



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 08:35 PM JST

PDB ID : 8IOG / pdb_00008iog
EMDB ID : EMD-35618
Title : Cryo-EM structure of porcine bc1 complex in isolated state
Authors : Wang, Y.X.; Dong, J.Q.; Yang, G.F.
Deposited on : 2023-03-11
Resolution : 2.88 Å(reported)
Based on initial model : 5GUP

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

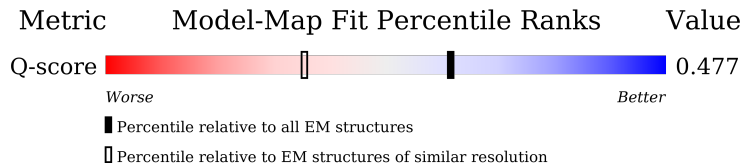
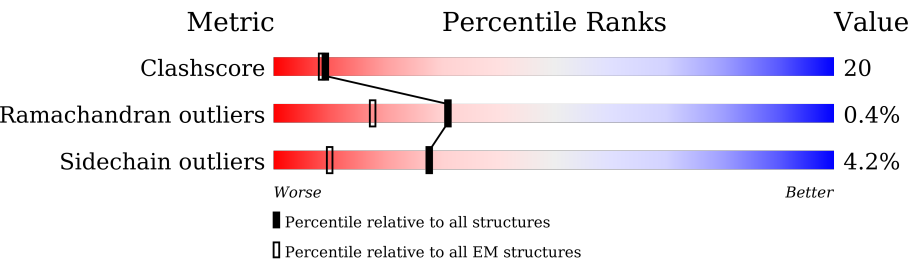
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12111 (2.38 - 3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	379	56% 32% 9% .
1	a	379	6% 50% 37% 11% .
2	B	326	16% 41% 27% . 26%
2	b	326	19% 51% 21% . 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	196	
3	c	196	
4	D	480	
4	d	480	
5	E	453	
5	e	453	
6	F	91	
6	f	91	
7	G	111	
7	g	111	
8	H	82	
8	h	82	
9	I	64	
9	i	64	
10	J	56	
10	j	56	
11	K	78	
11	k	78	

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
15	FES	C	301	-	-	X	-
15	FES	c	301	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 33413 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		
1	a	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	SER	GLY	variant	UNP P24964
a	314	SER	GLY	variant	UNP P24964

- Molecule 2 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	241	Total	C	N	O	S	0	0
			1920	1225	330	349	16		
2	b	239	Total	C	N	O	S	0	0
			1904	1214	327	347	16		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1502	946	261	288	7		
3	c	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	445	Total	C	N	O	S	0	0
			3452	2157	604	672	19		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		
5	e	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
6	f	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
7	g	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	71	Total	C	N	O	S	0	0
			608	399	112	95	2		
8	h	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	62	Total	C	N	O	0	0
			507	331	90	86		
9	i	62	Total	C	N	O	0	0
			507	331	90	86		

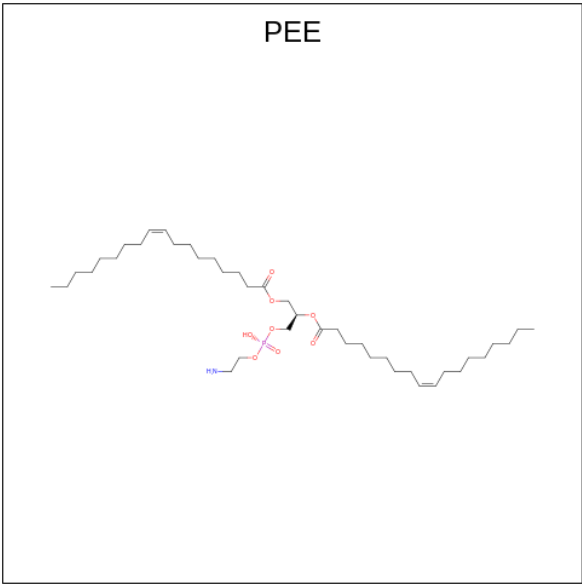
- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 10 | J | 49 | Total
405 | C
269 | N
71 | O
63 | S
2 | 0 | 0 |
| 10 | j | 51 | Total
421 | C
281 | N
74 | O
65 | S
1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 11 | K | 57 | Total
404 | C
252 | N
74 | O
76 | S
2 | 0 | 0 |
| 11 | k | 57 | Total
404 | C
252 | N
74 | O
76 | S
2 | 0 | 0 |

- # HEM

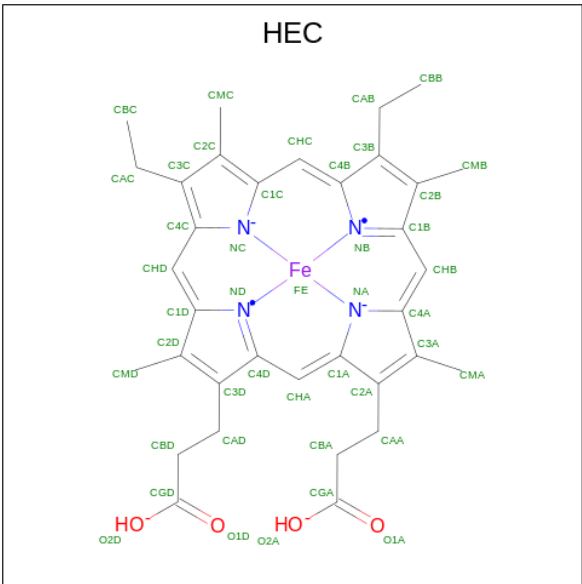
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	a	1	Total 43	C 34	Fe 1	N 4	O 4	0

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



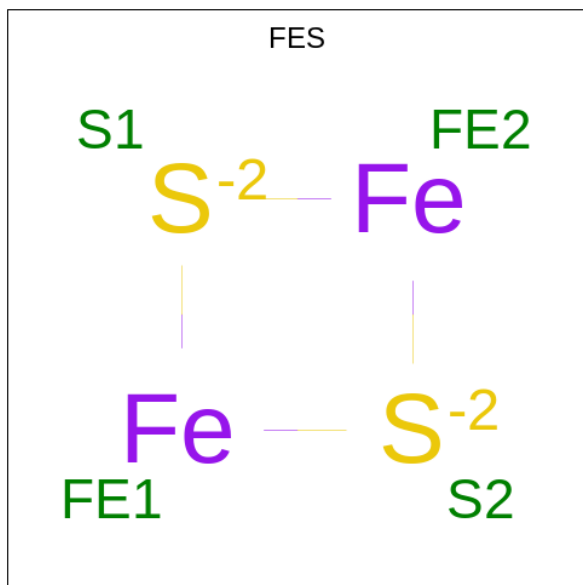
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
13	a	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 14 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



Mol	Chain	Residues	Atoms			AltConf
15	C	1	Total	Fe	S	0
			4	2	2	
15	c	1	Total	Fe	S	0
			4	2	2	

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).

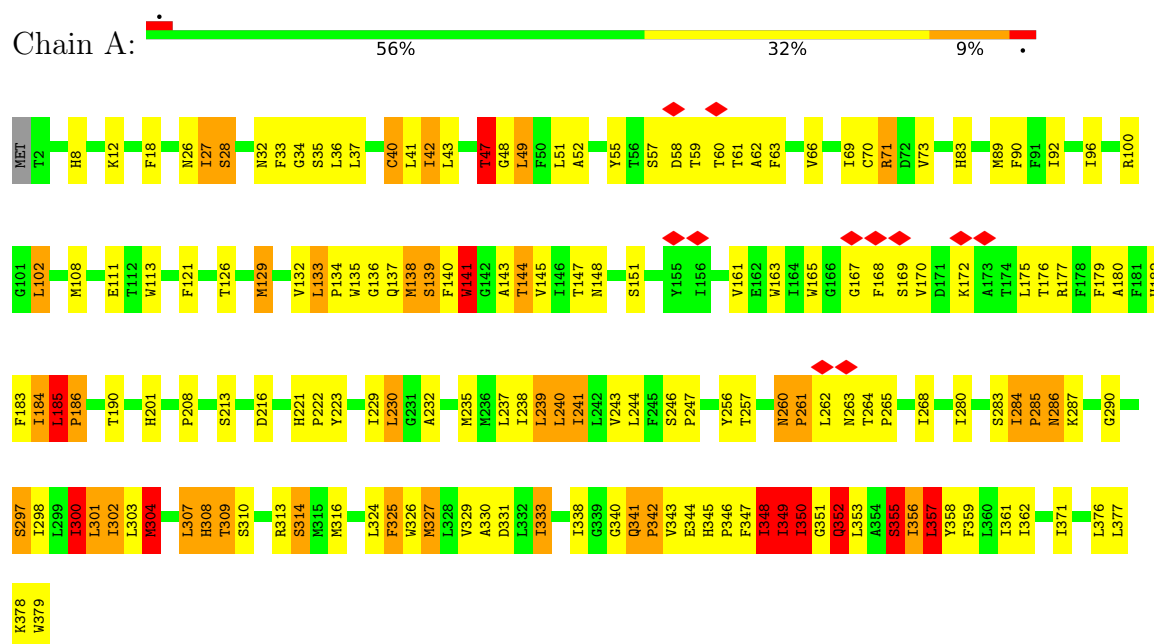


Mol	Chain	Residues	Atoms				AltConf
16	D	1	Total 64	C 45	O 17	P 2	0
16	a	1	Total 64	C 45	O 17	P 2	0

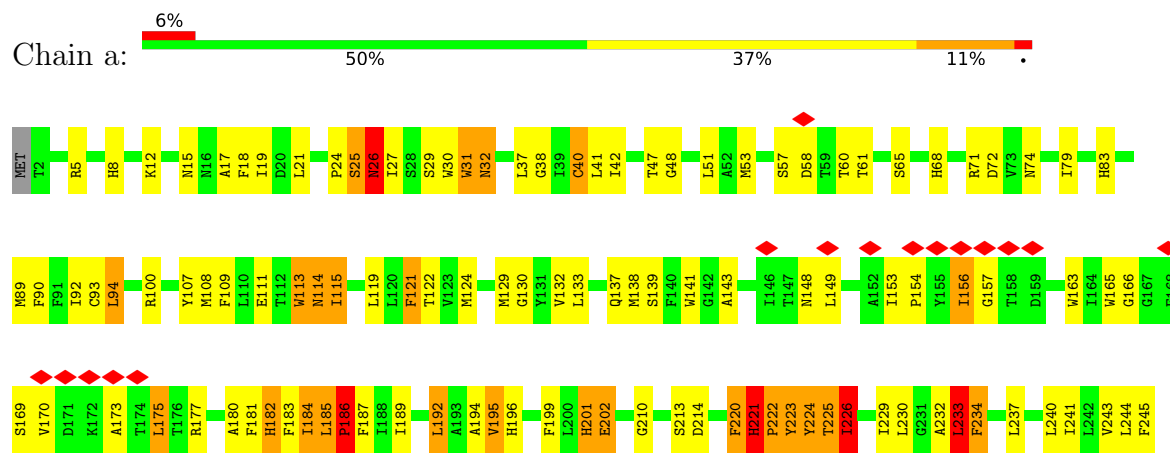
3 Residue-property plots

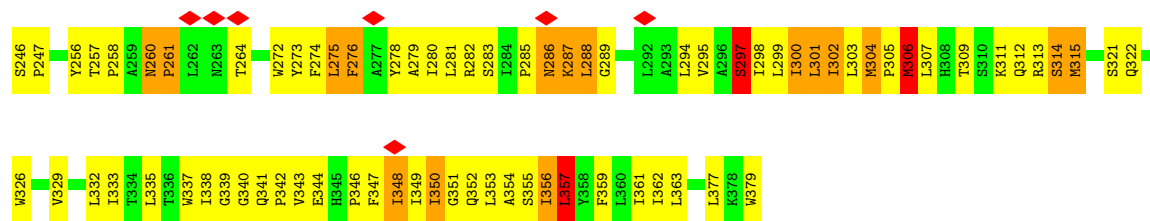
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome b

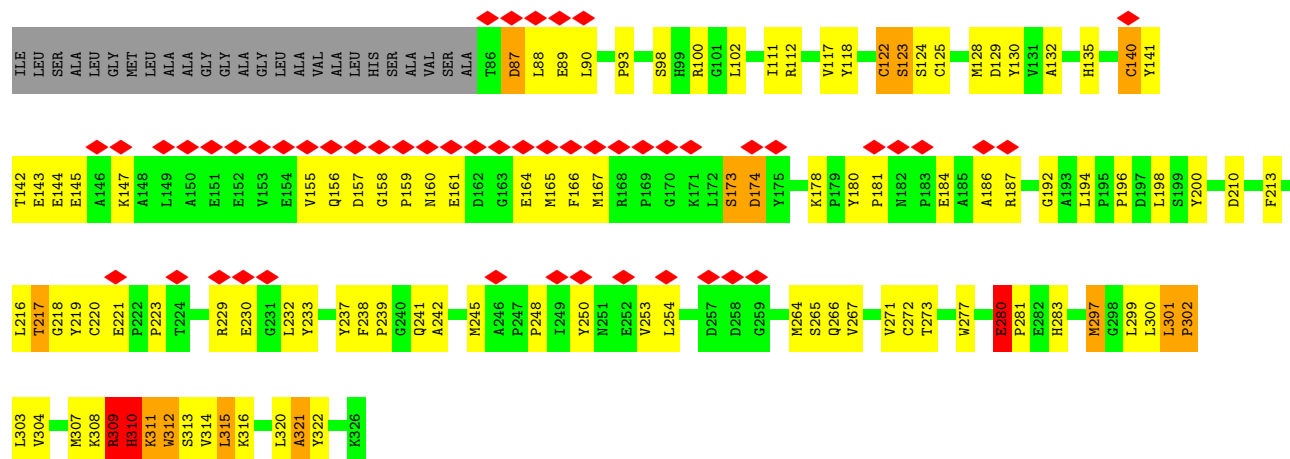
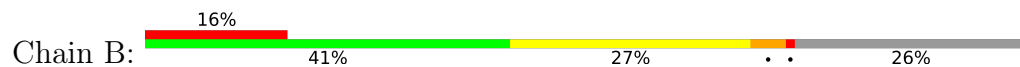


• Molecule 1: Cytochrome b

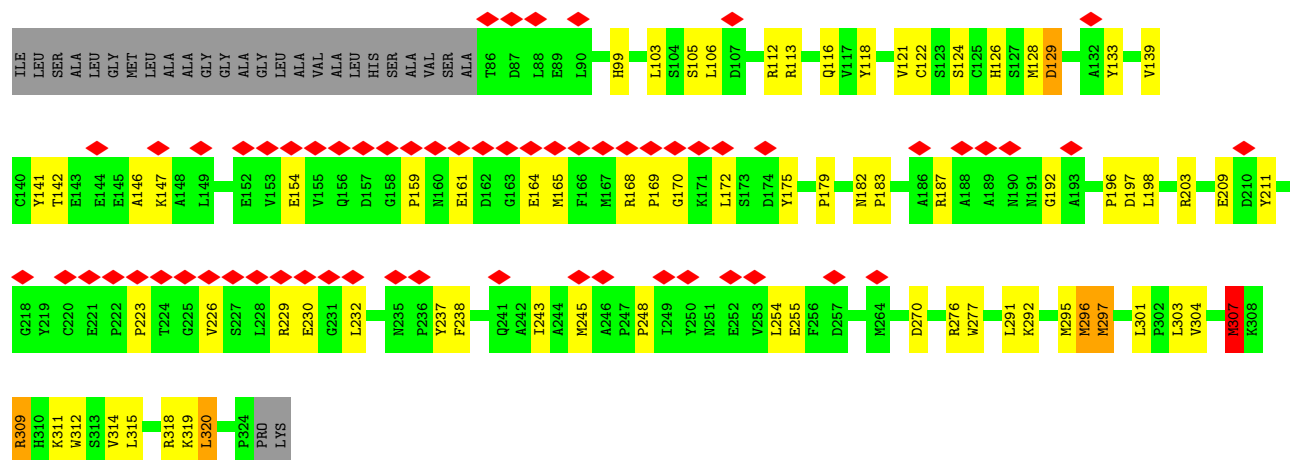




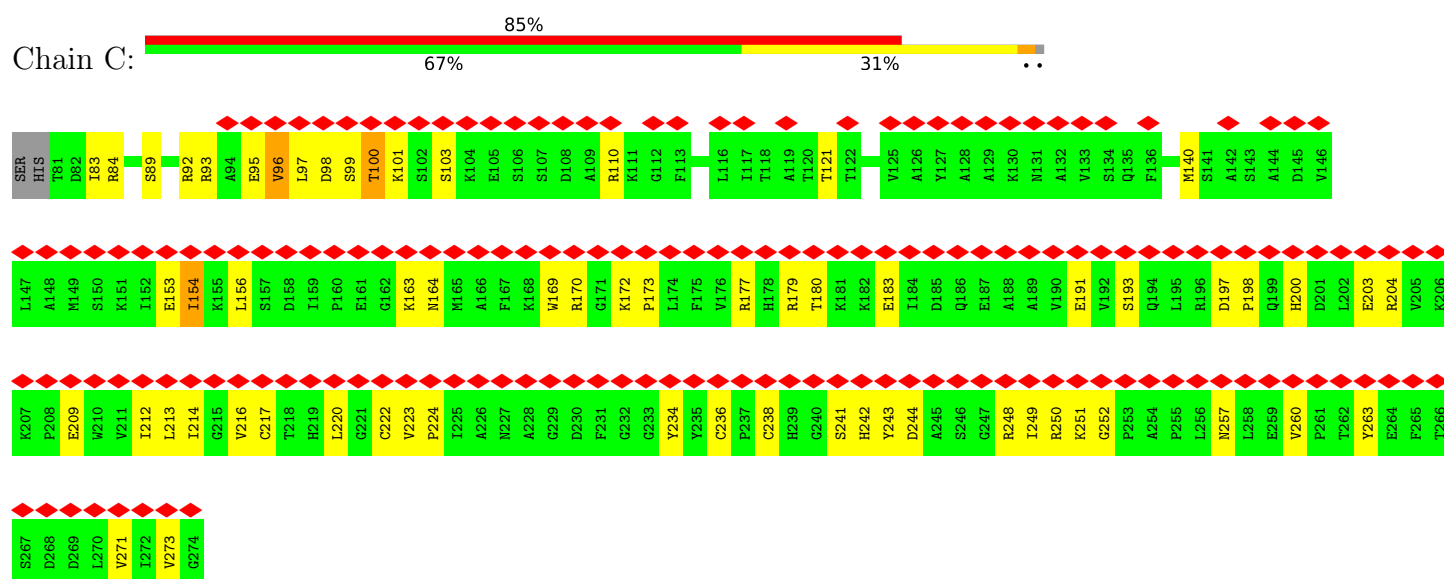
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



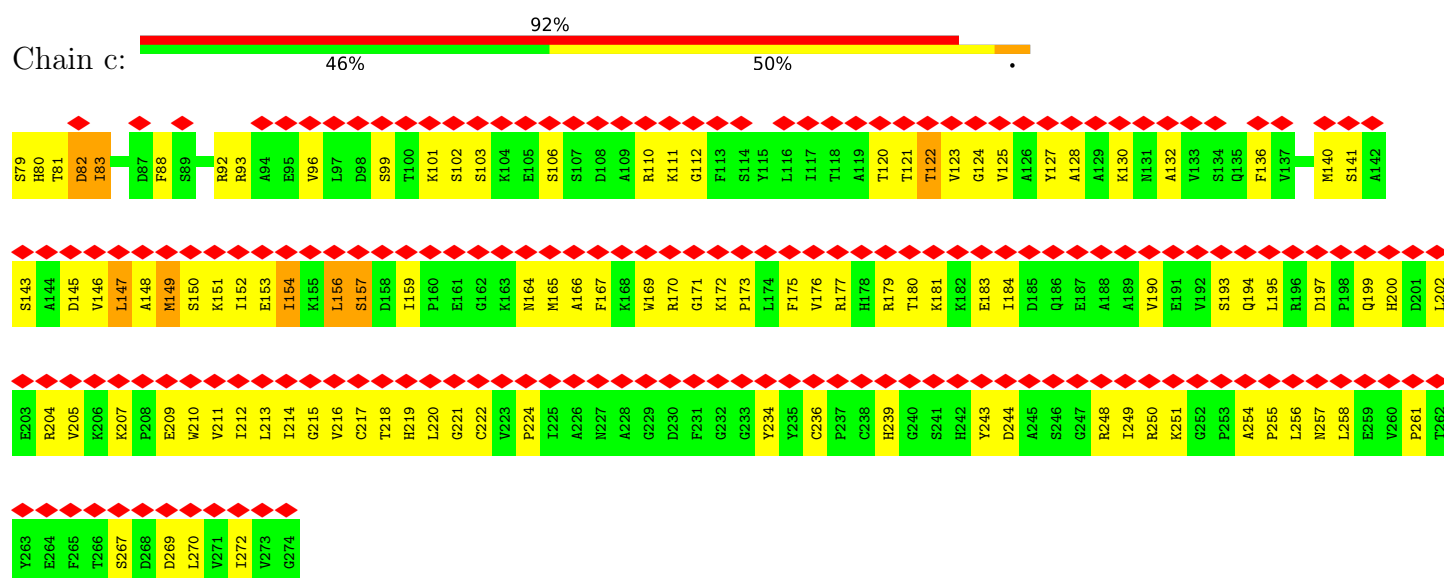
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



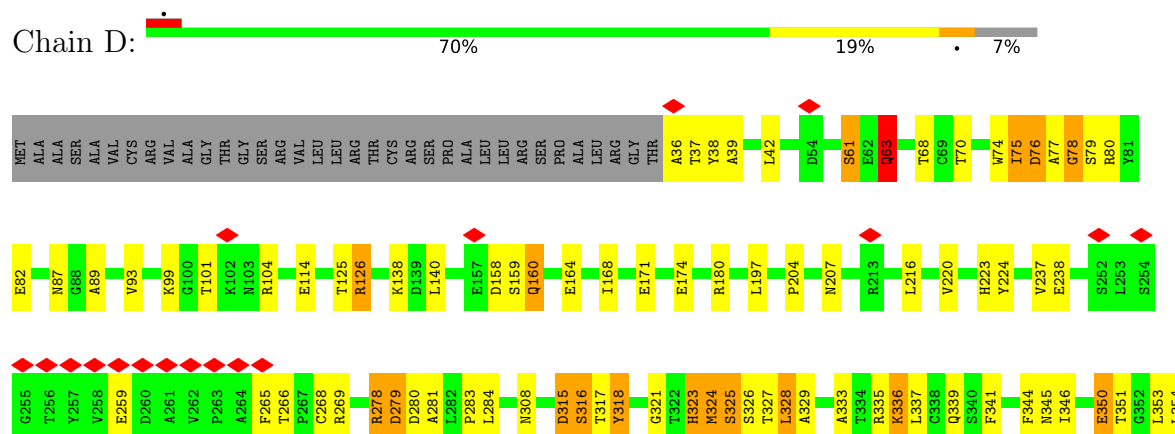
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

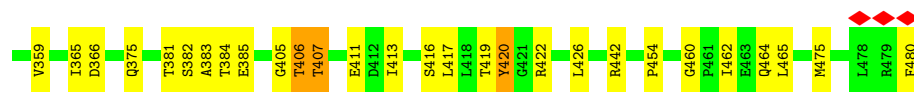


• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

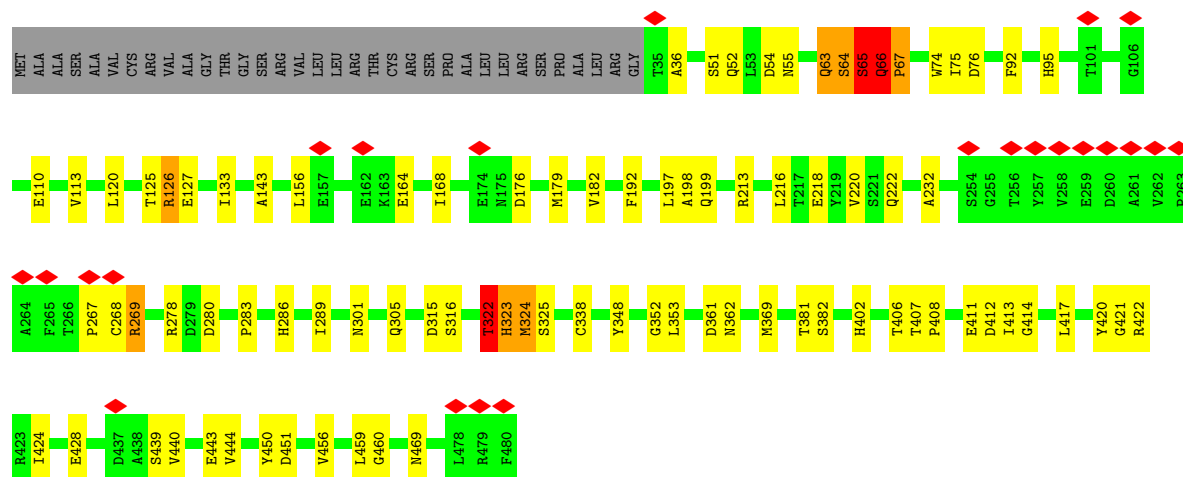
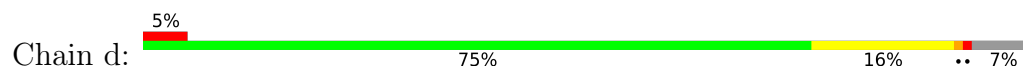


• Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

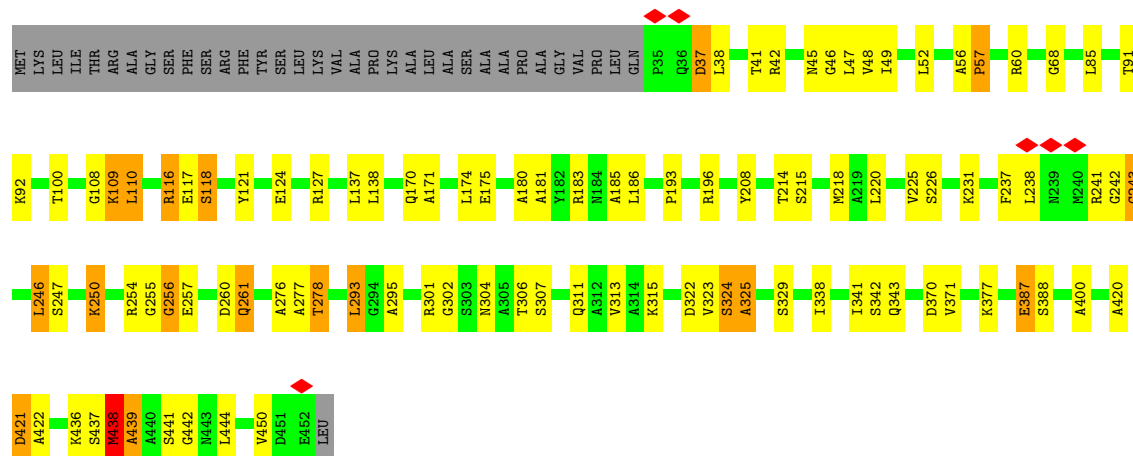




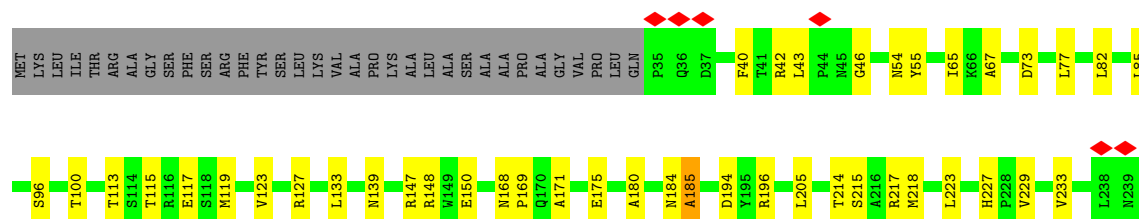
- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

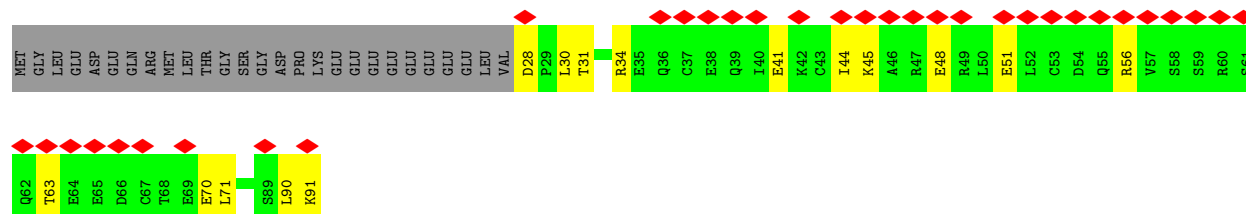


- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

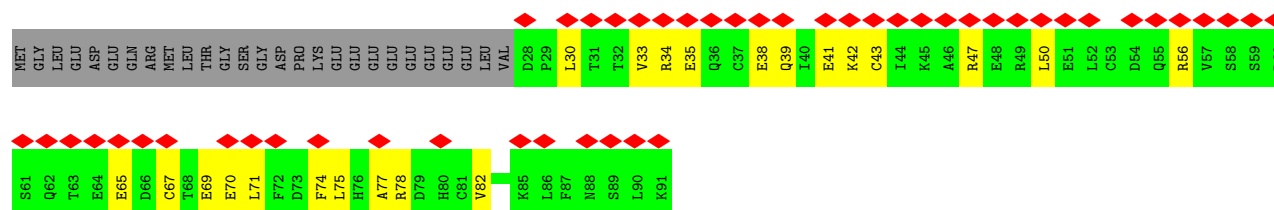




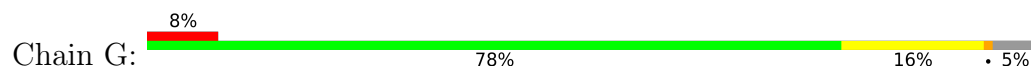
• Molecule 6: Cytochrome b-c1 complex subunit 6



• Molecule 6: Cytochrome b-c1 complex subunit 6



• Molecule 7: Cytochrome b-c1 complex subunit 7

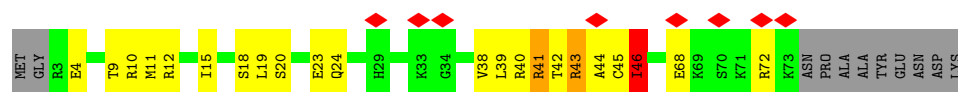


• Molecule 7: Cytochrome b-c1 complex subunit 7

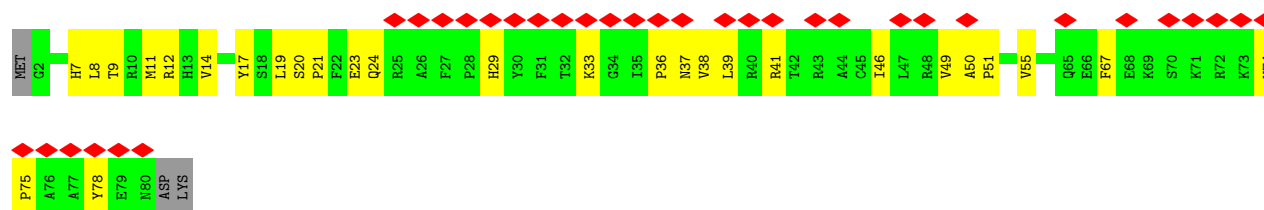
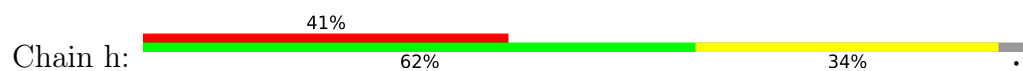


• Molecule 8: Cytochrome b-c1 complex subunit 8

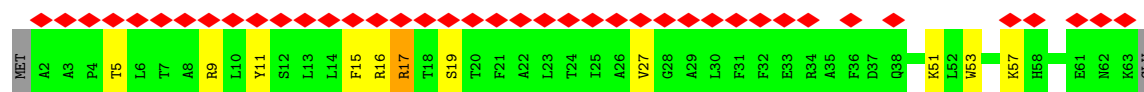




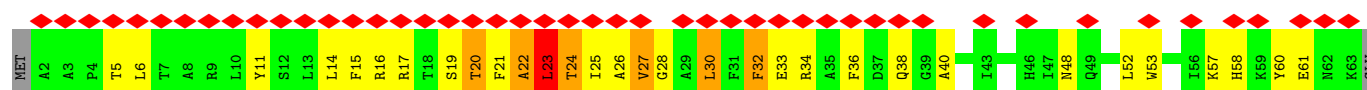
- Molecule 8: Cytochrome b-c1 complex subunit 8



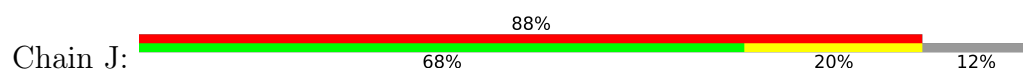
- Molecule 9: Complex III subunit 9



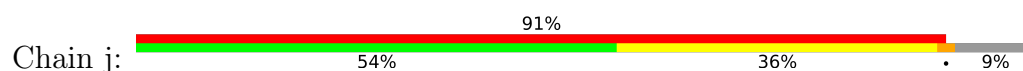
- Molecule 9: Complex III subunit 9



- Molecule 10: Cytochrome b-c1 complex subunit 10

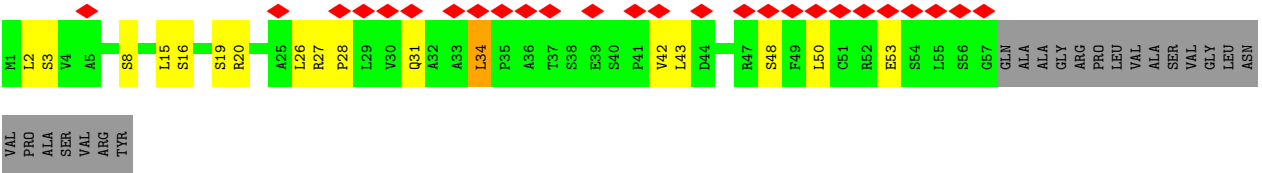


- Molecule 10: Cytochrome b-c1 complex subunit 10



- Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98300	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.21	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.627	Depositor
Minimum map value	-2.368	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	240.8, 240.8, 240.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	41/3115 (1.3%)	1.23	49/4259 (1.2%)
1	a	1.06	36/3115 (1.2%)	1.19	52/4259 (1.2%)
2	B	0.98	16/1978 (0.8%)	1.00	19/2684 (0.7%)
2	b	0.52	2/1961 (0.1%)	0.68	3/2661 (0.1%)
3	C	0.22	0/1534	0.61	2/2075 (0.1%)
3	c	0.22	0/1549	0.57	1/2095 (0.0%)
4	D	0.65	7/3524 (0.2%)	0.82	16/4783 (0.3%)
4	d	0.57	7/3531 (0.2%)	0.73	8/4793 (0.2%)
5	E	0.80	14/3187 (0.4%)	0.96	22/4314 (0.5%)
5	e	0.64	9/3187 (0.3%)	0.88	17/4314 (0.4%)
6	F	0.15	0/534	0.41	0/714
6	f	0.17	0/534	0.44	0/714
7	G	0.38	0/941	0.60	0/1262
7	g	0.66	2/941 (0.2%)	0.77	4/1262 (0.3%)
8	H	0.54	0/628	0.88	1/848 (0.1%)
8	h	0.28	0/688	0.62	0/931
9	I	0.18	0/520	0.51	0/701
9	i	0.52	1/520 (0.2%)	0.87	3/701 (0.4%)
10	J	0.16	0/420	0.44	0/576
10	j	0.18	0/437	0.54	1/598 (0.2%)
11	K	0.31	0/410	0.88	1/556 (0.2%)
11	k	0.28	0/410	0.83	1/556 (0.2%)
All	All	0.71	135/33664 (0.4%)	0.88	200/45656 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
4	D	0	2
4	d	0	3
8	h	0	1
9	I	0	1
11	K	0	2
All	All	0	14

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	311	LYS	C-O	-13.89	1.05	1.24
2	B	308	LYS	C-O	-13.68	1.07	1.24
1	a	196	HIS	C-O	-11.92	1.10	1.24
5	e	438	MET	CA-C	10.99	1.67	1.52
1	a	195	VAL	C-O	-10.41	1.12	1.24
1	A	304	MET	N-CA	9.42	1.53	1.46
1	a	196	HIS	CA-C	-9.39	1.40	1.52
1	a	115	ILE	C-O	-9.29	1.11	1.24
2	B	308	LYS	CA-C	-9.08	1.41	1.52
2	B	314	VAL	C-O	-8.91	1.14	1.24
1	a	221	HIS	C-O	-8.90	1.12	1.24
2	B	280	GLU	C-N	8.81	1.40	1.33
1	A	345	HIS	C-N	8.76	1.40	1.33
1	a	194	ALA	C-O	-8.50	1.13	1.24
1	a	220	PHE	C-O	-8.48	1.12	1.24
4	d	412	ASP	C-O	-8.47	1.14	1.24
2	B	315	LEU	C-O	-8.25	1.13	1.24
1	a	260	ASN	C-N	8.12	1.41	1.33
1	a	223	TYR	C-O	-8.08	1.14	1.24
1	A	27	ILE	C-O	-8.00	1.16	1.24
2	B	93	PRO	CG-CD	-8.00	1.23	1.50
5	e	258	ILE	C-O	-7.94	1.15	1.24
5	E	325	ALA	C-O	-7.81	1.15	1.23
1	A	327	MET	CA-CB	-7.64	1.41	1.53
1	A	26	ASN	N-CA	-7.61	1.37	1.46
1	a	300	ILE	C-O	-7.48	1.15	1.24
1	a	222	PRO	C-O	-7.48	1.14	1.24
4	d	413	ILE	C-O	-7.44	1.15	1.24
5	E	441	SER	C-O	-7.34	1.15	1.23
1	A	333	ILE	C-O	-7.32	1.15	1.24
1	A	359	PHE	C-O	-7.25	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	118	SER	C-O	-7.21	1.15	1.23
5	E	438	MET	CA-C	7.10	1.61	1.52
1	a	185	LEU	C-O	-7.08	1.18	1.24
1	A	302	ILE	C-O	-7.06	1.15	1.24
5	E	110	LEU	C-O	-7.00	1.15	1.24
4	d	125	THR	C-O	-6.98	1.16	1.24
1	A	330	ALA	C-O	-6.96	1.15	1.24
1	A	304	MET	C-O	-6.94	1.18	1.24
1	a	301	LEU	C-O	-6.89	1.16	1.24
1	a	221	HIS	CA-C	-6.81	1.44	1.52
9	i	23	LEU	CA-C	6.79	1.61	1.52
2	B	314	VAL	CA-CB	-6.78	1.46	1.54
5	E	250	LYS	CA-C	6.72	1.61	1.52
1	A	48	GLY	C-O	-6.68	1.16	1.24
4	d	325	SER	C-O	-6.67	1.15	1.24
1	A	34	GLY	C-O	-6.67	1.15	1.23
1	a	202	GLU	C-O	-6.67	1.15	1.24
1	a	233	LEU	C-O	-6.66	1.14	1.24
5	E	116	ARG	C-O	-6.64	1.15	1.24
1	A	308	HIS	C-O	-6.64	1.16	1.24
2	B	304	VAL	C-O	-6.63	1.16	1.24
5	e	441	SER	CA-C	6.63	1.61	1.52
2	B	310	HIS	C-O	-6.61	1.15	1.24
1	a	196	HIS	CA-CB	-6.60	1.43	1.53
2	B	312	TRP	N-CA	-6.59	1.38	1.46
5	e	436	LYS	CA-C	6.59	1.62	1.53
2	b	311	LYS	CA-C	6.55	1.62	1.52
1	A	327	MET	C-O	-6.55	1.16	1.24
7	g	110	LYS	CA-C	-6.54	1.44	1.52
1	A	331	ASP	C-O	-6.43	1.15	1.24
1	a	194	ALA	CA-C	-6.41	1.43	1.52
4	d	323	HIS	N-CA	-6.38	1.38	1.46
2	b	312	TRP	CB-CG	-6.30	1.30	1.50
2	B	309	ARG	C-O	-6.26	1.16	1.24
1	a	232	ALA	CA-C	-6.24	1.44	1.52
5	E	438	MET	CA-CB	-6.19	1.44	1.53
1	A	239	LEU	C-O	-6.12	1.16	1.24
5	e	438	MET	CA-CB	-6.11	1.45	1.53
1	a	229	ILE	CA-CB	-6.10	1.46	1.54
1	A	341	GLN	C-N	6.09	1.41	1.33
5	e	437	SER	CA-CB	-6.09	1.43	1.53
2	B	314	VAL	CA-C	-6.09	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	185	ALA	C-O	-6.08	1.16	1.23
5	E	442	GLY	C-O	-6.08	1.15	1.23
1	a	300	ILE	CA-C	-6.06	1.45	1.52
1	a	113	TRP	CA-CB	-5.98	1.43	1.53
4	D	78	GLY	CA-C	-5.97	1.46	1.51
1	A	28	SER	C-O	-5.96	1.17	1.23
5	e	260	ASP	C-O	-5.93	1.17	1.23
1	A	304	MET	CA-C	5.91	1.59	1.52
1	A	357	LEU	C-O	-5.86	1.16	1.24
4	D	335	ARG	C-O	-5.82	1.16	1.24
1	A	284	ILE	C-N	5.80	1.41	1.33
5	E	437	SER	CA-CB	-5.80	1.45	1.53
1	a	25	SER	N-CA	-5.77	1.37	1.45
2	B	311	LYS	C-N	-5.76	1.26	1.33
1	A	301	LEU	C-O	-5.75	1.17	1.24
1	A	34	GLY	CA-C	-5.74	1.46	1.52
1	a	232	ALA	C-O	-5.73	1.17	1.24
4	D	405	GLY	C-O	-5.71	1.18	1.24
1	a	185	LEU	CA-C	-5.70	1.46	1.52
1	a	222	PRO	N-CD	5.69	1.55	1.47
4	d	324	MET	CA-C	-5.68	1.45	1.52
4	D	315	ASP	C-O	-5.64	1.17	1.23
1	a	225	THR	CB-CG2	-5.62	1.34	1.52
1	A	36	LEU	C-O	-5.60	1.17	1.24
4	D	61	SER	C-O	-5.60	1.17	1.23
2	B	307	MET	CA-CB	-5.59	1.44	1.53
1	A	342	PRO	N-CD	5.55	1.55	1.47
1	A	350	ILE	C-O	-5.54	1.17	1.24
1	A	241	ILE	C-O	-5.51	1.16	1.24
5	e	439	ALA	CA-C	5.50	1.59	1.52
1	A	37	LEU	C-O	-5.45	1.17	1.24
1	A	327	MET	CA-C	-5.45	1.46	1.52
5	E	181	ALA	C-O	-5.45	1.17	1.24
1	a	261	PRO	N-CD	5.41	1.55	1.47
4	D	407	THR	C-N	5.40	1.41	1.34
5	E	57	PRO	N-CD	5.39	1.55	1.47
1	A	43	LEU	C-O	-5.37	1.17	1.24
1	a	247	PRO	N-CD	5.36	1.55	1.47
1	a	301	LEU	N-CA	5.36	1.52	1.46
1	A	326	TRP	CE2-CZ2	-5.35	1.28	1.39
1	A	352	GLN	C-O	-5.35	1.17	1.24
1	A	247	PRO	N-CD	5.35	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	PRO	N-CD	5.34	1.55	1.47
1	A	186	PRO	N-CD	5.32	1.55	1.47
1	a	233	LEU	CA-C	-5.28	1.43	1.52
1	a	229	ILE	C-O	-5.26	1.18	1.24
1	A	240	LEU	C-O	-5.24	1.17	1.24
1	a	246	SER	C-N	5.22	1.41	1.34
2	B	281	PRO	N-CD	5.20	1.55	1.47
4	D	317	THR	C-O	-5.16	1.16	1.23
4	d	414	GLY	C-O	-5.16	1.17	1.23
1	a	305	PRO	N-CD	5.14	1.54	1.47
1	A	185	LEU	C-N	5.14	1.41	1.34
1	A	246	SER	C-N	5.13	1.41	1.34
1	A	260	ASN	C-N	5.12	1.41	1.34
7	g	110	LYS	C-O	-5.11	1.17	1.24
1	A	261	PRO	N-CD	5.11	1.54	1.47
5	E	181	ALA	CA-CB	-5.06	1.46	1.54
1	a	113	TRP	C-O	-5.06	1.18	1.24
1	A	47	THR	C-O	-5.05	1.18	1.24
5	E	420	ALA	CA-C	-5.01	1.46	1.52
1	a	224	TYR	C-O	-5.00	1.17	1.24

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	440	ALA	N-CA-C	-14.98	86.76	107.88
1	a	297	SER	N-CA-C	14.41	126.70	111.14
5	e	245	GLY	N-CA-C	14.23	129.01	112.50
1	A	304	MET	N-CA-C	13.42	130.66	112.55
5	e	242	GLY	N-CA-C	13.16	129.62	112.77
1	a	224	TYR	N-CA-C	-12.43	98.24	113.41
1	a	223	TYR	N-CA-C	12.20	124.66	111.36
4	D	337	LEU	N-CA-C	11.91	124.34	111.36
1	a	301	LEU	N-CA-C	11.84	124.19	111.28
2	B	93	PRO	N-CD-CG	-11.70	85.65	103.20
5	E	246	LEU	N-CA-C	10.80	122.81	111.14
5	e	439	ALA	N-CA-C	-10.72	91.03	108.07
5	e	244	LEU	N-CA-C	10.58	125.57	110.23
1	A	304	MET	CA-C-N	10.27	130.58	119.28
1	A	304	MET	C-N-CA	10.27	130.58	119.28
2	B	307	MET	CB-CG-SD	-9.90	83.00	112.70
5	E	325	ALA	N-CA-C	-9.77	95.20	108.38
5	e	276	ALA	N-CA-C	9.72	124.67	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	72	ASP	N-CA-C	9.62	121.77	111.28
1	a	32	ASN	N-CA-C	9.32	121.52	111.36
9	i	23	LEU	N-CA-C	9.29	122.36	111.02
5	E	420	ALA	N-CA-C	-9.23	96.81	110.48
1	A	359	PHE	N-CA-C	8.99	121.16	111.36
1	A	229	ILE	N-CA-C	8.98	119.01	110.30
4	d	325	SER	N-CA-C	8.84	123.16	112.38
5	E	277	ALA	N-CA-C	8.79	122.89	110.50
5	e	436	LYS	N-CA-C	8.73	123.90	110.36
1	a	196	HIS	CA-C-O	-8.66	111.37	120.55
1	a	196	HIS	CB-CA-C	-8.61	96.50	110.79
1	a	196	HIS	CA-C-N	8.54	135.21	120.68
1	a	196	HIS	C-N-CA	8.54	135.21	120.68
1	a	184	ILE	CB-CA-C	8.53	125.28	111.29
1	a	306	MET	CA-C-N	8.37	135.05	121.99
1	a	306	MET	C-N-CA	8.37	135.05	121.99
5	E	117	GLU	N-CA-C	8.34	123.25	112.41
1	a	226	ILE	N-CA-C	8.30	119.08	110.62
3	C	103	SER	N-CA-C	8.26	120.36	111.36
5	e	438	MET	N-CA-C	-8.10	97.69	109.18
1	A	141	TRP	N-CA-C	8.07	123.17	113.16
1	A	235	MET	N-CA-C	8.03	120.12	111.36
4	d	65	SER	N-CA-C	8.00	122.72	111.52
4	D	325	SER	CA-C-N	-7.96	111.00	122.94
4	D	325	SER	C-N-CA	-7.96	111.00	122.94
5	e	227	HIS	N-CA-C	7.96	124.46	113.16
1	A	327	MET	CB-CG-SD	-7.91	88.97	112.70
1	A	27	ILE	CG1-CB-CG2	-7.79	87.33	110.70
3	c	149	MET	N-CA-C	7.77	119.75	111.28
4	D	318	TYR	CA-C-N	-7.76	115.63	121.61
4	D	318	TYR	C-N-CA	-7.76	115.63	121.61
5	e	437	SER	N-CA-C	-7.72	95.55	108.75
1	a	225	THR	N-CA-CB	7.46	120.80	109.91
1	a	300	ILE	CB-CA-C	-7.37	102.19	112.14
1	A	349	ILE	N-CA-C	7.25	117.35	110.53
5	E	436	LYS	N-CA-C	7.20	121.19	109.59
2	B	320	LEU	CA-C-N	7.20	135.30	121.54
2	B	320	LEU	C-N-CA	7.20	135.30	121.54
5	E	247	SER	N-CA-C	7.09	121.18	111.39
9	i	22	ALA	O-C-N	-7.08	114.73	122.09
5	E	276	ALA	CA-C-N	7.06	132.03	120.94
5	E	276	ALA	C-N-CA	7.06	132.03	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	100	THR	N-CA-C	7.06	121.91	113.16
4	D	78	GLY	N-CA-C	-7.00	101.04	110.56
5	E	243	GLY	N-CA-C	6.89	119.85	111.93
1	A	348	ILE	N-CA-C	6.87	117.66	110.72
1	a	157	GLY	N-CA-C	6.87	120.98	112.73
8	H	45	CYS	N-CA-C	6.84	120.71	107.71
1	A	341	GLN	CA-C-N	-6.78	113.70	120.21
1	A	341	GLN	C-N-CA	-6.78	113.70	120.21
1	A	284	ILE	CA-C-N	-6.77	113.01	119.85
1	A	284	ILE	C-N-CA	-6.77	113.01	119.85
1	A	33	PHE	N-CA-C	6.77	120.80	112.54
2	b	315	LEU	N-CA-C	6.77	121.55	113.16
2	B	93	PRO	CA-CB-CG	-6.76	91.66	104.50
1	a	224	TYR	CB-CA-C	6.73	121.02	109.24
1	A	42	ILE	N-CA-C	6.72	121.45	112.04
1	A	133	LEU	CA-C-N	6.70	127.24	119.47
1	A	133	LEU	C-N-CA	6.70	127.24	119.47
4	d	324	MET	N-CA-C	-6.64	99.09	109.72
4	D	278	ARG	N-CA-C	6.62	121.69	111.56
5	E	185	ALA	N-CA-C	6.61	118.49	111.28
1	A	26	ASN	N-CA-C	6.59	120.24	112.72
2	B	312	TRP	N-CA-C	-6.57	104.58	112.59
2	B	308	LYS	N-CA-C	-6.56	104.21	111.36
4	d	64	SER	N-CA-C	6.51	121.28	112.88
5	E	278	THR	N-CA-C	6.45	119.59	110.23
1	A	238	ILE	N-CA-C	6.44	117.19	110.62
1	a	260	ASN	CA-C-N	-6.44	113.10	120.89
1	a	260	ASN	C-N-CA	-6.44	113.10	120.89
2	B	280	GLU	CA-C-N	-6.37	113.33	121.04
2	B	280	GLU	C-N-CA	-6.37	113.33	121.04
5	e	184	ASN	N-CA-C	6.26	124.14	110.80
5	e	439	ALA	O-C-N	-6.22	117.81	123.41
2	B	123	SER	N-CA-C	6.20	118.04	111.28
1	A	133	LEU	N-CA-C	6.19	123.48	109.81
5	e	441	SER	N-CA-C	-6.19	97.62	110.80
1	A	27	ILE	CA-C-N	6.17	132.99	122.12
1	A	27	ILE	C-N-CA	6.17	132.99	122.12
1	A	345	HIS	CA-C-N	-6.16	113.58	121.04
1	A	345	HIS	C-N-CA	-6.16	113.58	121.04
5	E	293	LEU	N-CA-C	6.13	118.04	111.36
1	a	186	PRO	CA-C-O	-6.12	109.46	120.60
4	D	63	GLN	N-CA-C	6.11	119.09	108.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	MET	N-CA-C	6.07	117.70	111.14
1	a	187	PHE	N-CA-C	6.07	117.89	111.28
1	A	262	LEU	N-CA-C	6.03	117.85	111.28
4	D	77	ALA	N-CA-C	-6.03	100.24	108.38
2	B	122	CYS	N-CA-C	5.97	117.79	111.28
1	a	114	ASN	N-CA-C	5.97	118.75	111.82
4	d	127	GLU	N-CA-C	5.93	121.43	113.72
7	g	101	GLU	O-C-N	-5.92	114.35	122.46
1	A	355	SER	N-CA-C	5.90	117.39	111.07
5	e	258	ILE	CA-C-O	-5.90	114.97	120.22
10	j	41	ILE	N-CA-C	-5.85	107.80	113.53
1	A	325	PHE	N-CA-C	-5.83	104.11	111.11
2	B	314	VAL	CB-CA-C	-5.82	104.43	111.88
1	a	186	PRO	CA-C-N	-5.80	112.51	120.28
1	a	186	PRO	C-N-CA	-5.80	112.51	120.28
4	D	316	SER	N-CA-C	5.78	120.07	113.19
5	E	295	ALA	N-CA-C	5.76	119.51	111.74
11	k	27	ARG	N-CA-C	-5.75	97.11	109.81
7	g	48	ILE	N-CA-C	-5.75	107.21	112.96
4	d	408	PRO	CA-N-CD	-5.72	103.99	112.00
2	B	100	ARG	N-CA-C	5.72	117.51	111.28
4	D	324	MET	N-CA-C	5.69	117.24	110.19
4	D	336	LYS	N-CA-C	5.68	119.41	111.74
1	A	35	SER	N-CA-C	5.67	118.23	111.71
1	A	260	ASN	CA-C-N	-5.67	112.76	119.05
1	A	260	ASN	C-N-CA	-5.67	112.76	119.05
1	a	156	ILE	N-CA-C	5.64	116.41	110.72
1	a	226	ILE	N-CA-CB	5.63	118.19	110.54
4	d	414	GLY	N-CA-C	5.59	119.93	112.77
1	a	186	PRO	CA-N-CD	-5.59	104.17	112.00
2	b	320	LEU	N-CA-C	5.58	117.44	110.91
7	g	106	GLU	N-CA-C	5.58	117.16	111.14
5	E	37	ASP	N-CA-C	5.57	117.35	111.28
11	K	8	SER	N-CA-C	5.54	117.39	110.91
2	B	297	MET	N-CA-C	-5.52	105.27	111.28
2	B	321	ALA	CA-C-N	5.52	132.08	121.54
2	B	321	ALA	C-N-CA	5.52	132.08	121.54
2	B	216	LEU	N-CA-C	5.51	117.37	111.36
5	E	438	MET	CB-CG-SD	-5.50	96.21	112.70
1	A	358	TYR	CA-C-N	5.50	128.09	120.29
1	A	358	TYR	C-N-CA	5.50	128.09	120.29
9	i	27	VAL	N-CA-C	5.49	116.22	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	220	PHE	CB-CA-C	5.48	119.53	109.99
4	D	89	ALA	N-CA-C	5.48	117.25	111.28
1	A	287	LYS	N-CA-C	5.45	117.30	111.36
1	A	145	VAL	N-CA-C	5.44	115.58	110.30
1	A	185	LEU	CA-C-N	-5.42	113.03	119.05
1	A	185	LEU	C-N-CA	-5.42	113.03	119.05
5	E	118	SER	N-CA-C	5.41	117.61	109.23
1	A	356	ILE	N-CA-CB	5.40	117.89	110.54
5	E	436	LYS	CA-C-N	5.37	130.13	122.72
5	E	436	LYS	C-N-CA	5.37	130.13	122.72
5	E	256	GLY	N-CA-C	5.36	118.10	111.93
1	a	233	LEU	CA-CB-CG	5.36	135.07	116.30
1	a	186	PRO	N-CA-C	5.35	123.49	112.47
1	A	184	ILE	N-CA-C	5.33	116.05	110.62
1	a	246	SER	CA-C-N	-5.32	113.14	119.05
1	a	246	SER	C-N-CA	-5.32	113.14	119.05
4	D	279	ASP	N-CA-C	5.32	118.73	111.39
4	d	66	GLN	C-N-CD	-5.32	103.18	125.00
2	B	174	ASP	N-CA-C	5.31	117.94	110.23
1	a	357	LEU	N-CA-C	5.31	118.92	112.23
1	a	224	TYR	CA-C-N	-5.30	113.66	120.65
1	a	224	TYR	C-N-CA	-5.30	113.66	120.65
5	e	441	SER	CA-C-N	5.29	131.79	121.41
5	e	441	SER	C-N-CA	5.29	131.79	121.41
1	A	246	SER	CA-C-N	-5.29	113.18	119.05
1	A	246	SER	C-N-CA	-5.29	113.18	119.05
1	A	62	ALA	N-CA-C	5.29	116.72	111.07
4	D	407	THR	CA-C-N	-5.29	113.47	118.97
4	D	407	THR	C-N-CA	-5.29	113.47	118.97
1	a	31	TRP	CA-C-N	5.28	127.79	120.29
1	a	31	TRP	C-N-CA	5.28	127.79	120.29
2	b	307	MET	CB-CG-SD	-5.28	96.87	112.70
1	a	24	PRO	CA-C-N	-5.27	113.76	121.99
1	a	24	PRO	C-N-CA	-5.27	113.76	121.99
1	a	19	ILE	N-CA-C	5.26	115.98	110.62
1	a	187	PHE	CB-CA-C	5.26	119.52	110.79
1	A	49	LEU	CB-CA-C	-5.25	102.60	110.90
1	A	284	ILE	N-CA-C	5.25	113.86	107.61
5	E	421	ASP	N-CA-C	-5.23	103.49	110.55
1	a	221	HIS	CA-C-N	-5.21	113.32	119.84
1	a	221	HIS	C-N-CA	-5.21	113.32	119.84
1	a	223	TYR	O-C-N	-5.21	116.21	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	26	ASN	N-CA-C	5.20	119.31	112.92
1	a	300	ILE	N-CA-CB	5.19	117.59	110.54
1	a	185	LEU	CA-C-N	-5.18	113.36	119.84
1	a	185	LEU	C-N-CA	-5.18	113.36	119.84
1	a	276	PHE	N-CA-C	5.15	116.70	111.14
7	g	107	GLU	N-CA-CB	5.14	118.14	110.22
1	a	301	LEU	CA-CB-CG	5.13	134.25	116.30
5	E	323	VAL	CB-CA-C	-5.12	102.61	110.50
1	A	300	ILE	N-CA-C	5.08	119.15	112.04
1	A	232	ALA	N-CA-C	5.07	117.54	111.71
1	A	28	SER	CB-CA-C	-5.05	101.12	113.15
5	e	437	SER	CA-CB-OG	-5.01	101.07	111.10
2	B	173	SER	N-CA-C	5.01	116.74	111.28
1	a	234	PHE	N-CA-C	5.00	119.36	113.16

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	GLN	Peptide
1	A	141	TRP	Peptide
4	D	160	GLN	Peptide
4	D	420	TYR	Peptide
9	I	17	ARG	Peptide
11	K	26	LEU	Peptide
11	K	34	LEU	Peptide
1	a	133	LEU	Peptide
1	a	221	HIS	Peptide
1	a	306	MET	Peptide
4	d	322	THR	Peptide
4	d	338	CYS	Peptide
4	d	420	TYR	Peptide
8	h	55	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	3078	235	0
1	a	3017	0	3078	261	0
2	B	1920	0	1869	104	0
2	b	1904	0	1849	99	0
3	C	1502	0	1488	71	0
3	c	1517	0	1495	219	0
4	D	3452	0	3343	116	0
4	d	3459	0	3350	84	0
5	E	3134	0	3112	79	0
5	e	3134	0	3112	70	0
6	F	528	0	510	11	0
6	f	528	0	510	18	0
7	G	921	0	917	15	0
7	g	921	0	917	21	0
8	H	608	0	616	17	0
8	h	666	0	663	25	0
9	I	507	0	509	11	0
9	i	507	0	509	51	0
10	J	405	0	405	11	0
10	j	421	0	418	18	0
11	K	404	0	425	17	0
11	k	404	0	425	18	0
12	A	86	0	60	8	0
12	a	86	0	60	12	0
13	A	45	0	67	2	0
13	D	49	0	75	1	0
13	a	49	0	75	3	0
14	B	43	0	32	3	0
14	b	43	0	32	7	0
15	C	4	0	0	2	0
15	c	4	0	0	5	0
16	D	64	0	72	3	0
16	a	64	0	72	4	0
All	All	33413	0	33143	1358	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 20.

All (1358) 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)
2:b:122:CYS:CB	14:b:401:HEC:HAB	1.38	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:327:THR:HG21	4:D:375:GLN:NE2	1.32	1.39
3:c:80:HIS:NE2	4:d:182:VAL:HG12	1.39	1.33
3:c:82:ASP:O	3:c:83:ILE:HG23	1.14	1.31
3:C:220:LEU:HB2	15:C:301:FES:S2	1.72	1.28
3:c:239:HIS:HD2	15:c:301:FES:S2	1.59	1.26
1:A:121:PHE:CE2	1:A:298:ILE:HG21	1.73	1.22
3:c:239:HIS:CD2	15:c:301:FES:S2	2.33	1.21
3:c:123:VAL:CG1	9:i:25:ILE:HA	1.72	1.18
1:A:121:PHE:CE2	1:A:298:ILE:CG2	2.26	1.18
1:A:284:ILE:HD11	1:A:290:GLY:CA	1.75	1.15
1:a:129:MET:SD	1:a:181:PHE:HB3	1.85	1.15
1:a:348:ILE:O	1:a:352:GLN:HG3	1.45	1.14
9:i:22:ALA:O	9:i:25:ILE:HG12	1.45	1.14
3:c:99:SER:HA	4:d:269:ARG:HH11	1.15	1.11
9:i:17:ARG:HB2	9:i:20:THR:OG1	1.51	1.11
1:A:300:ILE:HD12	1:A:362:ILE:HD12	1.29	1.10
3:c:99:SER:HA	4:d:269:ARG:NH1	1.66	1.10
2:b:122:CYS:CB	14:b:401:HEC:CAB	2.29	1.10
2:b:122:CYS:HB3	14:b:401:HEC:HAB	1.23	1.10
1:A:141:TRP:NE1	3:c:222:CYS:HA	1.66	1.09
4:D:328:LEU:HB3	4:D:341:PHE:CZ	1.86	1.09
1:A:300:ILE:CD1	1:A:362:ILE:HD12	1.81	1.09
7:g:111:LYS:OXT	7:g:111:LYS:HG2	1.52	1.09
1:a:230:LEU:HD13	2:b:304:VAL:HG12	1.34	1.08
3:c:123:VAL:HG12	9:i:25:ILE:O	1.54	1.08
4:D:326:SER:HB2	4:D:329:ALA:HB3	1.23	1.07
2:b:122:CYS:HB3	14:b:401:HEC:CAB	1.85	1.07
1:a:275:LEU:HD22	1:a:340:GLY:N	1.70	1.07
2:b:122:CYS:HB2	14:b:401:HEC:HAB	1.26	1.07
3:c:150:SER:HA	3:c:153:GLU:HB3	1.09	1.07
3:c:150:SER:HB3	3:c:153:GLU:CD	1.79	1.06
9:i:24:THR:HA	9:i:27:VAL:HG23	1.38	1.05
1:a:132:VAL:HG13	1:a:139:SER:O	1.57	1.05
1:A:344:GLU:CB	1:A:347:PHE:HB2	1.88	1.04
1:a:58:ASP:HB2	1:a:61:THR:HB	1.38	1.04
3:c:82:ASP:O	3:c:83:ILE:CG2	2.05	1.04
3:c:150:SER:HA	3:c:153:GLU:CB	1.89	1.02
1:A:283:SER:OG	1:A:352:GLN:HB2	1.59	1.01
4:D:381:THR:HG22	4:D:382:SER:H	1.25	1.01
3:c:220:LEU:HD12	15:c:301:FES:S2	1.99	1.01
3:c:120:THR:O	3:c:123:VAL:HG22	1.61	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:CD2	1:A:298:ILE:HG21	1.97	1.00
3:c:80:HIS:NE2	4:d:182:VAL:CG1	2.25	0.99
1:A:280:ILE:HD13	1:A:355:SER:OG	1.63	0.99
4:D:326:SER:HB2	4:D:329:ALA:CB	1.92	0.99
1:a:129:MET:CE	1:a:181:PHE:HB3	1.92	0.99
3:c:156:LEU:CD2	3:c:269:ASP:HA	1.92	0.99
1:A:47:THR:HG22	1:A:83:HIS:ND1	1.76	0.99
1:A:180:ALA:O	1:A:184:ILE:HG12	1.61	0.98
1:A:223:TYR:CE2	2:B:315:LEU:CD2	2.46	0.98
1:a:201:HIS:O	1:a:202:GLU:HG2	1.60	0.98
1:a:299:LEU:O	1:a:302:ILE:HD11	1.61	0.98
3:c:156:LEU:HD11	3:c:210:TRP:CH2	1.99	0.97
1:A:284:ILE:CD1	1:A:290:GLY:HA2	1.92	0.97
1:A:344:GLU:HB2	1:A:347:PHE:CB	1.93	0.97
1:A:284:ILE:HD11	1:A:290:GLY:HA2	0.96	0.96
1:A:344:GLU:HB2	1:A:347:PHE:HB2	0.98	0.96
3:C:156:LEU:HB2	3:C:271:VAL:HG11	1.45	0.96
3:c:123:VAL:HG13	9:i:25:ILE:HA	1.47	0.96
4:D:327:THR:HG21	4:D:375:GLN:CD	1.90	0.95
3:c:80:HIS:CD2	4:d:182:VAL:HG12	2.01	0.95
5:e:214:THR:HG21	5:e:244:LEU:HA	1.48	0.95
3:c:123:VAL:HG12	9:i:25:ILE:HA	1.48	0.95
1:a:275:LEU:CD2	1:a:340:GLY:N	2.31	0.94
3:c:123:VAL:HG12	9:i:25:ILE:C	1.91	0.94
1:a:119:LEU:HD11	1:a:192:LEU:HB3	1.50	0.94
3:c:123:VAL:HG12	9:i:25:ILE:CA	1.96	0.94
1:A:338:ILE:HD11	1:A:350:ILE:HD11	1.49	0.93
1:a:111:GLU:HB3	1:a:199:PHE:CD2	2.01	0.93
4:D:327:THR:CG2	4:D:375:GLN:NE2	2.29	0.93
1:A:348:ILE:HD13	1:A:349:ILE:N	1.83	0.93
1:A:58:ASP:N	1:A:175:LEU:HD23	1.84	0.92
3:c:122:THR:HB	9:i:25:ILE:HG21	1.52	0.92
3:C:220:LEU:CB	15:C:301:FES:S2	2.58	0.91
3:C:222:CYS:SG	3:C:238:CYS:SG	2.68	0.91
2:B:112:ARG:HA	2:B:140:CYS:SG	2.11	0.91
5:e:438:MET:HG3	5:e:439:ALA:H	1.31	0.91
1:A:140:PHE:C	1:A:141:TRP:HE3	1.79	0.91
1:a:119:LEU:HD12	1:a:192:LEU:HD23	1.52	0.90
3:c:150:SER:O	3:c:153:GLU:HG2	1.72	0.90
2:b:118:TYR:HA	2:b:122:CYS:SG	2.11	0.90
1:A:348:ILE:HD13	1:A:349:ILE:H	1.33	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:245:MET:HE1	2:b:248:PRO:HG3	1.51	0.90
3:c:122:THR:HB	9:i:25:ILE:CG2	2.01	0.90
2:B:245:MET:HE2	2:B:248:PRO:HG2	1.51	0.90
1:a:315:MET:HE1	1:a:322:GLN:HA	1.54	0.89
1:a:121:PHE:CD1	1:a:298:ILE:HG21	2.06	0.89
1:A:223:TYR:CE2	2:B:315:LEU:HD21	2.07	0.89
1:a:297:SER:O	1:a:300:ILE:HG22	1.73	0.89
3:c:157:SER:OG	3:c:210:TRP:HZ3	1.55	0.89
2:b:303:LEU:HD21	3:c:120:THR:HB	1.54	0.89
5:e:240:MET:HE2	5:e:241:ARG:NH1	1.88	0.88
1:A:141:TRP:HE1	3:c:222:CYS:HA	1.35	0.88
1:A:165:TRP:CD2	1:A:169:SER:HA	2.08	0.88
1:A:59:THR:HB	1:A:172:LYS:HA	1.55	0.88
1:A:223:TYR:OH	2:B:315:LEU:CD1	2.22	0.88
1:a:111:GLU:HB3	1:a:199:PHE:CE2	2.09	0.87
3:c:148:ALA:O	3:c:152:ILE:HG12	1.75	0.87
1:a:149:LEU:HA	1:a:287:LYS:NZ	1.89	0.87
1:a:285:PRO:O	1:a:286:ASN:HB2	1.75	0.87
3:c:123:VAL:CG1	9:i:25:ILE:CA	2.51	0.87
1:A:223:TYR:OH	2:B:315:LEU:HD11	1.75	0.87
1:A:343:VAL:HG12	1:A:348:ILE:HG22	1.56	0.86
3:c:101:LYS:HD3	4:d:267:PRO:HG2	1.56	0.86
1:A:141:TRP:CD1	1:A:265:PRO:CG	2.57	0.86
3:C:93:ARG:HH11	3:C:110:ARG:HB2	1.39	0.86
3:c:120:THR:O	3:c:123:VAL:CG2	2.24	0.86
3:c:149:MET:HB2	3:c:169:TRP:CH2	2.11	0.85
5:E:306:THR:HG21	5:E:377:LYS:NZ	1.91	0.85
1:A:223:TYR:HE2	2:B:315:LEU:CD2	1.90	0.85
5:E:278:THR:HB	5:E:329:SER:OG	1.74	0.85
3:c:156:LEU:HD23	3:c:269:ASP:HA	1.57	0.85
1:a:130:GLY:HA3	1:a:182:HIS:CE1	2.11	0.85
1:A:280:ILE:CD1	1:A:355:SER:OG	2.25	0.85
1:a:183:PHE:HB3	1:a:184:ILE:HD13	1.59	0.85
1:A:300:ILE:HD12	1:A:362:ILE:CD1	2.06	0.84
1:A:141:TRP:CD1	1:A:265:PRO:HG2	2.13	0.84
9:i:17:ARG:HB2	9:i:20:THR:HG1	1.42	0.84
10:j:41:ILE:HA	10:j:44:TRP:HD1	1.40	0.84
1:A:47:THR:CG2	1:A:83:HIS:ND1	2.40	0.84
3:C:89:SER:HA	3:C:92:ARG:HG2	1.59	0.84
1:A:223:TYR:CE2	2:B:315:LEU:CD1	2.61	0.84
1:a:153:ILE:HG21	1:a:156:ILE:CG1	2.07	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:323:HIS:O	4:d:323:HIS:ND1	2.11	0.83
5:E:438:MET:HG3	5:E:439:ALA:H	1.43	0.82
9:i:24:THR:HA	9:i:27:VAL:CG2	2.08	0.82
2:B:112:ARG:CA	2:B:140:CYS:SG	2.67	0.82
1:a:275:LEU:CD2	1:a:339:GLY:C	2.52	0.82
4:d:156:LEU:HD22	4:d:213:ARG:HG3	1.62	0.82
1:A:141:TRP:NE1	3:c:222:CYS:CA	2.41	0.82
3:c:156:LEU:HD11	3:c:210:TRP:HH2	1.39	0.82
1:A:298:ILE:H	1:A:298:ILE:HD12	1.45	0.82
5:E:421:ASP:OD1	5:E:422:ALA:N	2.11	0.82
1:a:129:MET:HE2	1:a:181:PHE:HB3	1.61	0.82
8:H:43:ARG:C	8:H:43:ARG:HD2	2.05	0.82
3:c:157:SER:HG	3:c:210:TRP:HZ3	0.83	0.81
1:A:141:TRP:HE1	3:c:222:CYS:CA	1.92	0.81
1:A:165:TRP:CG	1:A:169:SER:HA	2.14	0.81
2:B:245:MET:HE2	2:B:248:PRO:CG	2.09	0.81
5:e:240:MET:HB2	5:e:241:ARG:NH1	1.96	0.81
4:D:321:GLY:O	4:D:333:ALA:CB	2.29	0.81
1:A:52:ALA:HA	1:A:55:TYR:HB3	1.63	0.81
2:B:310:HIS:O	2:B:310:HIS:ND1	2.14	0.81
1:a:230:LEU:HD13	2:b:304:VAL:CG1	2.11	0.81
2:B:229:ARG:HB3	2:B:232:LEU:HG	1.62	0.81
1:a:230:LEU:CD1	2:b:304:VAL:HG12	2.10	0.81
2:b:303:LEU:HD21	3:c:120:THR:CG2	2.11	0.81
1:a:27:ILE:CG2	1:a:31:TRP:HB2	2.11	0.80
1:A:51:LEU:O	1:A:55:TYR:HB2	1.82	0.80
5:e:244:LEU:H	5:e:244:LEU:CD2	1.94	0.80
9:i:22:ALA:O	9:i:25:ILE:CG1	2.29	0.80
2:b:303:LEU:HD21	3:c:120:THR:CB	2.11	0.80
1:A:141:TRP:CE2	3:c:222:CYS:HA	2.17	0.80
4:D:328:LEU:HB3	4:D:341:PHE:HZ	1.45	0.80
2:b:128:MET:CE	2:b:198:LEU:HB2	2.12	0.80
1:A:223:TYR:CE2	2:B:315:LEU:HD22	2.18	0.79
2:B:112:ARG:N	2:B:140:CYS:SG	2.56	0.79
2:B:217:THR:HG23	2:B:264:MET:HE3	1.65	0.79
1:A:59:THR:H	1:A:172:LYS:HD2	1.48	0.78
1:A:297:SER:O	1:A:300:ILE:HG22	1.84	0.78
1:a:304:MET:HE3	1:a:362:ILE:O	1.84	0.78
3:c:156:LEU:HD23	3:c:269:ASP:CA	2.12	0.78
1:A:140:PHE:CD2	1:A:141:TRP:HZ3	2.01	0.78
1:A:161:VAL:O	1:A:165:TRP:CE3	2.37	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:CE2	2:B:315:LEU:HD13	2.19	0.78
2:b:122:CYS:SG	14:b:401:HEC:HAB	2.22	0.78
1:A:121:PHE:CZ	1:A:298:ILE:HB	2.18	0.78
4:D:265:PHE:CD2	4:D:350:GLU:OE1	2.37	0.78
1:a:299:LEU:O	1:a:302:ILE:CD1	2.31	0.77
3:c:150:SER:CB	3:c:153:GLU:CD	2.56	0.77
5:E:306:THR:HG21	5:E:377:LYS:HZ3	1.49	0.77
1:a:182:HIS:HD2	12:a:401:HEM:NC	1.81	0.77
1:a:122:THR:HG22	1:a:189:ILE:HD11	1.66	0.77
5:e:244:LEU:H	5:e:244:LEU:HD23	1.48	0.77
1:a:298:ILE:O	1:a:299:LEU:HD12	1.85	0.77
2:b:209:GLU:OE1	2:b:276:ARG:HD2	1.84	0.77
1:A:126:THR:OG1	1:A:185:LEU:HD23	1.84	0.77
11:K:31:GLN:H	11:K:34:LEU:HG	1.50	0.77
1:A:141:TRP:O	1:A:268:ILE:HD12	1.85	0.77
2:B:161:GLU:HA	2:b:182:ASN:HD21	1.49	0.76
9:i:17:ARG:CB	9:i:20:THR:OG1	2.33	0.76
4:D:125:THR:HG22	4:D:126:ARG:H	1.49	0.76
4:D:278:ARG:O	4:D:460:GLY:HA3	1.85	0.76
1:A:52:ALA:HA	1:A:55:TYR:CB	2.16	0.76
1:a:210:GLY:C	1:a:313:ARG:HD3	2.11	0.76
1:a:119:LEU:CD1	1:a:192:LEU:HD23	2.15	0.76
4:D:327:THR:HG21	4:D:375:GLN:HE22	1.45	0.76
1:a:129:MET:SD	1:a:181:PHE:CB	2.70	0.76
3:c:122:THR:CB	9:i:25:ILE:HG21	2.16	0.76
1:a:38:GLY:O	1:a:42:ILE:HD12	1.86	0.75
3:c:150:SER:HB3	3:c:153:GLU:OE1	1.86	0.75
3:c:219:HIS:HB2	3:c:254:ALA:HA	1.68	0.75
5:E:306:THR:CG2	5:E:377:LYS:NZ	2.50	0.75
2:B:88:LEU:HD11	8:H:72:ARG:HG2	1.67	0.75
1:a:210:GLY:HA3	1:a:313:ARG:HG3	1.69	0.75
9:i:14:LEU:HD12	9:i:24:THR:HG21	1.69	0.75
5:e:185:ALA:HB3	5:e:251:ALA:HB2	1.69	0.75
3:c:80:HIS:CD2	4:d:182:VAL:CG1	2.66	0.75
1:A:141:TRP:HE1	3:c:222:CYS:CB	1.99	0.74
1:a:27:ILE:CG2	1:a:31:TRP:CG	2.70	0.74
1:a:27:ILE:HG23	1:a:31:TRP:CD2	2.22	0.74
1:A:344:GLU:HG3	1:A:347:PHE:CD2	2.21	0.74
5:E:45:ASN:ND2	5:E:238:LEU:HD23	2.02	0.74
2:B:87:ASP:OD2	2:B:241:GLN:NE2	2.21	0.74
1:a:302:ILE:N	1:a:302:ILE:HD12	2.02	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:102:ARG:HG3	7:g:105:ARG:NH2	2.02	0.73
3:c:122:THR:HG21	9:i:25:ILE:HD13	1.70	0.73
2:B:250:TYR:O	2:B:253:VAL:HG23	1.88	0.73
1:A:141:TRP:HD1	1:A:265:PRO:HG2	1.48	0.73
4:D:324:MET:HE3	4:D:329:ALA:HB1	1.71	0.72
3:c:156:LEU:CD1	3:c:210:TRP:CH2	2.71	0.72
1:a:132:VAL:HA	1:a:139:SER:HB3	1.71	0.72
1:A:300:ILE:HG12	1:A:300:ILE:O	1.89	0.72
1:A:223:TYR:HE2	2:B:315:LEU:HD22	1.53	0.72
2:B:303:LEU:HB3	3:C:121:THR:OG1	1.90	0.72
4:D:70:THR:HG22	4:D:406:THR:HG23	1.72	0.71
4:D:324:MET:CE	4:D:329:ALA:HB1	2.20	0.71
1:a:315:MET:CE	1:a:322:GLN:HA	2.20	0.71
1:A:143:ALA:O	1:A:147:THR:HG23	1.91	0.71
1:A:223:TYR:CZ	2:B:315:LEU:HD11	2.24	0.71
1:a:27:ILE:HG22	1:a:31:TRP:HB2	1.72	0.71
3:c:220:LEU:CD1	15:c:301:FES:S2	2.77	0.71
4:d:66:GLN:HB3	4:d:67:PRO:HD2	1.70	0.71
1:A:121:PHE:CE2	1:A:298:ILE:HG22	2.22	0.71
3:c:101:LYS:HD3	4:d:267:PRO:CG	2.19	0.71
6:f:35:GLU:O	6:f:39:GLN:NE2	2.22	0.71
1:A:167:GLY:HA3	3:c:147:LEU:HD11	1.73	0.71
3:C:234:TYR:HB2	3:C:243:TYR:HB2	1.71	0.71
1:a:27:ILE:HG23	1:a:31:TRP:CG	2.25	0.71
1:a:183:PHE:O	1:a:184:ILE:HD12	1.91	0.71
4:D:321:GLY:O	4:D:333:ALA:HB3	1.90	0.71
1:a:153:ILE:HG21	1:a:156:ILE:HD12	1.71	0.71
1:a:58:ASP:CB	1:a:61:THR:HB	2.17	0.71
1:a:153:ILE:CG2	1:a:154:PRO:HD2	2.21	0.70
1:A:223:TYR:HE2	2:B:315:LEU:HD13	1.56	0.70
1:a:288:LEU:C	1:a:288:LEU:HD23	2.15	0.70
3:c:224:PRO:HG2	3:c:234:TYR:HB3	1.73	0.70
10:j:38:TRP:HE1	10:j:40:LEU:HB2	1.56	0.70
4:D:78:GLY:HA3	4:D:126:ARG:O	1.90	0.70
3:C:173:PRO:HD3	1:a:261:PRO:HB2	1.74	0.70
12:A:402:HEM:HBC2	12:A:402:HEM:HHD	1.72	0.70
3:C:156:LEU:HB2	3:C:271:VAL:CG1	2.19	0.70
1:a:315:MET:HE1	1:a:322:GLN:CA	2.21	0.70
3:c:199:GLN:HB2	3:c:257:ASN:HD22	1.56	0.70
4:D:75:ILE:HG12	4:D:76:ASP:N	2.05	0.70
4:D:99:LYS:NZ	5:E:301:ARG:O	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:27:ILE:CG2	1:a:31:TRP:CB	2.69	0.70
1:a:356:ILE:HG13	1:a:357:LEU:N	2.05	0.70
3:C:172:LYS:NZ	1:a:169:SER:OG	2.25	0.70
5:E:324:SER:OG	5:E:325:ALA:N	2.24	0.70
2:B:233:TYR:O	2:B:242:ALA:HA	1.92	0.70
2:b:147:LYS:NZ	3:c:154:ILE:HD13	2.07	0.70
1:A:223:TYR:CZ	2:B:315:LEU:CD1	2.75	0.69
1:a:201:HIS:O	1:a:202:GLU:CG	2.36	0.69
4:D:70:THR:CG2	4:D:406:THR:CG2	2.70	0.69
1:a:153:ILE:HG21	1:a:156:ILE:CD1	2.22	0.69
1:A:223:TYR:HE2	2:B:315:LEU:CD1	2.03	0.69
4:D:265:PHE:HB3	4:D:350:GLU:OE2	1.93	0.69
4:D:70:THR:HG22	4:D:406:THR:CG2	2.22	0.69
5:E:438:MET:HG3	5:E:439:ALA:N	2.04	0.69
1:a:233:LEU:O	1:a:233:LEU:HD23	1.92	0.69
5:e:438:MET:HG3	5:e:439:ALA:N	1.96	0.69
1:A:309:THR:HG21	1:A:371:ILE:HG13	1.74	0.69
4:d:95:HIS:ND1	4:d:164:GLU:OE1	2.25	0.69
10:j:18:ILE:HG13	10:j:19:PRO:HD3	1.75	0.69
4:D:454:PRO:HG3	4:D:475:MET:HE3	1.73	0.69
1:a:5:ARG:NH1	1:a:15:ASN:OD1	2.24	0.69
2:b:113:ARG:NH1	2:b:270:ASP:OD2	2.26	0.69
7:G:76:LEU:HG	7:G:77:PRO:HD2	1.75	0.68
1:a:148:ASN:O	1:a:287:LYS:NZ	2.26	0.68
1:a:149:LEU:HA	1:a:287:LYS:HZ3	1.58	0.68
4:d:280:ASP:H	8:h:12:ARG:HG3	1.58	0.68
5:E:214:THR:HG23	5:E:242:GLY:O	1.93	0.68
3:c:156:LEU:O	3:c:156:LEU:HD12	1.94	0.68
3:C:217:CYS:SG	3:C:222:CYS:N	2.66	0.68
4:D:204:PRO:HG2	4:D:207:ASN:HB2	1.76	0.68
5:E:254:ARG:HG2	5:E:255:GLY:N	2.08	0.68
1:a:121:PHE:CD1	1:a:298:ILE:CG2	2.76	0.68
2:B:89:GLU:OE1	2:B:89:GLU:N	2.26	0.68
3:c:150:SER:CB	3:c:153:GLU:OE1	2.42	0.68
1:A:264:THR:HG23	1:A:264:THR:O	1.92	0.68
5:e:85:LEU:HD23	11:k:15:LEU:HD21	1.76	0.68
11:k:27:ARG:HG3	11:k:28:PRO:HD2	1.75	0.68
3:C:197:ASP:O	3:C:257:ASN:ND2	2.25	0.67
4:D:93:VAL:HG23	4:D:216:LEU:HD12	1.76	0.67
1:A:313:ARG:O	1:A:314:SER:HB3	1.94	0.67
1:a:210:GLY:O	1:a:313:ARG:HD3	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:HE2	1:A:298:ILE:CG2	2.06	0.67
1:A:141:TRP:HE3	1:A:141:TRP:N	1.92	0.67
6:f:47:ARG:HB2	6:f:74:PHE:HE2	1.60	0.67
1:a:346:PRO:HA	1:a:349:ILE:CG1	2.25	0.67
1:a:183:PHE:C	1:a:184:ILE:HD12	2.20	0.67
3:c:156:LEU:HD23	3:c:269:ASP:C	2.20	0.67
4:d:381:THR:HG22	4:d:382:SER:H	1.60	0.67
1:a:359:PHE:O	1:a:363:LEU:HB2	1.95	0.67
3:C:93:ARG:HB3	3:C:96:VAL:CG2	2.24	0.67
12:a:402:HEM:HBC2	12:a:402:HEM:HHD	1.76	0.67
3:c:156:LEU:HD23	3:c:269:ASP:O	1.94	0.67
5:e:304:ASN:O	5:e:311:GLN:NE2	2.27	0.67
1:A:141:TRP:NE1	3:c:222:CYS:CB	2.58	0.67
10:j:38:TRP:NE1	10:j:40:LEU:HB2	2.10	0.67
1:A:71:ARG:HH21	2:B:200:TYR:HE1	1.42	0.67
4:d:450:TYR:O	9:i:16:ARG:NH2	2.27	0.67
4:d:323:HIS:CE1	5:e:100:THR:HG21	2.30	0.66
1:A:300:ILE:CD1	1:A:362:ILE:CD1	2.68	0.66
4:D:381:THR:HG22	4:D:382:SER:N	2.04	0.66
7:G:9:ALA:O	7:G:12:LYS:NZ	2.29	0.66
1:A:308:HIS:HD2	1:A:310:SER:H	1.43	0.66
4:D:68:THR:HB	5:E:387:GLU:OE2	1.95	0.66
2:b:128:MET:HE1	2:b:198:LEU:HB2	1.77	0.66
2:b:133:TYR:HB2	2:b:172:LEU:O	1.95	0.66
16:D:501:CDL:H331	13:D:502:PEE:H20	1.76	0.66
3:c:175:PHE:HB2	3:c:213:LEU:HB2	1.78	0.66
8:h:20:SER:O	8:h:24:GLN:NE2	2.27	0.66
12:A:402:HEM:HBD2	12:A:402:HEM:HHA	1.76	0.66
3:c:150:SER:HB3	3:c:153:GLU:OE2	1.96	0.66
4:d:289:ILE:HG22	4:d:456:VAL:HG22	1.78	0.66
1:a:74:ASN:N	3:c:145:ASP:OD2	2.29	0.66
1:a:210:GLY:CA	1:a:313:ARG:HD3	2.26	0.65
1:a:288:LEU:HD23	1:a:289:GLY:N	2.11	0.65
1:a:313:ARG:O	1:a:314:SER:HB3	1.95	0.65
5:E:257:GLU:OE1	5:E:450:VAL:HG12	1.95	0.65
1:a:352:GLN:O	1:a:356:ILE:HG23	1.96	0.65
1:a:230:LEU:CD1	2:b:304:VAL:CG1	2.71	0.65
8:h:20:SER:HB3	8:h:23:GLU:OE1	1.97	0.65
1:a:149:LEU:HA	1:a:287:LYS:CE	2.26	0.65
5:e:241:ARG:HG2	5:e:241:ARG:HH11	1.60	0.65
1:A:141:TRP:O	1:A:268:ILE:CD1	2.45	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:O	3:c:171:GLY:HA2	1.97	0.65
2:B:220:CYS:SG	2:B:221:GLU:N	2.69	0.65
1:A:58:ASP:H	1:A:175:LEU:HD23	1.62	0.65
1:A:141:TRP:CD1	3:c:222:CYS:HB3	2.32	0.65
1:a:29:SER:O	1:a:32:ASN:N	2.26	0.65
1:a:37:LEU:HD21	1:a:93:CYS:CB	2.26	0.65
2:B:300:LEU:O	2:B:300:LEU:HD23	1.97	0.64
5:e:214:THR:HB	5:e:217:ARG:HD3	1.79	0.64
1:a:275:LEU:HD21	1:a:340:GLY:CA	2.27	0.64
1:a:377:LEU:O	7:g:34:ARG:NH1	2.29	0.64
11:k:27:ARG:HE	11:k:28:PRO:HD3	1.62	0.64
5:e:214:THR:HG21	5:e:244:LEU:CA	2.25	0.64
1:A:100:ARG:HD2	1:A:100:ARG:C	2.23	0.64
1:a:275:LEU:HD21	1:a:340:GLY:HA2	1.79	0.64
12:a:401:HEM:HMC1	12:a:401:HEM:HBC2	1.79	0.64
3:c:156:LEU:HD12	3:c:156:LEU:C	2.22	0.64
10:J:38:TRP:HE1	10:J:40:LEU:HB2	1.62	0.64
3:c:167:PHE:O	3:c:173:PRO:HA	1.96	0.64
1:A:63:PHE:CZ	1:A:256:TYR:O	2.50	0.64
1:a:132:VAL:HG11	1:a:143:ALA:HB2	1.79	0.64
3:C:100:THR:O	3:C:101:LYS:HD3	1.98	0.64
1:a:210:GLY:O	1:a:313:ARG:CD	2.46	0.64
2:b:126:HIS:ND1	2:b:196:PRO:O	2.29	0.64
1:A:18:PHE:HE2	16:D:501:CDL:H362	1.63	0.63
1:a:214:ASP:HB3	8:h:8:LEU:HD12	1.78	0.63
1:a:302:ILE:HD12	1:a:302:ILE:H	1.62	0.63
2:b:128:MET:SD	2:b:198:LEU:O	2.56	0.63
7:g:111:LYS:OXT	7:g:111:LYS:CG	2.36	0.63
3:C:156:LEU:HD13	3:C:271:VAL:HB	1.78	0.63
4:D:63:GLN:HG3	4:D:63:GLN:O	1.96	0.63
1:a:329:VAL:HB	13:a:403:PEE:H32	1.80	0.63
1:A:57:SER:HA	1:A:175:LEU:CD2	2.28	0.63
5:E:170:GLN:HE22	11:K:28:PRO:HG3	1.63	0.63
2:b:303:LEU:CD2	3:c:120:THR:HG22	2.28	0.63
4:d:63:GLN:HG3	4:d:63:GLN:O	1.98	0.63
3:C:93:ARG:NH2	8:H:24:GLN:O	2.31	0.63
1:a:165:TRP:CZ3	1:a:170:VAL:HG22	2.32	0.63
3:C:93:ARG:O	3:C:96:VAL:HG23	1.99	0.63
1:a:153:ILE:HG21	1:a:156:ILE:HG13	1.81	0.63
2:b:122:CYS:HB2	14:b:401:HEC:CAB	2.09	0.63
4:d:381:THR:HG22	4:d:382:SER:N	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASN:ND2	1:A:263:ASN:OD1	2.31	0.63
1:A:141:TRP:CD1	1:A:265:PRO:HG3	2.33	0.63
1:a:306:MET:O	1:a:307:LEU:HD22	1.99	0.63
1:a:304:MET:CE	1:a:362:ILE:O	2.47	0.62
3:C:200:HIS:HB3	3:C:203:GLU:HG2	1.80	0.62
1:A:144:THR:HG21	3:c:216:VAL:HG13	1.81	0.62
2:B:301:LEU:N	2:B:302:PRO:CD	2.62	0.62
4:D:158:ASP:O	4:D:159:SER:HB3	1.98	0.62
2:b:183:PRO:HB2	2:b:187:ARG:HH12	1.63	0.62
2:b:229:ARG:HB3	2:b:232:LEU:HB2	1.81	0.62
1:a:221:HIS:O	1:a:223:TYR:N	2.32	0.62
11:k:42:VAL:HG22	11:k:43:LEU:H	1.64	0.62
1:A:69:ILE:HG13	1:A:73:VAL:HG21	1.80	0.62
1:A:343:VAL:HG12	1:A:348:ILE:CG2	2.30	0.62
12:A:401:HEM:HBA1	12:A:401:HEM:HHA	1.80	0.62
2:B:321:ALA:HB3	8:H:15:ILE:H	1.63	0.62
4:D:413:ILE:O	4:D:417:LEU:HD23	2.00	0.62
3:c:99:SER:CA	4:d:269:ARG:NH1	2.55	0.62
3:c:157:SER:OG	3:c:210:TRP:CZ3	2.40	0.62
3:C:98:ASP:O	4:D:269:ARG:NH1	2.32	0.62
1:a:121:PHE:CE1	1:a:298:ILE:HB	2.34	0.62
1:a:153:ILE:CG2	1:a:156:ILE:HG13	2.30	0.62
3:C:93:ARG:O	3:C:96:VAL:CG2	2.48	0.62
3:c:156:LEU:CD2	3:c:269:ASP:CA	2.72	0.62
2:B:186:ALA:HB3	2:B:194:LEU:HD23	1.80	0.62
1:a:312:GLN:HG2	7:g:37:THR:O	2.00	0.62
1:A:300:ILE:HD11	1:A:362:ILE:HD12	1.79	0.61
1:a:346:PRO:HA	1:a:349:ILE:HG12	1.82	0.61
3:c:152:ILE:HA	3:c:272:ILE:HG23	1.81	0.61
5:e:297:PRO:HD2	11:k:29:LEU:HB2	1.81	0.61
6:f:74:PHE:HE1	6:f:78:ARG:HD2	1.65	0.61
4:D:365:ILE:CD1	4:D:462:ILE:HG22	2.30	0.61
4:d:156:LEU:O	4:d:213:ARG:NH1	2.33	0.61
5:e:293:LEU:HD22	5:e:309:LEU:HD23	1.81	0.61
1:A:63:PHE:CE1	1:A:256:TYR:O	2.54	0.61
3:c:172:LYS:HB2	3:c:214:ILE:HD11	1.80	0.61
1:A:121:PHE:CE2	1:A:298:ILE:CB	2.82	0.61
5:E:306:THR:CG2	5:E:377:LYS:HZ1	2.13	0.61
1:a:153:ILE:CG2	1:a:156:ILE:HB	2.30	0.61
4:D:382:SER:HB3	10:J:16:ASN:HB3	1.82	0.61
1:a:37:LEU:HD21	1:a:93:CYS:HB3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:238:PHE:CZ	2:b:243:ILE:HD13	2.35	0.61
3:c:172:LYS:HG3	3:c:216:VAL:HG23	1.81	0.61
3:c:193:SER:OG	3:c:194:GLN:OE1	2.19	0.61
5:e:180:ALA:O	5:e:256:GLY:HA3	2.00	0.61
3:c:121:THR:O	3:c:125:VAL:HG23	2.00	0.61
3:c:177:ARG:HH22	3:c:183:GLU:HG3	1.66	0.61
5:e:240:MET:HB2	5:e:241:ARG:HH11	1.63	0.61
2:b:106:LEU:HD21	2:b:276:ARG:NH1	2.15	0.61
3:c:120:THR:C	3:c:123:VAL:HG22	2.25	0.61
3:C:89:SER:HA	3:C:92:ARG:CG	2.30	0.60
4:D:384:THR:HG21	10:J:9:ARG:HD2	1.83	0.60
1:a:132:VAL:HG13	1:a:139:SER:C	2.26	0.60
4:d:417:LEU:HD12	4:d:421:GLY:HA2	1.83	0.60
3:c:106:SER:O	3:c:110:ARG:NH1	2.34	0.60
1:a:237:LEU:CD1	2:b:297:MET:HE1	2.31	0.60
5:e:240:MET:HE2	5:e:241:ARG:CZ	2.30	0.60
5:e:245:GLY:O	5:e:246:LEU:HD23	2.00	0.60
1:A:121:PHE:CZ	1:A:298:ILE:CB	2.84	0.60
3:c:244:ASP:OD2	3:c:248:ARG:NH2	2.35	0.60
8:h:75:PRO:HA	8:h:78:TYR:HB2	1.84	0.60
1:A:140:PHE:CE2	3:c:172:LYS:HE3	2.36	0.60
4:D:327:THR:CG2	4:D:375:GLN:CD	2.70	0.60
1:a:237:LEU:HD13	2:b:297:MET:CE	2.32	0.60
1:a:346:PRO:HA	1:a:349:ILE:HD11	1.84	0.60
1:a:346:PRO:O	1:a:349:ILE:HG13	2.02	0.60
4:d:322:THR:O	4:d:323:HIS:HB3	2.00	0.60
8:H:46:ILE:HG23	8:H:46:ILE:O	2.01	0.60
2:B:111:ILE:C	2:B:140:CYS:SG	2.84	0.60
7:G:68:ASP:OD2	7:G:72:ARG:NH2	2.35	0.60
11:K:2:LEU:O	11:K:3:SER:OG	2.16	0.60
1:a:149:LEU:HG	1:a:287:LYS:HE2	1.83	0.60
3:c:216:VAL:HG13	3:c:221:GLY:HA2	1.83	0.60
1:a:121:PHE:HD1	1:a:298:ILE:HG21	1.65	0.60
1:a:315:MET:HE1	1:a:321:SER:C	2.26	0.60
3:c:143:SER:O	3:c:147:LEU:HB2	2.01	0.60
4:d:66:GLN:HB3	4:d:67:PRO:CD	2.31	0.60
10:j:8:PRO:O	10:j:12:GLU:HG3	2.01	0.60
1:A:329:VAL:HG22	13:A:403:PEE:H33	1.84	0.60
1:A:340:GLY:C	1:A:341:GLN:HG2	2.26	0.60
3:c:99:SER:HA	4:d:269:ARG:HD2	1.84	0.60
3:c:154:ILE:HG22	3:c:270:LEU:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:217:CYS:SG	3:c:221:GLY:N	2.72	0.60
1:a:121:PHE:CE1	1:a:298:ILE:CG2	2.85	0.59
3:c:149:MET:O	3:c:153:GLU:HB3	2.02	0.59
5:E:121:TYR:HB3	5:E:137:LEU:HD11	1.84	0.59
5:E:214:THR:HG21	5:E:243:GLY:O	2.00	0.59
1:a:153:ILE:HG21	1:a:156:ILE:HB	1.82	0.59
3:c:99:SER:O	4:d:269:ARG:HD3	2.03	0.59
3:c:156:LEU:CD1	3:c:210:TRP:CZ3	2.85	0.59
3:C:110:ARG:NH2	8:H:23:GLU:OE2	2.34	0.59
4:D:265:PHE:HD2	4:D:350:GLU:OE1	1.85	0.59
1:a:29:SER:O	1:a:32:ASN:HB2	2.03	0.59
1:a:29:SER:O	1:a:32:ASN:CB	2.50	0.59
1:a:353:LEU:HA	1:a:356:ILE:HG12	1.84	0.59
2:b:99:HIS:NE2	2:b:209:GLU:OE1	2.35	0.59
3:c:175:PHE:HE2	3:c:215:GLY:HA2	1.68	0.59
11:k:42:VAL:HG13	11:k:43:LEU:HD13	1.84	0.59
1:A:379:TRP:OXT	7:G:34:ARG:NH1	2.35	0.59
5:E:304:ASN:O	5:E:311:GLN:NE2	2.36	0.59
1:a:65:SER:O	1:a:68:HIS:ND1	2.36	0.59
2:b:303:LEU:CD2	3:c:120:THR:CG2	2.81	0.59
5:e:115:THR:HG23	5:e:117:GLU:H	1.67	0.59
1:A:140:PHE:HB3	1:A:141:TRP:CE3	2.38	0.59
1:A:280:ILE:CD1	1:A:355:SER:HG	2.16	0.59
1:a:89:MET:HA	1:a:92:ILE:HD12	1.83	0.59
3:c:151:LYS:HG3	3:c:152:ILE:HG23	1.84	0.59
4:d:66:GLN:CB	4:d:67:PRO:CD	2.79	0.59
3:C:99:SER:HA	4:D:269:ARG:HD3	1.84	0.59
4:D:280:ASP:HB2	8:H:11:MET:O	2.03	0.59
3:c:150:SER:HA	3:c:153:GLU:CG	2.33	0.59
7:g:111:LYS:OXT	7:g:111:LYS:NZ	2.30	0.59
9:i:5:THR:HG22	9:i:6:LEU:H	1.68	0.59
7:G:69:LEU:HD11	7:G:76:LEU:HD13	1.84	0.59
1:A:183:PHE:O	1:A:186:PRO:HD2	2.03	0.59
1:a:153:ILE:HG21	1:a:156:ILE:CB	2.33	0.59
5:e:297:PRO:HG3	11:k:31:GLN:HG2	1.83	0.59
6:f:74:PHE:CE1	6:f:78:ARG:HD2	2.38	0.59
1:A:177:ARG:NH2	3:c:140:MET:O	2.22	0.58
3:C:100:THR:O	3:C:100:THR:HG22	2.03	0.58
2:b:183:PRO:HB2	2:b:187:ARG:NH1	2.18	0.58
1:A:121:PHE:HE2	1:A:298:ILE:HG22	1.65	0.58
1:a:298:ILE:C	1:a:299:LEU:HD12	2.28	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:182:ASN:HB2	2:b:183:PRO:HD2	1.85	0.58
1:A:133:LEU:N	1:A:134:PRO:HD2	2.18	0.58
2:B:218:GLY:O	2:B:219:TYR:C	2.46	0.58
2:b:303:LEU:HD21	3:c:120:THR:HG22	1.83	0.58
1:a:210:GLY:HA3	1:a:313:ARG:CG	2.32	0.58
4:d:110:GLU:HA	4:d:113:VAL:HG12	1.85	0.58
5:E:306:THR:CG2	5:E:377:LYS:HZ3	2.11	0.58
2:b:128:MET:HE2	2:b:198:LEU:HB2	1.84	0.58
1:a:100:ARG:HH22	12:a:402:HEM:HBD2	1.68	0.58
1:a:130:GLY:HA3	1:a:182:HIS:ND1	2.16	0.58
2:b:164:GLU:O	2:b:165:MET:HG2	2.04	0.58
3:c:172:LYS:HG3	3:c:216:VAL:CG2	2.34	0.58
3:c:207:LYS:HD3	3:c:210:TRP:CD1	2.39	0.58
5:e:217:ARG:HD2	5:e:244:LEU:HB3	1.86	0.58
1:a:275:LEU:CD2	1:a:340:GLY:CA	2.81	0.58
5:e:241:ARG:HH11	5:e:241:ARG:CG	2.17	0.58
1:a:27:ILE:HG21	1:a:31:TRP:CB	2.33	0.58
1:a:132:VAL:CG1	1:a:139:SER:O	2.44	0.58
1:A:140:PHE:CD2	1:A:141:TRP:CZ3	2.90	0.57
1:A:223:TYR:OH	2:B:315:LEU:HD13	2.04	0.57
1:A:342:PRO:HG2	1:A:344:GLU:HG2	1.85	0.57
2:B:309:ARG:HH11	2:B:309:ARG:CG	2.17	0.57
4:d:278:ARG:NH1	8:h:11:MET:SD	2.77	0.57
4:d:315:ASP:OD1	4:d:316:SER:N	2.34	0.57
2:B:112:ARG:NH2	2:B:145:GLU:OE1	2.36	0.57
5:E:37:ASP:O	5:E:38:LEU:HG	2.03	0.57
9:I:5:THR:O	9:I:9:ARG:NH1	2.33	0.57
1:a:153:ILE:HG23	1:a:154:PRO:HD2	1.85	0.57
1:a:237:LEU:HD12	2:b:297:MET:HE1	1.85	0.57
3:c:177:ARG:HB3	3:c:211:VAL:HG12	1.85	0.57
4:D:160:GLN:NE2	4:D:164:GLU:OE2	2.37	0.57
4:D:464:GLN:O	4:D:465:LEU:C	2.48	0.57
1:a:183:PHE:C	1:a:184:ILE:CD1	2.78	0.57
5:e:323:VAL:HG13	5:e:340:THR:HG22	1.86	0.57
3:c:82:ASP:OD1	3:c:82:ASP:N	2.34	0.57
3:C:93:ARG:HB3	3:C:96:VAL:HG21	1.84	0.57
4:D:140:LEU:HD11	4:D:237:VAL:HG12	1.86	0.57
2:b:124:SER:O	2:b:179:PRO:CB	2.53	0.57
2:b:318:ARG:NH2	7:g:68:ASP:OD2	2.37	0.57
3:c:204:ARG:HG2	3:c:205:VAL:HG23	1.85	0.57
1:A:208:PRO:O	1:A:316:MET:SD	2.63	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:401:HEM:HBC2	12:A:401:HEM:HHD	1.87	0.57
1:a:153:ILE:HG22	1:a:154:PRO:HD2	1.87	0.57
1:a:21:LEU:HD12	1:a:21:LEU:O	2.05	0.57
1:a:47:THR:HG23	1:a:79:ILE:HG23	1.86	0.57
1:a:121:PHE:HE1	1:a:298:ILE:HB	1.69	0.57
1:A:143:ALA:O	1:A:147:THR:CG2	2.52	0.56
4:D:383:ALA:H	4:D:442:ARG:HH11	1.52	0.56
1:a:40:CYS:HB3	1:a:90:PHE:HD1	1.70	0.56
2:b:112:ARG:HH12	9:i:60:TYR:HE2	1.52	0.56
2:B:159:PRO:HA	2:B:164:GLU:HB2	1.86	0.56
4:D:308:ASN:HD22	4:D:345:ASN:HD21	1.52	0.56
5:E:324:SER:OG	5:E:325:ALA:O	2.24	0.56
11:K:16:SER:OG	11:K:19:SER:O	2.23	0.56
4:D:125:THR:HG22	4:D:126:ARG:N	2.18	0.56
1:a:275:LEU:HD22	1:a:340:GLY:H	1.63	0.56
8:h:36:PRO:HA	8:h:39:LEU:HD12	1.87	0.56
9:i:23:LEU:O	9:i:26:ALA:HB3	2.06	0.56
9:i:25:ILE:HG13	9:i:26:ALA:N	2.21	0.56
1:A:141:TRP:N	1:A:141:TRP:CE3	2.73	0.56
1:A:168:PHE:HD2	3:c:170:ARG:HA	1.71	0.56
4:D:328:LEU:CB	4:D:341:PHE:CZ	2.77	0.56
5:E:45:ASN:HD21	5:E:238:LEU:HD23	1.68	0.56
5:E:260:ASP:O	5:E:444:LEU:HD11	2.05	0.56
3:c:209:GLU:HG2	3:c:210:TRP:CD1	2.40	0.56
1:A:165:TRP:CE2	1:A:169:SER:HA	2.40	0.56
4:D:281:ALA:HB3	8:H:12:ARG:HH12	1.70	0.56
5:E:108:GLY:O	5:E:109:LYS:HG2	2.05	0.56
2:b:121:VAL:HG23	2:b:254:LEU:HD13	1.87	0.56
9:i:30:LEU:HD12	10:j:48:ILE:HD11	1.87	0.56
4:D:140:LEU:CD1	4:D:237:VAL:HG12	2.35	0.56
4:D:266:THR:OG1	4:D:268:CYS:SG	2.63	0.56
3:c:99:SER:O	4:d:269:ARG:CD	2.54	0.56
4:d:133:ILE:HD11	4:d:143:ALA:HB1	1.88	0.56
5:E:214:THR:CG2	5:E:242:GLY:O	2.54	0.56
8:h:37:ASN:HB3	8:h:41:ARG:HH21	1.71	0.56
1:A:135:TRP:CZ2	1:A:140:PHE:CE1	2.93	0.56
5:E:47:LEU:HD12	5:E:218:MET:O	2.06	0.56
1:a:26:ASN:OD1	1:a:26:ASN:N	2.39	0.56
1:a:315:MET:HE1	1:a:322:GLN:N	2.21	0.56
3:c:80:HIS:HB3	4:d:176:ASP:OD1	2.05	0.56
2:B:187:ARG:HB3	2:B:192:GLY:HA2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:301:ASN:O	4:d:305:GLN:HG2	2.06	0.56
4:d:402:HIS:O	4:d:402:HIS:ND1	2.39	0.56
4:d:439:SER:O	4:d:443:GLU:HG3	2.05	0.56
5:E:45:ASN:CG	5:E:238:LEU:HD23	2.31	0.55
1:a:153:ILE:HB	1:a:156:ILE:HB	1.89	0.55
11:k:52:ARG:HH21	11:k:55:LEU:HD11	1.70	0.55
1:A:57:SER:C	1:A:175:LEU:HD23	2.30	0.55
2:B:164:GLU:HG2	2:B:165:MET:HG2	1.87	0.55
5:E:214:THR:CG2	5:E:243:GLY:O	2.54	0.55
1:a:57:SER:HA	1:a:175:LEU:CD2	2.36	0.55
1:a:201:HIS:O	1:a:202:GLU:CB	2.54	0.55
3:c:181:LYS:HA	3:c:184:ILE:HD13	1.88	0.55
1:a:241:ILE:O	1:a:245:PHE:HB2	2.06	0.55
1:a:315:MET:HE2	1:a:322:GLN:CG	2.36	0.55
1:a:111:GLU:OE1	1:a:199:PHE:CE2	2.59	0.55
4:d:120:LEU:HG	4:d:133:ILE:HG22	1.87	0.55
2:B:112:ARG:CZ	2:B:141:TYR:CE1	2.90	0.55
1:A:201:HIS:O	1:A:201:HIS:ND1	2.40	0.55
3:C:93:ARG:N	3:C:96:VAL:CG2	2.70	0.55
3:C:244:ASP:HB2	3:C:250:ARG:HD3	1.89	0.55
5:E:91:THR:HG22	5:E:92:LYS:H	1.72	0.55
3:c:205:VAL:HG12	3:c:207:LYS:H	1.72	0.55
1:A:168:PHE:CD2	3:c:170:ARG:HG2	2.41	0.55
1:A:237:LEU:HD13	2:B:297:MET:HG3	1.88	0.55
4:D:87:ASN:C	4:D:87:ASN:HD22	2.12	0.55
4:d:65:SER:O	4:d:65:SER:OG	2.22	0.55
9:i:21:PHE:C	9:i:21:PHE:CD1	2.85	0.55
4:D:419:THR:HG22	4:D:420:TYR:CD1	2.42	0.55
7:g:14:LEU:O	7:g:17:ILE:HG22	2.07	0.55
4:D:384:THR:HG22	4:D:385:GLU:H	1.72	0.55
2:b:314:VAL:HG22	8:h:21:PRO:HG3	1.87	0.55
1:A:140:PHE:C	1:A:141:TRP:CE3	2.72	0.55
1:A:167:GLY:CA	3:c:147:LEU:HD11	2.37	0.55
2:B:309:ARG:HH11	2:B:309:ARG:HG3	1.72	0.55
1:A:169:SER:HB3	3:c:172:LYS:H	1.71	0.54
2:B:266:GLN:HE21	6:F:90:LEU:HG	1.72	0.54
5:E:421:ASP:O	5:E:422:ALA:HB3	2.07	0.54
3:c:224:PRO:HG3	3:c:236:CYS:SG	2.47	0.54
11:K:42:VAL:HG22	11:K:43:LEU:HD13	1.88	0.54
1:a:183:PHE:CE1	12:a:401:HEM:HBC1	2.43	0.54
1:a:240:LEU:HA	1:a:243:VAL:HG12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:275:LEU:HD22	1:a:339:GLY:C	2.22	0.54
1:a:303:LEU:O	1:a:303:LEU:HG	2.06	0.54
1:a:122:THR:HG21	1:a:189:ILE:HG12	1.88	0.54
5:E:214:THR:HG21	5:E:243:GLY:C	2.32	0.54
5:e:260:ASP:O	5:e:441:SER:HA	2.07	0.54
2:B:302:PRO:O	2:B:303:LEU:HD23	2.08	0.54
1:a:346:PRO:HA	1:a:349:ILE:CD1	2.37	0.54
1:A:344:GLU:HB3	1:A:346:PRO:HD2	1.89	0.54
3:C:93:ARG:HB3	3:C:96:VAL:HG22	1.90	0.54
1:a:210:GLY:HA2	1:a:313:ARG:HD3	1.89	0.54
7:g:33:MET:SD	7:g:62:ARG:NH1	2.81	0.54
7:g:43:ASP:OD2	7:g:102:ARG:NH1	2.40	0.54
1:A:357:LEU:HD12	1:A:361:ILE:HG13	1.89	0.54
4:D:345:ASN:OD1	4:D:354:LEU:HD23	2.06	0.54
3:c:122:THR:CG2	9:i:25:ILE:CD1	2.85	0.54
3:C:89:SER:CA	3:C:92:ARG:HG2	2.35	0.54
4:D:323:HIS:HB3	5:E:100:THR:HG21	1.90	0.54
2:b:168:ARG:HD2	2:b:170:GLY:H	1.72	0.54
3:c:149:MET:CB	3:c:169:TRP:CH2	2.87	0.54
4:d:113:VAL:HG21	4:d:120:LEU:HD11	1.88	0.54
7:g:86:GLU:O	7:g:88:LYS:NZ	2.37	0.54
1:A:148:ASN:O	1:A:151:SER:HB3	2.08	0.54
3:c:79:SER:OG	7:g:57:ASN:ND2	2.36	0.54
1:A:223:TYR:CD2	2:B:315:LEU:CD2	2.91	0.54
5:E:138:LEU:HD11	5:E:237:PHE:HB2	1.89	0.54
1:a:38:GLY:O	1:a:42:ILE:CD1	2.54	0.54
1:a:182:HIS:O	1:a:186:PRO:HD2	2.08	0.54
4:d:75:ILE:HG22	4:d:76:ASP:H	1.72	0.54
5:E:225:VAL:HG12	5:E:226:SER:H	1.72	0.53
1:A:303:LEU:O	1:A:307:LEU:HD12	2.08	0.53
4:D:382:SER:HB3	10:J:16:ASN:CB	2.38	0.53
1:a:37:LEU:HD21	1:a:93:CYS:HB2	1.90	0.53
6:f:34:ARG:HG2	6:f:78:ARG:HH21	1.73	0.53
3:C:99:SER:HA	4:D:269:ARG:CD	2.39	0.53
4:D:79:SER:O	4:D:82:GLU:HG2	2.08	0.53
3:c:111:LYS:NZ	4:d:451:ASP:O	2.41	0.53
5:e:40:PHE:CE1	5:e:406:TYR:HB2	2.44	0.53
4:D:70:THR:CG2	4:D:406:THR:HG22	2.37	0.53
8:H:68:GLU:OE2	8:H:72:ARG:HD3	2.09	0.53
1:a:61:THR:HG22	1:a:61:THR:O	2.07	0.53
2:b:147:LYS:HE2	2:b:172:LEU:HD11	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:23:LEU:O	9:i:26:ALA:N	2.42	0.53
1:A:283:SER:HG	1:A:352:GLN:HB2	1.67	0.53
1:A:102:LEU:HD12	1:A:113:TRP:HH2	1.72	0.53
3:C:156:LEU:CB	3:C:271:VAL:CG1	2.86	0.53
4:D:442:ARG:CZ	10:J:16:ASN:HD21	2.22	0.53
5:E:324:SER:OG	11:K:27:ARG:NH2	2.42	0.53
5:e:379:LYS:HG2	5:e:413:LEU:HD22	1.90	0.53
1:A:338:ILE:HD11	1:A:350:ILE:CD1	2.31	0.53
2:B:141:TYR:HD1	2:B:145:GLU:CD	2.17	0.53
4:d:74:TRP:CZ2	4:d:411:GLU:HA	2.44	0.53
1:A:102:LEU:CD1	1:A:113:TRP:HH2	2.22	0.53
1:A:163:TRP:O	1:A:177:ARG:NH1	2.39	0.53
1:A:378:LYS:O	1:A:379:TRP:HB2	2.09	0.53
2:B:198:LEU:HD11	14:B:401:HEC:HHB	1.91	0.53
1:a:30:TRP:NE1	16:a:404:CDL:O1	2.38	0.53
3:c:122:THR:HG21	9:i:25:ILE:CD1	2.37	0.53
3:C:99:SER:HA	4:D:269:ARG:NE	2.24	0.52
1:a:153:ILE:CB	1:a:156:ILE:HB	2.39	0.52
5:e:244:LEU:HD23	5:e:244:LEU:N	2.19	0.52
7:g:97:GLU:OE1	7:g:100:ARG:NH1	2.42	0.52
1:A:165:TRP:CD1	1:A:169:SER:HA	2.44	0.52
1:A:342:PRO:O	1:A:344:GLU:CG	2.57	0.52
3:c:150:SER:O	3:c:153:GLU:CG	2.51	0.52
5:e:241:ARG:NH1	5:e:241:ARG:CG	2.72	0.52
1:A:144:THR:O	1:A:148:ASN:HB2	2.10	0.52
1:A:165:TRP:CD1	1:A:169:SER:C	2.87	0.52
1:A:298:ILE:HD12	1:A:298:ILE:N	2.20	0.52
2:B:220:CYS:SG	2:B:221:GLU:HG3	2.49	0.52
2:b:223:PRO:HD2	2:b:226:VAL:HG11	1.91	0.52
1:A:170:VAL:O	3:c:171:GLY:CA	2.56	0.52
3:c:88:PHE:O	3:c:92:ARG:HG2	2.09	0.52
10:j:14:ALA:O	10:j:18:ILE:HG23	2.09	0.52
1:A:179:PHE:O	1:A:183:PHE:HB2	2.09	0.52
1:a:65:SER:HA	1:a:68:HIS:ND1	2.25	0.52
2:b:154:GLU:HG2	2:b:169:PRO:HA	1.90	0.52
2:b:295:MET:HE2	9:i:36:PHE:CE1	2.44	0.52
3:c:248:ARG:HG3	3:c:257:ASN:ND2	2.25	0.52
2:b:292:LYS:HE2	9:i:40:ALA:HB3	1.92	0.52
3:c:164:ASN:OD1	3:c:175:PHE:HB3	2.09	0.52
6:f:69:GLU:N	6:f:69:GLU:OE1	2.43	0.52
1:A:176:THR:HG23	1:a:53:MET:HG2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:THR:CG2	4:D:406:THR:HG23	2.33	0.52
4:D:80:ARG:NE	4:D:197:LEU:HD13	2.25	0.52
1:a:315:MET:CE	1:a:322:GLN:CA	2.84	0.52
3:c:122:THR:HB	9:i:25:ILE:CB	2.39	0.52
2:B:238:PHE:CD1	2:B:239:PRO:HD2	2.45	0.52
3:C:97:LEU:HG	3:C:98:ASP:N	2.25	0.52
3:C:236:CYS:HB2	3:C:241:SER:H	1.73	0.52
5:E:306:THR:HG22	5:E:377:LYS:HZ1	1.73	0.52
1:a:177:ARG:O	1:a:180:ALA:HB3	2.09	0.52
2:b:211:TYR:OH	2:b:237:TYR:O	2.26	0.52
2:b:296:MET:SD	3:c:127:TYR:CE2	3.02	0.52
3:c:249:ILE:HG12	3:c:254:ALA:HB3	1.90	0.52
1:A:177:ARG:NH2	3:c:141:SER:OG	2.43	0.52
1:A:264:THR:O	1:A:264:THR:CG2	2.58	0.52
2:B:118:TYR:HA	2:B:122:CYS:SG	2.50	0.52
3:C:180:THR:N	3:C:183:GLU:OE1	2.40	0.52
1:a:243:VAL:HG13	1:a:244:LEU:HD13	1.92	0.52
1:a:304:MET:HE1	1:a:307:LEU:HG	1.92	0.52
1:a:304:MET:SD	1:a:307:LEU:HB2	2.50	0.52
9:i:30:LEU:O	9:i:34:ARG:HG3	2.10	0.52
1:A:167:GLY:CA	3:c:147:LEU:CD1	2.88	0.52
2:B:156:GLN:HA	2:B:167:MET:SD	2.50	0.52
5:e:301:ARG:HA	11:k:34:LEU:HD22	1.92	0.52
2:b:296:MET:HE1	3:c:128:ALA:HA	1.92	0.51
1:A:343:VAL:O	1:A:344:GLU:HB2	2.08	0.51
5:E:171:ALA:O	5:E:175:GLU:HG2	2.10	0.51
1:a:210:GLY:CA	1:a:313:ARG:HG3	2.40	0.51
3:c:146:VAL:O	3:c:146:VAL:HG22	2.10	0.51
3:c:200:HIS:HD2	3:c:202:LEU:H	1.59	0.51
5:e:180:ALA:O	5:e:256:GLY:CA	2.58	0.51
3:C:153:GLU:HG2	3:C:273:VAL:HG23	1.91	0.51
3:C:173:PRO:CD	1:a:261:PRO:HB2	2.41	0.51
3:C:198:PRO:HA	3:C:248:ARG:HD3	1.92	0.51
1:a:361:ILE:HG22	1:a:362:ILE:HG23	1.92	0.51
8:h:7:HIS:O	8:h:8:LEU:HD22	2.09	0.51
1:A:283:SER:OG	1:A:352:GLN:CB	2.46	0.51
1:a:281:LEU:HD13	1:a:294:LEU:HB2	1.92	0.51
12:a:401:HEM:HBC2	12:a:401:HEM:CMC	2.40	0.51
3:c:102:SER:OG	3:c:103:SER:N	2.44	0.51
3:c:172:LYS:HE2	3:c:216:VAL:HG22	1.91	0.51
4:d:422:ARG:O	4:d:424:ILE:HG13	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:171:ALA:O	5:e:175:GLU:HG2	2.10	0.51
5:e:223:LEU:HD21	5:e:389:SER:HB2	1.92	0.51
7:g:10:SER:O	7:g:13:TRP:HB2	2.11	0.51
1:A:223:TYR:CZ	2:B:315:LEU:HD13	2.44	0.51
2:B:309:ARG:CG	2:B:309:ARG:NH1	2.72	0.51
1:a:237:LEU:HD13	2:b:297:MET:HE3	1.91	0.51
3:c:166:ALA:HB1	3:c:173:PRO:HB3	1.93	0.51
10:j:41:ILE:HA	10:j:44:TRP:CD1	2.32	0.51
5:E:41:THR:HG21	5:E:231:LYS:HE2	1.93	0.51
4:D:383:ALA:H	4:D:442:ARG:NH1	2.08	0.51
5:E:342:SER:OG	5:E:343:GLN:N	2.43	0.51
1:a:129:MET:HE2	1:a:181:PHE:CB	2.36	0.51
2:b:124:SER:O	2:b:179:PRO:CG	2.58	0.51
7:g:11:SER:O	7:g:15:GLU:HG2	2.11	0.51
1:A:58:ASP:OD1	1:A:172:LYS:HE2	2.11	0.51
1:A:284:ILE:HD11	1:A:290:GLY:N	2.26	0.51
2:B:217:THR:HG23	2:B:264:MET:CE	2.39	0.51
3:c:173:PRO:HB2	3:c:175:PHE:CE1	2.46	0.51
5:E:48:VAL:HG11	5:E:400:ALA:HB1	1.92	0.51
6:F:41:GLU:HA	6:F:44:ILE:HG12	1.93	0.51
1:A:223:TYR:CD2	2:B:315:LEU:HD21	2.45	0.50
1:a:341:GLN:HG2	1:a:347:PHE:HE2	1.76	0.50
2:b:296:MET:HE3	3:c:127:TYR:HD2	1.75	0.50
3:c:197:ASP:OD2	3:c:256:LEU:HB2	2.11	0.50
5:e:139:ASN:O	5:e:139:ASN:ND2	2.44	0.50
1:A:121:PHE:CE2	1:A:298:ILE:HB	2.45	0.50
1:A:136:GLY:C	1:A:138:MET:H	2.18	0.50
3:C:241:SER:OG	3:C:252:GLY:O	2.23	0.50
1:a:149:LEU:HG	1:a:287:LYS:CE	2.41	0.50
3:c:122:THR:CG2	9:i:25:ILE:HD13	2.40	0.50
6:f:50:LEU:HA	6:f:70:GLU:HG3	1.94	0.50
11:k:42:VAL:HG23	11:k:46:LYS:HG3	1.92	0.50
1:A:284:ILE:CD1	1:A:290:GLY:CA	2.68	0.50
3:C:153:GLU:HG2	3:C:273:VAL:CG2	2.41	0.50
3:c:80:HIS:NE2	4:d:182:VAL:CB	2.74	0.50
3:c:177:ARG:HB3	3:c:211:VAL:CG1	2.42	0.50
1:A:132:VAL:HA	1:A:139:SER:HB3	1.92	0.50
1:a:121:PHE:CE1	1:a:298:ILE:HG21	2.46	0.50
1:A:52:ALA:CB	1:A:179:PHE:HZ	2.24	0.50
2:B:157:ASP:OD1	2:B:158:GLY:N	2.39	0.50
7:g:96:LYS:HE2	7:g:100:ARG:HH21	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:PRO:HD3	14:B:401:HEC:HBD2	1.93	0.50
4:D:79:SER:O	4:D:82:GLU:CG	2.60	0.50
5:E:91:THR:HG22	5:E:92:LYS:N	2.27	0.50
2:b:254:LEU:HG	2:b:255:GLU:H	1.77	0.50
2:b:314:VAL:HG21	4:d:469:ASN:ND2	2.27	0.50
9:i:24:THR:CA	9:i:27:VAL:HG23	2.28	0.50
1:A:59:THR:HG22	1:A:172:LYS:HD3	1.94	0.50
1:A:108:MET:HE2	1:A:308:HIS:ND1	2.26	0.50
4:D:266:THR:O	4:D:268:CYS:N	2.45	0.50
3:c:122:THR:HG22	9:i:25:ILE:HD12	1.93	0.50
4:D:284:LEU:HB2	11:K:43:LEU:HD23	1.93	0.49
1:a:350:ILE:O	1:a:351:GLY:C	2.51	0.49
2:b:116:GLN:NE2	2:b:141:TYR:OH	2.45	0.49
2:b:118:TYR:HD1	2:b:122:CYS:SG	2.34	0.49
7:g:96:LYS:HE2	7:g:100:ARG:NH2	2.27	0.49
5:E:183:ARG:HE	5:E:254:ARG:HB2	1.77	0.49
2:b:124:SER:O	2:b:179:PRO:HG2	2.12	0.49
2:b:139:VAL:HG21	2:b:277:TRP:CZ2	2.47	0.49
5:e:438:MET:CG	5:e:439:ALA:N	2.72	0.49
6:f:35:GLU:OE2	6:f:39:GLN:NE2	2.44	0.49
1:A:57:SER:HA	1:A:175:LEU:HD23	1.94	0.49
5:e:43:LEU:HB2	5:e:46:GLY:O	2.12	0.49
1:A:333:ILE:HG22	1:A:333:ILE:O	2.12	0.49
5:E:254:ARG:HG2	5:E:255:GLY:H	1.76	0.49
1:a:260:ASN:OD1	1:a:261:PRO:HD2	2.11	0.49
1:a:300:ILE:HD11	1:a:363:LEU:HD21	1.93	0.49
10:j:6:LEU:HA	10:j:11:ARG:HH12	1.77	0.49
1:A:168:PHE:H	3:c:147:LEU:HD21	1.78	0.49
2:B:312:TRP:O	2:B:316:LYS:HB2	2.13	0.49
9:i:11:TYR:HA	9:i:15:PHE:HB2	1.94	0.49
1:A:52:ALA:HA	1:A:55:TYR:HB2	1.91	0.49
1:A:61:THR:HG22	1:A:61:THR:O	2.13	0.49
1:A:126:THR:HG1	1:A:185:LEU:HD23	1.74	0.49
2:B:129:ASP:OD1	2:B:130:TYR:N	2.46	0.49
1:a:185:LEU:O	1:a:189:ILE:HG13	2.13	0.49
2:b:129:ASP:O	2:b:175:TYR:CD2	2.66	0.49
5:e:217:ARG:HD2	5:e:244:LEU:CB	2.42	0.49
1:a:60:THR:O	1:a:60:THR:HG22	2.12	0.49
1:a:113:TRP:HE3	12:a:402:HEM:HMD1	1.78	0.49
1:a:213:SER:O	1:a:213:SER:OG	2.24	0.49
3:c:92:ARG:NH2	4:d:269:ARG:NH2	2.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TRP:CZ2	1:A:140:PHE:HE1	2.31	0.49
4:D:70:THR:HG21	4:D:406:THR:HG22	1.95	0.49
3:c:149:MET:CG	3:c:169:TRP:CH2	2.96	0.49
12:A:402:HEM:HMB1	12:A:402:HEM:HBB2	1.93	0.49
2:B:245:MET:CE	2:B:248:PRO:HG2	2.32	0.49
10:j:38:TRP:CD1	10:j:40:LEU:HB2	2.47	0.49
2:B:301:LEU:H	2:B:302:PRO:CD	2.25	0.49
1:a:163:TRP:O	1:a:177:ARG:NH1	2.45	0.49
1:A:102:LEU:HD12	1:A:113:TRP:CH2	2.48	0.48
1:A:342:PRO:O	1:A:344:GLU:HG3	2.12	0.48
3:c:156:LEU:CD1	3:c:156:LEU:C	2.86	0.48
4:d:54:ASP:OD1	4:d:55:ASN:N	2.46	0.48
8:h:11:MET:HE2	8:h:14:VAL:HG11	1.95	0.48
1:A:132:VAL:O	1:A:132:VAL:HG12	2.13	0.48
12:A:401:HEM:HMB1	12:A:401:HEM:HBB2	1.95	0.48
4:D:366:ASP:OD1	4:D:366:ASP:N	2.46	0.48
3:c:190:VAL:HG11	3:c:195:LEU:HD21	1.95	0.48
4:d:323:HIS:ND1	5:e:100:THR:HG21	2.28	0.48
1:a:111:GLU:OE1	1:a:199:PHE:CZ	2.66	0.48
6:f:34:ARG:HG2	6:f:78:ARG:NH2	2.27	0.48
1:A:52:ALA:HB2	1:A:179:PHE:HZ	1.79	0.48
1:A:223:TYR:CE2	2:B:315:LEU:HD11	2.42	0.48
1:a:344:GLU:OE1	1:a:347:PHE:CE2	2.66	0.48
2:B:144:GLU:HA	2:B:147:LYS:HB3	1.95	0.48
1:a:357:LEU:C	1:a:359:PHE:N	2.69	0.48
3:c:92:ARG:HH22	4:d:269:ARG:NH2	2.09	0.48
1:A:41:LEU:HD21	1:A:190:THR:HG22	1.96	0.48
4:D:324:MET:HE2	4:D:329:ALA:HB1	1.96	0.48
11:K:20:ARG:NE	11:K:53:GLU:OE2	2.46	0.48
1:A:309:THR:HG22	1:A:309:THR:O	2.13	0.48
1:A:324:LEU:O	1:A:325:PHE:C	2.56	0.48
3:C:179:ARG:HH21	3:C:183:GLU:HB3	1.77	0.48
3:C:200:HIS:O	3:C:204:ARG:HB2	2.14	0.48
1:a:237:LEU:CD1	2:b:297:MET:CE	2.92	0.48
1:A:216:ASP:OD1	1:A:216:ASP:N	2.47	0.48
11:K:31:GLN:HA	11:K:34:LEU:HB2	1.96	0.48
1:a:302:ILE:CD1	1:a:302:ILE:H	2.23	0.48
2:b:319:LYS:HB2	8:h:17:TYR:HD1	1.78	0.48
4:d:278:ARG:O	4:d:460:GLY:HA3	2.14	0.48
1:A:167:GLY:HA2	3:c:147:LEU:CD1	2.43	0.48
2:B:265:SER:HB2	6:F:30:LEU:HD23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:210:GLY:CA	1:a:313:ARG:CG	2.91	0.48
1:a:315:MET:CE	1:a:322:GLN:N	2.76	0.48
1:A:141:TRP:NE1	3:c:222:CYS:HB3	2.28	0.48
1:A:261:PRO:HB3	3:c:173:PRO:HG3	1.96	0.48
2:B:90:LEU:HD23	2:B:237:TYR:CE1	2.48	0.48
2:b:320:LEU:O	2:b:320:LEU:HD23	2.14	0.48
9:I:53:TRP:NE1	9:I:57:LYS:HD3	2.29	0.47
11:K:27:ARG:O	11:K:27:ARG:NE	2.47	0.47
1:a:285:PRO:O	1:a:286:ASN:CB	2.53	0.47
3:c:176:VAL:HG22	3:c:212:ILE:HG22	1.96	0.47
3:c:179:ARG:N	3:c:209:GLU:O	2.47	0.47
2:B:98:SER:O	9:I:51:LYS:NZ	2.47	0.47
2:B:223:PRO:HG3	6:F:71:LEU:HD22	1.96	0.47
10:J:21:ALA:HA	10:J:24:TRP:HD1	1.78	0.47
1:a:137:GLN:NE2	1:a:258:PRO:O	2.48	0.47
16:a:404:CDL:H132	8:h:46:ILE:HD12	1.96	0.47
3:c:214:ILE:O	3:c:258:LEU:HD11	2.14	0.47
5:e:54:ASN:OD1	5:e:55:TYR:N	2.39	0.47
1:A:167:GLY:HA3	3:c:147:LEU:CD1	2.42	0.47
2:b:296:MET:SD	3:c:127:TYR:HE2	2.37	0.47
5:e:240:MET:C	5:e:241:ARG:HG2	2.36	0.47
1:A:344:GLU:HG3	1:A:347:PHE:CG	2.50	0.47
11:K:20:ARG:HH11	11:K:48:SER:CB	2.28	0.47
6:f:30:LEU:HA	6:f:33:VAL:HG22	1.97	0.47
9:i:5:THR:HG22	9:i:6:LEU:N	2.29	0.47
1:A:168:PHE:N	3:c:147:LEU:HD21	2.29	0.47
1:A:213:SER:O	1:A:213:SER:OG	2.20	0.47
3:C:153:GLU:O	3:C:273:VAL:HG22	2.13	0.47
4:D:38:TYR:CD1	5:E:57:PRO:HB2	2.48	0.47
1:a:153:ILE:HD13	1:a:156:ILE:HD12	1.95	0.47
1:a:362:ILE:HG13	1:a:363:LEU:HD22	1.96	0.47
2:b:126:HIS:CG	2:b:198:LEU:HG	2.49	0.47
4:d:192:PHE:HB2	4:d:198:ALA:HB2	1.96	0.47
5:e:399:GLN:HB2	11:k:2:LEU:HD12	1.96	0.47
2:B:266:GLN:HE22	6:F:91:LYS:HB2	1.79	0.47
4:D:42:LEU:HD12	4:D:426:LEU:HB3	1.97	0.47
4:D:114:GLU:OE1	5:E:306:THR:HG21	2.15	0.47
5:E:46:GLY:O	5:E:215:SER:O	2.32	0.47
9:I:27:VAL:HG22	10:J:30:VAL:HG11	1.96	0.47
1:a:224:TYR:O	1:a:225:THR:C	2.55	0.47
3:c:267:SER:HB3	3:c:270:LEU:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:280:ASP:HB2	8:h:11:MET:O	2.15	0.47
11:k:40:SER:O	11:k:40:SER:OG	2.32	0.47
1:A:261:PRO:CB	3:c:173:PRO:HG3	2.44	0.47
2:B:112:ARG:NH1	2:B:141:TYR:CE1	2.83	0.47
2:B:267:VAL:O	2:B:271:VAL:HG23	2.15	0.47
2:B:310:HIS:O	2:B:310:HIS:CG	2.68	0.47
4:D:238:GLU:O	4:D:238:GLU:HG2	2.15	0.47
4:D:324:MET:HE3	4:D:329:ALA:CB	2.41	0.47
5:E:183:ARG:CG	5:E:254:ARG:HB2	2.45	0.47
9:i:17:ARG:C	9:i:19:SER:H	2.23	0.47
10:j:45:VAL:HG22	10:j:47:TYR:HB2	1.97	0.47
1:A:141:TRP:CE3	1:A:141:TRP:CA	2.98	0.47
5:E:47:LEU:HD22	5:E:238:LEU:HD11	1.97	0.47
5:E:225:VAL:HG12	5:E:226:SER:N	2.30	0.47
1:a:37:LEU:CD2	1:a:93:CYS:CB	2.92	0.47
1:a:279:ALA:O	1:a:283:SER:HB2	2.15	0.47
3:c:250:ARG:C	3:c:251:LYS:HD2	2.39	0.47
4:d:36:ALA:O	5:e:127:ARG:HD3	2.15	0.47
8:h:50:ALA:HB3	8:h:51:PRO:HD3	1.97	0.47
1:A:298:ILE:H	1:A:298:ILE:CD1	2.22	0.47
3:C:164:ASN:HB2	3:C:177:ARG:HD3	1.96	0.47
4:D:462:ILE:HG13	4:D:462:ILE:O	2.15	0.47
10:J:7:GLY:O	10:J:11:ARG:NE	2.48	0.47
4:d:361:ASP:CG	4:d:362:ASN:H	2.23	0.47
5:e:245:GLY:O	5:e:246:LEU:CD2	2.63	0.47
5:E:170:GLN:OE1	11:K:28:PRO:HD3	2.14	0.46
4:d:179:MET:HE3	4:d:286:HIS:ND1	2.30	0.46
5:e:73:ASP:O	5:e:77:LEU:HD12	2.16	0.46
5:e:113:THR:HB	11:k:14:VAL:HG23	1.96	0.46
4:d:218:GLU:O	4:d:222:GLN:HG3	2.14	0.46
1:A:66:VAL:O	1:A:69:ILE:HG22	2.16	0.46
1:A:96:ILE:HD13	13:A:403:PEE:H25	1.98	0.46
3:C:93:ARG:NH1	3:C:110:ARG:HB2	2.19	0.46
3:c:150:SER:HG	3:c:169:TRP:CG	2.33	0.46
1:A:165:TRP:CG	1:A:169:SER:CA	2.94	0.46
2:B:184:GLU:HB3	2:b:161:GLU:HB2	1.96	0.46
5:E:56:ALA:H	5:E:127:ARG:HH21	1.62	0.46
5:E:246:LEU:N	5:E:246:LEU:CD1	2.78	0.46
1:a:94:LEU:HD12	1:a:94:LEU:HA	1.79	0.46
1:a:129:MET:HE1	1:a:181:PHE:O	2.15	0.46
1:a:315:MET:HE2	1:a:322:GLN:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:122:THR:CG2	9:i:25:ILE:HD12	2.45	0.46
3:C:223:VAL:HG11	1:a:261:PRO:O	2.16	0.46
4:D:308:ASN:ND2	4:D:345:ASN:HD21	2.14	0.46
5:E:293:LEU:O	5:E:307:SER:HB3	2.15	0.46
7:G:46:GLU:OE2	7:G:49:ARG:NH1	2.48	0.46
5:e:42:ARG:HG3	5:e:43:LEU:N	2.31	0.46
3:C:179:ARG:HB2	3:C:209:GLU:HA	1.98	0.46
3:C:243:TYR:CZ	3:C:249:ILE:HD13	2.50	0.46
1:a:311:LYS:HE2	1:a:379:TRP:HB3	1.97	0.46
1:A:169:SER:OG	3:c:172:LYS:HG2	2.16	0.46
1:A:356:ILE:HG13	1:A:357:LEU:N	2.29	0.46
5:E:250:LYS:O	5:E:250:LYS:HD3	2.16	0.46
1:a:302:ILE:HD12	1:a:303:LEU:N	2.30	0.46
3:c:239:HIS:NE2	15:c:301:FES:S2	2.86	0.46
5:e:259:ARG:HB3	5:e:444:LEU:HD13	1.98	0.46
5:e:370:ASP:OD1	5:e:371:VAL:N	2.48	0.46
2:B:277:TRP:O	2:B:280:GLU:O	2.34	0.46
1:a:121:PHE:HD1	1:a:298:ILE:CG2	2.27	0.46
11:k:34:LEU:HB2	11:k:35:PRO:HD3	1.98	0.46
1:a:27:ILE:HG21	1:a:31:TRP:CG	2.51	0.46
1:a:347:PHE:CD1	1:a:347:PHE:N	2.84	0.46
3:c:82:ASP:C	3:c:83:ILE:HG23	2.17	0.46
3:c:255:PRO:HG2	3:c:256:LEU:HD23	1.97	0.46
8:h:8:LEU:HB3	8:h:9:THR:H	1.67	0.46
2:B:210:ASP:OD1	2:B:210:ASP:N	2.44	0.46
4:D:138:LYS:H	4:D:138:LYS:HD2	1.80	0.46
4:D:308:ASN:ND2	4:D:345:ASN:OD1	2.49	0.46
5:e:42:ARG:HG3	5:e:43:LEU:H	1.81	0.46
3:C:170:ARG:O	3:C:170:ARG:HG2	2.16	0.45
5:E:49:ILE:HA	5:E:220:LEU:O	2.15	0.45
5:E:60:ARG:NH1	5:E:124:GLU:OE1	2.49	0.45
1:a:182:HIS:HD2	12:a:401:HEM:C4C	2.35	0.45
1:a:256:TYR:OH	2:b:203:ARG:NH2	2.48	0.45
1:a:280:ILE:HD12	1:a:355:SER:OG	2.16	0.45
1:a:309:THR:O	1:a:309:THR:HG22	2.15	0.45
1:a:335:LEU:HD12	1:a:354:ALA:HB1	1.97	0.45
2:b:223:PRO:HB3	6:f:67:CYS:HB2	1.98	0.45
3:c:154:ILE:HB	3:c:270:LEU:HD22	1.96	0.45
3:c:250:ARG:HB2	3:c:251:LYS:HD2	1.98	0.45
4:d:126:ARG:NH1	4:d:199:GLN:O	2.49	0.45
1:A:136:GLY:O	1:A:138:MET:N	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLY:O	1:A:341:GLN:OE1	2.35	0.45
1:A:377:LEU:HD23	7:G:21:TYR:HE1	1.80	0.45
2:B:301:LEU:N	2:B:302:PRO:HD2	2.30	0.45
4:D:454:PRO:HG3	4:D:475:MET:CE	2.42	0.45
9:I:16:ARG:HB3	9:I:17:ARG:HD3	1.97	0.45
3:c:93:ARG:HB2	3:c:96:VAL:HG22	1.98	0.45
3:c:217:CYS:HB2	3:c:243:TYR:CE2	2.51	0.45
1:A:58:ASP:H	1:A:175:LEU:CD2	2.29	0.45
2:B:245:MET:HE2	2:B:248:PRO:HG3	1.94	0.45
2:B:250:TYR:H	2:B:253:VAL:HG21	1.80	0.45
6:F:44:ILE:HG13	6:F:45:LYS:N	2.30	0.45
1:a:122:THR:HG22	1:a:189:ILE:CD1	2.39	0.45
1:a:332:LEU:CD1	13:a:403:PEE:H38	2.45	0.45
3:c:99:SER:CA	4:d:269:ARG:HD2	2.45	0.45
1:A:243:VAL:HG23	1:A:244:LEU:HD12	1.98	0.45
5:E:170:GLN:O	5:E:174:LEU:HD13	2.16	0.45
1:a:300:ILE:HG23	1:a:301:LEU:N	2.31	0.45
12:a:402:HEM:HMB1	12:a:402:HEM:HBB2	1.99	0.45
3:c:83:ILE:HG13	3:c:83:ILE:O	2.16	0.45
5:e:433:SER:O	5:e:433:SER:OG	2.34	0.45
2:B:164:GLU:OE1	2:B:164:GLU:N	2.49	0.45
3:C:93:ARG:N	3:C:96:VAL:HG23	2.30	0.45
5:E:260:ASP:C	5:E:444:LEU:HD11	2.42	0.45
1:a:347:PHE:N	1:a:347:PHE:HD1	2.14	0.45
2:b:106:LEU:HD21	2:b:276:ARG:HH12	1.81	0.45
3:c:80:HIS:HB3	4:d:176:ASP:CG	2.42	0.45
5:E:180:ALA:HB1	5:E:256:GLY:O	2.17	0.45
5:E:241:ARG:O	5:E:241:ARG:HG2	2.17	0.45
5:E:306:THR:HG22	5:E:306:THR:O	2.16	0.45
3:c:218:THR:OG1	3:c:243:TYR:OH	2.34	0.45
4:d:422:ARG:HH12	4:d:428:GLU:CD	2.25	0.45
4:d:440:VAL:O	4:d:444:VAL:HG22	2.17	0.45
1:A:169:SER:HB3	3:c:172:LYS:N	2.30	0.45
4:D:422:ARG:O	4:D:422:ARG:HG3	2.16	0.45
1:a:300:ILE:HG13	1:a:300:ILE:O	2.15	0.45
3:c:120:THR:O	3:c:123:VAL:HG23	2.14	0.45
7:g:59:ARG:HD2	7:g:90:TYR:OH	2.17	0.45
1:A:285:PRO:O	1:A:286:ASN:HB2	2.17	0.45
3:C:83:ILE:O	3:C:84:ARG:NE	2.49	0.45
3:C:224:PRO:HG2	3:C:234:TYR:HB3	1.98	0.45
4:D:36:ALA:O	5:E:127:ARG:HD3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:19:LEU:HD12	8:H:20:SER:H	1.81	0.45
9:I:16:ARG:HG2	9:I:17:ARG:HD3	1.99	0.45
1:a:210:GLY:CA	1:a:313:ARG:CD	2.95	0.45
1:a:302:ILE:HD12	1:a:303:LEU:H	1.82	0.45
3:c:177:ARG:NH2	3:c:183:GLU:HG3	2.30	0.45
5:e:229:VAL:O	5:e:233:VAL:HG13	2.17	0.45
1:A:144:THR:CG2	3:c:216:VAL:CG1	2.95	0.45
4:D:74:TRP:CZ2	4:D:411:GLU:HA	2.51	0.45
4:D:384:THR:HG22	4:D:385:GLU:N	2.31	0.45
5:E:438:MET:CG	5:E:439:ALA:N	2.74	0.45
4:D:158:ASP:O	4:D:159:SER:CB	2.61	0.45
5:E:313:VAL:O	5:E:315:LYS:O	2.34	0.45
2:b:209:GLU:CD	2:b:276:ARG:HD2	2.42	0.45
3:c:156:LEU:CD2	3:c:269:ASP:C	2.88	0.45
4:D:328:LEU:HD12	4:D:328:LEU:HA	1.79	0.44
6:F:28:ASP:O	6:F:31:THR:OG1	2.21	0.44
3:c:150:SER:CA	3:c:153:GLU:CD	2.90	0.44
3:C:222:CYS:HA	1:a:264:THR:HG21	1.99	0.44
4:D:315:ASP:HB3	4:D:318:TYR:CE1	2.53	0.44
5:e:67:ALA:O	5:e:119:MET:HG3	2.17	0.44
6:f:38:GLU:O	6:f:43:CYS:HB2	2.18	0.44
1:A:167:GLY:HA2	3:c:147:LEU:CD2	2.47	0.44
1:A:223:TYR:CD2	2:B:315:LEU:HD22	2.51	0.44
4:D:281:ALA:CB	8:H:12:ARG:HH12	2.30	0.44
2:b:147:LYS:HZ1	3:c:154:ILE:HD13	1.82	0.44
2:b:147:LYS:HZ3	3:c:154:ILE:HD13	1.81	0.44
3:c:217:CYS:H	3:c:221:GLY:HA2	1.81	0.44
6:f:56:ARG:NH2	6:f:65:GLU:HG2	2.32	0.44
2:B:142:THR:HG22	2:B:143:GLU:H	1.83	0.44
1:a:129:MET:HE1	1:a:181:PHE:C	2.42	0.44
3:c:159:ILE:HD12	3:c:159:ILE:H	1.82	0.44
3:C:154:ILE:HG23	3:C:271:VAL:O	2.18	0.44
4:D:381:THR:CG2	4:D:382:SER:H	2.10	0.44
1:a:137:GLN:OE1	1:a:257:THR:OG1	2.33	0.44
2:b:296:MET:HE3	3:c:127:TYR:CD2	2.52	0.44
3:c:149:MET:SD	3:c:169:TRP:HH2	2.41	0.44
5:e:168:ASN:HA	5:e:169:PRO:HD3	1.89	0.44
9:i:28:GLY:O	9:i:32:PHE:N	2.36	0.44
1:A:59:THR:HG23	1:A:60:THR:N	2.32	0.44
3:C:93:ARG:O	3:C:96:VAL:HG22	2.17	0.44
9:I:53:TRP:HE1	9:I:57:LYS:HD3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:114:ASN:OD1	1:a:302:ILE:HG22	2.18	0.44
2:b:129:ASP:OD1	2:b:129:ASP:N	2.41	0.44
4:d:315:ASP:OD2	11:k:20:ARG:HD3	2.18	0.44
1:A:165:TRP:CD1	1:A:170:VAL:N	2.86	0.44
2:B:111:ILE:HG12	2:B:273:THR:HG22	1.99	0.44
4:D:315:ASP:OD1	4:D:316:SER:N	2.51	0.44
10:J:38:TRP:HD1	10:J:39:ARG:N	2.16	0.44
1:a:51:LEU:HD13	12:a:401:HEM:HBD1	1.99	0.44
1:a:303:LEU:O	1:a:307:LEU:HD23	2.18	0.44
3:c:179:ARG:HH22	3:c:211:VAL:HG21	1.82	0.44
4:d:269:ARG:H	4:d:269:ARG:HG2	1.57	0.44
5:e:65:ILE:HG12	5:e:218:MET:HG2	1.99	0.44
8:h:38:VAL:HA	8:h:41:ARG:HG2	2.00	0.44
4:D:125:THR:CG2	4:D:126:ARG:H	2.27	0.44
1:a:344:GLU:HG2	8:h:67:PHE:CE1	2.52	0.44
3:c:150:SER:CA	3:c:153:GLU:CG	2.96	0.44
1:A:176:THR:O	1:A:180:ALA:HB2	2.18	0.44
4:D:138:LYS:HD2	4:D:138:LYS:N	2.33	0.44
5:E:193:PRO:O	5:E:196:ARG:HB3	2.18	0.44
7:G:41:ASP:OD1	7:G:41:ASP:N	2.44	0.44
2:b:168:ARG:HD2	2:b:170:GLY:N	2.33	0.44
3:c:130:LYS:HG2	10:j:34:TRP:HE1	1.83	0.44
2:B:232:LEU:O	2:B:233:TYR:HD1	2.01	0.43
1:a:121:PHE:CE1	1:a:298:ILE:CB	3.00	0.43
5:e:180:ALA:HB1	5:e:256:GLY:O	2.18	0.43
3:C:212:ILE:O	3:C:212:ILE:HG13	2.18	0.43
8:H:18:SER:OG	8:H:19:LEU:N	2.51	0.43
1:a:37:LEU:CD2	1:a:93:CYS:HB3	2.46	0.43
1:a:40:CYS:HB3	1:a:90:PHE:CD1	2.51	0.43
1:a:111:GLU:CB	1:a:199:PHE:CD2	2.88	0.43
2:b:126:HIS:HB3	2:b:197:ASP:HA	1.99	0.43
5:e:194:ASP:C	5:e:196:ARG:H	2.26	0.43
1:A:144:THR:HG21	3:c:216:VAL:CG1	2.47	0.43
1:A:342:PRO:O	1:A:344:GLU:HG2	2.19	0.43
1:A:344:GLU:CG	1:A:347:PHE:CG	3.01	0.43
7:G:102:ARG:HD2	10:j:4:ARG:HH22	1.83	0.43
12:a:401:HEM:HBA2	12:a:401:HEM:HHA	2.00	0.43
3:c:175:PHE:CE2	3:c:215:GLY:HA2	2.50	0.43
4:d:283:PRO:HD3	11:k:43:LEU:HG	2.00	0.43
4:d:451:ASP:OD2	9:i:11:TYR:OH	2.36	0.43
2:B:123:SER:O	2:B:125:CYS:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:THR:HG23	4:D:104:ARG:H	1.83	0.43
1:a:124:MET:HG3	1:a:274:PHE:CE1	2.53	0.43
2:b:159:PRO:HA	2:b:164:GLU:HB2	1.99	0.43
1:A:140:PHE:HE2	3:c:172:LYS:CE	2.32	0.43
1:A:177:ARG:O	1:A:180:ALA:HB3	2.18	0.43
2:B:283:HIS:O	2:B:283:HIS:ND1	2.52	0.43
4:D:259:GLU:O	4:D:259:GLU:HG2	2.18	0.43
4:D:327:THR:CB	4:D:375:GLN:CD	2.91	0.43
5:E:85:LEU:CD2	11:K:15:LEU:HD13	2.48	0.43
5:E:302:GLY:O	11:K:31:GLN:NE2	2.51	0.43
2:b:309:ARG:HH11	2:b:309:ARG:CG	2.32	0.43
1:A:301:LEU:O	1:A:304:MET:HB2	2.18	0.43
2:B:303:LEU:HD23	2:B:303:LEU:HA	1.84	0.43
1:a:115:ILE:O	1:a:115:ILE:CG2	2.66	0.43
1:a:329:VAL:O	1:a:333:ILE:HG12	2.18	0.43
3:c:159:ILE:CG1	3:c:165:MET:HB3	2.49	0.43
8:h:29:HIS:O	8:h:33:LYS:HG2	2.17	0.43
1:A:18:PHE:CE2	16:D:501:CDL:H362	2.49	0.43
1:A:343:VAL:O	1:A:347:PHE:HB2	2.19	0.43
2:B:88:LEU:CD1	8:H:72:ARG:HG2	2.45	0.43
3:C:243:TYR:CE2	3:C:249:ILE:HD13	2.53	0.43
4:D:283:PRO:HG2	11:K:43:LEU:O	2.19	0.43
4:D:365:ILE:HD11	4:D:462:ILE:HG22	1.98	0.43
1:a:138:MET:HE2	1:a:138:MET:HB2	1.92	0.43
1:a:230:LEU:HD12	2:b:304:VAL:HG11	2.00	0.43
1:a:233:LEU:CD2	2:b:301:LEU:HD12	2.48	0.43
3:c:123:VAL:HG23	3:c:124:GLY:N	2.34	0.43
4:d:51:SER:OG	4:d:52:GLN:N	2.52	0.43
6:f:69:GLU:HG2	6:f:70:GLU:H	1.84	0.43
1:A:168:PHE:CD2	3:c:170:ARG:HA	2.52	0.43
1:A:256:TYR:O	1:A:257:THR:C	2.61	0.43
4:D:37:THR:C	4:D:39:ALA:N	2.77	0.43
4:D:328:LEU:HD23	4:D:341:PHE:CE1	2.54	0.43
4:D:480:PHE:CD2	9:I:17:ARG:HG2	2.54	0.43
5:E:37:ASP:O	5:E:52:LEU:HD12	2.19	0.43
1:a:124:MET:HG3	1:a:274:PHE:HE1	1.83	0.43
1:a:341:GLN:HG3	1:a:342:PRO:HD2	2.01	0.43
4:d:322:THR:O	4:d:322:THR:OG1	2.31	0.43
4:D:38:TYR:CE1	4:D:42:LEU:HD21	2.53	0.43
5:E:322:ASP:HB3	5:E:341:ILE:HB	2.00	0.43
2:b:230:GLU:CD	2:b:230:GLU:H	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:88:PHE:CD2	8:h:19:LEU:HG	2.54	0.43
5:e:351:ILE:C	5:e:353:SER:H	2.27	0.43
10:j:51:LYS:HA	10:j:51:LYS:HD3	1.76	0.43
1:A:176:THR:HG23	1:a:53:MET:CG	2.49	0.43
6:F:56:ARG:HD2	6:F:63:THR:HG21	2.00	0.43
5:e:180:ALA:O	5:e:256:GLY:N	2.52	0.43
7:g:96:LYS:O	7:g:96:LYS:HG3	2.19	0.43
3:C:93:ARG:CB	3:C:96:VAL:CG2	2.96	0.42
1:a:89:MET:HA	1:a:92:ILE:CD1	2.49	0.42
1:a:166:GLY:HA3	1:a:173:ALA:HB1	2.00	0.42
1:A:140:PHE:CE2	3:c:172:LYS:CE	3.02	0.42
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.79	0.42
3:C:93:ARG:CA	3:C:96:VAL:CG2	2.97	0.42
4:D:220:VAL:O	4:D:224:TYR:HB2	2.19	0.42
7:G:102:ARG:HD2	10:j:4:ARG:NH2	2.33	0.42
1:a:226:ILE:O	1:a:226:ILE:HG13	2.18	0.42
4:d:197:LEU:HD21	4:d:348:TYR:CD2	2.54	0.42
4:d:216:LEU:O	4:d:220:VAL:HG23	2.19	0.42
4:d:422:ARG:NH1	4:d:428:GLU:OE1	2.52	0.42
5:e:123:VAL:HG21	5:e:133:LEU:HB3	2.01	0.42
5:e:240:MET:HB2	5:e:241:ARG:HH12	1.79	0.42
6:f:71:LEU:O	6:f:75:LEU:HD23	2.18	0.42
10:j:7:GLY:O	10:j:11:ARG:HD3	2.19	0.42
1:A:348:ILE:HD13	1:A:348:ILE:C	2.36	0.42
10:J:21:ALA:O	10:J:24:TRP:N	2.50	0.42
1:a:153:ILE:CG2	1:a:156:ILE:CG1	2.82	0.42
3:c:212:ILE:HD12	3:c:261:PRO:HG2	2.02	0.42
1:A:186:PRO:HG3	12:A:402:HEM:HMC2	2.01	0.42
3:C:163:LYS:HA	3:C:163:LYS:HD3	1.81	0.42
4:D:70:THR:HG21	4:D:406:THR:CG2	2.46	0.42
5:E:38:LEU:HD23	5:E:52:LEU:HB2	2.00	0.42
2:b:103:LEU:HD11	2:b:291:LEU:HD12	2.00	0.42
2:b:164:GLU:O	2:b:165:MET:CG	2.67	0.42
3:c:149:MET:CG	3:c:169:TRP:HH2	2.31	0.42
1:A:309:THR:CG2	1:A:371:ILE:HG13	2.45	0.42
2:B:301:LEU:O	2:B:301:LEU:HG	2.19	0.42
3:C:242:HIS:ND1	3:C:251:LYS:HD3	2.35	0.42
9:I:11:TYR:HA	9:I:15:PHE:HD2	1.84	0.42
9:I:19:SER:HB3	10:J:23:MET:CE	2.49	0.42
1:a:21:LEU:HD12	1:a:21:LEU:C	2.44	0.42
1:a:107:TYR:HE1	1:a:108:MET:HE2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:278:TYR:CD2	1:a:278:TYR:O	2.72	0.42
1:a:303:LEU:O	1:a:304:MET:SD	2.78	0.42
1:a:337:TRP:CE3	1:a:338:ILE:HD13	2.54	0.42
3:c:101:LYS:CD	4:d:267:PRO:CG	2.95	0.42
9:i:52:LEU:HD23	9:i:53:TRP:N	2.34	0.42
1:A:57:SER:CA	1:A:175:LEU:HD23	2.49	0.42
1:A:268:ILE:HG21	3:c:220:LEU:HD13	2.01	0.42
1:A:344:GLU:CG	1:A:347:PHE:CD2	2.97	0.42
2:B:117:VAL:HG22	2:B:254:LEU:HD22	2.02	0.42
8:H:4:GLU:N	8:H:4:GLU:OE1	2.53	0.42
4:d:280:ASP:N	8:h:12:ARG:HG3	2.31	0.42
5:e:147:ARG:HB2	5:e:150:GLU:OE1	2.19	0.42
10:j:33:VAL:HG13	10:j:38:TRP:HB3	2.00	0.42
3:C:169:TRP:O	3:C:170:ARG:HB3	2.19	0.42
4:D:308:ASN:HD22	4:D:345:ASN:ND2	2.16	0.42
7:G:91:LEU:O	7:G:91:LEU:HG	2.20	0.42
11:K:27:ARG:HB3	11:K:28:PRO:HD3	2.02	0.42
1:a:153:ILE:CG2	1:a:156:ILE:CB	2.95	0.42
1:a:185:LEU:HD23	1:a:185:LEU:HA	1.80	0.42
3:c:248:ARG:HG3	3:c:257:ASN:CG	2.44	0.42
4:d:278:ARG:HG2	8:h:11:MET:HG3	2.02	0.42
5:e:214:THR:HG21	5:e:244:LEU:N	2.35	0.42
5:e:215:SER:HB3	5:e:241:ARG:O	2.20	0.42
5:e:245:GLY:O	5:e:246:LEU:CG	2.68	0.42
9:i:58:HIS:HA	9:i:61:GLU:HG2	2.02	0.42
1:A:168:PHE:HB2	3:c:170:ARG:HA	2.01	0.42
2:B:178:LYS:NZ	2:B:181:PRO:O	2.53	0.42
3:C:140:MET:HB2	1:a:163:TRP:CZ2	2.55	0.42
1:a:357:LEU:C	1:a:359:PHE:H	2.27	0.42
2:b:245:MET:CE	2:b:248:PRO:HG3	2.37	0.42
6:f:78:ARG:O	6:f:82:VAL:HG23	2.19	0.42
7:g:58:ASP:HB3	7:g:62:ARG:HH21	1.85	0.42
11:k:1:MET:HE3	11:k:7:ARG:HH21	1.84	0.42
1:A:129:MET:HE3	1:A:182:HIS:N	2.35	0.42
4:D:38:TYR:CE1	5:E:57:PRO:HB2	2.54	0.42
4:D:164:GLU:O	4:D:168:ILE:HG12	2.19	0.42
1:a:41:LEU:HD12	1:a:41:LEU:HA	1.95	0.42
1:a:132:VAL:CA	1:a:139:SER:HB3	2.46	0.42
1:a:223:TYR:N	1:a:223:TYR:CD2	2.88	0.42
1:a:288:LEU:C	1:a:288:LEU:CD2	2.86	0.42
16:a:404:CDL:H142	16:a:404:CDL:H112	1.69	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:66:GLN:OE1	5:e:387:GLU:OE1	2.37	0.42
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.89	0.42
2:B:128:MET:SD	2:B:198:LEU:HB2	2.60	0.42
4:D:75:ILE:HD11	4:D:223:HIS:O	2.19	0.42
2:b:106:LEU:HA	2:b:106:LEU:HD23	1.86	0.42
4:D:339:GLN:HB2	4:D:359:VAL:HG13	2.02	0.41
1:a:48:GLY:CA	1:a:83:HIS:CE1	3.03	0.41
13:a:403:PEE:H53	16:a:404:CDL:H552	2.01	0.41
3:c:112:GLY:CA	9:i:11:TYR:HB2	2.49	0.41
4:d:459:LEU:HD12	4:d:460:GLY:H	1.85	0.41
2:B:118:TYR:CD1	2:B:122:CYS:HB2	2.55	0.41
4:D:346:ILE:HD12	4:D:353:LEU:HD12	2.02	0.41
1:a:153:ILE:HG22	1:a:156:ILE:HG13	2.02	0.41
1:a:332:LEU:HD23	1:a:332:LEU:HA	1.89	0.41
9:i:25:ILE:HG13	9:i:26:ALA:H	1.83	0.41
11:k:52:ARG:NH2	11:k:55:LEU:HD11	2.34	0.41
1:A:141:TRP:CZ2	3:c:222:CYS:HA	2.55	0.41
1:A:221:HIS:HA	1:A:222:PRO:HA	1.75	0.41
2:B:123:SER:C	2:B:125:CYS:H	2.27	0.41
2:B:160:ASN:CG	2:B:161:GLU:H	2.29	0.41
2:B:229:ARG:HG2	2:B:230:GLU:N	2.34	0.41
8:H:9:THR:HG22	8:H:10:ARG:N	2.36	0.41
9:I:9:ARG:HH11	9:I:9:ARG:HG3	1.85	0.41
1:a:57:SER:HA	1:a:175:LEU:HD21	2.02	0.41
1:a:107:TYR:C	1:a:109:PHE:N	2.76	0.41
4:d:369:MET:HE2	4:d:369:MET:HB2	1.89	0.41
1:A:185:LEU:HD12	1:A:185:LEU:HA	1.83	0.41
3:C:191:GLU:OE1	3:C:193:SER:N	2.52	0.41
3:C:214:ILE:HG12	3:C:216:VAL:H	1.85	0.41
4:D:80:ARG:CZ	4:D:197:LEU:HD13	2.51	0.41
6:F:70:GLU:OE2	6:F:70:GLU:N	2.44	0.41
7:G:52:PRO:HD3	5:e:148:ARG:NH2	2.35	0.41
2:b:105:SER:HB2	9:i:48:ASN:ND2	2.36	0.41
3:c:101:LYS:HD3	3:c:101:LYS:HA	1.94	0.41
3:c:180:THR:O	3:c:184:ILE:HD12	2.21	0.41
3:c:200:HIS:CD2	3:c:202:LEU:H	2.39	0.41
8:h:74:ASN:N	8:h:75:PRO:HD2	2.35	0.41
1:A:40:CYS:HB3	1:A:90:PHE:HD1	1.85	0.41
3:C:93:ARG:CB	3:C:96:VAL:HG22	2.51	0.41
1:a:234:PHE:CD1	2:b:301:LEU:HD11	2.55	0.41
4:d:323:HIS:HE1	5:e:96:SER:O	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LEU:O	7:G:18:ARG:HG2	2.20	0.41
3:C:173:PRO:HD3	1:a:261:PRO:CB	2.48	0.41
4:D:344:PHE:CD1	4:D:344:PHE:C	2.99	0.41
5:E:108:GLY:C	5:E:109:LYS:CG	2.93	0.41
5:E:370:ASP:OD1	5:E:371:VAL:N	2.53	0.41
7:G:92:GLU:OE2	7:G:96:LYS:NZ	2.33	0.41
2:b:296:MET:HE1	3:c:128:ALA:CA	2.50	0.41
2:b:303:LEU:HD12	2:b:303:LEU:HA	1.85	0.41
2:b:303:LEU:HD23	3:c:121:THR:HA	2.01	0.41
1:A:168:PHE:HB2	3:c:170:ARG:C	2.46	0.41
1:A:350:ILE:HG12	1:A:351:GLY:N	2.36	0.41
3:C:212:ILE:HD11	3:C:263:TYR:HB3	2.01	0.41
5:E:68:GLY:O	5:E:208:TYR:OH	2.39	0.41
1:a:137:GLN:O	1:a:141:TRP:HD1	2.03	0.41
4:d:352:GLY:O	4:d:353:LEU:HG	2.20	0.41
5:e:245:GLY:O	5:e:246:LEU:HG	2.20	0.41
1:A:223:TYR:HE2	2:B:315:LEU:CG	2.33	0.41
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.87	0.41
1:A:352:GLN:O	1:A:352:GLN:HG2	2.21	0.41
12:A:402:HEM:HHA	12:A:402:HEM:HBA1	2.03	0.41
2:B:122:CYS:SG	14:B:401:HEC:CAB	3.09	0.41
3:c:99:SER:HA	4:d:269:ARG:CD	2.50	0.41
3:c:99:SER:C	4:d:269:ARG:HD2	2.46	0.41
1:A:132:VAL:O	1:A:132:VAL:CG1	2.69	0.41
2:B:132:ALA:H	2:B:135:HIS:CE1	2.38	0.41
2:B:178:LYS:NZ	2:B:180:TYR:O	2.34	0.41
2:B:264:MET:HA	2:B:267:VAL:HG22	2.03	0.41
3:C:93:ARG:C	3:C:96:VAL:HG22	2.46	0.41
4:D:70:THR:HG21	4:D:406:THR:O	2.21	0.41
5:E:42:ARG:HD3	5:E:47:LEU:O	2.20	0.41
5:E:45:ASN:HD21	5:E:238:LEU:CD2	2.33	0.41
1:a:8:HIS:O	1:a:12:LYS:HG3	2.21	0.41
1:a:17:ALA:O	1:a:21:LEU:HD23	2.20	0.41
1:a:272:TRP:CE2	1:a:273:TYR:HD2	2.38	0.41
2:b:142:THR:O	2:b:146:ALA:N	2.54	0.41
3:c:122:THR:HB	9:i:25:ILE:HB	2.01	0.41
4:d:92:PHE:CE1	4:d:168:ILE:HG13	2.56	0.41
4:d:323:HIS:O	4:d:323:HIS:CG	2.70	0.41
6:f:41:GLU:OE2	6:f:42:LYS:HG2	2.21	0.41
6:f:42:LYS:HB3	6:f:77:ALA:HB1	2.02	0.41
9:i:38:GLN:NE2	9:i:38:GLN:H	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:53:TRP:CD1	9:i:57:LYS:HB2	2.55	0.41
9:i:57:LYS:HG2	9:i:61:GLU:HB3	2.02	0.41
4:D:278:ARG:HB3	8:H:12:ARG:O	2.21	0.41
7:G:92:GLU:HB3	7:G:93:PRO:HD3	2.03	0.41
1:a:119:LEU:HD11	1:a:192:LEU:CB	2.37	0.41
1:a:275:LEU:HD23	1:a:339:GLY:C	2.43	0.41
2:b:318:ARG:HA	8:h:17:TYR:O	2.21	0.41
4:d:74:TRP:CZ3	4:d:232:ALA:HB3	2.56	0.41
10:j:26:ALA:O	10:j:30:VAL:HG23	2.21	0.41
1:A:8:HIS:O	1:A:12:LYS:HB2	2.21	0.40
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.82	0.40
1:A:89:MET:O	1:A:92:ILE:HG22	2.21	0.40
2:B:160:ASN:HB3	2:B:166:PHE:HE1	1.86	0.40
4:D:171:GLU:O	4:D:174:GLU:HG3	2.21	0.40
1:a:221:HIS:HB3	1:a:222:PRO:HD3	2.02	0.40
4:D:75:ILE:HG12	4:D:76:ASP:H	1.81	0.40
4:D:326:SER:HB2	4:D:329:ALA:HB2	1.95	0.40
1:a:295:VAL:O	1:a:295:VAL:HG12	2.21	0.40
1:a:326:TRP:CE2	8:h:49:VAL:HG22	2.56	0.40
12:a:402:HEM:HBD1	12:a:402:HEM:HHA	2.03	0.40
3:c:197:ASP:O	3:c:257:ASN:ND2	2.50	0.40
1:A:175:LEU:HD12	1:A:175:LEU:HA	1.83	0.40
4:D:180:ARG:O	4:D:180:ARG:HG2	2.21	0.40
6:F:30:LEU:O	6:F:34:ARG:HG3	2.21	0.40
3:c:172:LYS:HE2	3:c:216:VAL:CG2	2.51	0.40
7:g:95:LEU:C	7:g:97:GLU:H	2.29	0.40
1:A:144:THR:CG2	3:c:216:VAL:HG13	2.50	0.40
2:B:213:PHE:HB2	2:B:272:CYS:SG	2.61	0.40
5:E:246:LEU:N	5:E:246:LEU:HD12	2.36	0.40
5:E:261:GLN:O	5:E:261:GLN:HG3	2.22	0.40
6:F:48:GLU:O	6:F:51:GLU:HG3	2.22	0.40
11:K:50:LEU:HD23	11:K:50:LEU:O	2.21	0.40
1:a:132:VAL:O	1:a:132:VAL:HG12	2.21	0.40
2:b:187:ARG:O	2:b:192:GLY:N	2.50	0.40
2:b:307:MET:C	2:b:307:MET:SD	3.04	0.40
2:b:309:ARG:HH11	2:b:309:ARG:HG3	1.85	0.40
3:c:200:HIS:NE2	3:c:202:LEU:HD13	2.36	0.40
4:d:113:VAL:HG21	4:d:120:LEU:CD1	2.51	0.40
5:e:82:LEU:HD23	5:e:205:LEU:HD11	2.04	0.40
1:A:239:LEU:HA	1:A:239:LEU:HD12	1.87	0.40
3:C:213:LEU:HD21	3:C:260:VAL:HG22	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:ARG:HD2	8:H:44:ALA:N	2.33	0.40
1:a:18:PHE:O	1:a:220:PHE:HD1	2.05	0.40
1:a:282:ARG:HH22	1:a:343:VAL:HG21	1.86	0.40
3:c:132:ALA:O	3:c:136:PHE:HD2	2.05	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 PDB entries followed by that with respect to all EM entries.

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	376/379 (99%)	352 (94%)	22 (6%)	2 (0%)	24	51
1	a	376/379 (99%)	340 (90%)	32 (8%)	4 (1%)	11	33
2	B	239/326 (73%)	215 (90%)	20 (8%)	4 (2%)	7	23
2	b	237/326 (73%)	217 (92%)	20 (8%)	0	100	100
3	C	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
3	c	194/196 (99%)	177 (91%)	16 (8%)	1 (0%)	24	51
4	D	443/480 (92%)	424 (96%)	19 (4%)	0	100	100
4	d	444/480 (92%)	400 (90%)	42 (10%)	2 (0%)	24	51
5	E	416/453 (92%)	387 (93%)	28 (7%)	1 (0%)	43	70
5	e	416/453 (92%)	375 (90%)	40 (10%)	1 (0%)	43	70
6	F	62/91 (68%)	59 (95%)	3 (5%)	0	100	100
6	f	62/91 (68%)	59 (95%)	3 (5%)	0	100	100
7	G	104/111 (94%)	95 (91%)	9 (9%)	0	100	100
7	g	104/111 (94%)	90 (86%)	14 (14%)	0	100	100
8	H	69/82 (84%)	56 (81%)	11 (16%)	2 (3%)	3	13
8	h	77/82 (94%)	64 (83%)	13 (17%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	60/64 (94%)	49 (82%)	11 (18%)	0	100	100
9	i	60/64 (94%)	57 (95%)	3 (5%)	0	100	100
10	J	47/56 (84%)	47 (100%)	0	0	100	100
10	j	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
11	K	55/78 (70%)	33 (60%)	22 (40%)	0	100	100
11	k	55/78 (70%)	34 (62%)	21 (38%)	0	100	100
All	All	4137/4632 (89%)	3763 (91%)	357 (9%)	17 (0%)	31	56

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	302	PRO
1	a	221	HIS
3	c	83	ILE
4	d	66	GLN
4	d	67	PRO
2	B	322	TYR
8	H	41	ARG
1	a	286	ASN
5	e	241	ARG
1	A	286	ASN
2	B	124	SER
5	E	439	ALA
8	H	46	ILE
1	A	314	SER
1	a	314	SER
1	a	304	MET
2	B	301	LEU

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 PDB entries followed by that with respect to all EM entries.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/332 (100%)	299 (90%)	32 (10%)	8	23
1	a	331/332 (100%)	305 (92%)	26 (8%)	11	32
2	B	206/259 (80%)	193 (94%)	13 (6%)	16	42
2	b	204/259 (79%)	199 (98%)	5 (2%)	42	72
3	C	164/166 (99%)	161 (98%)	3 (2%)	51	78
3	c	165/166 (99%)	158 (96%)	7 (4%)	26	58
4	D	371/397 (94%)	356 (96%)	15 (4%)	28	60
4	d	372/397 (94%)	362 (97%)	10 (3%)	39	70
5	E	327/354 (92%)	316 (97%)	11 (3%)	32	64
5	e	327/354 (92%)	320 (98%)	7 (2%)	47	75
6	F	61/85 (72%)	61 (100%)	0	100	100
6	f	61/85 (72%)	61 (100%)	0	100	100
7	G	95/99 (96%)	94 (99%)	1 (1%)	65	86
7	g	95/99 (96%)	91 (96%)	4 (4%)	26	58
8	H	65/73 (89%)	58 (89%)	7 (11%)	6	19
8	h	70/73 (96%)	70 (100%)	0	100	100
9	I	50/52 (96%)	50 (100%)	0	100	100
9	i	50/52 (96%)	44 (88%)	6 (12%)	5	14
10	J	40/46 (87%)	40 (100%)	0	100	100
10	j	41/46 (89%)	41 (100%)	0	100	100
11	K	44/59 (75%)	44 (100%)	0	100	100
11	k	44/59 (75%)	44 (100%)	0	100	100
All	All	3514/3844 (91%)	3367 (96%)	147 (4%)	28	58

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	28	SER
1	A	32	ASN
1	A	40	CYS
1	A	42	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	47	THR
1	A	49	LEU
1	A	70	CYS
1	A	71	ARG
1	A	102	LEU
1	A	111	GLU
1	A	129	MET
1	A	138	MET
1	A	139	SER
1	A	141	TRP
1	A	144	THR
1	A	185	LEU
1	A	230	LEU
1	A	297	SER
1	A	300	ILE
1	A	302	ILE
1	A	304	MET
1	A	307	LEU
1	A	309	THR
1	A	327	MET
1	A	348	ILE
1	A	349	ILE
1	A	350	ILE
1	A	352	GLN
1	A	353	LEU
1	A	355	SER
1	A	357	LEU
2	B	87	ASP
2	B	102	LEU
2	B	140	CYS
2	B	155	VAL
2	B	173	SER
2	B	174	ASP
2	B	217	THR
2	B	280	GLU
2	B	299	LEU
2	B	309	ARG
2	B	310	HIS
2	B	311	LYS
2	B	313	SER
3	C	95	GLU
3	C	96	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	154	ILE
4	D	61	SER
4	D	63	GLN
4	D	75	ILE
4	D	76	ASP
4	D	126	ARG
4	D	279	ASP
4	D	323	HIS
4	D	325	SER
4	D	328	LEU
4	D	336	LYS
4	D	350	GLU
4	D	351	THR
4	D	406	THR
4	D	407	THR
4	D	416	SER
5	E	109	LYS
5	E	110	LEU
5	E	116	ARG
5	E	118	SER
5	E	186	LEU
5	E	261	GLN
5	E	324	SER
5	E	338	ILE
5	E	387	GLU
5	E	388	SER
5	E	438	MET
7	G	76	LEU
8	H	38	VAL
8	H	39	LEU
8	H	40	ARG
8	H	41	ARG
8	H	42	THR
8	H	43	ARG
8	H	46	ILE
1	a	25	SER
1	a	26	ASN
1	a	40	CYS
1	a	71	ARG
1	a	94	LEU
1	a	121	PHE
1	a	175	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	182	HIS
1	a	186	PRO
1	a	192	LEU
1	a	195	VAL
1	a	201	HIS
1	a	226	ILE
1	a	233	LEU
1	a	275	LEU
1	a	276	PHE
1	a	287	LYS
1	a	288	LEU
1	a	297	SER
1	a	302	ILE
1	a	306	MET
1	a	315	MET
1	a	348	ILE
1	a	350	ILE
1	a	356	ILE
1	a	357	LEU
2	b	129	ASP
2	b	296	MET
2	b	297	MET
2	b	307	MET
2	b	309	ARG
3	c	81	THR
3	c	82	ASP
3	c	122	THR
3	c	147	LEU
3	c	154	ILE
3	c	156	LEU
3	c	157	SER
4	d	63	GLN
4	d	64	SER
4	d	65	SER
4	d	126	ARG
4	d	268	CYS
4	d	269	ARG
4	d	322	THR
4	d	324	MET
4	d	406	THR
4	d	407	THR
5	e	241	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	e	244	LEU
5	e	257	GLU
5	e	260	ASP
5	e	275	SER
5	e	438	MET
5	e	441	SER
7	g	103	LYS
7	g	104	GLU
7	g	107	GLU
7	g	111	LYS
9	i	20	THR
9	i	23	LEU
9	i	24	THR
9	i	30	LEU
9	i	32	PHE
9	i	33	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	ASN
1	A	44	GLN
1	A	68	HIS
1	A	97	HIS
1	A	137	GLN
1	A	221	HIS
1	A	341	GLN
2	B	116	GLN
2	B	182	ASN
2	B	190	ASN
2	B	241	GLN
2	B	266	GLN
3	C	131	ASN
3	C	186	GLN
4	D	308	ASN
4	D	345	ASN
4	D	464	GLN
5	E	232	GLN
5	E	319	GLN
9	I	55	HIS
1	a	83	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	221	HIS
2	b	116	GLN
2	b	266	GLN
3	c	200	HIS
3	c	239	HIS
4	d	40	GLN
4	d	63	GLN
4	d	160	GLN
4	d	223	HIS
4	d	239	HIS
4	d	286	HIS
4	d	469	ASN
5	e	155	GLN
5	e	170	GLN
5	e	284	ASN
6	f	55	GLN
9	i	38	GLN
9	i	55	HIS

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](#)

13 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	$\# Z > 2$
14	HEC	b	401	2	50,50,50	1.77	6 (12%)	68,82,82	1.31	5 (7%)
16	CDL	a	404	-	63,63,99	1.10	8 (12%)	69,75,111	1.12	4 (5%)
15	FES	c	301	-	0,4,4	-	-	-	-	-
16	CDL	D	501	-	63,63,99	1.08	8 (12%)	69,75,111	1.20	4 (5%)
14	HEC	B	401	2	50,50,50	1.64	3 (6%)	68,82,82	1.54	10 (14%)
13	PEE	D	502	-	48,48,50	1.58	8 (16%)	51,53,55	1.20	3 (5%)
13	PEE	A	403	-	44,44,50	1.56	7 (15%)	46,49,55	1.25	3 (6%)
12	HEM	a	402	1	50,50,50	1.51	8 (16%)	66,82,82	1.40	13 (19%)
12	HEM	A	401	1	50,50,50	1.47	8 (16%)	66,82,82	1.82	21 (31%)
12	HEM	A	402	1	50,50,50	1.41	7 (14%)	66,82,82	1.76	19 (28%)
12	HEM	a	401	1	50,50,50	1.33	5 (10%)	66,82,82	1.27	6 (9%)
13	PEE	a	403	-	48,48,50	1.53	5 (10%)	51,53,55	1.16	3 (5%)
15	FES	C	301	3	0,4,4	-	-	-	-	-

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
14	HEC	b	401	2	-	3/14/54/54	-
16	CDL	a	404	-	-	38/74/74/110	-
15	FES	c	301	-	-	-	0/1/1/1
16	CDL	D	501	-	-	36/74/74/110	-
14	HEC	B	401	2	-	5/14/54/54	-
13	PEE	D	502	-	-	17/52/52/54	-
13	PEE	A	403	-	-	24/48/48/54	-
12	HEM	a	402	1	-	4/14/54/54	-
12	HEM	A	401	1	-	8/14/54/54	-
12	HEM	A	402	1	-	9/14/54/54	-
12	HEM	a	401	1	-	4/14/54/54	-
13	PEE	a	403	-	-	23/52/52/54	-
15	FES	C	301	3	-	-	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	401	HEC	C3D-C2D	8.38	1.54	1.36
14	b	401	HEC	C3D-C2D	7.69	1.53	1.36
12	a	402	HEM	FE-NC	4.72	2.11	1.95
13	a	403	PEE	C18-C19	4.47	1.57	1.31
13	D	502	PEE	C18-C19	4.43	1.57	1.31
13	A	403	PEE	C18-C19	4.42	1.57	1.31
14	b	401	HEC	FE-ND	4.25	2.08	1.94
12	a	401	HEM	FE-NB	4.10	2.07	1.94
12	A	401	HEM	FE-ND	4.09	2.07	1.94
13	D	502	PEE	C39-C38	4.09	1.55	1.31
13	a	403	PEE	C39-C38	4.05	1.55	1.31
13	A	403	PEE	C39-C38	4.01	1.55	1.31
14	b	401	HEC	FE-NC	3.89	2.08	1.95
12	A	401	HEM	FE-NC	3.85	2.08	1.95
12	A	402	HEM	FE-NB	3.84	2.06	1.94
14	b	401	HEC	FE-NB	3.80	2.06	1.94
13	D	502	PEE	O3-C30	3.73	1.44	1.33
13	a	403	PEE	O3-C30	3.60	1.43	1.33
12	a	402	HEM	FE-NB	3.44	2.05	1.94
13	A	403	PEE	O3-C30	3.41	1.43	1.33
13	D	502	PEE	O2-C10	3.33	1.43	1.34
13	A	403	PEE	O2-C10	3.18	1.43	1.34
13	a	403	PEE	O2-C10	3.06	1.42	1.34
12	A	401	HEM	CAB-C3B	2.95	1.55	1.47
12	A	402	HEM	CAB-C3B	2.89	1.55	1.47
12	a	402	HEM	CAB-C3B	2.87	1.55	1.47
12	a	401	HEM	CAB-C3B	2.85	1.55	1.47
12	A	402	HEM	FE-ND	2.84	2.03	1.94
12	a	402	HEM	FE-ND	2.75	2.03	1.94
12	a	401	HEM	FE-ND	2.73	2.03	1.94
16	D	501	CDL	OA6-CA4	-2.70	1.39	1.46
12	A	402	HEM	CAC-C3C	2.66	1.54	1.47
14	B	401	HEC	FE-NB	2.63	2.03	1.94
12	A	401	HEM	C3C-C2C	-2.56	1.32	1.37
14	B	401	HEC	FE-ND	2.55	2.02	1.94
12	a	401	HEM	CAC-C3C	2.54	1.54	1.47
16	a	404	CDL	OB6-CB4	-2.53	1.40	1.46
12	A	401	HEM	C2A-C3A	-2.53	1.32	1.38
12	A	402	HEM	FE-NC	2.49	2.03	1.95
13	A	403	PEE	O2-C2	-2.48	1.40	1.46
16	D	501	CDL	OB6-CB4	-2.47	1.40	1.46
12	A	402	HEM	FE-NA	2.44	2.03	1.95
12	A	402	HEM	C3C-C2C	-2.43	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	402	HEM	C3C-C2C	-2.41	1.32	1.37
12	a	401	HEM	FE-NA	2.40	2.03	1.95
13	a	403	PEE	O2-C2	-2.40	1.40	1.46
13	D	502	PEE	C11-C10	2.38	1.57	1.50
16	D	501	CDL	OB8-CB7	2.37	1.40	1.33
16	D	501	CDL	OA8-CA7	2.36	1.40	1.33
12	a	402	HEM	C2A-C3A	-2.36	1.32	1.38
12	A	401	HEM	FE-NA	2.35	2.03	1.95
16	a	404	CDL	OA6-CA4	-2.35	1.40	1.46
16	a	404	CDL	OB6-CB5	2.34	1.40	1.34
16	a	404	CDL	OA6-CA5	2.32	1.40	1.34
12	A	401	HEM	FE-NB	2.31	2.02	1.94
16	a	404	CDL	OB8-CB7	2.29	1.40	1.33
16	a	404	CDL	OA8-CA7	2.29	1.40	1.33
16	a	404	CDL	OB8-CB6	-2.29	1.39	1.45
13	D	502	PEE	O2-C2	-2.26	1.41	1.46
13	D	502	PEE	P-O3P	2.23	1.68	1.59
12	a	402	HEM	C3D-C2D	-2.21	1.32	1.36
16	D	501	CDL	OB6-CB5	2.17	1.40	1.34
12	A	401	HEM	CAC-C3C	2.15	1.53	1.47
16	D	501	CDL	OA6-CA5	2.12	1.40	1.34
16	a	404	CDL	OA8-CA6	-2.12	1.40	1.45
16	D	501	CDL	OB8-CB6	-2.12	1.40	1.45
13	D	502	PEE	P-O4P	2.11	1.67	1.59
16	D	501	CDL	OA8-CA6	-2.11	1.40	1.45
12	a	402	HEM	CMA-C3A	2.06	1.55	1.50
13	A	403	PEE	P-O3P	2.06	1.67	1.59
14	b	401	HEC	CMC-C2C	2.02	1.55	1.50
13	A	403	PEE	C11-C10	2.01	1.56	1.50
14	b	401	HEC	CMB-C2B	2.00	1.55	1.50

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	401	HEC	C1D-ND-C4D	5.96	111.23	105.07
14	b	401	HEC	C1D-ND-C4D	5.73	110.99	105.07
12	A	402	HEM	CAD-C3D-C4D	5.12	133.60	124.66
12	A	402	HEM	CAD-C3D-C2D	-4.73	119.07	127.88
12	A	401	HEM	C4D-ND-C1D	4.33	109.55	105.07
13	D	502	PEE	O2-C10-C11	4.27	120.70	111.50
16	D	501	CDL	OB6-CB5-C51	4.18	120.52	111.50
16	D	501	CDL	OA6-CA5-C11	4.18	120.52	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	404	CDL	OA6-CA5-C11	4.08	120.30	111.50
12	A	401	HEM	CAA-C2A-C1A	3.86	132.48	124.89
14	B	401	HEC	C4A-CHB-C1B	-3.74	117.99	126.06
13	a	403	PEE	O2-C10-C11	3.67	119.40	111.50
16	a	404	CDL	OB6-CB5-C51	3.66	119.39	111.50
14	B	401	HEC	C4C-NC-C1C	3.65	108.92	105.35
12	A	401	HEM	CAD-C3D-C2D	-3.57	121.23	127.88
12	a	402	HEM	C4C-NC-C1C	3.56	108.84	105.35
13	A	403	PEE	O2-C10-C11	3.49	119.02	111.50
12	A	401	HEM	C3D-C4D-ND	-3.46	106.31	110.17
12	A	402	HEM	CAD-CBD-CGD	-3.32	106.45	113.60
12	A	401	HEM	CAD-C3D-C4D	3.31	130.44	124.66
12	a	401	HEM	CHC-C1C-NC	3.30	128.00	124.44
12	A	402	HEM	C4A-NA-C1A	3.27	108.55	105.35
12	A	401	HEM	CAA-C2A-C3A	-3.18	119.79	127.07
12	A	402	HEM	C4D-ND-C1D	3.13	108.31	105.07
12	A	401	HEM	C4C-NC-C1C	3.07	108.35	105.35
13	A	403	PEE	O3-C30-C31	3.05	121.49	111.91
12	A	401	HEM	C2A-C1A-NA	-2.99	106.80	110.15
16	D	501	CDL	OA8-CA7-C31	2.99	121.30	111.91
13	a	403	PEE	O3-C30-C31	2.97	121.24	111.91
12	A	401	HEM	C2D-C1D-ND	-2.96	106.33	109.88
12	A	401	HEM	CAC-C3C-C4C	2.96	132.05	124.90
16	a	404	CDL	OB8-CB7-C71	2.93	121.11	111.91
12	a	402	HEM	C4D-ND-C1D	2.92	108.09	105.07
12	A	402	HEM	CHD-C1D-ND	2.87	127.54	124.42
12	a	402	HEM	CHC-C1C-NC	2.85	127.52	124.44
12	a	402	HEM	C2D-C1D-ND	-2.80	106.53	109.88
12	A	402	HEM	C2A-C1A-NA	-2.77	107.06	110.15
12	a	401	HEM	C4A-NA-C1A	2.75	108.04	105.35
12	A	401	HEM	CAC-C3C-C2C	-2.74	119.58	128.60
14	B	401	HEC	CAD-CBD-CGD	-2.71	107.77	113.60
12	A	401	HEM	C4A-NA-C1A	2.69	107.98	105.35
12	a	401	HEM	C4D-ND-C1D	2.69	107.85	105.07
16	D	501	CDL	OB8-CB7-C71	2.68	120.33	111.91
12	A	401	HEM	CHD-C1D-ND	2.67	127.32	124.42
14	b	401	HEC	CAA-CBA-CGA	-2.66	107.87	113.60
12	A	402	HEM	C4C-NC-C1C	2.66	107.95	105.35
14	B	401	HEC	C4B-NB-C1B	2.64	107.80	105.07
12	A	401	HEM	CHD-C4C-C3C	2.62	129.75	125.26
13	D	502	PEE	O3-C30-C31	2.61	120.09	111.91
12	A	402	HEM	C1B-NB-C4B	2.60	107.75	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	401	HEC	C4C-NC-C1C	2.58	107.88	105.35
14	b	401	HEC	CAD-CBD-CGD	-2.58	108.06	113.60
16	a	404	CDL	OA8-CA7-C31	2.54	119.87	111.91
14	B	401	HEC	CAA-CBA-CGA	-2.53	108.15	113.60
12	A	401	HEM	CHC-C1C-NC	2.51	127.16	124.44
12	A	401	HEM	C1D-C2D-C3D	2.40	109.48	106.96
12	a	402	HEM	C4C-C3C-C2C	2.35	108.69	106.75
12	a	401	HEM	C2A-C1A-NA	-2.35	107.52	110.15
12	A	401	HEM	O2D-CGD-CBD	2.33	121.51	114.03
12	A	402	HEM	C3D-C4D-ND	-2.33	107.58	110.17
12	a	402	HEM	C1D-C2D-C3D	2.30	109.38	106.96
14	B	401	HEC	C4A-NA-C1A	2.28	107.58	105.35
12	A	402	HEM	CAC-C3C-C4C	2.27	130.39	124.90
14	B	401	HEC	C2A-C1A-NA	-2.27	108.11	110.32
14	B	401	HEC	C3C-C4C-NC	-2.27	107.61	110.15
12	A	402	HEM	C1D-C2D-C3D	2.25	109.33	106.96
12	a	402	HEM	CMB-C2B-C1B	-2.25	121.61	125.04
14	b	401	HEC	C3C-C4C-NC	-2.25	107.63	110.15
12	A	401	HEM	CAA-CBA-CGA	-2.18	108.91	113.60
12	A	401	HEM	CHA-C1A-C2A	2.14	130.03	125.36
12	a	402	HEM	CAC-C3C-C2C	-2.14	121.57	128.60
12	a	402	HEM	CHD-C4C-C3C	2.13	128.89	125.26
12	a	401	HEM	CAA-CBA-CGA	-2.12	109.04	113.60
12	A	402	HEM	CHC-C1C-NC	2.12	126.73	124.44
12	a	402	HEM	CHD-C1D-C2D	2.12	128.29	124.98
12	A	402	HEM	CAA-C2A-C1A	2.12	129.06	124.89
12	A	402	HEM	C3C-C2C-C1C	2.10	109.08	107.08
12	A	401	HEM	O1D-CGD-CBD	-2.10	116.34	123.08
12	a	401	HEM	C3B-C2B-C1B	2.10	108.04	106.49
14	B	401	HEC	C3B-C4B-NB	-2.10	107.83	110.17
12	A	402	HEM	CHA-C4D-C3D	2.09	129.25	125.33
12	A	402	HEM	C3B-C2B-C1B	2.06	108.02	106.49
13	D	502	PEE	C17-C18-C19	-2.06	108.93	124.73
13	A	403	PEE	C3-C2-C1	-2.05	106.93	111.79
12	a	402	HEM	CAA-CBA-CGA	-2.05	109.20	113.60
12	A	402	HEM	CAC-C3C-C2C	-2.04	121.88	128.60
12	A	402	HEM	C2D-C1D-ND	-2.03	107.45	109.88
12	a	402	HEM	CMD-C2D-C1D	2.02	128.11	125.04
12	a	402	HEM	CAC-C3C-C4C	2.01	129.74	124.90
13	a	403	PEE	C17-C18-C19	-2.01	109.34	124.73
12	A	401	HEM	C3C-C2C-C1C	2.00	108.99	107.08

There are no chirality outliers.

All (171) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	402	HEM	C1A-C2A-CAA-CBA
12	A	402	HEM	C2D-C3D-CAD-CBD
12	A	402	HEM	C4D-C3D-CAD-CBD
12	a	401	HEM	C1A-C2A-CAA-CBA
12	a	401	HEM	C3D-CAD-CBD-CGD
13	A	403	PEE	C17-C18-C19-C20
13	A	403	PEE	C1-O3P-P-O2P
13	A	403	PEE	C1-O3P-P-O1P
13	A	403	PEE	C4-O4P-P-O1P
13	A	403	PEE	O4P-C4-C5-N
13	A	403	PEE	C38-C39-C40-C41
13	D	502	PEE	C37-C38-C39-C40
13	a	403	PEE	C4-O4P-P-O3P
13	a	403	PEE	C4-O4P-P-O2P
13	a	403	PEE	C4-O4P-P-O1P
14	B	401	HEC	C2D-C3D-CAD-CBD
14	B	401	HEC	C4D-C3D-CAD-CBD
16	D	501	CDL	CA2-C1-CB2-OB2
16	D	501	CDL	OA6-CA4-CA6-OA8
16	D	501	CDL	C11-CA5-OA6-CA4
16	D	501	CDL	CB2-OB2-PB2-OB3
16	D	501	CDL	CB2-OB2-PB2-OB4
16	D	501	CDL	CB2-OB2-PB2-OB5
16	D	501	CDL	CB3-OB5-PB2-OB3
16	D	501	CDL	CB3-OB5-PB2-OB4
16	D	501	CDL	OB5-CB3-CB4-OB6
16	a	404	CDL	CB2-C1-CA2-OA2
16	a	404	CDL	C11-CA5-OA6-CA4
16	a	404	CDL	CB2-OB2-PB2-OB3
13	A	403	PEE	O5-C30-O3-C3
16	D	501	CDL	OA7-CA5-OA6-CA4
16	a	404	CDL	OA7-CA5-OA6-CA4
13	A	403	PEE	C31-C30-O3-C3
16	D	501	CDL	C31-CA7-OA8-CA6
16	D	501	CDL	C71-CB7-OB8-CB6
12	A	401	HEM	C4D-C3D-CAD-CBD
16	D	501	CDL	OA9-CA7-OA8-CA6
16	D	501	CDL	OB9-CB7-OB8-CB6
16	D	501	CDL	O1-C1-CB2-OB2
16	a	404	CDL	O1-C1-CA2-OA2
12	A	401	HEM	C1A-C2A-CAA-CBA
12	A	402	HEM	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	A	401	HEM	C3A-C2A-CAA-CBA
12	A	402	HEM	C3A-C2A-CAA-CBA
16	a	404	CDL	C31-CA7-OA8-CA6
16	a	404	CDL	C71-CB7-OB8-CB6
16	D	501	CDL	CB7-C71-C72-C73
13	a	403	PEE	C30-C31-C32-C33
16	D	501	CDL	CB5-C51-C52-C53
16	a	404	CDL	OA9-CA7-OA8-CA6
12	A	401	HEM	C2D-C3D-CAD-CBD
13	A	403	PEE	C1-O3P-P-O4P
13	D	502	PEE	C1-O3P-P-O4P
16	D	501	CDL	CB3-OB5-PB2-OB2
16	a	404	CDL	CA3-OA5-PA1-OA2
13	D	502	PEE	C10-C11-C12-C13
16	D	501	CDL	C32-C33-C34-C35
13	D	502	PEE	C21-C22-C23-C24
13	D	502	PEE	C40-C41-C42-C43
16	D	501	CDL	C74-C75-C76-C77
13	D	502	PEE	C11-C12-C13-C14
13	a	403	PEE	C37-C38-C39-C40
13	A	403	PEE	C12-C13-C14-C15
13	a	403	PEE	C33-C34-C35-C36
16	a	404	CDL	OB9-CB7-OB8-CB6
16	a	404	CDL	C14-C15-C16-C17
13	a	403	PEE	C34-C35-C36-C37
13	A	403	PEE	C14-C15-C16-C17
13	D	502	PEE	C34-C35-C36-C37
13	D	502	PEE	C31-C32-C33-C34
16	a	404	CDL	C74-C75-C76-C77
13	D	502	PEE	C22-C23-C24-C25
12	a	401	HEM	C3A-C2A-CAA-CBA
13	A	403	PEE	C19-C20-C21-C22
13	D	502	PEE	C23-C24-C25-C26
16	a	404	CDL	C54-C55-C56-C57
12	A	402	HEM	C3D-CAD-CBD-CGD
16	D	501	CDL	C11-C12-C13-C14
13	a	403	PEE	C39-C40-C41-C42
13	a	403	PEE	C22-C23-C24-C25
16	a	404	CDL	C72-C73-C74-C75
16	a	404	CDL	C51-C52-C53-C54
16	a	404	CDL	C32-C33-C34-C35
16	a	404	CDL	C52-C53-C54-C55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	D	502	PEE	C15-C16-C17-C18
12	a	402	HEM	C4D-C3D-CAD-CBD
16	D	501	CDL	C71-C72-C73-C74
13	A	403	PEE	C30-C31-C32-C33
16	D	501	CDL	OB5-CB3-CB4-CB6
13	a	403	PEE	C11-C12-C13-C14
16	D	501	CDL	C73-C74-C75-C76
13	D	502	PEE	C13-C14-C15-C16
13	a	403	PEE	C1-C2-C3-O3
16	D	501	CDL	C13-C14-C15-C16
13	a	403	PEE	C35-C36-C37-C38
16	D	501	CDL	C51-C52-C53-C54
13	A	403	PEE	C23-C24-C25-C26
12	a	402	HEM	C2D-C3D-CAD-CBD
16	a	404	CDL	O1-C1-CB2-OB2
16	D	501	CDL	C12-C13-C14-C15
16	a	404	CDL	C12-C13-C14-C15
16	a	404	CDL	C75-C76-C77-C78
13	A	403	PEE	C4-O4P-P-O3P
13	D	502	PEE	C32-C33-C34-C35
13	A	403	PEE	O2-C2-C3-O3
13	D	502	PEE	C42-C43-C44-C45
12	A	401	HEM	C3D-CAD-CBD-CGD
16	a	404	CDL	OB5-CB3-CB4-CB6
13	D	502	PEE	C39-C40-C41-C42
13	a	403	PEE	C32-C33-C34-C35
13	a	403	PEE	C42-C43-C44-C45
13	A	403	PEE	C1-C2-C3-O3
16	D	501	CDL	CA3-CA4-CA6-OA8
16	a	404	CDL	OB5-CB3-CB4-OB6
12	A	401	HEM	C4C-C3C-CAC-CBC
12	A	402	HEM	C4C-C3C-CAC-CBC
13	a	403	PEE	C41-C42-C43-C44
13	A	403	PEE	C15-C16-C17-C18
13	A	403	PEE	C2-C3-O3-C30
13	a	403	PEE	C13-C14-C15-C16
16	D	501	CDL	CB4-CB3-OB5-PB2
13	A	403	PEE	C4-O4P-P-O2P
13	D	502	PEE	C1-O3P-P-O2P
16	a	404	CDL	CA3-OA5-PA1-OA3
16	a	404	CDL	CA3-OA5-PA1-OA4
16	a	404	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	a	404	CDL	CA5-C11-C12-C13
14	B	401	HEC	C2B-C3B-CAB-CBB
13	a	403	PEE	C5-C4-O4P-P
16	a	404	CDL	OA5-CA3-CA4-OA6
13	a	403	PEE	C40-C41-C42-C43
13	a	403	PEE	O2-C2-C3-O3
13	A	403	PEE	C31-C32-C33-C34
16	D	501	CDL	C75-C76-C77-C78
16	a	404	CDL	OA5-CA3-CA4-CA6
16	a	404	CDL	C31-C32-C33-C34
16	D	501	CDL	CA2-OA2-PA1-OA5
16	D	501	CDL	CA3-OA5-PA1-OA2
16	a	404	CDL	CA2-OA2-PA1-OA5
16	a	404	CDL	CB2-OB2-PB2-OB5
12	a	402	HEM	CAD-CBD-CGD-O2D
16	a	404	CDL	OB6-CB4-CB6-OB8
16	D	501	CDL	C15-C16-C17-C18
16	a	404	CDL	CA2-C1-CB2-OB2
14	B	401	HEC	C4B-C3B-CAB-CBB
12	A	401	HEM	CAD-CBD-CGD-O1D
12	a	402	HEM	CAD-CBD-CGD-O1D
16	a	404	CDL	C71-C72-C73-C74
14	B	401	HEC	C2C-C3C-CAC-CBC
13	D	502	PEE	C38-C39-C40-C41
13	a	403	PEE	C14-C15-C16-C17
13	a	403	PEE	C38-C39-C40-C41
13	A	403	PEE	C22-C23-C24-C25
14	b	401	HEC	CAD-CBD-CGD-O2D
13	A	403	PEE	C36-C37-C38-C39
13	a	403	PEE	C18-C19-C20-C21
12	A	401	HEM	CAD-CBD-CGD-O2D
13	a	403	PEE	C36-C37-C38-C39
14	b	401	HEC	CAD-CBD-CGD-O1D
16	D	501	CDL	C54-C55-C56-C57
16	D	501	CDL	OB6-CB4-CB6-OB8
16	D	501	CDL	CB3-CB4-CB6-OB8
16	a	404	CDL	CB3-OB5-PB2-OB2
14	b	401	HEC	CAA-CBA-CGA-O2A
16	a	404	CDL	CA2-OA2-PA1-OA3
16	a	404	CDL	C11-C12-C13-C14
12	a	401	HEM	CAD-CBD-CGD-O2D
12	A	402	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	a	404	CDL	C12-C11-CA5-OA6
13	A	403	PEE	C18-C19-C20-C21
12	A	402	HEM	CAD-CBD-CGD-O2D

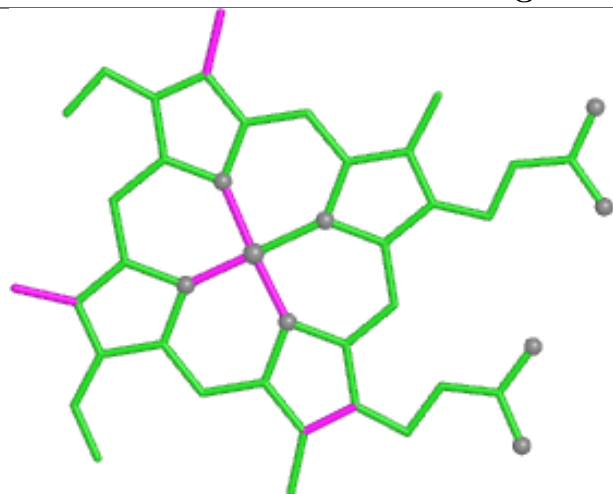
There are no ring outliers.

13 monomers are involved in 48 short contacts:

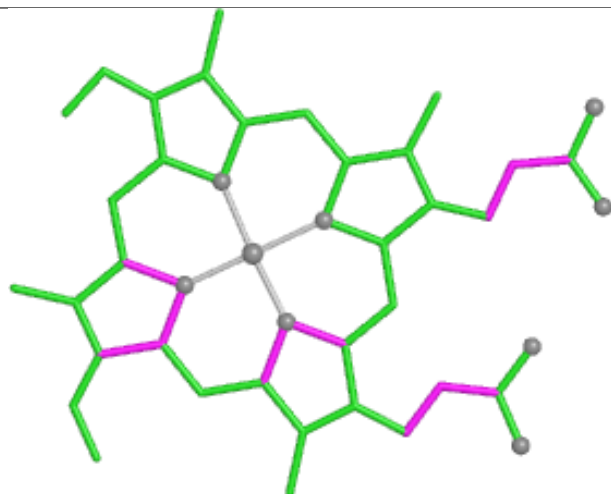
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	401	HEC	7	0
16	a	404	CDL	4	0
15	c	301	FES	5	0
16	D	501	CDL	3	0
14	B	401	HEC	3	0
13	D	502	PEE	1	0
13	A	403	PEE	2	0
12	a	402	HEM	5	0
12	A	401	HEM	3	0
12	A	402	HEM	5	0
12	a	401	HEM	7	0
13	a	403	PEE	3	0
15	C	301	FES	2	0

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.

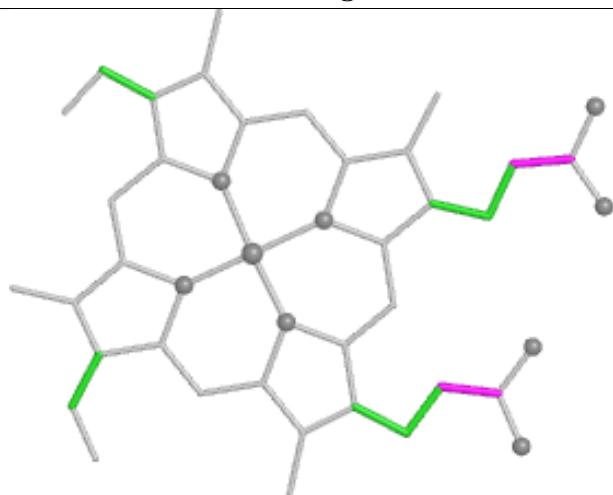
Ligand HEC b 401



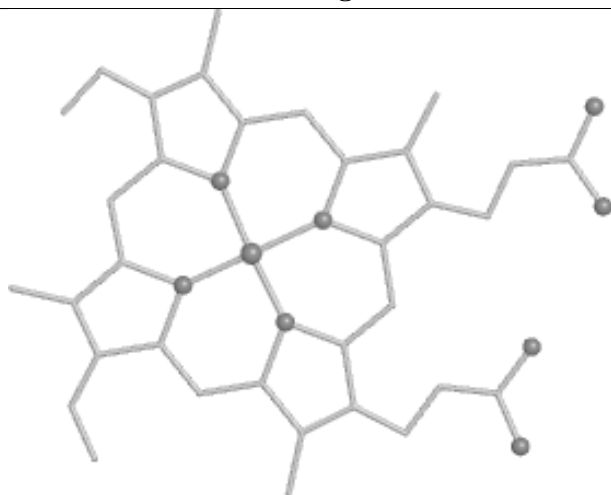
Bond lengths



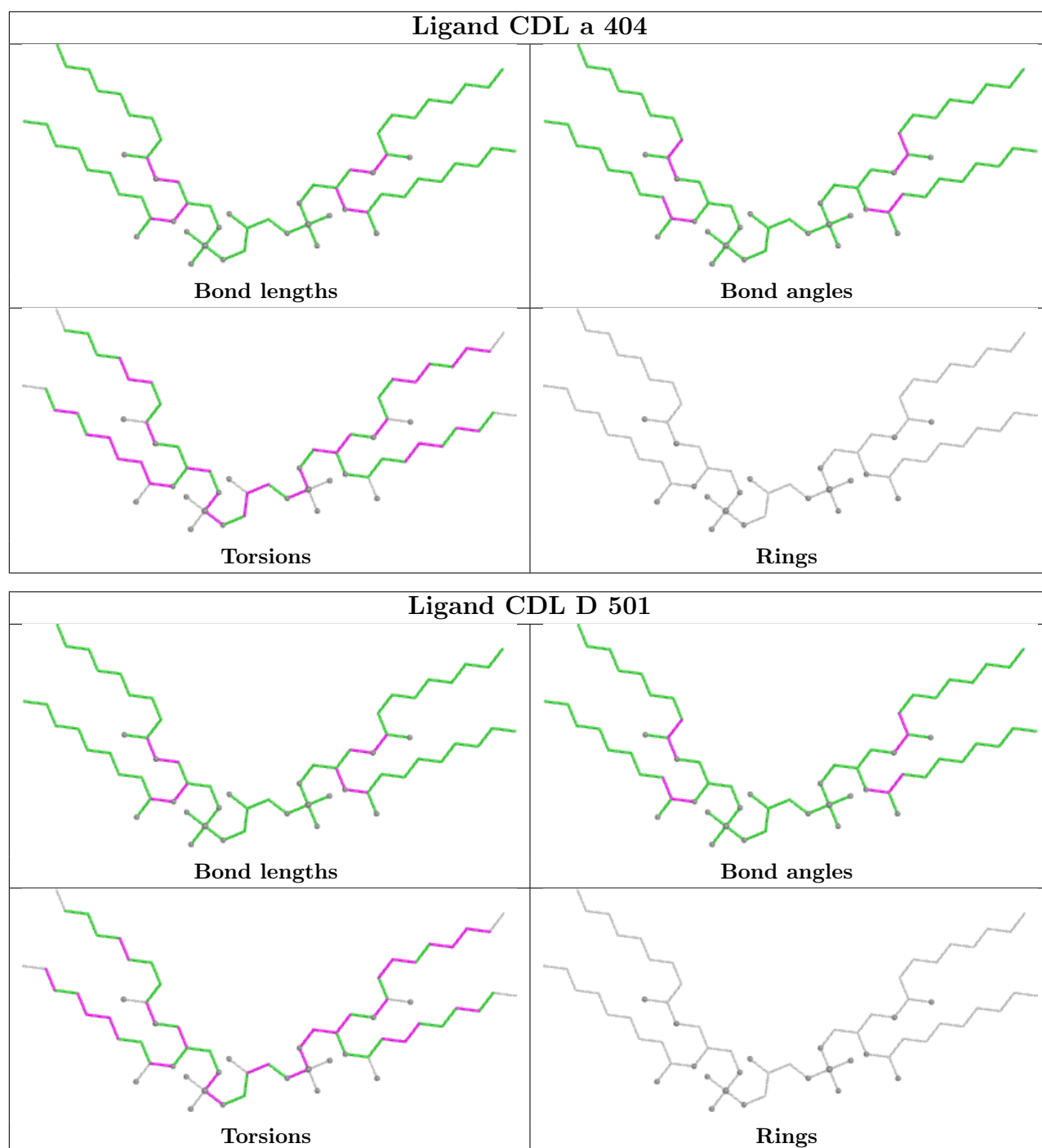
Bond angles



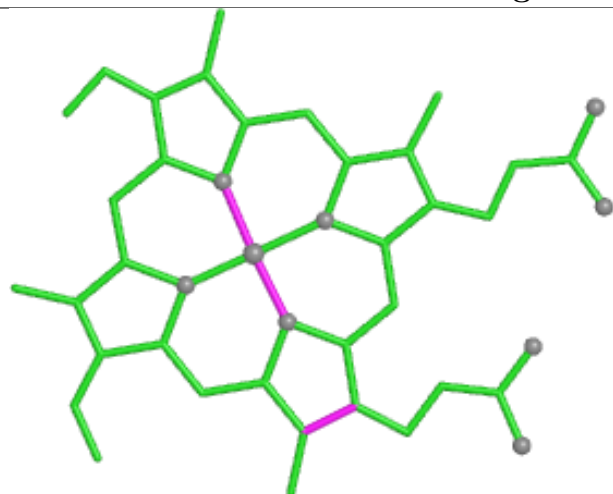
Torsions



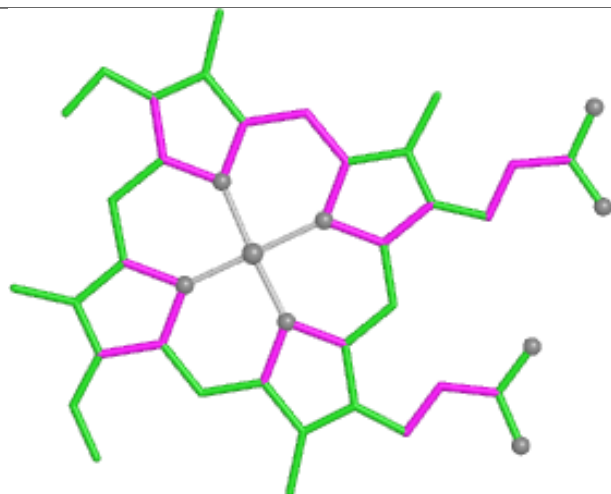
Rings



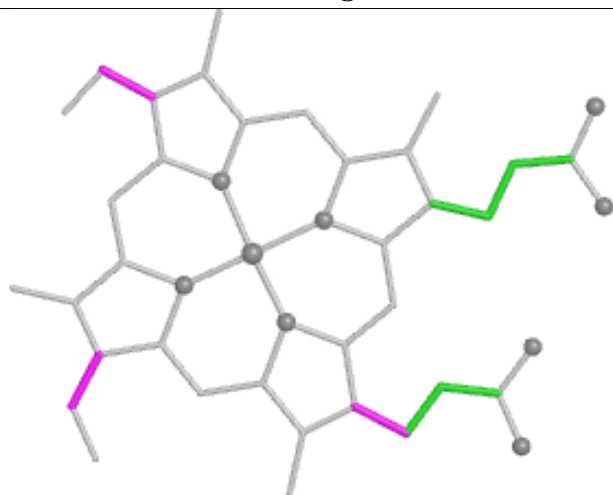
Ligand HEC B 401



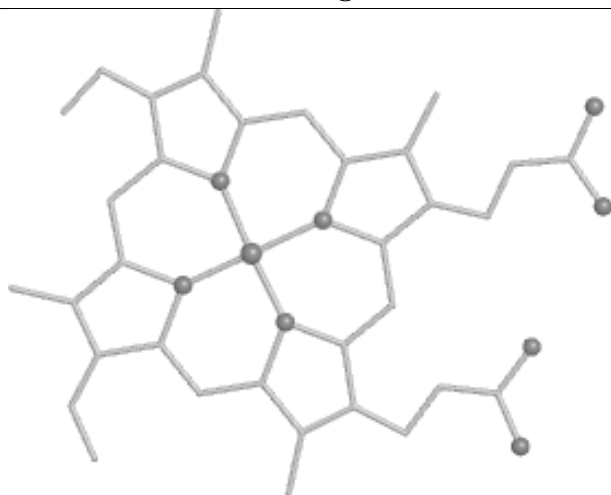
Bond lengths



Bond angles

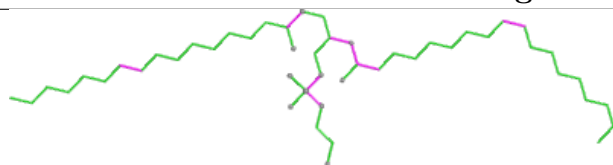


Torsions

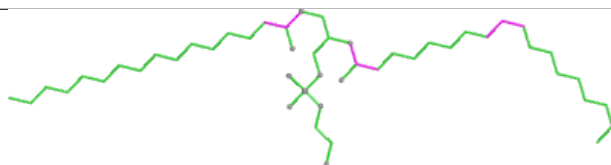


Rings

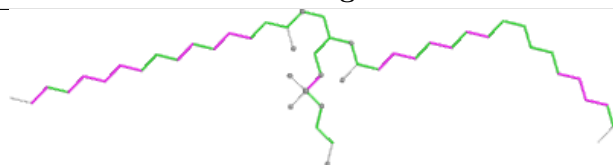
Ligand PEE D 502



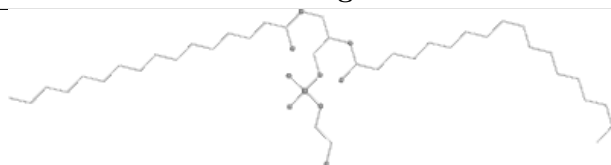
Bond lengths



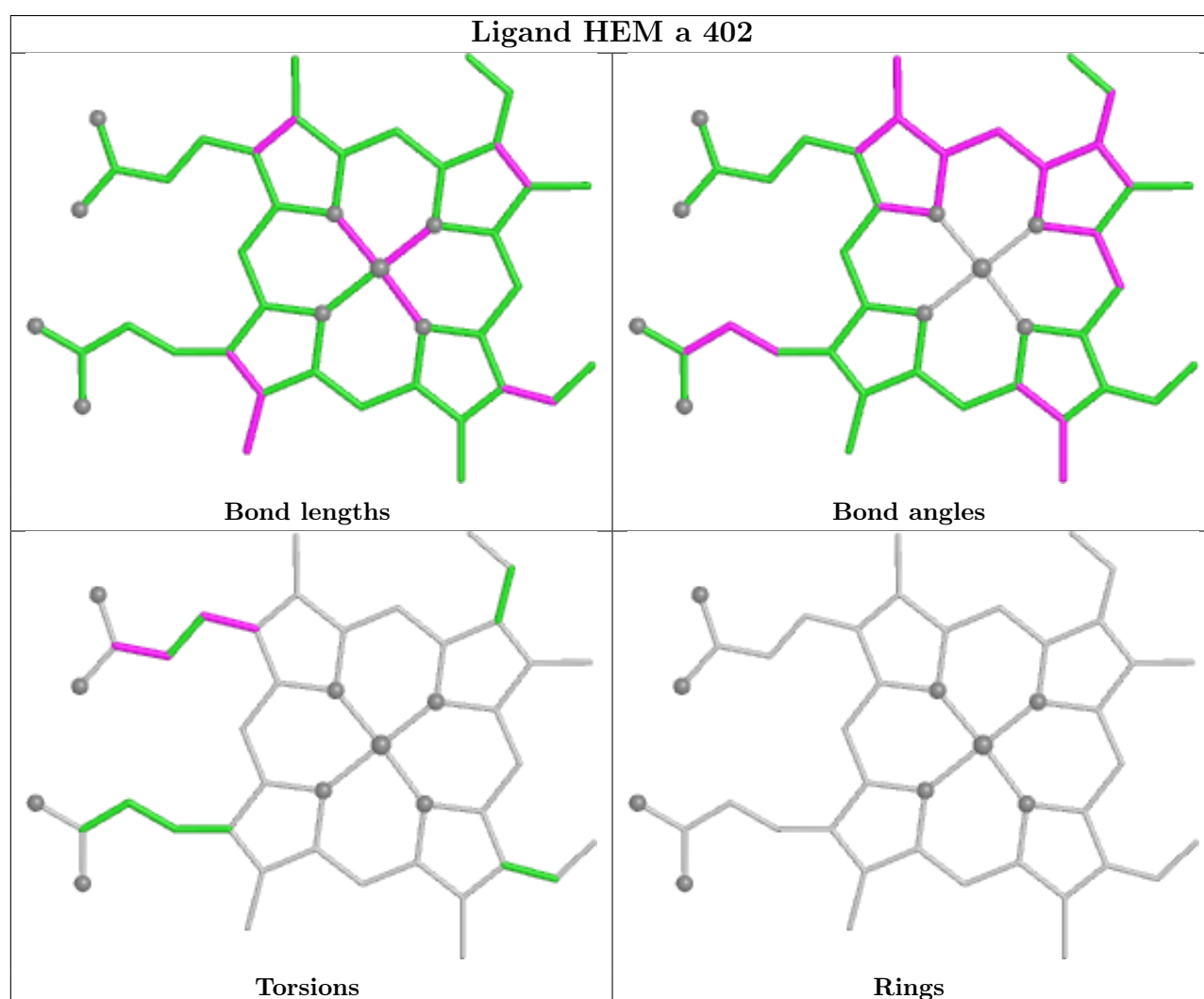
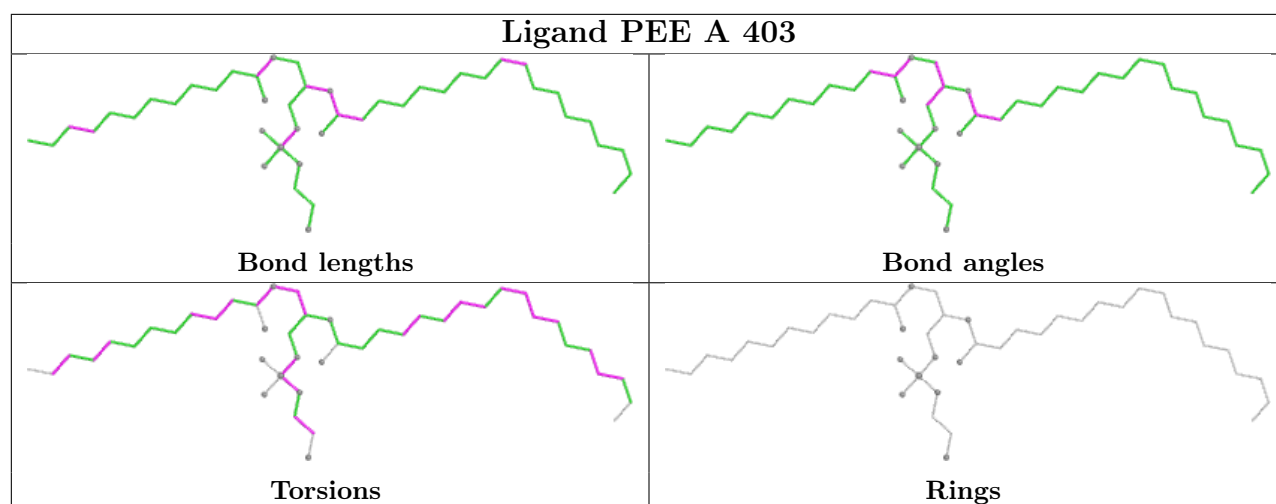
Bond angles

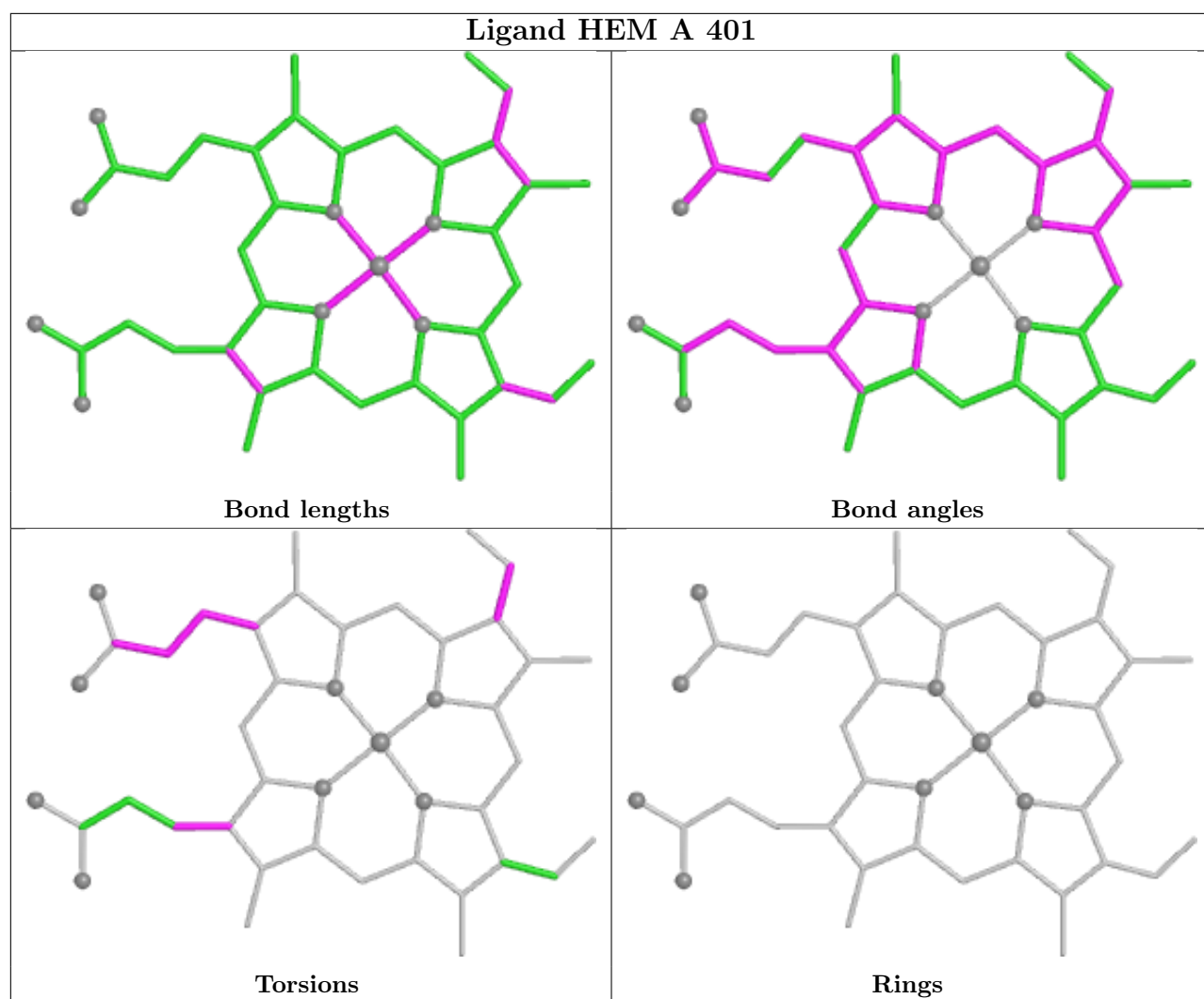


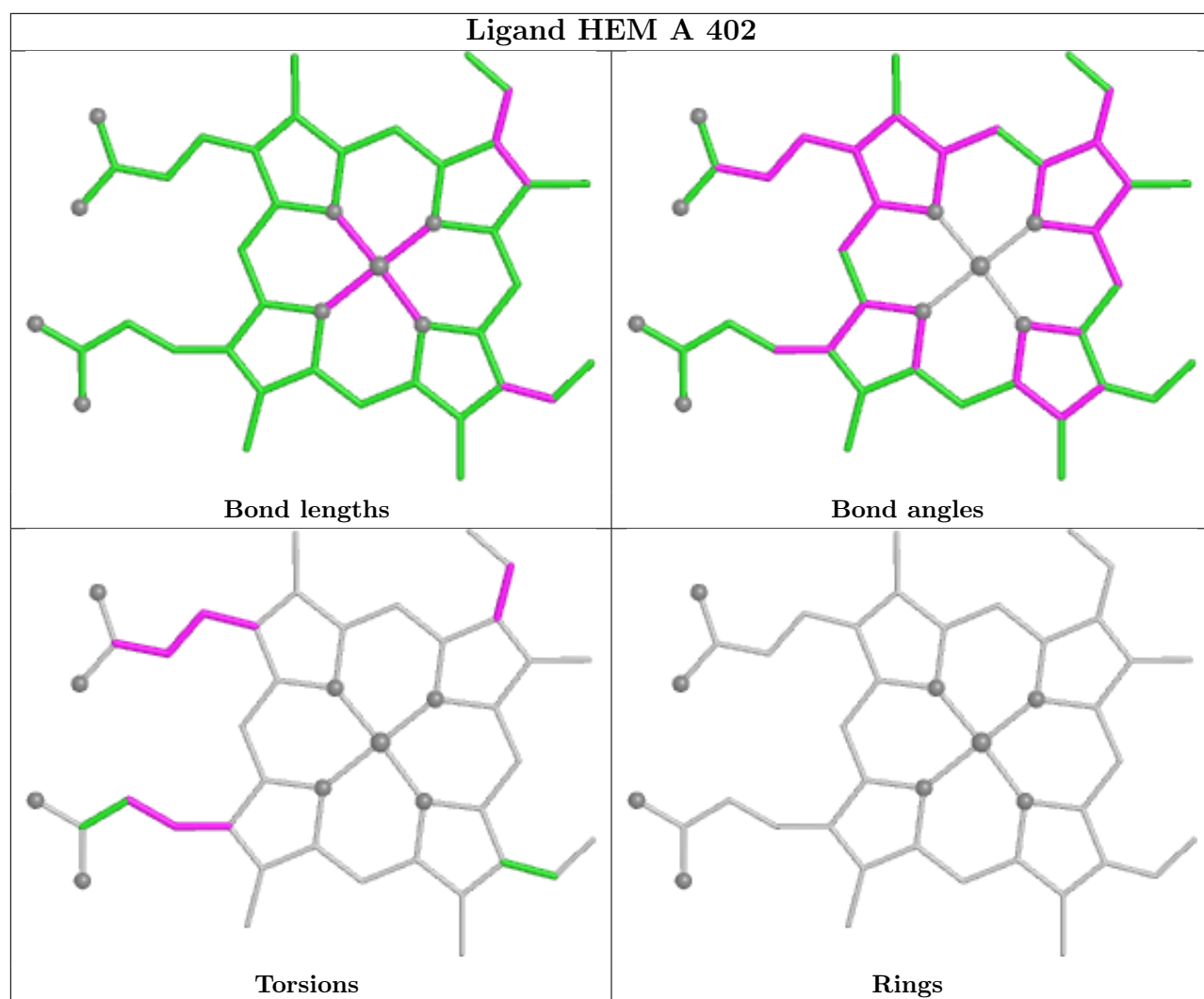
Torsions

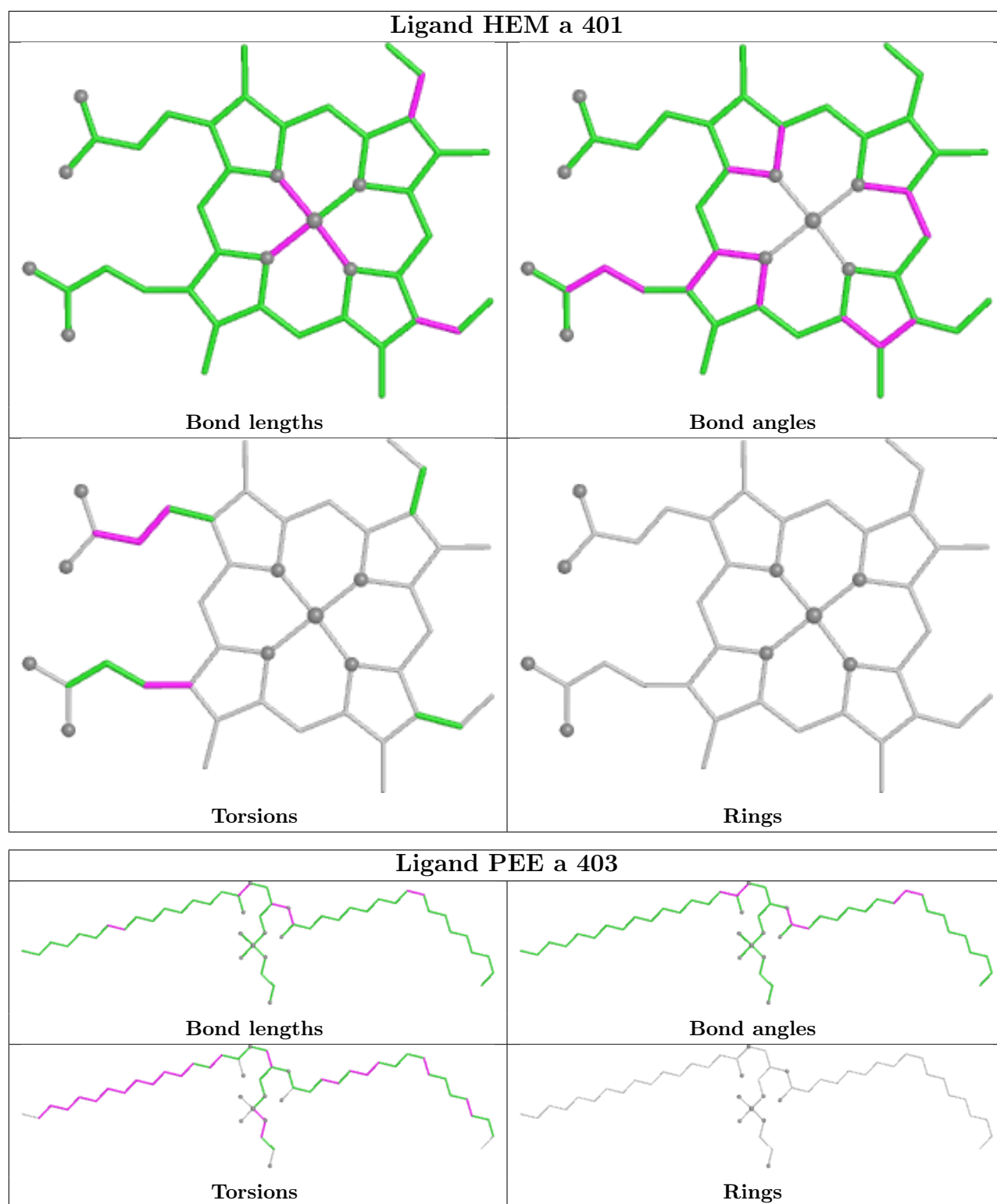


Rings









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

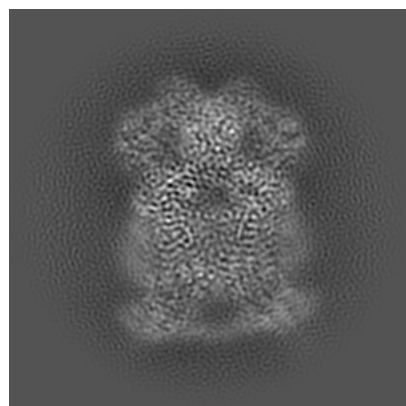
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35618. These allow visual inspection of the internal detail of the map and identification of artifacts.

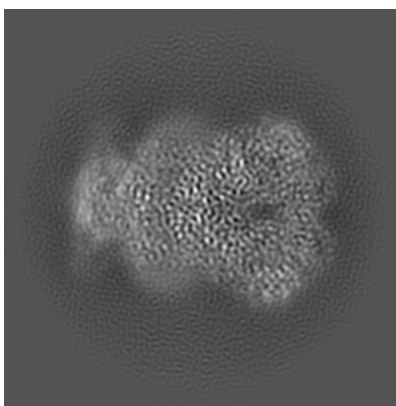
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

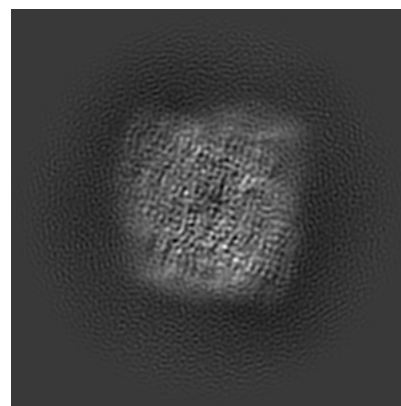
6.1.1 Primary map



X

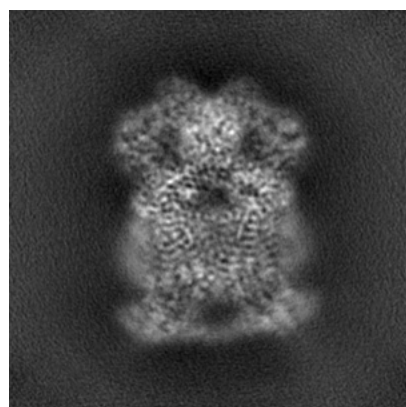


Y

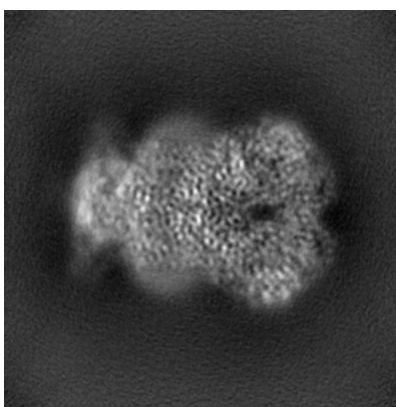


Z

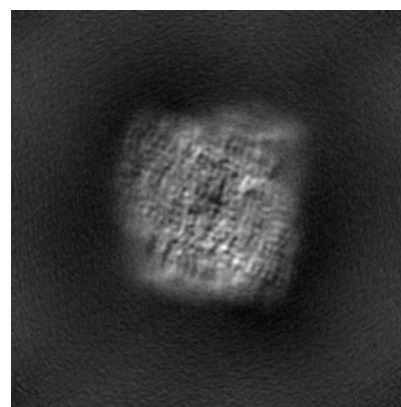
6.1.2 Raw map



X



Y

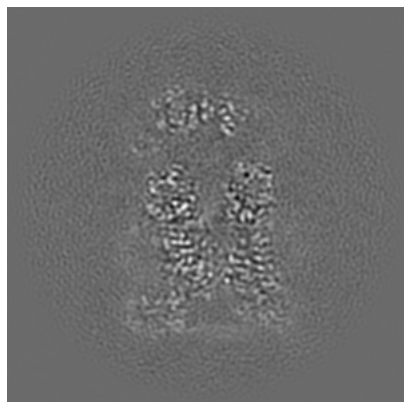


Z

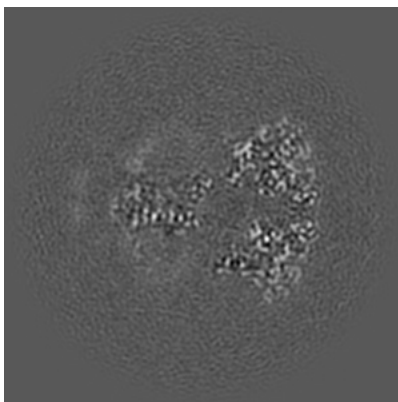
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

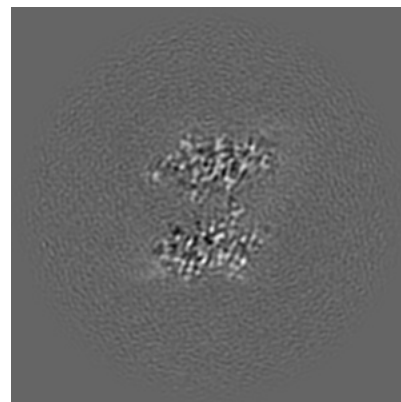
6.2.1 Primary map



X Index: 140

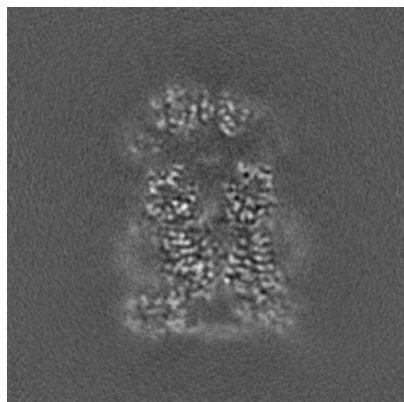


Y Index: 140

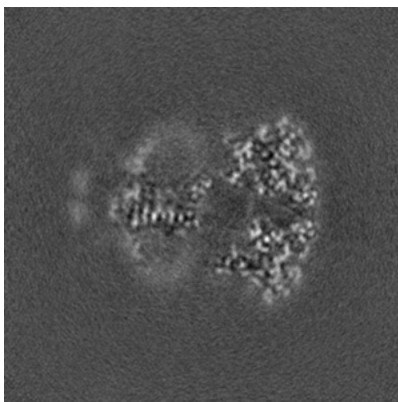


Z Index: 140

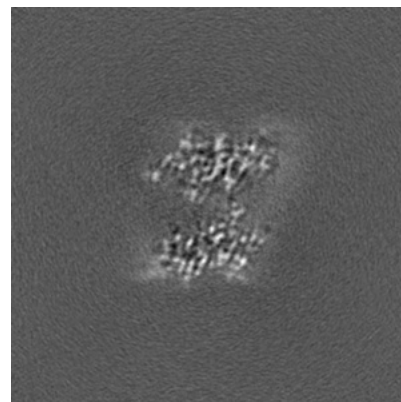
6.2.2 Raw map



X Index: 140



Y Index: 140

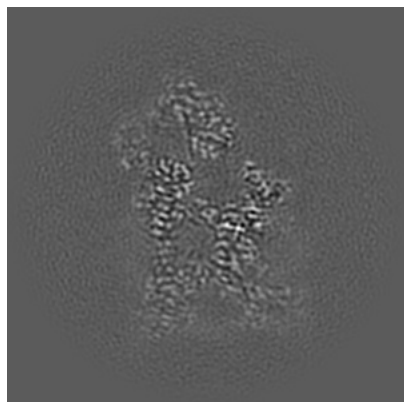


Z Index: 140

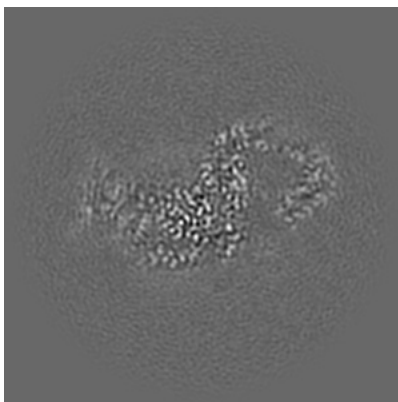
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

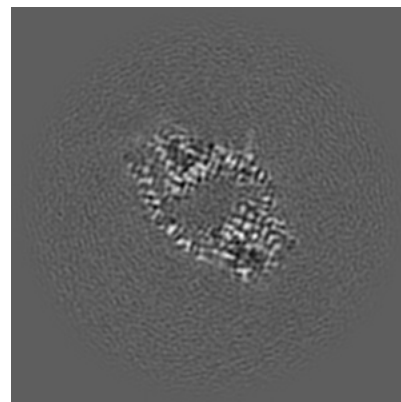
6.3.1 Primary map



X Index: 153

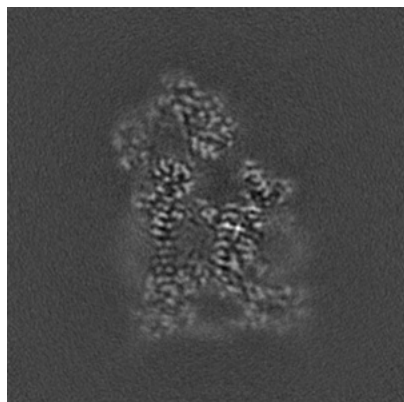


Y Index: 117

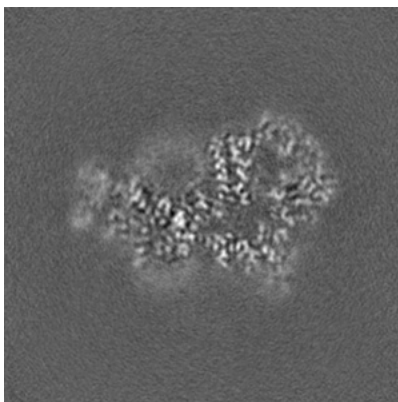


Z Index: 164

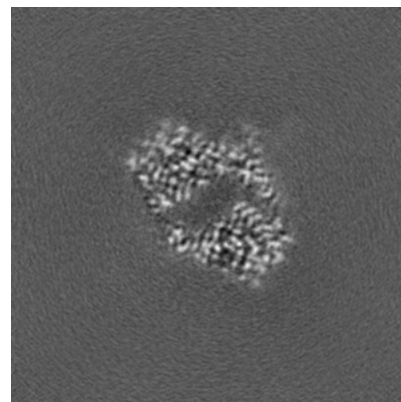
6.3.2 Raw map



X Index: 153



Y Index: 125

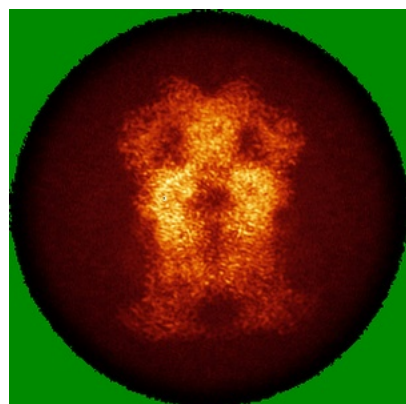


Z Index: 160

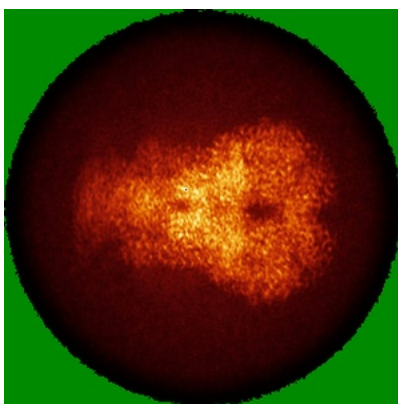
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

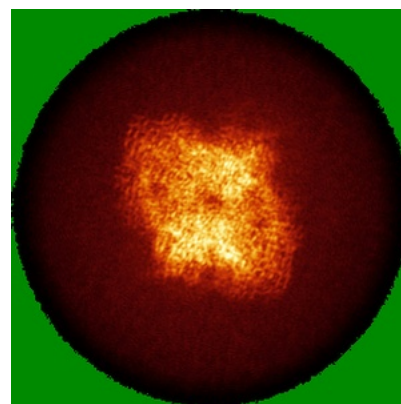
6.4.1 Primary map



X

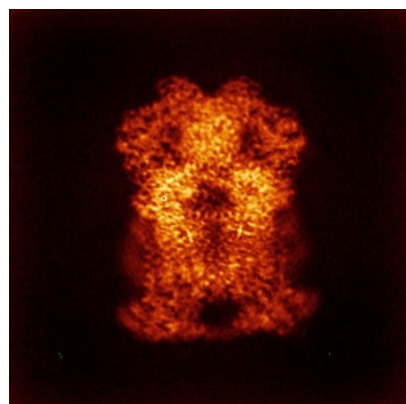


Y

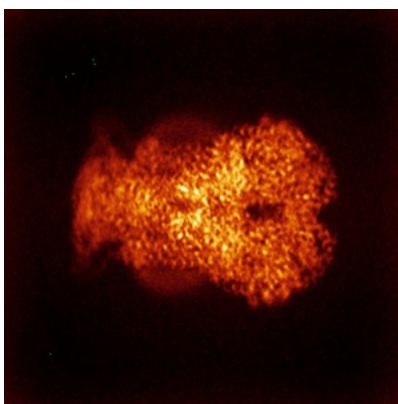


Z

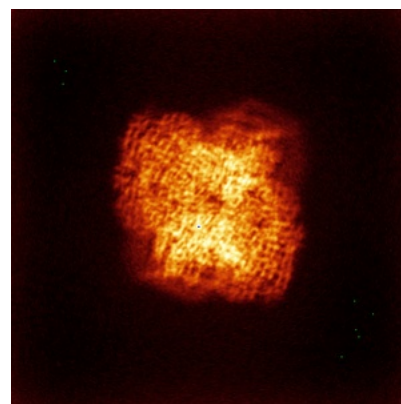
6.4.2 Raw map



X



Y

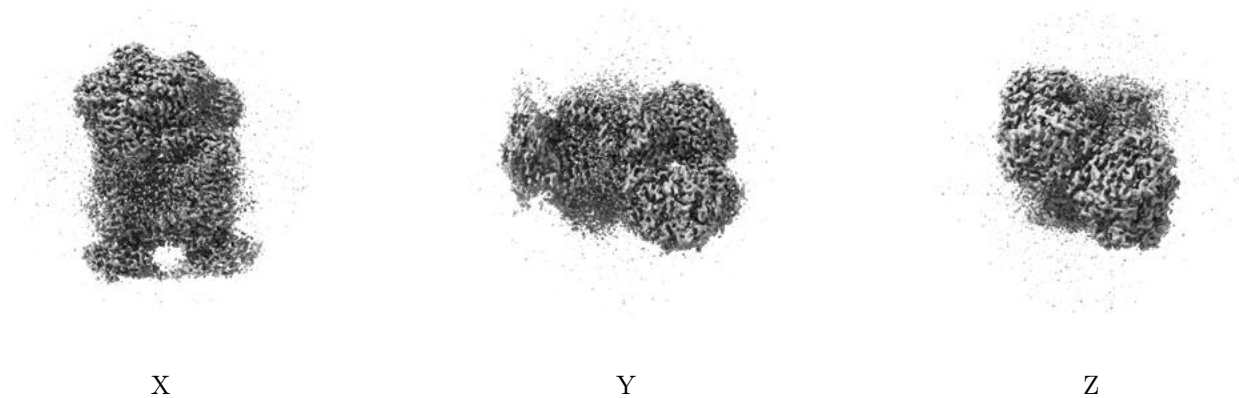


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

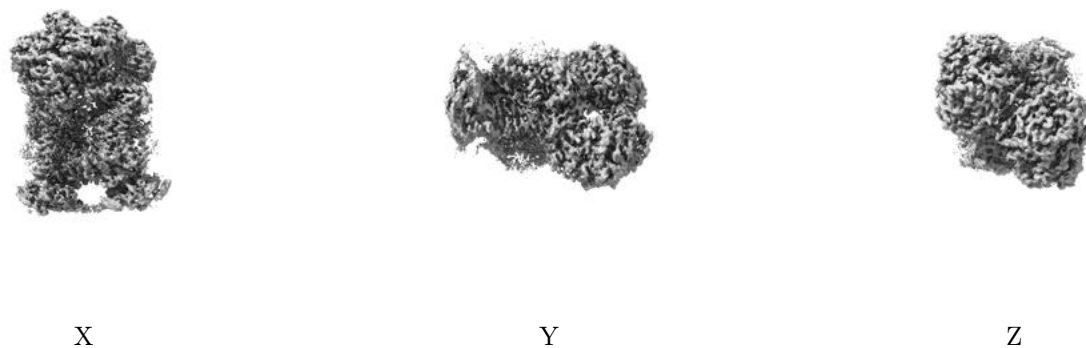
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

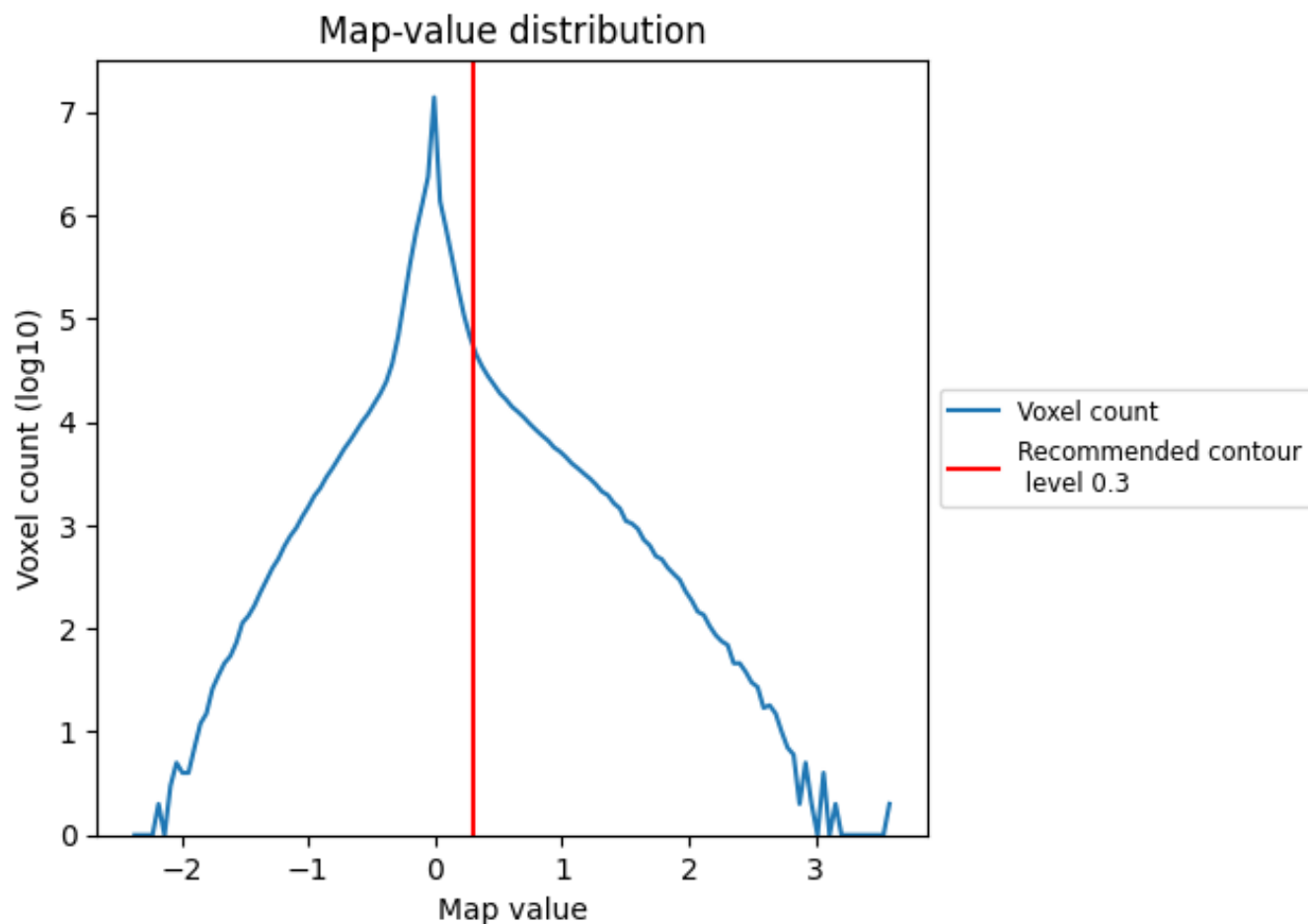
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

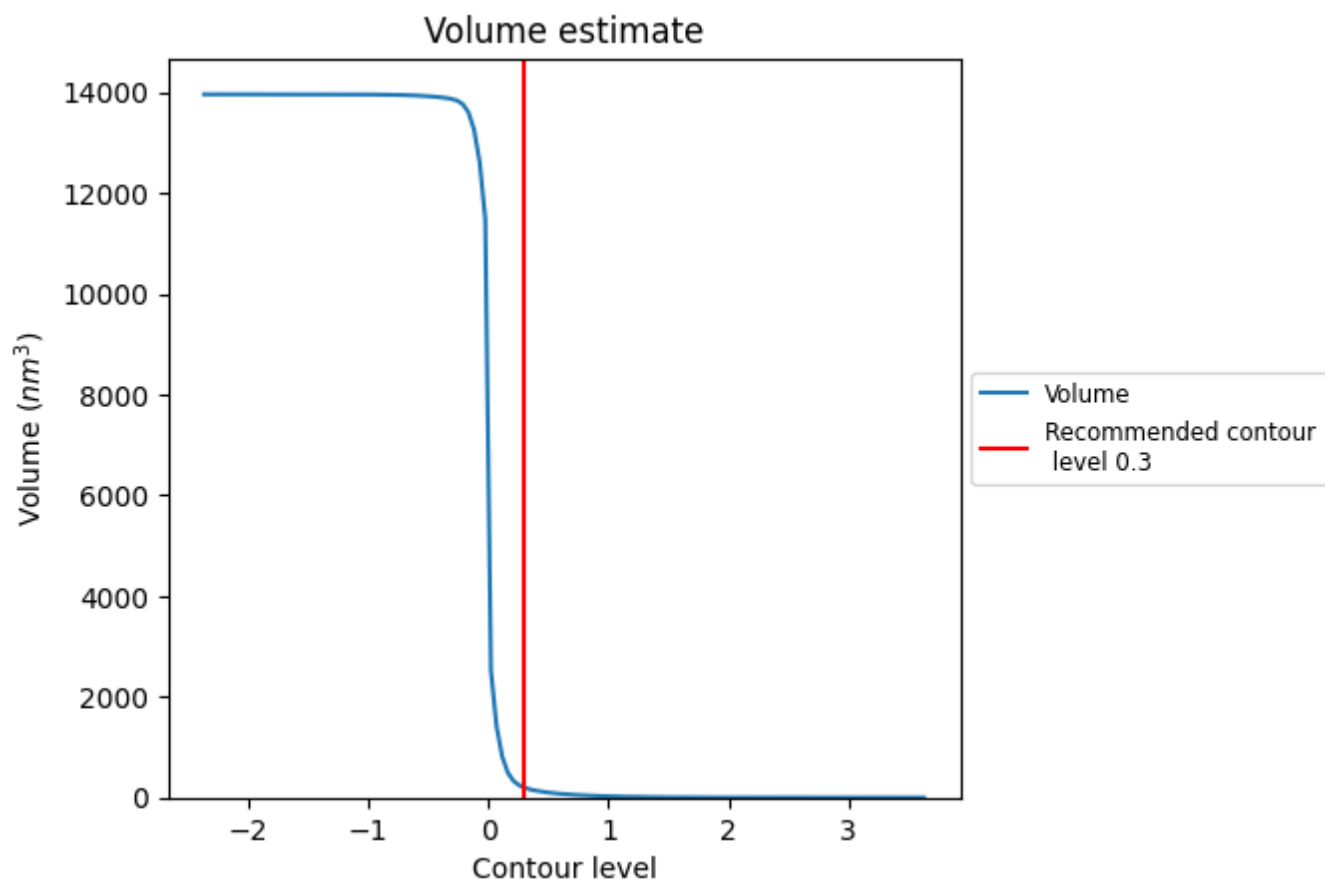
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

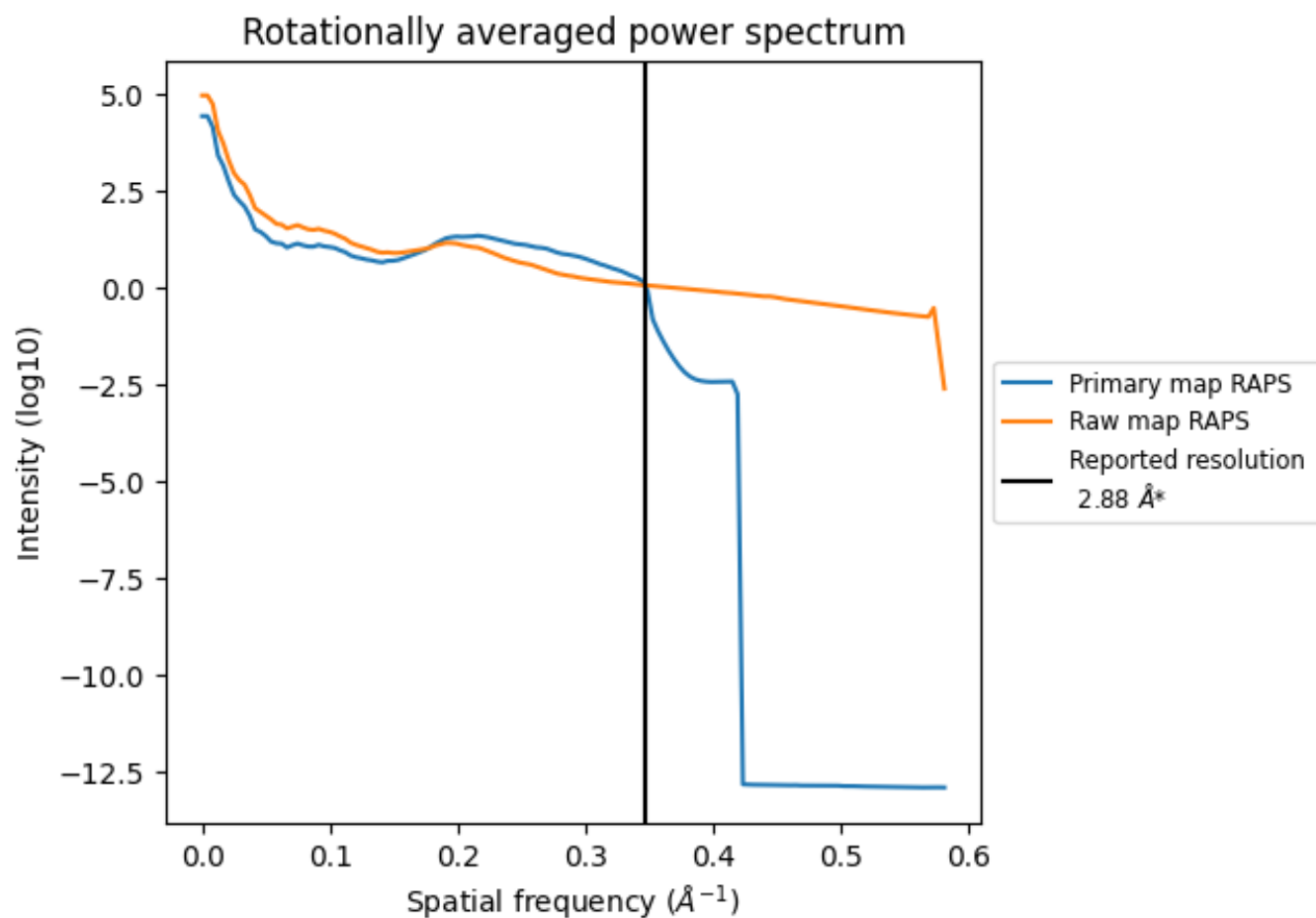
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm³; this corresponds to an approximate mass of 177 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

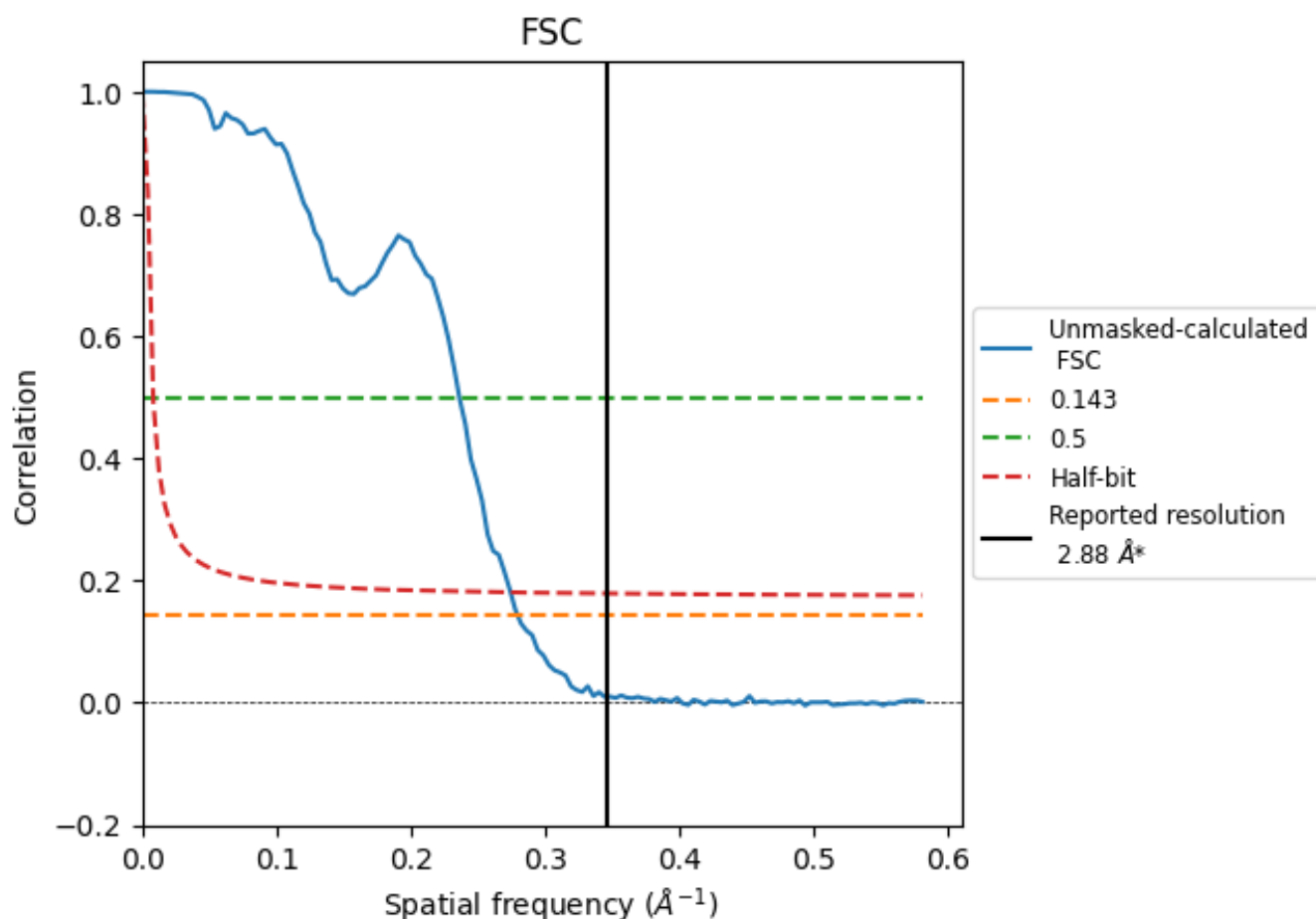


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.347 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

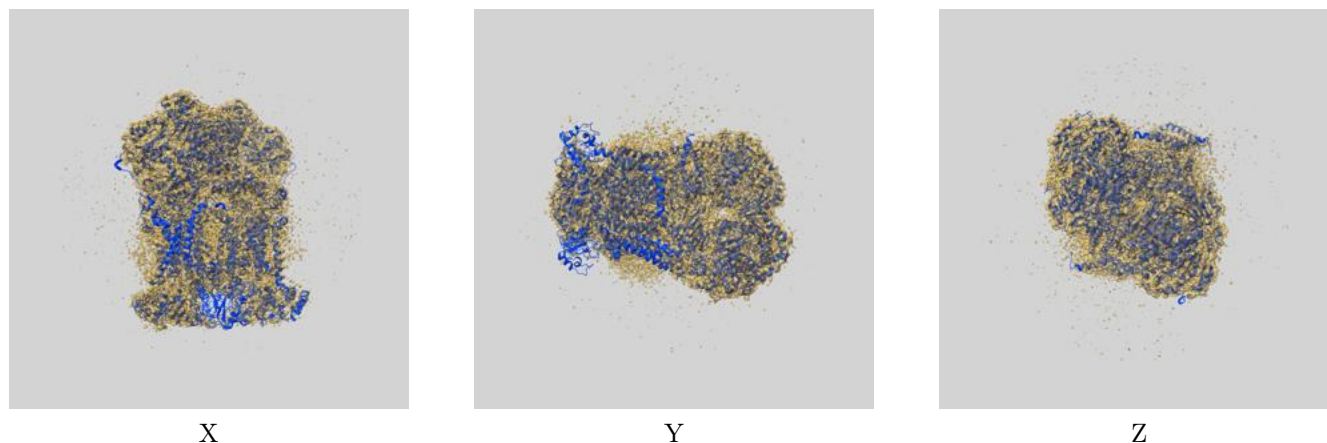
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	4.23	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 2.88 by more than 10 %

9 Map-model fit [i](#)

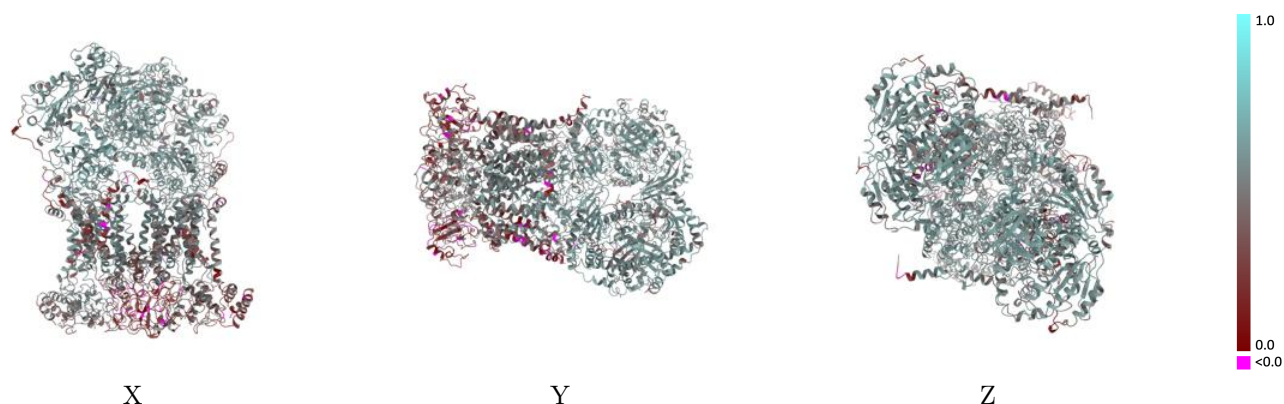
This section contains information regarding the fit between EMDB map EMD-35618 and PDB model 8IOG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



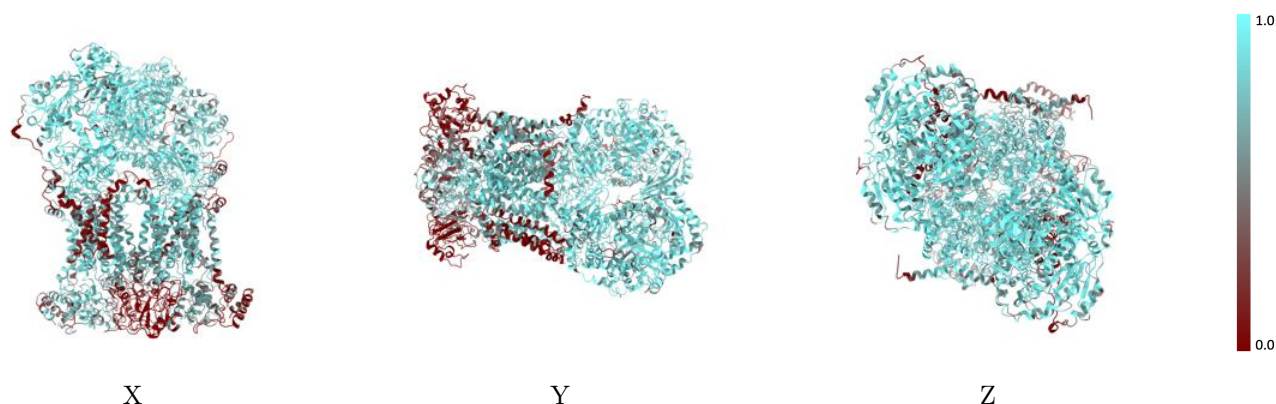
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



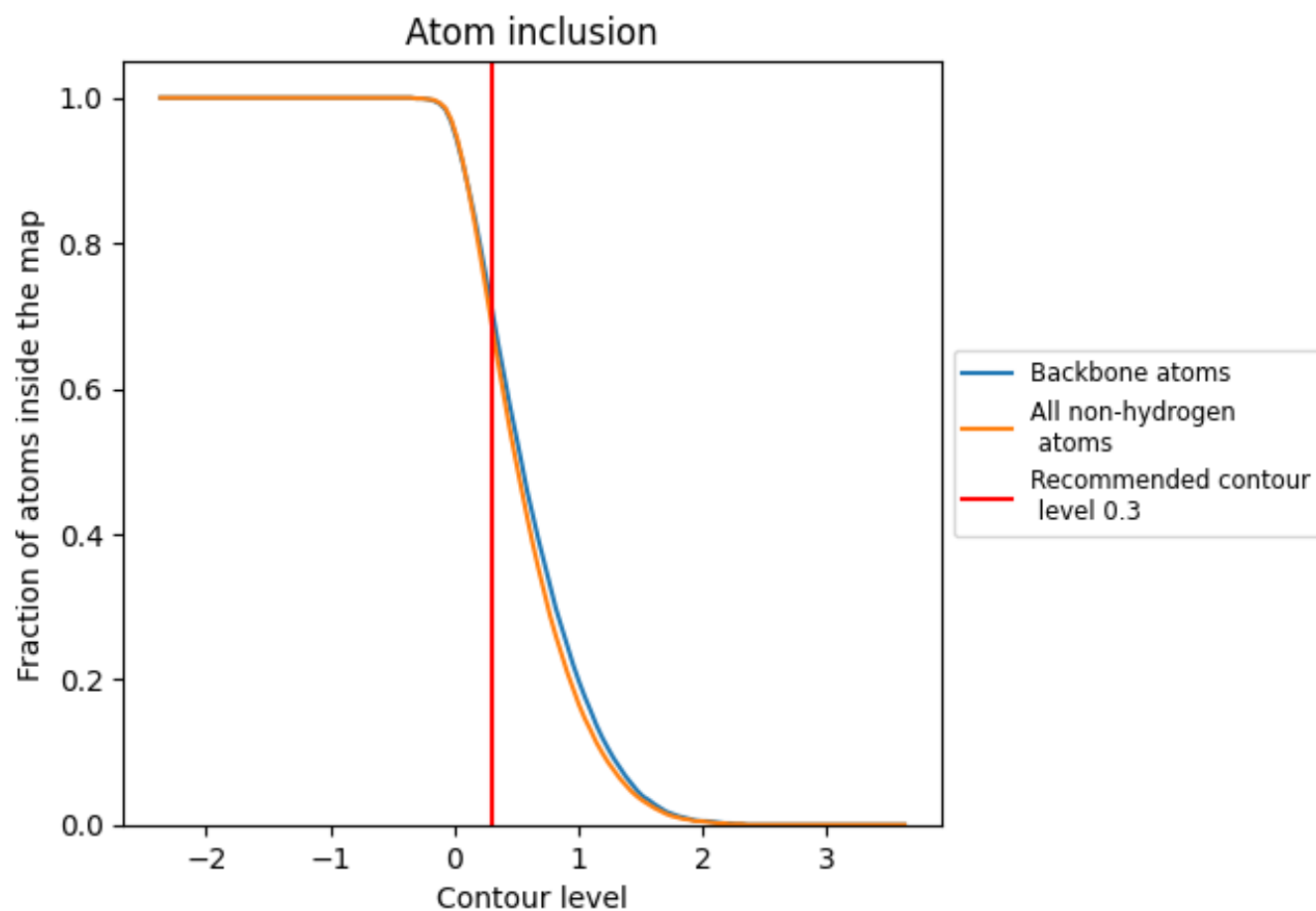
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.4770
A	 0.8720	 0.5310
B	 0.6660	 0.4620
C	 0.1280	 0.2640
D	 0.8340	 0.5480
E	 0.8810	 0.5630
F	 0.4340	 0.3910
G	 0.8770	 0.5590
H	 0.7710	 0.5100
I	 0.3130	 0.3820
J	 0.0360	 0.2290
K	 0.4540	 0.3630
a	 0.8170	 0.5000
b	 0.6050	 0.4310
c	 0.0930	 0.2300
d	 0.8480	 0.5490
e	 0.8870	 0.5660
f	 0.2460	 0.3040
g	 0.8050	 0.5230
h	 0.4910	 0.4020
i	 0.2080	 0.3260
j	 0.0250	 0.1960
k	 0.4090	 0.3600

