F:91:GLU:HG2	6:F:95:LYS:HE3	1.89	0.52
1:A:253:VAL:O	1:A:323:TYR:HD1	1.92	0.52
2:B:361:LYS:NZ	2:B:403:ASP:HA	2.25	0.52
3:C:342:GLN:HE21	3:C:342:GLN:HA	1.73	0.52
1:A:88:ALA:CB	1:A:96:ALA:O	2.48	0.52
3:C:103:LEU:HD13	3:C:103:LEU:C	2.34	0.52
5:E:78:LEU:CD1	5:E:187:PHE:HE1	2.21	0.52
8:H:47:ARG:HD3	8:H:48:SER:N	2.17	0.52
1:A:114:ALA:HB2	1:A:216:PHE:CE1	2.45	0.52
1:A:281:ASP:C	1:A:283:THR:H	2.17	0.52
1:A:293:PRO:O	1:A:297:ILE:N	2.37	0.52
2:B:40:ASN:O	2:B:41:TYR:HB2	2.09	0.52
1:A:274:ASN:O	1:A:309:THR:HG21	2.09	0.52
2:B:66:SER:O	2:B:69:LEU:HB3	2.09	0.52
2:B:199:PHE:CA	2:B:204:MET:HE3	2.39	0.52
2:B:248:ASN:C	2:B:248:ASN:ND2	2.67	0.52
2:B:280:GLY:O	2:B:283:PRO:HG2	2.08	0.52
3:C:157:ILE:O	3:C:161:LEU:HG	2.09	0.52
3:C:206:SER:HB2	12:C:383:U10:H3M1	1.92	0.52
1:A:286:GLY:HA3	1:A:289:HIS:NE2	2.24	0.52
1:A:297:ILE:HG22	1:A:303:LEU:HD11	1.92	0.52
1:A:366:VAL:C	1:A:368:HIS:H	2.17	0.52
2:B:202:ALA:HB2	2:B:229:GLY:HA2	1.92	0.52
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.92	0.52
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.44	0.52
1:A:250:LEU:HB2	1:A:326:CYS:O	2.10	0.52
2:B:258:VAL:CG1	2:B:259:ALA:N	2.71	0.52
2:B:264:ILE:HG12	2:B:316:TYR:C	2.35	0.52
3:C:261:ASN:ND2	3:C:264:VAL:HG23	2.25	0.52
5:E:118:ARG:HB3	5:E:118:ARG:HH11	1.75	0.52
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.38	0.52
1:A:171:SER:O	1:A:175:ARG:HG3	2.10	0.52
1:A:431:LEU:HD23	1:A:432:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASP:C	1:A:268:VAL:N	2.66	0.51
1:A:350:SER:OG	1:A:353:GLU:HG3	2.09	0.51
3:C:164:TRP:CD1	3:C:165:ALA:N	2.78	0.51
4:D:12:TRP:HB3	4:D:14:HIS:CE1	2.46	0.51
7:G:77:TYR:CZ	8:H:52:GLU:HB2	2.45	0.51
2:B:113:ARG:HG3	2:B:114:ASP:H	1.75	0.51
2:B:150:VAL:HG23	2:B:151:ALA:N	2.24	0.51
2:B:399:LEU:CA	2:B:402:ILE:HG22	2.40	0.51
3:C:3:PRO:O	3:C:5:ILE:HG13	2.10	0.51
4:D:149:PHE:CE1	4:D:156:GLN:HB3	2.46	0.51
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.46	0.51
4:D:231:LYS:HA	6:F:70:MET:HE1	1.91	0.51
4:D:117:VAL:HG23	4:D:190:LEU:HB3	1.92	0.51
6:F:16:ILE:O	6:F:19:TRP:N	2.43	0.51
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.11	0.51
1:A:178:SER:O	1:A:182:LEU:HD23	2.11	0.51
2:B:259:ALA:O	2:B:260:GLU:C	2.53	0.51
1:A:102:LEU:C	1:A:104:LYS:N	2.67	0.51
2:B:262:ALA:O	2:B:263:ALA:HB2	2.10	0.51
3:C:233:LEU:O	3:C:237:LEU:HB2	2.10	0.51
4:D:29:GLY:O	4:D:32:VAL:HG13	2.11	0.51
5:E:86:ASN:ND2	5:E:156:TYR:HE2	2.09	0.51
1:A:250:LEU:CD2	1:A:325:VAL:HG13	2.40	0.51
1:A:438:ARG:C	1:A:440:GLY:H	2.19	0.51
2:B:132:PHE:CD2	2:B:191:LEU:CB	2.94	0.51
3:C:48:THR:O	3:C:52:LEU:HB2	2.11	0.51
4:D:3:LEU:HD22	8:H:59:PHE:HE2	1.75	0.51
4:D:5:LEU:HB2	8:H:59:PHE:CD1	2.46	0.51
1:A:86:LEU:O	9:I:312:UNK:O	2.28	0.51
1:A:382:GLU:HG2	1:A:389:ARG:HD2	1.91	0.51
1:A:388:ARG:HG2	1:A:389:ARG:N	2.26	0.51
4:D:37:CYS:O	4:D:39:SER:N	2.43	0.51
4:D:57:THR:HB	4:D:60:GLU:HB2	1.93	0.51
1:A:343:MET:O	1:A:347:THR:HG22	2.11	0.51
1:A:444:LEU:O	1:A:445:ARG:O	2.28	0.51
2:B:162:ASN:CB	2:B:244:ILE:HD11	2.34	0.51
2:B:166:ALA:HB1	2:B:242:GLY:C	2.36	0.51
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.41	0.51
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.26	0.51
1:A:19:LEU:C	1:A:21:ASN:H	2.18	0.51
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:VAL:O	2:B:282:ASN:ND2	2.44	0.51
3:C:372:THR:O	3:C:375:ASN:N	2.43	0.51
3:C:373:LEU:HD23	3:C:373:LEU:C	2.36	0.51
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.46	0.51
5:E:78:LEU:HD21	5:E:193:VAL:HB	1.93	0.51
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.11	0.51
1:A:100:LYS:HE3	2:B:370:MET:CE	2.41	0.50
1:A:444:LEU:C	1:A:445:ARG:O	2.54	0.50
2:B:245:ARG:HB3	2:B:430:LEU:HD13	1.93	0.50
3:C:142:TRP:HA	3:C:145:THR:OG1	2.11	0.50
3:C:146:VAL:HG23	3:C:147:ILE:H	1.76	0.50
4:D:72:ASP:O	4:D:73:GLY:O	2.29	0.50
10:J:4:THR:O	10:J:5:LEU:C	2.53	0.50
1:A:42:ASP:CB	1:A:194:ARG:HB3	2.30	0.50
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.41	0.50
1:A:153:LEU:HD23	1:A:153:LEU:C	2.36	0.50
1:A:252:HIS:HB2	1:A:425:PRO:HD2	1.93	0.50
2:B:207:VAL:HG12	2:B:208:GLY:H	1.76	0.50
3:C:281:ILE:HG22	3:C:281:ILE:O	2.10	0.50
10:J:59:TYR:CD1	10:J:59:TYR:N	2.78	0.50
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.94	0.50
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.93	0.50
3:C:377:MET:HE2	6:F:20:TYR:CG	2.46	0.50
5:E:117:LEU:HD12	5:E:121:GLN:H	1.74	0.50
4:D:28:ARG:HD2	4:D:171:PHE:CE2	2.46	0.50
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.93	0.50
5:E:38:LEU:O	5:E:42:VAL:HG23	2.12	0.50
1:A:4:TYR:HB2	2:B:113:ARG:CB	2.40	0.50
1:A:106:VAL:HG21	1:A:203:VAL:CG1	2.40	0.50
1:A:106:VAL:CG2	1:A:203:VAL:HG22	2.41	0.50
2:B:109:VAL:HG13	2:B:109:VAL:O	2.11	0.50
2:B:368:TYR:O	2:B:372:VAL:HG23	2.12	0.50
4:D:227:TRP:O	4:D:228:SER:C	2.52	0.50
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.93	0.50
1:A:15:GLN:HB3	1:A:205:HIS:CE1	2.47	0.50
1:A:49:SER:N	1:A:52:ASN:HB3	2.16	0.50
1:A:253:VAL:HG11	1:A:335:MET:CE	2.41	0.50
2:B:135:TRP:H	2:B:135:TRP:CD1	2.30	0.50
5:E:12:ASP:N	5:E:20:TYR:HE2	2.10	0.50
8:H:73:LEU:C	8:H:73:LEU:CD2	2.84	0.50
1:A:245:GLU:C	1:A:247:GLY:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:LEU:HG	2:B:233:SER:N	2.23	0.50
3:C:86:ASN:OD1	3:C:244:ALA:HA	2.12	0.50
1:A:95:THR:HG22	1:A:96:ALA:N	2.27	0.50
1:A:444:LEU:HD12	1:A:444:LEU:H	1.76	0.50
2:B:62:ASN:O	2:B:65:THR:CG2	2.59	0.50
5:E:9:ASN:HD21	5:E:11:SER:HB3	1.76	0.50
5:E:14:ARG:HG2	5:E:14:ARG:NH1	2.17	0.50
9:I:313:UNK:CB	9:I:314:UNK:CD	2.90	0.50
2:B:131:GLU:O	2:B:131:GLU:HG3	2.11	0.49
1:A:292:SER:N	1:A:293:PRO:CD	2.71	0.49
4:D:37:CYS:C	4:D:39:SER:H	2.20	0.49
5:E:136:ILE:HG22	5:E:138:VAL:HG23	1.92	0.49
6:F:25:GLY:C	6:F:27:ASN:H	2.21	0.49
7:G:24:ARG:HB2	7:G:27:PRO:HB3	1.94	0.49
10:J:57:HIS:HB2	10:J:62:LYS:CB	2.42	0.49
1:A:106:VAL:HB	1:A:107:PRO:CD	2.42	0.49
1:A:339:GLN:OE1	1:A:437:ILE:O	2.30	0.49
3:C:9:HIS:HD2	3:C:10:PRO:CD	2.23	0.49
4:D:43:MET:CE	4:D:46:VAL:HG21	2.37	0.49
4:D:150:ASN:O	4:D:156:GLN:HA	2.13	0.49
1:A:391:PRO:O	1:A:392:LEU:C	2.53	0.49
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.18	0.49
1:A:349:ILE:HG22	1:A:408:ARG:HG3	1.93	0.49
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.75	0.49
4:D:27:ARG:CZ	10:J:59:TYR:CE2	2.95	0.49
4:D:180:SER:HB2	8:H:17:LEU:HB2	1.94	0.49
5:E:135:LEU:HD13	5:E:180:LEU:HD12	1.95	0.49
5:E:147:ILE:HD11	5:E:159:PRO:HG3	1.94	0.49
8:H:73:LEU:C	8:H:73:LEU:HD23	2.38	0.49
3:C:369:THR:C	3:C:371:GLY:N	2.67	0.49
5:E:29:ASP:OD1	5:E:32:ARG:HB2	2.13	0.49
5:E:60:SER:C	5:E:62:MET:N	2.61	0.49
5:E:109:GLU:CD	5:E:166:ASP:HB2	2.38	0.49
1:A:106:VAL:N	1:A:107:PRO:HD2	2.27	0.49
1:A:338:LEU:O	1:A:341:GLN:N	2.45	0.49
2:B:170:ASN:H	2:B:170:ASN:HD22	1.60	0.49
3:C:112:GLU:CD	3:C:112:GLU:H	2.13	0.49
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.77	0.49
3:C:318:PHE:CG	6:F:26:PHE:HB3	2.48	0.49
3:C:377:MET:CE	6:F:20:TYR:HB2	2.43	0.49
1:A:48:GLU:CD	1:A:54:GLY:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:O	1:A:106:VAL:C	2.55	0.49
2:B:56:ARG:O	2:B:56:ARG:HD3	2.13	0.49
2:B:372:VAL:O	2:B:378:PHE:HB2	2.13	0.49
3:C:141:PHE:HE1	3:C:171:VAL:O	1.96	0.49
3:C:147:ILE:HD11	3:C:271:PRO:HB3	1.94	0.49
8:H:49:GLN:O	8:H:49:GLN:HG2	2.11	0.49
2:B:24:LEU:HD23	2:B:24:LEU:N	2.27	0.49
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.95	0.49
3:C:120:LEU:CD1	3:C:190:ILE:HG23	2.43	0.49
5:E:42:VAL:O	5:E:45:LEU:HB3	2.13	0.49
5:E:136:ILE:HG13	5:E:181:GLU:CG	2.41	0.49
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.46	0.49
1:A:74:ALA:O	1:A:75:LEU:C	2.55	0.48
1:A:240:GLN:OE1	1:A:434:TYR:HB2	2.13	0.48
1:A:320:PHE:CE2	1:A:415:ILE:HD11	2.48	0.48
2:B:58:GLU:OE2	2:B:65:THR:HG22	2.13	0.48
3:C:130:VAL:HG13	3:C:179:PHE:CG	2.48	0.48
4:D:97:ASN:O	4:D:100:ALA:HB3	2.12	0.48
5:E:15:ARG:NH1	5:E:19:ASP:HB3	2.28	0.48
7:G:73:ASN:O	7:G:75:ALA:N	2.46	0.48
2:B:61:SER:O	2:B:62:ASN:OD1	2.31	0.48
3:C:125:MET:O	3:C:126:ALA:C	2.57	0.48
3:C:130:VAL:HG13	3:C:179:PHE:CB	2.42	0.48
3:C:283:ARG:NH2	3:C:339:ILE:O	2.46	0.48
4:D:181:GLN:C	4:D:181:GLN:NE2	2.71	0.48
1:A:288:LEU:HD22	2:B:83:PHE:CD1	2.45	0.48
1:A:305:GLN:O	1:A:306:SER:HB3	2.13	0.48
2:B:187:THR:OG1	2:B:190:GLU:HG3	2.13	0.48
2:B:429:ASN:O	2:B:430:LEU:HB2	2.13	0.48
4:D:21:LEU:CD1	4:D:26:ILE:HD11	2.42	0.48
5:E:19:ASP:C	5:E:20:TYR:CD1	2.91	0.48
8:H:37:LEU:HD13	8:H:37:LEU:C	2.37	0.48
2:B:89:ILE:CD1	2:B:96:LEU:HB2	2.44	0.48
3:C:220:PRO:HG2	3:C:223:PRO:CG	2.43	0.48
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.48	0.48
3:C:333:LEU:HD11	3:C:359:TYR:CE1	2.48	0.48
7:G:29:TYR:CD1	7:G:29:TYR:N	2.80	0.48
1:A:19:LEU:C	1:A:21:ASN:N	2.69	0.48
1:A:40:TRP:HZ3	1:A:377:GLU:CD	2.21	0.48
1:A:431:LEU:HD23	1:A:432:PRO:CD	2.43	0.48
2:B:399:LEU:O	2:B:402:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:TYR:CB	3:C:113:THR:HG23	2.44	0.48
3:C:344:VAL:HG23	3:C:344:VAL:O	2.12	0.48
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.95	0.48
5:E:21:SER:O	5:E:22:THR:OG1	2.23	0.48
5:E:35:PHE:O	5:E:38:LEU:HB3	2.13	0.48
6:F:13:LEU:N	6:F:13:LEU:HD12	2.28	0.48
8:H:62:LEU:O	8:H:66:ASP:OD1	2.32	0.48
1:A:391:PRO:O	1:A:394:GLU:N	2.40	0.48
2:B:72:ALA:O	2:B:73:SER:C	2.56	0.48
3:C:312:LYS:HG2	3:C:375:ASN:OD1	2.13	0.48
4:D:153:PHE:CG	4:D:158:ILE:HG12	2.49	0.48
4:D:211:MET:CG	14:D:242:BOG:H5'1	2.42	0.48
5:E:11:SER:CA	5:E:15:ARG:HD2	2.40	0.48
1:A:288:LEU:HD13	2:B:83:PHE:HA	1.96	0.48
1:A:366:VAL:C	1:A:368:HIS:N	2.71	0.48
1:A:408:ARG:O	1:A:409:GLU:C	2.56	0.48
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.96	0.48
2:B:112:LEU:O	2:B:113:ARG:C	2.57	0.48
3:C:329:LEU:O	3:C:330:VAL:C	2.57	0.48
2:B:232:LEU:CG	2:B:233:SER:H	2.20	0.48
2:B:63:LEU:C	2:B:65:THR:H	2.22	0.48
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.29	0.48
4:D:68:VAL:HG11	4:D:92:PRO:CG	2.44	0.48
4:D:220:TYR:O	4:D:224:ARG:HG2	2.13	0.48
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.24	0.48
1:A:65:LYS:HZ3	9:I:311:UNK:HA	1.78	0.48
2:B:39:GLU:HG3	2:B:41:TYR:CD1	2.48	0.48
2:B:141:GLN:N	2:B:142:PRO:HD2	2.29	0.48
2:B:360:ALA:O	2:B:361:LYS:C	2.57	0.48
3:C:280:ALA:C	3:C:282:LEU:N	2.71	0.48
4:D:29:GLY:O	4:D:30:PHE:C	2.57	0.48
8:H:50:THR:CG2	8:H:52:GLU:H	2.23	0.48
1:A:59:LEU:HD12	1:A:59:LEU:O	2.14	0.47
1:A:444:LEU:HD12	1:A:444:LEU:N	2.29	0.47
2:B:430:LEU:O	2:B:433:THR:N	2.36	0.47
4:D:220:TYR:CZ	4:D:224:ARG:HD3	2.49	0.47
5:E:29:ASP:N	5:E:30:PRO:HD2	2.28	0.47
7:G:38:TRP:C	7:G:40:ARG:N	2.69	0.47
1:A:146:ARG:HG3	1:A:323:TYR:OH	2.15	0.47
2:B:166:ALA:HB1	2:B:242:GLY:CA	2.44	0.47
2:B:214:PRO:HG2	2:B:215:VAL:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.94	0.47
3:C:285:ILE:HG23	3:C:291:GLY:HA2	1.97	0.47
4:D:141:VAL:HG21	8:H:55:THR:HG23	1.95	0.47
4:D:222:MET:CE	5:E:40:THR:HG23	2.45	0.47
8:H:20:VAL:HG12	8:H:20:VAL:O	2.13	0.47
1:A:373:THR:N	1:A:374:PRO:HD2	2.29	0.47
2:B:114:ASP:C	2:B:116:VAL:H	2.22	0.47
8:H:72:LYS:O	8:H:73:LEU:C	2.56	0.47
1:A:254:ALA:O	1:A:422:VAL:HA	2.14	0.47
1:A:292:SER:O	1:A:295:ALA:N	2.44	0.47
1:A:349:ILE:CD1	1:A:407:VAL:HG11	2.44	0.47
1:A:397:GLU:O	1:A:398:ARG:C	2.57	0.47
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.49	0.47
2:B:395:PRO:CA	2:B:398:VAL:HG12	2.44	0.47
3:C:108:TYR:HB3	3:C:114:TRP:CE3	2.48	0.47
3:C:118:VAL:HB	3:C:303:PHE:CE1	2.49	0.47
8:H:59:PHE:O	8:H:60:ASP:C	2.57	0.47
1:A:65:LYS:NZ	9:I:311:UNK:N	2.63	0.47
2:B:31:ASN:HB3	2:B:201:SER:CB	2.43	0.47
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.15	0.47
3:C:148:THR:HG21	3:C:166:TRP:CE3	2.50	0.47
3:C:326:PHE:O	3:C:329:LEU:HB3	2.15	0.47
7:G:57:LEU:HD22	7:G:57:LEU:H	1.79	0.47
1:A:418:GLN:O	1:A:420:PRO:HD3	2.14	0.47
2:B:75:LEU:HD11	2:B:140:LEU:HD22	1.96	0.47
2:B:258:VAL:HG11	2:B:321:LEU:CB	2.37	0.47
3:C:325:LEU:CD2	3:C:362:ILE:HG23	2.42	0.47
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.27	0.47
4:D:204:MET:HE2	14:D:242:BOG:H1	1.96	0.47
5:E:123:ASP:HA	5:E:126:ARG:HD3	1.97	0.47
2:B:24:LEU:HD11	2:B:392:TYR:CG	2.50	0.47
2:B:170:ASN:H	2:B:170:ASN:ND2	2.13	0.47
2:B:361:LYS:O	2:B:365:LYS:HG3	2.14	0.47
3:C:78:TRP:CG	4:D:197:GLU:HG2	2.50	0.47
3:C:292:VAL:O	3:C:295:LEU:HB3	2.15	0.47
3:C:342:GLN:HB3	3:C:343:PRO:HD2	1.97	0.47
5:E:14:ARG:NH1	5:E:14:ARG:CG	2.74	0.47
5:E:124:LEU:HA	5:E:127:VAL:HG22	1.96	0.47
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.97	0.47
7:G:41:LEU:O	7:G:41:LEU:HD13	2.15	0.47
1:A:149:VAL:HG13	1:A:150:PHE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:O	1:A:164:ALA:HB2	2.15	0.47
1:A:178:SER:C	1:A:180:ALA:N	2.68	0.47
4:D:102:ARG:HG2	4:D:109:LEU:HB2	1.96	0.47
4:D:165:TYR:O	4:D:168:VAL:CG2	2.63	0.47
2:B:252:LEU:HD23	2:B:252:LEU:N	2.29	0.47
2:B:317:SER:OG	2:B:318:ASP:N	2.47	0.47
3:C:51:LEU:HG	3:C:80:ILE:HD13	1.97	0.47
3:C:278:ALA:HB1	3:C:295:LEU:HD12	1.96	0.47
4:D:3:LEU:HD22	8:H:59:PHE:CE2	2.49	0.47
6:F:82:LYS:O	6:F:83:TYR:C	2.57	0.47
10:J:5:LEU:O	10:J:6:THR:C	2.57	0.47
1:A:240:GLN:NE2	1:A:242:ARG:HE	2.13	0.47
2:B:281:ALA:O	2:B:285:VAL:HB	2.15	0.47
3:C:103:LEU:HD12	3:C:326:PHE:CE1	2.50	0.47
4:D:75:ASN:CB	4:D:77:ASP:H	2.27	0.47
7:G:25:PRO:C	7:G:27:PRO:HD3	2.40	0.47
1:A:40:TRP:HZ3	1:A:377:GLU:OE2	1.97	0.46
2:B:323:GLY:O	2:B:324:PHE:HB3	2.15	0.46
2:B:338:LYS:O	2:B:341:TYR:HB3	2.16	0.46
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.51	0.46
5:E:16:PRO:O	5:E:18:ASP:N	2.47	0.46
6:F:60:PHE:CD1	7:G:13:LEU:HD22	2.49	0.46
1:A:382:GLU:HA	1:A:386:TYR:HD2	1.79	0.46
2:B:68:LEU:HD23	2:B:186:VAL:HG11	1.96	0.46
4:D:28:ARG:O	4:D:29:GLY:C	2.58	0.46
4:D:197:GLU:O	4:D:198:HIS:C	2.58	0.46
5:E:17:PRO:HD3	7:G:24:ARG:HH21	1.80	0.46
1:A:144:SER:O	1:A:146:ARG:N	2.48	0.46
2:B:70:ARG:HD3	2:B:100:SER:CB	2.45	0.46
2:B:146:ILE:O	2:B:147:ASP:C	2.57	0.46
3:C:38:LEU:HD11	3:C:95:ILE:HA	1.97	0.46
3:C:330:VAL:HG23	3:C:331:ALA:N	2.30	0.46
4:D:54:VAL:HG11	4:D:192:TRP:CH2	2.50	0.46
4:D:178:THR:O	4:D:179:MET:C	2.57	0.46
6:F:52:GLU:O	6:F:53:ASN:C	2.58	0.46
1:A:27:SER:HA	1:A:199:ALA:O	2.15	0.46
2:B:84:LYS:O	2:B:88:GLY:N	2.48	0.46
4:D:221:TYR:CE1	7:G:25:PRO:HG2	2.51	0.46
5:E:99:ARG:HB3	5:E:133:VAL:HG11	1.96	0.46
5:E:129:LYS:HA	5:E:130:PRO:HD3	1.73	0.46
5:E:163:SER:OG	5:E:176:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:OE1	1:A:53:ASN:ND2	2.49	0.46
2:B:57:TYR:N	2:B:57:TYR:CD1	2.84	0.46
2:B:379:LEU:O	2:B:382:VAL:HG22	2.16	0.46
3:C:346:HIS:ND1	3:C:346:HIS:C	2.72	0.46
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.80	0.46
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.45	0.46
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.84	0.46
2:B:170:ASN:HD22	2:B:170:ASN:C	2.24	0.46
2:B:433:THR:HG23	2:B:434:PRO:HD2	1.98	0.46
3:C:150:LEU:O	3:C:151:PHE:C	2.59	0.46
1:A:72:GLN:O	1:A:73:ASN:C	2.59	0.46
1:A:268:VAL:CG1	1:A:399:LEU:HB3	2.45	0.46
1:A:362:ARG:NH2	2:B:113:ARG:NH1	2.63	0.46
2:B:258:VAL:HG12	2:B:259:ALA:H	1.80	0.46
2:B:258:VAL:HG13	2:B:322:PHE:N	2.30	0.46
2:B:405:VAL:CG1	2:B:406:ALA:H	2.26	0.46
5:E:163:SER:HA	5:E:174:GLY:HA3	1.97	0.46
6:F:62:ILE:O	6:F:66:LEU:HG	2.15	0.46
8:H:73:LEU:HD23	8:H:73:LEU:O	2.16	0.46
3:C:350:ILE:HD13	3:C:350:ILE:N	2.31	0.46
1:A:24:ARG:HG3	1:A:24:ARG:HH11	1.81	0.46
1:A:156:THR:HG23	1:A:157:ALA:N	2.30	0.46
1:A:410:VAL:O	1:A:411:CYS:C	2.59	0.46
2:B:282:ASN:HB2	2:B:283:PRO:CD	2.46	0.46
5:E:141:HIS:HA	5:E:177:PRO:HD2	1.97	0.46
1:A:48:GLU:OE2	1:A:54:GLY:N	2.44	0.46
2:B:59:ASN:C	2:B:61:SER:H	2.22	0.46
3:C:280:ALA:C	3:C:282:LEU:H	2.24	0.46
3:C:301:ILE:HD11	3:C:364:LEU:CD1	2.45	0.46
3:C:348:PHE:O	3:C:349:ILE:C	2.59	0.46
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.51	0.46
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.84	0.46
4:D:124:GLU:O	4:D:125:ASP:C	2.59	0.46
4:D:132:THR:HG21	4:D:180:SER:HA	1.97	0.46
5:E:123:ASP:H	5:E:170:ARG:NH1	2.14	0.46
8:H:59:PHE:O	8:H:62:LEU:N	2.49	0.46
2:B:168:TYR:CE2	2:B:172:LEU:HD23	2.50	0.45
2:B:258:VAL:HG11	2:B:321:LEU:HD22	1.98	0.45
2:B:397:THR:HA	2:B:400:GLN:CB	2.46	0.45
4:D:98:PRO:O	4:D:101:ALA:N	2.48	0.45
5:E:17:PRO:HG3	7:G:24:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:CG2	1:A:100:LYS:HB3	2.38	0.45
1:A:65:LYS:HD2	1:A:65:LYS:N	2.30	0.45
2:B:137:VAL:CG2	2:B:138:ALA:N	2.78	0.45
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.35	0.45
4:D:75:ASN:OD1	4:D:79:GLU:HB2	2.16	0.45
5:E:52:LYS:O	5:E:56:THR:HG23	2.17	0.45
1:A:430:GLN:O	1:A:430:GLN:HG2	2.15	0.45
2:B:258:VAL:CG1	2:B:259:ALA:H	2.30	0.45
3:C:164:TRP:O	3:C:165:ALA:C	2.60	0.45
3:C:366:LEU:O	3:C:367:PHE:C	2.60	0.45
4:D:43:MET:HE3	4:D:46:VAL:CG2	2.40	0.45
4:D:231:LYS:HD3	6:F:70:MET:HE1	1.97	0.45
1:A:116:ILE:C	1:A:118:GLN:H	2.25	0.45
1:A:192:ALA:N	1:A:193:PRO:HD2	2.31	0.45
1:A:249:PRO:HG2	1:A:250:LEU:HD13	1.98	0.45
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.98	0.45
2:B:130:PRO:HB3	2:B:132:PHE:CE1	2.51	0.45
2:B:361:LYS:HZ1	2:B:403:ASP:HA	1.79	0.45
3:C:137:GLY:H	3:C:140:SER:HB2	1.81	0.45
3:C:327:TRP:HZ2	13:C:384:PEE:H7	1.81	0.45
5:E:12:ASP:N	5:E:20:TYR:CE2	2.84	0.45
5:E:78:LEU:HD11	5:E:187:PHE:HE1	1.80	0.45
1:A:261:GLY:O	1:A:262:TRP:C	2.60	0.45
1:A:405:ARG:CA	1:A:408:ARG:HH21	2.30	0.45
2:B:171:ALA:C	2:B:173:ALA:N	2.75	0.45
3:C:20:ILE:C	3:C:22:LEU:N	2.74	0.45
3:C:210:LEU:O	3:C:212:ILE:HG23	2.16	0.45
3:C:287:ASN:O	3:C:288:LYS:C	2.58	0.45
4:D:164:ILE:O	4:D:179:MET:HG3	2.17	0.45
3:C:40:VAL:HG21	3:C:233:LEU:HD21	1.98	0.45
4:D:28:ARG:O	4:D:31:GLN:HB2	2.17	0.45
5:E:11:SER:C	5:E:13:TYR:N	2.75	0.45
7:G:36:ASN:HA	7:G:39:ARG:HB2	1.99	0.45
1:A:178:SER:O	1:A:179:ARG:C	2.58	0.45
1:A:250:LEU:C	1:A:250:LEU:CD2	2.90	0.45
1:A:306:SER:HB2	9:I:206:UNK:CB	2.47	0.45
1:A:365:LEU:HD22	1:A:365:LEU:O	2.17	0.45
3:C:27:ASN:CB	6:F:69:ASN:HD22	2.29	0.45
4:D:1:SER:C	4:D:3:LEU:H	2.24	0.45
7:G:38:TRP:C	7:G:40:ARG:H	2.23	0.45
4:D:118:ARG:HD3	4:D:191:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:181:GLN:CG	8:H:77:LEU:HD22	2.47	0.45
5:E:78:LEU:HD11	5:E:187:PHE:CE1	2.52	0.45
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.51	0.45
5:E:121:GLN:OE1	5:E:126:ARG:NH1	2.44	0.45
1:A:36:THR:HG23	1:A:372:THR:OG1	2.17	0.45
1:A:92:ARG:HH12	1:A:166:SER:HA	1.81	0.45
1:A:170:PRO:HG2	1:A:173:ASN:HB2	1.97	0.45
3:C:59:ASP:O	3:C:60:THR:C	2.60	0.45
3:C:295:LEU:O	3:C:298:SER:OG	2.32	0.45
10:J:33:ARG:O	10:J:37:GLN:HG3	2.17	0.45
1:A:62:LEU:CD1	1:A:127:ILE:HG12	2.45	0.45
1:A:239:SER:O	1:A:421:ALA:HA	2.16	0.45
1:A:245:GLU:C	1:A:247:GLY:N	2.73	0.45
1:A:396:GLU:O	1:A:400:ALA:N	2.50	0.45
2:B:137:VAL:HG23	2:B:138:ALA:N	2.30	0.45
3:C:261:ASN:ND2	3:C:264:VAL:CG2	2.80	0.45
4:D:81:PHE:CD1	4:D:81:PHE:C	2.95	0.45
4:D:231:LYS:HD3	6:F:70:MET:CE	2.47	0.45
5:E:9:ASN:OD1	5:E:11:SER:HB2	2.17	0.45
5:E:182:VAL:HA	5:E:183:PRO:HD2	1.83	0.45
6:F:34:ASP:OD2	6:F:90:LEU:HB3	2.17	0.45
1:A:281:ASP:C	1:A:283:THR:N	2.75	0.44
2:B:232:LEU:O	2:B:233:SER:HB3	2.16	0.44
3:C:27:ASN:CB	6:F:69:ASN:ND2	2.77	0.44
3:C:319:ARG:NH1	3:C:374:GLU:HB3	2.32	0.44
4:D:116:ILE:CG2	4:D:190:LEU:HD13	2.47	0.44
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.52	0.44
5:E:69:LEU:O	5:E:72:SER:HB3	2.17	0.44
1:A:410:VAL:O	1:A:413:LYS:N	2.49	0.44
2:B:65:THR:O	2:B:69:LEU:HB2	2.17	0.44
2:B:70:ARG:NE	9:I:107:UNK:CB	2.80	0.44
2:B:399:LEU:HA	2:B:402:ILE:CG2	2.43	0.44
3:C:145:THR:O	3:C:149:ASN:HB2	2.18	0.44
3:C:361:THR:HA	3:C:365:ILE:HG22	2.00	0.44
4:D:32:VAL:CG2	4:D:186:VAL:HG22	2.47	0.44
4:D:138:PRO:HB3	8:H:58:LEU:HD22	1.99	0.44
5:E:59:VAL:O	5:E:59:VAL:CG1	2.66	0.44
1:A:365:LEU:CD1	1:A:392:LEU:HD22	2.47	0.44
2:B:24:LEU:HD11	2:B:392:TYR:CD1	2.52	0.44
2:B:59:ASN:O	2:B:61:SER:O	2.35	0.44
2:B:89:ILE:HD11	2:B:96:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:TYR:CD2	3:C:316:MET:HB2	2.52	0.44
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.45	0.44
5:E:55:VAL:O	5:E:59:VAL:HG23	2.17	0.44
5:E:121:GLN:NE2	5:E:126:ARG:HG3	2.32	0.44
1:A:65:LYS:NZ	9:I:311:UNK:HA	2.32	0.44
1:A:114:ALA:CB	1:A:216:PHE:CE1	3.01	0.44
1:A:153:LEU:C	1:A:153:LEU:CD2	2.90	0.44
1:A:369:LEU:HD21	1:A:378:ASP:OD2	2.18	0.44
2:B:61:SER:C	2:B:63:LEU:H	2.26	0.44
2:B:402:ILE:HD13	2:B:402:ILE:O	2.17	0.44
3:C:150:LEU:C	3:C:152:SER:N	2.76	0.44
6:F:93:TYR:O	6:F:94:LEU:C	2.60	0.44
1:A:123:GLU:HG3	1:A:125:SER:OG	2.18	0.44
1:A:349:ILE:HG22	1:A:408:ARG:CD	2.47	0.44
2:B:96:LEU:HD23	2:B:96:LEU:C	2.42	0.44
2:B:143:GLN:O	2:B:146:ILE:HG12	2.18	0.44
3:C:41:CYS:SG	3:C:91:PHE:HA	2.57	0.44
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.99	0.44
4:D:178:THR:O	4:D:182:VAL:HG12	2.17	0.44
1:A:266:ASP:O	1:A:268:VAL:N	2.50	0.44
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.98	0.44
4:D:57:THR:HG22	4:D:58:GLU:N	2.32	0.44
4:D:175:THR:HA	4:D:176:PRO:HD3	1.73	0.44
5:E:171:ILE:HG12	5:E:176:ALA:O	2.18	0.44
6:F:29:TYR:HB2	6:F:31:LEU:CD2	2.48	0.44
7:G:24:ARG:HA	7:G:25:PRO:HD3	1.68	0.44
1:A:114:ALA:HA	1:A:216:PHE:HE1	1.82	0.44
2:B:170:ASN:HD22	2:B:170:ASN:N	2.15	0.44
3:C:161:LEU:O	3:C:164:TRP:HD1	2.00	0.44
3:C:227:PHE:CE1	4:D:222:MET:HE2	2.53	0.44
4:D:55:CYS:SG	4:D:56:TYR:HD2	2.40	0.44
4:D:116:ILE:CG2	4:D:117:VAL:H	2.30	0.44
8:H:63:HIS:O	8:H:63:HIS:ND1	2.51	0.44
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.18	0.44
1:A:276:ILE:CD1	1:A:349:ILE:HD11	2.48	0.44
1:A:346:CYS:HB2	1:A:412:SER:N	2.33	0.44
3:C:92:PHE:O	3:C:95:ILE:HG22	2.18	0.44
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.47	0.44
3:C:311:SER:CB	3:C:316:MET:HE1	2.47	0.44
3:C:327:TRP:NE1	7:G:48:VAL:HG22	2.33	0.44
3:C:359:TYR:HD2	3:C:360:PHE:CE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:LEU:C	4:D:54:VAL:HG12	2.42	0.44
4:D:147:LEU:HD22	4:D:147:LEU:N	2.32	0.44
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.83	0.44
1:A:64:PHE:O	1:A:66:GLY:N	2.51	0.44
1:A:85:HIS:ND1	2:B:370:MET:HE1	2.33	0.44
1:A:228:VAL:O	1:A:228:VAL:HG13	2.17	0.44
1:A:281:ASP:O	1:A:284:TYR:CD1	2.71	0.44
1:A:373:THR:HB	1:A:374:PRO:CD	2.47	0.44
2:B:332:TYR:O	2:B:336:VAL:HG23	2.18	0.44
3:C:311:SER:HB2	3:C:316:MET:HE1	1.99	0.44
2:B:241:GLY:CA	2:B:421:GLN:HE21	2.12	0.43
2:B:250:ASP:O	2:B:251:SER:CB	2.66	0.43
2:B:424:MET:HG2	2:B:425:ALA:H	1.78	0.43
3:C:329:LEU:O	3:C:332:ASN:HB3	2.18	0.43
3:C:346:HIS:ND1	3:C:347:PRO:N	2.65	0.43
5:E:16:PRO:HG3	5:E:32:ARG:HH11	1.82	0.43
5:E:134:ILE:HD12	5:E:185:TYR:CE2	2.53	0.43
5:E:136:ILE:HG12	5:E:181:GLU:O	2.17	0.43
7:G:36:ASN:HA	7:G:39:ARG:CB	2.48	0.43
1:A:284:TYR:HD2	1:A:289:HIS:CE1	2.37	0.43
1:A:349:ILE:CG2	1:A:408:ARG:HG3	2.48	0.43
2:B:150:VAL:CG2	2:B:151:ALA:N	2.81	0.43
2:B:194:PHE:O	2:B:198:HIS:ND1	2.40	0.43
3:C:121:LEU:HD11	3:C:125:MET:HE3	2.00	0.43
3:C:344:VAL:O	3:C:349:ILE:HD11	2.18	0.43
4:D:28:ARG:O	4:D:31:GLN:N	2.51	0.43
5:E:29:ASP:C	5:E:31:SER:N	2.72	0.43
6:F:70:MET:HE2	6:F:71:ARG:N	2.32	0.43
1:A:41:ILE:HD12	1:A:195:MET:SD	2.59	0.43
1:A:438:ARG:C	1:A:438:ARG:HD3	2.43	0.43
2:B:150:VAL:HA	2:B:153:GLN:HE21	1.84	0.43
4:D:181:GLN:C	4:D:181:GLN:HE21	2.26	0.43
6:F:101:ARG:HG3	6:F:104:ARG:HH21	1.82	0.43
1:A:410:VAL:O	1:A:413:LYS:HB3	2.18	0.43
2:B:24:LEU:H	2:B:24:LEU:CD2	2.29	0.43
3:C:166:TRP:O	3:C:167:GLY:C	2.61	0.43
5:E:53:ASN:O	5:E:54:VAL:C	2.60	0.43
8:H:35:GLU:C	8:H:37:LEU:N	2.76	0.43
2:B:260:GLU:O	2:B:261:SER:CB	2.66	0.43
2:B:405:VAL:CG1	2:B:406:ALA:N	2.81	0.43
4:D:21:LEU:HB3	4:D:26:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:230:LEU:HB3	6:F:70:MET:SD	2.58	0.43
5:E:118:ARG:HH11	5:E:118:ARG:CB	2.31	0.43
1:A:24:ARG:HG3	1:A:24:ARG:NH1	2.33	0.43
2:B:109:VAL:HG13	2:B:119:LEU:CD2	2.49	0.43
3:C:285:ILE:CG2	3:C:291:GLY:HA2	2.48	0.43
3:C:319:ARG:CZ	3:C:374:GLU:OE1	2.66	0.43
1:A:293:PRO:O	1:A:294:LEU:C	2.61	0.43
2:B:89:ILE:CD1	2:B:96:LEU:HD12	2.49	0.43
2:B:192:HIS:O	2:B:196:GLN:HG3	2.19	0.43
3:C:9:HIS:HA	3:C:10:PRO:HD2	1.90	0.43
4:D:102:ARG:HA	4:D:108:ALA:O	2.18	0.43
10:J:12:LEU:C	10:J:13:LEU:HD12	2.43	0.43
1:A:53:ASN:ND2	1:A:53:ASN:C	2.77	0.43
3:C:153:ALA:O	3:C:154:ILE:C	2.61	0.43
7:G:56:TYR:O	7:G:57:LEU:C	2.61	0.43
7:G:75:ALA:C	7:G:77:TYR:N	2.75	0.43
1:A:149:VAL:HG13	1:A:150:PHE:H	1.84	0.43
1:A:153:LEU:HD23	1:A:157:ALA:HB2	2.01	0.43
3:C:51:LEU:HD11	5:E:61:SER:OG	2.19	0.43
3:C:55:HIS:HE1	5:E:61:SER:O	2.01	0.43
3:C:101:ARG:HD2	3:C:101:ARG:C	2.43	0.43
3:C:103:LEU:HD13	3:C:104:TYR:HD1	1.84	0.43
3:C:234:THR:OG1	4:D:216:VAL:HG12	2.18	0.43
4:D:10:TYR:N	4:D:10:TYR:CD1	2.87	0.43
5:E:45:LEU:HD21	10:J:28:ALA:CA	2.49	0.43
5:E:52:LYS:C	5:E:52:LYS:CD	2.92	0.43
5:E:118:ARG:CB	5:E:118:ARG:NH1	2.82	0.43
5:E:166:ASP:OD1	5:E:168:SER:N	2.50	0.43
2:B:50:PHE:HZ	2:B:379:LEU:HD13	1.84	0.43
2:B:135:TRP:CD1	2:B:135:TRP:N	2.87	0.43
2:B:170:ASN:O	2:B:171:ALA:O	2.36	0.43
2:B:202:ALA:HB3	2:B:229:GLY:C	2.44	0.43
3:C:201:LEU:O	3:C:203:GLU:N	2.52	0.43
1:A:65:LYS:HZ3	9:I:311:UNK:CA	2.32	0.42
1:A:93:GLU:O	1:A:94:HIS:HB2	2.19	0.42
1:A:320:PHE:HE2	1:A:415:ILE:HD11	1.83	0.42
2:B:113:ARG:HG3	2:B:114:ASP:N	2.34	0.42
2:B:353:SER:OG	2:B:355:GLU:HB3	2.19	0.42
4:D:32:VAL:HG21	4:D:186:VAL:HG21	2.01	0.42
5:E:45:LEU:HA	5:E:45:LEU:HD22	1.83	0.42
7:G:26:PHE:HE1	7:G:29:TYR:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:HIS:HB2	1:A:100:LYS:HG2	1.97	0.42
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.19	0.42
1:A:159:GLN:NE2	5:E:7:VAL:HG11	2.33	0.42
1:A:250:LEU:CD2	1:A:325:VAL:CG1	2.97	0.42
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.54	0.42
2:B:22:GLN:O	2:B:23:ASP:C	2.63	0.42
2:B:339:ALA:O	2:B:340:ALA:C	2.62	0.42
2:B:415:LYS:O	2:B:416:LYS:C	2.61	0.42
3:C:350:ILE:O	3:C:351:ILE:C	2.62	0.42
3:C:369:THR:C	3:C:371:GLY:H	2.27	0.42
4:D:102:ARG:HH11	4:D:109:LEU:HB2	1.84	0.42
4:D:132:THR:HA	4:D:179:MET:CE	2.46	0.42
5:E:17:PRO:CD	7:G:24:ARG:HH21	2.32	0.42
5:E:45:LEU:C	5:E:45:LEU:CD1	2.91	0.42
5:E:105:GLU:O	5:E:109:GLU:HG2	2.19	0.42
1:A:15:GLN:O	1:A:26:ALA:HA	2.19	0.42
1:A:338:LEU:C	1:A:340:GLY:N	2.76	0.42
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.01	0.42
2:B:198:HIS:NE2	2:B:232:LEU:CD2	2.83	0.42
3:C:92:PHE:HA	3:C:95:ILE:CG2	2.43	0.42
3:C:101:ARG:O	3:C:105:TYR:HD2	2.02	0.42
3:C:104:TYR:OH	3:C:316:MET:HG3	2.19	0.42
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.82	0.42
3:C:237:LEU:HD12	3:C:240:PHE:HD2	1.83	0.42
3:C:293:LEU:N	3:C:293:LEU:CD2	2.81	0.42
3:C:362:ILE:HA	3:C:366:LEU:HB2	2.01	0.42
5:E:17:PRO:HA	5:E:20:TYR:HE1	1.83	0.42
2:B:312:PHE:H	2:B:324:PHE:HA	1.84	0.42
2:B:385:GLN:NE2	2:B:392:TYR:HA	2.35	0.42
2:B:405:VAL:O	2:B:406:ALA:CB	2.67	0.42
3:C:75:GLN:C	3:C:77:GLY:N	2.78	0.42
3:C:145:THR:HG23	3:C:171:VAL:HB	2.00	0.42
4:D:46:VAL:HG12	4:D:47:ALA:N	2.34	0.42
5:E:12:ASP:CA	5:E:20:TYR:OH	2.67	0.42
5:E:153:PHE:CE2	5:E:172:ARG:NH1	2.87	0.42
1:A:65:LYS:N	1:A:65:LYS:CD	2.83	0.42
1:A:134:ILE:C	1:A:136:ARG:N	2.76	0.42
1:A:339:GLN:HG2	1:A:440:GLY:O	2.20	0.42
1:A:434:TYR:O	1:A:435:ASN:C	2.61	0.42
2:B:75:LEU:HD11	2:B:140:LEU:CD2	2.50	0.42
2:B:135:TRP:O	2:B:136:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:LEU:O	2:B:365:LYS:C	2.63	0.42
4:D:55:CYS:O	4:D:56:TYR:CD2	2.72	0.42
7:G:44:CYS:O	7:G:45:ILE:C	2.62	0.42
2:B:56:ARG:O	2:B:171:ALA:HB1	2.19	0.42
2:B:272:PHE:O	2:B:273:SER:C	2.62	0.42
3:C:130:VAL:HG13	3:C:179:PHE:HB3	2.01	0.42
4:D:54:VAL:HG13	4:D:55:CYS:N	2.34	0.42
5:E:86:ASN:HB2	5:E:99:ARG:NE	2.35	0.42
6:F:31:LEU:HD23	6:F:31:LEU:H	1.84	0.42
1:A:274:ASN:ND2	1:A:320:PHE:CZ	2.88	0.42
3:C:268:HIS:CD2	3:C:268:HIS:N	2.87	0.42
3:C:332:ASN:C	3:C:332:ASN:ND2	2.74	0.42
10:J:20:PHE:CE1	10:J:24:ILE:HD11	2.55	0.42
1:A:343:MET:HE2	1:A:343:MET:CA	2.49	0.42
2:B:284:HIS:O	2:B:286:LYS:N	2.48	0.42
3:C:2:ALA:HB1	3:C:3:PRO:HD2	2.01	0.42
8:H:40:CYS:C	8:H:54:CYS:SG	3.03	0.42
8:H:72:LYS:HA	8:H:75:ASN:HD21	1.85	0.42
1:A:48:GLU:HB3	1:A:53:ASN:HA	2.02	0.42
1:A:61:HIS:NE2	1:A:137:GLU:OE1	2.40	0.42
1:A:282:ARG:HD3	9:I:203:UNK:CB	2.50	0.42
1:A:365:LEU:HD13	1:A:392:LEU:HD22	2.02	0.42
3:C:98:HIS:HD2	11:C:382:HEM:C1C	2.38	0.42
4:D:98:PRO:O	4:D:99:GLU:C	2.61	0.42
9:I:107:UNK:HA	9:I:115:UNK:O	2.19	0.42
1:A:64:PHE:C	1:A:66:GLY:H	2.28	0.42
1:A:244:ARG:NE	7:G:10:VAL:HB	2.35	0.42
1:A:250:LEU:HD21	1:A:325:VAL:CG1	2.49	0.42
2:B:374:SER:O	2:B:375:SER:C	2.62	0.42
3:C:46:ILE:O	3:C:50:LEU:HB2	2.19	0.42
4:D:218:LEU:HD22	5:E:39:VAL:HG13	2.02	0.42
1:A:134:ILE:O	1:A:135:VAL:C	2.61	0.41
1:A:424:GLY:HA2	1:A:425:PRO:HD3	1.73	0.41
2:B:275:LEU:O	2:B:279:LEU:HB2	2.19	0.41
3:C:99:ILE:O	3:C:100:GLY:C	2.63	0.41
3:C:238:THR:HB	4:D:212:MET:HG3	2.01	0.41
3:C:276:LEU:O	3:C:277:PHE:C	2.62	0.41
1:A:102:LEU:H	1:A:102:LEU:CD1	2.31	0.41
3:C:9:HIS:HD2	3:C:10:PRO:HG2	1.86	0.41
3:C:250:LEU:HD13	3:C:250:LEU:O	2.20	0.41
4:D:75:ASN:ND2	4:D:81:PHE:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:176:ALA:HA	5:E:177:PRO:HD2	1.85	0.41
1:A:391:PRO:HG2	1:A:394:GLU:HB2	2.02	0.41
1:A:399:LEU:HD12	1:A:399:LEU:C	2.44	0.41
2:B:189:VAL:O	2:B:192:HIS:N	2.53	0.41
2:B:258:VAL:HG13	2:B:322:PHE:O	2.21	0.41
2:B:424:MET:HE3	2:B:436:VAL:CG1	2.50	0.41
3:C:92:PHE:CA	3:C:95:ILE:HG22	2.43	0.41
12:C:383:U10:H8	12:C:383:U10:C1M	2.50	0.41
4:D:70:VAL:HG21	4:D:89:ASP:OD2	2.20	0.41
4:D:208:MET:SD	4:D:208:MET:C	3.03	0.41
5:E:32:ARG:HD2	5:E:32:ARG:HA	1.76	0.41
1:A:142:ASP:OD2	5:E:1:SER:HA	2.20	0.41
1:A:145:MET:HA	1:A:148:VAL:HG13	2.00	0.41
5:E:177:PRO:C	5:E:178:LEU:HD23	2.46	0.41
1:A:28:GLU:O	1:A:200:ALA:HA	2.21	0.41
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.73	0.41
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.50	0.41
1:A:189:HIS:HD2	1:A:194:ARG:HH12	1.69	0.41
1:A:394:GLU:C	1:A:396:GLU:N	2.77	0.41
1:A:433:ASP:OD1	1:A:436:ARG:HG2	2.20	0.41
2:B:264:ILE:HG23	2:B:315:SER:O	2.20	0.41
3:C:5:ILE:O	3:C:5:ILE:CG2	2.66	0.41
3:C:16:ASN:OD1	3:C:16:ASN:O	2.39	0.41
3:C:285:ILE:HA	3:C:286:PRO:HD3	1.83	0.41
3:C:311:SER:C	3:C:313:GLN:H	2.27	0.41
4:D:41:HIS:HB3	4:D:113:LEU:HD13	2.02	0.41
4:D:144:ARG:HG3	4:D:147:LEU:HD23	2.02	0.41
4:D:232:SER:OG	5:E:14:ARG:HG3	2.20	0.41
5:E:68:VAL:C	5:E:70:ALA:N	2.76	0.41
6:F:84:GLU:H	6:F:84:GLU:CD	2.29	0.41
10:J:25:VAL:O	10:J:28:ALA:N	2.52	0.41
10:J:54:HIS:CD2	10:J:54:HIS:N	2.88	0.41
1:A:123:GLU:C	1:A:125:SER:N	2.77	0.41
1:A:191:THR:C	1:A:193:PRO:HD2	2.46	0.41
1:A:241:ILE:O	1:A:241:ILE:HG23	2.19	0.41
1:A:250:LEU:N	1:A:250:LEU:CD1	2.83	0.41
2:B:280:GLY:C	2:B:283:PRO:HD2	2.45	0.41
2:B:407:ASP:OD1	2:B:408:ALA:N	2.52	0.41
3:C:101:ARG:C	3:C:101:ARG:CD	2.93	0.41
4:D:161:ALA:O	4:D:163:PRO:HD3	2.21	0.41
2:B:269:ALA:C	2:B:271:ALA:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:70:MET:CE	6:F:71:ARG:HG2	2.50	0.41
1:A:260:PRO:HD3	1:A:414:TYR:CE2	2.55	0.41
1:A:402:VAL:HA	1:A:406:MET:SD	2.61	0.41
2:B:50:PHE:CD1	2:B:50:PHE:N	2.89	0.41
2:B:189:VAL:C	2:B:191:LEU:N	2.78	0.41
2:B:318:ASP:O	2:B:319:SER:HB2	2.20	0.41
2:B:385:GLN:C	2:B:387:LEU:H	2.27	0.41
3:C:166:TRP:O	3:C:167:GLY:O	2.39	0.41
3:C:348:PHE:O	3:C:350:ILE:N	2.54	0.41
6:F:60:PHE:O	6:F:61:ARG:C	2.62	0.41
1:A:90:SER:HB3	1:A:95:THR:HG23	2.03	0.41
1:A:108:LYS:HA	1:A:108:LYS:CE	2.50	0.41
1:A:289:HIS:O	1:A:290:SER:C	2.63	0.41
2:B:269:ALA:O	2:B:271:ALA:N	2.54	0.41
2:B:277:HIS:C	2:B:279:LEU:N	2.78	0.41
2:B:374:SER:O	2:B:376:GLU:N	2.54	0.41
3:C:151:PHE:HB2	3:C:162:VAL:CG2	2.51	0.41
3:C:156:TYR:O	3:C:158:GLY:N	2.51	0.41
3:C:200:PHE:O	3:C:201:LEU:C	2.62	0.41
3:C:257:PHE:HD2	4:D:115:TYR:HB3	1.86	0.41
3:C:273:TRP:CD2	3:C:274:TYR:N	2.89	0.41
3:C:305:ILE:HB	3:C:306:PRO:HD3	2.02	0.41
4:D:17:PRO:O	4:D:202:LYS:HD3	2.21	0.41
5:E:17:PRO:HD3	7:G:24:ARG:NH2	2.35	0.41
5:E:74:ILE:O	5:E:194:ILE:HA	2.21	0.41
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.21	0.41
5:E:158:CYS:HA	5:E:159:PRO:HD2	1.76	0.41
6:F:26:PHE:C	6:F:26:PHE:CD1	2.99	0.41
6:F:89:TYR:CD1	6:F:89:TYR:C	2.98	0.41
1:A:144:SER:C	1:A:146:ARG:H	2.29	0.41
1:A:264:HIS:HD2	1:A:266:ASP:HB2	1.86	0.41
2:B:254:HIS:O	2:B:426:ALA:HA	2.20	0.41
2:B:414:ALA:O	2:B:418:VAL:HG23	2.20	0.41
3:C:120:LEU:HA	3:C:120:LEU:HD13	1.87	0.41
3:C:166:TRP:CD1	3:C:166:TRP:C	2.99	0.41
3:C:253:ASP:HA	3:C:254:PRO:HD2	1.90	0.41
3:C:258:THR:O	3:C:259:PRO:C	2.63	0.41
3:C:325:LEU:HD22	3:C:362:ILE:CG2	2.44	0.41
8:H:24:CYS:C	8:H:26:GLN:H	2.28	0.41
8:H:69:VAL:O	8:H:73:LEU:HB2	2.21	0.41
1:A:389:ARG:HD2	1:A:390:ILE:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:HG	2:B:24:LEU:O	2.21	0.40
2:B:160:ILE:HG23	2:B:164:HIS:CE1	2.57	0.40
3:C:75:GLN:C	3:C:77:GLY:H	2.29	0.40
3:C:305:ILE:HD11	3:C:363:LEU:HD22	2.03	0.40
11:C:381:HEM:HHA	11:C:381:HEM:O2D	2.20	0.40
4:D:172:ASP:C	4:D:174:GLY:N	2.79	0.40
1:A:53:ASN:ND2	1:A:54:GLY:N	2.67	0.40
1:A:245:GLU:HA	7:G:11:ARG:HA	2.04	0.40
2:B:183:ILE:HG22	2:B:184:GLY:N	2.36	0.40
2:B:399:LEU:C	2:B:401:GLN:N	2.79	0.40
3:C:37:LEU:O	3:C:41:CYS:HB2	2.21	0.40
3:C:105:TYR:HA	3:C:315:THR:HG22	2.03	0.40
3:C:239:PRO:O	3:C:240:PHE:C	2.63	0.40
5:E:89:PHE:O	5:E:95:PRO:HA	2.20	0.40
5:E:165:TYR:HE2	5:E:179:ASN:HA	1.86	0.40
6:F:64:ARG:O	6:F:68:LEU:HD13	2.21	0.40
1:A:349:ILE:HG12	1:A:350:SER:N	2.36	0.40
2:B:92:VAL:O	2:B:92:VAL:HG12	2.21	0.40
2:B:95:LYS:HB2	2:B:110:GLU:HG3	2.01	0.40
2:B:109:VAL:O	2:B:109:VAL:CG1	2.69	0.40
2:B:273:SER:O	2:B:276:GLN:HB3	2.21	0.40
2:B:382:VAL:HG23	2:B:383:GLY:N	2.36	0.40
3:C:71:CYS:SG	3:C:81:ARG:HD3	2.62	0.40
3:C:150:LEU:O	3:C:152:SER:N	2.55	0.40
4:D:118:ARG:NH1	4:D:195:GLU:OE1	2.54	0.40
8:H:40:CYS:O	8:H:44:VAL:HG23	2.22	0.40
10:J:40:ASP:O	10:J:41:ALA:C	2.65	0.40
1:A:89:TYR:CD1	1:A:89:TYR:C	3.00	0.40
1:A:235:ARG:NH1	5:E:15:ARG:CZ	2.84	0.40
2:B:51:ILE:HG22	2:B:52:LYS:N	2.35	0.40
3:C:101:ARG:HD2	3:C:101:ARG:O	2.21	0.40
4:D:99:GLU:CD	4:D:99:GLU:H	2.28	0.40
4:D:141:VAL:HG23	8:H:53:ASP:HB3	2.03	0.40
4:D:161:ALA:O	4:D:162:PRO:C	2.64	0.40
4:D:218:LEU:O	4:D:222:MET:HG3	2.21	0.40
5:E:100:HIS:HD2	5:E:131:GLU:O	2.04	0.40
8:H:55:THR:O	8:H:56:GLU:C	2.64	0.40
1:A:182:LEU:N	1:A:182:LEU:HD22	2.36	0.40
3:C:11:LEU:O	3:C:14:MET:HB2	2.22	0.40
4:D:164:ILE:O	4:D:164:ILE:HG23	2.22	0.40
5:E:19:ASP:O	5:E:20:TYR:CG	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:GLU:HA	5:E:100:HIS:CB	2.46	0.40
7:G:29:TYR:O	7:G:34:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/446 (99%)	348 (79%)	73 (17%)	19 (4%)	2	13
2	B	404/422 (96%)	291 (72%)	74 (18%)	39 (10%)	0	2
3	C	377/380 (99%)	299 (79%)	64 (17%)	14 (4%)	2	15
4	D	239/241 (99%)	195 (82%)	31 (13%)	13 (5%)	1	9
5	E	194/196 (99%)	167 (86%)	23 (12%)	4 (2%)	5	26
6	F	98/109 (90%)	83 (85%)	15 (15%)	0	100	100
7	G	76/81 (94%)	61 (80%)	10 (13%)	5 (7%)	1	6
8	H	64/78 (82%)	50 (78%)	14 (22%)	0	100	100
10	J	57/62 (92%)	43 (75%)	12 (21%)	2 (4%)	3	16
All	All	1949/2015 (97%)	1537 (79%)	316 (16%)	96 (5%)	1	11

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	65	LYS
1	A	103	SER
1	A	282	ARG
1	A	291	SER
2	B	113	ARG

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Mol	Chain	Res	Type
2	B	171	ALA
2	B	183	ILE
2	B	228	GLY
2	B	263	ALA
2	B	286	LYS
2	B	330	ALA
2	B	375	SER
2	B	407	ASP
4	D	73	GLY
4	D	198	HIS
4	D	228	SER
4	D	233	ARG
5	E	21	SER
1	A	145	MET
2	B	23	ASP
2	B	109	VAL
2	B	111	CYS
2	B	233	SER
2	B	404	ALA
2	B	431	GLY
3	C	21	ASP
3	C	157	ILE
3	C	167	GLY
3	C	171	VAL
3	C	202	HIS
4	D	8	PRO
4	D	38	SER
4	D	75	ASN
5	E	17	PRO
5	E	106	ILE
7	G	43	ALA
10	J	5	LEU
1	A	71	PRO
1	A	128	GLU
2	B	21	PRO
2	B	63	LEU
2	B	261	SER
2	B	270	ASN
2	B	317	SER
2	B	345	LYS
2	B	349	GLN
2	B	354	ASN

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Mol	Chain	Res	Type
2	B	406	ALA
2	B	408	ALA
2	B	420	ARG
3	C	63	ALA
3	C	346	HIS
3	C	349	ILE
4	D	168	VAL
10	J	61	ASN
1	A	72	GLN
1	A	281	ASP
1	A	382	GLU
1	A	396	GLU
1	A	408	ARG
2	B	201	SER
2	B	269	ALA
2	B	361	LYS
2	B	372	VAL
3	C	60	THR
3	C	287	ASN
4	D	9	SER
4	D	67	GLU
4	D	176	PRO
5	E	13	TYR
1	A	405	ARG
2	B	19	PRO
2	B	20	HIS
2	B	260	GLU
2	B	262	ALA
2	B	331	ALA
3	C	47	LEU
7	G	25	PRO
7	G	50	PRO
1	A	56	GLY
1	A	113	LEU
1	A	267	LEU
2	B	62	ASN
2	B	232	LEU
3	C	3	PRO
3	C	36	SER
7	G	74	PRO
1	A	127	ILE
1	A	286	GLY

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Mol	Chain	Res	Type
2	B	64	GLY
3	C	5	ILE
4	D	133	GLY
7	G	33	GLY
4	D	98	PRO
2	B	305	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/376 (96%)	340 (95%)	19 (5%)	20	49
2	B	307/336 (91%)	289 (94%)	18 (6%)	18	45
3	C	326/329 (99%)	309 (95%)	17 (5%)	21	49
4	D	201/207 (97%)	191 (95%)	10 (5%)	22	50
5	E	165/169 (98%)	154 (93%)	11 (7%)	15	42
6	F	90/98 (92%)	84 (93%)	6 (7%)	15	42
7	G	60/72 (83%)	54 (90%)	6 (10%)	7	27
8	H	51/74 (69%)	50 (98%)	1 (2%)	48	68
10	J	41/52 (79%)	41 (100%)	0	100	100
All	All	1600/1713 (93%)	1512 (94%)	88 (6%)	19	47

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LYS
1	A	102	LEU
1	A	108	LYS
1	A	148	VAL
1	A	153	LEU
1	A	168	GLU
1	A	204	GLU
1	A	250	LEU

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Mol	Chain	Res	Type
1	A	316	GLU
1	A	361	LEU
1	A	365	LEU
1	A	368	HIS
1	A	382	GLU
1	A	384	LEU
1	A	388	ARG
1	A	395	TRP
1	A	409	GLU
1	A	431	LEU
1	A	443	TRP
2	B	56	ARG
2	B	57	TYR
2	B	62	ASN
2	B	85	ILE
2	B	112	LEU
2	B	135	TRP
2	B	170	ASN
2	B	221	GLU
2	B	225	ASN
2	B	247	GLN
2	B	248	ASN
2	B	252	LEU
2	B	264	ILE
2	B	307	PHE
2	B	325	TYR
2	B	402	ILE
2	B	434	PRO
2	B	437	ASP
3	C	40	VAL
3	C	43	MET
3	C	47	LEU
3	C	104	TYR
3	C	113	THR
3	C	120	LEU
3	C	124	LEU
3	C	136	TRP
3	C	145	THR
3	C	164	TRP
3	C	175	THR
3	C	217	ASP
3	C	323	GLN

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Mol	Chain	Res	Type
3	C	325	LEU
3	C	330	VAL
3	C	350	ILE
3	C	354	MET
4	D	24	THR
4	D	32	VAL
4	D	36	VAL
4	D	82	MET
4	D	99	GLU
4	D	136	GLU
4	D	143	VAL
4	D	163	PRO
4	D	181	GLN
4	D	192	TRP
5	E	17	PRO
5	E	19	ASP
5	E	71	MET
5	E	78	LEU
5	E	87	MET
5	E	90	LYS
5	E	113	GLU
5	E	145	VAL
5	E	186	GLU
5	E	188	THR
5	E	194	ILE
6	F	12	TRP
6	F	31	LEU
6	F	37	ILE
6	F	59	MET
6	F	68	LEU
6	F	70	MET
7	G	4	PHE
7	G	27	PRO
7	G	28	HIS
7	G	29	TYR
7	G	41	LEU
7	G	77	TYR
8	H	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	53	ASN
1	A	69	ASN
1	A	118	GLN
1	A	141	ASN
1	A	151	ASN
1	A	165	GLN
1	A	207	GLN
1	A	240	GLN
1	A	274	ASN
1	A	289	HIS
1	A	339	GLN
1	A	341	GLN
1	A	363	ASN
1	A	435	ASN
2	B	22	GLN
2	B	31	ASN
2	B	141	GLN
2	B	153	GLN
2	B	170	ASN
2	B	196	GLN
2	B	225	ASN
2	B	248	ASN
2	B	282	ASN
2	B	343	GLN
2	B	349	GLN
2	B	351	ASN
2	B	356	ASN
2	B	393	ASN
2	B	401	GLN
2	B	421	GLN
2	B	429	ASN
3	C	4	ASN
3	C	9	HIS
3	C	55	HIS
3	C	73	ASN
3	C	82	ASN
3	C	261	ASN
3	C	287	ASN
3	C	313	GLN
3	C	323	GLN
3	C	342	GLN
3	C	379	ASN

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Mol	Chain	Res	Type
4	D	35	GLN
4	D	75	ASN
4	D	156	GLN
4	D	181	GLN
5	E	86	ASN
5	E	122	HIS
5	E	164	HIS
6	F	69	ASN
6	F	72	GLN
7	G	12	HIS
7	G	23	GLN
7	G	64	GLN
8	H	75	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	HEM	C	382	3	50,50,50	1.81	12 (24%)	67,82,82	2.37	22 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HEM	D	243	4	50,50,50	1.80	12 (24%)	67,82,82	2.18	24 (35%)
15	FES	E	197	5	0,4,4	-	-	-		
14	BOG	D	242	-	20,20,20	0.74	0	25,25,25	0.94	1 (4%)
12	U10	C	383	-	29,29,63	2.30	8 (27%)	36,38,79	1.73	11 (30%)
11	HEM	C	381	3	50,50,50	1.54	11 (22%)	67,82,82	2.26	21 (31%)
13	PEE	C	384	-	48,48,50	2.57	12 (25%)	51,53,55	4.31	18 (35%)
13	PEE	E	198	-	48,48,50	2.51	11 (22%)	51,53,55	4.34	17 (33%)

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
11	HEM	C	382	3	-	7/14/54/54	-
11	HEM	D	243	4	-	8/14/54/54	-
15	FES	E	197	5	-	-	0/1/1/1
14	BOG	D	242	-	-	5/11/31/31	0/1/1/1
12	U10	C	383	-	-	8/23/47/87	0/1/1/1
11	HEM	C	381	3	-	5/14/54/54	-
13	PEE	C	384	-	1/1/4/8	21/52/52/54	-
13	PEE	E	198	-	1/1/4/8	27/52/52/54	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	198	PEE	O5-C30	11.44	1.56	1.22
13	C	384	PEE	O5-C30	11.17	1.55	1.22
12	C	383	U10	C6-C1	7.62	1.48	1.35
11	C	382	HEM	FE-ND	-5.60	1.77	1.94
11	D	243	HEM	FE-ND	-5.13	1.79	1.94
13	C	384	PEE	C18-C19	5.03	1.60	1.31
13	E	198	PEE	O2-C10	5.02	1.48	1.34
13	C	384	PEE	C39-C38	5.01	1.60	1.31
12	C	383	U10	C7-C6	4.92	1.60	1.51
13	E	198	PEE	C39-C38	4.76	1.58	1.31
13	E	198	PEE	C18-C19	4.72	1.58	1.31
13	C	384	PEE	O2-C10	4.44	1.46	1.34
11	D	243	HEM	CBB-CAB	4.41	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	382	HEM	CHA-C1A	-4.40	1.29	1.39
11	D	243	HEM	CBC-CAC	4.19	1.50	1.30
11	C	381	HEM	FE-NB	-4.16	1.82	1.94
13	C	384	PEE	C11-C10	3.96	1.62	1.50
13	E	198	PEE	C21-C22	-3.66	1.33	1.51
12	C	383	U10	C18-C19	3.62	1.41	1.33
13	E	198	PEE	C42-C41	-3.57	1.34	1.51
11	C	381	HEM	CAB-C3B	-3.56	1.37	1.47
13	E	198	PEE	C11-C10	3.48	1.60	1.50
13	C	384	PEE	C21-C22	-3.46	1.34	1.51
13	C	384	PEE	C42-C41	-3.39	1.34	1.51
13	C	384	PEE	C1-C2	3.39	1.61	1.50
11	C	381	HEM	FE-NA	-3.34	1.84	1.95
12	C	383	U10	C13-C14	3.15	1.40	1.33
13	E	198	PEE	C31-C30	-3.07	1.41	1.50
11	C	382	HEM	FE-NC	-3.04	1.85	1.95
11	C	382	HEM	CHB-C1B	-3.03	1.32	1.38
11	C	382	HEM	CHA-C4D	-2.88	1.32	1.38
11	D	243	HEM	FE-NA	-2.87	1.85	1.95
11	C	382	HEM	CAC-C3C	-2.84	1.39	1.47
13	C	384	PEE	C31-C30	-2.84	1.42	1.50
13	C	384	PEE	P-O3P	2.81	1.70	1.59
11	D	243	HEM	CHB-C4A	-2.67	1.33	1.39
11	C	381	HEM	FE-NC	-2.62	1.86	1.95
12	C	383	U10	C3-C2	-2.61	1.41	1.48
11	C	381	HEM	CHD-C4C	-2.56	1.33	1.38
11	D	243	HEM	C1B-NB	-2.56	1.35	1.40
11	C	382	HEM	CAB-C3B	-2.53	1.40	1.47
11	D	243	HEM	CHB-C1B	-2.52	1.33	1.38
12	C	383	U10	C8-C9	2.51	1.38	1.33
11	D	243	HEM	C2A-C3A	-2.39	1.32	1.38
13	C	384	PEE	O2-C2	-2.37	1.41	1.46
11	C	382	HEM	C1A-NA	-2.37	1.35	1.39
11	D	243	HEM	CHD-C1D	-2.36	1.33	1.39
12	C	383	U10	O4-C4M	-2.29	1.40	1.45
11	C	381	HEM	CAC-C3C	-2.28	1.41	1.47
11	C	382	HEM	C4D-ND	-2.23	1.36	1.40
11	D	243	HEM	C3C-C2C	-2.23	1.32	1.37
11	C	381	HEM	CHA-C4D	-2.20	1.34	1.38
11	C	382	HEM	FE-NA	-2.20	1.87	1.95
11	C	381	HEM	C2A-C3A	-2.19	1.33	1.38
11	C	381	HEM	CHA-C1A	-2.19	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	384	PEE	C23-C24	2.17	1.62	1.51
11	D	243	HEM	CHA-C1A	-2.13	1.34	1.39
13	E	198	PEE	O2-C2	-2.13	1.41	1.46
11	D	243	HEM	FE-NC	-2.13	1.88	1.95
13	E	198	PEE	C1-C2	2.12	1.57	1.50
12	C	383	U10	C16-C14	2.11	1.55	1.51
11	C	381	HEM	CHD-C1D	-2.10	1.34	1.39
13	E	198	PEE	C5-C4	2.07	1.58	1.49
11	C	382	HEM	C3D-C2D	-2.04	1.32	1.36
11	C	381	HEM	CHC-C4B	-2.03	1.34	1.39
11	C	382	HEM	CBC-CAC	2.02	1.40	1.30

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	198	PEE	O4-C10-C11	-18.60	51.02	123.78
13	C	384	PEE	O4-C10-C11	-18.58	51.11	123.78
13	E	198	PEE	O3-C30-C31	13.17	151.98	111.83
13	C	384	PEE	O3-C30-C31	12.89	151.15	111.83
13	C	384	PEE	O3-C30-O5	-11.49	94.89	123.63
13	E	198	PEE	O3-C30-O5	-11.34	95.27	123.63
13	E	198	PEE	O2-C2-C3	7.95	136.86	108.34
13	C	384	PEE	O2-C2-C3	7.84	136.47	108.34
13	E	198	PEE	O2-C10-C11	7.16	126.96	111.48
13	C	384	PEE	O2-C10-O4	-6.66	108.13	123.70
11	C	382	HEM	C2A-C1A-NA	6.45	117.31	110.15
13	E	198	PEE	C12-C11-C10	-6.44	90.09	113.69
13	C	384	PEE	O2-C10-C11	6.43	125.40	111.48
13	E	198	PEE	O2-C10-O4	-6.42	108.69	123.70
11	D	243	HEM	C3B-C4B-NB	6.14	113.88	109.47
11	C	381	HEM	C3B-C4B-NB	6.05	113.81	109.47
13	C	384	PEE	C12-C11-C10	-5.95	91.91	113.69
11	C	382	HEM	C3D-C4D-ND	5.65	116.37	110.17
11	C	382	HEM	C2B-C1B-NB	5.63	116.32	109.84
11	C	382	HEM	C4D-ND-C1D	-5.58	98.60	105.21
11	C	381	HEM	CAD-C3D-C4D	5.42	134.14	124.70
13	C	384	PEE	O3-C3-C2	5.09	123.07	108.40
11	D	243	HEM	CMA-C3A-C4A	5.09	133.16	125.42
11	C	381	HEM	CAD-C3D-C2D	-5.08	118.36	127.87
13	E	198	PEE	O3-C3-C2	4.70	121.94	108.40
11	D	243	HEM	CAD-C3D-C4D	4.58	132.68	124.70
11	C	382	HEM	C4A-NA-C1A	-4.55	98.40	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	382	HEM	CBD-CAD-C3D	4.52	125.04	112.53
11	C	381	HEM	C4C-C3C-C2C	-4.36	103.03	106.81
12	C	383	U10	C1-C6-C5	-4.25	115.49	119.62
11	C	382	HEM	CBA-CAA-C2A	4.18	124.09	112.53
11	D	243	HEM	C2B-C1B-NB	4.16	114.62	109.84
11	C	382	HEM	C3B-C2B-C1B	-4.15	103.30	106.41
11	C	381	HEM	C2D-C1D-ND	4.08	114.62	109.90
11	C	381	HEM	C4D-ND-C1D	-4.01	100.45	105.21
11	D	243	HEM	C1B-NB-C4B	-3.98	100.49	105.21
11	C	381	HEM	C2A-C1A-NA	3.86	114.44	110.15
12	C	383	U10	C10-C9-C8	-3.83	113.79	123.63
11	C	382	HEM	C1B-NB-C4B	-3.83	100.67	105.21
11	C	382	HEM	C3B-C4B-NB	3.75	112.16	109.47
11	C	381	HEM	C4C-NC-C1C	-3.68	99.83	105.82
11	D	243	HEM	CMD-C2D-C1D	3.59	130.64	125.03
14	D	242	BOG	C1'-O1-C1	3.58	119.79	113.68
11	C	381	HEM	C3B-C2B-C1B	-3.53	103.76	106.41
11	D	243	HEM	C4D-ND-C1D	-3.53	101.03	105.21
11	C	382	HEM	C2D-C1D-ND	3.50	113.95	109.90
13	C	384	PEE	C42-C41-C40	3.44	130.40	113.86
13	E	198	PEE	C22-C21-C20	3.41	130.27	113.86
11	D	243	HEM	CAD-C3D-C2D	-3.41	121.48	127.87
11	D	243	HEM	CBB-CAB-C3B	-3.40	110.52	127.53
11	C	382	HEM	CHD-C1D-ND	-3.38	120.79	124.42
11	C	381	HEM	CMB-C2B-C1B	3.36	130.29	125.03
13	E	198	PEE	C42-C41-C40	3.36	130.01	113.86
11	C	381	HEM	C2B-C1B-NB	3.28	113.62	109.84
11	C	381	HEM	C1B-NB-C4B	-3.28	101.33	105.21
13	C	384	PEE	C22-C21-C20	3.24	129.43	113.86
11	D	243	HEM	C3D-C4D-ND	3.19	113.67	110.17
13	E	198	PEE	C33-C32-C31	3.11	124.56	113.13
11	D	243	HEM	C2D-C1D-ND	3.10	113.49	109.90
11	C	381	HEM	CBA-CAA-C2A	3.10	121.10	112.53
11	D	243	HEM	CMC-C2C-C1C	3.05	130.09	124.73
13	E	198	PEE	C34-C33-C32	-3.04	99.00	114.37
11	C	381	HEM	C4A-NA-C1A	-3.03	100.88	105.82
13	C	384	PEE	C12-C13-C14	-3.03	99.07	114.37
11	C	382	HEM	C1A-C2A-C3A	-3.03	102.19	106.87
11	C	381	HEM	CMD-C2D-C1D	2.95	129.64	125.03
13	C	384	PEE	C33-C32-C31	2.91	123.81	113.13
11	D	243	HEM	C4A-NA-C1A	-2.88	101.13	105.82
12	C	383	U10	C15-C14-C13	-2.87	116.26	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	384	PEE	C34-C33-C32	-2.84	99.99	114.37
13	E	198	PEE	O5-C30-C31	-2.82	112.74	123.78
11	C	381	HEM	CHD-C4C-C3C	-2.76	120.55	125.21
11	D	243	HEM	C4C-NC-C1C	-2.71	101.39	105.82
11	D	243	HEM	C2A-C1A-NA	2.69	113.14	110.15
12	C	383	U10	C15-C14-C16	2.68	119.89	115.23
11	D	243	HEM	CHD-C4C-NC	-2.68	121.53	124.45
11	C	382	HEM	CHA-C4D-C3D	-2.68	120.29	125.23
13	E	198	PEE	C12-C13-C14	-2.67	100.87	114.37
11	C	381	HEM	C3D-C4D-ND	2.63	113.05	110.17
11	C	382	HEM	C4C-NC-C1C	-2.55	101.67	105.82
11	C	382	HEM	CAA-C2A-C1A	2.53	129.89	124.94
13	C	384	PEE	O5-C30-C31	-2.53	113.88	123.78
11	C	381	HEM	C1D-C2D-C3D	-2.52	104.33	106.98
12	C	383	U10	C10-C9-C11	2.52	119.60	115.23
11	C	381	HEM	CHA-C4D-ND	-2.43	121.36	124.37
12	C	383	U10	C11-C9-C8	2.42	126.61	121.17
11	D	243	HEM	CBD-CAD-C3D	2.42	119.21	112.53
11	D	243	HEM	CHC-C4B-NB	-2.41	121.83	124.42
11	C	382	HEM	CMD-C2D-C1D	2.41	128.80	125.03
11	C	382	HEM	CHD-C4C-NC	-2.40	121.84	124.45
13	C	384	PEE	O2-C2-C1	2.39	116.92	108.34
11	C	381	HEM	C2C-C1C-NC	2.38	114.03	109.64
12	C	383	U10	O2-C2-C3	-2.38	116.00	121.03
11	C	382	HEM	C4D-C3D-C2D	-2.38	103.43	106.89
11	D	243	HEM	C3A-C4A-NA	2.36	113.93	110.14
13	E	198	PEE	O2-C2-C1	2.34	116.73	108.34
11	C	382	HEM	CMC-C2C-C1C	2.32	128.81	124.73
13	E	198	PEE	C3-C2-C1	-2.31	106.40	111.78
11	C	382	HEM	C3A-C4A-NA	2.28	113.80	110.14
11	C	382	HEM	CHB-C1B-C2B	-2.27	120.48	126.95
11	D	243	HEM	C4B-C3B-C2B	-2.27	105.19	107.28
11	D	243	HEM	CMC-C2C-C3C	-2.25	122.98	128.43
12	C	383	U10	C20-C19-C18	-2.25	117.86	123.63
13	C	384	PEE	C3-C2-C1	-2.24	106.57	111.78
12	C	383	U10	O5-C5-C4	-2.23	116.30	121.03
11	C	381	HEM	CAA-C2A-C1A	2.21	129.26	124.94
11	D	243	HEM	C4A-C3A-C2A	-2.20	104.30	106.82
13	C	384	PEE	C3-O3-C30	-2.20	109.09	117.12
11	D	243	HEM	C4D-C3D-C2D	-2.19	103.70	106.89
12	C	383	U10	C8-C7-C6	2.16	117.40	112.08
13	C	384	PEE	C14-C15-C16	-2.11	103.71	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	198	PEE	C36-C35-C34	-2.09	103.81	114.37
12	C	383	U10	C7-C8-C9	2.05	130.37	126.83
11	D	243	HEM	CAA-C2A-C1A	2.02	128.88	124.94

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	384	PEE	C2
13	E	198	PEE	C2

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	HEM	C2B-C3B-CAB-CBB
11	C	381	HEM	C4B-C3B-CAB-CBB
12	C	383	U10	C5-C6-C7-C8
12	C	383	U10	C14-C16-C17-C18
13	C	384	PEE	O4-C10-O2-C2
13	E	198	PEE	O4-C10-O2-C2
13	E	198	PEE	O5-C30-O3-C3
13	E	198	PEE	C31-C30-O3-C3
13	C	384	PEE	O5-C30-O3-C3
12	C	383	U10	C12-C11-C9-C10
13	C	384	PEE	C37-C38-C39-C40
13	E	198	PEE	C22-C23-C24-C25
11	C	382	HEM	C4D-C3D-CAD-CBD
13	C	384	PEE	C22-C23-C24-C25
13	C	384	PEE	C31-C30-O3-C3
13	C	384	PEE	C17-C18-C19-C20
13	E	198	PEE	C37-C38-C39-C40
12	C	383	U10	C12-C11-C9-C8
14	D	242	BOG	C2-C1-O1-C1'
13	E	198	PEE	C30-C31-C32-C33
14	D	242	BOG	O5-C1-O1-C1'
13	C	384	PEE	C3-C2-O2-C10
13	E	198	PEE	C17-C18-C19-C20
13	E	198	PEE	C35-C36-C37-C38
13	E	198	PEE	C12-C13-C14-C15
13	E	198	PEE	C31-C32-C33-C34
13	E	198	PEE	C21-C22-C23-C24
13	C	384	PEE	C20-C21-C22-C23
13	E	198	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	D	243	HEM	C2D-C3D-CAD-CBD
12	C	383	U10	C1-C6-C7-C8
13	E	198	PEE	C33-C34-C35-C36
11	D	243	HEM	C2B-C3B-CAB-CBB
13	C	384	PEE	C13-C14-C15-C16
14	D	242	BOG	C2'-C3'-C4'-C5'
13	E	198	PEE	C39-C40-C41-C42
13	E	198	PEE	C11-C12-C13-C14
14	D	242	BOG	C3'-C4'-C5'-C6'
13	E	198	PEE	C1-C2-C3-O3
13	E	198	PEE	C19-C20-C21-C22
13	C	384	PEE	C12-C13-C14-C15
13	C	384	PEE	C40-C41-C42-C43
13	E	198	PEE	O3P-C1-C2-O2
13	C	384	PEE	C39-C40-C41-C42
13	C	384	PEE	C14-C15-C16-C17
13	E	198	PEE	C41-C42-C43-C44
12	C	383	U10	C9-C11-C12-C13
13	C	384	PEE	C23-C24-C25-C26
13	C	384	PEE	C41-C42-C43-C44
11	C	382	HEM	C2C-C3C-CAC-CBC
11	D	243	HEM	C2C-C3C-CAC-CBC
13	C	384	PEE	O3P-C1-C2-O2
13	C	384	PEE	O2-C2-C3-O3
13	C	384	PEE	C4-O4P-P-O1P
13	E	198	PEE	O4P-C4-C5-N
13	E	198	PEE	C36-C37-C38-C39
13	E	198	PEE	C40-C41-C42-C43
11	C	382	HEM	C2B-C3B-CAB-CBB
11	C	382	HEM	CAA-CBA-CGA-O1A
11	C	381	HEM	CAA-CBA-CGA-O1A
11	C	382	HEM	CAA-CBA-CGA-O2A
11	C	381	HEM	CAA-CBA-CGA-O2A
13	C	384	PEE	C16-C17-C18-C19
13	E	198	PEE	C20-C21-C22-C23
11	C	382	HEM	CAD-CBD-CGD-O2D
11	C	382	HEM	CAD-CBD-CGD-O1D
13	C	384	PEE	C36-C37-C38-C39
13	E	198	PEE	C42-C43-C44-C45
14	D	242	BOG	C4'-C5'-C6'-C7'
11	D	243	HEM	CAA-CBA-CGA-O2A
13	E	198	PEE	C38-C39-C40-C41

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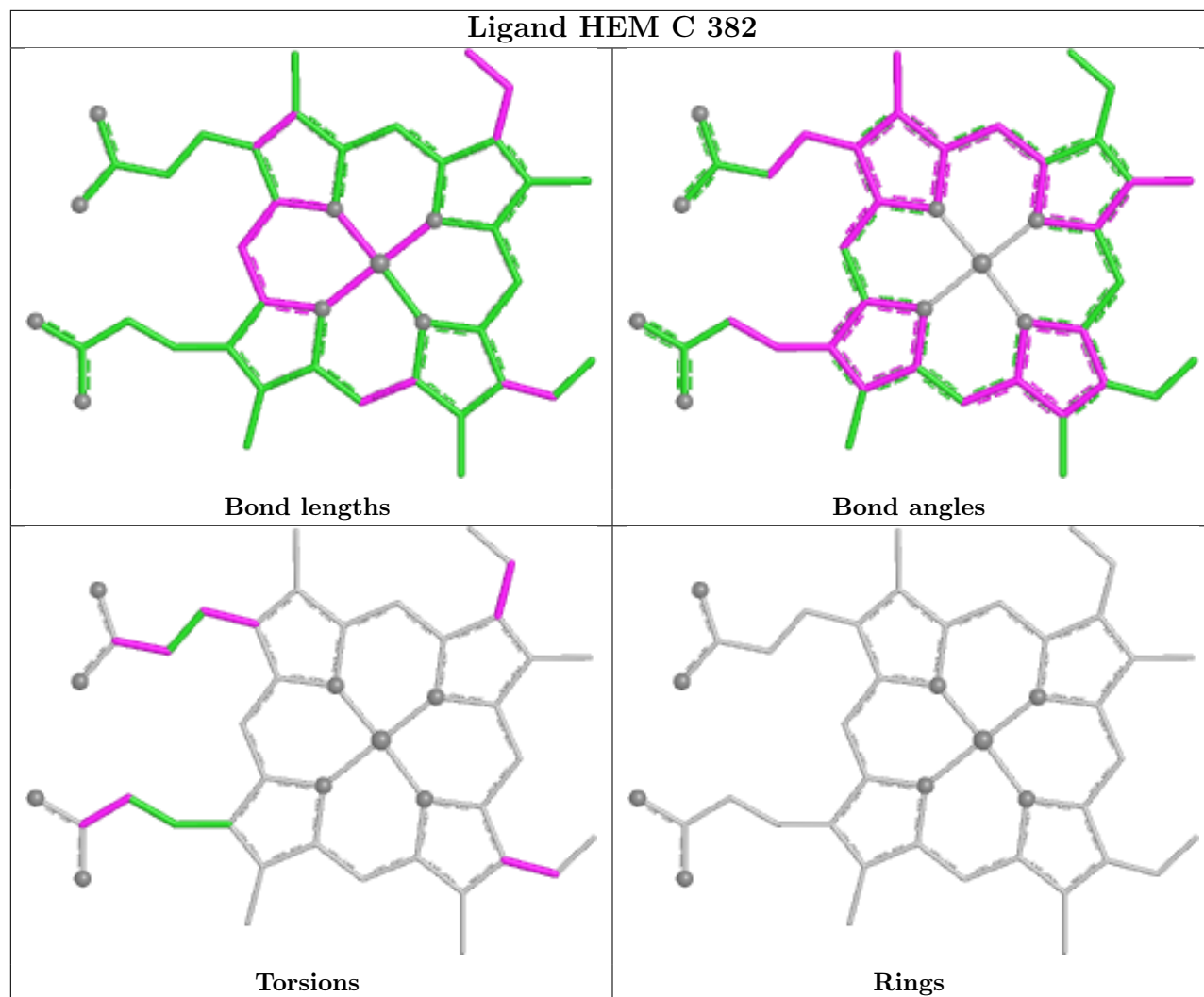
Mol	Chain	Res	Type	Atoms
11	D	243	HEM	C4B-C3B-CAB-CBB
11	D	243	HEM	C4C-C3C-CAC-CBC
11	C	381	HEM	C3D-CAD-CBD-CGD
13	C	384	PEE	O3P-C1-C2-C3
11	D	243	HEM	CAA-CBA-CGA-O1A
13	E	198	PEE	C3-C2-O2-C10
12	C	383	U10	C6-C7-C8-C9
12	C	383	U10	C16-C17-C18-C19
13	E	198	PEE	O3-C30-C31-C32
11	D	243	HEM	CAD-CBD-CGD-O2D

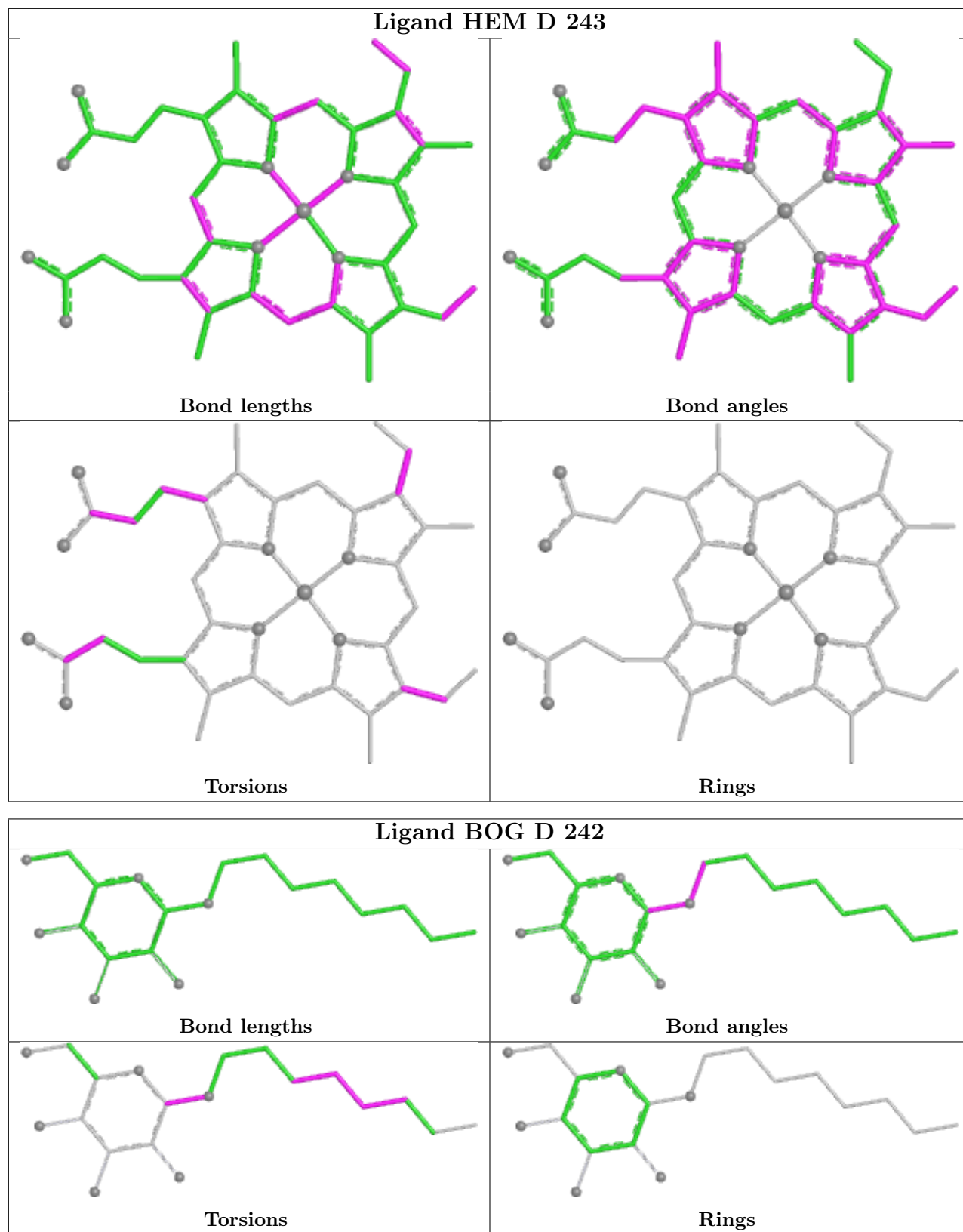
There are no ring outliers.

7 monomers are involved in 21 short contacts:

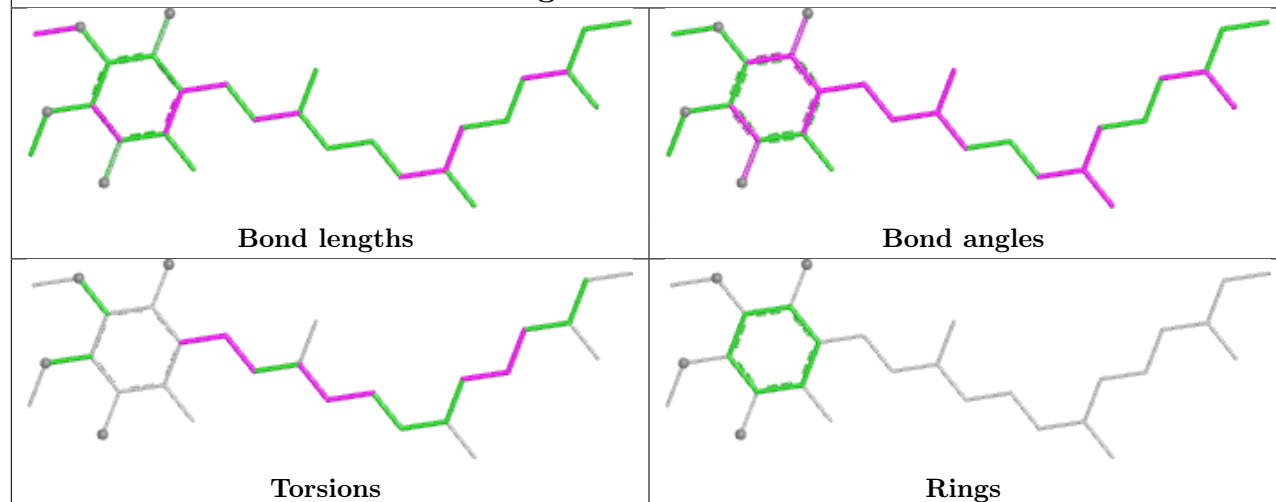
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	382	HEM	7	0
15	E	197	FES	1	0
14	D	242	BOG	3	0
12	C	383	U10	2	0
11	C	381	HEM	5	0
13	C	384	PEE	2	0
13	E	198	PEE	1	0

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

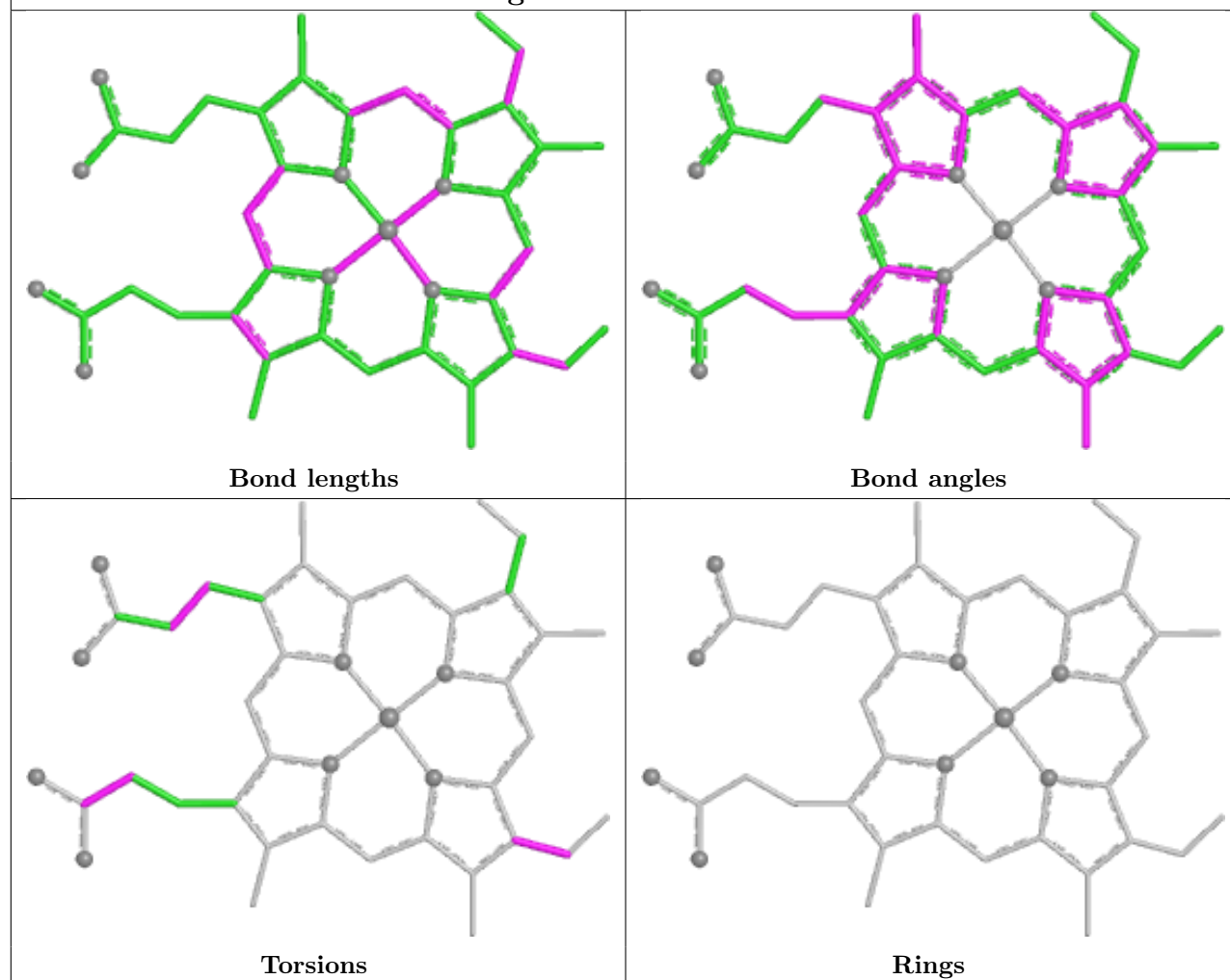


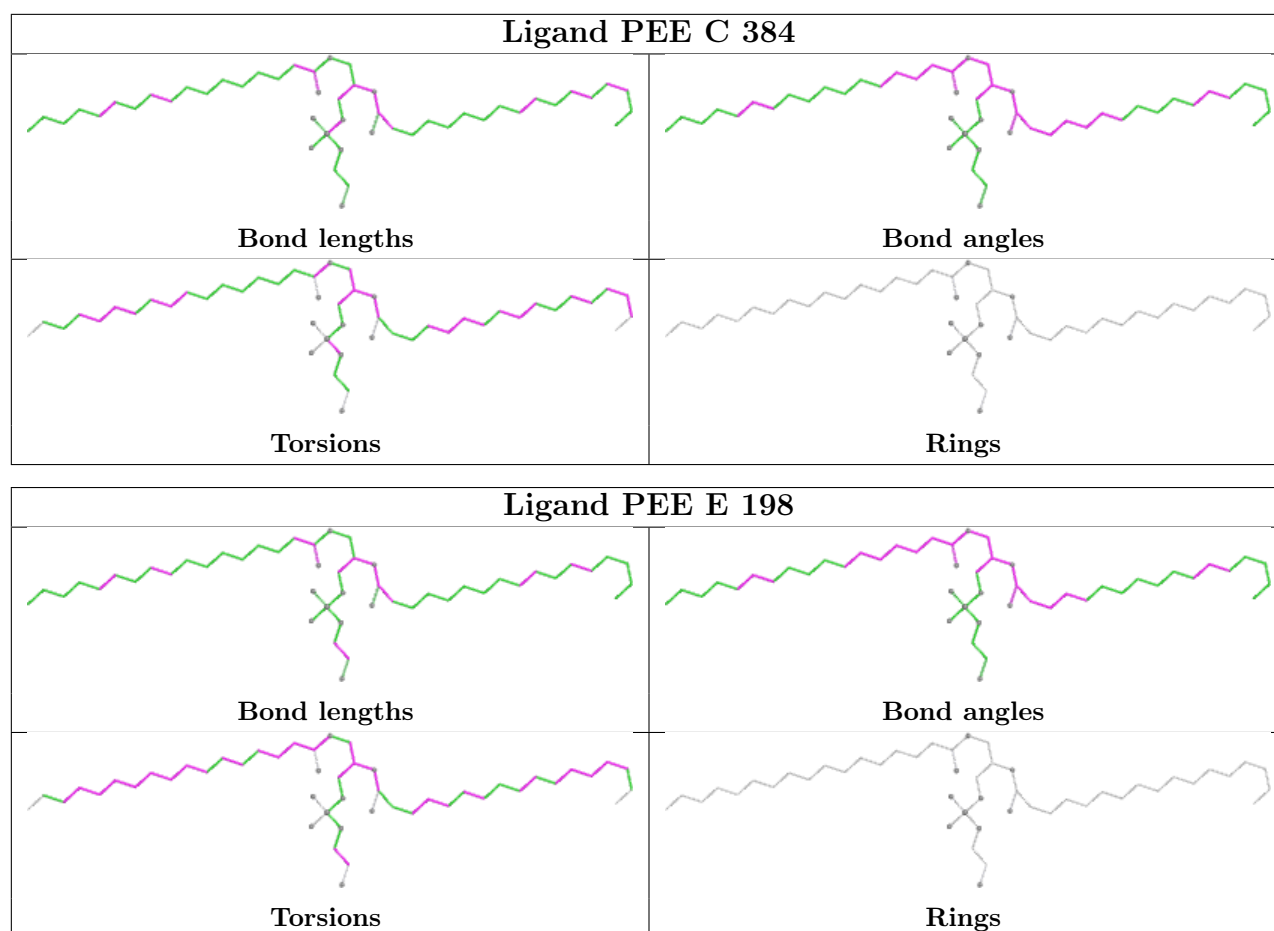


Ligand U10 C 383



Ligand HEM C 381





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	210:UNK	C	309:UNK	N	33.23
1	I	121:UNK	C	202:UNK	N	29.43

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	442/446 (99%)	1.38	113 (25%) 1 1	47, 84, 100, 100	0
2	B	406/422 (96%)	1.61	115 (28%) 1 1	60, 93, 100, 100	0
3	C	379/380 (99%)	0.89	46 (12%) 8 5	33, 64, 96, 100	0
4	D	241/241 (100%)	1.16	38 (15%) 5 3	50, 76, 99, 100	0
5	E	196/196 (100%)	2.43	113 (57%) 0 0	54, 100, 100, 100	0
6	F	100/109 (91%)	1.14	16 (16%) 5 3	50, 73, 98, 100	0
7	G	78/81 (96%)	1.31	18 (23%) 2 2	51, 85, 100, 100	0
8	H	66/78 (84%)	1.79	30 (45%) 0 1	76, 95, 99, 100	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	1.47	15 (25%) 1 1	66, 80, 99, 100	0
All	All	1967/2048 (96%)	1.41	504 (25%) 1 1	33, 83, 100, 100	0

All (504) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	163	SER	7.7
5	E	162	GLY	7.6
5	E	114	VAL	7.5
4	D	75	ASN	6.8
5	E	141	HIS	6.5
5	E	174	GLY	6.3
5	E	117	LEU	6.2
1	A	32	GLN	6.2
1	A	220	PRO	6.2
5	E	111	ALA	6.1
5	E	124	LEU	5.9
5	E	191	ASP	5.9
5	E	189	SER	5.9
5	E	115	SER	5.6

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Mol	Chain	Res	Type	RSRZ
2	B	23	ASP	5.5
5	E	84	GLY	5.5
4	D	72	ASP	5.4
2	B	114	ASP	5.3
1	A	202	GLY	5.3
2	B	222	GLN	5.3
5	E	121	GLN	5.3
1	A	380	GLY	5.2
5	E	150	ALA	5.2
8	H	26	GLN	5.1
1	A	96	ALA	5.0
2	B	423	SER	4.9
2	B	170	ASN	4.9
5	E	102	THR	4.9
2	B	305	ASN	4.9
2	B	212	SER	4.8
5	E	177	PRO	4.8
5	E	139	CYS	4.8
5	E	155	GLY	4.8
2	B	20	HIS	4.8
1	A	20	ASP	4.8
10	J	8	ARG	4.7
10	J	61	ASN	4.7
5	E	159	PRO	4.7
5	E	171	ILE	4.7
2	B	419	SER	4.6
2	B	40	ASN	4.6
1	A	101	ALA	4.5
3	C	35	GLY	4.5
6	F	91	GLU	4.4
1	A	412	SER	4.4
2	B	260	GLU	4.4
7	G	26	PHE	4.4
4	D	139	THR	4.4
1	A	120	CYS	4.4
5	E	98	VAL	4.3
5	E	87	MET	4.3
5	E	169	GLY	4.3
1	A	147	GLU	4.3
4	D	31	GLN	4.2
5	E	192	MET	4.2
5	E	161	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
5	E	188	THR	4.2
4	D	228	SER	4.2
2	B	273	SER	4.1
4	D	65	ALA	4.1
3	C	158	GLY	4.1
5	E	165	TYR	4.1
5	E	158	CYS	4.1
5	E	146	PRO	4.0
5	E	110	ALA	4.0
4	D	180	SER	3.9
5	E	176	ALA	3.9
2	B	375	SER	3.9
2	B	18	PRO	3.9
4	D	239	PRO	3.9
3	C	48	THR	3.8
8	H	36	ARG	3.8
5	E	127	VAL	3.8
2	B	129	ALA	3.8
4	D	125	ASP	3.8
5	E	140	THR	3.8
1	A	437	ILE	3.7
10	J	19	THR	3.7
5	E	79	SER	3.7
2	B	181	TYR	3.7
2	B	397	THR	3.7
5	E	194	ILE	3.7
5	E	151	GLY	3.7
5	E	153	PHE	3.7
4	D	67	GLU	3.6
5	E	195	VAL	3.6
5	E	109	GLU	3.6
1	A	15	GLN	3.6
3	C	371	GLY	3.6
5	E	160	CYS	3.6
7	G	31	SER	3.6
1	A	223	TYR	3.6
1	A	118	GLN	3.5
5	E	112	VAL	3.5
2	B	224	LEU	3.5
2	B	226	ILE	3.5
5	E	108	GLN	3.5
2	B	281	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
8	H	53	ASP	3.5
5	E	132	TRP	3.5
3	C	5	ILE	3.5
2	B	431	GLY	3.5
4	D	16	GLY	3.5
5	E	122	HIS	3.5
5	E	76	ILE	3.4
5	E	181	GLU	3.4
2	B	60	SER	3.4
2	B	100	SER	3.4
2	B	353	SER	3.4
1	A	403	ASP	3.4
5	E	113	GLU	3.4
2	B	200	THR	3.4
3	C	157	ILE	3.4
5	E	157	TYR	3.4
1	A	7	ALA	3.4
3	C	160	THR	3.4
2	B	370	MET	3.4
1	A	264	HIS	3.4
3	C	361	THR	3.4
2	B	197	ASN	3.3
1	A	281	ASP	3.3
2	B	439	LEU	3.3
8	H	15	ASP	3.3
1	A	52	ASN	3.3
5	E	96	LEU	3.3
4	D	80	MET	3.3
2	B	371	SER	3.3
1	A	119	ASN	3.3
7	G	77	TYR	3.2
2	B	19	PRO	3.2
2	B	134	PRO	3.2
1	A	8	LEU	3.2
2	B	408	ALA	3.2
1	A	187	SER	3.2
4	D	108	ALA	3.2
5	E	100	HIS	3.2
2	B	438	GLU	3.2
5	E	142	LEU	3.2
6	F	16	ILE	3.2
10	J	18	SER	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	167	ALA	3.2
8	H	25	GLU	3.1
1	A	73	ASN	3.1
5	E	187	PHE	3.1
2	B	118	ILE	3.1
4	D	158	ILE	3.1
6	F	72	GLN	3.1
5	E	106	ILE	3.1
2	B	175	SER	3.1
8	H	23	GLN	3.1
5	E	72	SER	3.1
1	A	221	PHE	3.1
1	A	195	MET	3.1
1	A	390	ILE	3.1
5	E	86	ASN	3.1
6	F	22	ASN	3.1
8	H	46	SER	3.1
1	A	71	PRO	3.1
2	B	288	GLY	3.0
1	A	76	GLU	3.0
2	B	61	SER	3.0
6	F	14	GLU	3.0
2	B	263	ALA	3.0
4	D	100	ALA	3.0
6	F	21	TYR	3.0
1	A	151	ASN	3.0
3	C	17	ASN	3.0
5	E	85	LYS	3.0
1	A	140	GLU	3.0
1	A	102	LEU	3.0
10	J	49	GLY	3.0
2	B	26	ILE	3.0
6	F	70	MET	3.0
4	D	99	GLU	3.0
5	E	95	PRO	3.0
5	E	178	LEU	3.0
10	J	44	GLU	3.0
7	G	76	ALA	3.0
10	J	54	HIS	3.0
1	A	367	SER	2.9
5	E	173	LYS	2.9
2	B	235	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	359	ALA	2.9
1	A	27	SER	2.9
3	C	156	TYR	2.9
1	A	42	ASP	2.9
5	E	29	ASP	2.9
5	E	80	ASP	2.9
8	H	31	VAL	2.9
2	B	119	LEU	2.9
2	B	123	LEU	2.9
5	E	152	ASP	2.9
4	D	203	ARG	2.9
5	E	128	LYS	2.9
5	E	60	SER	2.8
5	E	148	ALA	2.8
2	B	346	THR	2.8
8	H	52	GLU	2.8
6	F	24	ALA	2.8
4	D	84	PRO	2.8
2	B	398	VAL	2.8
2	B	29	LEU	2.8
2	B	198	HIS	2.8
2	B	396	SER	2.8
4	D	102	ARG	2.8
2	B	405	VAL	2.8
1	A	413	LYS	2.8
4	D	136	GLU	2.8
10	J	45	HIS	2.8
1	A	214	LYS	2.8
1	A	134	ILE	2.8
1	A	368	HIS	2.8
2	B	36	ALA	2.8
1	A	370	ASP	2.7
8	H	41	ASP	2.7
6	F	53	ASN	2.7
4	D	118	ARG	2.7
6	F	102	LYS	2.7
1	A	11	VAL	2.7
1	A	444	LEU	2.7
5	E	147	ILE	2.7
3	C	4	ASN	2.7
5	E	129	LYS	2.7
10	J	7	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	204	GLU	2.7
3	C	168	GLY	2.7
3	C	6	ARG	2.7
5	E	190	ASP	2.7
2	B	341	TYR	2.7
6	F	87	VAL	2.7
2	B	400	GLN	2.7
2	B	111	CYS	2.7
1	A	103	SER	2.7
2	B	220	ALA	2.7
5	E	145	VAL	2.7
8	H	67	HIS	2.7
2	B	82	SER	2.7
3	C	206	SER	2.7
2	B	171	ALA	2.7
8	H	64	ALA	2.7
1	A	384	LEU	2.7
2	B	282	ASN	2.7
1	A	12	PRO	2.6
2	B	153	GLN	2.6
5	E	30	PRO	2.6
5	E	175	PRO	2.6
5	E	131	GLU	2.6
1	A	191	THR	2.6
2	B	330	ALA	2.6
8	H	33	ALA	2.6
5	E	166	ASP	2.6
2	B	104	ASN	2.6
2	B	395	PRO	2.6
6	F	92	PRO	2.6
10	J	62	LYS	2.6
3	C	131	GLY	2.6
5	E	143	GLY	2.6
8	H	28	GLU	2.6
7	G	63	THR	2.6
1	A	79	VAL	2.6
2	B	267	ALA	2.6
2	B	233	SER	2.6
8	H	45	SER	2.6
5	E	185	TYR	2.6
6	F	71	ARG	2.6
2	B	342	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	179	ASN	2.6
1	A	261	GLY	2.6
8	H	51	GLU	2.6
2	B	106	ALA	2.6
5	E	168	SER	2.6
7	G	28	HIS	2.6
4	D	167	ASP	2.6
1	A	208	LEU	2.6
1	A	196	VAL	2.6
2	B	219	VAL	2.6
5	E	5	ILE	2.6
4	D	88	SER	2.6
5	E	183	PRO	2.6
1	A	206	GLN	2.6
3	C	379	ASN	2.6
1	A	394	GLU	2.6
2	B	404	ALA	2.6
7	G	30	PHE	2.5
10	J	20	PHE	2.5
2	B	386	ALA	2.5
3	C	335	ILE	2.5
3	C	346	HIS	2.5
5	E	156	TYR	2.5
4	D	5	LEU	2.5
1	A	263	ALA	2.5
1	A	378	ASP	2.5
1	A	409	GLU	2.5
3	C	2	ALA	2.5
1	A	329	MET	2.5
4	D	33	TYR	2.5
8	H	32	LYS	2.5
5	E	65	SER	2.5
6	F	73	GLN	2.5
3	C	63	ALA	2.5
1	A	111	GLU	2.5
1	A	87	ASN	2.5
3	C	287	ASN	2.5
1	A	57	TYR	2.5
2	B	192	HIS	2.5
2	B	227	ARG	2.5
7	G	29	TYR	2.5
3	C	138	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	275	ALA	2.5
2	B	81	SER	2.5
3	C	255	GLU	2.5
1	A	332	ASP	2.5
2	B	31	ASN	2.5
3	C	13	LYS	2.5
2	B	66	SER	2.4
1	A	358	LYS	2.4
2	B	225	ASN	2.4
5	E	99	ARG	2.4
5	E	126	ARG	2.4
2	B	27	THR	2.4
3	C	10	PRO	2.4
2	B	323	GLY	2.4
5	E	154	GLY	2.4
5	E	11	SER	2.4
7	G	42	ARG	2.4
3	C	11	LEU	2.4
7	G	8	THR	2.4
2	B	213	HIS	2.4
2	B	285	VAL	2.4
2	B	389	ALA	2.4
5	E	88	ALA	2.4
5	E	172	ARG	2.4
1	A	211	LEU	2.4
7	G	73	ASN	2.4
3	C	106	GLY	2.4
7	G	33	GLY	2.4
2	B	39	GLU	2.4
3	C	373	LEU	2.4
8	H	27	LEU	2.4
8	H	62	LEU	2.4
5	E	24	SER	2.4
1	A	376	CYS	2.4
8	H	68	CYS	2.4
1	A	391	PRO	2.4
2	B	432	HIS	2.4
4	D	103	ALA	2.4
8	H	49	GLN	2.4
2	B	379	LEU	2.4
8	H	39	LEU	2.4
1	A	28	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	10	SER	2.4
1	A	160	GLY	2.3
1	A	317	THR	2.3
5	E	3	THR	2.3
2	B	248	ASN	2.3
2	B	388	ALA	2.3
1	A	225	ASP	2.3
1	A	341	GLN	2.3
2	B	216	LEU	2.3
5	E	105	GLU	2.3
6	F	52	GLU	2.3
1	A	285	GLY	2.3
4	D	78	GLY	2.3
1	A	313	CYS	2.3
2	B	246	GLU	2.3
1	A	77	LYS	2.3
4	D	85	GLY	2.3
4	D	211	MET	2.3
1	A	186	LEU	2.3
1	A	369	LEU	2.3
1	A	399	LEU	2.3
3	C	256	ASN	2.3
3	C	375	ASN	2.3
1	A	29	GLN	2.3
8	H	44	VAL	2.3
4	D	144	ARG	2.3
7	G	47	ARG	2.3
2	B	229	GLY	2.3
3	C	358	SER	2.3
2	B	112	LEU	2.3
8	H	63	HIS	2.3
5	E	94	LYS	2.3
1	A	397	GLU	2.3
5	E	15	ARG	2.3
1	A	201	GLY	2.3
2	B	173	ALA	2.3
6	F	13	LEU	2.3
7	G	66	PHE	2.3
1	A	363	ASN	2.3
1	A	18	GLN	2.3
1	A	100	LYS	2.3
2	B	203	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	329	GLN	2.3
8	H	60	ASP	2.3
2	B	377	GLY	2.2
3	C	167	GLY	2.2
10	J	30	LEU	2.2
3	C	284	SER	2.2
1	A	179	ARG	2.2
4	D	83	ARG	2.2
8	H	47	ARG	2.2
1	A	53	ASN	2.2
1	A	207	GLN	2.2
2	B	276	GLN	2.2
3	C	16	ASN	2.2
5	E	138	VAL	2.2
1	A	227	ALA	2.2
8	H	13	LEU	2.2
8	H	37	LEU	2.2
2	B	385	GLN	2.2
5	E	144	CYS	2.2
2	B	24	LEU	2.2
4	D	240	PRO	2.2
7	G	25	PRO	2.2
1	A	336	PHE	2.2
2	B	307	PHE	2.2
1	A	143	THR	2.2
1	A	222	THR	2.2
3	C	113	THR	2.2
2	B	325	TYR	2.2
1	A	366	VAL	2.2
2	B	59	ASN	2.2
2	B	430	LEU	2.2
3	C	163	GLU	2.2
2	B	318	ASP	2.2
1	A	189	HIS	2.2
5	E	182	VAL	2.2
2	B	146	ILE	2.2
5	E	116	GLN	2.2
3	C	334	LEU	2.2
1	A	48	GLU	2.2
5	E	70	ALA	2.2
5	E	149	ASN	2.2
7	G	43	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	73	GLY	2.2
5	E	34	GLY	2.2
5	E	77	LYS	2.2
5	E	90	LYS	2.2
5	E	118	ARG	2.2
8	H	54	CYS	2.2
1	A	372	THR	2.1
3	C	177	THR	2.1
5	E	22	THR	2.1
1	A	90	SER	2.1
1	A	292	SER	2.1
2	B	28	LYS	2.1
2	B	188	SER	2.1
1	A	184	GLU	2.1
1	A	210	GLU	2.1
2	B	262	ALA	2.1
2	B	317	SER	2.1
3	C	345	GLU	2.1
2	B	351	ASN	2.1
1	A	115	ASP	2.1
5	E	56	THR	2.1
4	D	109	LEU	2.1
1	A	6	GLN	2.1
2	B	230	LEU	2.1
3	C	354	MET	2.1
1	A	5	ALA	2.1
3	C	144	ALA	2.1
1	A	291	SER	2.1
2	B	97	SER	2.1
1	A	359	ASN	2.1
7	G	53	LEU	2.1
2	B	343	GLN	2.1
3	C	352	GLY	2.1
8	H	38	GLU	2.1
5	E	21	SER	2.1
2	B	287	ARG	2.1
3	C	166	TRP	2.1
10	J	15	ARG	2.1
5	E	119	ASP	2.1
2	B	76	THR	2.1
3	C	14	MET	2.1
5	E	20	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
10	J	37	GLN	2.1
1	A	427	PRO	2.1
4	D	138	PRO	2.1
5	E	27	GLU	2.1
5	E	75	GLU	2.1
7	G	74	PRO	2.1
3	C	298	SER	2.0
2	B	277	HIS	2.0
4	D	212	MET	2.0
1	A	185	TYR	2.0
1	A	357	GLY	2.0
5	E	89	PHE	2.0
4	D	58	GLU	2.0
1	A	194	ARG	2.0
1	A	209	LEU	2.0
5	E	92	ARG	2.0
1	A	315	SER	2.0
5	E	184	SER	2.0
10	J	11	SER	2.0
3	C	164	TRP	2.0
2	B	138	ALA	2.0
2	B	168	TYR	2.0
4	D	77	ASP	2.0
1	A	68	LYS	2.0
1	A	326	CYS	2.0
2	B	113	ARG	2.0
1	A	182	LEU	2.0
1	A	297	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

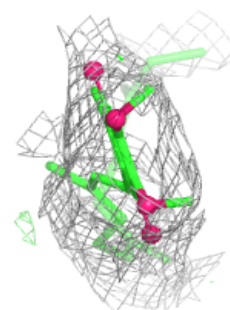
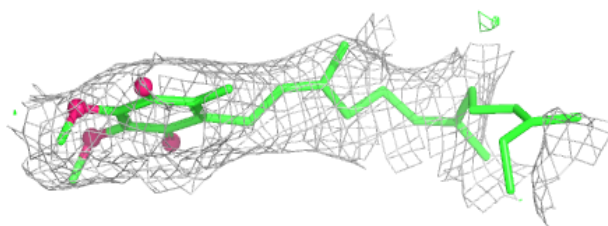
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	U10	C	383	29/63	0.63	0.21	77,83,100,100	29
13	PEE	E	198	49/51	0.76	0.18	24,45,64,65	49
14	BOG	D	242	20/20	0.81	0.13	37,59,70,72	20
13	PEE	C	384	49/51	0.84	0.12	20,39,54,55	49
11	HEM	C	382	43/43	0.94	0.13	43,46,59,62	0
11	HEM	C	381	43/43	0.95	0.10	43,51,59,62	0
11	HEM	D	243	43/43	0.95	0.10	46,58,69,74	0
15	FES	E	197	4/4	0.96	0.17	100,100,100,100	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.

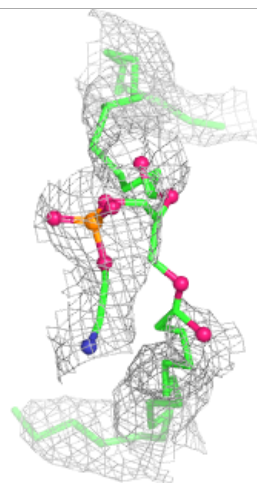
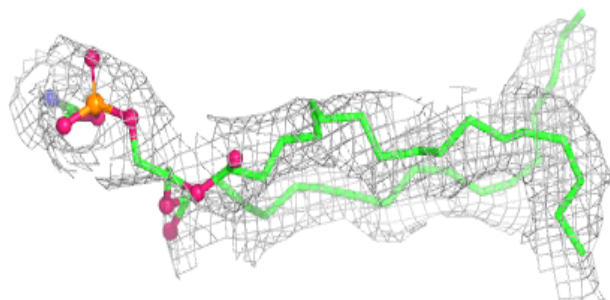
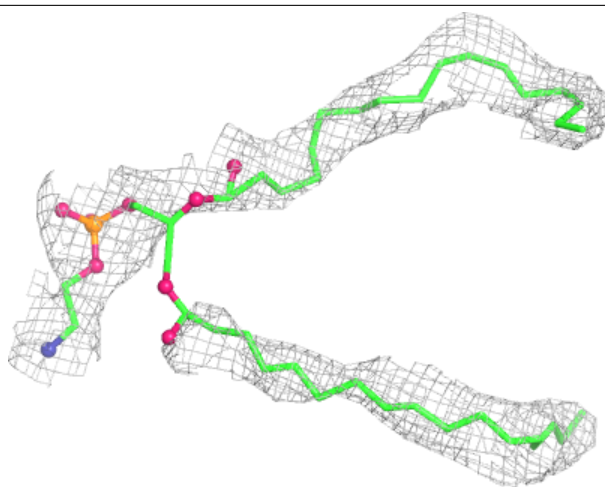
Electron density around U10 C 383:

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



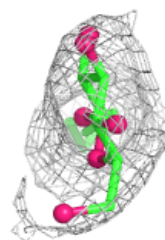
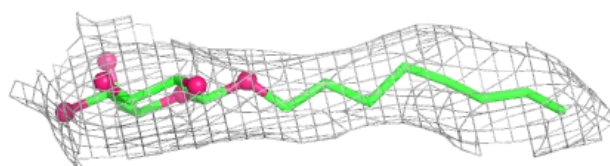
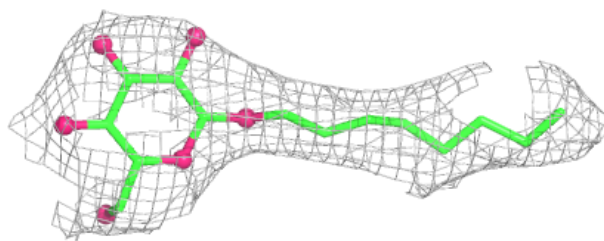
Electron density around PEE E 198:

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

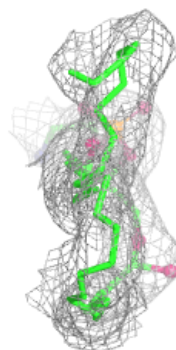
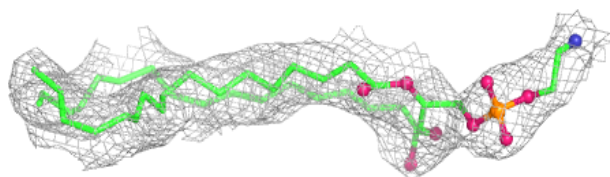
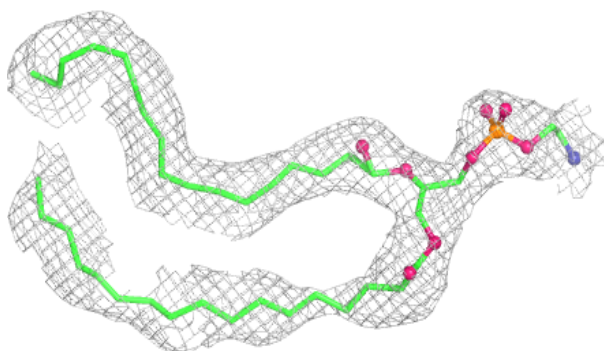


Electron density around BOG D 242:

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

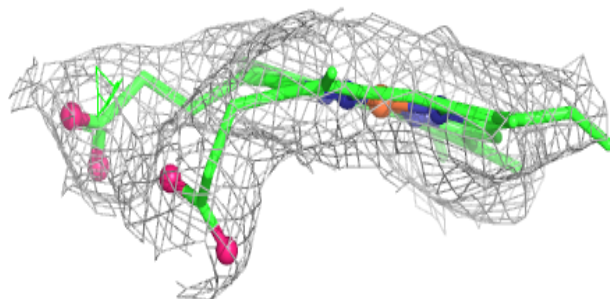
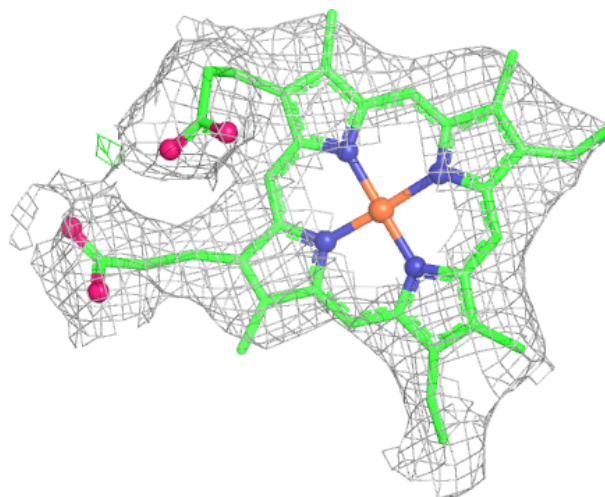
**Electron density around PEE C 384:**

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



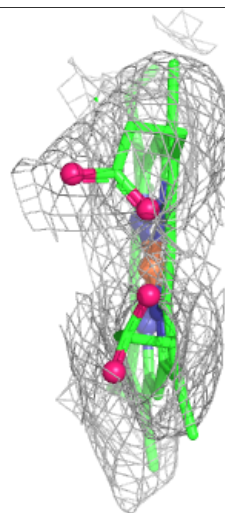
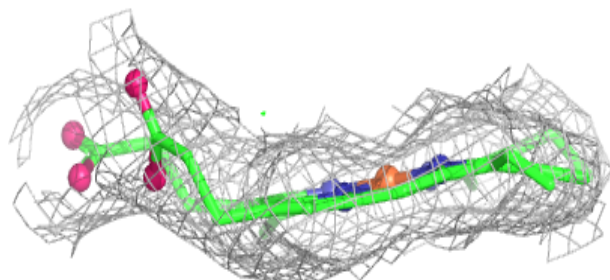
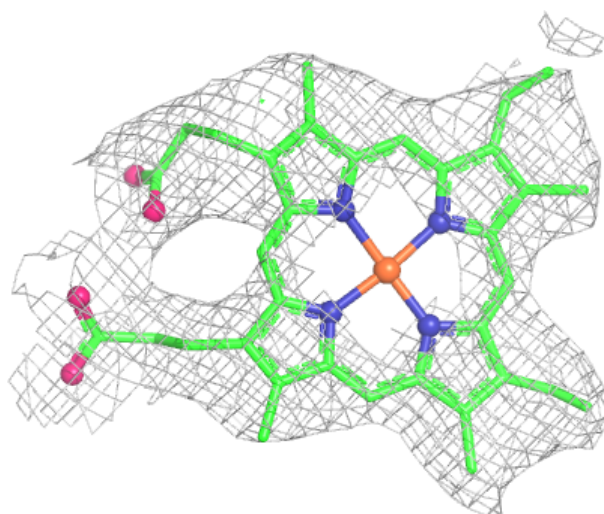
Electron density around HEM C 382:

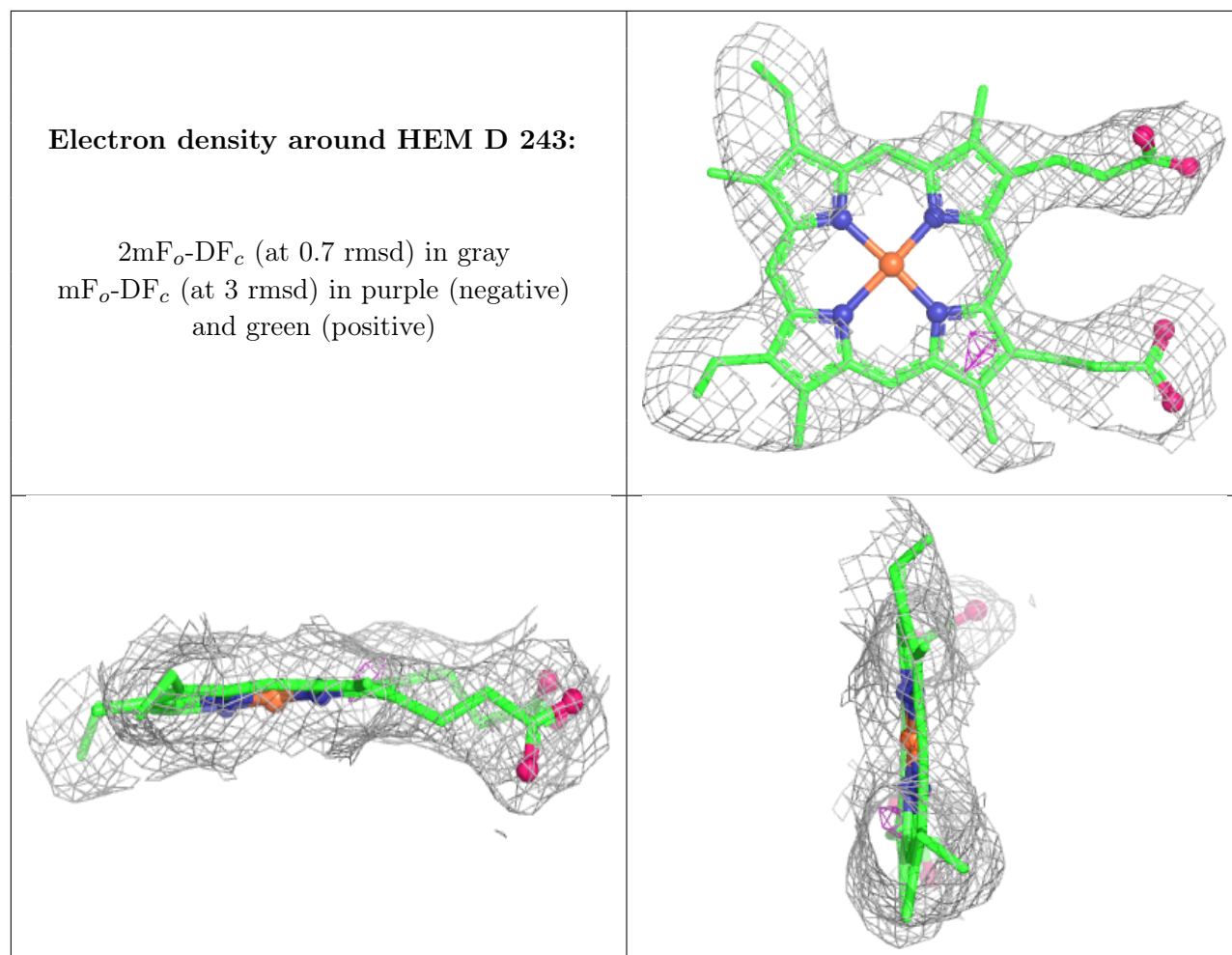
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 381:

$2mF_o-DF_c$ (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.