



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:34 AM UTC

PDB ID : 2E76 / pdb_00002e76
Title : Crystal Structure of the Cytochrome b6f Complex with tridecyl-stigmatellin (TDS) from *M.laminosus*
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.
Deposited on : 2007-01-05
Resolution : 3.41 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

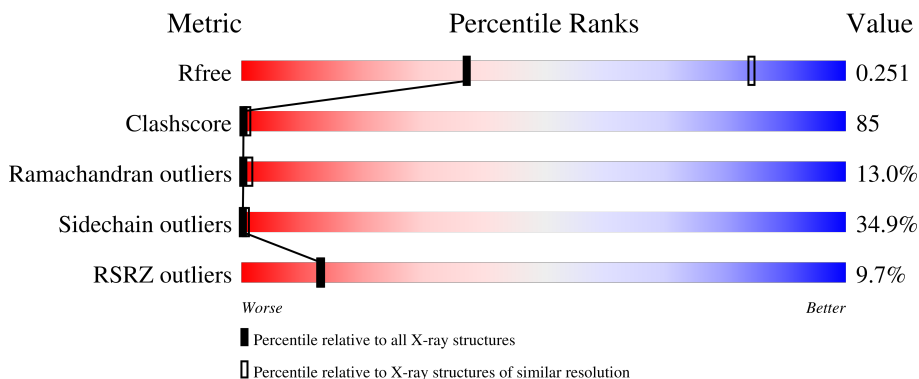
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 Å.

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




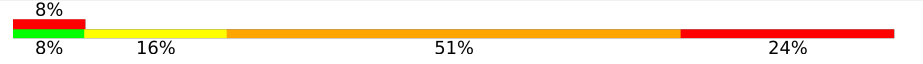

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	215	
2	B	160	
3	C	289	
4	D	179	
5	E	32	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	35	
7	G	37	
8	H	29	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HEM	A	302	-	-	X	-
11	HEC	A	303	-	-	X	-
11	HEC	C	301	-	-	X	-
12	OPC	B	1001	-	X	-	-
13	UMQ	A	1101	X	-	-	-
13	UMQ	A	1102	X	-	-	-
13	UMQ	A	1103	X	-	-	-
13	UMQ	A	1104	X	-	-	-
14	CLA	B	201	X	-	-	-
15	TDS	B	1201	-	X	-	-
15	TDS	B	1202	-	X	-	-
17	SQD	D	201	X	X	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 8112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b6.

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

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

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

- Molecule 3 is a protein called Apocytochrome f.

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

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

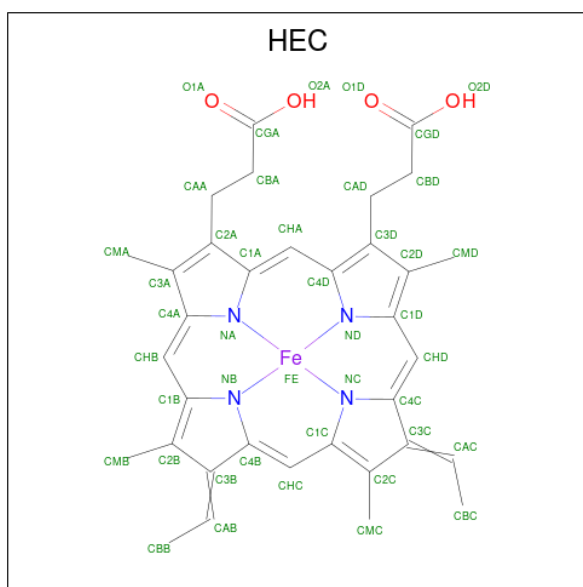
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	168	1288	823	221	237	7	0	0	0

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

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

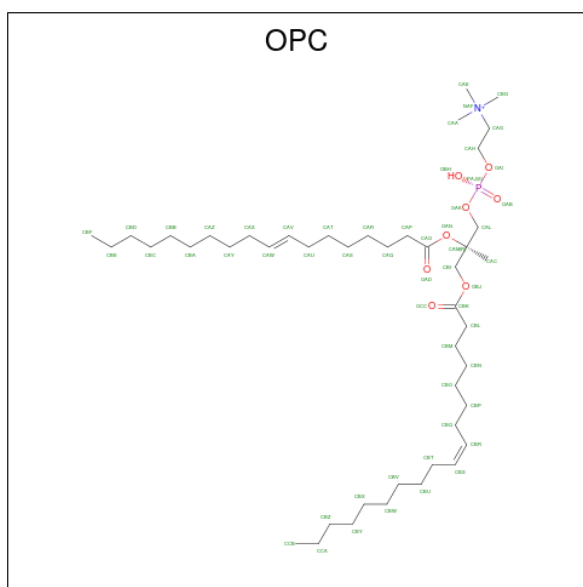
- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

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



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

- Molecule 12 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: C₄₅H₈₇NO₈P).



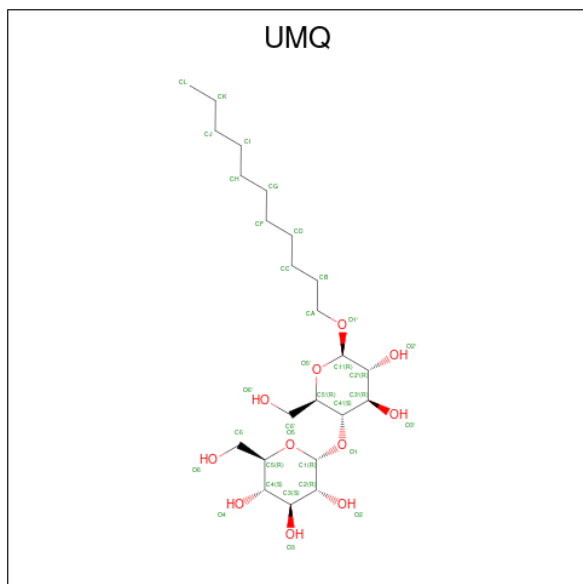
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
12	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

Continued on next page...

Continued from previous page...

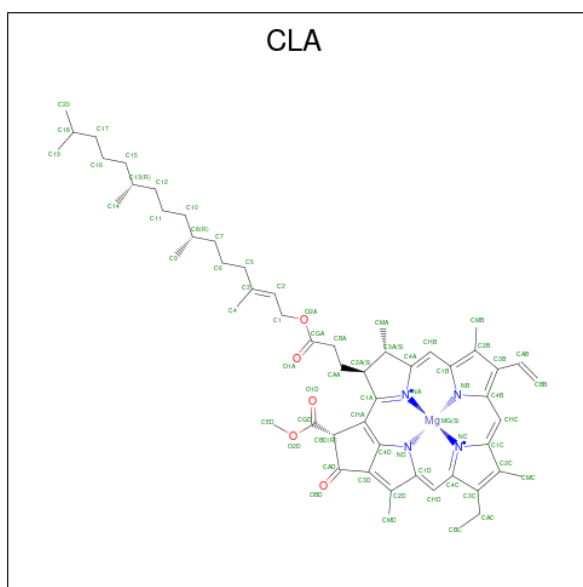
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
12	B	1	54	44	1	8	1	0	0

- Molecule 13 is UNDECYL-MALTOSE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).



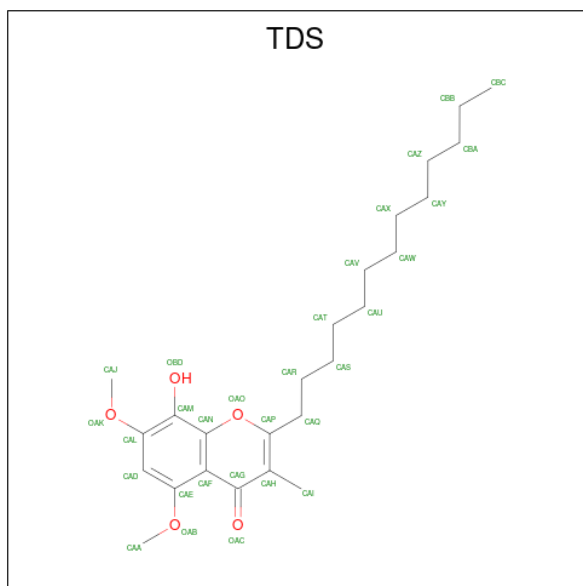
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	A	1	34	23	11	0	0
13	A	1	34	23	11	0	0
13	A	1	34	23	11	0	0
13	A	1	34	23	11	0	0

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



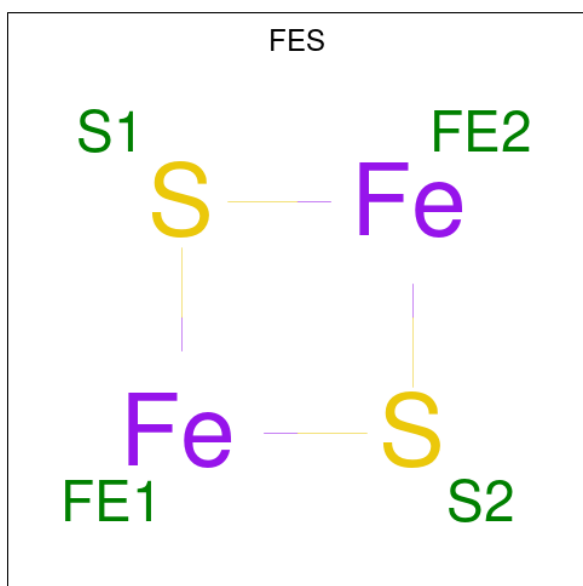
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 15 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (CCD ID: TDS) (formula: $C_{25}H_{38}O_5$).



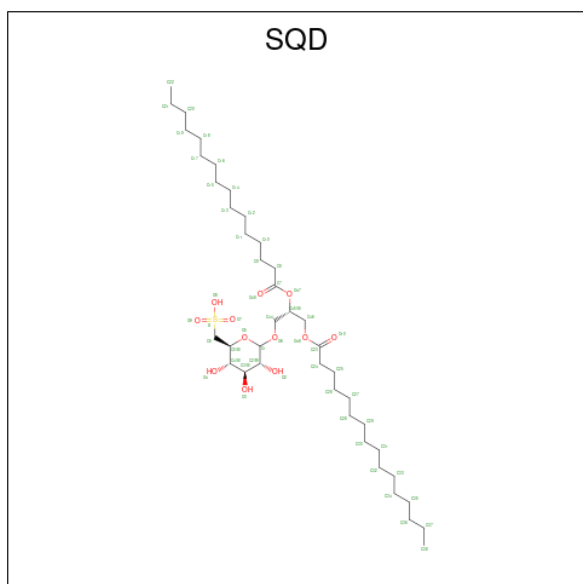
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			30	25	5		
15	B	1	Total	C	O	0	0
			30	25	5		

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



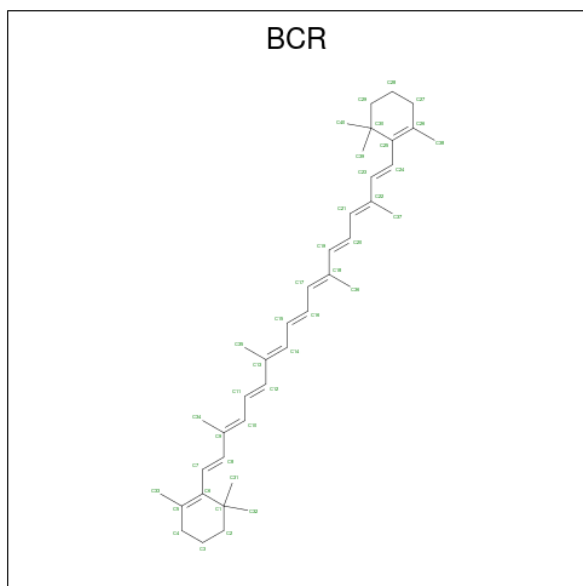
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
16	D	1	4	2	2	0	0

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



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

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

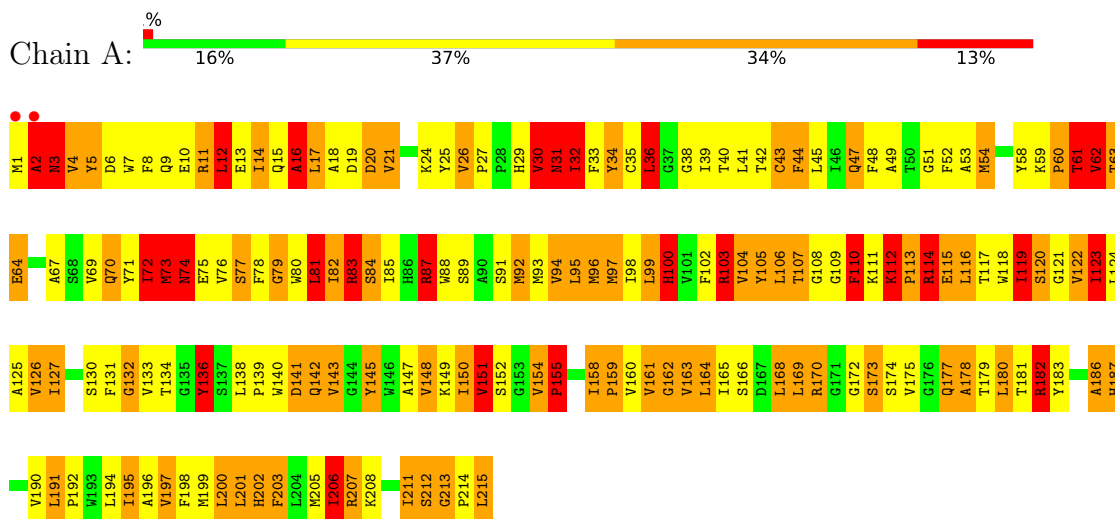
- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	2	Total O 2 2	0	0
19	B	2	Total O 2 2	0	0
19	C	1	Total O 1 1	0	0

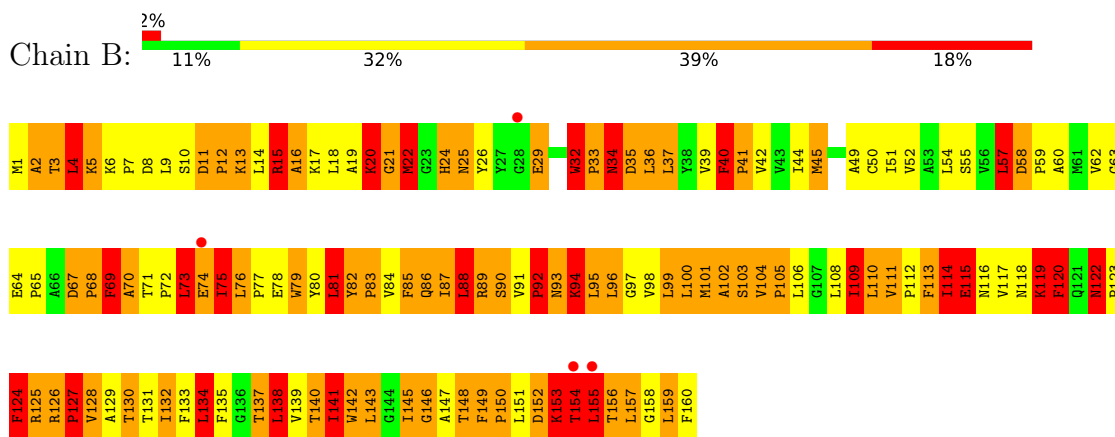
3 Residue-property plots

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

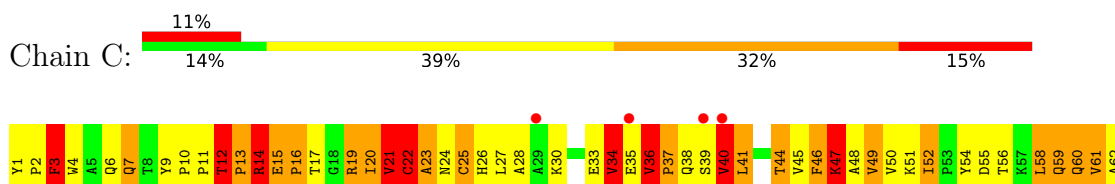
- Molecule 1: Cytochrome b6

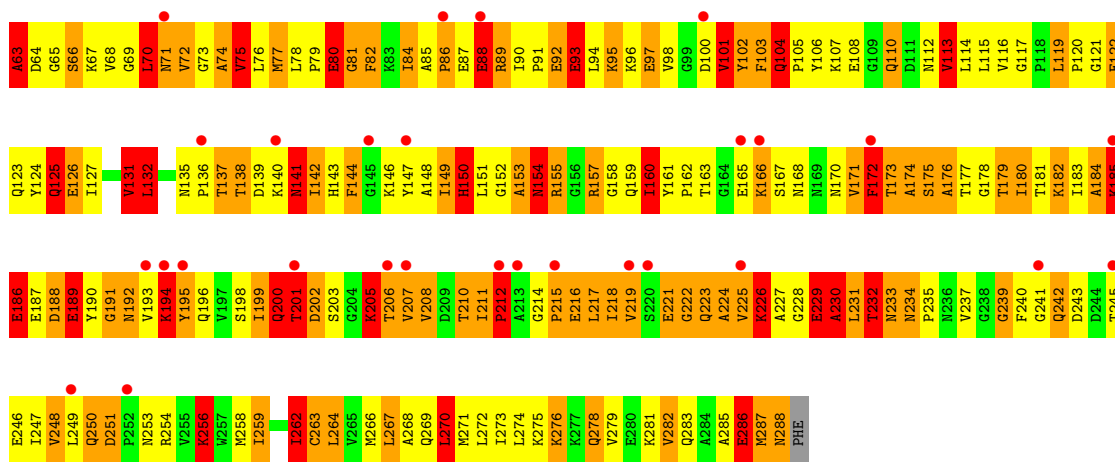


- Molecule 2: Cytochrome b6-f complex subunit 4

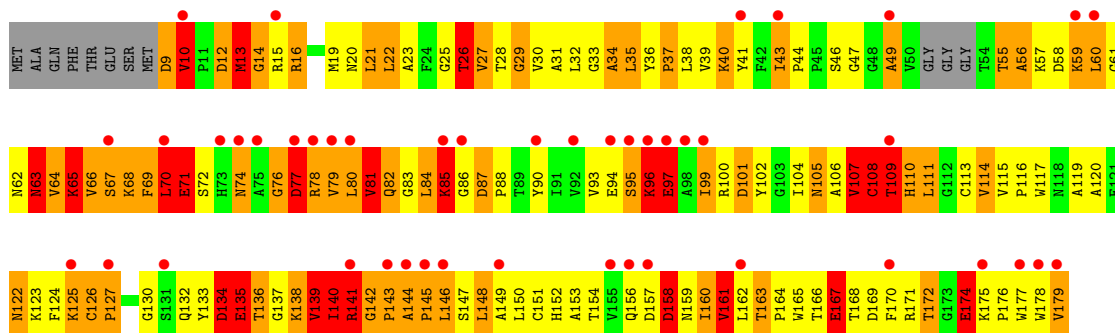


- Molecule 3: Apocytochrome f





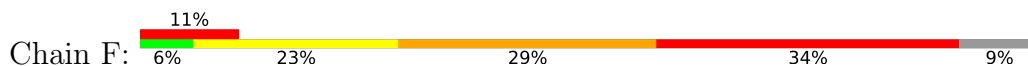
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



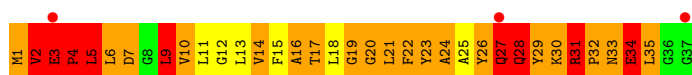
• Molecule 5: Cytochrome b6-f complex subunit 6



• Molecule 6: Cytochrome b6-f complex subunit 7

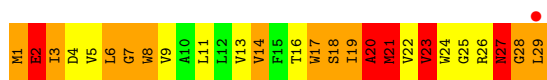


• Molecule 7: Cytochrome b6-f complex subunit 5



- Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:  3% 10% 34% 38% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.23Å 157.23Å 363.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.27 – 3.41 41.27 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.27-3.41) 99.7 (41.27-3.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.256 0.182 , 0.251	Depositor DCC
R_{free} test set	1852 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	92.6	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 95.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8112	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OPC, SQD, CLA, TDS, HEM, UMQ, CD, HEC, FES, BCR

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	2.17	63/1763 (3.6%)	2.44	123/2405 (5.1%)
2	B	2.20	39/1288 (3.0%)	2.58	110/1765 (6.2%)
3	C	1.81	45/2264 (2.0%)	2.10	111/3082 (3.6%)
4	D	1.72	18/1320 (1.4%)	2.06	58/1798 (3.2%)
5	E	2.21	10/253 (4.0%)	2.58	19/340 (5.6%)
6	F	2.39	15/246 (6.1%)	2.33	13/331 (3.9%)
7	G	2.38	16/289 (5.5%)	2.32	17/391 (4.3%)
8	H	2.23	12/236 (5.1%)	2.13	8/323 (2.5%)
All	All	2.02	218/7659 (2.8%)	2.30	459/10435 (4.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	3
3	C	0	7
4	D	0	5
5	E	0	1
6	F	0	3
7	G	0	2
8	H	0	2
All	All	0	27

All (218) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	THR	CA-CB	-13.55	1.31	1.53
1	A	67	ALA	CA-CB	-13.26	1.31	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	44	PRO	CA-C	-11.17	1.45	1.51
2	B	141	ILE	CA-CB	-10.98	1.39	1.54
1	A	186	ALA	CA-CB	-10.94	1.36	1.53
3	C	40	VAL	CA-CB	-10.13	1.40	1.54
4	D	107	VAL	CA-CB	-10.05	1.41	1.54
1	A	165	ILE	CA-CB	-9.76	1.43	1.54
7	G	3	GLU	CG-CD	9.71	1.76	1.52
1	A	85	ILE	CA-CB	-9.34	1.44	1.54
3	C	256	LYS	CG-CD	9.20	1.80	1.52
1	A	62	VAL	CA-CB	-9.11	1.41	1.54
6	F	2	THR	CA-CB	9.09	1.68	1.53
6	F	29	ILE	CA-CB	9.03	1.66	1.54
2	B	117	VAL	CA-CB	9.00	1.66	1.54
3	C	148	ALA	CA-CB	-8.97	1.38	1.53
3	C	207	VAL	CA-CB	8.96	1.63	1.54
4	D	10	VAL	CA-CB	8.88	1.63	1.53
1	A	62	VAL	CA-C	-8.55	1.40	1.52
2	B	49	ALA	CA-CB	-8.53	1.39	1.53
2	B	15	ARG	CZ-NH1	8.49	1.44	1.32
3	C	49	VAL	CA-CB	-8.47	1.44	1.53
3	C	256	LYS	CE-NZ	8.27	1.74	1.49
1	A	72	ILE	CA-CB	-8.26	1.45	1.54
2	B	119	LYS	N-CA	-8.24	1.37	1.46
4	D	141	ARG	N-CA	8.17	1.57	1.45
2	B	150	PRO	CA-C	-8.16	1.44	1.52
1	A	160	VAL	CA-CB	8.06	1.64	1.54
3	C	16	PRO	C-O	8.05	1.34	1.24
4	D	27	VAL	CA-CB	-8.04	1.44	1.54
3	C	84	ILE	CA-CB	-7.93	1.45	1.54
6	F	2	THR	N-CA	7.92	1.55	1.46
1	A	175	VAL	CA-CB	-7.85	1.46	1.54
6	F	25	LEU	CG-CD1	7.52	1.77	1.52
7	G	3	GLU	CA-CB	7.46	1.63	1.53
7	G	24	ALA	CA-CB	7.43	1.65	1.53
1	A	113	PRO	N-CA	7.38	1.56	1.47
1	A	114	ARG	CA-C	7.37	1.62	1.52
3	C	286	GLU	N-CA	7.33	1.55	1.46
2	B	120	PHE	CA-C	-7.32	1.43	1.52
8	H	26	ARG	CZ-NH1	7.26	1.43	1.32
6	F	20	TRP	C-O	7.26	1.33	1.24
3	C	246	GLU	CD-OE2	7.21	1.39	1.25
3	C	131	VAL	CA-C	-7.14	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246	GLU	CG-CD	7.13	1.69	1.52
1	A	120	SER	C-O	7.12	1.32	1.24
3	C	147	TYR	C-O	7.09	1.32	1.23
1	A	178	ALA	CA-CB	-7.08	1.41	1.53
1	A	30	VAL	CA-CB	7.05	1.61	1.53
2	B	149	PHE	N-CA	7.00	1.54	1.45
6	F	3	GLU	CB-CG	6.97	1.73	1.52
2	B	134	LEU	N-CA	6.95	1.55	1.46
7	G	1	MET	SD-CE	6.94	1.97	1.79
2	B	114	ILE	C-O	-6.83	1.16	1.24
1	A	140	TRP	CA-CB	-6.82	1.42	1.53
1	A	59	LYS	C-O	-6.79	1.16	1.24
2	B	20	LYS	C-O	6.73	1.32	1.24
3	C	40	VAL	CA-C	-6.68	1.44	1.52
2	B	138	LEU	CG-CD1	6.66	1.74	1.52
1	A	34	TYR	CA-C	6.64	1.61	1.52
2	B	115	GLU	CG-CD	6.63	1.68	1.52
7	G	2	VAL	N-CA	6.55	1.54	1.46
3	C	22	CYS	CA-C	6.51	1.61	1.52
5	E	4	GLY	C-O	6.49	1.32	1.23
1	A	120	SER	CA-C	6.48	1.61	1.52
2	B	40	PHE	CE2-CZ	6.47	1.58	1.38
3	C	81	GLY	N-CA	6.45	1.54	1.45
2	B	73	LEU	N-CA	6.45	1.54	1.45
5	E	26	ILE	CA-CB	6.45	1.63	1.54
1	A	190	VAL	CA-CB	-6.44	1.47	1.54
2	B	143	LEU	C-O	6.39	1.32	1.24
1	A	13	GLU	CB-CG	6.37	1.71	1.52
2	B	140	THR	CA-CB	6.36	1.64	1.53
3	C	48	ALA	CA-CB	-6.35	1.44	1.53
7	G	1	MET	N-CA	6.32	1.58	1.46
2	B	72	PRO	CA-C	-6.29	1.46	1.52
1	A	154	VAL	N-CA	-6.29	1.38	1.46
1	A	73	MET	C-O	6.27	1.31	1.24
5	E	2	ILE	C-O	6.26	1.31	1.24
3	C	142	ILE	C-O	6.26	1.30	1.24
6	F	14	GLY	C-O	6.25	1.31	1.23
7	G	26	TYR	N-CA	-6.24	1.40	1.46
5	E	13	ALA	CA-CB	-6.21	1.43	1.53
1	A	136	TYR	CA-C	-6.16	1.44	1.52
3	C	248	VAL	CA-CB	-6.16	1.47	1.54
6	F	8	ALA	CA-CB	-6.15	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	ILE	CA-C	6.14	1.60	1.52
5	E	12	ILE	C-O	6.06	1.30	1.24
3	C	201	THR	N-CA	6.06	1.54	1.46
8	H	17	TRP	C-O	6.06	1.31	1.24
7	G	3	GLU	CB-CG	6.05	1.70	1.52
2	B	64	GLU	C-O	-6.03	1.15	1.23
7	G	27	GLN	CA-C	6.02	1.60	1.52
1	A	32	ILE	N-CA	6.01	1.53	1.46
2	B	71	THR	CA-C	6.00	1.59	1.52
2	B	98	VAL	CA-CB	-5.99	1.47	1.54
8	H	23	VAL	CA-CB	-5.99	1.46	1.54
2	B	12	PRO	CA-C	-5.98	1.44	1.52
4	D	60	LEU	CA-C	5.97	1.61	1.52
3	C	176	ALA	N-CA	5.95	1.50	1.46
1	A	16	ALA	CA-CB	-5.93	1.43	1.53
1	A	186	ALA	CA-C	-5.89	1.45	1.52
1	A	119	ILE	CA-CB	-5.83	1.46	1.54
8	H	23	VAL	CA-C	5.83	1.60	1.52
1	A	61	THR	CA-C	-5.82	1.45	1.52
1	A	114	ARG	N-CA	5.80	1.53	1.46
1	A	213	GLY	C-O	5.79	1.31	1.24
3	C	13	PRO	CA-C	5.78	1.60	1.52
1	A	141	ASP	N-CA	-5.77	1.38	1.45
3	C	144	PHE	CA-CB	-5.77	1.43	1.53
2	B	83	PRO	CA-C	-5.77	1.44	1.52
1	A	174	SER	CA-C	5.77	1.59	1.52
3	C	262	ILE	CA-CB	-5.75	1.47	1.54
1	A	112	LYS	CG-CD	5.75	1.69	1.52
2	B	114	ILE	CA-C	5.74	1.60	1.52
2	B	148	THR	CB-CG2	5.74	1.71	1.52
2	B	16	ALA	CA-CB	-5.74	1.43	1.53
5	E	19	ALA	CA-CB	-5.73	1.43	1.53
1	A	87	ARG	CG-CD	5.72	1.69	1.52
4	D	97	GLU	N-CA	5.72	1.53	1.46
1	A	169	LEU	CG-CD2	5.72	1.71	1.52
2	B	75	ILE	C-O	-5.68	1.18	1.24
8	H	28	GLY	N-CA	5.67	1.52	1.45
4	D	140	ILE	CA-C	5.66	1.60	1.52
5	E	9	ILE	CA-CB	-5.66	1.47	1.54
2	B	142	TRP	N-CA	-5.66	1.39	1.46
6	F	3	GLU	CG-CD	5.65	1.66	1.52
3	C	256	LYS	CB-CG	5.63	1.69	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	THR	CB-CG2	-5.63	1.33	1.52
1	A	213	GLY	C-N	5.62	1.40	1.33
1	A	123	ILE	C-O	5.61	1.31	1.24
1	A	179	THR	C-O	5.60	1.30	1.24
3	C	246	GLU	CB-CG	5.60	1.69	1.52
1	A	75	GLU	N-CA	5.59	1.53	1.46
6	F	27	LEU	CA-C	-5.59	1.46	1.53
4	D	174	GLU	CA-C	5.58	1.60	1.52
2	B	70	ALA	CA-CB	-5.58	1.43	1.53
7	G	22	PHE	N-CA	5.58	1.53	1.46
1	A	13	GLU	N-CA	5.57	1.53	1.46
3	C	15	GLU	N-CA	5.55	1.52	1.46
2	B	15	ARG	CG-CD	5.55	1.69	1.52
1	A	113	PRO	CB-CG	5.54	1.77	1.49
2	B	34	ASN	N-CA	-5.52	1.39	1.46
4	D	74	ASN	CA-C	5.51	1.56	1.53
5	E	27	LYS	CE-NZ	5.51	1.65	1.49
3	C	263	CYS	CA-C	-5.51	1.45	1.52
3	C	143	HIS	CA-C	-5.49	1.46	1.52
2	B	111	VAL	C-O	-5.49	1.17	1.24
4	D	134	ASP	N-CA	5.48	1.52	1.45
1	A	127	ILE	CA-CB	-5.46	1.47	1.54
3	C	176	ALA	CA-C	5.46	1.56	1.53
7	G	1	MET	CG-SD	5.45	1.94	1.80
1	A	60	PRO	CA-C	-5.45	1.44	1.52
1	A	105	TYR	C-O	-5.44	1.17	1.24
2	B	68	PRO	N-CA	-5.42	1.40	1.47
7	G	1	MET	CB-CG	5.42	1.68	1.52
1	A	70	GLN	C-O	5.41	1.30	1.24
1	A	45	LEU	CA-C	5.40	1.60	1.52
1	A	206	ILE	CA-CB	-5.39	1.47	1.54
1	A	13	GLU	CG-CD	5.37	1.65	1.52
3	C	154	ASN	CA-C	-5.37	1.46	1.52
1	A	2	ALA	N-CA	5.36	1.53	1.46
3	C	36	VAL	C-O	-5.36	1.17	1.24
3	C	226	LYS	N-CA	5.35	1.53	1.46
4	D	40	LYS	N-CA	-5.35	1.39	1.46
7	G	21	LEU	C-O	5.34	1.30	1.24
3	C	153	ALA	N-CA	5.33	1.52	1.45
8	H	20	ALA	CA-CB	-5.33	1.44	1.53
8	H	1	MET	N-CA	5.31	1.56	1.46
8	H	29	LEU	CB-CG	5.30	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1	MET	CA-C	5.29	1.64	1.52
1	A	73	MET	CA-C	5.29	1.59	1.52
5	E	29	ILE	CG1-CD1	5.28	1.72	1.51
2	B	85	PHE	C-O	5.27	1.30	1.24
6	F	22	LEU	CA-C	5.27	1.59	1.52
1	A	70	GLN	CA-CB	-5.25	1.45	1.53
1	A	61	THR	N-CA	-5.24	1.39	1.46
1	A	3	ASN	N-CA	5.23	1.52	1.46
1	A	103	ARG	N-CA	5.23	1.52	1.46
4	D	99	ILE	CA-CB	5.23	1.61	1.54
1	A	30	VAL	C-O	5.23	1.30	1.23
8	H	1	MET	CG-SD	5.22	1.93	1.80
8	H	8	TRP	CB-CG	-5.21	1.34	1.50
7	G	17	THR	CA-C	5.21	1.57	1.52
3	C	89	ARG	CB-CG	-5.20	1.36	1.52
6	F	30	GLN	CA-C	-5.17	1.45	1.52
3	C	148	ALA	N-CA	5.17	1.52	1.45
4	D	158	ASP	CA-C	5.17	1.60	1.52
3	C	25	CYS	CA-C	-5.17	1.45	1.52
4	D	136	THR	CA-C	5.16	1.58	1.52
7	G	1	MET	CA-CB	5.15	1.63	1.53
4	D	135	GLU	CA-C	5.14	1.59	1.52
1	A	26	VAL	CA-C	5.12	1.57	1.53
3	C	185	LYS	N-CA	5.12	1.53	1.46
2	B	145	ILE	CA-CB	-5.12	1.47	1.54
1	A	112	LYS	CB-CG	5.12	1.67	1.52
3	C	40	VAL	N-CA	-5.12	1.40	1.46
3	C	166	LYS	N-CA	5.09	1.52	1.45
4	D	34	ALA	CA-CB	-5.09	1.45	1.53
6	F	13	PHE	CA-C	5.08	1.59	1.52
3	C	142	ILE	CA-CB	-5.07	1.47	1.54
3	C	153	ALA	CA-C	-5.07	1.46	1.52
1	A	48	PHE	CA-CB	-5.07	1.45	1.53
5	E	2	ILE	CA-CB	5.07	1.60	1.54
2	B	127	PRO	CA-C	-5.06	1.45	1.52
7	G	10	VAL	CA-CB	-5.06	1.47	1.54
3	C	226	LYS	CA-C	5.06	1.59	1.52
4	D	166	THR	CA-CB	5.05	1.61	1.53
2	B	114	ILE	CA-CB	-5.04	1.47	1.54
3	C	80	GLU	CA-C	5.04	1.59	1.52
1	A	145	TYR	CA-CB	-5.03	1.44	1.53
3	C	208	VAL	CA-C	5.03	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	MET	CB-CG	5.03	1.67	1.52
2	B	93	ASN	CA-C	5.02	1.59	1.52
2	B	60	ALA	N-CA	5.02	1.52	1.46
8	H	29	LEU	CG-CD2	5.02	1.69	1.52
1	A	168	LEU	C-O	5.01	1.29	1.24
6	F	9	ALA	CA-C	5.00	1.59	1.52

All (459) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	23	ILE	CB-CA-C	-17.53	89.90	111.81
2	B	70	ALA	CA-C-N	-15.15	100.36	120.67
2	B	70	ALA	C-N-CA	-15.15	100.36	120.67
1	A	26	VAL	N-CA-C	14.30	122.90	107.60
5	E	23	ILE	N-CA-CB	14.04	125.93	110.62
3	C	239	GLY	N-CA-C	13.24	125.45	112.08
4	D	74	ASN	N-CA-C	12.60	120.85	108.75
2	B	153	LYS	N-CA-C	-12.52	98.91	112.93
1	A	112	LYS	CA-C-N	-12.52	104.19	119.84
1	A	112	LYS	C-N-CA	-12.52	104.19	119.84
1	A	158	ILE	CA-C-N	12.34	131.80	118.97
1	A	158	ILE	C-N-CA	12.34	131.80	118.97
2	B	111	VAL	CA-C-N	-12.14	106.32	119.19
2	B	111	VAL	C-N-CA	-12.14	106.32	119.19
3	C	205	LYS	N-CA-C	11.45	125.33	111.02
4	D	109	THR	N-CA-C	-11.45	96.44	113.61
4	D	87	ASP	CA-C-N	-11.35	107.99	119.90
4	D	87	ASP	C-N-CA	-11.35	107.99	119.90
1	A	74	ASN	N-CA-C	11.34	134.96	110.80
4	D	163	THR	CA-C-N	-10.93	108.75	119.90
4	D	163	THR	C-N-CA	-10.93	108.75	119.90
2	B	11	ASP	CA-C-N	10.91	133.48	119.84
2	B	11	ASP	C-N-CA	10.91	133.48	119.84
1	A	59	LYS	CA-C-N	-10.82	106.32	119.84
1	A	59	LYS	C-N-CA	-10.82	106.32	119.84
2	B	63	GLY	N-CA-C	-10.67	99.99	112.79
6	F	4	GLU	N-CA-C	-10.58	99.05	112.90
2	B	82	TYR	CA-C-N	10.52	132.99	119.84
2	B	82	TYR	C-N-CA	10.52	132.99	119.84
1	A	191	LEU	CA-C-N	-10.24	108.01	119.28
1	A	191	LEU	C-N-CA	-10.24	108.01	119.28
1	A	159	PRO	CA-C-N	-10.22	110.29	122.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	PRO	C-N-CA	-10.22	110.29	122.35
2	B	67	ASP	CA-C-N	10.20	131.30	119.47
2	B	67	ASP	C-N-CA	10.20	131.30	119.47
2	B	154	THR	N-CA-C	10.18	122.07	110.97
2	B	149	PHE	N-CA-C	10.15	122.49	110.31
2	B	71	THR	CA-C-N	-10.10	107.81	120.23
2	B	71	THR	C-N-CA	-10.10	107.81	120.23
4	D	44	PRO	CA-C-N	10.04	130.67	119.83
4	D	44	PRO	C-N-CA	10.04	130.67	119.83
7	G	3	GLU	CA-C-N	9.81	132.10	119.84
7	G	3	GLU	C-N-CA	9.81	132.10	119.84
1	A	62	VAL	CB-CA-C	-9.64	96.65	112.26
3	C	70	LEU	N-CA-C	9.59	121.97	108.74
2	B	4	LEU	N-CA-C	9.56	123.68	109.24
4	D	107	VAL	CB-CA-C	-9.42	98.91	111.15
1	A	187	HIS	N-CA-C	-9.40	100.91	111.82
1	A	3	ASN	N-CA-C	9.39	130.81	110.80
3	C	90	ILE	CA-C-N	-9.29	108.23	119.84
3	C	90	ILE	C-N-CA	-9.29	108.23	119.84
3	C	10	PRO	N-CA-C	9.26	121.99	110.70
3	C	176	ALA	N-CA-C	9.20	116.32	108.78
3	C	41	LEU	CA-C-N	-9.20	111.42	120.52
3	C	41	LEU	C-N-CA	-9.20	111.42	120.52
2	B	22	MET	N-CA-C	9.11	130.19	110.80
2	B	104	VAL	CA-C-N	9.07	131.18	119.84
2	B	104	VAL	C-N-CA	9.07	131.18	119.84
2	B	72	PRO	CB-CA-C	-9.06	101.69	111.56
2	B	24	HIS	N-CA-C	9.06	123.43	112.38
1	A	114	ARG	N-CA-C	9.00	129.98	110.80
3	C	101	VAL	CA-C-N	-8.84	109.36	123.23
3	C	101	VAL	C-N-CA	-8.84	109.36	123.23
4	D	126	CYS	CA-C-N	8.80	129.54	120.04
4	D	126	CYS	C-N-CA	8.80	129.54	120.04
3	C	102	TYR	CA-C-N	-8.75	108.26	122.26
3	C	102	TYR	C-N-CA	-8.75	108.26	122.26
7	G	28	GLN	N-CA-C	-8.62	101.71	113.18
1	A	63	THR	CB-CA-C	-8.49	97.48	110.90
2	B	62	VAL	CA-C-N	-8.46	112.61	122.85
2	B	62	VAL	C-N-CA	-8.46	112.61	122.85
3	C	229	GLU	N-CA-C	8.46	121.75	109.14
7	G	9	LEU	CA-CB-CG	-8.42	86.84	116.30
1	A	109	GLY	N-CA-C	-8.39	104.01	114.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	ARG	N-CA-C	8.39	123.74	113.17
7	G	2	VAL	CA-C-N	-8.37	112.86	123.16
7	G	2	VAL	C-N-CA	-8.37	112.86	123.16
3	C	12	THR	N-CA-C	8.35	118.88	108.11
2	B	15	ARG	N-CA-C	-8.26	102.23	111.07
2	B	58	ASP	CA-C-N	8.23	129.33	120.11
2	B	58	ASP	C-N-CA	8.23	129.33	120.11
2	B	69	PHE	CA-C-N	-8.18	110.78	123.13
2	B	69	PHE	C-N-CA	-8.18	110.78	123.13
2	B	41	PRO	N-CA-C	-8.17	102.17	113.53
3	C	167	SER	N-CA-C	-8.15	97.48	109.63
2	B	82	TYR	N-CA-CB	8.10	118.08	110.39
5	E	11	PHE	N-CA-C	-8.06	102.57	111.36
2	B	40	PHE	CA-C-N	8.06	128.00	119.05
2	B	40	PHE	C-N-CA	8.06	128.00	119.05
4	D	85	LYS	N-CA-C	-8.04	103.97	113.38
7	G	2	VAL	CB-CA-C	-8.01	99.31	111.08
3	C	39	SER	CA-C-N	-8.00	110.68	122.68
3	C	39	SER	C-N-CA	-8.00	110.68	122.68
3	C	104	GLN	CA-C-N	8.00	128.29	119.90
3	C	104	GLN	C-N-CA	8.00	128.29	119.90
1	A	110	PHE	CB-CA-C	-7.99	98.95	111.17
2	B	126	ARG	CA-C-N	7.93	129.76	119.84
2	B	126	ARG	C-N-CA	7.93	129.76	119.84
8	H	18	SER	N-CA-C	-7.93	101.01	111.24
4	D	44	PRO	O-C-N	7.92	124.95	121.31
5	E	7	PHE	N-CA-C	-7.89	102.68	111.28
4	D	79	VAL	N-CA-C	7.82	119.06	108.11
3	C	185	LYS	N-CA-C	7.81	119.63	110.41
4	D	144	ALA	CA-C-N	7.77	129.56	119.84
4	D	144	ALA	C-N-CA	7.77	129.56	119.84
3	C	148	ALA	N-CA-C	7.75	121.01	110.55
1	A	151	VAL	CA-C-N	-7.74	108.03	121.66
1	A	151	VAL	C-N-CA	-7.74	108.03	121.66
3	C	226	LYS	N-CA-C	7.70	127.21	110.80
4	D	97	GLU	N-CA-C	7.69	127.18	110.80
2	B	82	TYR	O-C-N	7.66	125.55	120.27
8	H	3	ILE	N-CA-C	-7.65	102.82	110.62
4	D	95	SER	N-CA-C	7.64	122.00	113.21
1	A	26	VAL	CA-C-N	7.63	128.24	120.38
1	A	26	VAL	C-N-CA	7.63	128.24	120.38
2	B	72	PRO	CA-C-O	-7.63	112.00	120.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	160	ILE	N-CA-C	7.62	119.73	108.45
2	B	81	LEU	N-CA-C	7.60	122.40	113.20
3	C	286	GLU	N-CA-C	7.59	122.73	113.17
1	A	136	TYR	CA-C-N	-7.58	110.78	122.60
1	A	136	TYR	C-N-CA	-7.58	110.78	122.60
3	C	51	LYS	N-CA-C	7.52	121.50	109.24
4	D	140	ILE	CB-CA-C	7.51	121.76	111.92
1	A	165	ILE	CB-CA-C	-7.49	102.30	111.88
1	A	175	VAL	CB-CA-C	-7.49	99.16	111.51
5	E	10	VAL	CB-CA-C	-7.48	100.14	112.26
2	B	59	PRO	CA-C-N	7.46	131.34	120.82
2	B	59	PRO	C-N-CA	7.46	131.34	120.82
1	A	44	PHE	N-CA-C	7.41	119.00	111.07
1	A	64	GLU	N-CA-C	7.38	122.28	113.28
4	D	108	CYS	N-CA-CB	7.37	120.55	110.38
6	F	15	LEU	N-CA-C	-7.37	103.75	112.89
5	E	23	ILE	N-CA-C	-7.37	103.16	110.30
3	C	39	SER	N-CA-C	7.34	121.36	109.40
1	A	172	GLY	N-CA-C	-7.33	99.64	111.59
5	E	31	LEU	N-CA-C	-7.33	103.44	113.18
3	C	49	VAL	N-CA-C	7.28	119.09	107.73
1	A	63	THR	CA-CB-CG2	-7.25	98.18	110.50
3	C	80	GLU	N-CA-C	7.24	126.23	110.80
3	C	92	GLU	N-CA-C	7.23	120.57	111.24
1	A	177	GLN	CA-C-N	-7.23	109.83	120.38
1	A	177	GLN	C-N-CA	-7.23	109.83	120.38
7	G	1	MET	CG-SD-CE	7.22	116.77	100.90
4	D	125	LYS	N-CA-C	7.21	120.17	108.34
1	A	72	ILE	CB-CA-C	-7.20	102.67	111.88
3	C	3	PHE	CB-CA-C	7.19	122.32	110.81
8	H	21	MET	CB-CG-SD	-7.17	91.20	112.70
8	H	1	MET	CB-CG-SD	7.12	134.06	112.70
1	A	4	VAL	N-CA-C	7.11	117.62	110.23
3	C	123	GLN	N-CA-C	-7.11	104.48	113.72
1	A	25	TYR	CA-C-N	-7.09	110.22	123.34
1	A	25	TYR	C-N-CA	-7.09	110.22	123.34
3	C	88	GLU	CA-C-N	-7.08	111.25	122.08
3	C	88	GLU	C-N-CA	-7.08	111.25	122.08
2	B	110	LEU	CA-CB-CG	-7.06	91.60	116.30
2	B	62	VAL	O-C-N	-7.05	115.56	123.10
4	D	71	GLU	N-CA-C	7.04	125.79	110.80
5	E	12	ILE	O-C-N	6.93	129.36	121.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	GLY	CA-C-N	-6.92	109.48	121.66
2	B	146	GLY	C-N-CA	-6.92	109.48	121.66
3	C	200	GLN	N-CA-C	6.90	125.50	110.80
1	A	32	ILE	N-CA-C	6.88	123.64	109.34
1	A	202	HIS	CA-C-N	-6.87	110.53	120.29
1	A	202	HIS	C-N-CA	-6.87	110.53	120.29
4	D	12	ASP	N-CA-C	6.87	119.32	108.67
3	C	202	ASP	N-CA-C	6.86	125.41	110.80
1	A	105	TYR	CA-C-N	-6.85	111.49	122.66
1	A	105	TYR	C-N-CA	-6.85	111.49	122.66
1	A	190	VAL	N-CA-C	6.84	116.94	110.30
1	A	43	CYS	CA-C-N	-6.83	111.56	120.44
1	A	43	CYS	C-N-CA	-6.83	111.56	120.44
5	E	29	ILE	N-CA-C	-6.82	95.15	109.34
1	A	126	VAL	N-CA-C	6.82	117.58	110.62
2	B	155	LEU	N-CA-C	-6.82	102.22	112.04
3	C	125	GLN	N-CA-C	-6.81	103.31	111.69
1	A	79	GLY	N-CA-C	-6.78	104.59	112.73
2	B	15	ARG	CB-CG-CD	6.73	126.78	111.30
4	D	13	MET	CB-CG-SD	-6.73	92.52	112.70
3	C	93	GLU	N-CA-C	-6.73	105.04	113.18
4	D	81	VAL	CB-CA-C	-6.72	100.27	111.29
4	D	29	GLY	CA-C-N	-6.71	111.26	120.46
4	D	29	GLY	C-N-CA	-6.71	111.26	120.46
5	E	26	ILE	CB-CA-C	6.71	121.23	112.24
3	C	15	GLU	N-CA-CB	6.67	117.03	109.49
5	E	12	ILE	N-CA-CB	6.67	118.19	110.65
4	D	139	VAL	CB-CA-C	-6.67	100.36	111.29
1	A	63	THR	N-CA-C	6.66	118.33	111.14
2	B	149	PHE	CB-CA-C	-6.65	99.98	109.96
3	C	127	ILE	CB-CA-C	-6.61	100.68	110.33
2	B	26	TYR	N-CA-C	-6.59	105.78	113.88
2	B	15	ARG	NE-CZ-NH2	-6.58	113.27	119.20
1	A	49	ALA	N-CA-C	6.58	118.14	110.97
1	A	212	SER	N-CA-C	-6.57	96.81	110.80
2	B	142	TRP	N-CA-C	-6.56	103.33	112.45
3	C	246	GLU	N-CA-C	-6.55	99.62	110.17
1	A	170	ARG	CA-C-O	6.53	126.19	118.69
2	B	76	LEU	CA-C-N	-6.52	111.69	119.84
2	B	76	LEU	C-N-CA	-6.52	111.69	119.84
1	A	100	HIS	CB-CA-C	6.52	121.11	110.88
5	E	6	VAL	N-CA-C	6.50	116.61	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	134	ASP	N-CA-C	6.50	118.91	110.53
3	C	44	THR	CA-C-N	-6.48	111.99	121.71
3	C	44	THR	C-N-CA	-6.48	111.99	121.71
6	F	23	GLY	N-CA-C	6.47	120.33	112.49
3	C	46	PHE	CA-C-N	-6.47	112.51	122.09
3	C	46	PHE	C-N-CA	-6.47	112.51	122.09
1	A	197	VAL	N-CA-C	-6.47	103.57	110.36
3	C	157	ARG	N-CA-C	6.46	119.61	110.50
3	C	262	ILE	N-CA-C	6.46	117.98	110.62
2	B	117	VAL	CA-C-N	-6.46	109.21	121.54
2	B	117	VAL	C-N-CA	-6.46	109.21	121.54
2	B	104	VAL	CA-C-O	6.45	123.01	118.69
2	B	52	VAL	N-CA-C	-6.43	104.37	110.42
1	A	160	VAL	N-CA-CB	6.43	122.11	110.86
3	C	172	PHE	N-CA-C	6.43	119.98	109.76
1	A	119	ILE	CB-CA-C	-6.41	100.78	111.29
4	D	113	CYS	CA-CB-SG	-6.41	99.66	114.40
2	B	70	ALA	N-CA-C	6.38	120.52	107.69
4	D	35	LEU	N-CA-C	6.38	119.05	111.33
1	A	69	VAL	CB-CA-C	-6.35	103.72	112.04
3	C	36	VAL	N-CA-C	-6.35	95.17	108.88
5	E	14	LEU	CD1-CG-CD2	6.34	124.75	110.80
5	E	9	ILE	N-CA-C	6.34	117.84	110.62
3	C	10	PRO	CA-C-N	-6.33	113.69	120.47
3	C	10	PRO	C-N-CA	-6.33	113.69	120.47
2	B	119	LYS	CA-C-N	-6.33	111.88	122.64
2	B	119	LYS	C-N-CA	-6.33	111.88	122.64
7	G	33	ASN	N-CA-C	6.33	124.28	110.80
6	F	3	GLU	N-CA-C	-6.31	104.04	112.94
1	A	92	MET	CA-CB-CG	-6.29	101.52	114.10
4	D	107	VAL	N-CA-C	6.29	117.19	108.89
3	C	192	ASN	N-CA-C	6.29	124.19	110.80
2	B	120	PHE	N-CA-CB	6.27	120.85	110.63
1	A	58	TYR	O-C-N	-6.26	115.86	123.19
2	B	32	TRP	CA-C-N	6.25	127.66	119.84
2	B	32	TRP	C-N-CA	6.25	127.66	119.84
1	A	113	PRO	CA-C-N	6.18	133.35	121.54
1	A	113	PRO	C-N-CA	6.18	133.35	121.54
6	F	22	LEU	CB-CA-C	6.18	120.70	110.81
3	C	262	ILE	CB-CA-C	-6.17	103.96	112.04
5	E	26	ILE	N-CA-C	-6.16	104.28	111.00
4	D	39	VAL	N-CA-C	-6.10	105.78	111.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	7	ASP	CB-CA-C	6.09	120.91	110.79
3	C	113	VAL	CB-CA-C	-6.09	103.08	110.99
1	A	203	PHE	N-CA-C	6.08	117.99	111.36
3	C	113	VAL	N-CA-CB	-6.08	104.23	111.90
7	G	34	GLU	N-CA-C	6.08	123.76	110.80
1	A	91	SER	CA-CB-OG	-6.08	98.94	111.10
7	G	26	TYR	N-CA-C	-6.06	102.31	111.34
3	C	34	VAL	CB-CA-C	-6.06	101.35	111.29
2	B	122	ASN	N-CA-C	6.05	123.19	109.81
1	A	64	GLU	CA-CB-CG	-6.05	101.99	114.10
1	A	160	VAL	CB-CA-C	-6.05	104.59	111.55
3	C	103	PHE	N-CA-C	6.03	119.02	108.52
1	A	62	VAL	CG1-CB-CG2	6.03	124.07	110.80
1	A	197	VAL	CA-C-N	-6.03	110.44	120.68
1	A	197	VAL	C-N-CA	-6.03	110.44	120.68
4	D	175	LYS	N-CA-C	6.02	117.29	109.64
1	A	186	ALA	CB-CA-C	-6.02	101.69	110.96
4	D	70	LEU	N-CA-C	-6.02	97.98	110.80
3	C	37	PRO	CB-CA-C	-6.01	102.15	111.22
1	A	149	LYS	N-CA-C	5.97	117.48	110.97
1	A	169	LEU	CB-CG-CD1	-5.97	92.78	110.70
1	A	58	TYR	CA-C-N	-5.96	111.72	122.28
1	A	58	TYR	C-N-CA	-5.96	111.72	122.28
3	C	201	THR	N-CA-C	5.96	123.50	110.80
1	A	132	GLY	N-CA-C	5.96	127.31	113.18
1	A	180	LEU	N-CA-C	-5.96	104.79	111.28
3	C	263	CYS	N-CA-C	-5.96	104.72	112.23
3	C	137	THR	CB-CA-C	-5.93	98.77	110.27
2	B	21	GLY	CA-C-N	-5.92	110.24	121.54
2	B	21	GLY	C-N-CA	-5.92	110.24	121.54
1	A	83	ARG	CG-CD-NE	-5.91	99.00	112.00
5	E	12	ILE	CB-CA-C	-5.91	104.25	111.87
4	D	46	SER	CA-C-N	5.90	126.49	120.00
4	D	46	SER	C-N-CA	5.90	126.49	120.00
1	A	123	ILE	N-CA-C	-5.90	103.54	111.44
1	A	114	ARG	CA-C-N	-5.89	111.17	120.60
1	A	114	ARG	C-N-CA	-5.89	111.17	120.60
2	B	141	ILE	N-CA-C	5.88	121.58	109.34
1	A	141	ASP	N-CA-CB	-5.88	101.04	110.51
2	B	20	LYS	CA-C-O	5.88	125.60	119.14
4	D	139	VAL	N-CA-C	5.87	121.55	109.34
7	G	5	LEU	CA-CB-CG	-5.87	95.77	116.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	125	ARG	N-CA-C	5.86	123.28	110.80
2	B	130	THR	CB-CA-C	5.85	122.06	110.42
7	G	2	VAL	O-C-N	-5.84	116.60	122.62
3	C	217	LEU	N-CA-C	-5.83	100.39	109.72
1	A	63	THR	OG1-CB-CG2	5.82	120.94	109.30
6	F	10	LEU	CA-C-N	-5.82	110.81	121.52
6	F	10	LEU	C-N-CA	-5.82	110.81	121.52
1	A	134	THR	N-CA-C	5.81	118.09	111.11
1	A	136	TYR	CB-CA-C	-5.81	98.86	110.42
1	A	186	ALA	O-C-N	5.80	128.06	122.03
6	F	3	GLU	CB-CG-CD	5.79	122.44	112.60
3	C	138	THR	CA-C-N	-5.77	115.34	122.84
3	C	138	THR	C-N-CA	-5.77	115.34	122.84
3	C	149	ILE	CB-CA-C	-5.77	101.62	110.50
3	C	102	TYR	N-CA-C	5.75	119.03	107.41
3	C	182	LYS	N-CA-C	5.75	118.03	108.13
3	C	194	LYS	N-CA-C	5.75	123.04	110.80
2	B	57	LEU	CA-C-N	-5.74	116.66	122.74
2	B	57	LEU	C-N-CA	-5.74	116.66	122.74
1	A	12	LEU	N-CA-C	5.73	120.41	113.41
1	A	177	GLN	N-CA-CB	5.73	118.55	110.12
2	B	34	ASN	N-CA-C	5.73	123.00	110.80
2	B	22	MET	CA-C-N	-5.72	110.19	121.41
2	B	22	MET	C-N-CA	-5.72	110.19	121.41
8	H	21	MET	N-CA-C	5.72	119.07	111.75
4	D	26	THR	N-CA-CB	5.71	120.03	110.32
3	C	246	GLU	CB-CA-C	5.70	119.13	109.50
3	C	256	LYS	CB-CG-CD	5.70	124.40	111.30
2	B	152	ASP	CA-C-N	-5.69	113.20	122.65
2	B	152	ASP	C-N-CA	-5.69	113.20	122.65
4	D	37	PRO	N-CA-C	-5.68	106.13	113.57
5	E	14	LEU	N-CA-CB	-5.66	101.51	109.94
3	C	89	ARG	NE-CZ-NH1	-5.66	115.84	121.50
3	C	14	ARG	CA-C-N	-5.62	113.37	122.48
3	C	14	ARG	C-N-CA	-5.62	113.37	122.48
2	B	99	LEU	CA-CB-CG	-5.62	96.63	116.30
1	A	62	VAL	N-CA-CB	5.62	120.94	110.77
1	A	85	ILE	CB-CA-C	-5.61	104.70	111.88
1	A	31	ASN	N-CA-C	-5.60	101.91	110.14
3	C	47	LYS	CA-C-N	-5.60	115.10	123.00
3	C	47	LYS	C-N-CA	-5.60	115.10	123.00
1	A	134	THR	CB-CA-C	-5.59	101.86	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	141	ASN	CA-C-N	5.58	131.24	122.70
3	C	141	ASN	C-N-CA	5.58	131.24	122.70
3	C	256	LYS	N-CA-CB	5.58	118.05	109.91
4	D	63	ASN	N-CA-C	5.57	122.67	110.80
3	C	132	LEU	CB-CG-CD2	-5.57	93.98	110.70
1	A	191	LEU	CA-CB-CG	-5.57	96.81	116.30
4	D	27	VAL	CB-CA-C	5.56	119.31	112.02
3	C	150	HIS	CB-CA-C	-5.56	99.64	109.70
4	D	136	THR	CB-CA-C	-5.56	101.89	109.28
4	D	43	ILE	CA-C-N	5.56	123.72	119.66
4	D	43	ILE	C-N-CA	5.56	123.72	119.66
2	B	138	LEU	CD1-CG-CD2	5.54	123.00	110.80
4	D	158	ASP	N-CA-C	5.54	119.99	113.23
2	B	11	ASP	CB-CA-C	5.52	116.30	110.17
2	B	29	GLU	CB-CA-C	5.52	117.37	109.26
3	C	63	ALA	CA-C-N	5.52	128.23	120.28
3	C	63	ALA	C-N-CA	5.52	128.23	120.28
6	F	5	MET	CA-CB-CG	-5.52	103.06	114.10
2	B	141	ILE	CB-CA-C	-5.51	102.25	111.29
2	B	62	VAL	N-CA-C	-5.50	100.26	108.46
2	B	41	PRO	CA-C-N	-5.50	113.56	120.77
2	B	41	PRO	C-N-CA	-5.50	113.56	120.77
2	B	50	CYS	N-CA-C	5.49	118.03	111.71
3	C	21	VAL	CB-CA-C	-5.49	104.64	112.22
7	G	2	VAL	N-CA-C	5.49	118.46	109.78
1	A	62	VAL	CA-CB-CG1	-5.49	101.07	110.40
3	C	86	PRO	N-CA-C	-5.49	102.51	111.68
2	B	65	PRO	N-CD-CG	-5.49	94.97	103.20
1	A	169	LEU	CD1-CG-CD2	5.48	122.86	110.80
1	A	133	VAL	CB-CA-C	-5.48	104.87	111.88
1	A	126	VAL	CA-CB-CG2	-5.48	101.09	110.40
3	C	147	TYR	CA-C-N	-5.47	109.83	121.32
3	C	147	TYR	C-N-CA	-5.47	109.83	121.32
1	A	173	SER	CA-CB-OG	-5.47	100.16	111.10
3	C	75	VAL	CB-CA-C	-5.45	103.43	110.84
3	C	246	GLU	CB-CG-CD	5.43	121.84	112.60
3	C	52	ILE	CB-CA-C	-5.43	101.48	111.36
1	A	187	HIS	CA-C-N	-5.42	113.64	122.26
1	A	187	HIS	C-N-CA	-5.42	113.64	122.26
1	A	26	VAL	CB-CA-C	5.41	117.40	111.18
4	D	142	GLY	N-CA-C	-5.41	101.31	112.34
3	C	71	ASN	N-CA-C	5.41	117.90	108.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	27	LEU	O-C-N	5.40	128.53	122.32
3	C	11	PRO	CA-C-N	-5.39	112.21	122.08
3	C	11	PRO	C-N-CA	-5.39	112.21	122.08
2	B	69	PHE	N-CA-C	5.38	119.47	113.02
2	B	128	VAL	N-CA-C	5.37	116.15	110.72
4	D	130	GLY	N-CA-C	5.37	125.91	113.18
1	A	10	GLU	CA-C-N	5.37	131.79	121.54
1	A	10	GLU	C-N-CA	5.37	131.79	121.54
3	C	97	GLU	N-CA-C	-5.37	106.73	113.28
1	A	105	TYR	CB-CA-C	-5.36	101.84	110.74
2	B	120	PHE	O-C-N	5.35	129.25	123.10
4	D	135	GLU	N-CA-C	5.32	122.13	110.80
2	B	153	LYS	CB-CG-CD	5.32	123.52	111.30
1	A	83	ARG	CA-CB-CG	-5.31	103.48	114.10
3	C	38	GLN	CA-C-N	-5.31	114.97	122.94
3	C	38	GLN	C-N-CA	-5.31	114.97	122.94
2	B	71	THR	N-CA-C	5.30	117.30	109.50
2	B	117	VAL	N-CA-CB	5.30	119.98	111.23
4	D	62	ASN	N-CA-C	5.30	118.46	109.76
3	C	253	ASN	N-CA-C	5.30	116.74	111.07
8	H	14	VAL	CB-CA-C	-5.29	104.91	112.22
2	B	92	PRO	CA-C-N	-5.29	113.60	122.17
2	B	92	PRO	C-N-CA	-5.29	113.60	122.17
1	A	54	MET	CA-C-N	-5.28	110.72	121.18
1	A	54	MET	C-N-CA	-5.28	110.72	121.18
3	C	234	ASN	N-CA-C	5.28	121.49	109.81
4	D	55	THR	N-CA-C	5.27	117.34	109.59
3	C	25	CYS	CA-C-N	-5.27	115.41	122.42
3	C	25	CYS	C-N-CA	-5.27	115.41	122.42
4	D	27	VAL	N-CA-C	5.27	115.48	110.53
4	D	76	GLY	N-CA-C	-5.26	107.74	114.37
8	H	14	VAL	N-CA-CB	5.26	118.47	110.58
3	C	93	GLU	N-CA-CB	5.26	119.25	110.41
7	G	24	ALA	N-CA-CB	5.25	118.39	110.30
2	B	122	ASN	CA-C-N	-5.22	113.31	119.84
2	B	122	ASN	C-N-CA	-5.22	113.31	119.84
3	C	90	ILE	N-CA-C	-5.22	97.60	108.88
1	A	122	VAL	CA-C-N	-5.22	111.31	120.29
1	A	122	VAL	C-N-CA	-5.22	111.31	120.29
2	B	59	PRO	O-C-N	5.22	128.97	122.71
3	C	250	GLN	CB-CG-CD	-5.22	103.73	112.60
2	B	81	LEU	CB-CG-CD2	-5.21	95.06	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	106	ALA	N-CA-C	5.21	119.49	113.18
8	H	8	TRP	N-CA-C	5.21	117.36	111.11
2	B	45	MET	N-CA-C	5.21	117.64	111.33
1	A	63	THR	CA-C-N	-5.20	112.39	122.06
1	A	63	THR	C-N-CA	-5.20	112.39	122.06
2	B	74	GLU	CA-C-N	-5.19	116.17	123.13
2	B	74	GLU	C-N-CA	-5.19	116.17	123.13
3	C	127	ILE	CA-C-N	-5.19	115.49	122.91
3	C	127	ILE	C-N-CA	-5.19	115.49	122.91
4	D	161	VAL	N-CA-C	5.18	114.96	106.72
1	A	20	ASP	CA-C-N	-5.18	112.26	120.55
1	A	20	ASP	C-N-CA	-5.18	112.26	120.55
2	B	125	ARG	CA-C-O	-5.17	113.12	120.51
3	C	248	VAL	CB-CA-C	-5.17	103.81	110.84
1	A	119	ILE	CB-CG1-CD1	-5.17	102.95	113.80
2	B	111	VAL	N-CA-C	5.16	120.03	108.88
1	A	102	PHE	CA-C-N	-5.16	113.37	120.28
1	A	102	PHE	C-N-CA	-5.16	113.37	120.28
3	C	270	LEU	N-CA-C	-5.16	105.57	111.14
5	E	14	LEU	N-CA-C	5.15	117.29	111.11
1	A	67	ALA	N-CA-CB	-5.14	102.30	110.22
3	C	126	GLU	N-CA-C	-5.14	101.50	109.72
1	A	24	LYS	N-CA-C	-5.13	101.51	109.72
1	A	94	VAL	N-CA-CB	5.12	116.88	110.47
2	B	127	PRO	CA-CB-CG	-5.12	94.77	104.50
4	D	127	PRO	N-CA-C	-5.12	107.36	114.27
2	B	29	GLU	CA-C-N	-5.10	114.66	119.76
2	B	29	GLU	C-N-CA	-5.10	114.66	119.76
6	F	26	LEU	O-C-N	5.10	128.01	122.20
1	A	113	PRO	CA-N-CD	5.10	119.14	112.00
5	E	29	ILE	N-CA-CB	5.10	119.64	111.23
3	C	14	ARG	N-CA-C	5.10	117.27	109.07
3	C	82	PHE	N-CA-C	-5.09	102.95	110.48
1	A	182	ARG	NE-CZ-NH1	-5.08	116.42	121.50
6	F	25	LEU	CB-CG-CD2	-5.08	95.45	110.70
1	A	81	LEU	CB-CG-CD2	-5.08	95.47	110.70
1	A	105	TYR	N-CA-C	5.06	119.72	111.37
1	A	103	ARG	N-CA-CB	5.05	117.54	110.12
4	D	80	LEU	N-CA-C	5.05	117.04	110.43
6	F	18	VAL	CB-CA-C	-5.05	105.42	111.88
2	B	127	PRO	CA-C-N	-5.03	113.27	120.42
2	B	127	PRO	C-N-CA	-5.03	113.27	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	7	ASP	CB-CG-OD1	5.03	129.97	118.40
1	A	162	GLY	N-CA-C	5.03	125.09	113.18
2	B	109	ILE	CB-CA-C	-5.03	103.05	111.29
3	C	142	ILE	N-CA-CB	-5.03	104.55	111.99
4	D	35	LEU	CA-CB-CG	-5.02	98.73	116.30
3	C	232	THR	N-CA-C	5.02	117.52	111.40
1	A	87	ARG	CB-CG-CD	5.00	122.80	111.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LYS	Peptide
1	A	161	VAL	Peptide
1	A	2	ALA	Peptide
1	A	73	MET	Peptide
2	B	124	PHE	Peptide
2	B	2	ALA	Peptide
2	B	32	TRP	Peptide
3	C	191	GLY	Peptide
3	C	200	GLN	Peptide
3	C	216	GLU	Peptide
3	C	222	GLY	Peptide
3	C	225	VAL	Peptide
3	C	230	ALA	Peptide
3	C	81	GLY	Peptide
4	D	108	CYS	Peptide
4	D	158	ASP	Peptide
4	D	65	LYS	Peptide
4	D	96	LYS	Peptide
4	D	97	GLU	Peptide
5	E	28	SER	Peptide
6	F	26	LEU	Peptide
6	F	27	LEU	Peptide
6	F	9	ALA	Peptide
7	G	27	GLN	Peptide
7	G	31	ARG	Peptide
8	H	2	GLU	Peptide
8	H	27	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1711	0	1736	315	0
2	B	1249	0	1308	265	0
3	C	2216	0	2233	417	1
4	D	1288	0	1273	236	0
5	E	248	0	284	41	0
6	F	242	0	260	63	0
7	G	283	0	289	76	1
8	H	230	0	239	52	0
9	A	1	0	0	0	0
10	A	86	0	60	41	0
11	A	43	0	31	23	0
11	C	43	0	32	29	0
12	A	54	0	79	17	0
12	B	54	0	83	2	0
13	A	136	0	165	6	0
14	B	65	0	72	6	0
15	B	60	0	70	38	0
16	D	4	0	0	1	0
17	D	54	0	53	9	0
18	G	40	0	52	9	0
19	A	2	0	0	0	0
19	B	2	0	0	0	0
19	C	1	0	0	0	0
All	All	8112	0	8319	1392	1

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 85.

All (1392) 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)
6:F:25:LEU:CD1	6:F:25:LEU:CG	1.77	1.62
3:C:256:LYS:CG	3:C:256:LYS:CD	1.80	1.59
2:B:138:LEU:CG	2:B:138:LEU:CD1	1.74	1.59
7:G:3:GLU:CD	7:G:3:GLU:CG	1.76	1.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:256:LYS:CE	3:C:256:LYS:NZ	1.74	1.50
1:A:92:MET:CE	12:A:1002:OPC:HCB2	1.37	1.48
1:A:113:PRO:CG	1:A:113:PRO:CB	1.77	1.46
7:G:29:TYR:O	7:G:29:TYR:CD2	1.69	1.44
1:A:92:MET:HE3	12:A:1002:OPC:CCB	1.45	1.43
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	1.35	1.37
3:C:22:CYS:HB2	11:C:301:HEC:CAB	1.55	1.35
6:F:29:ILE:O	6:F:29:ILE:CD1	1.75	1.35
6:F:29:ILE:O	6:F:29:ILE:HD12	1.20	1.33
4:D:85:LYS:NZ	4:D:85:LYS:HB2	1.17	1.31
2:B:93:ASN:OD1	2:B:96:LEU:HB2	1.25	1.28
6:F:7:TYR:O	6:F:11:LEU:CD1	1.83	1.27
4:D:122:ASN:HB3	4:D:135:GLU:OE2	1.33	1.26
3:C:65:GLY:O	3:C:66:SER:O	1.52	1.26
2:B:9:LEU:O	2:B:15:ARG:HD2	1.31	1.24
3:C:200:GLN:HG3	3:C:205:LYS:O	1.37	1.24
4:D:111:LEU:N	4:D:111:LEU:CD1	2.04	1.19
3:C:15:GLU:HB3	3:C:16:PRO:HD2	1.23	1.19
13:A:1104:UMQ:H31	13:A:1104:UMQ:H6'2	1.20	1.15
2:B:142:TRP:CH2	2:B:155:LEU:O	1.99	1.15
4:D:85:LYS:NZ	4:D:85:LYS:CB	2.11	1.14
3:C:157:ARG:HB2	11:C:301:HEC:HAD2	1.25	1.14
4:D:111:LEU:N	4:D:111:LEU:HD13	1.51	1.14
10:A:301:HEM:CBB	10:A:301:HEM:HMB2	1.77	1.13
1:A:54:MET:CE	10:A:301:HEM:HBD1	1.78	1.13
4:D:139:VAL:HG22	4:D:147:SER:CA	1.77	1.13
2:B:34:ASN:ND2	3:C:283:GLN:HE22	1.47	1.12
3:C:93:GLU:N	3:C:93:GLU:OE1	1.83	1.11
3:C:188:ASP:O	3:C:190:TYR:N	1.81	1.11
6:F:11:LEU:HB3	6:F:15:LEU:HD12	1.32	1.11
4:D:109:THR:CG2	4:D:144:ALA:HB1	1.80	1.11
4:D:146:LEU:HD12	4:D:177:TRP:CD2	1.84	1.11
2:B:95:LEU:O	2:B:95:LEU:HD23	1.49	1.11
3:C:19:ARG:O	3:C:20:ILE:HB	1.46	1.11
3:C:211:ILE:O	3:C:211:ILE:HG13	1.38	1.10
2:B:152:ASP:HA	2:B:154:THR:HG22	1.12	1.10
6:F:7:TYR:O	6:F:11:LEU:HD12	0.92	1.10
1:A:39:ILE:HD11	18:G:101:BCR:H312	1.17	1.09
4:D:109:THR:HG22	4:D:144:ALA:CB	1.82	1.09
2:B:96:LEU:HD13	2:B:100:LEU:CD1	1.81	1.09
12:A:1002:OPC:HBV1	7:G:9:LEU:HD21	1.34	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:1202:TDS:HAA3	15:B:1202:TDS:OAC	1.51	1.08
1:A:163:VAL:HG12	1:A:164:LEU:N	1.58	1.08
3:C:171:VAL:HG12	3:C:235:PRO:HD2	1.11	1.08
3:C:171:VAL:HG12	3:C:235:PRO:CD	1.84	1.08
2:B:91:VAL:HG12	2:B:91:VAL:O	1.29	1.07
7:G:2:VAL:CG1	7:G:4:PRO:HD3	1.84	1.07
3:C:22:CYS:CB	11:C:301:HEC:HAB	1.83	1.07
7:G:26:TYR:O	7:G:28:GLN:N	1.86	1.07
1:A:97:MET:HE1	1:A:125:ALA:HA	1.10	1.06
1:A:97:MET:CE	1:A:125:ALA:HA	1.83	1.06
2:B:124:PHE:HE1	7:G:26:TYR:HB2	1.20	1.06
3:C:171:VAL:CG1	3:C:235:PRO:HD2	1.85	1.06
1:A:54:MET:HE3	10:A:301:HEM:HBD1	1.22	1.06
4:D:137:GLY:HA3	4:D:171:ARG:NH1	1.71	1.06
1:A:92:MET:HB3	12:A:1002:OPC:HCB1	1.38	1.05
3:C:70:LEU:N	3:C:70:LEU:HD23	1.69	1.05
3:C:144:PHE:CZ	3:C:251:ASP:HB2	1.91	1.05
1:A:7:TRP:CE2	1:A:11:ARG:NH2	2.24	1.04
4:D:139:VAL:H	4:D:147:SER:HB3	1.16	1.04
2:B:132:ILE:HD12	2:B:132:ILE:H	1.22	1.03
1:A:36:LEU:HB3	1:A:100:HIS:HB2	1.38	1.03
10:A:302:HEM:HBC2	10:A:302:HEM:HMC2	1.40	1.03
1:A:106:LEU:HD21	2:B:133:PHE:CE1	1.93	1.02
1:A:207:ARG:HG3	1:A:207:ARG:HH11	1.24	1.02
4:D:122:ASN:CB	4:D:135:GLU:OE2	2.07	1.02
7:G:29:TYR:O	7:G:29:TYR:CG	2.10	1.02
6:F:11:LEU:HB3	6:F:15:LEU:CD1	1.89	1.02
10:A:301:HEM:CMB	10:A:301:HEM:CBB	2.30	1.01
3:C:70:LEU:HD23	3:C:70:LEU:H	1.18	1.01
3:C:84:ILE:HD11	3:C:114:LEU:HD13	1.42	1.01
6:F:13:PHE:CE2	6:F:17:PHE:HE1	1.79	1.01
1:A:47:GLN:HE21	1:A:47:GLN:CA	1.74	1.01
2:B:96:LEU:HD13	2:B:100:LEU:HD11	1.39	1.00
4:D:139:VAL:CG2	4:D:147:SER:HB3	1.90	1.00
1:A:113:PRO:HG3	2:B:21:GLY:HA3	1.39	1.00
3:C:70:LEU:N	3:C:70:LEU:CD2	2.25	0.99
4:D:133:TYR:CE2	4:D:148:LEU:HD23	1.96	0.99
1:A:61:THR:HA	1:A:177:GLN:HE22	1.25	0.99
1:A:103:ARG:HD2	1:A:103:ARG:C	1.86	0.98
3:C:171:VAL:CG1	3:C:234:ASN:HD22	1.75	0.98
1:A:41:LEU:HD23	11:A:303:HEC:CBC	1.93	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HG22	1:A:33:PHE:CD2	1.99	0.97
5:E:22:ILE:O	5:E:26:ILE:HB	1.63	0.97
2:B:128:VAL:O	2:B:132:ILE:CD1	2.12	0.97
3:C:28:ALA:HB3	3:C:239:GLY:HA3	1.45	0.97
3:C:15:GLU:CB	3:C:16:PRO:HD2	1.95	0.97
1:A:110:PHE:HD1	2:B:112:PRO:HB3	1.26	0.97
1:A:150:ILE:HD13	15:B:1201:TDS:CAA	1.95	0.96
5:E:18:ILE:O	5:E:22:ILE:HG22	1.63	0.96
3:C:176:ALA:HB1	3:C:205:LYS:NZ	1.80	0.96
1:A:26:VAL:HG21	1:A:30:VAL:HG11	1.47	0.96
1:A:110:PHE:H	1:A:110:PHE:HD2	1.09	0.96
2:B:91:VAL:O	2:B:91:VAL:CG1	2.07	0.96
3:C:189:GLU:O	3:C:190:TYR:CD2	2.18	0.96
3:C:273:ILE:HG13	8:H:21:MET:HG3	1.44	0.96
2:B:82:TYR:N	2:B:83:PRO:HD2	1.78	0.96
2:B:142:TRP:HH2	2:B:155:LEU:O	1.45	0.96
3:C:120:PRO:HD2	3:C:124:TYR:HD1	1.30	0.96
11:A:303:HEC:HBB2	11:A:303:HEC:HMB3	1.46	0.95
6:F:20:TRP:O	6:F:24:VAL:HG23	1.65	0.95
2:B:128:VAL:O	2:B:132:ILE:HD12	1.65	0.95
1:A:150:ILE:HD13	15:B:1201:TDS:HAA3	1.48	0.95
10:A:301:HEM:O2D	10:A:301:HEM:HBA2	1.66	0.95
3:C:15:GLU:HB3	3:C:16:PRO:CD	1.96	0.95
4:D:84:LEU:HD12	4:D:84:LEU:H	1.31	0.95
2:B:34:ASN:HD21	3:C:283:GLN:NE2	1.65	0.95
3:C:141:ASN:N	3:C:141:ASN:HD22	1.59	0.95
1:A:163:VAL:CG1	1:A:164:LEU:N	2.30	0.95
2:B:40:PHE:CB	2:B:41:PRO:HD3	1.95	0.95
7:G:2:VAL:HG13	7:G:4:PRO:HD3	1.46	0.94
1:A:39:ILE:HD11	18:G:101:BCR:C31	1.97	0.94
2:B:25:ASN:HD22	2:B:25:ASN:H	1.15	0.94
3:C:170:ASN:O	3:C:235:PRO:HG3	1.67	0.94
4:D:146:LEU:CD1	4:D:177:TRP:CG	2.50	0.94
1:A:31:ASN:C	1:A:31:ASN:HD22	1.74	0.94
1:A:147:ALA:HB2	15:B:1201:TDS:HAJ3	1.46	0.94
10:A:301:HEM:HBB2	10:A:301:HEM:HMB2	0.95	0.94
2:B:152:ASP:CA	2:B:154:THR:HG22	1.97	0.94
2:B:93:ASN:OD1	2:B:96:LEU:CB	2.17	0.93
6:F:29:ILE:O	6:F:29:ILE:HD13	1.67	0.93
1:A:70:GLN:O	1:A:74:ASN:HB2	1.69	0.93
4:D:66:VAL:HG23	4:D:158:ASP:O	1.69	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:285:ALA:C	3:C:286:GLU:OE1	2.11	0.93
4:D:109:THR:HG22	4:D:144:ALA:HB1	0.94	0.93
2:B:109:ILE:O	2:B:112:PRO:HD2	1.69	0.93
3:C:288:ASN:C	3:C:288:ASN:HD22	1.76	0.93
3:C:200:GLN:CG	3:C:205:LYS:O	2.16	0.93
3:C:193:VAL:O	3:C:194:LYS:HG2	1.69	0.92
3:C:178:GLY:O	3:C:224:ALA:HA	1.69	0.92
2:B:79:TRP:CD1	2:B:80:TYR:N	2.38	0.92
11:A:303:HEC:CGA	15:B:1202:TDS:HAA2	2.00	0.92
3:C:170:ASN:O	3:C:235:PRO:CG	2.17	0.92
6:F:29:ILE:HD12	6:F:29:ILE:C	1.96	0.91
3:C:180:ILE:HD11	3:C:183:ILE:CD1	2.00	0.91
3:C:141:ASN:HD22	3:C:141:ASN:H	1.12	0.91
1:A:103:ARG:NH1	1:A:104:VAL:HG23	1.86	0.91
3:C:144:PHE:CE2	3:C:251:ASP:HB2	2.05	0.91
1:A:39:ILE:CD1	18:G:101:BCR:H312	2.01	0.90
2:B:96:LEU:CD1	2:B:100:LEU:HD11	2.01	0.90
1:A:47:GLN:HE21	1:A:47:GLN:HA	1.31	0.90
1:A:112:LYS:O	1:A:113:PRO:C	2.12	0.90
4:D:94:GLU:OE2	4:D:100:ARG:HG2	1.70	0.90
3:C:200:GLN:O	3:C:205:LYS:HG2	1.70	0.90
7:G:11:LEU:N	7:G:11:LEU:HD23	1.85	0.90
2:B:115:GLU:OE2	2:B:126:ARG:NH1	2.04	0.90
4:D:146:LEU:HD12	4:D:177:TRP:CG	2.06	0.90
1:A:26:VAL:CG2	1:A:30:VAL:HG11	2.02	0.90
11:A:303:HEC:O2A	15:B:1202:TDS:HAA2	1.71	0.90
2:B:57:LEU:HD12	8:H:8:TRP:CE3	2.06	0.90
2:B:138:LEU:CD1	2:B:138:LEU:HG	2.01	0.90
4:D:139:VAL:HG22	4:D:147:SER:CB	2.01	0.90
3:C:211:ILE:O	3:C:212:PRO:O	1.91	0.89
3:C:119:LEU:CD2	3:C:124:TYR:CD1	2.55	0.89
2:B:88:LEU:HD13	15:B:1201:TDS:CAI	2.03	0.89
2:B:124:PHE:CE1	7:G:26:TYR:HB2	2.07	0.89
1:A:30:VAL:HG22	1:A:34:TYR:CG	2.08	0.89
1:A:47:GLN:HA	1:A:47:GLN:NE2	1.87	0.89
4:D:139:VAL:HG23	4:D:147:SER:HB3	1.54	0.89
3:C:40:VAL:HG12	8:H:1:MET:HE1	1.56	0.89
3:C:60:GLN:HE22	3:C:157:ARG:HG2	1.36	0.89
1:A:108:GLY:HA2	1:A:110:PHE:CE2	2.07	0.88
4:D:85:LYS:HB2	4:D:85:LYS:HZ3	1.06	0.88
7:G:10:VAL:HG12	7:G:11:LEU:HD23	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ASP:HA	2:B:154:THR:CG2	2.03	0.88
6:F:6:LEU:O	6:F:10:LEU:HB2	1.74	0.88
7:G:29:TYR:O	7:G:29:TYR:HD2	1.55	0.88
4:D:139:VAL:HG22	4:D:147:SER:HA	1.54	0.88
3:C:171:VAL:HG11	3:C:234:ASN:HD22	1.36	0.88
1:A:103:ARG:HH12	1:A:104:VAL:HG23	1.38	0.87
3:C:22:CYS:HB2	11:C:301:HEC:HAB	0.89	0.87
3:C:71:ASN:HB2	11:C:301:HEC:O2A	1.74	0.87
2:B:118:ASN:HD22	2:B:120:PHE:H	1.22	0.87
1:A:100:HIS:HE1	10:A:302:HEM:C1A	1.93	0.87
3:C:119:LEU:HD23	3:C:124:TYR:CD1	2.10	0.87
4:D:110:HIS:HB3	16:D:200:FES:S2	2.14	0.87
2:B:4:LEU:H	3:C:287:MET:CE	1.87	0.86
2:B:79:TRP:CG	2:B:80:TYR:N	2.43	0.86
3:C:52:ILE:O	3:C:52:ILE:HG22	1.75	0.86
1:A:163:VAL:HG12	1:A:164:LEU:H	1.40	0.86
4:D:109:THR:HG21	4:D:146:LEU:O	1.74	0.86
6:F:22:LEU:HD13	6:F:22:LEU:C	1.99	0.86
4:D:85:LYS:CB	4:D:85:LYS:HZ3	1.83	0.86
4:D:134:ASP:OD1	4:D:134:ASP:C	2.18	0.86
1:A:61:THR:HG22	1:A:64:GLU:H	1.41	0.86
3:C:22:CYS:CB	11:C:301:HEC:CAB	2.50	0.86
3:C:211:ILE:O	3:C:211:ILE:CG1	2.22	0.86
3:C:219:VAL:HG12	3:C:219:VAL:O	1.73	0.86
6:F:25:LEU:CD1	6:F:25:LEU:HG	2.05	0.86
3:C:223:GLN:HG3	3:C:224:ALA:H	1.41	0.85
4:D:21:LEU:HD11	17:D:201:SQD:H301	1.58	0.85
4:D:102:TYR:HA	4:D:151:CYS:O	1.76	0.85
4:D:69:PHE:HD2	4:D:69:PHE:C	1.83	0.85
1:A:26:VAL:CG2	1:A:30:VAL:CG1	2.54	0.85
1:A:39:ILE:HG22	1:A:96:MET:HG3	1.56	0.85
3:C:226:LYS:HB3	3:C:226:LYS:HZ3	1.40	0.85
6:F:13:PHE:CE2	6:F:17:PHE:CE1	2.64	0.85
3:C:60:GLN:NE2	3:C:157:ARG:HG2	1.90	0.85
3:C:71:ASN:N	11:C:301:HEC:O2A	2.10	0.85
3:C:28:ALA:HB3	3:C:239:GLY:CA	2.07	0.85
2:B:77:PRO:HB3	15:B:1201:TDS:CAM	2.07	0.85
4:D:68:LYS:HA	4:D:71:GLU:HB2	1.59	0.85
2:B:95:LEU:HD23	2:B:95:LEU:C	2.02	0.84
3:C:259:ILE:HD12	8:H:6:LEU:HD13	1.57	0.84
4:D:110:HIS:C	4:D:111:LEU:CD1	2.50	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ILE:HG22	2:B:115:GLU:N	1.90	0.84
6:F:5:MET:HG2	6:F:6:LEU:N	1.92	0.84
14:B:201:CLA:HBB1	14:B:201:CLA:HMB1	1.57	0.84
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.13	0.83
1:A:142:GLN:OE1	1:A:142:GLN:HA	1.78	0.83
11:C:301:HEC:HMC1	11:C:301:HEC:HBC3	1.60	0.83
11:A:303:HEC:HBB2	11:A:303:HEC:CMB	2.09	0.83
2:B:34:ASN:HD21	3:C:283:GLN:HE22	0.88	0.83
2:B:79:TRP:CD1	2:B:79:TRP:C	2.57	0.83
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.59	0.83
1:A:103:ARG:HD2	1:A:103:ARG:O	1.79	0.83
4:D:143:PRO:O	4:D:145:PRO:HD3	1.79	0.82
1:A:92:MET:CB	12:A:1002:OPC:HCB1	2.08	0.82
5:E:5:ALA:O	5:E:9:ILE:HG13	1.80	0.82
2:B:159:LEU:O	2:B:160:PHE:CD2	2.33	0.82
1:A:215:LEU:HD13	2:B:122:ASN:HA	1.61	0.82
2:B:70:ALA:HB1	3:C:17:THR:HG22	1.61	0.82
4:D:111:LEU:N	4:D:111:LEU:HD12	1.90	0.82
4:D:139:VAL:H	4:D:147:SER:CB	1.92	0.82
4:D:133:TYR:CD2	4:D:148:LEU:HD23	2.15	0.81
4:D:21:LEU:CD1	17:D:201:SQD:H301	2.10	0.81
1:A:26:VAL:HG21	1:A:30:VAL:CG1	2.10	0.81
4:D:102:TYR:OH	4:D:136:THR:HG22	1.80	0.81
1:A:108:GLY:HA2	1:A:110:PHE:HE2	1.45	0.81
3:C:229:GLU:HA	3:C:229:GLU:OE1	1.78	0.81
3:C:13:PRO:O	3:C:21:VAL:HG22	1.81	0.81
2:B:130:THR:CG2	7:G:22:PHE:HE2	1.93	0.81
2:B:82:TYR:N	2:B:83:PRO:CD	2.44	0.81
3:C:139:ASP:OD1	3:C:139:ASP:C	2.19	0.81
3:C:119:LEU:CD2	3:C:124:TYR:CE1	2.64	0.81
4:D:80:LEU:C	4:D:81:VAL:HG23	2.05	0.81
1:A:155:PRO:HD3	15:B:1201:TDS:HAX2	1.63	0.80
3:C:171:VAL:CG1	3:C:234:ASN:HA	2.11	0.80
5:E:10:VAL:O	5:E:14:LEU:HB2	1.81	0.80
10:A:302:HEM:HMC2	10:A:302:HEM:CBC	2.11	0.80
4:D:12:ASP:O	4:D:13:MET:C	2.23	0.80
4:D:137:GLY:HA3	4:D:171:ARG:HH11	1.46	0.80
2:B:57:LEU:HD12	8:H:8:TRP:CD2	2.17	0.80
3:C:250:GLN:HG3	3:C:251:ASP:N	1.97	0.80
2:B:118:ASN:ND2	2:B:120:PHE:H	1.78	0.80
2:B:90:SER:O	2:B:91:VAL:HG23	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LEU:CD1	8:H:8:TRP:CD2	2.64	0.80
4:D:139:VAL:HG22	4:D:147:SER:HB3	1.60	0.80
4:D:139:VAL:HG22	4:D:147:SER:N	1.97	0.80
2:B:91:VAL:O	2:B:93:ASN:N	2.15	0.79
3:C:107:LYS:HE3	3:C:110:GLN:HE22	1.45	0.79
3:C:177:THR:HG21	3:C:226:LYS:HD2	1.62	0.79
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.17	0.79
6:F:24:VAL:O	6:F:27:LEU:HB2	1.81	0.79
1:A:7:TRP:NE1	1:A:11:ARG:NH2	2.29	0.79
3:C:84:ILE:HD11	3:C:114:LEU:CD1	2.12	0.79
1:A:110:PHE:CD1	2:B:112:PRO:HB3	2.15	0.79
3:C:226:LYS:HB3	3:C:226:LYS:NZ	1.96	0.79
4:D:105:ASN:HB3	4:D:149:ALA:HB3	1.63	0.79
7:G:26:TYR:C	7:G:28:GLN:H	1.91	0.79
2:B:104:VAL:O	2:B:108:LEU:HB2	1.81	0.79
4:D:85:LYS:HB2	4:D:85:LYS:HZ2	0.97	0.79
1:A:207:ARG:NH1	15:B:1202:TDS:HAI2	1.98	0.79
3:C:206:THR:CG2	3:C:206:THR:O	2.30	0.78
1:A:36:LEU:HD21	1:A:99:LEU:HB3	1.65	0.78
3:C:107:LYS:HE3	3:C:110:GLN:NE2	1.97	0.78
3:C:141:ASN:N	3:C:141:ASN:ND2	2.31	0.78
4:D:69:PHE:C	4:D:69:PHE:CD2	2.61	0.78
4:D:85:LYS:CB	4:D:85:LYS:HZ2	1.83	0.78
4:D:105:ASN:HD21	4:D:107:VAL:HG23	1.46	0.78
3:C:46:PHE:CZ	3:C:131:VAL:HG22	2.19	0.78
10:A:302:HEM:HHA	10:A:302:HEM:HBA1	1.66	0.78
1:A:83:ARG:HD2	10:A:301:HEM:O1D	1.84	0.78
3:C:171:VAL:CG1	3:C:234:ASN:ND2	2.46	0.78
3:C:199:ILE:O	3:C:200:GLN:HB2	1.82	0.78
3:C:120:PRO:HD2	3:C:124:TYR:CD1	2.18	0.77
3:C:107:LYS:CE	3:C:110:GLN:HE22	1.96	0.77
3:C:219:VAL:O	3:C:219:VAL:CG1	2.32	0.77
3:C:286:GLU:OE1	3:C:286:GLU:N	2.17	0.77
4:D:21:LEU:HD12	17:D:201:SQD:H282	1.66	0.77
2:B:40:PHE:HB2	2:B:41:PRO:HD3	1.64	0.77
6:F:29:ILE:CD1	6:F:29:ILE:C	2.57	0.77
3:C:176:ALA:HB1	3:C:205:LYS:HZ1	1.49	0.77
3:C:19:ARG:O	3:C:20:ILE:CB	2.20	0.77
3:C:180:ILE:HD11	3:C:183:ILE:HD12	1.67	0.77
1:A:103:ARG:HA	7:G:21:LEU:HD21	1.67	0.77
10:A:301:HEM:HBB2	10:A:301:HEM:HMB3	1.63	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:LEU:HD23	3:C:124:TYR:CE1	2.19	0.77
3:C:270:LEU:HA	8:H:21:MET:CE	2.15	0.77
4:D:80:LEU:C	4:D:81:VAL:CG2	2.56	0.77
5:E:29:ILE:HG22	5:E:29:ILE:O	1.85	0.77
3:C:171:VAL:HG11	3:C:234:ASN:HA	1.64	0.77
4:D:110:HIS:C	4:D:111:LEU:HD12	2.08	0.77
4:D:139:VAL:CG2	4:D:147:SER:N	2.48	0.77
1:A:207:ARG:HH11	1:A:207:ARG:CG	1.97	0.77
2:B:16:ALA:O	2:B:19:ALA:HB3	1.85	0.77
3:C:178:GLY:O	3:C:224:ALA:CA	2.32	0.77
3:C:178:GLY:O	3:C:224:ALA:CB	2.33	0.76
12:A:1002:OPC:CBV	7:G:9:LEU:HD21	2.13	0.76
4:D:161:VAL:HG12	4:D:161:VAL:O	1.83	0.76
4:D:12:ASP:O	4:D:14:GLY:N	2.18	0.76
1:A:150:ILE:CD1	15:B:1201:TDS:CAA	2.64	0.76
2:B:10:SER:O	2:B:12:PRO:HD3	1.86	0.76
3:C:14:ARG:CZ	3:C:150:HIS:CD2	2.69	0.76
3:C:200:GLN:NE2	3:C:206:THR:OG1	2.19	0.76
6:F:13:PHE:HE2	6:F:17:PHE:CE1	2.02	0.76
4:D:69:PHE:O	4:D:70:LEU:O	2.03	0.76
4:D:108:CYS:HB2	4:D:133:TYR:OH	1.86	0.76
3:C:71:ASN:OD1	3:C:120:PRO:HA	1.86	0.75
3:C:270:LEU:HB2	8:H:21:MET:CE	2.16	0.75
4:D:139:VAL:CG2	4:D:147:SER:CB	2.60	0.75
4:D:150:LEU:HD21	4:D:171:ARG:NH1	2.01	0.75
2:B:152:ASP:C	2:B:154:THR:H	1.94	0.75
3:C:172:PHE:CD1	3:C:172:PHE:N	2.54	0.75
4:D:111:LEU:HD13	4:D:111:LEU:H	1.45	0.75
2:B:81:LEU:CD1	15:B:1201:TDS:HAR1	2.16	0.75
4:D:15:ARG:HB3	5:E:31:LEU:CD2	2.15	0.75
3:C:171:VAL:HG13	3:C:234:ASN:HD22	1.50	0.75
3:C:225:VAL:HG12	3:C:229:GLU:CG	2.17	0.75
4:D:64:VAL:HG13	4:D:69:PHE:HD1	1.51	0.75
11:C:301:HEC:CMB	11:C:301:HEC:HBB3	2.17	0.75
3:C:180:ILE:HD11	3:C:183:ILE:HD11	1.68	0.75
3:C:171:VAL:HG13	3:C:234:ASN:ND2	2.03	0.74
1:A:147:ALA:HB2	15:B:1201:TDS:CAJ	2.16	0.74
2:B:123:PRO:HA	2:B:126:ARG:HG3	1.69	0.74
3:C:270:LEU:HB2	8:H:21:MET:HE2	1.70	0.74
4:D:146:LEU:HD13	4:D:177:TRP:CG	2.23	0.74
4:D:66:VAL:HG23	4:D:158:ASP:C	2.13	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:HIS:O	1:A:206:ILE:HG13	1.87	0.74
1:A:150:ILE:CD1	15:B:1201:TDS:HAA3	2.18	0.74
2:B:25:ASN:H	2:B:25:ASN:ND2	1.86	0.74
11:A:303:HEC:O2A	15:B:1202:TDS:CAA	2.35	0.74
3:C:270:LEU:HA	8:H:21:MET:HE2	1.70	0.74
3:C:285:ALA:HB2	4:D:10:VAL:HG21	1.68	0.74
4:D:146:LEU:CD1	4:D:177:TRP:CD2	2.66	0.74
8:H:19:ILE:HG22	8:H:20:ALA:N	2.03	0.74
13:A:1101:UMQ:H51	13:A:1101:UMQ:H6'1	1.69	0.73
3:C:119:LEU:HD22	3:C:124:TYR:CD1	2.21	0.73
2:B:45:MET:HE1	4:D:27:VAL:HG22	1.70	0.73
3:C:4:TRP:CD2	3:C:162:PRO:HG3	2.23	0.73
3:C:221:GLU:OE1	3:C:222:GLY:N	2.22	0.73
3:C:229:GLU:CD	3:C:230:ALA:H	1.96	0.73
1:A:127:ILE:CG2	1:A:195:ILE:HG13	2.18	0.73
1:A:47:GLN:HE21	1:A:47:GLN:N	1.87	0.73
4:D:117:TRP:CH2	4:D:122:ASN:C	2.67	0.73
3:C:94:LEU:O	3:C:94:LEU:HD23	1.89	0.73
1:A:112:LYS:O	1:A:114:ARG:N	2.21	0.73
2:B:82:TYR:H	2:B:83:PRO:HD2	1.53	0.73
2:B:9:LEU:O	2:B:15:ARG:CD	2.25	0.73
7:G:2:VAL:HG12	7:G:2:VAL:O	1.87	0.73
3:C:226:LYS:NZ	3:C:226:LYS:CB	2.52	0.72
8:H:1:MET:O	8:H:2:GLU:HB3	1.87	0.72
1:A:7:TRP:NE1	1:A:11:ARG:HH21	1.83	0.72
2:B:124:PHE:HE1	7:G:26:TYR:CB	1.99	0.72
3:C:65:GLY:C	3:C:66:SER:O	2.32	0.72
1:A:33:PHE:CD1	7:G:21:LEU:HD13	2.24	0.72
2:B:88:LEU:HD13	15:B:1201:TDS:HAI3	1.72	0.72
3:C:23:ALA:HB2	3:C:240:PHE:CE2	2.24	0.72
3:C:189:GLU:O	3:C:190:TYR:HD2	1.70	0.72
1:A:100:HIS:CE1	10:A:302:HEM:C1A	2.76	0.72
1:A:111:LYS:O	1:A:113:PRO:HD2	1.90	0.72
2:B:14:LEU:HD11	2:B:18:LEU:HD11	1.71	0.72
5:E:10:VAL:HG12	5:E:14:LEU:HD12	1.69	0.72
8:H:23:VAL:HA	8:H:28:GLY:HA3	1.72	0.72
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.04	0.72
3:C:15:GLU:CB	3:C:16:PRO:CD	2.60	0.72
6:F:27:LEU:O	6:F:30:GLN:HG3	1.89	0.72
11:A:303:HEC:CHB	15:B:1202:TDS:OAK	2.37	0.72
2:B:126:ARG:N	2:B:127:PRO:HD3	2.04	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:TYR:HE1	3:C:70:LEU:HD21	1.54	0.72
2:B:132:ILE:HD12	2:B:132:ILE:N	2.00	0.72
3:C:237:VAL:HG22	3:C:237:VAL:O	1.88	0.72
2:B:149:PHE:HB3	2:B:150:PRO:CD	2.19	0.72
3:C:19:ARG:O	3:C:242:GLN:OE1	2.08	0.72
1:A:31:ASN:C	1:A:31:ASN:ND2	2.45	0.71
5:E:6:VAL:O	5:E:10:VAL:HG23	1.89	0.71
7:G:24:ALA:O	7:G:28:GLN:HB2	1.90	0.71
13:A:1104:UMQ:H31	13:A:1104:UMQ:C6'	2.10	0.71
1:A:36:LEU:HB3	1:A:100:HIS:CB	2.20	0.71
1:A:36:LEU:CD2	1:A:99:LEU:HB3	2.20	0.71
11:A:303:HEC:CBA	15:B:1202:TDS:HAA2	2.21	0.71
2:B:118:ASN:ND2	2:B:120:PHE:CD1	2.59	0.71
3:C:223:GLN:HG3	3:C:224:ALA:N	2.05	0.71
1:A:20:ASP:O	1:A:20:ASP:OD2	2.08	0.71
1:A:83:ARG:NH1	10:A:301:HEM:O2A	2.23	0.71
4:D:170:PHE:CE2	4:D:171:ARG:HG3	2.26	0.71
3:C:174:ALA:HB2	3:C:231:LEU:HD23	1.73	0.71
5:E:9:ILE:O	5:E:13:ALA:HB2	1.91	0.71
1:A:111:LYS:HE2	2:B:115:GLU:O	1.91	0.71
2:B:77:PRO:HA	15:B:1201:TDS:HAJ2	1.73	0.71
3:C:94:LEU:HD23	3:C:94:LEU:C	2.15	0.70
3:C:259:ILE:CD1	8:H:6:LEU:HD13	2.21	0.70
3:C:9:TYR:CG	3:C:21:VAL:HG11	2.26	0.70
6:F:16:ILE:HG22	6:F:17:PHE:N	2.05	0.70
1:A:32:ILE:CG2	1:A:33:PHE:N	2.54	0.70
3:C:275:LYS:HE2	4:D:20:ASN:OD1	1.90	0.70
1:A:54:MET:HE1	10:A:301:HEM:HBD1	1.70	0.70
1:A:54:MET:CE	10:A:301:HEM:CBD	2.66	0.70
2:B:79:TRP:CG	2:B:80:TYR:H	2.10	0.70
3:C:264:LEU:O	3:C:264:LEU:HD22	1.91	0.70
7:G:26:TYR:O	7:G:27:GLN:C	2.32	0.70
1:A:110:PHE:N	1:A:110:PHE:CD2	2.56	0.70
1:A:92:MET:CE	12:A:1002:OPC:CCB	2.27	0.70
13:A:1104:UMQ:O3'	13:A:1104:UMQ:H11	1.92	0.70
3:C:22:CYS:O	3:C:24:ASN:N	2.24	0.70
7:G:26:TYR:C	7:G:28:GLN:N	2.48	0.70
11:C:301:HEC:HBB3	11:C:301:HEC:HMB1	1.72	0.70
2:B:123:PRO:HD3	7:G:25:ALA:HB1	1.73	0.70
4:D:55:THR:HG23	4:D:159:ASN:HB3	1.74	0.70
6:F:11:LEU:O	6:F:15:LEU:HB2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:PHE:C	6:F:13:PHE:CD2	2.70	0.70
2:B:40:PHE:CB	2:B:41:PRO:CD	2.70	0.69
1:A:127:ILE:HG22	1:A:195:ILE:HG13	1.74	0.69
2:B:147:ALA:C	2:B:149:PHE:N	2.48	0.69
3:C:270:LEU:CA	8:H:21:MET:HE2	2.21	0.69
4:D:63:ASN:O	4:D:64:VAL:C	2.34	0.69
4:D:146:LEU:HD13	4:D:177:TRP:CB	2.23	0.69
1:A:39:ILE:CG2	1:A:96:MET:HG3	2.22	0.69
1:A:61:THR:HA	1:A:177:GLN:NE2	2.03	0.69
3:C:60:GLN:OE1	3:C:70:LEU:HB3	1.91	0.69
4:D:9:ASP:HA	5:E:30:LYS:NZ	2.07	0.69
14:B:201:CLA:HBB1	14:B:201:CLA:CMB	2.22	0.69
4:D:55:THR:HG21	4:D:63:ASN:OD1	1.92	0.69
5:E:26:ILE:CG2	5:E:32:ILE:HG13	2.22	0.69
2:B:57:LEU:HD11	8:H:8:TRP:HA	1.75	0.69
3:C:270:LEU:C	3:C:270:LEU:HD13	2.17	0.69
3:C:270:LEU:HD13	3:C:271:MET:N	2.08	0.69
4:D:178:TRP:CD1	4:D:179:VAL:HB	2.27	0.69
1:A:72:ILE:O	1:A:79:GLY:HA3	1.93	0.69
3:C:259:ILE:HD12	8:H:6:LEU:CD1	2.22	0.69
3:C:172:PHE:HD1	3:C:172:PHE:H	1.41	0.68
3:C:25:CYS:SG	11:C:301:HEC:CBC	2.81	0.68
3:C:180:ILE:CD1	3:C:183:ILE:HD11	2.23	0.68
3:C:176:ALA:HB1	3:C:205:LYS:HZ2	1.57	0.68
3:C:221:GLU:OE1	3:C:221:GLU:HA	1.93	0.68
5:E:14:LEU:O	5:E:18:ILE:HG12	1.92	0.68
2:B:4:LEU:H	3:C:287:MET:HE1	1.56	0.68
2:B:40:PHE:HZ	15:B:1202:TDS:HBD	1.41	0.68
2:B:42:VAL:HG13	3:C:269:GLN:HB3	1.75	0.68
3:C:188:ASP:C	3:C:190:TYR:H	1.99	0.68
6:F:11:LEU:CB	6:F:15:LEU:HD12	2.19	0.68
2:B:95:LEU:HD21	2:B:99:LEU:HD11	1.74	0.68
2:B:122:ASN:HD21	7:G:29:TYR:HB2	1.59	0.68
1:A:26:VAL:HG22	1:A:30:VAL:HG12	1.75	0.68
1:A:127:ILE:HG21	1:A:195:ILE:CG1	2.22	0.68
3:C:34:VAL:HG21	3:C:151:LEU:CB	2.24	0.68
15:B:1202:TDS:OAC	15:B:1202:TDS:CAA	2.38	0.67
4:D:104:ILE:HG22	4:D:148:LEU:HD12	1.77	0.67
11:C:301:HEC:HMC1	11:C:301:HEC:CBC	2.25	0.67
1:A:88:TRP:CZ3	2:B:54:LEU:HD13	2.29	0.67
3:C:23:ALA:HB2	3:C:240:PHE:CD2	2.29	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:32:LEU:O	4:D:33:GLY:C	2.36	0.67
4:D:110:HIS:C	4:D:111:LEU:HD13	2.15	0.67
3:C:14:ARG:NH2	3:C:150:HIS:CD2	2.63	0.67
4:D:65:LYS:CB	4:D:68:LYS:HZ1	2.08	0.67
4:D:117:TRP:CZ2	4:D:122:ASN:HA	2.28	0.67
4:D:100:ARG:NH1	4:D:102:TYR:OH	2.28	0.67
2:B:128:VAL:O	2:B:132:ILE:HD11	1.93	0.67
3:C:101:VAL:HG11	3:C:103:PHE:CE2	2.29	0.67
7:G:29:TYR:CD2	7:G:29:TYR:C	2.66	0.67
8:H:23:VAL:O	8:H:24:TRP:C	2.33	0.66
1:A:41:LEU:HD23	11:A:303:HEC:HBC1	1.76	0.66
2:B:21:GLY:O	2:B:22:MET:HB3	1.93	0.66
7:G:20:GLY:N	18:G:101:BCR:H363	2.10	0.66
1:A:82:ILE:HG12	4:D:41:TYR:CD1	2.31	0.66
3:C:288:ASN:C	3:C:288:ASN:ND2	2.48	0.66
3:C:41:LEU:HB2	8:H:1:MET:SD	2.36	0.66
3:C:215:PRO:HB3	3:C:232:THR:HG22	1.76	0.66
3:C:229:GLU:O	3:C:231:LEU:N	2.29	0.66
3:C:262:ILE:HG22	3:C:263:CYS:N	2.11	0.66
4:D:90:TYR:OH	4:D:116:PRO:HA	1.96	0.66
3:C:36:VAL:HG11	3:C:149:ILE:CD1	2.25	0.65
3:C:87:GLU:C	3:C:89:ARG:H	2.04	0.65
2:B:17:LYS:O	2:B:20:LYS:N	2.17	0.65
3:C:136:PRO:HB3	3:C:142:ILE:O	1.97	0.65
4:D:117:TRP:CH2	4:D:123:LYS:N	2.65	0.65
6:F:28:LYS:O	6:F:30:GLN:N	2.29	0.65
18:G:101:BCR:C8	18:G:101:BCR:H321	2.09	0.65
3:C:278:GLN:O	3:C:278:GLN:HG2	1.97	0.65
6:F:25:LEU:C	6:F:27:LEU:H	2.03	0.65
3:C:158:GLY:H	11:C:301:HEC:C3D	2.09	0.65
3:C:195:TYR:CD1	3:C:195:TYR:N	2.59	0.65
15:B:1202:TDS:CAS	15:B:1202:TDS:OAO	2.44	0.65
3:C:200:GLN:HG3	3:C:205:LYS:HB3	1.77	0.65
1:A:80:TRP:O	1:A:84:SER:HB2	1.97	0.65
1:A:195:ILE:CD1	1:A:199:MET:HE2	2.26	0.65
3:C:14:ARG:CZ	3:C:150:HIS:HD2	2.10	0.65
3:C:285:ALA:CB	4:D:10:VAL:HG21	2.26	0.65
4:D:65:LYS:HB3	4:D:68:LYS:NZ	2.12	0.64
4:D:161:VAL:O	4:D:161:VAL:CG1	2.44	0.64
4:D:139:VAL:N	4:D:147:SER:HB3	2.01	0.64
2:B:104:VAL:N	2:B:105:PRO:HD2	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:ASN:CB	11:C:301:HEC:O2A	2.45	0.64
3:C:206:THR:O	3:C:206:THR:HG22	1.97	0.64
4:D:150:LEU:HD21	4:D:171:ARG:CZ	2.28	0.64
1:A:95:LEU:O	1:A:96:MET:C	2.40	0.64
1:A:150:ILE:CD1	15:B:1201:TDS:HAA2	2.27	0.64
2:B:106:LEU:O	2:B:109:ILE:HB	1.96	0.64
4:D:69:PHE:HD2	4:D:69:PHE:O	1.78	0.64
1:A:207:ARG:NH1	15:B:1202:TDS:CAI	2.60	0.64
4:D:9:ASP:HA	5:E:30:LYS:HZ3	1.63	0.64
6:F:13:PHE:C	6:F:13:PHE:HD2	2.05	0.64
1:A:136:TYR:HE2	15:B:1201:TDS:CAJ	2.11	0.64
3:C:60:GLN:OE1	3:C:70:LEU:CB	2.46	0.64
3:C:279:VAL:C	3:C:281:LYS:H	2.05	0.64
4:D:25:GLY:HA3	17:D:201:SQD:H341	1.78	0.64
1:A:26:VAL:CG2	1:A:30:VAL:HG12	2.26	0.63
3:C:232:THR:O	3:C:233:ASN:HB3	1.97	0.63
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.28	0.63
6:F:14:GLY:O	6:F:17:PHE:HB2	1.97	0.63
7:G:13:LEU:O	7:G:14:VAL:C	2.41	0.63
1:A:41:LEU:HD23	11:A:303:HEC:HBC2	1.78	0.63
2:B:22:MET:HA	2:B:24:HIS:HD2	1.63	0.63
4:D:146:LEU:CD1	4:D:177:TRP:CB	2.76	0.63
7:G:24:ALA:C	7:G:26:TYR:H	2.06	0.63
3:C:2:PRO:HD3	11:C:301:HEC:CHB	2.28	0.63
3:C:71:ASN:HB2	11:C:301:HEC:CGA	2.29	0.63
3:C:94:LEU:O	3:C:98:VAL:HG23	1.99	0.63
2:B:118:ASN:HD22	2:B:120:PHE:N	1.94	0.63
2:B:58:ASP:OD2	2:B:58:ASP:C	2.42	0.63
3:C:25:CYS:SG	11:C:301:HEC:C3C	2.86	0.63
3:C:26:HIS:HD1	3:C:154:ASN:ND2	1.97	0.63
1:A:95:LEU:HD22	1:A:96:MET:HE2	1.80	0.62
2:B:45:MET:CE	4:D:27:VAL:HG13	2.28	0.62
1:A:8:PHE:HB3	1:A:14:ILE:HG12	1.81	0.62
1:A:63:THR:O	1:A:63:THR:HG22	1.91	0.62
1:A:211:ILE:C	1:A:212:SER:O	2.35	0.62
4:D:55:THR:CG2	4:D:63:ASN:OD1	2.47	0.62
7:G:2:VAL:HG13	7:G:3:GLU:N	2.09	0.62
1:A:29:HIS:CD2	1:A:213:GLY:O	2.52	0.62
3:C:180:ILE:HG12	3:C:181:THR:N	2.12	0.62
4:D:65:LYS:CB	4:D:68:LYS:NZ	2.62	0.62
7:G:17:THR:O	7:G:21:LEU:HB2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:HD2	1:A:106:LEU:HD23	1.64	0.62
3:C:19:ARG:HG2	3:C:19:ARG:HH11	1.64	0.62
4:D:63:ASN:O	4:D:64:VAL:O	2.17	0.62
4:D:137:GLY:HA3	4:D:171:ARG:HH12	1.63	0.62
4:D:150:LEU:O	4:D:151:CYS:HB3	2.00	0.62
1:A:30:VAL:CG2	1:A:34:TYR:CG	2.80	0.62
2:B:95:LEU:CD2	2:B:99:LEU:CD1	2.77	0.62
3:C:161:TYR:C	3:C:163:THR:H	2.07	0.62
3:C:225:VAL:HG12	3:C:229:GLU:HG2	1.81	0.62
3:C:74:ALA:H	11:C:301:HEC:HMB2	1.65	0.62
3:C:179:THR:HA	3:C:223:GLN:O	2.00	0.62
3:C:200:GLN:HE21	3:C:206:THR:HA	1.64	0.62
2:B:95:LEU:O	2:B:99:LEU:HD12	1.99	0.62
2:B:126:ARG:N	2:B:127:PRO:CD	2.63	0.62
3:C:62:ALA:HB2	3:C:68:VAL:HG12	1.81	0.62
3:C:119:LEU:HD22	3:C:124:TYR:CG	2.35	0.62
4:D:64:VAL:CG1	4:D:69:PHE:HD1	2.12	0.62
2:B:69:PHE:N	2:B:69:PHE:CD2	2.68	0.61
2:B:32:TRP:CD1	2:B:33:PRO:CD	2.84	0.61
3:C:180:ILE:HG22	3:C:223:GLN:HB3	1.83	0.61
6:F:17:PHE:O	6:F:20:TRP:HB3	2.00	0.61
2:B:57:LEU:CD1	8:H:8:TRP:CE3	2.81	0.61
3:C:282:VAL:HG11	4:D:16:ARG:HE	1.65	0.61
1:A:44:PHE:C	1:A:44:PHE:CD2	2.79	0.61
1:A:103:ARG:O	1:A:107:THR:HB	2.00	0.61
2:B:6:LYS:O	2:B:7:PRO:C	2.43	0.61
2:B:158:GLY:C	2:B:159:LEU:HD23	2.25	0.61
1:A:111:LYS:NZ	2:B:120:PHE:O	2.31	0.61
1:A:215:LEU:HD13	2:B:122:ASN:CA	2.29	0.61
1:A:215:LEU:HB3	2:B:122:ASN:HB2	1.81	0.61
4:D:90:TYR:HE1	4:D:115:VAL:O	1.84	0.61
4:D:170:PHE:CE2	4:D:171:ARG:CG	2.83	0.61
7:G:10:VAL:HG12	7:G:11:LEU:N	2.15	0.61
1:A:12:LEU:CB	1:A:14:ILE:CD1	2.79	0.61
3:C:34:VAL:HG21	3:C:151:LEU:HB2	1.82	0.61
3:C:186:GLU:HB2	3:C:194:LYS:HB2	1.83	0.61
5:E:29:ILE:O	5:E:29:ILE:CG2	2.49	0.61
1:A:32:ILE:HG23	1:A:33:PHE:N	2.14	0.61
3:C:1:TYR:HA	11:C:301:HEC:C4A	2.30	0.61
4:D:168:THR:HA	4:D:176:PRO:HD3	1.83	0.61
2:B:134:LEU:HD13	2:B:134:LEU:N	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:LEU:CD1	6:F:10:LEU:C	2.74	0.61
1:A:111:LYS:CE	2:B:115:GLU:O	2.48	0.60
2:B:151:LEU:O	2:B:154:THR:CG2	2.48	0.60
3:C:93:GLU:O	3:C:97:GLU:HG3	2.01	0.60
1:A:15:GLN:O	1:A:16:ALA:C	2.43	0.60
3:C:28:ALA:CB	3:C:239:GLY:HA3	2.25	0.60
3:C:54:TYR:HE1	3:C:70:LEU:CD2	2.13	0.60
4:D:65:LYS:HB3	4:D:68:LYS:HZ1	1.67	0.60
5:E:27:LYS:O	5:E:30:LYS:HA	2.02	0.60
2:B:75:ILE:HG23	2:B:75:ILE:O	2.01	0.60
3:C:62:ALA:HB2	3:C:68:VAL:CG1	2.31	0.60
3:C:173:THR:O	3:C:231:LEU:CD2	2.50	0.60
3:C:176:ALA:CB	3:C:205:LYS:HZ2	2.15	0.60
5:E:24:PHE:CE1	6:F:29:ILE:HD11	2.37	0.60
1:A:12:LEU:HB3	1:A:14:ILE:CD1	2.32	0.60
1:A:96:MET:HE2	1:A:96:MET:HA	1.84	0.60
4:D:132:GLN:OE1	4:D:141:ARG:HG2	2.02	0.60
3:C:54:TYR:CE1	3:C:70:LEU:HD21	2.35	0.60
3:C:173:THR:HB	3:C:228:GLY:C	2.26	0.60
3:C:286:GLU:OE1	3:C:286:GLU:CA	2.50	0.60
4:D:105:ASN:ND2	4:D:107:VAL:HG23	2.16	0.60
1:A:105:TYR:CD2	1:A:106:LEU:HD23	2.37	0.60
10:A:302:HEM:CMB	10:A:302:HEM:HBB2	2.31	0.60
3:C:271:MET:HE2	4:D:22:LEU:HD12	1.84	0.60
1:A:195:ILE:O	1:A:199:MET:HG3	2.02	0.59
3:C:19:ARG:HG2	3:C:19:ARG:NH1	2.17	0.59
1:A:211:ILE:CD1	1:A:212:SER:H	2.15	0.59
3:C:172:PHE:N	3:C:172:PHE:HD1	1.96	0.59
2:B:104:VAL:HB	2:B:105:PRO:CD	2.32	0.59
4:D:152:HIS:O	4:D:162:LEU:HA	2.01	0.59
6:F:23:GLY:O	6:F:26:LEU:HB2	2.02	0.59
1:A:32:ILE:CG2	1:A:33:PHE:CD2	2.82	0.59
1:A:87:ARG:HH11	1:A:87:ARG:HG2	1.67	0.59
3:C:158:GLY:C	3:C:159:GLN:NE2	2.60	0.59
4:D:64:VAL:HG13	4:D:69:PHE:CD1	2.35	0.59
1:A:211:ILE:HG23	1:A:212:SER:O	2.02	0.59
3:C:80:GLU:OE2	3:C:80:GLU:HA	2.02	0.59
1:A:200:LEU:C	1:A:200:LEU:HD22	2.28	0.59
13:A:1101:UMQ:HK2	4:D:34:ALA:HA	1.85	0.59
4:D:84:LEU:C	4:D:86:GLY:H	2.11	0.59
1:A:187:HIS:HE1	10:A:301:HEM:C1B	2.21	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1102:UMQ:O3'	13:A:1102:UMQ:H11	2.02	0.59
1:A:112:LYS:HA	1:A:115:GLU:OE2	2.02	0.59
2:B:91:VAL:C	2:B:93:ASN:N	2.58	0.59
4:D:78:ARG:HD2	4:D:117:TRP:CD1	2.37	0.59
4:D:156:GLN:O	4:D:157:ASP:HB2	2.03	0.59
1:A:120:SER:O	1:A:123:ILE:N	2.35	0.59
3:C:171:VAL:HG23	3:C:171:VAL:O	2.01	0.59
4:D:170:PHE:CD2	4:D:171:ARG:HG3	2.38	0.59
3:C:61:VAL:HG21	3:C:214:GLY:O	2.03	0.59
1:A:92:MET:HE2	12:A:1002:OPC:HCB2	1.70	0.58
2:B:25:ASN:HD22	2:B:25:ASN:N	1.87	0.58
2:B:95:LEU:HD23	2:B:99:LEU:HD12	1.84	0.58
3:C:155:ARG:O	3:C:155:ARG:HG2	2.01	0.58
11:A:303:HEC:HBC2	11:A:303:HEC:HHD	1.85	0.58
2:B:134:LEU:HD21	7:G:22:PHE:CZ	2.38	0.58
5:E:4:GLY:O	5:E:8:TYR:N	2.26	0.58
1:A:32:ILE:HG22	1:A:33:PHE:CE2	2.38	0.58
1:A:141:ASP:C	1:A:141:ASP:OD2	2.45	0.58
1:A:207:ARG:NH1	1:A:207:ARG:CG	2.61	0.58
10:A:302:HEM:HBA1	10:A:302:HEM:CHA	2.27	0.58
3:C:237:VAL:O	3:C:237:VAL:CG2	2.50	0.58
3:C:270:LEU:CB	8:H:21:MET:HE2	2.32	0.58
4:D:64:VAL:CG1	4:D:69:PHE:CD1	2.87	0.58
3:C:264:LEU:HD22	3:C:264:LEU:C	2.21	0.58
4:D:122:ASN:HB3	4:D:135:GLU:CD	2.24	0.58
4:D:165:TRP:CD1	4:D:165:TRP:C	2.82	0.58
1:A:36:LEU:HD23	1:A:99:LEU:C	2.28	0.58
6:F:23:GLY:HA2	6:F:26:LEU:HD23	1.84	0.58
3:C:171:VAL:O	3:C:171:VAL:CG2	2.51	0.58
4:D:22:LEU:N	4:D:22:LEU:HD23	2.17	0.58
4:D:105:ASN:ND2	4:D:105:ASN:C	2.62	0.58
4:D:105:ASN:O	4:D:148:LEU:HD13	2.03	0.58
4:D:117:TRP:NE1	4:D:119:ALA:HA	2.19	0.58
3:C:34:VAL:CG2	3:C:151:LEU:CB	2.81	0.58
1:A:95:LEU:C	1:A:95:LEU:HD23	2.28	0.58
3:C:26:HIS:CE1	11:C:301:HEC:NA	2.72	0.58
3:C:34:VAL:HG21	3:C:151:LEU:HB3	1.84	0.58
3:C:78:LEU:HB2	3:C:112:ASN:O	2.04	0.58
4:D:59:LYS:H	4:D:59:LYS:HD3	1.69	0.58
3:C:154:ASN:CG	3:C:155:ARG:N	2.62	0.57
6:F:27:LEU:HD11	8:H:27:ASN:HA	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:O	1:A:97:MET:N	2.36	0.57
2:B:81:LEU:HD11	15:B:1201:TDS:HAR1	1.85	0.57
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.85	0.57
3:C:60:GLN:HE22	3:C:157:ARG:H	1.52	0.57
3:C:87:GLU:C	3:C:89:ARG:N	2.59	0.57
2:B:149:PHE:CB	2:B:150:PRO:CD	2.82	0.57
3:C:94:LEU:C	3:C:94:LEU:CD2	2.77	0.57
4:D:133:TYR:CE2	4:D:148:LEU:CD2	2.80	0.57
6:F:27:LEU:O	6:F:30:GLN:CG	2.51	0.57
1:A:39:ILE:CD1	18:G:101:BCR:C31	2.74	0.57
1:A:87:ARG:CG	1:A:87:ARG:NH1	2.68	0.57
1:A:195:ILE:HD13	1:A:199:MET:HE2	1.86	0.57
3:C:221:GLU:OE1	3:C:221:GLU:CA	2.52	0.57
3:C:285:ALA:O	3:C:286:GLU:OE1	2.23	0.57
4:D:28:THR:O	4:D:29:GLY:C	2.45	0.57
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.69	0.57
1:A:103:ARG:HH21	1:A:211:ILE:HD11	1.69	0.57
3:C:79:PRO:HG2	3:C:82:PHE:CD1	2.39	0.57
3:C:183:ILE:HG22	3:C:183:ILE:O	2.05	0.57
4:D:133:TYR:HB3	4:D:137:GLY:O	2.04	0.57
1:A:127:ILE:CG2	1:A:195:ILE:CG1	2.81	0.57
1:A:177:GLN:O	1:A:178:ALA:C	2.39	0.57
4:D:102:TYR:H	4:D:102:TYR:HD2	1.52	0.57
2:B:85:PHE:HD2	15:B:1201:TDS:OAC	1.87	0.57
3:C:225:VAL:HG12	3:C:229:GLU:HG3	1.87	0.57
7:G:7:ASP:OD2	7:G:7:ASP:N	2.32	0.57
2:B:150:PRO:O	2:B:152:ASP:N	2.38	0.57
5:E:26:ILE:HG23	5:E:32:ILE:HG13	1.85	0.57
2:B:84:VAL:HG11	2:B:101:MET:HG3	1.86	0.57
3:C:171:VAL:CG1	3:C:233:ASN:O	2.52	0.57
3:C:172:PHE:N	3:C:232:THR:OG1	2.38	0.57
7:G:34:GLU:N	7:G:34:GLU:OE2	2.38	0.57
8:H:9:VAL:O	8:H:13:VAL:HG23	2.05	0.57
1:A:207:ARG:HH12	15:B:1202:TDS:CAI	2.18	0.56
1:A:27:PRO:HB2	1:A:29:HIS:CE1	2.40	0.56
1:A:96:MET:HE2	1:A:96:MET:CA	2.34	0.56
1:A:105:TYR:CZ	14:B:201:CLA:CBB	2.88	0.56
11:A:303:HEC:CMB	11:A:303:HEC:CBB	2.76	0.56
3:C:171:VAL:HG12	3:C:234:ASN:HA	1.87	0.56
3:C:200:GLN:NE2	3:C:205:LYS:O	2.39	0.56
4:D:78:ARG:CD	4:D:117:TRP:CG	2.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2:ILE:O	5:E:6:VAL:HG23	2.05	0.56
5:E:15:PHE:HA	5:E:18:ILE:HG13	1.87	0.56
6:F:25:LEU:C	6:F:27:LEU:N	2.62	0.56
1:A:168:LEU:O	1:A:182:ARG:HD3	2.05	0.56
3:C:271:MET:HE2	4:D:22:LEU:CD1	2.35	0.56
8:H:23:VAL:HG13	8:H:28:GLY:H	1.70	0.56
2:B:122:ASN:ND2	7:G:29:TYR:HB2	2.21	0.56
1:A:33:PHE:CD2	1:A:33:PHE:N	2.73	0.56
2:B:97:GLY:HA2	2:B:100:LEU:HB2	1.88	0.56
2:B:123:PRO:CD	7:G:25:ALA:HB1	2.35	0.56
3:C:193:VAL:HG12	3:C:194:LYS:N	2.21	0.56
3:C:210:THR:C	3:C:211:ILE:CG2	2.79	0.56
4:D:21:LEU:HD11	17:D:201:SQD:C30	2.32	0.56
7:G:34:GLU:C	7:G:35:LEU:HD23	2.31	0.56
1:A:92:MET:CG	12:A:1002:OPC:HCB1	2.35	0.56
1:A:96:MET:HE2	1:A:96:MET:N	2.20	0.56
3:C:34:VAL:HG23	3:C:151:LEU:CD2	2.36	0.56
4:D:110:HIS:O	4:D:111:LEU:HD12	2.05	0.56
1:A:33:PHE:H	1:A:33:PHE:HD2	1.51	0.56
1:A:87:ARG:HH11	1:A:87:ARG:CG	2.19	0.56
2:B:57:LEU:HD12	8:H:8:TRP:CZ3	2.41	0.56
3:C:54:TYR:HD2	3:C:125:GLN:HE22	1.53	0.56
3:C:223:GLN:O	3:C:224:ALA:HB2	2.04	0.56
4:D:139:VAL:CG2	4:D:147:SER:CA	2.66	0.56
4:D:165:TRP:HD1	4:D:165:TRP:O	1.89	0.56
8:H:23:VAL:HG12	8:H:24:TRP:N	2.13	0.56
3:C:181:THR:O	3:C:182:LYS:HG3	2.06	0.56
4:D:96:LYS:HB2	4:D:96:LYS:HZ3	1.70	0.56
5:E:26:ILE:O	5:E:31:LEU:HB2	2.06	0.56
7:G:2:VAL:HG12	7:G:4:PRO:HD3	1.83	0.56
1:A:100:HIS:HE1	10:A:302:HEM:CHA	2.19	0.55
3:C:270:LEU:HA	8:H:21:MET:HE3	1.87	0.55
7:G:30:LYS:C	7:G:32:PRO:HD3	2.31	0.55
1:A:94:VAL:HG11	2:B:80:TYR:CG	2.41	0.55
4:D:21:LEU:HD11	17:D:201:SQD:H312	1.88	0.55
8:H:8:TRP:O	8:H:9:VAL:C	2.45	0.55
1:A:83:ARG:O	1:A:83:ARG:HG3	2.05	0.55
1:A:205:MET:O	1:A:206:ILE:C	2.47	0.55
2:B:91:VAL:C	2:B:93:ASN:H	2.15	0.55
3:C:161:TYR:C	3:C:163:THR:N	2.64	0.55
3:C:206:THR:O	3:C:206:THR:HG23	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:HG22	1:A:34:TYR:CD2	2.41	0.55
11:C:301:HEC:CBC	11:C:301:HEC:CMC	2.83	0.55
4:D:69:PHE:O	4:D:70:LEU:C	2.48	0.55
1:A:82:ILE:HD13	1:A:82:ILE:N	2.21	0.55
10:A:302:HEM:HMB1	10:A:302:HEM:CBB	2.37	0.55
3:C:14:ARG:NE	3:C:150:HIS:HD2	2.05	0.55
3:C:170:ASN:O	3:C:235:PRO:CD	2.54	0.55
8:H:5:VAL:O	8:H:6:LEU:C	2.49	0.55
1:A:93:MET:O	1:A:94:VAL:C	2.47	0.55
1:A:155:PRO:HB2	1:A:166:SER:OG	2.06	0.55
1:A:211:ILE:HD12	1:A:212:SER:H	1.72	0.55
3:C:34:VAL:CG2	3:C:151:LEU:HB2	2.37	0.55
3:C:217:LEU:N	3:C:217:LEU:HD12	2.21	0.55
3:C:271:MET:HE2	4:D:22:LEU:HB3	1.87	0.55
1:A:80:TRP:H	1:A:80:TRP:CD1	2.25	0.55
2:B:87:ILE:HG22	2:B:88:LEU:N	2.22	0.55
2:B:96:LEU:O	2:B:99:LEU:HB2	2.07	0.55
4:D:66:VAL:CG2	4:D:158:ASP:C	2.79	0.55
7:G:15:PHE:O	7:G:17:THR:N	2.40	0.55
1:A:44:PHE:HB2	1:A:93:MET:SD	2.46	0.55
2:B:22:MET:HA	2:B:24:HIS:CD2	2.41	0.55
2:B:123:PRO:HD2	2:B:124:PHE:H	1.72	0.55
3:C:171:VAL:HB	3:C:232:THR:HB	1.87	0.55
3:C:270:LEU:CD1	3:C:271:MET:N	2.70	0.55
1:A:54:MET:HE1	10:A:301:HEM:CBD	2.33	0.55
1:A:143:VAL:HG13	1:A:143:VAL:O	2.07	0.55
2:B:4:LEU:H	3:C:287:MET:HE3	1.70	0.55
2:B:129:ALA:O	2:B:130:THR:C	2.49	0.55
2:B:130:THR:CG2	7:G:22:PHE:CE2	2.83	0.55
4:D:78:ARG:HD2	4:D:117:TRP:CG	2.42	0.55
6:F:10:LEU:C	6:F:10:LEU:HD13	2.30	0.55
1:A:35:CYS:SG	11:A:303:HEC:HMB3	2.47	0.55
1:A:72:ILE:HA	1:A:76:VAL:CG2	2.36	0.55
2:B:138:LEU:CD1	2:B:138:LEU:CB	2.76	0.55
4:D:47:GLY:C	4:D:49:ALA:H	2.14	0.55
1:A:6:ASP:O	1:A:9:GLN:N	2.40	0.54
2:B:147:ALA:C	2:B:149:PHE:H	2.15	0.54
11:A:303:HEC:HBD1	11:A:303:HEC:HHA	1.89	0.54
2:B:96:LEU:C	2:B:100:LEU:HD12	2.32	0.54
2:B:124:PHE:CE1	7:G:26:TYR:CB	2.83	0.54
2:B:151:LEU:O	2:B:154:THR:HG21	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:ALA:CB	3:C:205:LYS:NZ	2.63	0.54
3:C:266:MET:CE	5:E:15:PHE:CD1	2.90	0.54
1:A:97:MET:SD	10:A:302:HEM:HAB	2.47	0.54
1:A:108:GLY:HA2	1:A:110:PHE:CD2	2.43	0.54
2:B:11:ASP:OD1	2:B:13:LYS:HB2	2.08	0.54
2:B:151:LEU:HD13	2:B:151:LEU:C	2.32	0.54
3:C:54:TYR:CE1	3:C:70:LEU:HG	2.43	0.54
3:C:181:THR:HG22	3:C:182:LYS:HG3	1.88	0.54
2:B:151:LEU:O	2:B:151:LEU:HD13	2.08	0.54
2:B:114:ILE:O	2:B:116:ASN:N	2.41	0.54
3:C:47:LYS:HD2	3:C:49:VAL:CG2	2.38	0.54
6:F:22:LEU:HD12	8:H:20:ALA:CB	2.37	0.54
1:A:7:TRP:CD2	1:A:11:ARG:NH2	2.68	0.54
4:D:34:ALA:O	4:D:37:PRO:HD2	2.08	0.54
4:D:80:LEU:O	4:D:81:VAL:HG22	2.07	0.54
1:A:110:PHE:CE1	2:B:111:VAL:HG12	2.43	0.54
1:A:111:LYS:O	1:A:112:LYS:C	2.50	0.54
2:B:159:LEU:O	2:B:160:PHE:CG	2.61	0.54
3:C:9:TYR:CE1	3:C:21:VAL:HB	2.43	0.54
3:C:180:ILE:CG2	3:C:222:GLY:O	2.56	0.54
1:A:103:ARG:NH1	1:A:104:VAL:CG2	2.65	0.54
1:A:145:TYR:O	1:A:145:TYR:CD1	2.61	0.54
1:A:145:TYR:O	1:A:145:TYR:CG	2.59	0.53
2:B:79:TRP:O	2:B:82:TYR:N	2.40	0.53
2:B:96:LEU:HD13	2:B:100:LEU:HD12	1.80	0.53
2:B:114:ILE:HG22	2:B:115:GLU:H	1.73	0.53
1:A:54:MET:HE1	10:A:301:HEM:CGD	2.38	0.53
3:C:15:GLU:N	3:C:15:GLU:OE1	2.39	0.53
3:C:279:VAL:C	3:C:281:LYS:N	2.66	0.53
4:D:90:TYR:CE1	4:D:115:VAL:O	2.61	0.53
4:D:152:HIS:CE1	4:D:165:TRP:CE3	2.96	0.53
6:F:28:LYS:C	6:F:30:GLN:H	2.17	0.53
1:A:29:HIS:NE2	1:A:213:GLY:C	2.67	0.53
1:A:98:ILE:HD11	14:B:201:CLA:CED	2.38	0.53
2:B:81:LEU:HD23	2:B:81:LEU:N	2.14	0.53
3:C:40:VAL:HG12	8:H:1:MET:CE	2.35	0.53
3:C:54:TYR:HE1	3:C:70:LEU:CG	2.21	0.53
3:C:194:LYS:O	3:C:195:TYR:C	2.51	0.53
4:D:119:ALA:O	4:D:122:ASN:OD1	2.26	0.53
4:D:167:GLU:CD	4:D:167:GLU:H	2.15	0.53
1:A:31:ASN:ND2	1:A:33:PHE:H	2.06	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:GLY:H	11:C:301:HEC:CAD	2.21	0.53
1:A:7:TRP:CD1	1:A:11:ARG:NH2	2.76	0.53
3:C:200:GLN:CD	3:C:205:LYS:O	2.51	0.53
4:D:114:VAL:O	4:D:114:VAL:CG1	2.55	0.53
4:D:146:LEU:HD12	4:D:177:TRP:CE3	2.40	0.53
1:A:145:TYR:CD1	1:A:145:TYR:C	2.84	0.53
7:G:23:TYR:C	7:G:23:TYR:CD2	2.87	0.53
8:H:3:ILE:O	8:H:7:GLY:N	2.38	0.53
1:A:119:ILE:O	1:A:123:ILE:HD12	2.09	0.53
2:B:45:MET:HE2	4:D:30:VAL:HB	1.91	0.53
2:B:113:PHE:O	2:B:114:ILE:C	2.51	0.53
3:C:273:ILE:HG13	8:H:21:MET:CG	2.29	0.53
4:D:169:ASP:O	4:D:170:PHE:C	2.51	0.53
5:E:8:TYR:OH	5:E:12:ILE:HD11	2.09	0.53
12:A:1002:OPC:HBP2	6:F:8:ALA:HA	1.90	0.53
2:B:69:PHE:N	2:B:69:PHE:HD2	2.05	0.53
3:C:1:TYR:HB3	3:C:2:PRO:HD2	1.90	0.53
3:C:180:ILE:HG22	3:C:222:GLY:O	2.08	0.53
3:C:188:ASP:O	3:C:190:TYR:O	2.25	0.53
3:C:226:LYS:CB	3:C:226:LYS:HZ2	2.22	0.53
1:A:31:ASN:ND2	1:A:33:PHE:HD2	2.07	0.52
1:A:80:TRP:CD2	3:C:254:ARG:NH2	2.77	0.52
1:A:147:ALA:O	1:A:148:VAL:C	2.49	0.52
3:C:22:CYS:C	3:C:24:ASN:H	2.16	0.52
3:C:75:VAL:HG13	3:C:75:VAL:O	2.08	0.52
1:A:95:LEU:C	1:A:97:MET:N	2.67	0.52
3:C:159:GLN:C	3:C:160:ILE:HG13	2.34	0.52
1:A:72:ILE:HA	1:A:76:VAL:HG23	1.90	0.52
1:A:92:MET:CG	12:A:1002:OPC:CCB	2.87	0.52
2:B:119:LYS:O	2:B:119:LYS:HG2	2.10	0.52
2:B:134:LEU:HD13	2:B:134:LEU:H	1.74	0.52
3:C:171:VAL:HG11	3:C:234:ASN:ND2	2.15	0.52
8:H:2:GLU:HB2	8:H:5:VAL:CG2	2.39	0.52
2:B:118:ASN:ND2	2:B:120:PHE:HD1	2.06	0.52
1:A:12:LEU:HB2	1:A:14:ILE:CD1	2.39	0.52
2:B:134:LEU:CD2	7:G:22:PHE:CZ	2.93	0.52
4:D:165:TRP:CD1	4:D:165:TRP:O	2.62	0.52
3:C:25:CYS:SG	11:C:301:HEC:HBC3	2.49	0.52
3:C:55:ASP:C	3:C:55:ASP:OD1	2.52	0.52
3:C:200:GLN:CG	3:C:205:LYS:HB3	2.39	0.52
4:D:84:LEU:C	4:D:86:GLY:N	2.65	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:21:GLY:O	6:F:22:LEU:C	2.52	0.52
1:A:29:HIS:CD2	1:A:214:PRO:HA	2.45	0.52
1:A:38:GLY:HA3	11:A:303:HEC:C1C	2.40	0.52
2:B:40:PHE:HZ	15:B:1202:TDS:OBD	1.93	0.52
3:C:59:GLN:HB2	3:C:67:LYS:HE3	1.92	0.52
3:C:272:LEU:O	3:C:275:LYS:HB3	2.10	0.52
4:D:38:LEU:O	4:D:38:LEU:HG	2.09	0.52
2:B:154:THR:HG23	2:B:155:LEU:H	1.75	0.52
3:C:64:ASP:OD2	3:C:65:GLY:N	2.43	0.52
3:C:1:TYR:HA	11:C:301:HEC:NA	2.25	0.52
3:C:250:GLN:HE21	3:C:251:ASP:H	1.58	0.52
1:A:92:MET:HG3	12:A:1002:OPC:CCB	2.40	0.51
15:B:1202:TDS:OAO	15:B:1202:TDS:HAS1	2.09	0.51
3:C:160:ILE:O	11:C:301:HEC:HAC	2.10	0.51
1:A:18:ALA:O	1:A:21:VAL:N	2.39	0.51
3:C:200:GLN:HG2	3:C:201:THR:N	2.24	0.51
4:D:69:PHE:CD2	4:D:69:PHE:O	2.61	0.51
5:E:9:ILE:O	5:E:13:ALA:CB	2.57	0.51
1:A:103:ARG:CA	7:G:21:LEU:HD21	2.38	0.51
1:A:191:LEU:O	1:A:192:PRO:C	2.50	0.51
2:B:57:LEU:HD13	8:H:8:TRP:CD2	2.45	0.51
3:C:266:MET:SD	8:H:13:VAL:HG12	2.51	0.51
4:D:13:MET:O	4:D:15:ARG:N	2.43	0.51
1:A:105:TYR:CZ	14:B:201:CLA:HBB2	2.45	0.51
10:A:302:HEM:CMB	10:A:302:HEM:CBB	2.87	0.51
2:B:84:VAL:HG11	2:B:101:MET:SD	2.50	0.51
1:A:53:ALA:HB1	4:D:41:TYR:CE2	2.45	0.51
3:C:45:VAL:HG13	3:C:85:ALA:HB2	1.93	0.51
1:A:111:LYS:O	1:A:113:PRO:CD	2.57	0.51
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.45	0.51
2:B:155:LEU:C	2:B:157:LEU:H	2.18	0.51
7:G:10:VAL:HG12	7:G:11:LEU:CD2	2.34	0.51
1:A:163:VAL:O	1:A:164:LEU:C	2.53	0.51
4:D:132:GLN:OE1	4:D:141:ARG:NH1	2.44	0.51
6:F:15:LEU:HD23	8:H:16:THR:OG1	2.10	0.51
1:A:88:TRP:CE3	2:B:54:LEU:HD13	2.46	0.51
1:A:103:ARG:NH2	1:A:211:ILE:HD11	2.25	0.51
2:B:84:VAL:CG1	2:B:101:MET:SD	2.99	0.51
6:F:24:VAL:O	6:F:27:LEU:CB	2.55	0.51
2:B:45:MET:HE1	4:D:27:VAL:HG13	1.91	0.51
3:C:102:TYR:O	3:C:104:GLN:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:ASN:O	4:D:93:VAL:HG11	2.10	0.51
1:A:39:ILE:O	1:A:42:THR:N	2.43	0.50
2:B:34:ASN:O	3:C:276:LYS:HE3	2.10	0.50
3:C:144:PHE:CE1	3:C:251:ASP:HB2	2.41	0.50
3:C:180:ILE:CD1	3:C:183:ILE:CD1	2.79	0.50
3:C:232:THR:O	3:C:233:ASN:CB	2.59	0.50
1:A:15:GLN:O	1:A:18:ALA:N	2.45	0.50
1:A:15:GLN:O	1:A:17:LEU:N	2.44	0.50
1:A:80:TRP:CZ3	1:A:81:LEU:HG	2.45	0.50
1:A:207:ARG:HG3	1:A:207:ARG:NH1	2.05	0.50
3:C:87:GLU:O	3:C:89:ARG:N	2.44	0.50
4:D:167:GLU:O	4:D:176:PRO:HG3	2.11	0.50
6:F:4:GLU:HG2	7:G:5:LEU:HD12	1.94	0.50
7:G:24:ALA:C	7:G:26:TYR:N	2.68	0.50
3:C:34:VAL:CG2	3:C:151:LEU:HD22	2.42	0.50
3:C:117:GLY:HA2	3:C:119:LEU:HD12	1.93	0.50
4:D:80:LEU:O	4:D:81:VAL:CG2	2.59	0.50
2:B:130:THR:HG21	7:G:22:PHE:HE2	1.75	0.50
1:A:212:SER:HB3	10:A:302:HEM:O2D	2.12	0.50
3:C:159:GLN:CD	3:C:159:GLN:N	2.70	0.50
3:C:214:GLY:C	3:C:215:PRO:O	2.50	0.50
3:C:229:GLU:OE1	3:C:229:GLU:CA	2.51	0.50
6:F:22:LEU:HD12	8:H:20:ALA:HB1	1.94	0.50
2:B:147:ALA:O	2:B:148:THR:C	2.55	0.50
3:C:173:THR:O	3:C:231:LEU:HD23	2.12	0.50
3:C:184:ALA:HB3	3:C:196:GLN:HB2	1.94	0.50
4:D:13:MET:HA	4:D:16:ARG:HD3	1.94	0.50
8:H:5:VAL:C	8:H:7:GLY:N	2.68	0.50
1:A:106:LEU:HD12	7:G:21:LEU:HD23	1.94	0.50
3:C:186:GLU:OE2	3:C:196:GLN:HG3	2.12	0.50
5:E:26:ILE:HG22	5:E:32:ILE:HG13	1.91	0.50
1:A:103:ARG:HH12	1:A:104:VAL:CG2	2.18	0.50
1:A:71:TYR:O	1:A:72:ILE:C	2.50	0.49
1:A:147:ALA:CB	15:B:1201:TDS:HAJ3	2.32	0.49
3:C:268:ALA:HA	4:D:26:THR:OG1	2.12	0.49
1:A:124:LEU:HD21	1:A:199:MET:N	2.27	0.49
1:A:138:LEU:N	1:A:139:PRO:HD3	2.28	0.49
3:C:196:GLN:NE2	3:C:210:THR:HG23	2.28	0.49
4:D:146:LEU:CD1	4:D:177:TRP:HB2	2.42	0.49
5:E:20:VAL:HG12	5:E:21:GLY:N	2.26	0.49
3:C:80:GLU:OE2	3:C:80:GLU:CA	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:TRP:CZ2	4:D:122:ASN:CA	2.95	0.49
4:D:138:LYS:HA	4:D:147:SER:CB	2.43	0.49
1:A:29:HIS:CD2	1:A:213:GLY:C	2.90	0.49
2:B:16:ALA:C	2:B:19:ALA:HB3	2.38	0.49
2:B:118:ASN:HD22	2:B:119:LYS:N	2.11	0.49
2:B:118:ASN:OD1	12:B:1001:OPC:HAH2	2.13	0.49
2:B:151:LEU:HD13	2:B:152:ASP:HB3	1.93	0.49
15:B:1202:TDS:HAA3	15:B:1202:TDS:CAG	2.38	0.49
3:C:54:TYR:OH	3:C:121:GLY:HA3	2.12	0.49
2:B:155:LEU:C	2:B:157:LEU:N	2.68	0.49
3:C:86:PRO:O	3:C:86:PRO:HG2	2.11	0.49
4:D:25:GLY:CA	17:D:201:SQD:H341	2.43	0.49
4:D:172:THR:HG23	4:D:174:GLU:OE2	2.12	0.49
1:A:95:LEU:HD22	1:A:96:MET:CE	2.43	0.49
3:C:9:TYR:CD1	3:C:21:VAL:HB	2.47	0.49
3:C:101:VAL:CG1	3:C:103:PHE:CE2	2.95	0.49
4:D:163:THR:O	4:D:164:PRO:C	2.54	0.49
7:G:26:TYR:C	7:G:26:TYR:CD2	2.91	0.49
1:A:51:GLY:HA3	10:A:301:HEM:C3C	2.48	0.49
1:A:151:VAL:HG23	1:A:151:VAL:O	2.13	0.49
1:A:215:LEU:HD22	2:B:122:ASN:H	1.78	0.49
4:D:133:TYR:CD2	4:D:148:LEU:CD2	2.93	0.49
6:F:22:LEU:C	6:F:22:LEU:CD1	2.81	0.49
7:G:20:GLY:H	18:G:101:BCR:H363	1.77	0.49
1:A:122:VAL:O	1:A:125:ALA:HB3	2.13	0.49
2:B:159:LEU:O	2:B:160:PHE:CB	2.60	0.49
5:E:23:ILE:O	5:E:27:LYS:N	2.43	0.49
1:A:12:LEU:CB	1:A:14:ILE:HD11	2.43	0.49
2:B:95:LEU:C	2:B:95:LEU:CD2	2.78	0.49
7:G:6:LEU:O	7:G:9:LEU:HB2	2.12	0.49
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.95	0.48
3:C:77:MET:HB3	3:C:113:VAL:HG13	1.94	0.48
4:D:101:ASP:OD1	4:D:101:ASP:N	2.44	0.48
3:C:34:VAL:CG2	3:C:151:LEU:HB3	2.43	0.48
3:C:54:TYR:CE2	3:C:125:GLN:NE2	2.81	0.48
2:B:151:LEU:CD1	2:B:152:ASP:HB3	2.44	0.48
3:C:94:LEU:O	3:C:95:LYS:C	2.57	0.48
3:C:185:LYS:HB2	3:C:185:LYS:NZ	2.28	0.48
4:D:47:GLY:C	4:D:49:ALA:N	2.71	0.48
2:B:122:ASN:OD1	2:B:124:PHE:HB2	2.13	0.48
3:C:200:GLN:HG3	3:C:205:LYS:C	2.25	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:O	1:A:82:ILE:C	2.57	0.48
3:C:151:LEU:HG	3:C:152:GLY:N	2.23	0.48
4:D:83:GLY:HA2	4:D:162:LEU:CD1	2.43	0.48
1:A:12:LEU:CB	1:A:14:ILE:HD13	2.43	0.48
1:A:95:LEU:CD2	1:A:99:LEU:HG	2.43	0.48
2:B:40:PHE:N	2:B:41:PRO:CD	2.77	0.48
1:A:3:ASN:O	1:A:6:ASP:HB2	2.12	0.48
2:B:99:LEU:O	2:B:103:SER:OG	2.32	0.48
14:B:201:CLA:HMB1	14:B:201:CLA:CBB	2.38	0.48
7:G:35:LEU:HD23	7:G:35:LEU:N	2.29	0.48
1:A:196:ALA:O	1:A:197:VAL:C	2.56	0.48
2:B:113:PHE:O	2:B:116:ASN:HB2	2.13	0.48
4:D:28:THR:O	4:D:31:ALA:N	2.47	0.48
8:H:17:TRP:O	8:H:21:MET:HB2	2.14	0.48
1:A:4:VAL:O	1:A:5:TYR:C	2.57	0.48
1:A:119:ILE:HD13	2:B:109:ILE:HD13	1.95	0.48
3:C:13:PRO:O	3:C:20:ILE:HA	2.14	0.48
3:C:70:LEU:N	3:C:70:LEU:HD22	2.23	0.48
6:F:30:GLN:HG3	6:F:31:GLY:N	2.28	0.48
2:B:104:VAL:CB	2:B:105:PRO:CD	2.92	0.48
3:C:9:TYR:CD1	3:C:21:VAL:HG11	2.48	0.48
3:C:15:GLU:OE1	3:C:19:ARG:HB3	2.14	0.48
3:C:115:LEU:N	3:C:115:LEU:HD23	2.24	0.47
5:E:14:LEU:C	5:E:14:LEU:HD23	2.39	0.47
7:G:27:GLN:OE1	8:H:29:LEU:HD21	2.14	0.47
1:A:34:TYR:CE1	1:A:103:ARG:NE	2.75	0.47
1:A:80:TRP:CG	3:C:254:ARG:NH2	2.83	0.47
4:D:56:ALA:O	4:D:57:LYS:HG3	2.14	0.47
4:D:120:ALA:C	4:D:122:ASN:H	2.22	0.47
4:D:142:GLY:HA2	4:D:144:ALA:N	2.29	0.47
7:G:11:LEU:O	7:G:12:GLY:C	2.57	0.47
3:C:270:LEU:C	3:C:270:LEU:CD1	2.87	0.47
4:D:115:VAL:HG12	4:D:124:PHE:HB3	1.96	0.47
7:G:4:PRO:O	7:G:5:LEU:C	2.56	0.47
3:C:61:VAL:CG1	3:C:168:ASN:HD21	2.28	0.47
4:D:101:ASP:O	4:D:153:ALA:HB3	2.13	0.47
6:F:24:VAL:C	6:F:27:LEU:HB2	2.40	0.47
1:A:95:LEU:C	1:A:95:LEU:CD2	2.87	0.47
1:A:127:ILE:HG21	1:A:195:ILE:HG12	1.94	0.47
2:B:87:ILE:O	2:B:88:LEU:C	2.57	0.47
3:C:34:VAL:HG23	3:C:151:LEU:HD23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLY:O	3:C:74:ALA:HB2	2.15	0.47
3:C:139:ASP:OD1	3:C:140:LYS:N	2.46	0.47
3:C:263:CYS:O	3:C:267:LEU:HB2	2.15	0.47
4:D:142:GLY:HA2	4:D:144:ALA:H	1.79	0.47
1:A:62:VAL:HG23	1:A:63:THR:N	2.29	0.47
2:B:124:PHE:CE1	7:G:26:TYR:HD1	2.31	0.47
3:C:34:VAL:O	3:C:34:VAL:HG12	2.14	0.47
6:F:21:GLY:O	6:F:24:VAL:HB	2.15	0.47
6:F:22:LEU:HD13	6:F:23:GLY:N	2.30	0.47
1:A:12:LEU:HB2	1:A:14:ILE:HD11	1.96	0.47
2:B:12:PRO:HB2	2:B:13:LYS:HD3	1.97	0.47
3:C:14:ARG:NE	3:C:150:HIS:CD2	2.82	0.47
3:C:77:MET:HG3	3:C:150:HIS:HB2	1.97	0.47
4:D:134:ASP:OD1	4:D:134:ASP:O	2.31	0.47
3:C:23:ALA:HB2	3:C:240:PHE:HE2	1.78	0.47
3:C:107:LYS:HE2	3:C:110:GLN:HE22	1.77	0.47
4:D:29:GLY:O	4:D:30:VAL:C	2.53	0.47
6:F:20:TRP:CD1	6:F:24:VAL:CG2	2.98	0.47
8:H:19:ILE:O	8:H:20:ALA:C	2.58	0.47
1:A:183:TYR:O	1:A:186:ALA:HB3	2.15	0.46
12:A:1002:OPC:HBX1	12:A:1002:OPC:HBU2	1.44	0.46
2:B:41:PRO:O	2:B:42:VAL:C	2.56	0.46
3:C:44:THR:O	3:C:132:LEU:HA	2.15	0.46
3:C:62:ALA:O	3:C:63:ALA:C	2.57	0.46
3:C:136:PRO:HG3	3:C:142:ILE:HG22	1.97	0.46
4:D:16:ARG:O	4:D:20:ASN:N	2.45	0.46
4:D:144:ALA:HA	4:D:145:PRO:HD2	1.75	0.46
1:A:7:TRP:O	1:A:11:ARG:CG	2.62	0.46
5:E:10:VAL:O	5:E:10:VAL:HG12	2.14	0.46
8:H:2:GLU:C	8:H:2:GLU:OE1	2.59	0.46
1:A:33:PHE:C	1:A:35:CYS:H	2.22	0.46
2:B:157:LEU:O	2:B:159:LEU:HD23	2.14	0.46
3:C:171:VAL:HG12	3:C:233:ASN:O	2.14	0.46
3:C:251:ASP:OD2	3:C:251:ASP:C	2.57	0.46
2:B:57:LEU:CD2	3:C:258:MET:HE2	2.44	0.46
2:B:82:TYR:O	2:B:85:PHE:N	2.49	0.46
1:A:110:PHE:HD1	2:B:112:PRO:CB	2.13	0.46
2:B:11:ASP:HA	2:B:12:PRO:HD2	1.44	0.46
2:B:134:LEU:O	2:B:135:PHE:C	2.57	0.46
3:C:12:THR:OG1	3:C:13:PRO:CD	2.63	0.46
4:D:21:LEU:O	4:D:21:LEU:HG	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLY:HA3	10:A:302:HEM:C3C	2.51	0.46
2:B:156:THR:C	2:B:158:GLY:N	2.72	0.46
3:C:270:LEU:CB	8:H:21:MET:CE	2.91	0.46
4:D:115:VAL:HG13	4:D:116:PRO:HD2	1.98	0.46
4:D:126:CYS:HA	4:D:127:PRO:HD3	1.54	0.46
4:D:139:VAL:HG21	4:D:147:SER:N	2.29	0.46
2:B:109:ILE:O	2:B:112:PRO:CD	2.52	0.46
3:C:172:PHE:O	3:C:231:LEU:HG	2.16	0.46
3:C:219:VAL:HB	3:C:231:LEU:HA	1.98	0.46
4:D:102:TYR:HH	4:D:136:THR:HG22	1.79	0.46
6:F:28:LYS:C	6:F:30:GLN:N	2.73	0.46
1:A:14:ILE:CD1	1:A:14:ILE:N	2.78	0.46
1:A:150:ILE:HD13	15:B:1201:TDS:HAA2	1.80	0.46
1:A:195:ILE:HD13	1:A:199:MET:CE	2.45	0.46
1:A:202:HIS:HE1	10:A:302:HEM:C4C	2.33	0.46
2:B:84:VAL:O	2:B:87:ILE:HB	2.16	0.46
2:B:152:ASP:C	2:B:154:THR:N	2.60	0.46
3:C:274:LEU:HB3	4:D:19:MET:HE1	1.98	0.46
4:D:177:TRP:NE1	4:D:178:TRP:HE3	2.13	0.46
1:A:141:ASP:OD2	1:A:141:ASP:O	2.34	0.46
1:A:195:ILE:HG23	1:A:199:MET:HE3	1.97	0.46
1:A:206:ILE:HG21	11:A:303:HEC:HBD1	1.97	0.46
2:B:124:PHE:CZ	7:G:26:TYR:HD1	2.34	0.46
2:B:130:THR:HG23	7:G:22:PHE:HE2	1.76	0.46
2:B:153:LYS:NZ	2:B:153:LYS:HB3	2.30	0.46
3:C:4:TRP:HA	3:C:7:GLN:CB	2.45	0.46
3:C:153:ALA:O	3:C:240:PHE:CD1	2.69	0.46
2:B:110:LEU:HA	2:B:110:LEU:HD23	1.16	0.46
3:C:14:ARG:NH2	3:C:150:HIS:HD2	2.11	0.46
3:C:149:ILE:HB	3:C:245:THR:HG23	1.97	0.46
4:D:150:LEU:HD11	4:D:171:ARG:NE	2.31	0.46
5:E:27:LYS:O	5:E:30:LYS:N	2.47	0.46
1:A:29:HIS:CG	1:A:214:PRO:HA	2.51	0.45
1:A:30:VAL:CG2	1:A:34:TYR:CD1	2.98	0.45
1:A:92:MET:HE3	12:A:1002:OPC:HCB2	0.54	0.45
3:C:104:GLN:HA	3:C:105:PRO:HD3	1.69	0.45
1:A:35:CYS:O	1:A:36:LEU:C	2.58	0.45
1:A:103:ARG:C	1:A:103:ARG:CD	2.70	0.45
2:B:4:LEU:HG	2:B:5:LYS:H	1.81	0.45
2:B:122:ASN:OD1	2:B:122:ASN:C	2.59	0.45
8:H:11:LEU:C	8:H:11:LEU:HD12	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:CD	10:A:301:HEM:O1D	2.60	0.45
2:B:33:PRO:O	2:B:34:ASN:C	2.57	0.45
2:B:137:THR:O	2:B:141:ILE:HG13	2.16	0.45
3:C:273:ILE:HD12	8:H:25:GLY:HA3	1.98	0.45
4:D:21:LEU:CD1	17:D:201:SQD:C30	2.89	0.45
4:D:134:ASP:HB3	4:D:140:ILE:HD12	1.97	0.45
7:G:3:GLU:HA	7:G:4:PRO:HD2	1.72	0.45
3:C:65:GLY:O	3:C:66:SER:C	2.46	0.45
3:C:241:GLY:O	3:C:242:GLN:HG2	2.16	0.45
5:E:8:TYR:CD2	5:E:8:TYR:C	2.93	0.45
1:A:94:VAL:HG11	2:B:80:TYR:CD2	2.52	0.45
3:C:101:VAL:HG11	3:C:103:PHE:CZ	2.51	0.45
3:C:171:VAL:HA	3:C:232:THR:HG21	1.98	0.45
2:B:108:LEU:HD12	2:B:108:LEU:HA	1.74	0.45
2:B:156:THR:C	2:B:158:GLY:H	2.25	0.45
4:D:76:GLY:C	4:D:77:ASP:O	2.60	0.45
6:F:1:MET:HE3	6:F:1:MET:HB2	1.53	0.45
7:G:21:LEU:HD12	7:G:21:LEU:HA	1.73	0.45
2:B:18:LEU:HD23	2:B:18:LEU:HA	1.56	0.45
2:B:95:LEU:HD23	2:B:99:LEU:CD1	2.44	0.45
2:B:32:TRP:CD1	2:B:33:PRO:HD2	2.50	0.45
2:B:32:TRP:CG	2:B:33:PRO:CD	3.00	0.45
2:B:34:ASN:ND2	3:C:283:GLN:NE2	2.32	0.45
2:B:36:LEU:O	2:B:37:LEU:C	2.59	0.45
3:C:36:VAL:HG23	3:C:37:PRO:O	2.16	0.45
3:C:200:GLN:O	3:C:205:LYS:CG	2.53	0.45
2:B:85:PHE:CD2	15:B:1201:TDS:OAC	2.69	0.45
3:C:4:TRP:CG	3:C:162:PRO:HG3	2.52	0.45
4:D:141:ARG:CG	4:D:141:ARG:HH11	2.30	0.45
10:A:302:HEM:CBC	10:A:302:HEM:CMC	2.83	0.45
2:B:93:ASN:O	2:B:94:LYS:C	2.60	0.45
2:B:102:ALA:O	2:B:106:LEU:HG	2.16	0.45
3:C:1:TYR:O	3:C:2:PRO:C	2.60	0.45
3:C:271:MET:CE	4:D:22:LEU:HD12	2.47	0.45
4:D:59:LYS:HD3	4:D:59:LYS:N	2.32	0.45
5:E:11:PHE:HE2	5:E:15:PHE:CE1	2.35	0.45
5:E:24:PHE:O	5:E:25:ALA:C	2.61	0.45
1:A:5:TYR:O	1:A:6:ASP:C	2.59	0.44
1:A:80:TRP:CG	1:A:81:LEU:H	2.36	0.44
1:A:112:LYS:HB3	1:A:113:PRO:HD3	1.99	0.44
3:C:94:LEU:CD2	3:C:98:VAL:CG2	2.95	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:286:GLU:OE1	3:C:286:GLU:HA	2.17	0.44
4:D:117:TRP:HE1	4:D:119:ALA:HA	1.82	0.44
4:D:143:PRO:O	4:D:145:PRO:CD	2.58	0.44
6:F:20:TRP:CD1	6:F:24:VAL:HG21	2.52	0.44
1:A:80:TRP:CG	1:A:81:LEU:N	2.85	0.44
1:A:211:ILE:CD1	10:A:302:HEM:O2D	2.65	0.44
3:C:36:VAL:HG11	3:C:149:ILE:HD12	1.97	0.44
4:D:160:ILE:HG23	4:D:160:ILE:HD13	1.66	0.44
6:F:11:LEU:HD23	6:F:15:LEU:HD11	2.00	0.44
7:G:19:GLY:O	7:G:21:LEU:N	2.49	0.44
2:B:33:PRO:O	2:B:35:ASP:N	2.50	0.44
2:B:73:LEU:H	2:B:73:LEU:HG	1.46	0.44
15:B:1202:TDS:OAO	15:B:1202:TDS:HAS2	2.17	0.44
3:C:242:GLN:HE21	3:C:242:GLN:HB3	1.49	0.44
3:C:271:MET:O	4:D:23:ALA:HB2	2.17	0.44
2:B:84:VAL:HG11	2:B:101:MET:CG	2.46	0.44
2:B:131:THR:C	2:B:133:PHE:N	2.73	0.44
3:C:266:MET:HE2	5:E:15:PHE:CE1	2.53	0.44
4:D:74:ASN:O	4:D:93:VAL:CG1	2.66	0.44
1:A:114:ARG:CZ	1:A:212:SER:HA	2.47	0.44
2:B:40:PHE:HB3	2:B:41:PRO:HD3	1.92	0.44
2:B:134:LEU:N	2:B:134:LEU:CD1	2.70	0.44
2:B:150:PRO:O	2:B:151:LEU:C	2.61	0.44
3:C:36:VAL:HG11	3:C:149:ILE:HD13	1.99	0.44
3:C:210:THR:C	3:C:211:ILE:HG22	2.43	0.44
7:G:11:LEU:N	7:G:11:LEU:CD2	2.58	0.44
1:A:122:VAL:HG22	10:A:302:HEM:CBC	2.48	0.44
2:B:118:ASN:ND2	2:B:119:LYS:N	2.65	0.44
3:C:171:VAL:HB	3:C:233:ASN:O	2.18	0.44
3:C:193:VAL:CG1	3:C:194:LYS:N	2.80	0.44
4:D:65:LYS:HB2	4:D:68:LYS:NZ	2.31	0.44
1:A:104:VAL:HG21	10:A:302:HEM:C2D	2.53	0.44
2:B:151:LEU:O	2:B:151:LEU:HD22	2.16	0.44
2:B:159:LEU:O	2:B:160:PHE:HD2	1.95	0.44
18:G:101:BCR:H20C	18:G:101:BCR:H361	1.34	0.44
1:A:47:GLN:CA	1:A:47:GLN:NE2	2.45	0.44
1:A:117:THR:O	1:A:118:TRP:C	2.61	0.44
3:C:135:ASN:ND2	3:C:138:THR:HG23	2.33	0.44
4:D:81:VAL:O	4:D:83:GLY:N	2.51	0.44
5:E:27:LYS:O	5:E:30:LYS:CA	2.66	0.44
1:A:26:VAL:N	2:B:29:GLU:O	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1002:OPC:CBN	7:G:5:LEU:HD11	2.48	0.43
2:B:124:PHE:CE1	7:G:26:TYR:CD1	3.06	0.43
3:C:73:GLY:O	3:C:74:ALA:CB	2.66	0.43
3:C:264:LEU:HD23	3:C:264:LEU:HA	1.46	0.43
4:D:63:ASN:HD22	4:D:63:ASN:H	1.66	0.43
1:A:18:ALA:O	1:A:19:ASP:C	2.57	0.43
1:A:31:ASN:HD22	1:A:32:ILE:N	2.15	0.43
1:A:40:THR:HG22	10:A:302:HEM:HMB1	1.98	0.43
12:A:1002:OPC:HBN1	7:G:5:LEU:HD11	1.99	0.43
2:B:131:THR:O	2:B:133:PHE:N	2.51	0.43
3:C:278:GLN:HG3	5:E:31:LEU:O	2.18	0.43
1:A:103:ARG:HG3	1:A:103:ARG:HH11	1.83	0.43
1:A:154:VAL:HB	1:A:155:PRO:CD	2.48	0.43
1:A:118:TRP:O	1:A:119:ILE:C	2.56	0.43
2:B:106:LEU:HG	2:B:106:LEU:H	1.64	0.43
3:C:60:GLN:HG2	3:C:70:LEU:HB3	1.99	0.43
6:F:30:GLN:HE21	6:F:30:GLN:HB2	1.68	0.43
1:A:112:LYS:HB3	1:A:113:PRO:CD	2.49	0.43
11:A:303:HEC:C3C	2:B:40:PHE:CE2	3.01	0.43
2:B:120:PHE:CD1	2:B:120:PHE:N	2.85	0.43
3:C:34:VAL:CG2	3:C:151:LEU:CD2	2.96	0.43
11:C:301:HEC:CMB	11:C:301:HEC:CBB	2.94	0.43
4:D:178:TRP:O	4:D:179:VAL:HG23	2.19	0.43
1:A:11:ARG:H	1:A:11:ARG:HG2	1.19	0.43
1:A:77:SER:O	1:A:78:PHE:HB2	2.18	0.43
1:A:114:ARG:NH1	10:A:302:HEM:O1D	2.51	0.43
3:C:4:TRP:HA	3:C:7:GLN:HB2	1.99	0.43
3:C:76:LEU:HG	3:C:77:MET:N	2.34	0.43
3:C:258:MET:HE3	3:C:258:MET:HB3	1.93	0.43
4:D:122:ASN:HB2	4:D:135:GLU:OE2	2.08	0.43
1:A:30:VAL:HG22	1:A:34:TYR:CB	2.49	0.43
1:A:163:VAL:O	1:A:166:SER:N	2.51	0.43
11:A:303:HEC:C1C	2:B:40:PHE:CZ	3.02	0.43
2:B:33:PRO:HB2	2:B:34:ASN:H	1.13	0.43
3:C:46:PHE:CZ	3:C:131:VAL:CG2	2.95	0.43
3:C:171:VAL:HG11	3:C:234:ASN:CA	2.41	0.43
4:D:139:VAL:CG2	4:D:146:LEU:C	2.91	0.43
1:A:32:ILE:HG22	1:A:33:PHE:N	2.32	0.43
1:A:138:LEU:N	1:A:139:PRO:CD	2.82	0.43
1:A:142:GLN:HE22	2:B:67:ASP:HB3	1.84	0.43
2:B:80:TYR:CD1	2:B:80:TYR:C	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:GLU:HG3	12:B:1001:OPC:OCC	2.19	0.43
3:C:171:VAL:HG12	3:C:235:PRO:HD3	1.87	0.43
4:D:65:LYS:O	4:D:67:SER:N	2.52	0.43
1:A:7:TRP:O	1:A:11:ARG:HG3	2.19	0.43
2:B:11:ASP:C	2:B:13:LYS:N	2.72	0.43
2:B:88:LEU:HD12	2:B:101:MET:SD	2.59	0.43
3:C:3:PHE:O	3:C:6:GLN:HB3	2.18	0.43
3:C:4:TRP:CE2	3:C:162:PRO:HG3	2.53	0.43
4:D:107:VAL:HG23	4:D:107:VAL:H	1.37	0.43
2:B:41:PRO:O	2:B:45:MET:HB2	2.19	0.42
2:B:96:LEU:HD11	2:B:100:LEU:HD11	1.97	0.42
3:C:21:VAL:O	3:C:22:CYS:C	2.62	0.42
3:C:52:ILE:O	3:C:52:ILE:CG2	2.41	0.42
3:C:193:VAL:HG12	3:C:194:LYS:H	1.82	0.42
11:C:301:HEC:HHA	11:C:301:HEC:HAA2	1.74	0.42
8:H:6:LEU:HD23	8:H:6:LEU:HA	1.51	0.42
2:B:91:VAL:O	2:B:92:PRO:C	2.62	0.42
3:C:34:VAL:HG23	3:C:151:LEU:HD22	2.01	0.42
3:C:64:ASP:CG	3:C:65:GLY:N	2.77	0.42
4:D:21:LEU:HD11	17:D:201:SQD:C31	2.49	0.42
4:D:78:ARG:HD3	4:D:117:TRP:CG	2.54	0.42
1:A:103:ARG:HB2	7:G:21:LEU:HD11	2.00	0.42
3:C:158:GLY:H	11:C:301:HEC:HAD2	1.83	0.42
4:D:81:VAL:O	4:D:82:GLN:C	2.62	0.42
6:F:10:LEU:HD13	6:F:10:LEU:HA	1.61	0.42
7:G:14:VAL:HG12	7:G:15:PHE:N	2.34	0.42
1:A:180:LEU:O	1:A:181:THR:C	2.62	0.42
1:A:206:ILE:CG2	11:A:303:HEC:HBD1	2.50	0.42
3:C:61:VAL:CG1	3:C:168:ASN:ND2	2.82	0.42
3:C:267:LEU:HD22	3:C:267:LEU:HA	1.85	0.42
4:D:65:LYS:HD3	4:D:158:ASP:O	2.18	0.42
1:A:38:GLY:HA3	11:A:303:HEC:NC	2.35	0.42
1:A:82:ILE:HD13	1:A:82:ILE:H	1.84	0.42
1:A:88:TRP:O	1:A:92:MET:HG2	2.20	0.42
3:C:27:LEU:HA	3:C:27:LEU:HD23	1.82	0.42
3:C:36:VAL:HG23	3:C:37:PRO:N	2.34	0.42
3:C:155:ARG:HD2	3:C:239:GLY:O	2.19	0.42
7:G:15:PHE:O	7:G:16:ALA:C	2.62	0.42
8:H:3:ILE:HD12	8:H:3:ILE:HA	1.92	0.42
1:A:30:VAL:CG2	1:A:34:TYR:CD2	3.02	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:MET:HA	1:A:96:MET:CE	2.50	0.42
1:A:203:PHE:CD1	1:A:203:PHE:N	2.83	0.42
3:C:102:TYR:CD2	3:C:102:TYR:C	2.97	0.42
4:D:13:MET:O	4:D:16:ARG:N	2.52	0.42
1:A:104:VAL:HG12	1:A:118:TRP:HZ3	1.83	0.42
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.39	0.42
2:B:3:THR:HG21	3:C:283:GLN:OE1	2.20	0.42
3:C:122:GLU:H	3:C:122:GLU:HG2	1.18	0.42
4:D:12:ASP:O	4:D:15:ARG:N	2.50	0.42
4:D:36:TYR:OH	4:D:40:LYS:HE3	2.19	0.42
6:F:16:ILE:HG22	6:F:17:PHE:H	1.82	0.42
1:A:15:GLN:C	1:A:17:LEU:N	2.77	0.42
1:A:44:PHE:CE1	1:A:195:ILE:HG21	2.54	0.42
1:A:127:ILE:CD1	1:A:194:LEU:HB3	2.49	0.42
1:A:150:ILE:HD11	15:B:1201:TDS:HAA2	2.00	0.42
10:A:301:HEM:HBA2	10:A:301:HEM:CGD	2.46	0.42
2:B:93:ASN:OD1	2:B:96:LEU:N	2.52	0.42
3:C:58:LEU:CD1	3:C:58:LEU:C	2.93	0.42
4:D:15:ARG:HB3	5:E:31:LEU:HD23	1.96	0.42
1:A:139:PRO:HG3	10:A:301:HEM:O2D	2.20	0.42
2:B:129:ALA:O	2:B:131:THR:N	2.53	0.42
2:B:138:LEU:O	2:B:139:VAL:C	2.61	0.42
4:D:146:LEU:HD12	4:D:177:TRP:CE2	2.48	0.42
1:A:182:ARG:O	1:A:183:TYR:C	2.63	0.42
2:B:130:THR:HG23	7:G:22:PHE:CE2	2.54	0.42
4:D:58:ASP:O	4:D:61:GLY:N	2.53	0.42
4:D:172:THR:O	4:D:174:GLU:OE2	2.37	0.42
1:A:20:ASP:OD2	1:A:20:ASP:C	2.63	0.41
2:B:87:ILE:O	2:B:89:ARG:N	2.53	0.41
4:D:22:LEU:HD22	4:D:22:LEU:HA	1.62	0.41
4:D:170:PHE:CZ	4:D:171:ARG:HG2	2.54	0.41
6:F:22:LEU:CD1	8:H:20:ALA:HB1	2.50	0.41
1:A:106:LEU:CD2	2:B:133:PHE:CE1	2.83	0.41
3:C:54:TYR:CE1	3:C:70:LEU:CG	3.01	0.41
3:C:93:GLU:OE1	3:C:93:GLU:CA	2.66	0.41
3:C:223:GLN:O	3:C:224:ALA:CB	2.68	0.41
4:D:36:TYR:N	4:D:37:PRO:HD2	2.36	0.41
4:D:139:VAL:HG21	4:D:146:LEU:C	2.45	0.41
3:C:94:LEU:CD2	3:C:98:VAL:HG23	2.50	0.41
3:C:157:ARG:N	11:C:301:HEC:HBA1	2.35	0.41
6:F:20:TRP:O	6:F:24:VAL:CG2	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:GLU:O	7:G:35:LEU:HG	2.21	0.41
1:A:214:PRO:HD3	2:B:24:HIS:CE1	2.55	0.41
2:B:14:LEU:HD11	2:B:18:LEU:CD1	2.47	0.41
3:C:215:PRO:HB3	3:C:232:THR:CG2	2.49	0.41
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.50	0.41
7:G:31:ARG:O	7:G:32:PRO:O	2.38	0.41
1:A:158:ILE:HA	1:A:159:PRO:HD3	1.46	0.41
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.74	0.41
2:B:68:PRO:C	2:B:69:PHE:HD2	2.29	0.41
2:B:131:THR:O	2:B:132:ILE:C	2.59	0.41
3:C:94:LEU:C	3:C:96:LYS:N	2.74	0.41
3:C:189:GLU:N	3:C:189:GLU:OE1	2.54	0.41
3:C:279:VAL:O	3:C:281:LYS:N	2.54	0.41
3:C:72:VAL:H	3:C:72:VAL:HG13	1.46	0.41
4:D:169:ASP:O	4:D:171:ARG:N	2.54	0.41
1:A:38:GLY:HA3	11:A:303:HEC:C4C	2.51	0.41
2:B:152:ASP:CA	2:B:154:THR:H	2.32	0.41
3:C:94:LEU:HD23	3:C:98:VAL:HG23	2.02	0.41
3:C:189:GLU:OE1	3:C:189:GLU:CA	2.68	0.41
3:C:200:GLN:HG2	3:C:201:THR:HA	2.03	0.41
5:E:24:PHE:CZ	6:F:29:ILE:HD11	2.55	0.41
3:C:33:GLU:HA	3:C:243:ASP:OD2	2.21	0.41
3:C:174:ALA:HB3	3:C:229:GLU:H	1.86	0.41
3:C:229:GLU:CD	3:C:230:ALA:N	2.72	0.41
5:E:24:PHE:CZ	6:F:29:ILE:CD1	3.04	0.41
1:A:39:ILE:HD13	1:A:39:ILE:HG21	1.72	0.41
1:A:43:CYS:HB3	1:A:93:MET:HB2	2.02	0.41
1:A:105:TYR:OH	2:B:129:ALA:HB1	2.21	0.41
1:A:198:PHE:HA	1:A:201:LEU:HD12	2.03	0.41
11:A:303:HEC:CGA	15:B:1202:TDS:CAA	2.85	0.41
2:B:134:LEU:HA	2:B:134:LEU:HD12	1.12	0.41
3:C:214:GLY:N	3:C:215:PRO:CD	2.84	0.41
3:C:247:ILE:HD13	3:C:247:ILE:HG21	1.82	0.41
3:C:270:LEU:HB2	8:H:21:MET:HE1	1.98	0.41
4:D:87:ASP:HB3	4:D:105:ASN:OD1	2.21	0.41
4:D:105:ASN:HD21	4:D:107:VAL:CG2	2.23	0.41
4:D:114:VAL:O	4:D:114:VAL:HG12	2.19	0.41
7:G:18:LEU:O	7:G:22:PHE:HD1	2.03	0.41
3:C:151:LEU:CG	3:C:152:GLY:N	2.80	0.41
3:C:173:THR:O	3:C:231:LEU:HG	2.21	0.41
3:C:229:GLU:C	3:C:231:LEU:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ALA:O	3:C:232:THR:N	2.53	0.41
1:A:126:VAL:H	1:A:126:VAL:HG23	1.75	0.40
12:A:1002:OPC:HBZ2	18:G:101:BCR:H333	2.03	0.40
2:B:83:PRO:O	2:B:84:VAL:C	2.63	0.40
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.56	0.40
4:D:64:VAL:HG11	4:D:69:PHE:CD1	2.56	0.40
1:A:17:LEU:HA	1:A:17:LEU:HD13	1.67	0.40
1:A:117:THR:HG22	10:A:302:HEM:C2D	2.57	0.40
1:A:142:GLN:NE2	2:B:67:ASP:HB3	2.36	0.40
2:B:97:GLY:HA2	2:B:100:LEU:CD1	2.51	0.40
3:C:149:ILE:HB	3:C:245:THR:CG2	2.52	0.40
3:C:218:ILE:HD12	3:C:218:ILE:H	1.86	0.40
3:C:226:LYS:O	3:C:228:GLY:N	2.54	0.40
6:F:22:LEU:HD12	8:H:20:ALA:HB2	2.02	0.40
1:A:9:GLN:HA	1:A:9:GLN:OE1	2.21	0.40
1:A:80:TRP:CD2	1:A:81:LEU:N	2.89	0.40
3:C:72:VAL:O	3:C:72:VAL:HG22	2.20	0.40
3:C:79:PRO:HD3	3:C:149:ILE:HG12	2.03	0.40
3:C:178:GLY:O	3:C:224:ALA:HB1	2.20	0.40
3:C:285:ALA:HB2	4:D:10:VAL:CG2	2.46	0.40
4:D:87:ASP:O	4:D:88:PRO:C	2.62	0.40
1:A:26:VAL:HA	1:A:27:PRO:HD2	1.56	0.40
1:A:211:ILE:O	1:A:212:SER:O	2.40	0.40
10:A:302:HEM:HBB2	10:A:302:HEM:HMB1	2.00	0.40
11:A:303:HEC:HBA2	15:B:1202:TDS:HAA2	2.02	0.40
2:B:1:MET:HE2	2:B:1:MET:HB2	1.95	0.40
2:B:94:LYS:O	2:B:95:LEU:C	2.65	0.40
2:B:149:PHE:CB	2:B:150:PRO:HD3	2.50	0.40
3:C:274:LEU:HA	3:C:274:LEU:HD23	1.58	0.40
1:A:215:LEU:HB2	7:G:28:GLN:OE1	2.21	0.40
2:B:85:PHE:HE1	2:B:147:ALA:CB	2.34	0.40
2:B:159:LEU:HD23	2:B:159:LEU:N	2.35	0.40
3:C:115:LEU:HD23	3:C:115:LEU:HA	1.59	0.40
3:C:146:LYS:HG3	3:C:248:VAL:HG23	2.02	0.40
7:G:27:GLN:OE1	8:H:29:LEU:CD2	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:GLU:OE2	7:G:33:ASN:CB[8_565]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/215 (99%)	154 (72%)	41 (19%)	18 (8%)	0	4
2	B	158/160 (99%)	89 (56%)	43 (27%)	26 (16%)	0	0
3	C	286/289 (99%)	204 (71%)	51 (18%)	31 (11%)	0	3
4	D	164/179 (92%)	114 (70%)	28 (17%)	22 (13%)	0	1
5	E	30/32 (94%)	15 (50%)	11 (37%)	4 (13%)	0	1
6	F	30/35 (86%)	15 (50%)	8 (27%)	7 (23%)	0	0
7	G	35/37 (95%)	11 (31%)	15 (43%)	9 (26%)	0	0
8	H	27/29 (93%)	15 (56%)	6 (22%)	6 (22%)	0	0
All	All	943/976 (97%)	617 (65%)	203 (22%)	123 (13%)	0	1

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ALA
1	A	36	LEU
1	A	73	MET
1	A	74	ASN
1	A	112	LYS
1	A	162	GLY
2	B	22	MET
2	B	33	PRO
2	B	34	ASN
2	B	37	LEU
2	B	87	ILE
2	B	88	LEU
2	B	113	PHE
2	B	114	ILE
2	B	115	GLU
2	B	125	ARG
3	C	23	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	63	ALA
3	C	66	SER
3	C	74	ALA
3	C	173	THR
3	C	186	GLU
3	C	189	GLU
3	C	192	ASN
3	C	200	GLN
3	C	201	THR
3	C	202	ASP
3	C	212	PRO
3	C	224	ALA
3	C	226	LYS
3	C	227	ALA
3	C	230	ALA
4	D	13	MET
4	D	14	GLY
4	D	49	ALA
4	D	63	ASN
4	D	64	VAL
4	D	70	LEU
4	D	71	GLU
4	D	77	ASP
4	D	135	GLU
4	D	139	VAL
4	D	145	PRO
4	D	167	GLU
6	F	9	ALA
6	F	10	LEU
6	F	29	ILE
7	G	16	ALA
7	G	20	GLY
7	G	27	GLN
7	G	32	PRO
7	G	34	GLU
8	H	2	GLU
8	H	4	ASP
1	A	2	ALA
1	A	3	ASN
1	A	114	ARG
1	A	132	GLY
1	A	136	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	150	ILE
2	B	146	GLY
3	C	34	VAL
3	C	174	ALA
3	C	191	GLY
3	C	278	GLN
4	D	21	LEU
4	D	56	ALA
4	D	81	VAL
4	D	97	GLU
4	D	110	HIS
6	F	24	VAL
7	G	19	GLY
1	A	32	ILE
1	A	131	PHE
2	B	94	LYS
2	B	95	LEU
3	C	20	ILE
3	C	91	PRO
3	C	184	ALA
3	C	195	TYR
4	D	82	GLN
4	D	138	LYS
4	D	174	GLU
5	E	13	ALA
6	F	17	PHE
7	G	4	PRO
7	G	14	VAL
1	A	96	MET
2	B	78	GLU
2	B	134	LEU
2	B	145	ILE
3	C	175	SER
3	C	187	GLU
3	C	231	LEU
4	D	122	ASN
8	H	7	GLY
8	H	20	ALA
1	A	60	PRO
1	A	155	PRO
2	B	2	ALA
2	B	36	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	86	GLN
2	B	102	ALA
2	B	124	PHE
2	B	137	THR
2	B	141	ILE
3	C	194	LYS
5	E	17	GLY
5	E	19	ALA
6	F	6	LEU
7	G	31	ARG
2	B	92	PRO
2	B	105	PRO
2	B	122	ASN
3	C	88	GLU
3	C	215	PRO
1	A	206	ILE
5	E	18	ILE
6	F	16	ILE
8	H	19	ILE
8	H	23	VAL
3	C	69	GLY
4	D	143	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/184 (100%)	126 (68%)	58 (32%)	0	1
2	B	137/137 (100%)	90 (66%)	47 (34%)	0	1
3	C	242/243 (100%)	153 (63%)	89 (37%)	0	0
4	D	139/146 (95%)	94 (68%)	45 (32%)	0	1
5	E	25/25 (100%)	17 (68%)	8 (32%)	0	1
6	F	24/27 (89%)	11 (46%)	13 (54%)	0	0
7	G	28/28 (100%)	15 (54%)	13 (46%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	24/24 (100%)	17 (71%)	7 (29%)	0	1
All	All	803/814 (99%)	523 (65%)	280 (35%)	0	1

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	TYR
1	A	11	ARG
1	A	12	LEU
1	A	14	ILE
1	A	17	LEU
1	A	21	VAL
1	A	30	VAL
1	A	31	ASN
1	A	32	ILE
1	A	36	LEU
1	A	47	GLN
1	A	52	PHE
1	A	61	THR
1	A	62	VAL
1	A	72	ILE
1	A	77	SER
1	A	81	LEU
1	A	82	ILE
1	A	83	ARG
1	A	84	SER
1	A	87	ARG
1	A	95	LEU
1	A	97	MET
1	A	99	LEU
1	A	100	HIS
1	A	103	ARG
1	A	104	VAL
1	A	106	LEU
1	A	107	THR
1	A	110	PHE
1	A	112	LYS
1	A	114	ARG
1	A	115	GLU
1	A	116	LEU
1	A	119	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	123	ILE
1	A	130	SER
1	A	142	GLN
1	A	143	VAL
1	A	148	VAL
1	A	151	VAL
1	A	152	SER
1	A	155	PRO
1	A	161	VAL
1	A	163	VAL
1	A	164	LEU
1	A	169	LEU
1	A	173	SER
1	A	182	ARG
1	A	195	ILE
1	A	200	LEU
1	A	201	LEU
1	A	206	ILE
1	A	207	ARG
1	A	208	LYS
1	A	211	ILE
1	A	215	LEU
2	B	3	THR
2	B	4	LEU
2	B	5	LYS
2	B	8	ASP
2	B	13	LYS
2	B	15	ARG
2	B	20	LYS
2	B	25	ASN
2	B	35	ASP
2	B	39	VAL
2	B	40	PHE
2	B	44	ILE
2	B	51	ILE
2	B	55	SER
2	B	57	LEU
2	B	69	PHE
2	B	73	LEU
2	B	74	GLU
2	B	75	ILE
2	B	76	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	79	TRP
2	B	81	LEU
2	B	86	GLN
2	B	88	LEU
2	B	90	SER
2	B	94	LYS
2	B	96	LEU
2	B	100	LEU
2	B	101	MET
2	B	103	SER
2	B	109	ILE
2	B	115	GLU
2	B	119	LYS
2	B	120	PHE
2	B	127	PRO
2	B	132	ILE
2	B	134	LEU
2	B	138	LEU
2	B	140	THR
2	B	141	ILE
2	B	143	LEU
2	B	153	LYS
2	B	154	THR
2	B	155	LEU
2	B	156	THR
2	B	157	LEU
2	B	159	LEU
3	C	3	PHE
3	C	7	GLN
3	C	12	THR
3	C	14	ARG
3	C	19	ARG
3	C	21	VAL
3	C	22	CYS
3	C	30	LYS
3	C	35	GLU
3	C	36	VAL
3	C	40	VAL
3	C	47	LYS
3	C	50	VAL
3	C	56	THR
3	C	58	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	59	GLN
3	C	60	GLN
3	C	61	VAL
3	C	70	LEU
3	C	72	VAL
3	C	75	VAL
3	C	77	MET
3	C	80	GLU
3	C	88	GLU
3	C	92	GLU
3	C	93	GLU
3	C	95	LYS
3	C	100	ASP
3	C	101	VAL
3	C	104	GLN
3	C	110	GLN
3	C	113	VAL
3	C	116	VAL
3	C	119	LEU
3	C	122	GLU
3	C	125	GLN
3	C	126	GLU
3	C	131	VAL
3	C	132	LEU
3	C	137	THR
3	C	141	ASN
3	C	150	HIS
3	C	154	ASN
3	C	155	ARG
3	C	160	ILE
3	C	165	GLU
3	C	166	LYS
3	C	171	VAL
3	C	172	PHE
3	C	175	SER
3	C	179	THR
3	C	180	ILE
3	C	185	LYS
3	C	186	GLU
3	C	188	ASP
3	C	189	GLU
3	C	198	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	199	ILE
3	C	203	SER
3	C	205	LYS
3	C	206	THR
3	C	207	VAL
3	C	208	VAL
3	C	210	THR
3	C	211	ILE
3	C	212	PRO
3	C	216	GLU
3	C	218	ILE
3	C	219	VAL
3	C	221	GLU
3	C	223	GLN
3	C	226	LYS
3	C	229	GLU
3	C	232	THR
3	C	233	ASN
3	C	242	GLN
3	C	249	LEU
3	C	251	ASP
3	C	256	LYS
3	C	259	ILE
3	C	262	ILE
3	C	264	LEU
3	C	267	LEU
3	C	270	LEU
3	C	276	LYS
3	C	282	VAL
3	C	286	GLU
3	C	287	MET
3	C	288	ASN
4	D	9	ASP
4	D	10	VAL
4	D	13	MET
4	D	16	ARG
4	D	22	LEU
4	D	26	THR
4	D	35	LEU
4	D	43	ILE
4	D	59	LYS
4	D	60	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	65	LYS
4	D	66	VAL
4	D	67	SER
4	D	68	LYS
4	D	69	PHE
4	D	72	SER
4	D	77	ASP
4	D	78	ARG
4	D	79	VAL
4	D	84	LEU
4	D	85	LYS
4	D	95	SER
4	D	96	LYS
4	D	97	GLU
4	D	99	ILE
4	D	101	ASP
4	D	105	ASN
4	D	107	VAL
4	D	109	THR
4	D	111	LEU
4	D	114	VAL
4	D	125	LYS
4	D	134	ASP
4	D	139	VAL
4	D	140	ILE
4	D	141	ARG
4	D	146	LEU
4	D	148	LEU
4	D	154	THR
4	D	160	ILE
4	D	161	VAL
4	D	167	GLU
4	D	172	THR
4	D	174	GLU
4	D	179	VAL
5	E	9	ILE
5	E	12	ILE
5	E	14	LEU
5	E	18	ILE
5	E	26	ILE
5	E	29	ILE
5	E	30	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	32	ILE
6	F	1	MET
6	F	6	LEU
6	F	10	LEU
6	F	11	LEU
6	F	12	SER
6	F	15	LEU
6	F	16	ILE
6	F	22	LEU
6	F	25	LEU
6	F	26	LEU
6	F	27	LEU
6	F	29	ILE
6	F	30	GLN
7	G	1	MET
7	G	2	VAL
7	G	3	GLU
7	G	4	PRO
7	G	5	LEU
7	G	6	LEU
7	G	9	LEU
7	G	23	TYR
7	G	28	GLN
7	G	29	TYR
7	G	30	LYS
7	G	34	GLU
7	G	35	LEU
8	H	2	GLU
8	H	6	LEU
8	H	14	VAL
8	H	18	SER
8	H	21	MET
8	H	22	VAL
8	H	27	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
2	B	25	ASN
2	B	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	118	ASN
3	C	6	GLN
3	C	59	GLN
3	C	60	GLN
3	C	110	GLN
3	C	123	GLN
3	C	141	ASN
3	C	154	ASN
3	C	200	GLN
3	C	223	GLN
3	C	234	ASN
3	C	242	GLN
3	C	250	GLN
3	C	288	ASN
4	D	73	HIS
4	D	105	ASN
4	D	152	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](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	TDS	B	1201	-	31,31,31	4.17	15 (48%)	37,40,40	5.20	17 (45%)
11	HEC	C	301	3	46,50,50	2.47	19 (41%)	58,82,82	2.42	14 (24%)
18	BCR	G	101	-	41,41,41	3.48	23 (56%)	56,56,56	6.82	27 (48%)
10	HEM	A	302	1	50,50,50	2.16	18 (36%)	67,82,82	2.06	20 (29%)
15	TDS	B	1202	11	31,31,31	4.21	13 (41%)	37,40,40	5.50	23 (62%)
13	UMQ	A	1102	-	35,35,35	2.17	9 (25%)	46,46,46	3.03	18 (39%)
13	UMQ	A	1103	-	35,35,35	1.98	5 (14%)	46,46,46	2.59	13 (28%)
13	UMQ	A	1104	-	35,35,35	1.58	3 (8%)	46,46,46	3.04	19 (41%)
17	SQD	D	201	-	52,54,54	2.93	25 (48%)	62,65,65	5.06	31 (50%)
13	UMQ	A	1101	-	35,35,35	1.75	5 (14%)	46,46,46	3.05	24 (52%)
12	OPC	B	1001	-	53,53,54	2.28	23 (43%)	59,61,64	2.71	25 (42%)
10	HEM	A	301	1	50,50,50	2.42	15 (30%)	67,82,82	3.40	35 (52%)
12	OPC	A	1002	-	53,53,54	2.05	14 (26%)	59,61,64	2.88	20 (33%)
11	HEC	A	303	19,15,1	46,50,50	2.34	13 (28%)	58,82,82	2.29	20 (34%)
16	FES	D	200	4	0,4,4	-	-	-	-	-
14	CLA	B	201	19	69,73,73	2.10	20 (28%)	82,113,113	3.04	36 (43%)

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
15	TDS	B	1201	-	-	11/17/17/17	0/2/2/2
11	HEC	C	301	3	-	8/14/54/54	-
18	BCR	G	101	-	-	12/29/63/63	0/2/2/2
10	HEM	A	302	1	-	6/14/54/54	-
15	TDS	B	1202	11	-	11/17/17/17	0/2/2/2
13	UMQ	A	1104	-	2/2/10/10	13/20/60/60	0/2/2/2
13	UMQ	A	1102	-	2/2/10/10	12/20/60/60	0/2/2/2
13	UMQ	A	1103	-	2/2/10/10	11/20/60/60	0/2/2/2
17	SQD	D	201	-	3/3/9/9	27/49/69/69	0/1/1/1
13	UMQ	A	1101	-	2/2/10/10	11/20/60/60	0/2/2/2
12	OPC	B	1001	-	-	23/57/57/60	-
10	HEM	A	301	1	-	5/14/54/54	-
12	OPC	A	1002	-	-	32/57/57/60	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEC	A	303	19,15,1	-	6/14/54/54	-
16	FES	D	200	4	-	-	0/1/1/1
14	CLA	B	201	19	2/2/15/20	13/39/115/115	-

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1202	TDS	CAD-CAE	-10.82	1.20	1.38
18	G	101	BCR	C8-C9	-10.35	1.23	1.46
15	B	1202	TDS	CAD-CAL	-10.08	1.21	1.38
15	B	1201	TDS	CAD-CAE	-9.85	1.22	1.38
15	B	1202	TDS	CAM-CAN	9.63	1.54	1.39
15	B	1201	TDS	CAL-CAM	9.23	1.53	1.40
15	B	1201	TDS	CAD-CAL	-9.07	1.23	1.38
18	G	101	BCR	C26-C25	7.64	1.47	1.34
18	G	101	BCR	C23-C22	-7.34	1.30	1.46
13	A	1102	UMQ	O1'-C1'	7.32	1.52	1.40
13	A	1101	UMQ	C1'-C2'	-7.15	1.31	1.52
12	B	1001	OPC	OBJ-CBK	7.13	1.54	1.33
15	B	1201	TDS	CAM-CAN	7.09	1.50	1.39
10	A	301	HEM	FE-NB	-7.06	1.73	1.94
17	D	201	SQD	C4-C3	6.70	1.69	1.52
15	B	1201	TDS	CAR-CAQ	-6.66	1.27	1.52
13	A	1103	UMQ	O1'-C1'	6.63	1.51	1.40
15	B	1202	TDS	CAL-CAM	6.62	1.49	1.40
15	B	1202	TDS	CAR-CAQ	-6.45	1.28	1.52
17	D	201	SQD	O47-C7	6.40	1.52	1.34
17	D	201	SQD	C17-C16	-6.40	1.20	1.51
18	G	101	BCR	C30-C25	6.33	1.61	1.53
15	B	1201	TDS	OAB-CAE	6.16	1.47	1.37
11	C	301	HEC	CAC-C3C	6.16	1.55	1.35
10	A	301	HEM	C3D-C2D	6.00	1.49	1.36
15	B	1202	TDS	CAH-CAG	-5.96	1.33	1.47
14	B	201	CLA	C3C-C2C	5.86	1.49	1.36
13	A	1103	UMQ	C1'-C2'	-5.76	1.35	1.52
11	C	301	HEC	CAB-C3B	5.71	1.53	1.35
18	G	101	BCR	C38-C26	5.68	1.60	1.50
11	A	303	HEC	CAC-C3C	5.60	1.53	1.35
12	A	1002	OPC	OAN-CAO	5.55	1.50	1.34
17	D	201	SQD	O6-C1	5.49	1.49	1.40
10	A	301	HEM	CMC-C2C	5.48	1.62	1.50
17	D	201	SQD	C12-C11	-5.44	1.24	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	301	HEC	C3D-C2D	5.32	1.52	1.38
11	A	303	HEC	CAB-C3B	5.27	1.52	1.35
12	B	1001	OPC	CAG-CAH	-5.24	1.35	1.51
11	A	303	HEC	CBB-CAB	-5.20	1.30	1.49
10	A	302	HEM	C3D-C2D	5.19	1.48	1.36
13	A	1102	UMQ	C1'-C2'	-5.10	1.37	1.52
15	B	1201	TDS	CAF-CAE	5.08	1.49	1.40
14	B	201	CLA	OBD-CAD	5.02	1.31	1.22
11	A	303	HEC	C3D-C2D	5.00	1.52	1.38
17	D	201	SQD	C16-C15	-4.92	1.27	1.51
14	B	201	CLA	O2D-CGD	4.86	1.45	1.33
18	G	101	BCR	C7-C6	-4.85	1.28	1.45
17	D	201	SQD	O48-C23	4.84	1.47	1.33
11	C	301	HEC	CMB-C2B	4.83	1.60	1.50
18	G	101	BCR	C8-C7	-4.81	1.18	1.33
13	A	1104	UMQ	O1'-C1'	4.81	1.48	1.40
13	A	1104	UMQ	C1'-C2'	-4.76	1.38	1.52
17	D	201	SQD	C18-C17	-4.76	1.28	1.51
10	A	301	HEM	CMB-C2B	4.71	1.60	1.50
12	A	1002	OPC	CBP-CBQ	-4.66	1.32	1.52
15	B	1201	TDS	CAR-CAS	-4.64	1.28	1.51
15	B	1202	TDS	CAR-CAS	-4.62	1.28	1.51
15	B	1201	TDS	OAK-CAL	4.59	1.44	1.37
13	A	1102	UMQ	O5'-C1'	4.59	1.53	1.41
15	B	1202	TDS	OAB-CAE	4.57	1.44	1.37
14	B	201	CLA	CHC-C1C	4.55	1.47	1.38
17	D	201	SQD	C13-C12	-4.55	1.29	1.51
14	B	201	CLA	O2A-CGA	4.41	1.46	1.33
12	B	1001	OPC	CAV-CAW	4.33	1.56	1.31
11	C	301	HEC	CBC-CAC	-4.31	1.33	1.49
10	A	302	HEM	C3C-C2C	-4.30	1.28	1.37
12	B	1001	OPC	CAQ-CAP	-4.30	1.36	1.52
10	A	301	HEM	FE-NC	4.27	2.09	1.95
11	A	303	HEC	C3B-C2B	-4.26	1.26	1.41
12	A	1002	OPC	CAV-CAW	4.25	1.55	1.31
12	A	1002	OPC	CAQ-CAP	-4.24	1.36	1.52
14	B	201	CLA	C3D-C4D	-4.22	1.34	1.44
15	B	1201	TDS	CAH-CAG	-4.22	1.37	1.47
17	D	201	SQD	C11-C10	-4.21	1.30	1.51
15	B	1202	TDS	CAF-CAE	4.21	1.48	1.40
12	A	1002	OPC	CBP-CBO	-4.20	1.30	1.51
11	A	303	HEC	CBC-CAC	-4.19	1.34	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1002	OPC	CAG-CAH	-4.03	1.39	1.51
17	D	201	SQD	C21-C20	-4.01	1.26	1.51
10	A	301	HEM	CAD-C3D	3.89	1.61	1.51
18	G	101	BCR	C19-C18	-3.80	1.37	1.46
10	A	302	HEM	CHC-C1C	-3.79	1.30	1.38
15	B	1201	TDS	OBD-CAM	3.78	1.45	1.36
13	A	1101	UMQ	O1'-C1'	3.78	1.46	1.40
14	B	201	CLA	CHD-C4C	3.75	1.47	1.39
11	A	303	HEC	C3C-C2C	-3.75	1.28	1.41
12	A	1002	OPC	OBJ-CBK	3.71	1.44	1.33
10	A	302	HEM	C4C-NC	-3.60	1.32	1.39
11	A	303	HEC	O1A-CGA	3.58	1.33	1.22
12	B	1001	OPC	OAN-CAO	3.58	1.44	1.34
10	A	301	HEM	C2A-C3A	-3.57	1.29	1.38
18	G	101	BCR	C1-C6	-3.56	1.49	1.53
10	A	302	HEM	C1B-C2B	3.55	1.51	1.44
12	A	1002	OPC	CAQ-CAR	-3.53	1.34	1.51
11	C	301	HEC	CBB-CAB	-3.53	1.36	1.49
18	G	101	BCR	C24-C25	-3.53	1.33	1.45
11	C	301	HEC	C4A-NA	-3.46	1.33	1.39
12	A	1002	OPC	CAR-CAS	-3.45	1.34	1.51
17	D	201	SQD	C22-C21	-3.43	1.25	1.50
11	C	301	HEC	CMA-C3A	3.43	1.57	1.50
14	B	201	CLA	CHB-C1B	3.41	1.47	1.39
10	A	302	HEM	O1A-CGA	3.37	1.33	1.22
17	D	201	SQD	C20-C19	-3.37	1.35	1.51
10	A	301	HEM	CHA-C4D	-3.35	1.31	1.38
17	D	201	SQD	C19-C18	-3.34	1.35	1.51
10	A	302	HEM	O1D-CGD	3.34	1.33	1.22
18	G	101	BCR	C27-C26	3.32	1.57	1.51
15	B	1202	TDS	OBD-CAM	3.31	1.44	1.36
13	A	1103	UMQ	O5'-C1'	3.29	1.50	1.41
18	G	101	BCR	C12-C13	-3.27	1.38	1.46
10	A	302	HEM	CHD-C1D	-3.27	1.31	1.39
18	G	101	BCR	C36-C18	3.26	1.57	1.50
11	C	301	HEC	C4C-NC	-3.24	1.33	1.39
10	A	301	HEM	CHA-C1A	-3.24	1.32	1.39
15	B	1202	TDS	OAK-CAL	3.23	1.42	1.37
14	B	201	CLA	CHC-C4B	3.17	1.46	1.39
18	G	101	BCR	C24-C23	-3.17	1.23	1.33
13	A	1104	UMQ	O2'-C2'	-3.14	1.35	1.43
15	B	1201	TDS	CAF-CAG	-3.12	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	201	CLA	C1B-C2B	3.12	1.50	1.43
13	A	1101	UMQ	O2'-C2'	-3.11	1.35	1.43
17	D	201	SQD	C36-C35	-3.08	1.36	1.51
12	B	1001	OPC	CBL-CBK	3.07	1.59	1.50
12	A	1002	OPC	CBC-CBD	-3.06	1.36	1.51
10	A	302	HEM	C1C-NC	-3.05	1.33	1.39
13	A	1103	UMQ	O2'-C2'	-3.05	1.35	1.43
12	B	1001	OPC	CAG-NAF	-3.05	1.42	1.51
12	A	1002	OPC	CBT-CBS	-3.04	1.33	1.50
12	A	1002	OPC	CBQ-CBR	-3.01	1.33	1.50
12	B	1001	OPC	CAQ-CAR	-2.99	1.36	1.51
14	B	201	CLA	C4C-C3C	2.98	1.50	1.45
12	B	1001	OPC	CAR-CAS	-2.95	1.37	1.51
10	A	302	HEM	CAC-C3C	2.95	1.55	1.47
17	D	201	SQD	C15-C14	-2.94	1.37	1.51
15	B	1201	TDS	CAQ-CAP	-2.93	1.42	1.49
18	G	101	BCR	C39-C30	2.92	1.59	1.53
12	B	1001	OPC	CBC-CBD	-2.92	1.37	1.51
10	A	301	HEM	CHB-C4A	-2.91	1.32	1.39
14	B	201	CLA	C3D-C2D	2.89	1.46	1.39
12	B	1001	OPC	CBB-CBC	-2.88	1.37	1.51
10	A	302	HEM	C3B-C2B	-2.88	1.31	1.37
10	A	301	HEM	CBD-CGD	2.85	1.57	1.50
17	D	201	SQD	C14-C13	-2.85	1.37	1.51
15	B	1202	TDS	CAF-CAG	-2.84	1.39	1.46
10	A	302	HEM	CMB-C2B	2.82	1.56	1.50
13	A	1102	UMQ	C1-C2	2.82	1.60	1.52
13	A	1101	UMQ	O5'-C1'	2.80	1.49	1.41
12	A	1002	OPC	CBB-CBC	-2.79	1.37	1.51
11	C	301	HEC	C3C-C2C	-2.78	1.31	1.41
10	A	302	HEM	CMC-C2C	2.76	1.56	1.50
10	A	302	HEM	CHD-C4C	-2.74	1.33	1.38
11	A	303	HEC	C1B-NB	-2.74	1.34	1.39
10	A	301	HEM	CAC-C3C	2.71	1.54	1.47
14	B	201	CLA	C1D-ND	-2.68	1.34	1.37
11	C	301	HEC	CMD-C2D	2.68	1.56	1.50
17	D	201	SQD	C34-C33	-2.68	1.38	1.51
13	A	1102	UMQ	C3'-C4'	2.67	1.59	1.52
11	A	303	HEC	C3B-C4B	-2.64	1.41	1.46
10	A	302	HEM	CHC-C4B	-2.63	1.33	1.39
10	A	302	HEM	CHA-C1A	-2.61	1.33	1.39
11	A	303	HEC	C2A-C3A	-2.61	1.31	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1002	OPC	PAJ-OAI	2.60	1.69	1.59
10	A	302	HEM	CAB-C3B	2.59	1.54	1.47
11	A	303	HEC	CAD-C3D	2.56	1.57	1.51
17	D	201	SQD	C35-C34	-2.54	1.39	1.51
18	G	101	BCR	C20-C19	2.53	1.41	1.34
11	C	301	HEC	C1A-C2A	-2.52	1.40	1.45
12	B	1001	OPC	CBP-CBQ	-2.51	1.41	1.52
17	D	201	SQD	C37-C36	-2.50	1.36	1.51
17	D	201	SQD	C32-C31	-2.47	1.39	1.51
17	D	201	SQD	C1-C2	2.47	1.59	1.52
14	B	201	CLA	MG-NA	-2.47	2.00	2.06
17	D	201	SQD	C33-C32	-2.46	1.39	1.51
18	G	101	BCR	C17-C18	2.45	1.41	1.35
18	G	101	BCR	C40-C30	2.43	1.58	1.53
15	B	1202	TDS	CAQ-CAP	-2.43	1.43	1.49
11	A	303	HEC	O1D-CGD	2.43	1.30	1.22
10	A	301	HEM	C1A-NA	-2.43	1.35	1.39
18	G	101	BCR	C11-C10	-2.40	1.35	1.43
14	B	201	CLA	C1C-C2C	2.40	1.49	1.44
12	B	1001	OPC	CBZ-CBY	2.40	1.63	1.51
14	B	201	CLA	CHD-C1D	2.40	1.43	1.38
11	C	301	HEC	CHD-C4C	-2.40	1.33	1.38
17	D	201	SQD	C38-C37	-2.39	1.33	1.50
11	C	301	HEC	CHB-C4A	-2.39	1.33	1.38
14	B	201	CLA	C4-C3	2.37	1.56	1.50
13	A	1101	UMQ	C4-C5	2.35	1.58	1.53
13	A	1102	UMQ	O2'-C2'	-2.33	1.37	1.43
18	G	101	BCR	C21-C22	2.32	1.41	1.35
12	B	1001	OPC	CBP-CBO	-2.32	1.40	1.51
14	B	201	CLA	CBD-CGD	-2.30	1.45	1.52
11	C	301	HEC	C1B-NB	-2.30	1.35	1.39
12	B	1001	OPC	CBX-CBW	2.30	1.63	1.51
11	C	301	HEC	C1D-C2D	2.29	1.48	1.43
13	A	1102	UMQ	O2-C2	2.29	1.48	1.43
10	A	301	HEM	FE-NA	-2.28	1.87	1.95
12	B	1001	OPC	CBG-NAF	-2.28	1.43	1.50
11	C	301	HEC	O1A-CGA	2.26	1.29	1.22
18	G	101	BCR	C16-C17	-2.21	1.36	1.43
13	A	1103	UMQ	O5-C1	2.19	1.47	1.41
15	B	1201	TDS	CAH-CAP	2.19	1.38	1.34
10	A	301	HEM	C4D-C3D	2.19	1.48	1.45
18	G	101	BCR	C29-C28	2.17	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1001	OPC	CBW-CBV	2.17	1.62	1.51
15	B	1201	TDS	CBC-CBB	-2.16	1.34	1.50
12	B	1001	OPC	CBY-CBX	2.14	1.62	1.51
12	B	1001	OPC	CBI-CAM	2.13	1.57	1.50
14	B	201	CLA	C2-C3	2.11	1.37	1.33
18	G	101	BCR	C2-C1	2.10	1.58	1.54
13	A	1102	UMQ	O1-C1	2.09	1.47	1.41
12	B	1001	OPC	CBM-CBL	2.06	1.59	1.52
13	A	1102	UMQ	C4'-C5'	2.06	1.58	1.52
12	B	1001	OPC	CCA-CBZ	2.05	1.64	1.51
14	B	201	CLA	C6-C5	2.04	1.59	1.52
10	A	302	HEM	CBA-CGA	2.04	1.55	1.50
17	D	201	SQD	C4-C5	-2.03	1.48	1.53
11	C	301	HEC	CHB-C1B	-2.02	1.34	1.39
11	C	301	HEC	CHD-C1D	-2.01	1.34	1.39
12	B	1001	OPC	OCC-CBK	2.01	1.28	1.22
12	B	1001	OPC	CBV-CBU	2.00	1.61	1.51

All (342) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	101	BCR	C24-C23-C22	28.08	167.78	126.23
18	G	101	BCR	C7-C8-C9	26.41	165.30	126.23
15	B	1202	TDS	CAE-CAD-CAL	19.11	155.92	118.98
18	G	101	BCR	C8-C7-C6	18.66	176.84	127.00
15	B	1201	TDS	CAE-CAD-CAL	17.87	153.53	118.98
17	D	201	SQD	O3-C3-C4	-16.36	71.81	110.38
18	G	101	BCR	C23-C24-C25	15.79	169.18	127.00
17	D	201	SQD	O4-C4-C3	15.48	146.87	110.38
15	B	1202	TDS	OAK-CAL-CAM	13.30	128.44	114.53
15	B	1201	TDS	CAD-CAL-CAM	-12.30	108.90	120.59
17	D	201	SQD	C17-C16-C15	11.93	174.66	114.37
17	D	201	SQD	C18-C17-C16	11.78	173.90	114.37
15	B	1201	TDS	OAK-CAL-CAM	11.74	126.82	114.53
17	D	201	SQD	C12-C11-C10	11.00	169.96	114.37
12	A	1002	OPC	CAA-NAF-CAE	-10.84	80.51	108.98
15	B	1201	TDS	CAD-CAE-CAF	-10.76	103.06	121.79
15	B	1202	TDS	CAD-CAE-CAF	-10.64	103.27	121.79
15	B	1202	TDS	CAD-CAL-CAM	-10.41	110.70	120.59
11	C	301	HEC	CBB-CAB-C3B	-10.36	106.72	127.43
13	A	1104	UMQ	O1'-C1'-C2'	10.19	123.75	108.27
18	G	101	BCR	C32-C1-C6	-9.77	94.91	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	201	SQD	C13-C12-C11	9.76	163.68	114.37
18	G	101	BCR	C33-C5-C6	-9.58	114.03	124.48
17	D	201	SQD	C22-C21-C20	9.42	177.00	113.36
10	A	301	HEM	C3B-C2B-C1B	-9.25	99.46	106.41
17	D	201	SQD	O6-C1-C2	8.91	121.80	108.27
11	A	303	HEC	CBC-CAC-C3C	-8.65	110.14	127.43
13	A	1103	UMQ	CA-O1'-C1'	8.62	128.41	113.68
12	B	1001	OPC	CAA-NAF-CBG	-8.34	87.07	108.98
17	D	201	SQD	O47-C7-C8	8.26	129.35	111.48
15	B	1202	TDS	OAB-CAE-CAF	8.14	127.37	115.84
10	A	301	HEM	CAD-C3D-C4D	8.00	138.64	124.70
15	B	1202	TDS	CAL-CAM-CAN	-7.83	107.79	118.91
10	A	301	HEM	CHC-C1C-NC	-7.74	116.02	124.45
13	A	1104	UMQ	CA-O1'-C1'	7.70	126.84	113.68
10	A	301	HEM	C3C-C2C-C1C	-7.70	99.76	107.05
13	A	1101	UMQ	O2'-C2'-C3'	7.65	128.42	110.38
10	A	301	HEM	C4B-C3B-C2B	7.54	114.21	107.28
13	A	1102	UMQ	CA-O1'-C1'	7.52	126.53	113.68
13	A	1103	UMQ	O1'-C1'-C2'	7.19	119.19	108.27
18	G	101	BCR	C8-C9-C10	7.09	130.17	119.01
18	G	101	BCR	C20-C21-C22	7.06	137.18	127.28
14	B	201	CLA	C4-C3-C5	7.06	127.48	115.23
10	A	301	HEM	CHC-C4B-NB	7.01	131.96	124.42
11	C	301	HEC	CHA-C1A-NA	6.97	132.04	124.45
15	B	1201	TDS	OAB-CAE-CAF	6.79	125.47	115.84
17	D	201	SQD	O5-C5-C4	6.79	121.94	109.70
13	A	1101	UMQ	O5'-C1'-O1'	6.75	125.99	110.04
14	B	201	CLA	C4A-NA-C1A	6.61	109.69	106.68
14	B	201	CLA	C1D-ND-C4D	-6.56	101.71	106.31
15	B	1202	TDS	OAO-CAP-CAQ	6.56	124.04	110.12
15	B	1201	TDS	CAA-OAB-CAE	6.56	127.13	117.51
13	A	1103	UMQ	O5'-C1'-O1'	6.39	125.14	110.04
12	A	1002	OPC	CAA-NAF-CBG	-6.25	92.56	108.98
10	A	301	HEM	C4D-C3D-C2D	-6.21	97.85	106.89
12	B	1001	OPC	CBU-CBT-CBS	6.16	147.12	112.60
15	B	1201	TDS	CAL-CAM-CAN	-6.13	110.20	118.91
14	B	201	CLA	CMD-C2D-C1D	6.08	135.44	124.73
17	D	201	SQD	C15-C14-C13	5.99	144.65	114.37
12	A	1002	OPC	CAA-NAF-CAG	-5.95	86.24	109.91
12	B	1001	OPC	CAM-OAN-CAO	-5.93	103.60	117.80
13	A	1102	UMQ	C1'-O5'-C5'	5.89	125.23	113.72
14	B	201	CLA	C3C-C4C-NC	5.86	117.94	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	201	CLA	O2D-CGD-CBD	5.86	121.47	111.23
13	A	1104	UMQ	O5-C5-C4	5.82	120.19	109.70
12	A	1002	OPC	OAN-CAO-CAP	5.76	123.93	111.48
15	B	1202	TDS	CAJ-OAK-CAL	-5.70	109.14	117.51
13	A	1101	UMQ	O1-C4'-C5'	5.67	124.35	109.48
12	A	1002	OPC	CAH-CAG-NAF	5.62	133.85	115.82
13	A	1102	UMQ	O5-C5-C4	5.61	119.81	109.70
13	A	1103	UMQ	O2'-C2'-C3'	5.59	123.55	110.38
10	A	301	HEM	C3D-C4D-ND	5.58	116.29	110.17
13	A	1102	UMQ	O5'-C1'-O1'	5.55	123.15	110.04
14	B	201	CLA	C2D-C1D-ND	5.52	115.59	110.13
13	A	1102	UMQ	O1'-C1'-C2'	5.47	116.58	108.27
12	B	1001	OPC	CBG-NAF-CAG	5.44	131.52	109.91
14	B	201	CLA	CMB-C2B-C1B	5.42	133.67	125.42
11	C	301	HEC	CHD-C4C-NC	5.38	130.31	124.45
10	A	302	HEM	CMB-C2B-C1B	5.35	133.40	125.03
13	A	1104	UMQ	O5'-C1'-C2'	5.34	121.34	110.37
14	B	201	CLA	C2C-C1C-NC	5.32	115.57	109.98
11	A	303	HEC	CAD-C3D-C4D	5.32	135.33	124.94
10	A	302	HEM	C3B-C4B-NB	5.31	113.28	109.47
13	A	1101	UMQ	CA-O1'-C1'	5.29	122.72	113.68
12	A	1002	OPC	CBI-CAM-CAL	-5.16	99.75	111.78
14	B	201	CLA	CHD-C4C-C3C	-5.16	117.25	124.77
10	A	302	HEM	CAD-CBD-CGD	-5.14	100.02	113.67
18	G	101	BCR	C36-C18-C17	5.14	131.14	122.82
17	D	201	SQD	C14-C13-C12	5.13	140.32	114.37
12	B	1001	OPC	CAR-CAQ-CAP	5.12	131.93	113.13
13	A	1102	UMQ	O2'-C2'-C3'	5.10	122.39	110.38
14	B	201	CLA	C4C-C3C-C2C	-5.08	99.50	106.89
14	B	201	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
10	A	301	HEM	CBB-CAB-C3B	-5.03	102.37	127.53
13	A	1102	UMQ	C3-C4-C5	5.01	119.31	110.23
13	A	1104	UMQ	O2'-C2'-C1'	5.00	122.00	110.08
13	A	1102	UMQ	O1-C1-C2	5.00	120.38	108.09
12	A	1002	OPC	OAI-CAH-CAG	4.98	133.63	109.65
14	B	201	CLA	C5-C3-C2	-4.96	110.04	121.17
13	A	1101	UMQ	O2'-C2'-C1'	4.95	121.87	110.08
14	B	201	CLA	C2B-C1B-NB	4.94	115.45	110.33
10	A	301	HEM	CMB-C2B-C1B	4.93	132.73	125.03
18	G	101	BCR	C34-C9-C8	-4.90	110.60	118.09
13	A	1101	UMQ	O5-C5-C4	4.88	118.50	109.70
14	B	201	CLA	C6-C5-C3	-4.88	101.58	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	301	HEM	C4C-C3C-C2C	4.86	111.02	106.81
13	A	1102	UMQ	O5'-C1'-C2'	4.82	120.28	110.37
15	B	1202	TDS	OBD-CAM-CAL	-4.81	108.87	119.21
14	B	201	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
13	A	1102	UMQ	O2-C2-C1	4.71	121.31	110.08
11	A	303	HEC	CBB-CAB-C3B	-4.63	118.17	127.43
18	G	101	BCR	C2-C1-C6	4.63	117.16	110.44
13	A	1102	UMQ	C1'-C2'-C3'	4.63	119.74	110.01
13	A	1104	UMQ	C1'-C2'-C3'	4.62	119.74	110.01
13	A	1101	UMQ	O1-C1-C2	4.54	119.27	108.09
11	A	303	HEC	CMB-C2B-C1B	4.54	132.33	125.42
17	D	201	SQD	C16-C15-C14	4.52	137.22	114.37
15	B	1201	TDS	OAO-CAP-CAQ	4.50	119.66	110.12
13	A	1101	UMQ	O5'-C1'-C2'	4.49	119.58	110.37
14	B	201	CLA	CHD-C1D-ND	-4.47	118.50	124.80
11	A	303	HEC	CBA-CAA-C2A	-4.46	100.21	112.53
14	B	201	CLA	CED-O2D-CGD	-4.45	105.83	115.92
12	B	1001	OPC	OAN-CAO-OAD	-4.43	113.34	123.70
14	B	201	CLA	C3B-C4B-NB	4.43	114.48	110.53
10	A	301	HEM	C2B-C1B-NB	4.39	114.89	109.84
13	A	1101	UMQ	C2'-C3'-C4'	-4.38	99.73	109.68
12	A	1002	OPC	CAR-CAS-CAT	4.37	136.45	114.37
10	A	301	HEM	CHD-C1D-ND	4.33	129.08	124.42
13	A	1103	UMQ	O2'-C2'-C1'	4.32	120.37	110.08
13	A	1101	UMQ	O5-C1-C2	-4.32	101.50	110.37
11	C	301	HEC	CBD-CAD-C3D	-4.31	100.60	112.53
15	B	1201	TDS	OAO-CAP-CAH	4.29	125.59	121.81
12	B	1001	OPC	CBP-CBO-CBN	4.24	135.80	114.37
14	B	201	CLA	O2A-CGA-CBA	4.21	124.67	111.83
10	A	301	HEM	O2D-CGD-O1D	-4.15	112.67	123.33
18	G	101	BCR	C36-C18-C19	-4.12	111.79	118.09
17	D	201	SQD	C35-C34-C33	4.12	135.19	114.37
14	B	201	CLA	C3D-C4D-ND	4.10	116.66	109.99
15	B	1202	TDS	OAO-CAN-CAF	-3.99	115.16	121.19
13	A	1101	UMQ	O1'-C1'-C2'	3.99	114.33	108.27
13	A	1104	UMQ	C3'-C4'-C5'	-3.96	102.15	110.93
10	A	302	HEM	CMC-C2C-C1C	3.96	131.70	124.73
13	A	1102	UMQ	C3'-C4'-C5'	3.95	119.69	110.93
11	C	301	HEC	CBC-CAC-C3C	-3.95	119.54	127.43
13	A	1101	UMQ	C1-O1-C4'	-3.94	108.65	117.98
12	B	1001	OPC	OAN-CAO-CAP	3.91	119.94	111.48
12	A	1002	OPC	CAQ-CAR-CAS	3.88	134.00	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	201	SQD	O4-C4-C5	-3.88	99.77	109.32
15	B	1202	TDS	OAC-CAG-CAH	-3.87	115.36	120.45
12	B	1001	OPC	CBI-OBJ-CBK	3.86	131.21	117.12
17	D	201	SQD	O6-C44-C45	3.83	120.14	110.82
14	B	201	CLA	CAA-CBA-CGA	-3.81	102.39	113.21
12	B	1001	OPC	CAA-NAF-CAG	-3.79	94.86	109.91
14	B	201	CLA	CHB-C4A-NA	3.74	129.80	124.40
11	C	301	HEC	CAD-CBD-CGD	3.73	123.57	113.67
12	B	1001	OPC	CAR-CAS-CAT	3.72	133.19	114.37
18	G	101	BCR	C32-C1-C2	3.72	123.24	108.95
10	A	301	HEM	C1D-C2D-C3D	3.68	110.85	106.98
13	A	1102	UMQ	C1-O5-C5	3.68	120.90	113.72
10	A	301	HEM	O1A-CGA-CBA	-3.61	111.63	123.09
13	A	1104	UMQ	O3'-C3'-C2'	3.61	118.88	110.38
18	G	101	BCR	C33-C5-C4	3.60	121.28	113.60
10	A	302	HEM	CMB-C2B-C3B	-3.60	119.72	128.43
10	A	302	HEM	C2D-C1D-ND	3.60	114.06	109.90
18	G	101	BCR	C29-C28-C27	3.60	119.19	111.28
13	A	1104	UMQ	O1-C4'-C5'	3.59	118.90	109.48
15	B	1201	TDS	CAU-CAV-CAW	-3.59	96.24	114.37
15	B	1201	TDS	CAS-CAT-CAU	-3.57	96.32	114.37
15	B	1201	TDS	CAE-CAF-CAG	-3.54	117.82	123.49
13	A	1104	UMQ	C3-C4-C5	3.53	116.64	110.23
10	A	302	HEM	CAA-CBA-CGA	3.52	123.00	113.67
14	B	201	CLA	O1D-CGD-CBD	-3.48	117.66	124.52
15	B	1201	TDS	OAB-CAE-CAD	3.48	130.06	124.08
17	D	201	SQD	C32-C31-C30	3.47	131.92	114.37
10	A	302	HEM	CHB-C1B-NB	-3.46	120.08	124.37
18	G	101	BCR	C3-C4-C5	-3.46	107.88	114.06
17	D	201	SQD	O47-C45-C44	3.46	120.76	108.34
11	A	303	HEC	CMC-C2C-C1C	3.44	130.65	125.42
13	A	1104	UMQ	O1-C1-C2	3.42	116.51	108.09
11	C	301	HEC	CHC-C4B-NB	3.40	128.16	124.45
12	A	1002	OPC	CBP-CBQ-CBR	3.38	131.51	112.60
11	C	301	HEC	CHA-C1A-C2A	-3.37	119.55	124.86
12	A	1002	OPC	CAS-CAT-CAU	-3.35	97.74	113.86
15	B	1202	TDS	CAE-CAF-CAG	-3.35	118.13	123.49
13	A	1104	UMQ	O2'-C2'-C3'	3.35	118.26	110.38
10	A	301	HEM	O2A-CGA-CBA	3.33	124.51	114.00
13	A	1101	UMQ	O2-C2-C3	3.29	118.12	110.38
15	B	1201	TDS	CAT-CAU-CAV	3.27	130.88	114.37
13	A	1102	UMQ	O2'-C2'-C1'	3.26	117.85	110.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	302	HEM	CBA-CAA-C2A	-3.26	103.52	112.53
10	A	301	HEM	CMC-C2C-C1C	3.25	130.45	124.73
15	B	1201	TDS	CAV-CAW-CAX	3.24	130.72	114.37
12	B	1001	OPC	CBO-CBP-CBQ	3.23	129.39	113.86
18	G	101	BCR	C23-C22-C21	-3.21	113.96	119.01
10	A	301	HEM	C4A-NA-C1A	-3.21	100.59	105.82
17	D	201	SQD	O9-S-C6	3.19	111.52	106.76
11	C	301	HEC	CMD-C2D-C1D	3.19	130.27	125.42
13	A	1104	UMQ	C2'-C3'-C4'	-3.17	102.49	109.68
13	A	1102	UMQ	O5-C1-C2	3.16	116.86	110.37
12	A	1002	OPC	PAJ-OAI-CAH	3.16	136.28	121.26
17	D	201	SQD	C36-C35-C34	3.14	130.23	114.37
12	A	1002	OPC	OBJ-CBK-OCC	-3.13	115.81	123.63
14	B	201	CLA	CAC-C3C-C4C	3.12	128.85	124.79
10	A	301	HEM	CHA-C4D-ND	-3.12	120.50	124.37
10	A	301	HEM	C2C-C1C-NC	3.12	115.41	109.64
10	A	301	HEM	CMD-C2D-C1D	3.12	129.90	125.03
17	D	201	SQD	O2-C2-C1	3.11	117.50	110.08
18	G	101	BCR	C39-C30-C25	3.11	115.11	110.24
13	A	1104	UMQ	O2-C2-C3	3.10	117.69	110.38
17	D	201	SQD	C1-C2-C3	3.10	116.53	110.01
10	A	301	HEM	C4A-CHB-C1B	-3.09	118.99	126.25
13	A	1101	UMQ	C1-O5-C5	3.06	119.69	113.72
12	B	1001	OPC	CCB-CCA-CBZ	3.05	133.99	113.36
10	A	302	HEM	C3C-C2C-C1C	-3.05	104.16	107.05
18	G	101	BCR	C20-C19-C18	-3.03	118.07	126.36
12	A	1002	OPC	CAE-NAF-CAG	3.02	121.93	109.91
17	D	201	SQD	O5-C1-O6	3.02	117.19	110.04
15	B	1202	TDS	OAB-CAE-CAD	3.01	129.26	124.08
13	A	1102	UMQ	C2'-C3'-C4'	3.00	116.48	109.68
13	A	1101	UMQ	O2-C2-C1	2.95	117.09	110.08
12	A	1002	OPC	CBA-CBB-CBC	2.94	129.25	114.37
12	B	1001	OPC	OBJ-CBI-CAM	2.93	116.83	108.40
11	A	303	HEC	CAA-CBA-CGA	2.93	121.42	113.67
10	A	302	HEM	C1D-C2D-C3D	-2.92	103.91	106.98
14	B	201	CLA	C6-C7-C8	2.92	125.66	115.97
17	D	201	SQD	C33-C32-C31	2.92	129.11	114.37
12	B	1001	OPC	CBP-CBQ-CBR	2.89	128.81	112.60
13	A	1103	UMQ	O1-C1-C2	2.88	115.18	108.09
13	A	1103	UMQ	C1'-C2'-C3'	2.88	116.07	110.01
15	B	1202	TDS	CAT-CAU-CAV	2.84	128.71	114.37
10	A	301	HEM	C2A-C1A-NA	2.84	113.30	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	303	HEC	CMB-C2B-C3B	-2.83	119.91	126.55
10	A	301	HEM	CHC-C4B-C3B	-2.82	119.44	125.07
11	A	303	HEC	C4D-C3D-C2D	-2.82	102.50	106.87
13	A	1103	UMQ	C1-O5-C5	2.81	119.20	113.72
14	B	201	CLA	O2A-C1-C2	2.81	118.91	108.11
12	A	1002	OPC	CBG-NAF-CAE	2.79	116.31	108.98
13	A	1103	UMQ	O3'-C3'-C4'	2.78	117.07	109.94
10	A	302	HEM	CHC-C4B-C3B	-2.78	119.53	125.07
17	D	201	SQD	O49-C7-C8	-2.78	112.92	123.78
11	C	301	HEC	CMA-C3A-C4A	2.77	129.61	124.73
10	A	302	HEM	C4C-NC-C1C	-2.77	101.31	105.82
13	A	1101	UMQ	C1'-O5'-C5'	2.75	119.10	113.72
15	B	1202	TDS	CAR-CAQ-CAP	2.74	118.79	113.08
12	B	1001	OPC	CBW-CBV-CBU	2.74	128.22	114.37
10	A	302	HEM	C2C-C1C-NC	2.74	114.70	109.64
10	A	302	HEM	C4C-CHD-C1D	-2.73	120.21	126.02
15	B	1202	TDS	OAO-CAP-CAH	2.71	124.20	121.81
10	A	301	HEM	CHB-C4A-C3A	-2.70	119.60	127.43
12	A	1002	OPC	CBG-NAF-CAG	2.68	120.58	109.91
15	B	1202	TDS	OAC-CAG-CAF	2.67	126.89	122.06
10	A	302	HEM	CBD-CAD-C3D	2.66	119.89	112.53
11	A	303	HEC	CAA-C2A-C3A	-2.62	122.96	127.87
17	D	201	SQD	O47-C7-O49	-2.58	117.67	123.70
13	A	1103	UMQ	O5'-C1'-C2'	2.58	115.67	110.37
12	B	1001	OPC	CBY-CBX-CBW	2.57	127.36	114.37
13	A	1101	UMQ	O3'-C3'-C2'	2.56	116.40	110.38
10	A	301	HEM	CMD-C2D-C3D	-2.55	119.25	126.15
10	A	302	HEM	CHC-C4B-NB	2.55	127.17	124.42
13	A	1101	UMQ	C3'-C4'-C5'	-2.53	105.32	110.93
15	B	1201	TDS	CAS-CAR-CAQ	-2.52	103.85	113.13
11	A	303	HEC	CMA-C3A-C4A	2.52	129.17	124.73
15	B	1202	TDS	OAO-CAN-CAM	2.52	121.27	116.28
10	A	302	HEM	CHC-C1C-C2C	-2.51	120.26	125.49
17	D	201	SQD	C19-C18-C17	2.50	127.02	114.37
10	A	301	HEM	O2D-CGD-CBD	2.50	121.89	114.00
15	B	1202	TDS	CBC-CBB-CBA	2.50	130.21	113.36
17	D	201	SQD	C46-O48-C23	2.49	126.22	117.12
12	A	1002	OPC	CBY-CBX-CBW	-2.49	101.80	114.37
10	A	301	HEM	CAA-C2A-C1A	2.48	129.78	124.94
13	A	1101	UMQ	O4-C4-C3	-2.47	104.56	110.38
13	A	1102	UMQ	O6'-C6'-C5'	2.46	119.71	111.33
17	D	201	SQD	C34-C33-C32	2.46	126.79	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	301	HEC	CMC-C2C-C1C	2.46	129.16	125.42
10	A	301	HEM	CAB-C3B-C2B	-2.46	120.44	128.43
12	B	1001	OPC	CBZ-CBY-CBX	2.45	126.78	114.37
12	B	1001	OPC	OAI-CAH-CAG	2.42	121.28	109.65
18	G	101	BCR	C15-C16-C17	2.40	128.44	123.52
14	B	201	CLA	CHB-C1B-NB	-2.40	120.44	124.05
15	B	1201	TDS	CAR-CAS-CAT	2.40	126.49	114.37
18	G	101	BCR	C34-C9-C10	-2.40	118.93	122.82
13	A	1103	UMQ	O2-C2-C1	2.38	115.74	110.08
13	A	1104	UMQ	O3-C3-C2	2.37	115.95	110.38
11	A	303	HEC	O2A-CGA-O1A	2.37	129.41	123.33
10	A	301	HEM	C3A-C4A-NA	2.36	113.93	110.14
17	D	201	SQD	O8-S-C6	2.36	110.52	105.97
13	A	1104	UMQ	C6'-C5'-C4'	2.35	120.00	113.38
12	A	1002	OPC	CBU-CBT-CBS	2.35	125.74	112.60
15	B	1202	TDS	CAV-CAW-CAX	2.33	126.16	114.37
10	A	301	HEM	CAD-C3D-C2D	-2.33	123.51	127.87
15	B	1202	TDS	CAN-CAF-CAG	2.32	123.96	119.99
11	A	303	HEC	O1A-CGA-CBA	-2.31	115.75	123.09
13	A	1101	UMQ	C4-C3-C2	-2.31	106.78	110.83
11	C	301	HEC	CAA-C2A-C1A	-2.31	120.17	124.85
13	A	1102	UMQ	C4-C3-C2	2.29	114.85	110.83
14	B	201	CLA	C7-C6-C5	-2.28	107.18	113.26
12	B	1001	OPC	CBA-CBB-CBC	2.28	125.89	114.37
11	A	303	HEC	CHD-C4C-NC	-2.27	121.98	124.45
17	D	201	SQD	C45-O47-C7	-2.27	112.36	117.80
10	A	301	HEM	CAC-C3C-C4C	-2.27	119.41	124.82
11	A	303	HEC	C1D-CHD-C4C	2.26	131.63	124.66
12	B	1001	OPC	CBM-CBL-CBK	2.25	121.95	113.69
12	A	1002	OPC	CAQ-CAP-CAO	2.25	121.93	113.69
18	G	101	BCR	C37-C22-C23	2.25	121.52	118.09
13	A	1104	UMQ	O1-C4'-C3'	2.24	112.92	107.23
15	B	1202	TDS	CAY-CAZ-CBA	2.24	125.69	114.37
12	B	1001	OPC	CBT-CBS-CBR	2.24	141.61	124.83
13	A	1101	UMQ	C1-C2-C3	-2.22	105.33	110.01
14	B	201	CLA	CAC-C3C-C2C	2.22	131.64	127.56
14	B	201	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
14	B	201	CLA	C3A-C2A-C1A	2.21	104.64	101.34
11	A	303	HEC	CAD-C3D-C2D	-2.20	122.14	127.07
11	C	301	HEC	CHD-C4C-C3C	-2.19	121.51	125.21
10	A	302	HEM	C4A-CHB-C1B	-2.19	121.09	126.25
15	B	1202	TDS	CAS-CAR-CAQ	2.19	121.17	113.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	301	HEM	CHB-C1B-C2B	-2.19	120.74	126.95
14	B	201	CLA	CBA-CAA-C2A	-2.18	107.29	113.79
11	A	303	HEC	CHD-C1D-C2D	-2.18	121.10	127.43
13	A	1103	UMQ	O5-C5-C6	2.17	111.81	106.44
13	A	1104	UMQ	C1-O5-C5	2.16	117.94	113.72
13	A	1103	UMQ	C3-C4-C5	2.16	114.15	110.23
11	A	303	HEC	CHD-C1D-ND	2.15	127.76	123.86
13	A	1101	UMQ	C3-C4-C5	2.14	114.12	110.23
12	B	1001	OPC	CBO-CBN-CBM	2.14	125.17	114.37
18	G	101	BCR	C31-C1-C6	-2.14	106.89	110.24
13	A	1101	UMQ	O6-C6-C5	2.13	118.58	111.33
18	G	101	BCR	C30-C25-C26	2.12	125.53	122.64
11	A	303	HEC	CHA-C4D-ND	-2.12	120.02	123.86
14	B	201	CLA	CAA-C2A-C3A	-2.11	107.29	113.00
18	G	101	BCR	C32-C1-C31	-2.10	102.61	108.63
11	C	301	HEC	C4D-ND-C1D	2.10	109.25	105.82
14	B	201	CLA	C1C-C2C-C3C	-2.10	104.77	106.98
18	G	101	BCR	C7-C6-C5	2.09	126.37	121.56
13	A	1101	UMQ	CI-CH-CG	-2.09	103.81	114.37
14	B	201	CLA	C2A-C1A-CHA	-2.07	120.28	123.87
12	B	1001	OPC	CAY-CAZ-CBA	2.07	124.82	114.37
10	A	302	HEM	CAC-C3C-C4C	2.07	129.75	124.82
18	G	101	BCR	C27-C26-C25	-2.06	119.92	122.70
13	A	1104	UMQ	O5'-C1'-O1'	2.06	114.91	110.04
12	B	1001	OPC	CBX-CBW-CBV	2.03	124.62	114.37
11	A	303	HEC	CAA-C2A-C1A	2.02	128.96	124.85
10	A	301	HEM	C1B-NB-C4B	-2.01	102.83	105.21

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	1101	UMQ	C1'
13	A	1101	UMQ	C2'
13	A	1102	UMQ	C1'
13	A	1102	UMQ	C2'
13	A	1103	UMQ	C1'
13	A	1103	UMQ	C2'
13	A	1104	UMQ	C1'
13	A	1104	UMQ	C2'
14	B	201	CLA	ND
14	B	201	CLA	C8
17	D	201	SQD	C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	D	201	SQD	C3
17	D	201	SQD	C4

All (201) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	301	HEM	C1A-C2A-CAA-CBA
10	A	302	HEM	C1A-C2A-CAA-CBA
10	A	302	HEM	C2D-C3D-CAD-CBD
10	A	302	HEM	C4D-C3D-CAD-CBD
11	A	303	HEC	C2B-C3B-CAB-CBB
11	A	303	HEC	C4B-C3B-CAB-CBB
11	A	303	HEC	C2C-C3C-CAC-CBC
11	A	303	HEC	C4C-C3C-CAC-CBC
11	C	301	HEC	C2B-C3B-CAB-CBB
11	C	301	HEC	C4B-C3B-CAB-CBB
12	A	1002	OPC	OAN-CAM-CBI-OBJ
12	A	1002	OPC	CAM-CAL-OAK-PAJ
12	A	1002	OPC	CAL-OAK-PAJ-OBH
12	A	1002	OPC	CAL-OAK-PAJ-OAB
12	A	1002	OPC	CAL-OAK-PAJ-OAI
12	A	1002	OPC	CAH-OAI-PAJ-OBH
12	A	1002	OPC	CAH-OAI-PAJ-OAB
12	A	1002	OPC	NAF-CAG-CAH-OAI
12	A	1002	OPC	CBO-CBP-CBQ-CBR
12	B	1001	OPC	CAH-OAI-PAJ-OAK
12	B	1001	OPC	CAH-OAI-PAJ-OBH
12	B	1001	OPC	NAF-CAG-CAH-OAI
12	B	1001	OPC	CBO-CBP-CBQ-CBR
13	A	1101	UMQ	O5'-C1'-O1'-CA
13	A	1102	UMQ	C2'-C1'-O1'-CA
13	A	1103	UMQ	O5'-C1'-O1'-CA
13	A	1104	UMQ	C3'-C4'-O1'-C1
13	A	1104	UMQ	O5'-C1'-O1'-CA
14	B	201	CLA	O2A-C1-C2-C3
15	B	1202	TDS	CAP-CAQ-CAR-CAS
17	D	201	SQD	O5-C1-O6-C44
17	D	201	SQD	O5-C5-C6-S
17	D	201	SQD	C5-C6-S-O7
17	D	201	SQD	C5-C6-S-O8
17	D	201	SQD	C5-C6-S-O9
18	G	101	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	G	101	BCR	C5-C6-C7-C8
18	G	101	BCR	C6-C7-C8-C9
18	G	101	BCR	C7-C8-C9-C34
18	G	101	BCR	C23-C24-C25-C26
15	B	1202	TDS	CAF-CAE-OAB-CAA
13	A	1104	UMQ	O5-C1-O1-C4'
13	A	1104	UMQ	C2-C1-O1-C4'
15	B	1201	TDS	CAD-CAL-OAK-CAJ
13	A	1102	UMQ	C3'-C4'-O1-C1
15	B	1201	TDS	CAM-CAL-OAK-CAJ
17	D	201	SQD	C24-C23-O48-C46
14	B	201	CLA	CBD-CGD-O2D-CED
17	D	201	SQD	C8-C7-O47-C45
17	D	201	SQD	O10-C23-O48-C46
12	A	1002	OPC	CAQ-CAR-CAS-CAT
17	D	201	SQD	C33-C34-C35-C36
17	D	201	SQD	C31-C32-C33-C34
17	D	201	SQD	C12-C13-C14-C15
11	A	303	HEC	C4D-C3D-CAD-CBD
13	A	1102	UMQ	O5'-C5'-C6'-O6'
17	D	201	SQD	C13-C14-C15-C16
13	A	1103	UMQ	O5'-C5'-C6'-O6'
13	A	1104	UMQ	O5-C5-C6-O6
17	D	201	SQD	O49-C7-O47-C45
15	B	1202	TDS	CAS-CAT-CAU-CAV
13	A	1103	UMQ	C4'-C5'-C6'-O6'
15	B	1201	TDS	CAD-CAE-OAB-CAA
15	B	1202	TDS	CAD-CAE-OAB-CAA
18	G	101	BCR	C37-C22-C23-C24
18	G	101	BCR	C7-C8-C9-C10
18	G	101	BCR	C21-C22-C23-C24
12	A	1002	OPC	CBM-CBN-CBO-CBP
11	A	303	HEC	C2D-C3D-CAD-CBD
12	B	1001	OPC	CAZ-CBA-CBB-CBC
14	B	201	CLA	C8-C10-C11-C12
13	A	1101	UMQ	O5'-C5'-C6'-O6'
13	A	1104	UMQ	C4-C5-C6-O6
13	A	1101	UMQ	O1'-CA-CB-CC
15	B	1201	TDS	CAF-CAE-OAB-CAA
13	A	1104	UMQ	O1'-CA-CB-CC
14	B	201	CLA	C10-C11-C12-C13
18	G	101	BCR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	A	1002	OPC	CBU-CBV-CBW-CBX
13	A	1101	UMQ	C4'-C5'-C6'-O6'
13	A	1102	UMQ	C4'-C5'-C6'-O6'
12	B	1001	OPC	CAP-CAO-OAN-CAM
17	D	201	SQD	C10-C11-C12-C13
12	A	1002	OPC	CAH-CAG-NAF-CAA
14	B	201	CLA	O1D-CGD-O2D-CED
14	B	201	CLA	C15-C16-C17-C18
13	A	1102	UMQ	C4-C5-C6-O6
13	A	1102	UMQ	O5-C5-C6-O6
13	A	1104	UMQ	CB-CC-CD-CF
12	B	1001	OPC	CAY-CAZ-CBA-CBB
13	A	1102	UMQ	C5'-C4'-O1-C1
12	A	1002	OPC	CBL-CBM-CBN-CBO
12	A	1002	OPC	CBV-CBW-CBX-CBY
14	B	201	CLA	C3A-C2A-CAA-CBA
12	B	1001	OPC	CBT-CBU-CBV-CBW
12	A	1002	OPC	CBY-CBZ-CCA-CCB
13	A	1103	UMQ	CG-CH-CI-CJ
17	D	201	SQD	C29-C30-C31-C32
12	A	1002	OPC	CBT-CBU-CBV-CBW
15	B	1202	TDS	CAY-CAZ-CBA-CBB
17	D	201	SQD	C15-C16-C17-C18
12	B	1001	OPC	CAH-CAG-NAF-CAE
12	A	1002	OPC	CBW-CBX-CBY-CBZ
18	G	101	BCR	C23-C24-C25-C30
13	A	1102	UMQ	CI-CJ-CK-CL
12	B	1001	OPC	OAD-CAO-OAN-CAM
10	A	301	HEM	C3A-C2A-CAA-CBA
17	D	201	SQD	C11-C12-C13-C14
12	A	1002	OPC	CAZ-CBA-CBB-CBC
12	B	1001	OPC	CBC-CBD-CBE-CBF
13	A	1101	UMQ	CF-CG-CH-CI
17	D	201	SQD	C28-C29-C30-C31
13	A	1103	UMQ	CF-CG-CH-CI
15	B	1201	TDS	CAT-CAU-CAV-CAW
12	B	1001	OPC	CBU-CBV-CBW-CBX
15	B	1201	TDS	CAR-CAS-CAT-CAU
13	A	1103	UMQ	C4-C5-C6-O6
13	A	1101	UMQ	CA-CB-CC-CD
15	B	1201	TDS	CAW-CAX-CAY-CAZ
14	B	201	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	B	1001	OPC	CBK-CBL-CBM-CBN
15	B	1202	TDS	CAU-CAV-CAW-CAX
13	A	1102	UMQ	CC-CD-CF-CG
12	A	1002	OPC	CAW-CAX-CAY-CAZ
14	B	201	CLA	C4-C3-C5-C6
13	A	1104	UMQ	CH-CI-CJ-CK
13	A	1104	UMQ	CI-CJ-CK-CL
12	A	1002	OPC	CBC-CBD-CBE-CBF
13	A	1104	UMQ	CG-CH-CI-CJ
15	B	1202	TDS	CAR-CAS-CAT-CAU
15	B	1202	TDS	CAM-CAL-OAK-CAJ
17	D	201	SQD	C27-C28-C29-C30
17	D	201	SQD	C2-C1-O6-C44
14	B	201	CLA	C2-C3-C5-C6
17	D	201	SQD	C25-C26-C27-C28
13	A	1101	UMQ	CC-CD-CF-CG
17	D	201	SQD	C16-C17-C18-C19
15	B	1201	TDS	CAV-CAW-CAX-CAY
12	B	1001	OPC	CAS-CAT-CAU-CAV
12	B	1001	OPC	CAR-CAS-CAT-CAU
12	B	1001	OPC	CBL-CBM-CBN-CBO
12	A	1002	OPC	CAS-CAT-CAU-CAV
12	A	1002	OPC	CBX-CBY-CBZ-CCA
14	B	201	CLA	C11-C10-C8-C9
12	B	1001	OPC	CAH-CAG-NAF-CAA
13	A	1103	UMQ	CA-CB-CC-CD
13	A	1101	UMQ	O5-C1-O1-C4'
13	A	1101	UMQ	CB-CC-CD-CF
13	A	1102	UMQ	O1'-CA-CB-CC
13	A	1103	UMQ	CD-CF-CG-CH
15	B	1202	TDS	CAX-CAY-CAZ-CBA
12	A	1002	OPC	CBP-CBQ-CBR-CBS
12	A	1002	OPC	CBK-CBL-CBM-CBN
12	A	1002	OPC	CAL-CAM-CBI-OBJ
17	D	201	SQD	O6-C44-C45-C46
12	A	1002	OPC	CAH-OAI-PAJ-OAK
12	B	1001	OPC	CAH-OAI-PAJ-OAB
12	B	1001	OPC	CBP-CBQ-CBR-CBS
17	D	201	SQD	O6-C44-C45-O47
17	D	201	SQD	C14-C15-C16-C17
13	A	1102	UMQ	CB-CA-O1'-C1'
11	C	301	HEC	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

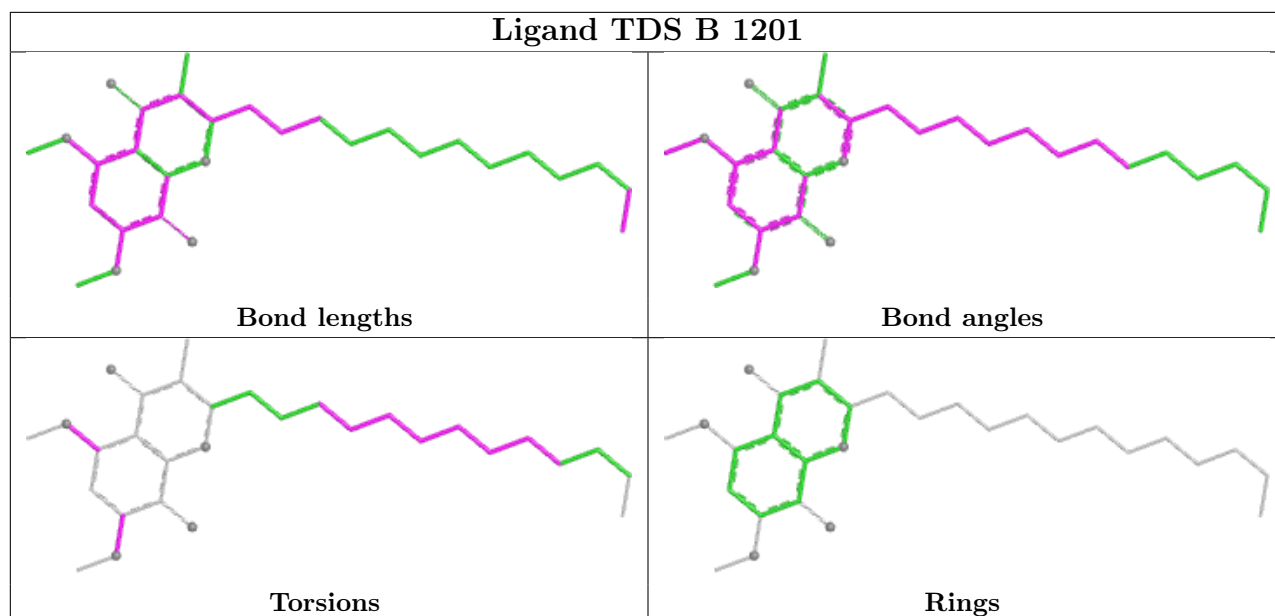
Mol	Chain	Res	Type	Atoms
10	A	301	HEM	C2A-CAA-CBA-CGA
15	B	1201	TDS	CAX-CAY-CAZ-CBA
11	C	301	HEC	C1A-C2A-CAA-CBA
12	A	1002	OPC	CAT-CAU-CAV-CAW
10	A	301	HEM	CAA-CBA-CGA-O2A
13	A	1104	UMQ	CC-CD-CF-CG
18	G	101	BCR	C11-C10-C9-C34
11	C	301	HEC	C3D-CAD-CBD-CGD
13	A	1102	UMQ	CF-CG-CH-CI
12	B	1001	OPC	CAL-CAM-CBI-OBJ
12	B	1001	OPC	CBS-CBT-CBU-CBV
12	B	1001	OPC	CBM-CBN-CBO-CBP
10	A	301	HEM	CAA-CBA-CGA-O1A
18	G	101	BCR	C11-C10-C9-C8
15	B	1201	TDS	CAU-CAV-CAW-CAX
14	B	201	CLA	C12-C13-C15-C16
10	A	302	HEM	C3A-C2A-CAA-CBA
13	A	1103	UMQ	CH-CI-CJ-CK
10	A	302	HEM	CAD-CBD-CGD-O2D
13	A	1101	UMQ	CG-CH-CI-CJ
12	A	1002	OPC	CAY-CAZ-CBA-CBB
11	C	301	HEC	CAD-CBD-CGD-O2D
13	A	1104	UMQ	CD-CF-CG-CH
11	C	301	HEC	CAD-CBD-CGD-O1D
10	A	302	HEM	CAD-CBD-CGD-O1D
12	A	1002	OPC	OAK-CAL-CAM-OAN
12	A	1002	OPC	CAH-CAG-NAF-CBG
17	D	201	SQD	C44-C45-C46-O48
13	A	1103	UMQ	O5-C5-C6-O6
15	B	1202	TDS	CAT-CAU-CAV-CAW
15	B	1201	TDS	CAS-CAT-CAU-CAV
13	A	1103	UMQ	CB-CA-O1'-C1'
17	D	201	SQD	O47-C7-C8-C9
12	A	1002	OPC	OAK-CAL-CAM-CBI
15	B	1202	TDS	CAD-CAL-OAK-CAJ
13	A	1101	UMQ	C2-C1-O1-C4'
11	C	301	HEC	CAA-CBA-CGA-O2A
14	B	201	CLA	C2-C1-O2A-CGA
12	B	1001	OPC	OAD-CAO-CAP-CAQ

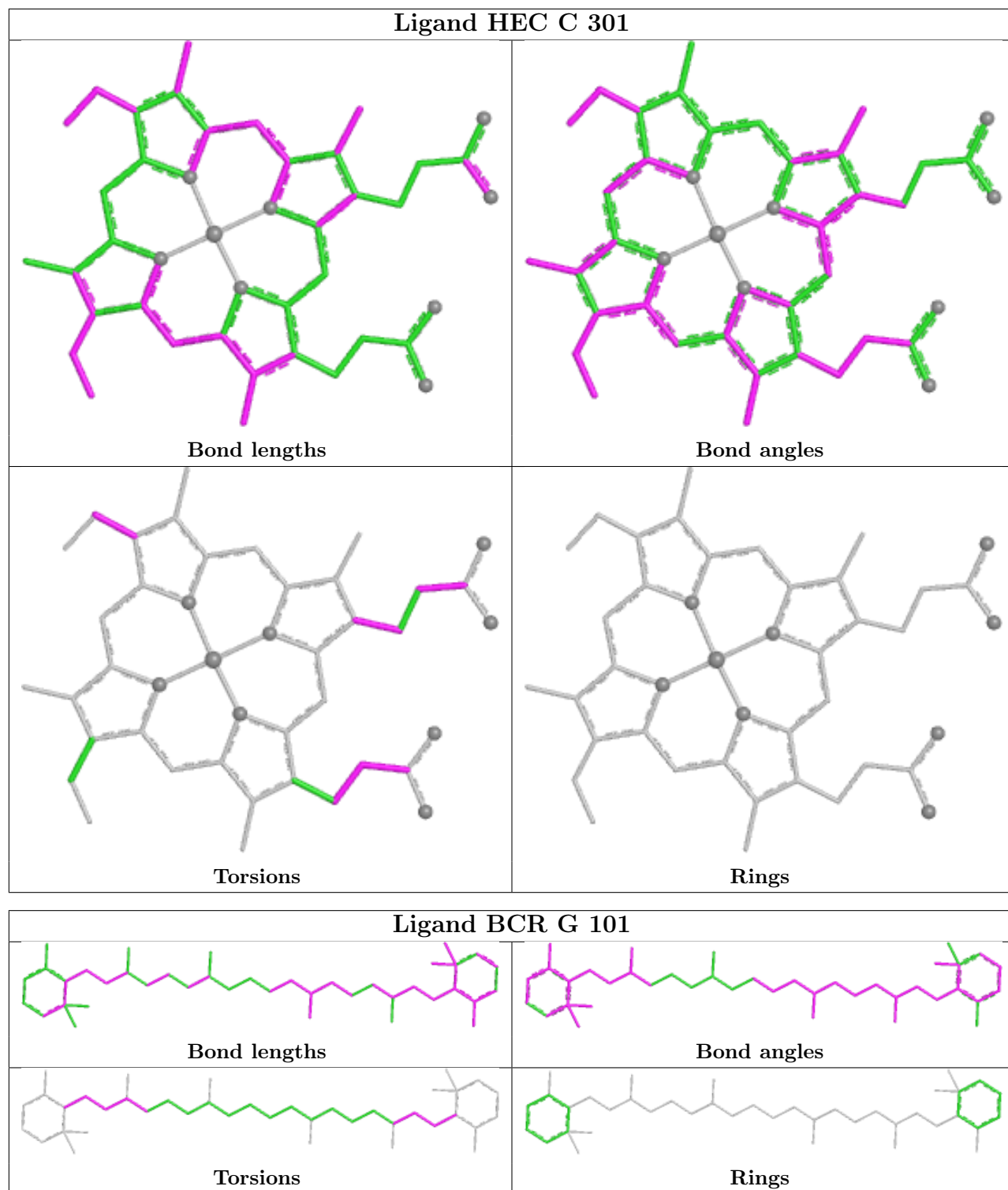
There are no ring outliers.

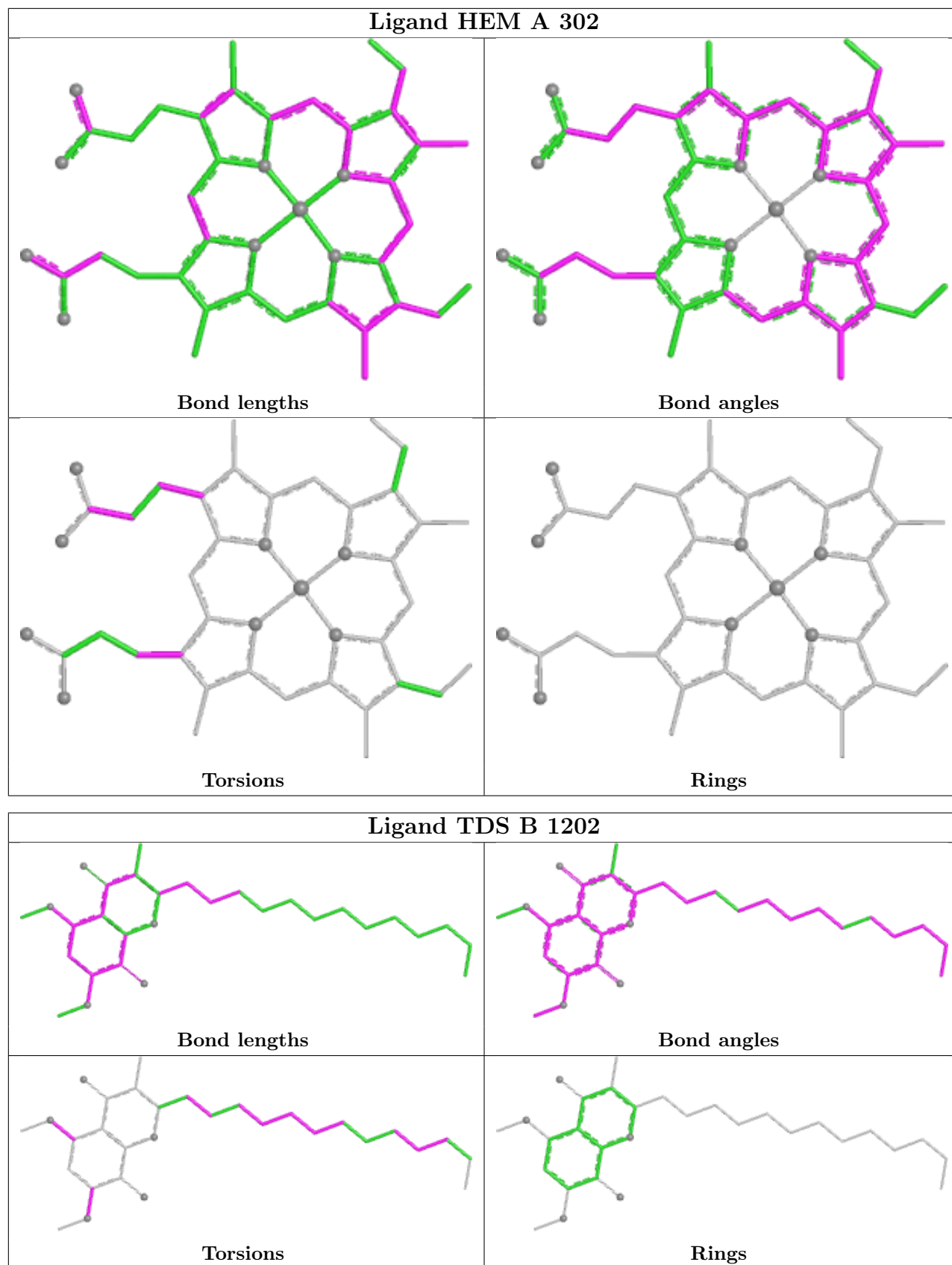
15 monomers are involved in 173 short contacts:

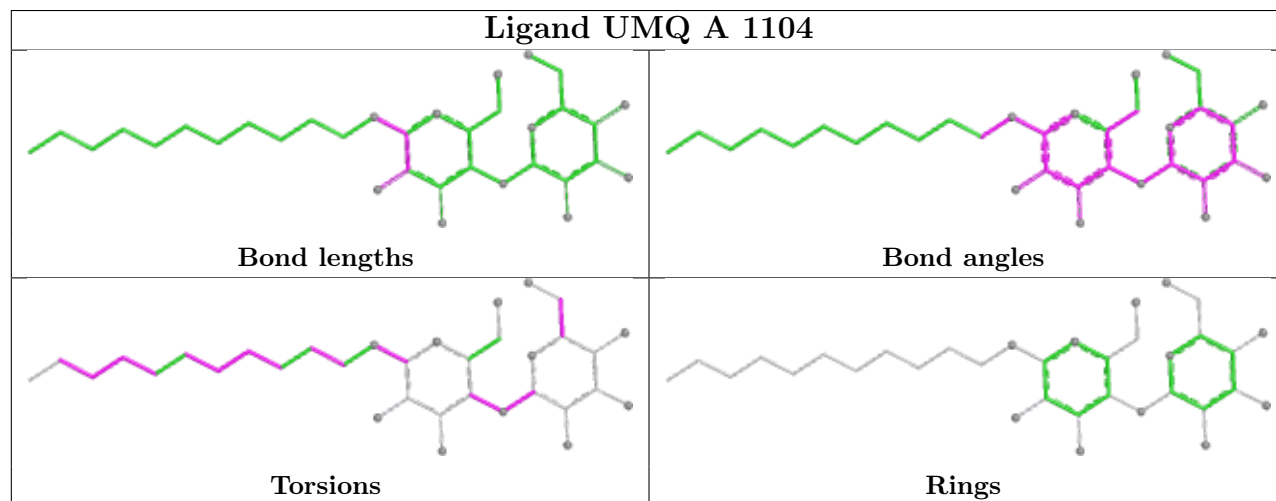
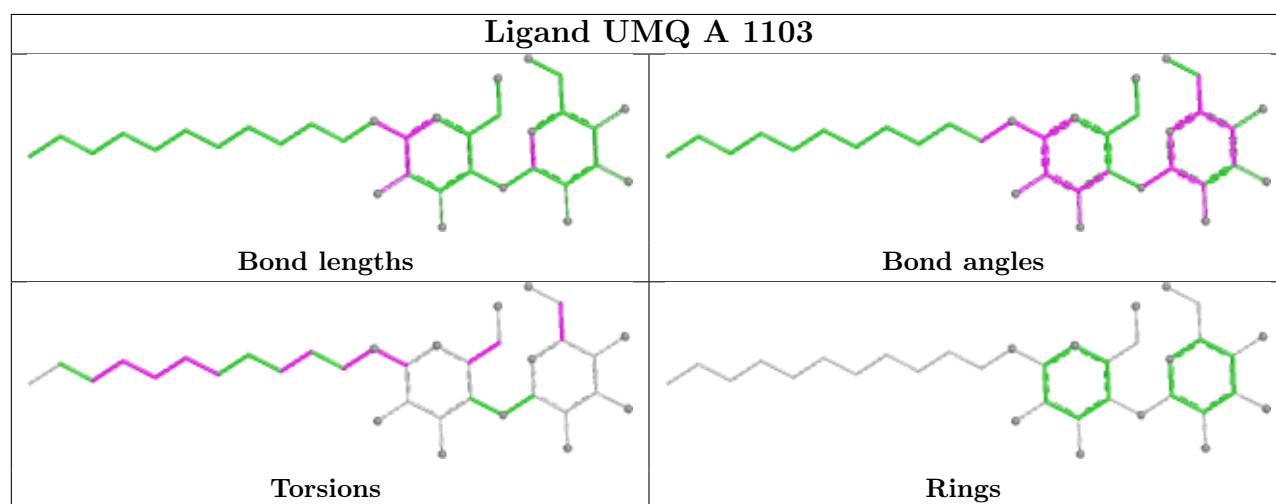
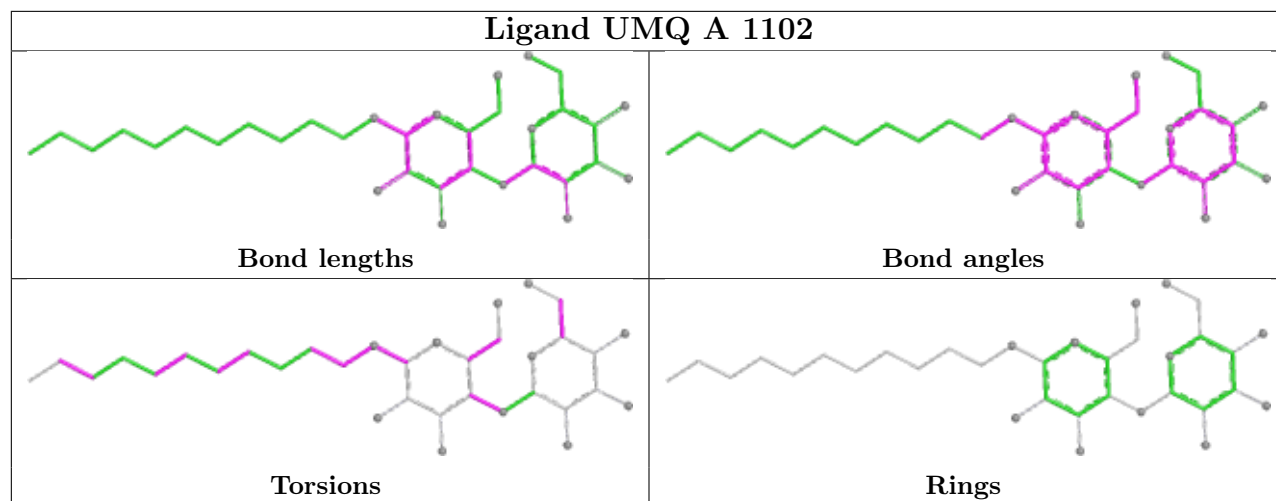
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1201	TDS	20	0
11	C	301	HEC	29	0
18	G	101	BCR	9	0
10	A	302	HEM	22	0
15	B	1202	TDS	18	0
13	A	1102	UMQ	1	0
13	A	1104	UMQ	3	0
17	D	201	SQD	9	0
13	A	1101	UMQ	2	0
12	B	1001	OPC	2	0
10	A	301	HEM	19	0
12	A	1002	OPC	17	0
11	A	303	HEC	23	0
16	D	200	FES	1	0
14	B	201	CLA	6	0

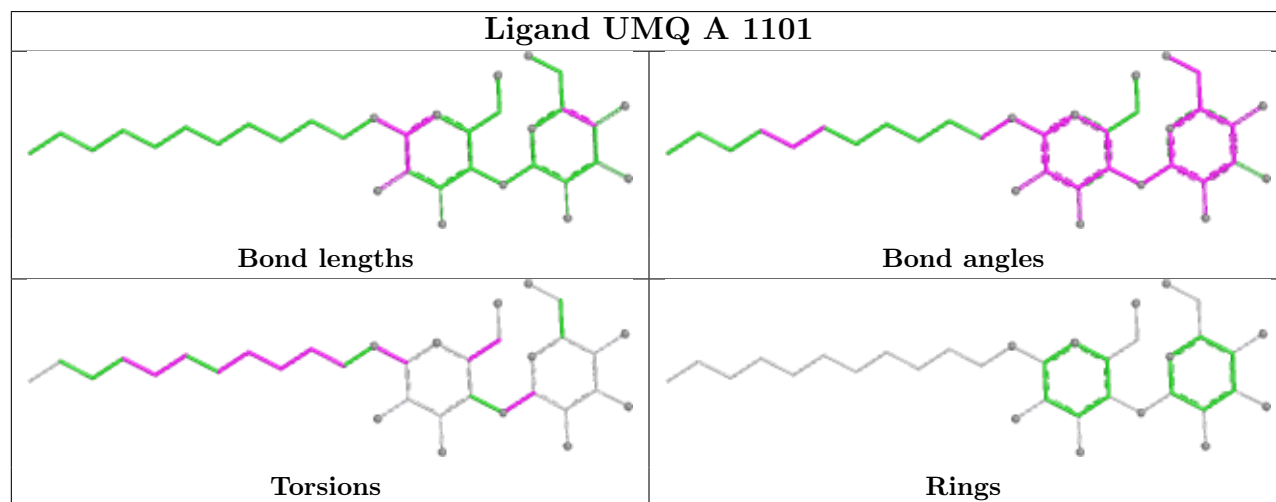
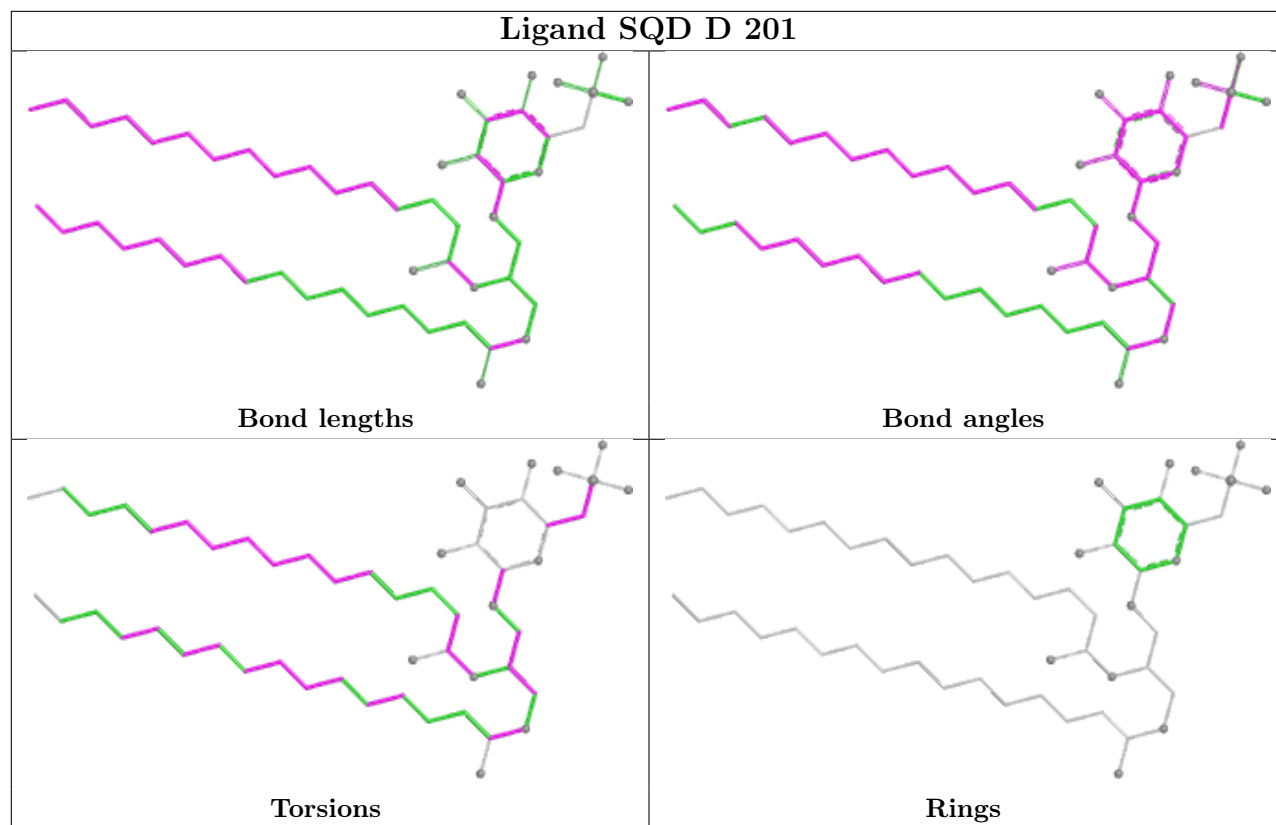
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

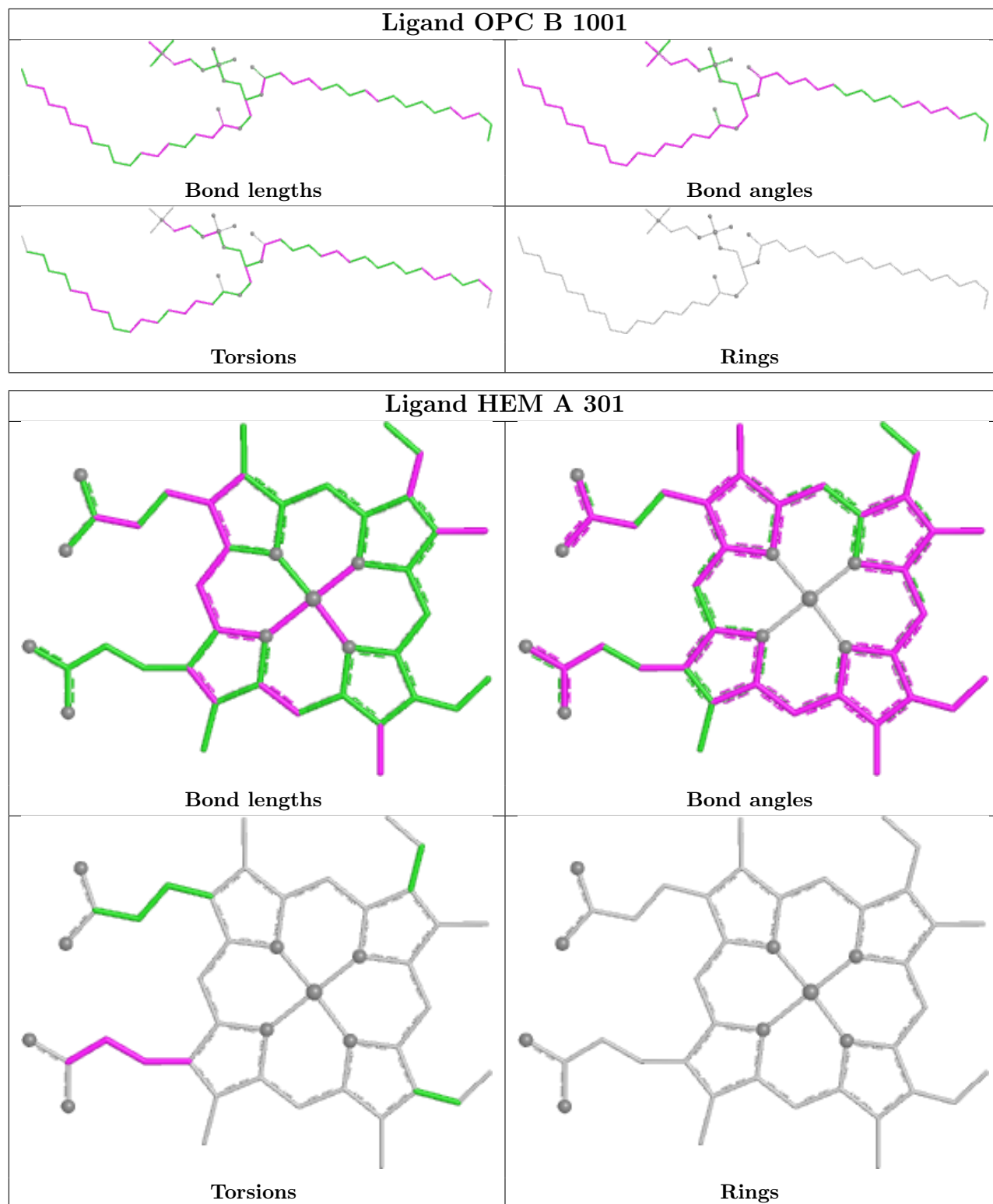


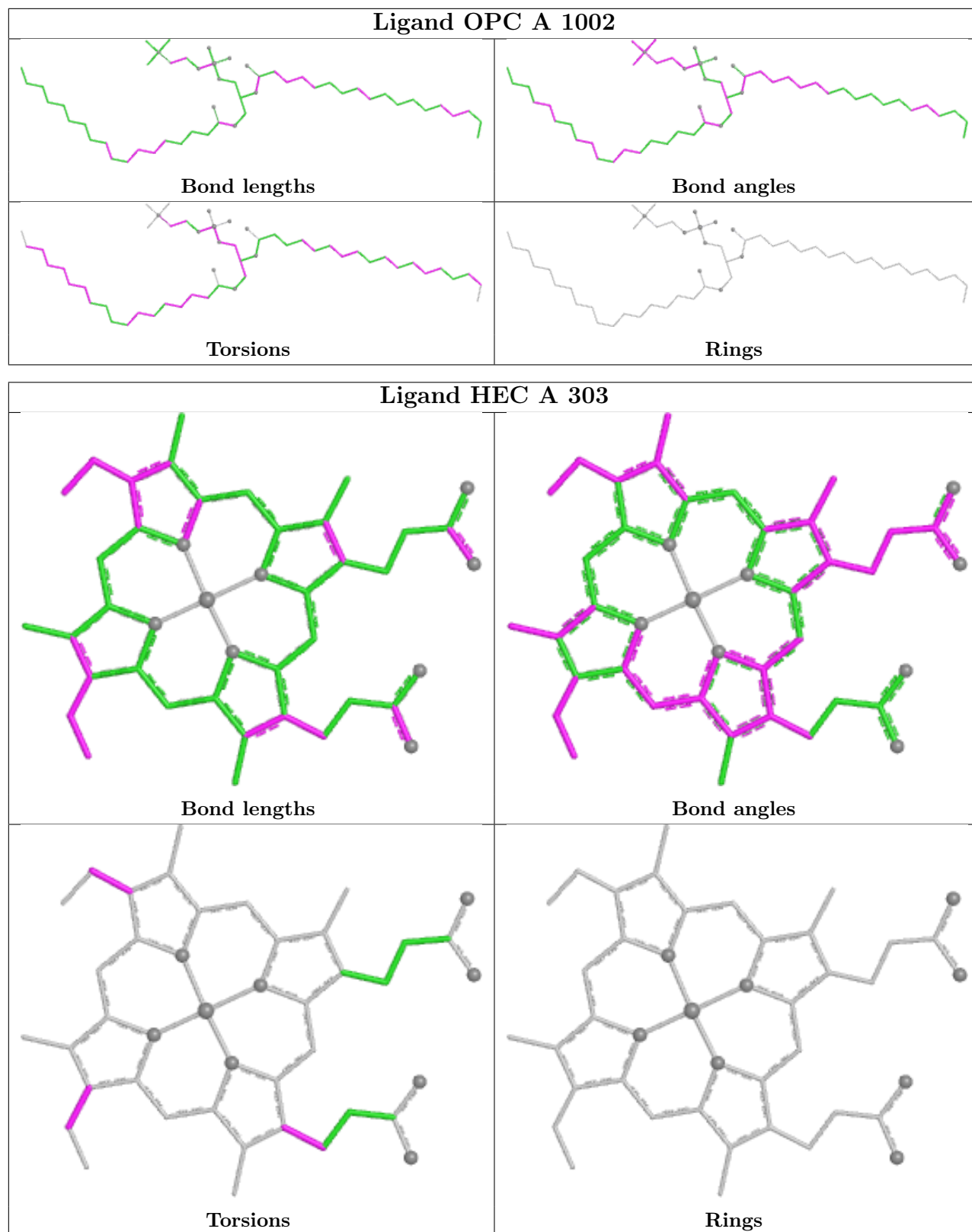


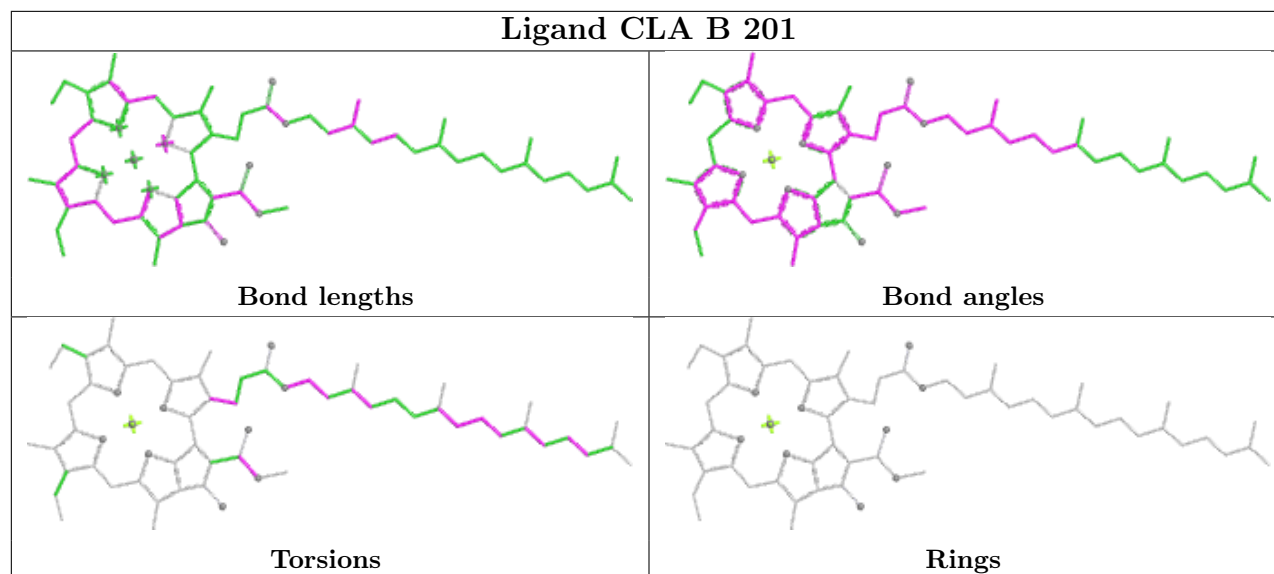












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/215 (100%)	-0.62	2 (0%) 81 69	5, 31, 72, 170	0
2	B	160/160 (100%)	-0.25	4 (2%) 58 43	22, 50, 97, 146	0
3	C	288/289 (99%)	0.85	32 (11%) 10 11	4, 55, 142, 159	1 (0%)
4	D	168/179 (93%)	1.49	45 (26%) 1 2	24, 90, 140, 156	0
5	E	32/32 (100%)	0.02	2 (6%) 26 20	39, 63, 93, 110	0
6	F	32/35 (91%)	0.15	4 (12%) 8 9	35, 50, 112, 121	0
7	G	37/37 (100%)	-0.08	3 (8%) 18 15	29, 44, 119, 138	0
8	H	29/29 (100%)	-0.42	1 (3%) 48 35	31, 42, 72, 95	0
All	All	961/976 (98%)	0.33	93 (9%) 13 13	4, 52, 132, 170	1 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	96	LYS	9.7
3	C	40	VAL	7.8
4	D	95	SER	7.5
4	D	141	ARG	7.0
4	D	157	ASP	7.0
3	C	88	GLU	6.4
3	C	220	SER	6.0
4	D	75	ALA	5.2
3	C	100	ASP	5.2
3	C	212	PRO	5.2
4	D	177	TRP	4.9
4	D	156	GLN	4.8
3	C	195	TYR	4.2
4	D	144	ALA	4.0
4	D	146	LEU	4.0
3	C	35	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	74	GLU	3.9
3	C	207	VAL	3.9
4	D	67	SER	3.8
3	C	201	THR	3.6
3	C	165	GLU	3.6
4	D	79	VAL	3.4
3	C	71	ASN	3.3
4	D	77	ASP	3.3
3	C	145	GLY	3.3
4	D	78	ARG	3.3
4	D	85	LYS	3.3
3	C	225	VAL	3.2
4	D	97	GLU	3.2
4	D	90	TYR	3.2
1	A	1	MET	3.1
4	D	70	LEU	3.0
4	D	127	PRO	3.0
3	C	140	LYS	3.0
3	C	206	THR	3.0
4	D	80	LEU	2.9
3	C	219	VAL	2.9
3	C	252	PRO	2.9
4	D	179	VAL	2.9
2	B	154	THR	2.8
4	D	145	PRO	2.8
2	B	155	LEU	2.8
6	F	3	GLU	2.8
4	D	41	TYR	2.7
4	D	125	LYS	2.7
3	C	249	LEU	2.7
1	A	2	ALA	2.7
3	C	213	ALA	2.7
3	C	29	ALA	2.7
4	D	170	PHE	2.6
6	F	4	GLU	2.6
4	D	10	VAL	2.6
5	E	1	MET	2.6
6	F	1	MET	2.6
3	C	194	LYS	2.6
3	C	39	SER	2.6
7	G	37	GLY	2.5
4	D	99	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	175	LYS	2.5
4	D	131	SER	2.4
4	D	149	ALA	2.4
4	D	74	ASN	2.4
2	B	28	GLY	2.4
4	D	49	ALA	2.4
4	D	94	GLU	2.4
4	D	155	VAL	2.4
4	D	60	LEU	2.3
8	H	29	LEU	2.3
3	C	215	PRO	2.3
3	C	185	LYS	2.3
6	F	31	GLY	2.3
3	C	86	PRO	2.3
3	C	136	PRO	2.3
3	C	172	PHE	2.3
4	D	178	TRP	2.3
5	E	2	ILE	2.2
4	D	143	PRO	2.2
4	D	162	LEU	2.2
3	C	241	GLY	2.2
3	C	245	THR	2.2
3	C	193	VAL	2.2
7	G	3	GLU	2.2
4	D	73	HIS	2.2
4	D	98	ALA	2.1
4	D	109	THR	2.1
7	G	27	GLN	2.1
4	D	86	GLY	2.1
3	C	166	LYS	2.1
4	D	15	ARG	2.1
3	C	147	TYR	2.0
4	D	59	LYS	2.0
4	D	92	VAL	2.0
4	D	43	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

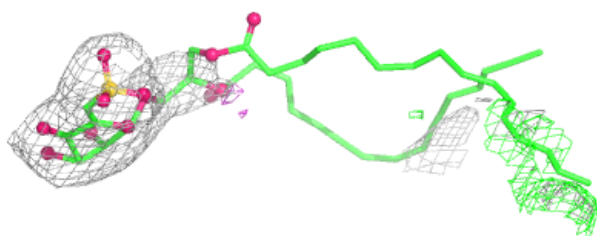
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	SQD	D	201	54/54	0.79	0.27	44,147,189,215	0
13	UMQ	A	1102	34/34	0.86	0.18	47,118,166,176	0
12	OPC	A	1002	54/55	0.86	0.22	19,84,180,191	0
13	UMQ	A	1104	34/34	0.87	0.15	61,129,164,178	0
13	UMQ	A	1103	34/34	0.88	0.14	58,109,133,141	0
18	BCR	G	101	40/40	0.90	0.19	24,63,149,159	0
15	TDS	B	1201	30/30	0.92	0.17	46,83,113,127	0
13	UMQ	A	1101	34/34	0.93	0.13	18,110,147,150	0
12	OPC	B	1001	54/55	0.95	0.14	28,80,117,123	0
15	TDS	B	1202	30/30	0.96	0.11	32,78,98,120	0
14	CLA	B	201	65/65	0.97	0.10	23,51,105,119	0
11	HEC	A	303	43/43	0.98	0.07	21,48,67,87	0
16	FES	D	200	4/4	0.98	0.08	59,69,70,72	0
10	HEM	A	301	43/43	0.99	0.06	2,21,41,74	0
10	HEM	A	302	43/43	0.99	0.07	6,26,45,63	0
9	CD	A	216	1/1	0.99	0.03	63,63,63,63	0
11	HEC	C	301	43/43	0.99	0.05	3,35,79,104	0

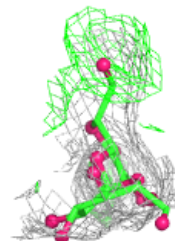
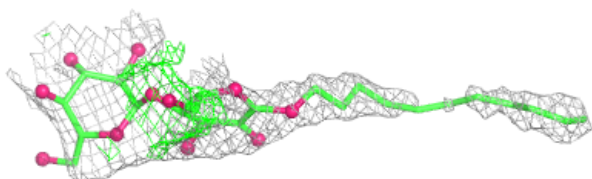
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SQD D 201:

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

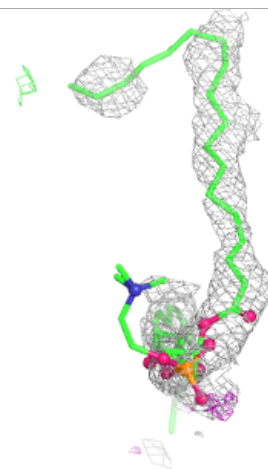
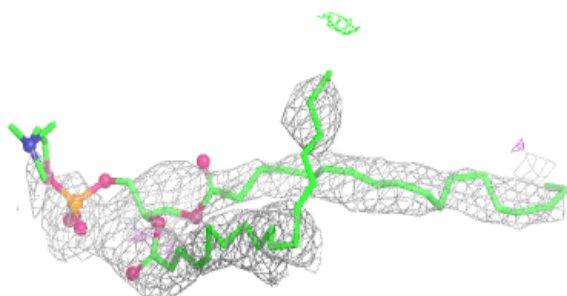
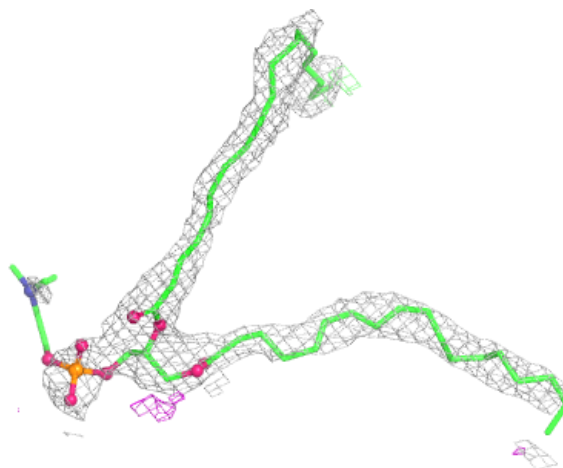
**Electron density around UMQ A 1102:**

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



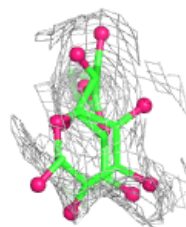
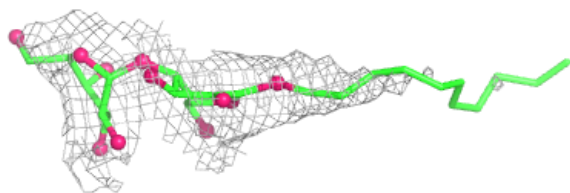
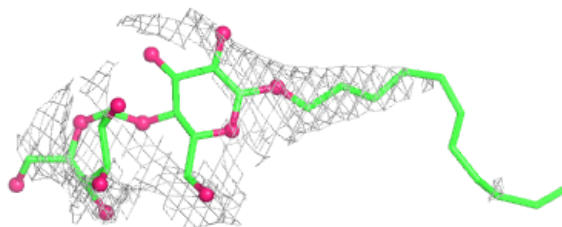
Electron density around OPC A 1002:

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

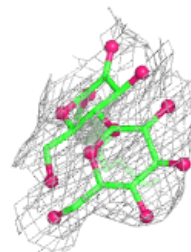
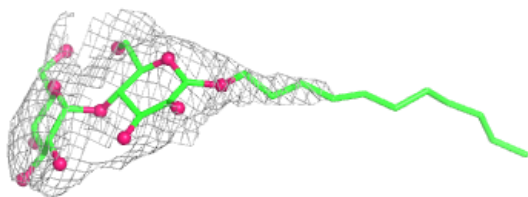
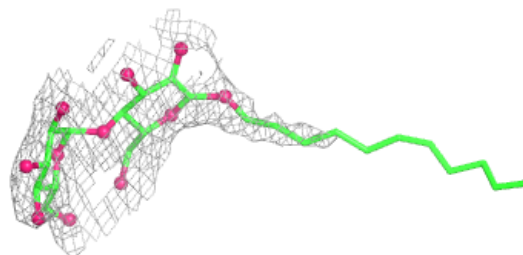


Electron density around UMQ A 1104:

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

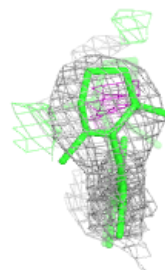
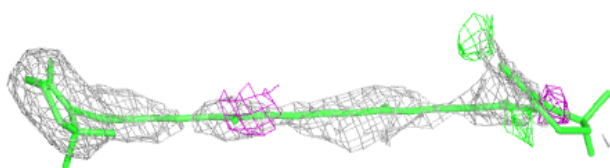
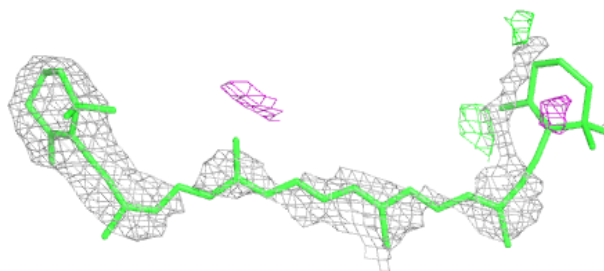
**Electron density around UMQ A 1103:**

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

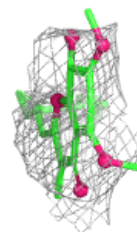
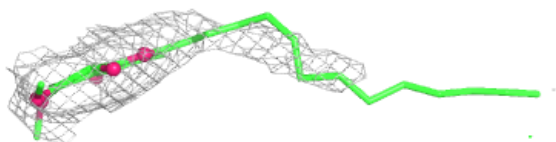
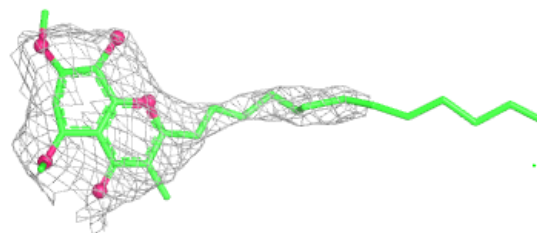


Electron density around BCR G 101:

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

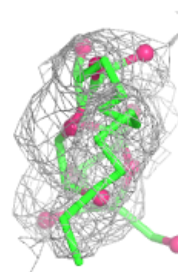
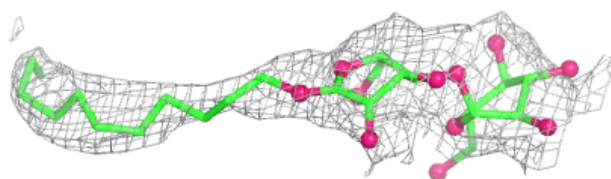
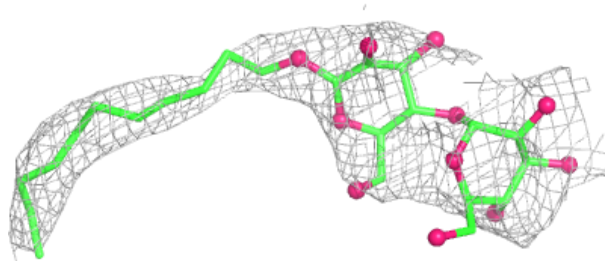
**Electron density around TDS B 1201:**

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

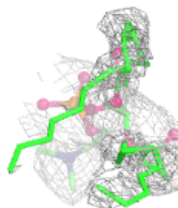
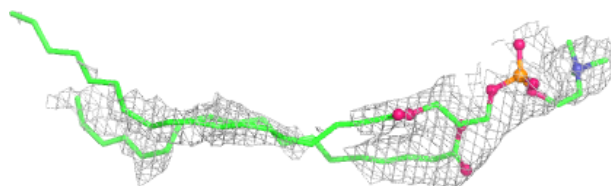
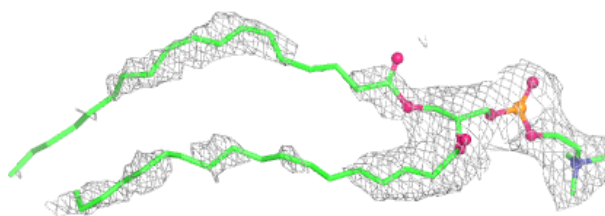


Electron density around UMQ A 1101:

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

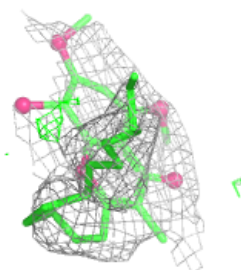
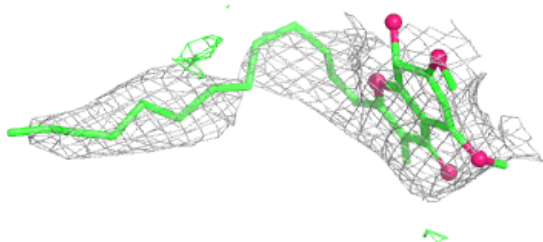
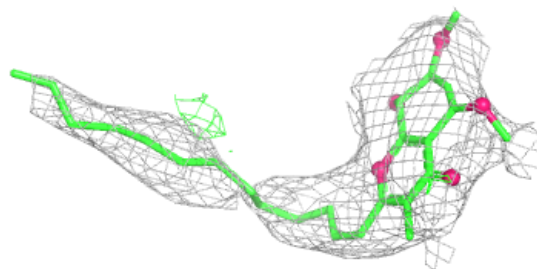
**Electron density around OPC B 1001:**

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

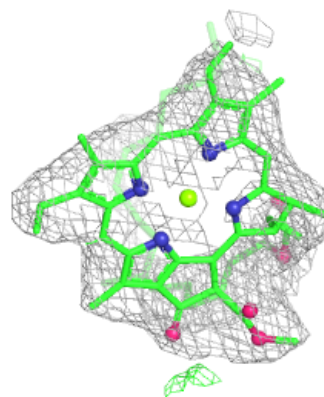
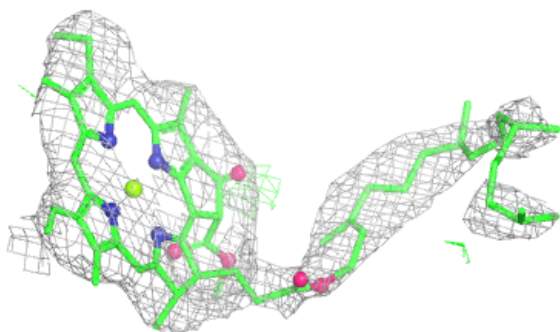
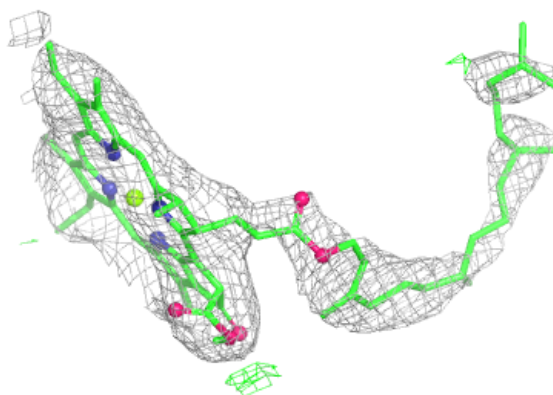


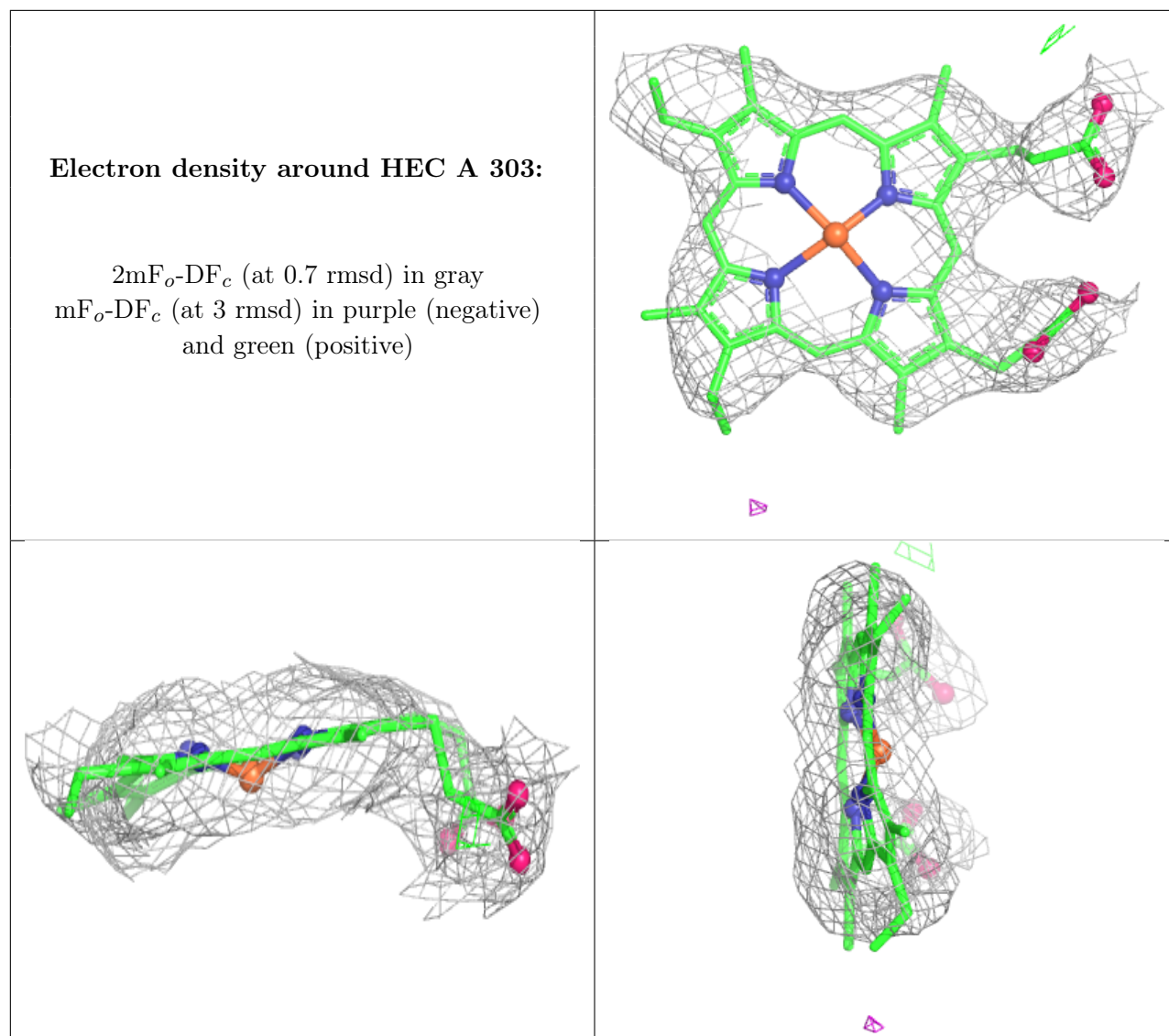
Electron density around TDS B 1202:

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

**Electron density around CLA B 201:**

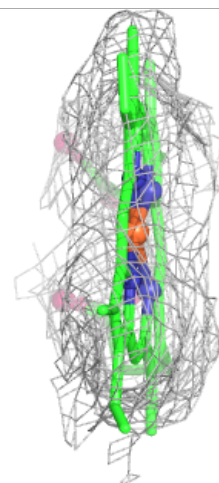
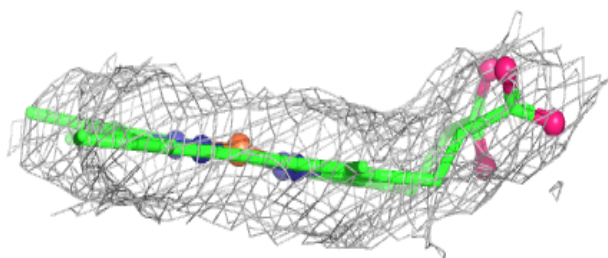
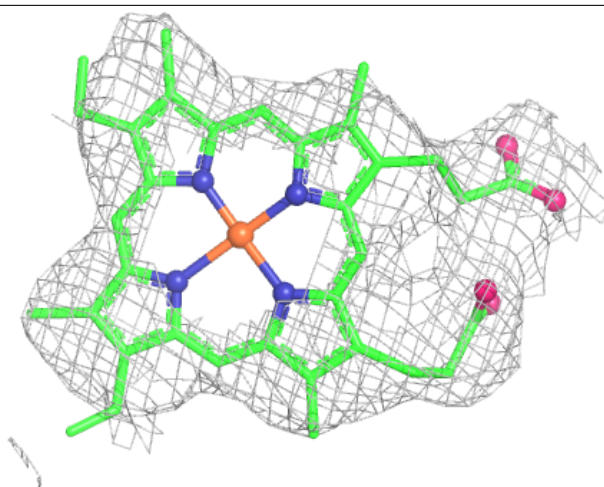
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





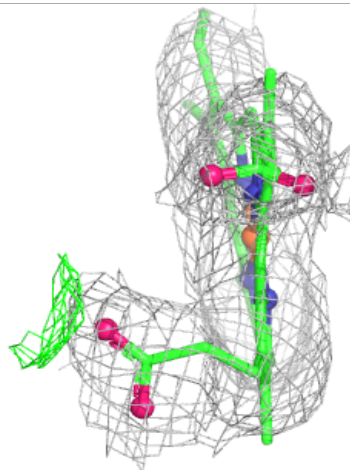
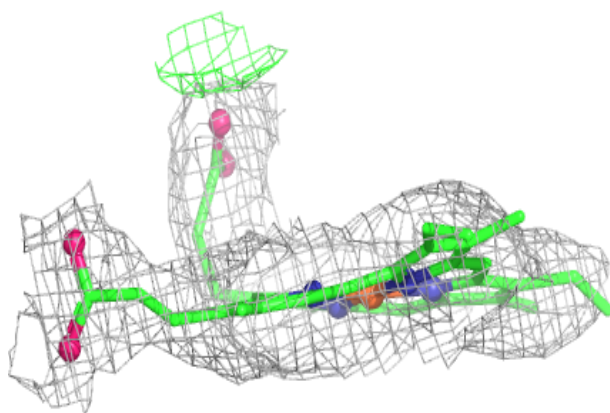
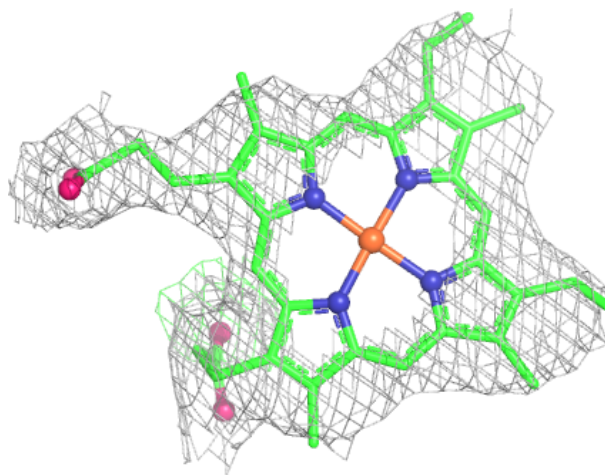
Electron density around HEM A 301:

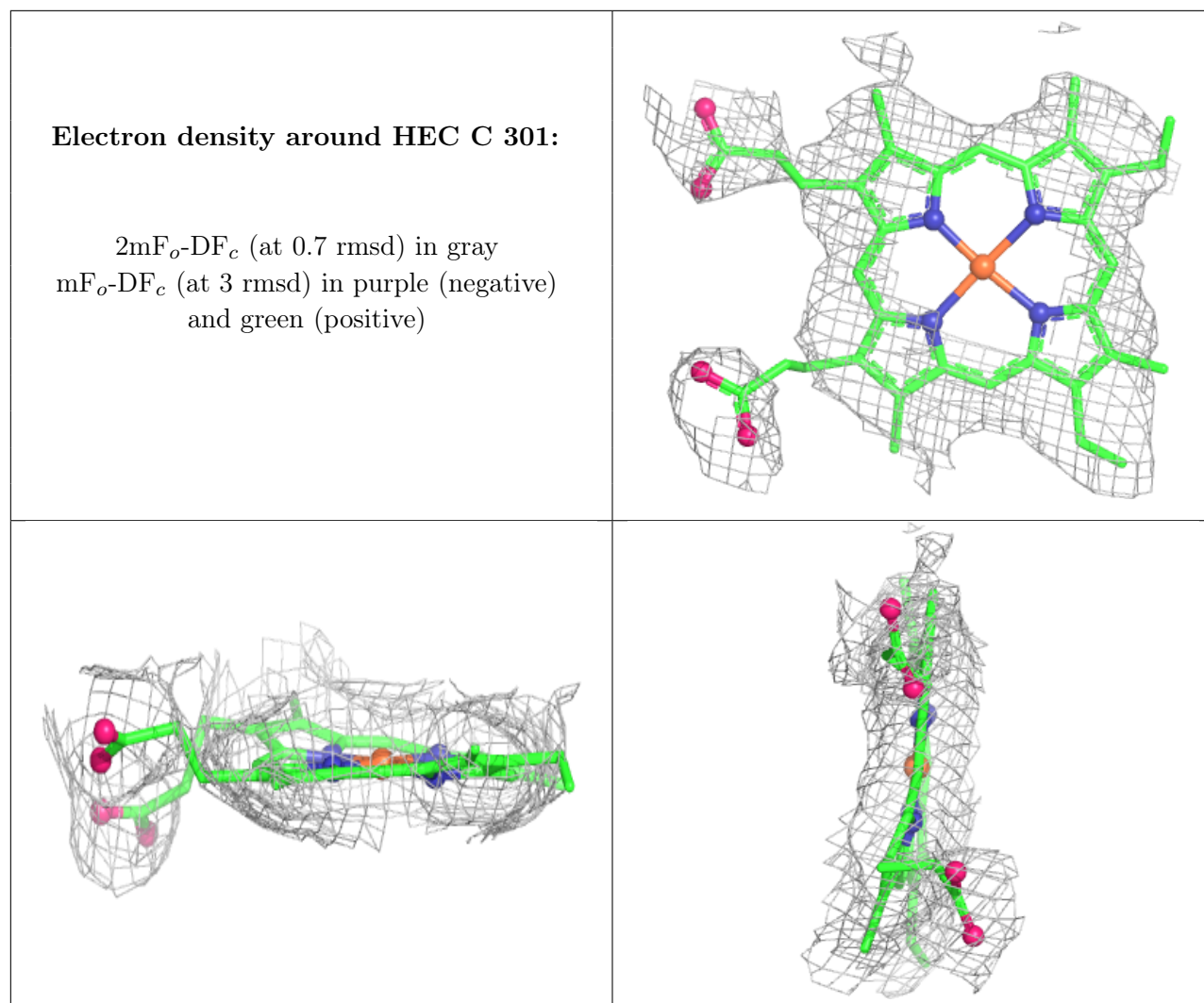
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 302:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.