



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:14 PM UTC

PDB ID : 3OFU / pdb_00003ofu
Title : Crystal Structure of Cytochrome P450 CYP101C1
Authors : Zhou, W.; Ma, M.; Bell, S.G.; Yang, W.; Hao, Y.; Rees, N.H.; Bartlam, M.;
Wong, L.-L.; Rao, Z.
Deposited on : 2010-08-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

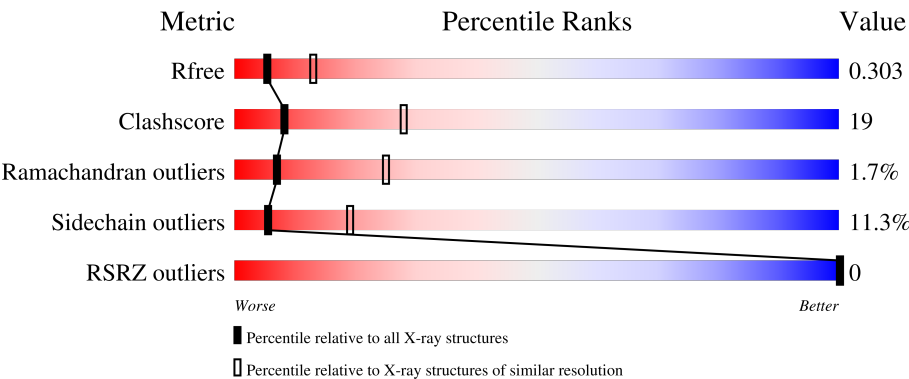
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	396	
1	B	396	
1	C	396	
1	D	396	
1	E	396	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	396	45% 36% 15% ••

2 Entry composition [i](#)

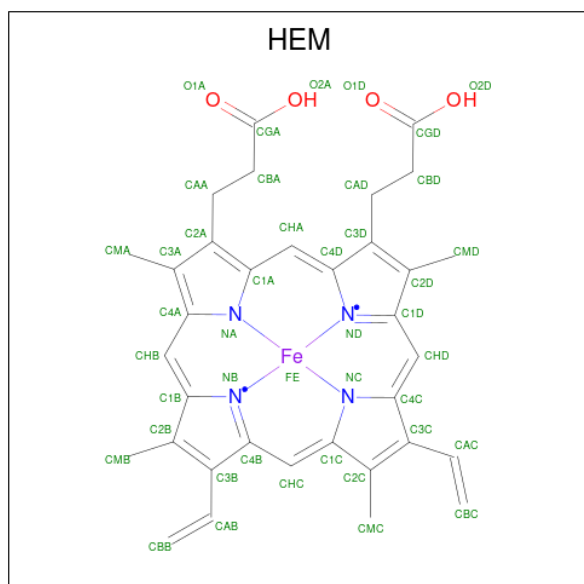
There are 4 unique types of molecules in this entry. The entry contains 18917 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P450.

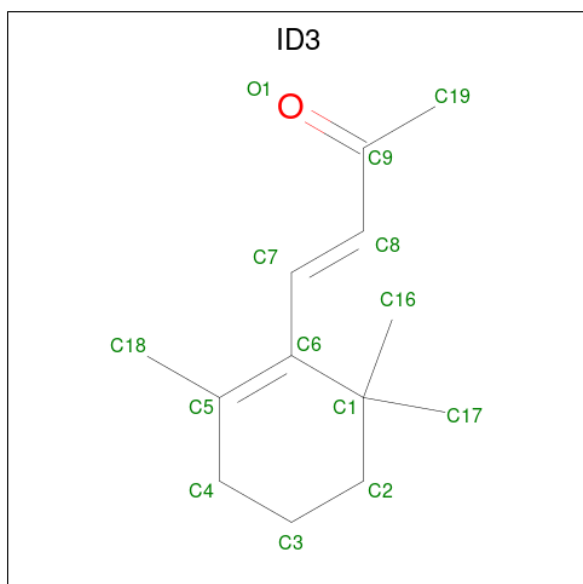
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3068	1950	552	547	19			
1	B	396	Total	C	N	O	S	0	0	0
			3068	1950	552	547	19			
1	C	396	Total	C	N	O	S	0	0	0
			3068	1950	552	547	19			
1	D	394	Total	C	N	O	S	0	0	0
			3053	1941	550	543	19			
1	E	390	Total	C	N	O	S	0	0	0
			3025	1926	543	537	19			
1	F	390	Total	C	N	O	S	0	0	0
			3025	1926	543	537	19			

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



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

- Molecule 3 is (3E)-4-(2,6,6-trimethylcyclohex-1-en-1-yl)but-3-en-2-one (CCD ID: ID3) (formula: C₁₃H₂₀O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 14	C 13	O 1	0	0
3	B	1	Total 14	C 13	O 1	0	0
3	C	1	Total 14	C 13	O 1	0	0

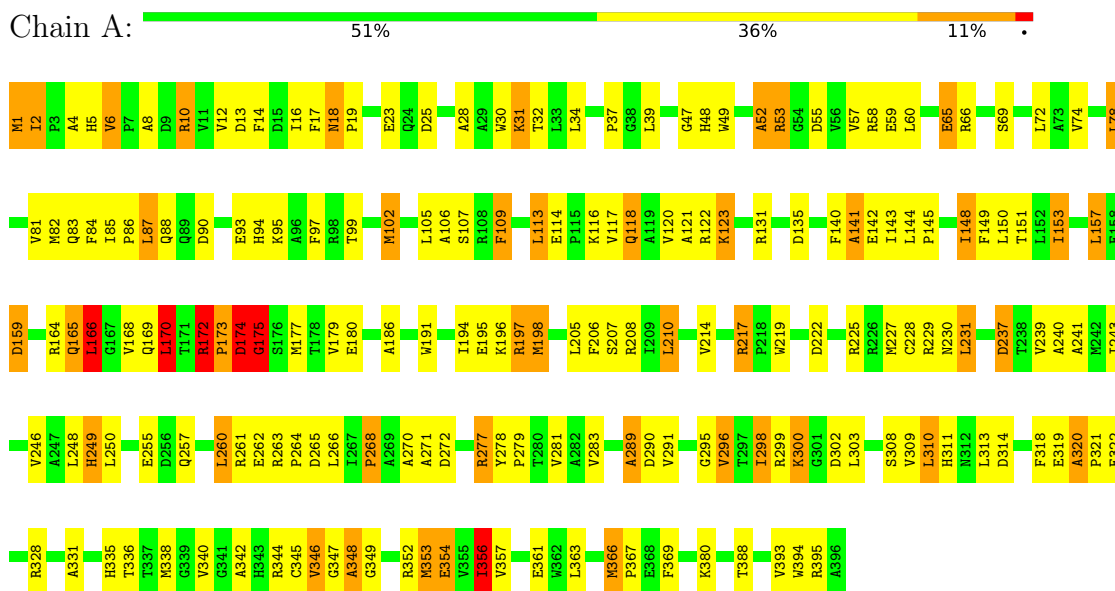
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total 51	O 51	0	0
4	B	62	Total 62	O 62	0	0
4	C	64	Total 64	O 64	0	0
4	D	52	Total 52	O 52	0	0
4	E	41	Total 41	O 41	0	0
4	F	40	Total 40	O 40	0	0

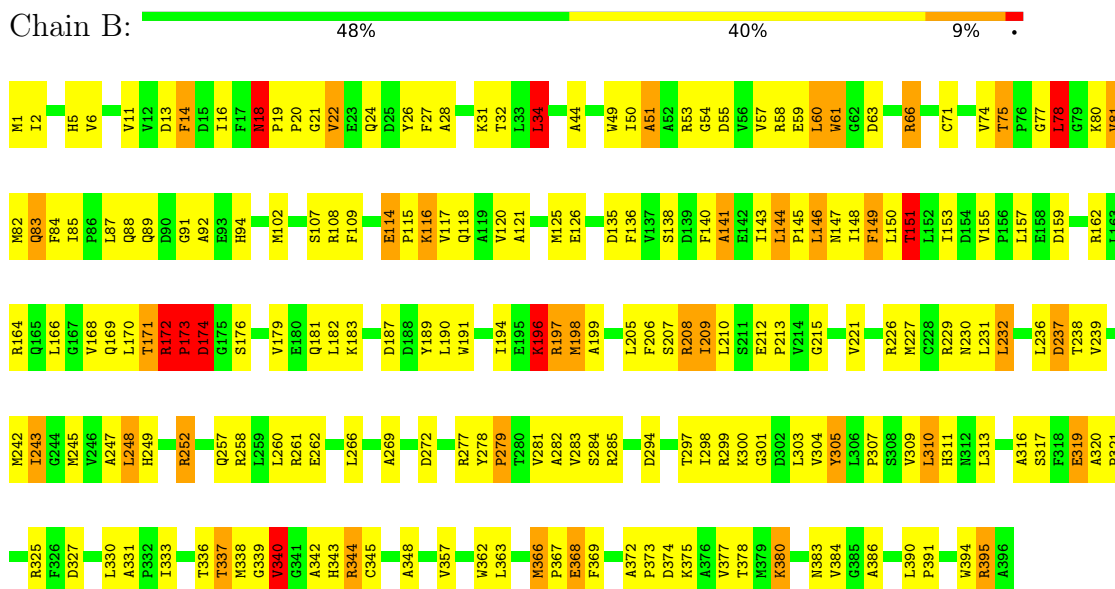
3 Residue-property plots

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.

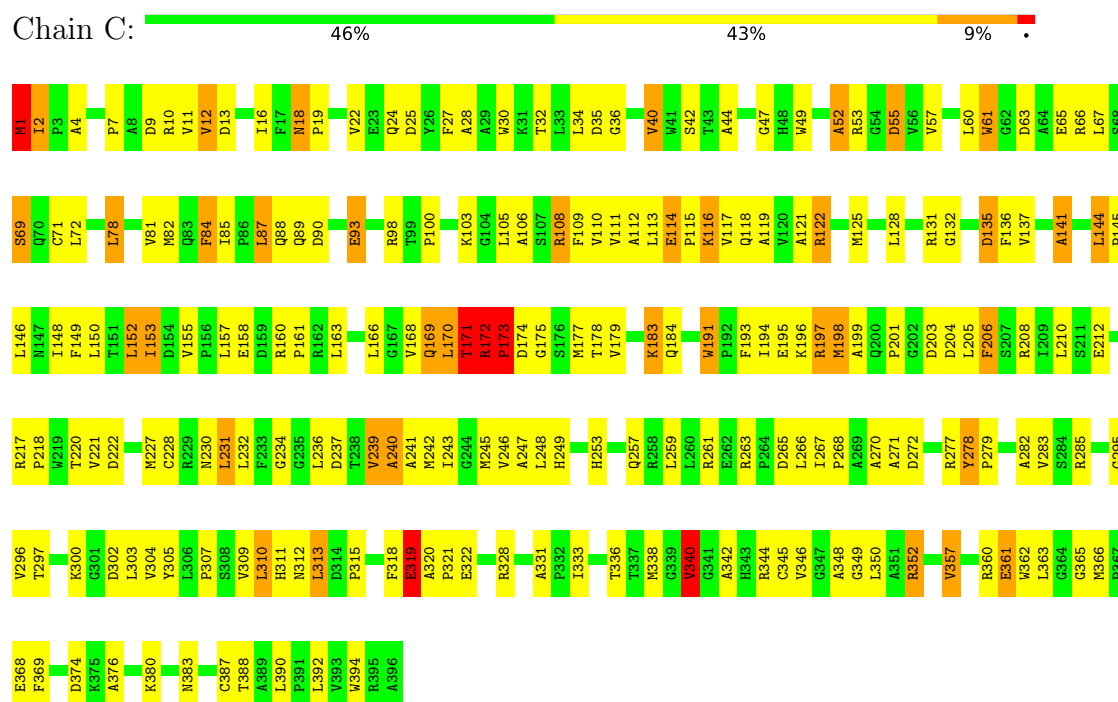
• Molecule 1: Cytochrome P450



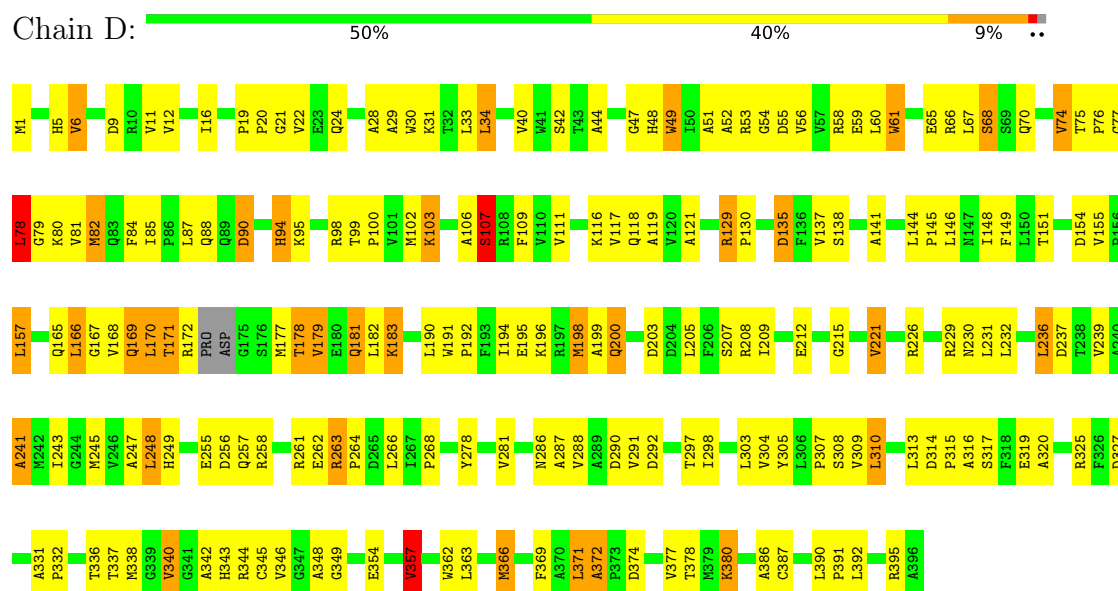
• Molecule 1: Cytochrome P450



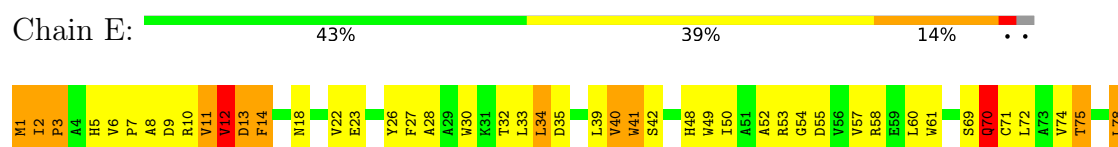
• Molecule 1: Cytochrome P450

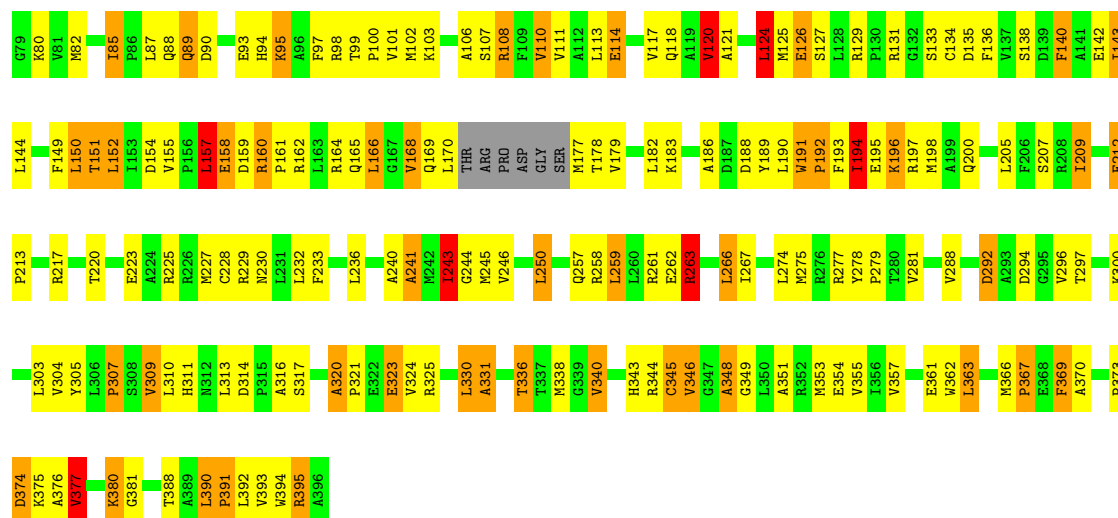


• Molecule 1: Cytochrome P450



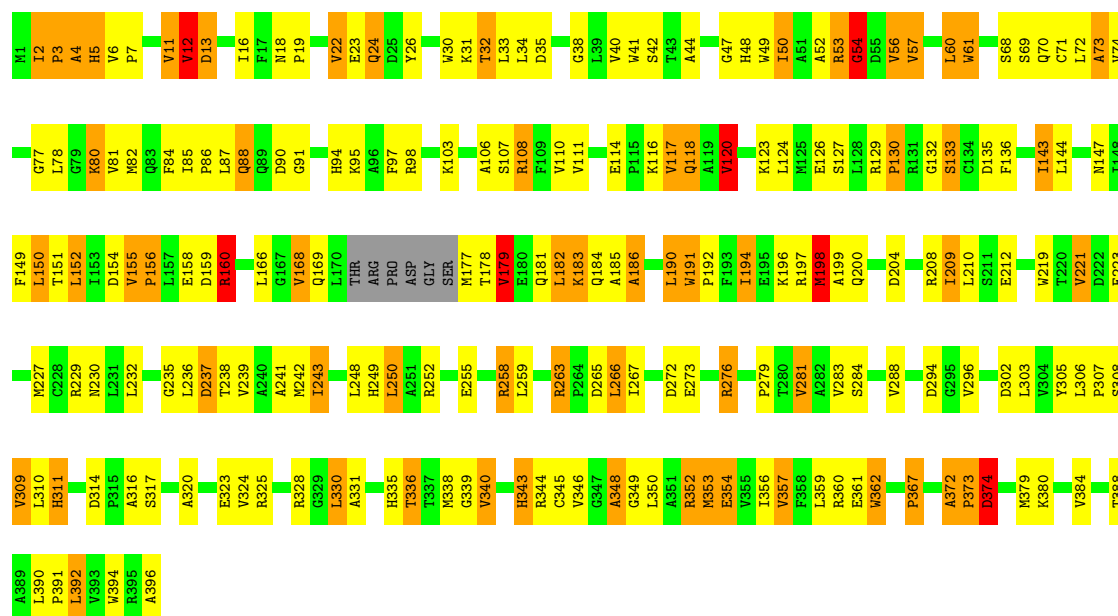
• Molecule 1: Cytochrome P450





• Molecule 1: Cytochrome P450

Chain F: 45% 36% 15% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.36Å 113.42Å 150.23Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.80) 98.3 (50.00-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.193 , 0.303 0.195 , 0.303	Depositor DCC
R_{free} test set	2829 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 9.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18917	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7644e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ID3

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	2.12	86/3140 (2.7%)	1.62	40/4269 (0.9%)
1	B	2.07	81/3140 (2.6%)	1.60	34/4269 (0.8%)
1	C	2.09	96/3140 (3.1%)	1.64	50/4269 (1.2%)
1	D	2.06	81/3123 (2.6%)	1.58	28/4243 (0.7%)
1	E	2.02	65/3095 (2.1%)	1.61	41/4206 (1.0%)
1	F	2.02	69/3095 (2.2%)	1.61	42/4206 (1.0%)
All	All	2.06	478/18733 (2.6%)	1.61	235/25462 (0.9%)

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	B	0	1
1	C	0	2
1	F	0	1
All	All	0	4

All (478) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	336	THR	CA-CB	12.26	1.70	1.53
1	F	336	THR	CA-CB	10.23	1.67	1.53
1	F	143	ILE	CA-CB	10.09	1.67	1.54
1	A	69	SER	N-CA	-9.95	1.35	1.46
1	A	296	VAL	CA-CB	9.93	1.68	1.54
1	A	140	PHE	CA-C	9.75	1.61	1.52
1	B	231	LEU	C-O	-9.55	1.13	1.24
1	E	320	ALA	C-O	-9.32	1.19	1.23
1	A	255	GLU	C-O	9.22	1.35	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	320	ALA	CA-CB	9.20	1.60	1.52
1	F	241	ALA	CA-CB	-8.95	1.39	1.53
1	C	13	ASP	C-O	-8.82	1.12	1.24
1	E	267	ILE	CA-CB	8.76	1.59	1.53
1	D	391	PRO	C-O	8.62	1.32	1.23
1	B	232	LEU	CA-C	-8.55	1.42	1.52
1	F	348	ALA	N-CA	8.49	1.56	1.46
1	F	22	VAL	CA-C	8.46	1.63	1.52
1	A	120	VAL	CA-CB	8.35	1.64	1.54
1	B	114	GLU	C-O	-8.30	1.16	1.24
1	C	160	ARG	C-O	-8.23	1.16	1.24
1	F	54	GLY	C-O	-8.10	1.12	1.23
1	F	374	ASP	CA-C	8.05	1.59	1.52
1	A	331	ALA	CA-CB	-8.04	1.41	1.53
1	C	4	ALA	CA-CB	-8.02	1.41	1.53
1	C	271	ALA	CA-C	7.92	1.63	1.52
1	F	143	ILE	CA-C	7.90	1.60	1.52
1	B	316	ALA	N-CA	7.86	1.56	1.46
1	C	203	ASP	CB-CG	7.79	1.71	1.52
1	C	240	ALA	CA-C	7.76	1.63	1.52
1	C	121	ALA	N-CA	-7.75	1.37	1.46
1	A	298	ILE	CA-CB	-7.75	1.44	1.54
1	B	262	GLU	CG-CD	7.74	1.71	1.52
1	C	220	THR	CA-CB	-7.72	1.40	1.53
1	F	391	PRO	N-CA	7.71	1.57	1.47
1	B	172	ARG	CA-C	7.69	1.62	1.52
1	B	198	MET	C-O	-7.68	1.14	1.24
1	F	252	ARG	CA-C	7.66	1.63	1.52
1	F	117	VAL	CA-CB	7.59	1.64	1.54
1	A	116	LYS	N-CA	-7.57	1.37	1.46
1	D	342	ALA	CA-C	7.55	1.62	1.52
1	E	209	ILE	CA-CB	7.49	1.63	1.54
1	D	307	PRO	CA-C	7.43	1.59	1.52
1	D	374	ASP	CG-OD2	7.43	1.39	1.25
1	A	8	ALA	CA-CB	-7.43	1.40	1.53
1	E	348	ALA	N-CA	7.40	1.55	1.46
1	C	357	VAL	CA-CB	-7.40	1.45	1.54
1	A	81	VAL	CA-CB	7.39	1.64	1.54
1	C	346	VAL	N-CA	7.39	1.55	1.46
1	A	393	VAL	C-O	7.36	1.31	1.23
1	F	309	VAL	CA-CB	-7.34	1.45	1.54
1	A	271	ALA	CA-C	7.32	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	286	ASN	C-O	7.32	1.32	1.24
1	C	297	THR	CA-CB	7.30	1.67	1.53
1	C	285	ARG	C-O	7.30	1.32	1.23
1	A	37	PRO	C-O	7.29	1.32	1.23
1	A	4	ALA	CA-CB	-7.25	1.42	1.53
1	E	117	VAL	CA-CB	7.25	1.64	1.54
1	B	60	LEU	C-O	-7.17	1.15	1.24
1	F	391	PRO	C-O	7.17	1.33	1.23
1	E	292	ASP	CA-C	-7.08	1.43	1.52
1	D	205	LEU	CA-C	7.06	1.62	1.52
1	F	360	ARG	CA-C	7.05	1.61	1.52
1	C	110	VAL	CA-CB	-7.05	1.46	1.54
1	E	110	VAL	C-O	-7.01	1.16	1.24
1	D	331	ALA	CA-CB	-6.98	1.43	1.53
1	A	135	ASP	CB-CG	6.95	1.69	1.52
1	D	6	VAL	CA-C	6.90	1.60	1.52
1	E	377	VAL	CA-CB	6.90	1.61	1.53
1	C	52	ALA	CA-CB	-6.87	1.42	1.53
1	D	357	VAL	C-O	-6.86	1.16	1.24
1	B	331	ALA	CA-CB	-6.85	1.41	1.53
1	C	100	PRO	N-CA	-6.85	1.38	1.47
1	C	173	PRO	N-CA	6.84	1.56	1.47
1	A	346	VAL	N-CA	6.83	1.54	1.46
1	B	11	VAL	C-O	6.83	1.31	1.23
1	B	395	ARG	CG-CD	6.83	1.73	1.52
1	F	320	ALA	CA-CB	6.82	1.64	1.53
1	B	231	LEU	CA-C	-6.82	1.44	1.52
1	C	28	ALA	CA-CB	-6.80	1.42	1.53
1	E	182	LEU	N-CA	6.79	1.54	1.46
1	C	267	ILE	CA-CB	6.77	1.62	1.54
1	F	60	LEU	CA-C	6.75	1.62	1.52
1	B	49	TRP	C-O	6.74	1.32	1.23
1	F	284	SER	CA-C	-6.74	1.44	1.52
1	B	121	ALA	CA-CB	-6.74	1.43	1.53
1	C	203	ASP	CG-OD1	6.73	1.38	1.25
1	E	263	ARG	CA-C	6.73	1.60	1.53
1	A	102	MET	N-CA	-6.72	1.38	1.46
1	C	111	VAL	C-O	-6.72	1.16	1.24
1	A	105	LEU	N-CA	-6.72	1.37	1.46
1	E	41	TRP	CA-C	6.68	1.60	1.52
1	B	377	VAL	CA-CB	6.68	1.61	1.54
1	D	196	LYS	CD-CE	6.65	1.72	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	359	LEU	CA-C	6.64	1.61	1.52
1	D	386	ALA	CA-C	-6.64	1.44	1.52
1	B	6	VAL	CA-C	6.62	1.58	1.53
1	C	84	PHE	N-CA	-6.62	1.37	1.46
1	B	285	ARG	N-CA	-6.61	1.37	1.45
1	B	386	ALA	CA-C	-6.60	1.44	1.52
1	D	281	VAL	CA-CB	-6.59	1.46	1.54
1	B	74	VAL	C-O	6.59	1.32	1.24
1	C	259	LEU	N-CA	-6.58	1.38	1.46
1	E	240	ALA	N-CA	6.58	1.54	1.46
1	A	283	VAL	N-CA	-6.57	1.38	1.46
1	D	209	ILE	CA-CB	-6.57	1.47	1.54
1	E	349	GLY	C-O	6.57	1.32	1.23
1	B	342	ALA	CA-CB	6.56	1.64	1.53
1	E	12	VAL	CA-CB	6.55	1.63	1.54
1	B	78	LEU	CA-C	6.54	1.61	1.52
1	D	292	ASP	N-CA	6.53	1.54	1.46
1	F	160	ARG	C-N	6.52	1.42	1.34
1	A	28	ALA	CA-CB	-6.51	1.43	1.53
1	A	186	ALA	C-O	-6.50	1.16	1.24
1	D	316	ALA	N-CA	6.49	1.54	1.46
1	C	90	ASP	CA-C	6.48	1.60	1.52
1	C	352	ARG	CZ-NH2	6.48	1.41	1.33
1	C	218	PRO	C-O	6.47	1.30	1.23
1	A	87	LEU	CA-C	-6.47	1.44	1.52
1	E	212	GLU	CA-C	-6.46	1.45	1.53
1	F	179	VAL	CA-CB	6.44	1.61	1.54
1	A	12	VAL	C-O	6.44	1.31	1.23
1	F	178	THR	CA-CB	6.43	1.63	1.53
1	A	279	PRO	CA-C	6.42	1.59	1.52
1	B	215	GLY	C-O	-6.42	1.17	1.24
1	C	360	ARG	CZ-NH2	6.42	1.41	1.33
1	D	288	VAL	CA-CB	-6.41	1.47	1.54
1	F	50	ILE	CA-CB	-6.41	1.46	1.54
1	C	22	VAL	CA-CB	-6.41	1.46	1.54
1	A	240	ALA	CA-CB	6.39	1.63	1.53
1	A	121	ALA	N-CA	-6.39	1.38	1.46
1	E	143	ILE	CA-CB	6.39	1.62	1.54
1	F	331	ALA	C-N	6.38	1.42	1.34
1	B	342	ALA	CA-C	6.38	1.61	1.52
1	D	198	MET	C-O	-6.37	1.15	1.24
1	C	12	VAL	C-O	6.36	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	ALA	N-CA	-6.36	1.38	1.46
1	C	135	ASP	CB-CG	6.36	1.68	1.52
1	D	181	GLN	CA-C	-6.35	1.43	1.52
1	E	120	VAL	CA-CB	6.35	1.61	1.54
1	A	356	ILE	CA-C	6.35	1.60	1.52
1	F	26	TYR	N-CA	6.34	1.54	1.46
1	A	17	PHE	CA-C	6.34	1.61	1.52
1	B	390	LEU	C-O	-6.34	1.17	1.24
1	C	241	ALA	N-CA	-6.34	1.38	1.46
1	E	281	VAL	CA-CB	6.33	1.63	1.54
1	A	142	GLU	C-O	-6.32	1.16	1.24
1	F	352	ARG	N-CA	6.32	1.53	1.46
1	B	92	ALA	CA-CB	-6.32	1.43	1.53
1	E	71	CYS	CA-C	6.31	1.61	1.52
1	F	296	VAL	CA-C	-6.30	1.44	1.52
1	B	367	PRO	N-CA	6.30	1.54	1.47
1	E	316	ALA	N-CA	6.30	1.54	1.46
1	F	343	HIS	CA-C	6.28	1.62	1.52
1	A	30	TRP	CA-C	-6.28	1.44	1.52
1	D	68	SER	CA-C	-6.28	1.44	1.52
1	B	248	LEU	N-CA	-6.27	1.38	1.46
1	B	285	ARG	CA-C	6.26	1.60	1.52
1	B	199	ALA	CA-CB	6.25	1.64	1.53
1	B	282	ALA	CA-C	6.23	1.60	1.52
1	D	44	ALA	CA-CB	-6.22	1.43	1.53
1	D	304	VAL	CA-CB	6.22	1.62	1.54
1	D	51	ALA	CA-C	-6.19	1.45	1.52
1	A	174	ASP	N-CA	6.18	1.54	1.46
1	F	19	PRO	CA-C	-6.17	1.48	1.51
1	D	137	VAL	CA-CB	-6.17	1.47	1.54
1	E	194	ILE	CA-CB	6.17	1.62	1.54
1	E	309	VAL	CA-CB	-6.17	1.46	1.54
1	F	311	HIS	CA-C	-6.16	1.47	1.52
1	E	14	PHE	CA-C	6.15	1.61	1.52
1	E	376	ALA	CA-CB	6.13	1.62	1.53
1	B	144	LEU	CA-C	-6.13	1.45	1.52
1	A	291	VAL	CA-CB	-6.12	1.46	1.54
1	B	269	ALA	CA-CB	6.10	1.62	1.53
1	A	118	GLN	CA-C	6.09	1.60	1.52
1	E	186	ALA	N-CA	6.09	1.54	1.46
1	C	222	ASP	N-CA	6.09	1.53	1.46
1	B	339	GLY	C-O	-6.09	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	HIS	C-O	6.09	1.31	1.24
1	F	283	VAL	N-CA	6.09	1.53	1.46
1	F	373	PRO	N-CA	6.09	1.55	1.47
1	E	60	LEU	CA-C	6.08	1.61	1.52
1	F	392	LEU	N-CA	6.08	1.53	1.45
1	B	281	VAL	CB-CG2	6.08	1.72	1.52
1	D	179	VAL	CA-C	6.07	1.60	1.52
1	D	82	MET	N-CA	6.07	1.53	1.46
1	E	70	GLN	CA-C	6.05	1.60	1.52
1	A	210	LEU	CA-CB	-6.05	1.43	1.53
1	C	114	GLU	CG-CD	-6.05	1.36	1.52
1	A	6	VAL	C-O	-6.04	1.16	1.24
1	A	219	TRP	CA-C	6.04	1.60	1.52
1	C	253	HIS	C-N	6.04	1.41	1.33
1	A	177	MET	CA-C	6.02	1.59	1.52
1	C	352	ARG	CZ-NH1	6.02	1.41	1.32
1	B	20	PRO	CA-C	6.02	1.58	1.52
1	D	247	ALA	CA-C	6.01	1.60	1.52
1	C	331	ALA	CA-CB	-6.01	1.42	1.53
1	F	307	PRO	C-O	6.00	1.31	1.24
1	C	36	GLY	C-N	-5.99	1.26	1.33
1	C	322	GLU	CA-C	5.99	1.60	1.52
1	B	187	ASP	CA-C	5.98	1.60	1.52
1	D	200	GLN	CG-CD	5.97	1.67	1.52
1	F	281	VAL	CA-C	-5.96	1.45	1.52
1	A	231	LEU	C-O	-5.95	1.17	1.24
1	C	146	LEU	CA-C	-5.94	1.45	1.52
1	A	388	THR	CA-C	-5.93	1.45	1.52
1	C	103	LYS	CD-CE	5.93	1.70	1.52
1	A	289	ALA	N-CA	5.93	1.53	1.45
1	E	305	TYR	C-O	5.93	1.31	1.24
1	D	146	LEU	N-CA	-5.92	1.38	1.46
1	C	18	ASN	C-O	-5.92	1.17	1.24
1	D	51	ALA	CA-CB	-5.92	1.43	1.53
1	C	114	GLU	C-O	-5.92	1.16	1.24
1	B	284	SER	C-O	-5.91	1.16	1.24
1	D	196	LYS	CG-CD	5.89	1.70	1.52
1	D	215	GLY	C-O	-5.88	1.16	1.23
1	F	221	VAL	CA-CB	5.86	1.61	1.54
1	E	331	ALA	C-N	5.85	1.42	1.34
1	D	378	THR	N-CA	5.84	1.53	1.45
1	B	373	PRO	CA-C	5.84	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	LEU	CA-C	-5.84	1.44	1.52
1	C	217	ARG	N-CA	5.83	1.53	1.45
1	D	65	GLU	CA-C	5.83	1.60	1.52
1	B	75	THR	N-CA	5.83	1.56	1.46
1	C	360	ARG	NE-CZ	5.83	1.39	1.33
1	C	208	ARG	NE-CZ	5.83	1.39	1.33
1	B	191	TRP	CA-C	5.82	1.60	1.52
1	C	194	ILE	CA-CB	-5.82	1.47	1.54
1	E	151	THR	CA-CB	5.81	1.62	1.53
1	A	148	ILE	CA-CB	5.80	1.61	1.54
1	D	121	ALA	N-CA	-5.80	1.39	1.46
1	E	307	PRO	C-O	5.79	1.31	1.24
1	D	392	LEU	CA-C	-5.79	1.45	1.52
1	F	308	SER	N-CA	5.78	1.53	1.46
1	F	328	ARG	C-O	-5.77	1.17	1.24
1	A	123	LYS	CG-CD	5.77	1.69	1.52
1	D	380	LYS	CA-C	-5.77	1.45	1.52
1	A	272	ASP	N-CA	-5.76	1.39	1.46
1	E	373	PRO	N-CA	5.76	1.55	1.47
1	F	19	PRO	N-CA	5.76	1.53	1.46
1	D	374	ASP	N-CA	5.76	1.53	1.46
1	A	246	VAL	CA-CB	5.75	1.61	1.54
1	A	279	PRO	N-CA	-5.75	1.40	1.47
1	C	212	GLU	CA-C	-5.74	1.46	1.53
1	B	196	LYS	CD-CE	5.72	1.69	1.52
1	D	303	LEU	C-O	-5.72	1.17	1.23
1	C	249	HIS	N-CA	-5.72	1.39	1.46
1	D	74	VAL	C-O	5.72	1.31	1.24
1	E	58	ARG	C-O	-5.72	1.17	1.24
1	C	30	TRP	CA-C	-5.72	1.44	1.52
1	B	91	GLY	N-CA	-5.71	1.38	1.45
1	C	106	ALA	N-CA	5.71	1.53	1.46
1	C	319	GLU	CG-CD	5.71	1.66	1.52
1	A	283	VAL	C-O	5.71	1.30	1.23
1	A	17	PHE	CE1-CZ	5.70	1.55	1.38
1	B	107	SER	N-CA	5.69	1.53	1.46
1	D	135	ASP	CG-OD2	5.69	1.36	1.25
1	C	93	GLU	N-CA	-5.69	1.39	1.46
1	C	297	THR	CA-C	-5.68	1.45	1.52
1	A	55	ASP	N-CA	5.68	1.53	1.46
1	B	317	SER	CA-C	5.68	1.60	1.52
1	D	390	LEU	CA-C	5.68	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	199	ALA	CA-C	5.67	1.59	1.52
1	D	258	ARG	NE-CZ	5.67	1.39	1.33
1	D	281	VAL	CA-C	-5.67	1.45	1.52
1	A	271	ALA	N-CA	5.66	1.52	1.46
1	C	174	ASP	CA-CB	5.65	1.60	1.53
1	E	258	ARG	C-O	5.65	1.30	1.24
1	D	297	THR	N-CA	-5.64	1.39	1.46
1	A	250	LEU	C-O	-5.64	1.17	1.24
1	A	353	MET	CA-C	5.63	1.59	1.52
1	B	126	GLU	N-CA	-5.63	1.39	1.46
1	D	183	LYS	CA-C	-5.63	1.45	1.52
1	F	179	VAL	CA-C	5.63	1.59	1.52
1	C	63	ASP	C-O	-5.62	1.17	1.23
1	A	66	ARG	N-CA	5.62	1.53	1.45
1	C	105	LEU	N-CA	-5.61	1.39	1.46
1	C	81	VAL	N-CA	-5.61	1.38	1.46
1	A	106	ALA	CA-C	5.60	1.60	1.52
1	F	12	VAL	CA-CB	5.60	1.62	1.54
1	D	106	ALA	C-O	5.60	1.30	1.23
1	F	306	LEU	CA-C	5.60	1.59	1.52
1	D	28	ALA	N-CA	5.60	1.53	1.46
1	C	374	ASP	CB-CG	5.59	1.66	1.52
1	E	69	SER	CA-C	-5.59	1.45	1.52
1	E	376	ALA	N-CA	5.58	1.53	1.46
1	A	272	ASP	CA-CB	-5.57	1.44	1.53
1	C	141	ALA	CA-C	-5.57	1.45	1.52
1	D	395	ARG	CA-C	-5.56	1.45	1.52
1	A	153	ILE	CA-CB	-5.56	1.47	1.54
1	C	183	LYS	CA-C	-5.56	1.45	1.52
1	D	199	ALA	C-O	5.56	1.28	1.23
1	B	232	LEU	C-O	-5.55	1.17	1.24
1	A	354	GLU	N-CA	-5.55	1.39	1.46
1	A	109	PHE	CG-CD1	5.55	1.50	1.38
1	E	377	VAL	CA-C	5.55	1.59	1.52
1	B	368	GLU	CA-C	5.54	1.60	1.52
1	C	44	ALA	CA-C	-5.54	1.45	1.53
1	C	392	LEU	N-CA	5.54	1.52	1.46
1	F	354	GLU	C-O	-5.54	1.17	1.24
1	B	49	TRP	CA-C	5.53	1.60	1.52
1	F	80	LYS	CG-CD	5.53	1.69	1.52
1	B	297	THR	N-CA	-5.53	1.40	1.46
1	C	282	ALA	CA-CB	-5.53	1.40	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	ALA	CA-CB	5.53	1.61	1.53
1	D	287	ALA	N-CA	5.53	1.52	1.46
1	F	82	MET	CA-C	-5.53	1.46	1.53
1	B	394	TRP	C-O	-5.52	1.17	1.23
1	F	353	MET	N-CA	-5.52	1.40	1.46
1	E	324	VAL	CA-CB	-5.51	1.47	1.54
1	B	116	LYS	CB-CG	5.51	1.69	1.52
1	B	71	CYS	CA-C	5.50	1.60	1.52
1	E	22	VAL	CA-C	5.50	1.59	1.52
1	E	275	MET	CA-C	5.50	1.60	1.52
1	B	22	VAL	C-O	-5.50	1.17	1.24
1	A	6	VAL	CA-CB	-5.49	1.47	1.54
1	B	32	THR	C-O	-5.49	1.17	1.24
1	C	172	ARG	N-CA	5.48	1.53	1.46
1	D	78	LEU	CA-C	5.48	1.60	1.52
1	B	304	VAL	CA-CB	5.47	1.61	1.54
1	C	169	GLN	CG-CD	5.47	1.65	1.52
1	A	249	HIS	N-CA	-5.47	1.39	1.46
1	D	268	PRO	C-O	-5.46	1.17	1.24
1	C	55	ASP	N-CA	5.46	1.52	1.46
1	C	67	LEU	CA-C	5.46	1.60	1.53
1	F	209	ILE	CA-CB	5.45	1.61	1.54
1	D	6	VAL	C-O	-5.44	1.17	1.24
1	F	69	SER	C-O	-5.44	1.16	1.24
1	D	1	MET	SD-CE	5.44	1.93	1.79
1	E	351	ALA	CA-CB	-5.44	1.45	1.53
1	F	263	ARG	N-CA	5.43	1.52	1.46
1	D	94	HIS	N-CA	-5.43	1.40	1.46
1	C	342	ALA	CA-CB	5.42	1.62	1.53
1	D	76	PRO	C-O	5.42	1.30	1.23
1	F	168	VAL	CA-CB	5.42	1.61	1.54
1	A	66	ARG	CA-C	-5.42	1.45	1.52
1	D	61	TRP	CA-C	-5.42	1.45	1.52
1	F	190	LEU	CA-C	-5.42	1.45	1.52
1	C	109	PHE	CD2-CE2	5.41	1.54	1.38
1	A	320	ALA	N-CA	5.41	1.50	1.46
1	F	61	TRP	CA-C	5.41	1.59	1.52
1	D	49	TRP	C-O	5.40	1.30	1.23
1	D	317	SER	CA-C	5.40	1.59	1.52
1	C	116	LYS	N-CA	-5.40	1.39	1.46
1	D	129	ARG	N-CA	-5.40	1.41	1.46
1	F	324	VAL	CA-CB	-5.40	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	196	LYS	CD-CE	5.40	1.68	1.52
1	C	112	ALA	N-CA	-5.39	1.39	1.46
1	D	231	LEU	C-O	-5.39	1.17	1.24
1	C	30	TRP	N-CA	-5.39	1.39	1.46
1	A	47	GLY	C-O	5.39	1.31	1.23
1	C	7	PRO	C-O	-5.39	1.17	1.24
1	A	291	VAL	C-O	-5.38	1.18	1.24
1	A	394	TRP	N-CA	-5.37	1.39	1.46
1	D	263	ARG	C-O	-5.37	1.17	1.24
1	E	143	ILE	CA-C	5.37	1.58	1.52
1	C	175	GLY	N-CA	5.37	1.49	1.44
1	E	241	ALA	CA-CB	-5.36	1.45	1.53
1	F	281	VAL	N-CA	5.36	1.52	1.46
1	A	113	LEU	N-CA	-5.35	1.39	1.46
1	C	302	ASP	CA-C	-5.35	1.46	1.52
1	A	342	ALA	CA-CB	5.35	1.62	1.53
1	D	371	LEU	N-CA	-5.35	1.39	1.46
1	B	301	GLY	C-O	5.34	1.30	1.24
1	C	328	ARG	N-CA	5.34	1.52	1.46
1	F	391	PRO	CA-C	5.34	1.58	1.52
1	E	261	ARG	CA-C	5.34	1.59	1.52
1	F	316	ALA	N-CA	5.33	1.53	1.46
1	B	279	PRO	CB-CG	5.32	1.76	1.49
1	E	233	PHE	CA-C	-5.32	1.46	1.52
1	E	296	VAL	C-O	-5.32	1.17	1.24
1	A	175	GLY	N-CA	5.32	1.54	1.45
1	C	270	ALA	C-O	5.32	1.30	1.24
1	B	173	PRO	N-CA	5.31	1.54	1.47
1	A	308	SER	N-CA	-5.31	1.39	1.46
1	A	37	PRO	N-CA	-5.30	1.40	1.47
1	B	209	ILE	CA-CB	-5.30	1.48	1.54
1	A	348	ALA	CA-CB	5.30	1.62	1.53
1	E	18	ASN	CA-CB	5.30	1.59	1.53
1	E	193	PHE	N-CA	5.29	1.52	1.46
1	E	124	LEU	C-O	5.29	1.30	1.24
1	F	308	SER	CA-C	-5.28	1.45	1.52
1	F	305	TYR	C-O	5.28	1.30	1.24
1	D	61	TRP	C-O	-5.28	1.17	1.24
1	D	107	SER	N-CA	5.27	1.52	1.46
1	E	140	PHE	C-O	5.27	1.30	1.24
1	E	314	ASP	C-O	-5.27	1.18	1.24
1	A	347	GLY	C-O	5.26	1.29	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	380	LYS	CA-CB	-5.26	1.44	1.53
1	A	356	ILE	CA-CB	-5.25	1.48	1.54
1	D	372	ALA	N-CA	5.25	1.53	1.46
1	A	270	ALA	CA-C	-5.24	1.45	1.52
1	E	40	VAL	C-O	5.23	1.29	1.24
1	B	81	VAL	CA-C	5.23	1.59	1.52
1	D	308	SER	N-CA	-5.23	1.39	1.46
1	B	272	ASP	C-O	5.23	1.30	1.24
1	B	298	ILE	N-CA	-5.22	1.39	1.46
1	D	30	TRP	N-CA	-5.22	1.39	1.46
1	F	18	ASN	CB-CG	5.21	1.65	1.52
1	B	283	VAL	C-O	5.21	1.29	1.23
1	C	13	ASP	C-N	-5.21	1.25	1.33
1	D	248	LEU	C-O	5.21	1.30	1.24
1	F	22	VAL	CA-CB	5.20	1.61	1.54
1	E	188	ASP	N-CA	5.20	1.52	1.46
1	A	114	GLU	C-O	-5.20	1.17	1.24
1	C	152	LEU	CA-C	5.20	1.59	1.52
1	D	304	VAL	C-O	5.20	1.30	1.24
1	D	40	VAL	CA-CB	5.19	1.62	1.54
1	E	391	PRO	N-CA	5.19	1.53	1.47
1	D	29	ALA	C-O	-5.19	1.18	1.24
1	B	61	TRP	CA-C	-5.18	1.46	1.52
1	A	272	ASP	C-O	5.18	1.30	1.24
1	D	232	LEU	C-O	-5.18	1.18	1.24
1	A	194	ILE	CA-CB	-5.18	1.47	1.54
1	C	376	ALA	CA-CB	5.17	1.61	1.53
1	F	126	GLU	CA-C	5.17	1.59	1.52
1	F	114	GLU	N-CA	5.16	1.53	1.46
1	A	52	ALA	CA-CB	-5.16	1.44	1.53
1	C	304	VAL	C-O	5.16	1.29	1.24
1	D	81	VAL	N-CA	-5.16	1.40	1.46
1	E	370	ALA	N-CA	-5.16	1.38	1.46
1	A	151	THR	N-CA	-5.16	1.39	1.46
1	B	114	GLU	CA-C	-5.16	1.46	1.52
1	C	228	CYS	CA-C	5.16	1.59	1.52
1	B	283	VAL	CA-C	5.15	1.58	1.52
1	B	190	LEU	N-CA	-5.15	1.39	1.46
1	F	111	VAL	CB-CG1	5.13	1.69	1.52
1	C	247	ALA	CA-CB	-5.13	1.45	1.53
1	A	99	THR	CA-CB	-5.12	1.45	1.53
1	F	267	ILE	CA-CB	5.12	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	ALA	CA-C	-5.12	1.46	1.52
1	B	44	ALA	CA-CB	-5.12	1.45	1.53
1	E	355	VAL	CA-CB	5.12	1.60	1.54
1	B	247	ALA	CA-C	5.12	1.59	1.52
1	C	177	MET	N-CA	5.12	1.52	1.46
1	A	109	PHE	CE2-CZ	5.11	1.53	1.38
1	A	281	VAL	CA-CB	5.11	1.61	1.54
1	A	59	GLU	N-CA	-5.10	1.39	1.46
1	C	47	GLY	N-CA	5.10	1.52	1.45
1	E	374	ASP	CA-C	5.10	1.58	1.52
1	F	111	VAL	CA-CB	5.10	1.60	1.54
1	B	2	ILE	CA-C	5.10	1.58	1.52
1	B	94	HIS	CA-C	5.10	1.59	1.52
1	E	179	VAL	CA-CB	5.10	1.60	1.54
1	C	271	ALA	CA-CB	-5.10	1.45	1.53
1	B	242	MET	CA-C	5.09	1.59	1.52
1	D	81	VAL	CA-CB	5.09	1.60	1.54
1	E	263	ARG	CA-CB	5.08	1.58	1.53
1	B	305	TYR	N-CA	5.08	1.52	1.46
1	D	137	VAL	N-CA	-5.08	1.40	1.46
1	B	26	TYR	C-O	-5.08	1.17	1.24
1	B	51	ALA	CA-CB	-5.07	1.44	1.53
1	C	240	ALA	CA-CB	5.06	1.61	1.53
1	A	81	VAL	C-O	-5.06	1.18	1.24
1	C	172	ARG	CA-C	5.06	1.59	1.52
1	A	177	MET	N-CA	5.06	1.52	1.46
1	B	149	PHE	CA-C	5.06	1.59	1.52
1	C	146	LEU	CA-CB	-5.05	1.45	1.53
1	C	69	SER	N-CA	-5.05	1.39	1.46
1	E	259	LEU	CG-CD1	5.04	1.69	1.52
1	C	247	ALA	C-O	5.04	1.29	1.24
1	D	95	LYS	CG-CD	5.04	1.67	1.52
1	C	108	ARG	NE-CZ	5.04	1.38	1.33
1	B	333	ILE	CA-CB	5.04	1.62	1.54
1	C	136	PHE	N-CA	-5.04	1.40	1.46
1	D	40	VAL	CA-C	-5.04	1.46	1.52
1	F	306	LEU	N-CA	5.03	1.52	1.46
1	E	159	ASP	CA-C	-5.03	1.46	1.52
1	D	286	ASN	CA-C	5.03	1.58	1.52
1	B	151	THR	C-O	-5.02	1.17	1.24
1	C	108	ARG	CD-NE	5.02	1.53	1.46
1	F	243	ILE	CA-CB	-5.02	1.48	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	ARG	C-O	5.02	1.30	1.23
1	E	120	VAL	N-CA	5.02	1.52	1.46
1	E	179	VAL	CA-C	5.02	1.58	1.52
1	F	379	MET	CA-C	5.02	1.58	1.52
1	F	178	THR	N-CA	5.02	1.52	1.45
1	B	372	ALA	N-CA	5.01	1.53	1.46
1	C	19	PRO	C-O	-5.00	1.18	1.24

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	MET	N-CA-C	-11.60	99.25	113.41
1	B	6	VAL	N-CA-C	10.56	117.17	107.56
1	F	191	TRP	CA-C-N	-10.34	107.91	119.28
1	F	191	TRP	C-N-CA	-10.34	107.91	119.28
1	E	266	LEU	CA-C-N	9.62	126.30	120.24
1	E	266	LEU	C-N-CA	9.62	126.30	120.24
1	E	198	MET	N-CA-C	-9.35	100.50	112.93
1	A	198	MET	N-CA-C	-9.31	99.51	112.45
1	C	172	ARG	N-CA-C	8.27	128.09	109.81
1	F	154	ASP	N-CA-C	8.27	122.79	111.54
1	A	153	ILE	N-CA-C	-8.14	104.77	112.83
1	F	272	ASP	N-CA-C	-8.06	102.47	111.82
1	A	10	ARG	NE-CZ-NH1	-7.92	113.58	121.50
1	C	32	THR	N-CA-C	-7.92	102.63	111.82
1	A	32	THR	N-CA-C	-7.87	103.13	112.89
1	D	99	THR	CA-C-N	-7.86	111.62	119.56
1	D	99	THR	C-N-CA	-7.86	111.62	119.56
1	A	65	GLU	N-CA-C	7.80	120.68	111.71
1	E	288	VAL	N-CA-C	-7.72	104.84	112.17
1	D	77	GLY	N-CA-C	7.71	125.77	115.59
1	A	19	PRO	CA-C-N	-7.63	111.75	119.99
1	A	19	PRO	C-N-CA	-7.63	111.75	119.99
1	E	191	TRP	CA-C-N	-7.47	110.80	119.32
1	E	191	TRP	C-N-CA	-7.47	110.80	119.32
1	B	18	ASN	CA-C-N	7.45	125.10	119.66
1	B	18	ASN	C-N-CA	7.45	125.10	119.66
1	B	198	MET	N-CA-C	-7.44	102.33	111.40
1	D	198	MET	N-CA-C	-7.37	103.24	112.90
1	D	65	GLU	N-CA-C	7.35	119.08	111.14
1	B	28	ALA	N-CA-C	-7.32	103.24	111.14
1	E	154	ASP	N-CA-C	7.27	121.19	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	212	GLU	N-CA-C	-7.21	100.34	110.29
1	E	159	ASP	N-CA-C	-7.20	102.62	111.40
1	A	246	VAL	N-CA-C	-7.17	103.87	110.82
1	F	209	ILE	N-CA-C	-7.08	103.95	110.82
1	F	186	ALA	N-CA-C	7.08	119.89	111.33
1	C	172	ARG	CA-C-N	7.07	128.68	119.84
1	C	172	ARG	C-N-CA	7.07	128.68	119.84
1	E	388	THR	N-CA-C	-7.05	103.93	114.64
1	E	34	LEU	N-CA-C	-7.00	104.70	113.18
1	A	66	ARG	NE-CZ-NH2	6.98	125.48	119.20
1	A	66	ARG	NE-CZ-NH1	-6.96	114.54	121.50
1	F	320	ALA	CA-C-N	6.92	126.55	119.56
1	F	320	ALA	C-N-CA	6.92	126.55	119.56
1	D	387	CYS	N-CA-C	-6.90	98.36	109.96
1	E	243	ILE	CB-CA-C	-6.86	103.10	111.88
1	C	90	ASP	N-CA-C	6.84	120.27	109.81
1	E	267	ILE	CB-CA-C	-6.83	107.11	114.35
1	D	205	LEU	N-CA-C	6.83	119.59	111.33
1	C	278	TYR	CA-C-N	-6.71	112.74	119.99
1	C	278	TYR	C-N-CA	-6.71	112.74	119.99
1	D	107	SER	N-CA-C	6.62	118.50	111.28
1	A	157	LEU	CA-CB-CG	6.61	139.44	116.30
1	A	270	ALA	N-CA-C	-6.58	103.30	112.45
1	A	191	TRP	CA-CB-CG	-6.57	101.12	113.60
1	A	260	LEU	N-CA-C	6.57	119.44	111.82
1	A	195	GLU	N-CA-C	-6.54	104.07	111.07
1	B	83	GLN	N-CA-C	6.54	120.43	111.54
1	F	5	HIS	N-CA-C	6.47	119.83	112.97
1	C	66	ARG	NE-CZ-NH2	6.42	124.97	119.20
1	D	11	VAL	N-CA-C	6.41	118.03	108.23
1	C	61	TRP	N-CA-C	-6.37	104.44	111.82
1	F	178	THR	N-CA-CB	6.31	119.39	110.36
1	B	298	ILE	N-CA-C	-6.30	101.42	109.30
1	F	13	ASP	N-CA-C	-6.25	104.24	113.61
1	C	10	ARG	NE-CZ-NH1	-6.24	115.27	121.50
1	C	315	PRO	N-CA-C	-6.23	106.07	113.86
1	A	69	SER	N-CA-C	-6.22	103.78	112.25
1	D	221	VAL	N-CA-C	6.22	116.96	110.62
1	E	192	PRO	CA-C-N	6.21	128.85	120.65
1	E	192	PRO	C-N-CA	6.21	128.85	120.65
1	C	65	GLU	N-CA-C	6.20	118.83	111.33
1	F	263	ARG	N-CA-C	6.16	119.65	109.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ALA	N-CA-C	-6.14	102.03	109.83
1	A	149	PHE	N-CA-C	-6.13	103.75	111.11
1	F	288	VAL	N-CA-C	-6.13	105.38	111.88
1	D	166	LEU	N-CA-C	6.12	121.80	113.97
1	E	70	GLN	N-CA-C	6.09	117.61	110.97
1	D	237	ASP	N-CA-C	6.07	118.86	111.82
1	B	18	ASN	O-C-N	6.05	124.90	121.27
1	C	246	VAL	N-CA-C	-6.05	104.95	110.82
1	A	123	LYS	N-CA-C	-6.04	104.61	111.14
1	C	66	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	D	82	MET	N-CA-C	6.02	118.63	111.71
1	E	129	ARG	CA-C-N	6.02	127.36	119.84
1	E	129	ARG	C-N-CA	6.02	127.36	119.84
1	C	153	ILE	N-CA-C	-6.02	105.88	112.80
1	F	199	ALA	N-CA-C	5.99	117.50	110.97
1	C	160	ARG	CA-C-N	-5.98	112.37	119.84
1	C	160	ARG	C-N-CA	-5.98	112.37	119.84
1	E	160	ARG	N-CA-C	5.93	122.92	109.81
1	C	363	LEU	N-CA-C	5.91	119.68	112.23
1	F	243	ILE	CB-CA-C	-5.90	104.17	112.14
1	A	18	ASN	N-CA-CB	5.90	119.12	111.40
1	C	340	VAL	N-CA-C	5.88	116.12	108.35
1	E	58	ARG	N-CA-C	5.87	118.16	111.11
1	A	93	GLU	N-CA-C	-5.87	104.79	111.07
1	C	30	TRP	N-CA-C	-5.86	106.26	113.41
1	F	126	GLU	N-CA-C	5.86	119.25	111.75
1	F	56	VAL	N-CA-C	5.86	116.59	110.62
1	B	6	VAL	CB-CA-C	-5.85	104.16	110.95
1	F	198	MET	N-CA-C	-5.83	103.64	112.04
1	E	220	THR	N-CA-CB	5.83	119.15	110.29
1	C	194	ILE	N-CA-C	5.79	117.22	110.62
1	A	174	ASP	CA-C-N	5.79	132.12	121.70
1	A	174	ASP	C-N-CA	5.79	132.12	121.70
1	B	205	LEU	N-CA-C	5.78	117.58	111.28
1	C	228	CYS	N-CA-C	5.78	118.04	111.11
1	C	2	ILE	N-CA-CB	-5.78	103.12	111.21
1	D	314	ASP	CA-C-N	5.76	125.38	119.56
1	D	314	ASP	C-N-CA	5.76	125.38	119.56
1	B	172	ARG	N-CA-C	5.76	122.54	109.81
1	E	75	THR	CA-C-N	-5.75	112.66	119.84
1	E	75	THR	C-N-CA	-5.75	112.66	119.84
1	F	73	ALA	N-CA-C	5.75	118.60	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	88	GLN	N-CA-C	5.74	120.40	113.17
1	A	166	LEU	CA-C-N	5.73	127.49	120.22
1	A	166	LEU	C-N-CA	5.73	127.49	120.22
1	C	283	VAL	N-CA-C	5.72	117.09	108.96
1	B	189	TYR	N-CA-C	5.70	118.23	111.33
1	E	126	GLU	N-CA-C	5.67	117.46	111.28
1	E	220	THR	N-CA-C	-5.65	102.11	110.48
1	E	323	GLU	N-CA-C	5.65	117.29	109.15
1	B	107	SER	N-CA-C	5.62	118.34	111.82
1	C	387	CYS	N-CA-C	-5.62	102.16	110.48
1	C	277	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	B	57	VAL	CB-CA-C	-5.61	102.09	111.29
1	D	349	GLY	CA-C-O	-5.61	115.28	121.05
1	C	270	ALA	N-CA-C	-5.60	104.67	112.45
1	B	208	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	F	265	ASP	N-CA-C	-5.59	105.96	112.89
1	A	328	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	E	369	PHE	N-CA-C	5.52	118.46	109.24
1	C	191	TRP	CA-CB-CG	-5.51	103.14	113.60
1	B	252	ARG	N-CA-C	-5.50	106.56	113.28
1	A	90	ASP	N-CA-C	5.50	118.23	110.14
1	D	315	PRO	N-CA-C	-5.50	106.98	113.86
1	A	388	THR	N-CA-C	-5.50	106.57	113.72
1	A	174	ASP	N-CA-C	5.48	122.47	110.80
1	F	258	ARG	N-CA-C	-5.45	104.37	111.02
1	B	340	VAL	N-CA-C	5.45	116.21	108.42
1	E	320	ALA	CA-C-N	5.45	125.09	119.05
1	E	320	ALA	C-N-CA	5.45	125.09	119.05
1	E	129	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	A	243	ILE	N-CA-C	-5.44	105.08	110.62
1	E	178	THR	CA-C-N	5.43	127.61	120.60
1	E	178	THR	C-N-CA	5.43	127.61	120.60
1	E	78	LEU	CA-CB-CG	5.42	135.26	116.30
1	C	19	PRO	CA-C-N	-5.41	112.95	120.25
1	C	19	PRO	C-N-CA	-5.41	112.95	120.25
1	F	237	ASP	CB-CA-C	5.40	120.69	109.95
1	F	60	LEU	N-CA-C	5.40	118.66	111.75
1	A	277	ARG	NE-CZ-NH2	5.39	124.06	119.20
1	C	204	ASP	N-CA-C	5.39	116.88	110.19
1	B	34	LEU	N-CA-C	-5.38	105.85	112.90
1	C	197	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	D	346	VAL	N-CA-CB	5.38	117.19	110.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ALA	N-CA-C	-5.38	105.11	110.97
1	B	208	ARG	CA-C-N	-5.37	113.68	120.56
1	B	208	ARG	C-N-CA	-5.37	113.68	120.56
1	F	11	VAL	N-CA-C	5.37	116.51	109.21
1	A	180	GLU	N-CA-C	5.37	116.81	111.07
1	F	120	VAL	N-CA-CB	5.36	116.46	110.51
1	B	344	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	C	361	GLU	N-CA-C	5.34	117.11	111.28
1	C	93	GLU	N-CA-C	-5.33	105.37	111.07
1	F	26	TYR	CA-C-N	5.32	127.68	120.44
1	F	26	TYR	C-N-CA	5.32	127.68	120.44
1	F	372	ALA	CA-C-N	5.31	126.48	119.84
1	F	372	ALA	C-N-CA	5.31	126.48	119.84
1	F	384	VAL	CA-C-N	-5.31	115.29	120.34
1	F	384	VAL	C-N-CA	-5.31	115.29	120.34
1	F	374	ASP	CA-C-N	5.29	128.22	120.71
1	F	374	ASP	C-N-CA	5.29	128.22	120.71
1	C	122	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	D	90	ASP	N-CA-C	5.27	118.15	109.72
1	F	276	ARG	CB-CG-CD	5.27	123.41	111.30
1	C	122	ARG	N-CA-C	5.26	116.70	111.07
1	D	195	GLU	CA-C-N	5.25	127.31	120.28
1	D	195	GLU	C-N-CA	5.25	127.31	120.28
1	D	157	LEU	N-CA-C	5.25	117.00	111.28
1	F	335	HIS	N-CA-C	-5.25	101.67	109.96
1	F	118	GLN	N-CA-C	-5.24	105.62	112.23
1	E	110	VAL	N-CA-C	-5.24	105.28	110.62
1	A	95	LYS	N-CA-C	5.23	117.66	111.33
1	C	12	VAL	CA-C-N	-5.23	114.35	122.67
1	C	12	VAL	C-N-CA	-5.23	114.35	122.67
1	C	40	VAL	N-CA-C	5.23	116.23	108.65
1	E	278	TYR	N-CA-C	5.23	118.15	109.79
1	C	374	ASP	N-CA-CB	-5.22	103.97	111.54
1	A	107	SER	N-CA-C	5.22	119.98	111.37
1	E	89	GLN	N-CA-CB	-5.21	102.13	110.63
1	C	144	LEU	CA-C-N	-5.19	113.29	119.05
1	C	144	LEU	C-N-CA	-5.19	113.29	119.05
1	C	245	MET	N-CA-C	-5.18	106.46	112.89
1	A	172	ARG	CA-C-N	5.17	126.30	119.84
1	A	172	ARG	C-N-CA	5.17	126.30	119.84
1	E	263	ARG	N-CA-C	5.16	118.36	108.97
1	B	294	ASP	N-CA-C	-5.16	104.53	111.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	TYR	CA-C-N	-5.15	113.30	120.25
1	A	278	TYR	C-N-CA	-5.15	113.30	120.25
1	C	232	LEU	N-CA-C	-5.15	105.36	110.97
1	C	239	VAL	N-CA-C	5.14	115.36	110.42
1	B	299	ARG	N-CA-C	5.14	118.13	110.52
1	B	66	ARG	NE-CZ-NH1	-5.13	116.36	121.50
1	E	363	LEU	N-CA-C	5.13	116.56	111.07
1	F	266	LEU	N-CA-CB	-5.13	102.60	110.44
1	D	100	PRO	N-CA-C	-5.12	107.46	113.86
1	B	243	ILE	N-CA-C	-5.10	105.42	110.62
1	C	9	ASP	N-CA-C	-5.10	105.80	111.36
1	B	116	LYS	N-CA-C	-5.10	105.64	111.14
1	F	388	THR	N-CA-C	-5.09	107.02	114.39
1	E	13	ASP	N-CA-C	-5.08	105.77	112.94
1	B	285	ARG	N-CA-CB	-5.08	102.97	111.20
1	A	210	LEU	O-C-N	-5.08	116.28	122.22
1	F	116	LYS	N-CA-C	5.08	117.71	111.82
1	D	119	ALA	N-CA-C	-5.07	106.35	112.54
1	A	335	HIS	CA-C-O	-5.06	115.71	121.68
1	C	119	ALA	N-CA-C	-5.05	105.90	111.71
1	E	250	LEU	CA-C-N	5.05	127.01	120.44
1	E	250	LEU	C-N-CA	5.05	127.01	120.44
1	C	1	MET	CG-SD-CE	5.05	112.01	100.90
1	D	181	GLN	N-CA-C	-5.04	106.29	112.90
1	D	192	PRO	CA-C-N	5.04	126.99	120.44
1	D	192	PRO	C-N-CA	5.04	126.99	120.44
1	D	56	VAL	N-CA-C	-5.04	105.68	110.42
1	B	337	THR	CA-C-N	-5.03	114.67	122.67
1	B	337	THR	C-N-CA	-5.03	114.67	122.67
1	F	367	PRO	N-CA-C	-5.03	102.11	112.47
1	B	155	VAL	CA-C-N	-5.01	114.75	119.76
1	B	155	VAL	C-N-CA	-5.01	114.75	119.76
1	B	300	LYS	N-CA-C	-5.01	102.87	110.24
1	F	324	VAL	CB-CA-C	-5.01	104.88	111.25
1	C	206	PHE	N-CA-C	-5.01	105.90	111.36
1	B	11	VAL	CB-CA-C	-5.00	105.83	111.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	172	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	171	THR	Peptide
1	C	172	ARG	Peptide
1	F	197	ARG	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	3068	0	3088	104	0
1	B	3068	0	3088	123	1
1	C	3068	0	3088	108	0
1	D	3053	0	3076	107	1
1	E	3025	0	3048	146	0
1	F	3025	0	3048	133	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
2	E	43	0	30	3	0
2	F	43	0	30	6	0
3	A	14	0	20	2	0
3	B	14	0	20	5	0
3	C	14	0	20	2	0
4	A	51	0	0	0	0
4	B	62	0	0	6	0
4	C	64	0	0	5	0
4	D	52	0	0	6	0
4	E	41	0	0	4	0
4	F	40	0	0	3	0
All	All	18917	0	18676	720	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 19.

All (720) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PRO:CG	1:B:279:PRO:CB	1.76	1.32
1:B:245:MET:HE3	1:B:245:MET:HA	1.23	1.12
1:C:172:ARG:HH22	1:C:237:ASP:HB3	1.03	1.12
1:C:257:GLN:HE21	1:C:261:ARG:NH2	1.46	1.11
1:A:172:ARG:NH1	1:A:237:ASP:HB3	1.66	1.09
1:B:172:ARG:NH2	1:B:237:ASP:HB3	1.65	1.09
1:B:172:ARG:C	1:B:174:ASP:H	1.57	1.08
1:C:172:ARG:NH2	1:C:237:ASP:HB3	1.70	1.06
1:B:53:ARG:HD2	1:B:55:ASP:OD1	1.55	1.05
1:A:172:ARG:H	1:A:173:PRO:CD	1.71	1.03
1:A:257:GLN:HE21	1:A:261:ARG:HH22	1.04	1.02
1:B:245:MET:HE3	1:B:245:MET:CA	1.90	0.98
1:A:153:ILE:O	1:A:197:ARG:NH1	1.97	0.97
1:C:84:PHE:H	1:C:88:GLN:NE2	1.64	0.95
1:E:232:LEU:O	1:E:236:LEU:HG	1.68	0.94
1:E:124:LEU:O	1:E:127:SER:HB3	1.68	0.92
1:B:172:ARG:HH22	1:B:237:ASP:HB3	1.22	0.92
1:F:204:ASP:O	1:F:208:ARG:HG3	1.70	0.92
1:A:257:GLN:HE21	1:A:261:ARG:NH2	1.68	0.91
1:C:153:ILE:O	1:C:197:ARG:NH1	2.02	0.91
1:D:53:ARG:HD2	1:D:55:ASP:OD1	1.73	0.89
1:D:245:MET:HE3	1:D:245:MET:HA	1.54	0.89
1:A:197:ARG:HG2	1:A:207:SER:OG	1.72	0.89
1:C:257:GLN:HE21	1:C:261:ARG:HH22	1.19	0.89
1:C:199:ALA:O	1:C:201:PRO:HD3	1.72	0.89
1:E:338:MET:HE2	1:E:348:ALA:HA	1.57	0.87
1:E:162:ARG:HG2	1:E:166:LEU:HD22	1.54	0.86
1:C:318:PHE:O	1:C:321:PRO:HD3	1.75	0.86
1:B:82:MET:O	1:B:229:ARG:NH1	2.09	0.85
1:B:245:MET:HA	1:B:245:MET:CE	2.05	0.85
1:F:196:LYS:O	1:F:200:GLN:N	2.09	0.85
1:B:153:ILE:O	1:B:197:ARG:NH1	2.09	0.85
1:E:196:LYS:O	1:E:200:GLN:N	2.11	0.84
1:A:169:GLN:O	1:A:170:LEU:HB3	1.78	0.83
1:B:84:PHE:H	1:B:88:GLN:NE2	1.77	0.83
1:C:118:GLN:HG3	1:C:357:VAL:HG13	1.59	0.82
1:D:84:PHE:H	1:D:88:GLN:NE2	1.78	0.82
1:F:3:PRO:O	1:F:5:HIS:N	2.13	0.81
1:B:309:VAL:CG2	1:B:313:LEU:HD12	2.10	0.81
1:E:279:PRO:HG2	1:E:309:VAL:HA	1.62	0.80
1:C:1:MET:HE2	1:C:1:MET:HA	1.63	0.80
1:E:99:THR:HB	1:E:100:PRO:HD3	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLN:HE21	1:B:261:ARG:NH2	1.80	0.80
1:D:84:PHE:H	1:D:88:GLN:HE21	1.25	0.80
1:E:362:TRP:O	1:E:366:MET:HB2	1.83	0.78
1:F:12:VAL:O	1:F:42:SER:HA	1.83	0.78
1:A:172:ARG:NH1	1:A:237:ASP:CB	2.45	0.77
1:E:1:MET:HE2	1:E:1:MET:N	1.99	0.77
1:F:323:GLU:OE1	1:F:325:ARG:HD3	1.84	0.77
1:D:290:ASP:O	1:E:395:ARG:NH1	2.18	0.77
1:B:172:ARG:C	1:B:174:ASP:N	2.34	0.76
2:D:417:HEM:CMB	2:D:417:HEM:HBB2	2.16	0.76
1:C:191:TRP:NE1	1:C:195:GLU:OE2	2.18	0.76
1:E:1:MET:HE2	1:E:1:MET:H1	1.50	0.76
1:E:157:LEU:HA	1:E:160:ARG:HD2	1.68	0.76
1:B:194:ILE:O	1:B:198:MET:HG3	1.85	0.76
1:E:40:VAL:HG22	1:E:50:ILE:HB	1.67	0.75
1:D:309:VAL:HG13	1:D:310:LEU:HD13	1.69	0.75
1:E:311:HIS:CD2	1:E:336:THR:OG1	2.40	0.75
1:C:257:GLN:HE21	1:C:261:ARG:HH21	1.35	0.74
1:F:232:LEU:O	1:F:236:LEU:HG	1.87	0.74
1:B:84:PHE:H	1:B:88:GLN:HE21	1.33	0.74
1:B:245:MET:HE1	1:B:248:LEU:HD23	1.70	0.74
1:B:362:TRP:CH2	1:B:366:MET:HE2	2.23	0.74
1:B:61:TRP:HB3	1:B:340:VAL:HG13	1.68	0.74
1:F:135:ASP:HB3	4:F:397:HOH:O	1.85	0.73
1:E:196:LYS:HE2	1:E:200:GLN:HB2	1.70	0.73
1:A:172:ARG:H	1:A:173:PRO:HD2	1.51	0.73
1:D:118:GLN:HG3	1:D:357:VAL:HG13	1.68	0.73
1:E:165:GLN:O	1:E:168:VAL:HG23	1.88	0.73
1:F:132:GLY:CA	1:F:396:ALA:HB2	2.18	0.73
1:E:6:VAL:HG11	1:E:41:TRP:HB3	1.70	0.73
1:C:171:THR:O	1:C:171:THR:CG2	2.36	0.73
1:A:172:ARG:HH12	1:A:237:ASP:CB	2.02	0.73
1:F:54:GLY:HA2	1:F:311:HIS:HA	1.70	0.73
1:E:98:ARG:NH1	1:E:346:VAL:CG1	2.52	0.72
1:A:172:ARG:HH22	1:A:237:ASP:HA	1.54	0.72
1:B:118:GLN:HG3	1:B:357:VAL:HG13	1.72	0.72
1:B:245:MET:CA	1:B:245:MET:CE	2.67	0.71
1:C:122:ARG:HG3	1:C:361:GLU:OE2	1.90	0.71
1:F:53:ARG:HH22	1:F:294:ASP:CG	1.97	0.71
1:A:366:MET:HG3	1:A:367:PRO:HD2	1.72	0.71
1:F:132:GLY:HA3	1:F:396:ALA:HB2	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLU:O	1:A:264:PRO:HD3	1.92	0.70
1:A:311:HIS:HD2	1:A:336:THR:OG1	1.75	0.69
1:E:367:PRO:HG2	1:E:394:TRP:HB2	1.74	0.69
1:B:85:ILE:C	1:B:230:ASN:HD22	2.00	0.69
1:F:311:HIS:CD2	1:F:336:THR:OG1	2.45	0.69
1:A:172:ARG:H	1:A:173:PRO:HD3	1.54	0.69
1:F:33:LEU:C	1:F:35:ASP:H	2.00	0.69
1:D:102:MET:CG	4:D:414:HOH:O	2.40	0.69
1:F:156:PRO:HG2	1:F:159:ASP:OD2	1.92	0.69
1:D:78:LEU:HG	1:D:179:VAL:HG21	1.75	0.69
1:A:1:MET:C	1:A:2:ILE:HD13	2.18	0.69
1:E:89:GLN:NE2	1:E:93:GLU:HG2	2.08	0.68
1:D:6:VAL:O	1:D:6:VAL:HG12	1.89	0.68
1:D:85:ILE:C	1:D:230:ASN:HD22	2.01	0.68
1:F:183:LYS:HD3	1:F:183:LYS:C	2.18	0.68
1:A:78:LEU:HG	1:A:179:VAL:HG21	1.74	0.68
1:A:290:ASP:OD1	1:A:300:LYS:HG2	1.93	0.68
1:A:169:GLN:O	1:A:170:LEU:CB	2.41	0.68
1:D:257:GLN:HE21	1:D:261:ARG:NH2	1.92	0.68
1:F:235:GLY:O	1:F:239:VAL:HG23	1.94	0.68
1:A:172:ARG:HH12	1:A:237:ASP:HB3	1.54	0.68
1:F:276:ARG:HD3	1:F:330:LEU:HD12	1.76	0.67
1:B:108:ARG:NH2	1:F:31:LYS:HE2	2.09	0.67
1:E:1:MET:H1	1:E:1:MET:CE	2.07	0.67
1:E:155:VAL:CG2	1:E:160:ARG:HG2	2.24	0.67
1:A:172:ARG:N	1:A:173:PRO:CD	2.49	0.67
1:E:12:VAL:O	1:E:42:SER:HA	1.94	0.67
1:C:171:THR:O	1:C:171:THR:HG22	1.95	0.67
1:E:196:LYS:HE2	1:E:200:GLN:CB	2.25	0.66
1:F:98:ARG:NH1	1:F:346:VAL:HG12	2.11	0.66
1:B:87:LEU:H	1:B:230:ASN:ND2	1.92	0.66
1:D:169:GLN:CD	1:D:169:GLN:H	2.02	0.66
1:E:263:ARG:HB3	1:E:266:LEU:HD23	1.78	0.66
1:F:124:LEU:HD21	1:F:143:ILE:HG22	1.77	0.66
1:B:63:ASP:OD2	1:B:66:ARG:HB2	1.95	0.66
1:D:362:TRP:CH2	1:D:366:MET:HE2	2.30	0.66
1:A:122:ARG:HG3	1:A:361:GLU:OE2	1.95	0.65
1:D:257:GLN:HE21	1:D:261:ARG:HH21	1.43	0.65
1:F:71:CYS:O	1:F:73:ALA:N	2.29	0.65
1:A:85:ILE:C	1:A:230:ASN:HD22	2.04	0.65
1:D:24:GLN:OE1	4:D:434:HOH:O	2.13	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:HIS:HD2	1:E:336:THR:OG1	1.79	0.65
1:F:151:THR:HA	1:F:160:ARG:HH22	1.62	0.65
1:E:162:ARG:CG	1:E:166:LEU:HD22	2.26	0.65
1:F:106:ALA:HB1	1:F:108:ARG:HH21	1.60	0.65
1:F:374:ASP:OD2	1:F:374:ASP:N	2.29	0.65
1:C:114:GLU:HB3	1:C:115:PRO:HD3	1.78	0.65
1:D:178:THR:HG22	1:D:181:GLN:OE1	1.96	0.65
1:E:95:LYS:HZ2	1:E:95:LYS:HB2	1.61	0.65
1:A:356:ILE:HG22	1:A:357:VAL:N	2.11	0.65
1:F:338:MET:HE2	1:F:348:ALA:HA	1.77	0.65
1:D:16:ILE:HD12	1:D:305:TYR:CZ	2.31	0.65
1:F:3:PRO:C	1:F:5:HIS:H	2.05	0.65
1:D:61:TRP:HB3	1:D:340:VAL:HG13	1.79	0.64
1:D:102:MET:HG2	4:D:414:HOH:O	1.95	0.64
1:D:338:MET:HE2	1:D:348:ALA:HA	1.78	0.64
1:D:344:ARG:O	1:D:345:CYS:C	2.41	0.64
1:D:98:ARG:NH2	1:D:344:ARG:O	2.27	0.64
1:F:87:LEU:H	1:F:230:ASN:HD21	1.46	0.64
1:B:78:LEU:HG	1:B:179:VAL:HG21	1.80	0.64
1:A:311:HIS:CD2	1:A:336:THR:OG1	2.51	0.64
1:A:227:MET:HE3	1:A:228:CYS:N	2.13	0.63
1:C:257:GLN:NE2	1:C:261:ARG:HH22	1.91	0.63
1:D:166:LEU:N	1:D:167:GLY:HA3	2.13	0.63
1:C:257:GLN:NE2	1:C:261:ARG:NH2	2.32	0.63
1:B:309:VAL:HG23	1:B:313:LEU:HD12	1.79	0.63
1:A:172:ARG:NH2	1:A:237:ASP:HA	2.13	0.63
1:C:117:VAL:HG13	1:C:148:ILE:HG12	1.79	0.63
1:C:312:ASN:C	1:C:313:LEU:HD23	2.23	0.63
1:D:165:GLN:O	1:D:169:GLN:NE2	2.32	0.63
2:D:417:HEM:HBB2	2:D:417:HEM:HMB1	1.80	0.63
1:E:98:ARG:NH1	1:E:346:VAL:HG13	2.13	0.63
1:F:24:GLN:H	1:F:24:GLN:CD	2.06	0.63
1:E:135:ASP:HB3	4:E:401:HOH:O	1.97	0.63
1:F:52:ALA:HA	1:F:310:LEU:HD23	1.79	0.63
1:C:84:PHE:HB2	1:C:88:GLN:HE21	1.63	0.63
1:E:98:ARG:HH12	1:E:346:VAL:CG1	2.12	0.63
1:E:194:ILE:O	1:E:196:LYS:N	2.32	0.63
1:F:32:THR:O	1:F:35:ASP:HB2	1.98	0.63
1:F:350:LEU:HD12	1:F:354:GLU:HG3	1.79	0.62
1:C:89:GLN:NE2	1:C:93:GLU:OE1	2.29	0.62
1:A:205:LEU:HD21	1:A:231:LEU:HD13	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:MET:HE2	1:B:348:ALA:HA	1.81	0.62
1:E:320:ALA:O	1:E:323:GLU:HB2	2.00	0.62
1:A:172:ARG:N	1:A:173:PRO:HD2	2.13	0.62
1:B:146:LEU:HD12	1:B:236:LEU:HD21	1.82	0.62
1:E:98:ARG:NH1	1:E:346:VAL:HG12	2.15	0.61
1:F:3:PRO:HB2	1:F:5:HIS:CD2	2.34	0.61
1:B:108:ARG:N	1:F:35:ASP:OD1	2.32	0.61
1:C:118:GLN:HA	1:C:357:VAL:CG1	2.30	0.61
1:E:40:VAL:CG2	1:E:50:ILE:HB	2.31	0.61
1:A:84:PHE:H	1:A:88:GLN:NE2	1.98	0.61
1:E:89:GLN:HE22	1:E:93:GLU:HG2	1.65	0.61
1:E:108:ARG:HB3	1:E:108:ARG:CZ	2.30	0.61
1:F:117:VAL:HG12	1:F:357:VAL:HG11	1.81	0.61
1:B:257:GLN:HE21	1:B:261:ARG:HH21	1.47	0.61
1:C:1:MET:HA	1:C:1:MET:CE	2.30	0.61
1:E:377:VAL:HG13	1:E:390:LEU:HD13	1.83	0.61
1:A:353:MET:O	1:A:354:GLU:C	2.44	0.60
1:E:263:ARG:HD3	1:E:266:LEU:CD2	2.30	0.60
1:F:6:VAL:HG11	1:F:41:TRP:CB	2.31	0.60
1:A:164:ARG:O	1:A:168:VAL:HG23	2.01	0.60
1:B:277:ARG:O	1:B:277:ARG:NH1	2.35	0.60
1:C:362:TRP:O	1:C:366:MET:HB2	2.02	0.60
1:B:141:ALA:O	1:B:145:PRO:CD	2.49	0.60
3:B:397:ID3:H8	3:B:397:ID3:H17	1.82	0.60
1:E:85:ILE:C	1:E:230:ASN:HD22	2.08	0.60
1:A:102:MET:HG3	1:A:346:VAL:HG12	1.83	0.60
1:E:53:ARG:NH2	1:E:294:ASP:OD1	2.28	0.60
1:F:84:PHE:HE1	1:F:229:ARG:HG2	1.67	0.60
1:B:196:LYS:NZ	1:B:197:ARG:HH21	2.00	0.60
1:B:108:ARG:HH22	1:F:31:LYS:HE2	1.66	0.60
1:E:14:PHE:CD1	1:E:33:LEU:HD21	2.36	0.60
1:A:16:ILE:HD11	1:A:74:VAL:HG21	1.83	0.59
1:A:227:MET:CE	1:A:228:CYS:SG	2.90	0.59
1:E:118:GLN:HG3	1:E:361:GLU:HG2	1.83	0.59
1:F:6:VAL:HG11	1:F:41:TRP:HB3	1.82	0.59
1:F:124:LEU:O	1:F:127:SER:HB3	2.02	0.59
1:B:171:THR:O	1:B:173:PRO:CD	2.50	0.59
1:F:367:PRO:HG2	1:F:394:TRP:HB2	1.84	0.59
1:B:135:ASP:HB3	4:B:445:HOH:O	2.03	0.59
1:D:319:GLU:O	1:D:320:ALA:C	2.45	0.59
1:D:117:VAL:HG13	1:D:148:ILE:HG12	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:O	1:A:345:CYS:C	2.45	0.59
1:D:169:GLN:CD	1:D:169:GLN:N	2.60	0.59
1:B:383:ASN:HB2	3:B:397:ID3:H17B	1.84	0.58
1:C:338:MET:HE2	1:C:348:ALA:HA	1.85	0.58
1:F:85:ILE:C	1:F:230:ASN:HD22	2.11	0.58
1:D:102:MET:HG3	4:D:414:HOH:O	2.03	0.58
1:C:311:HIS:CD2	1:C:336:THR:OG1	2.57	0.58
1:F:56:VAL:HG12	1:F:60:LEU:HD22	1.86	0.58
1:F:13:ASP:O	1:F:44:ALA:HB2	2.04	0.58
1:F:392:LEU:HB2	1:F:394:TRP:HZ3	1.69	0.58
1:B:319:GLU:O	1:B:320:ALA:C	2.44	0.57
1:B:109:PHE:HB2	1:B:208:ARG:NH2	2.19	0.57
1:C:12:VAL:O	1:C:42:SER:HA	2.04	0.57
1:E:196:LYS:HG3	1:E:200:GLN:HB2	1.86	0.57
1:D:129:ARG:HB3	1:D:130:PRO:HD3	1.87	0.57
1:B:61:TRP:HB3	1:B:340:VAL:CG1	2.34	0.57
1:E:95:LYS:HB2	1:E:95:LYS:NZ	2.19	0.57
1:E:97:PHE:CZ	1:E:223:GLU:HG2	2.40	0.57
1:F:259:LEU:O	1:F:263:ARG:HB2	2.05	0.57
1:C:198:MET:HG3	1:C:210:LEU:HD13	1.87	0.57
1:E:99:THR:HB	1:E:100:PRO:CD	2.33	0.57
1:F:30:TRP:HB3	1:F:310:LEU:CD1	2.35	0.57
1:A:78:LEU:HG	1:A:179:VAL:CG2	2.35	0.57
1:F:68:SER:OG	1:F:70:GLN:HB2	2.05	0.57
1:B:311:HIS:CD2	1:B:336:THR:OG1	2.58	0.56
1:C:344:ARG:O	1:C:345:CYS:C	2.48	0.56
1:D:48:HIS:HD2	1:D:49:TRP:O	1.87	0.56
1:E:120:VAL:O	1:E:121:ALA:C	2.46	0.56
1:E:98:ARG:HH11	1:E:98:ARG:HG2	1.69	0.56
1:F:56:VAL:O	1:F:60:LEU:HB2	2.05	0.56
1:A:257:GLN:NE2	1:A:261:ARG:NH2	2.46	0.56
1:B:172:ARG:O	1:B:174:ASP:N	2.34	0.56
1:F:48:HIS:HD2	1:F:49:TRP:O	1.88	0.56
1:F:311:HIS:HD2	1:F:336:THR:OG1	1.87	0.56
1:B:206:PHE:O	1:B:210:LEU:HD12	2.06	0.56
1:B:102:MET:CG	4:B:425:HOH:O	2.54	0.56
1:F:344:ARG:O	1:F:345:CYS:C	2.48	0.56
1:F:3:PRO:C	1:F:5:HIS:N	2.63	0.56
1:F:343:HIS:O	2:F:417:HEM:HAA2	2.06	0.56
1:C:84:PHE:H	1:C:88:GLN:HE21	1.52	0.55
1:E:190:LEU:O	1:E:194:ILE:HG13	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:MET:HE1	1:A:228:CYS:SG	2.46	0.55
1:C:172:ARG:HD2	1:C:173:PRO:N	2.21	0.55
1:D:53:ARG:HH11	1:D:55:ASP:CG	2.13	0.55
1:A:49:TRP:NE1	1:A:298:ILE:HG23	2.20	0.55
1:A:94:HIS:HE1	2:A:417:HEM:O2D	1.89	0.55
1:D:66:ARG:O	1:D:67:LEU:HD23	2.05	0.55
1:E:72:LEU:HD22	1:E:88:GLN:NE2	2.21	0.55
1:A:118:GLN:HA	1:A:357:VAL:CG1	2.37	0.55
1:B:311:HIS:HD2	1:B:336:THR:OG1	1.90	0.55
1:E:10:ARG:HD2	1:E:39:LEU:O	2.07	0.55
1:C:87:LEU:O	1:C:87:LEU:HG	2.07	0.55
1:E:113:LEU:HD13	1:E:152:LEU:CD2	2.37	0.55
1:E:133:SER:O	1:E:134:CYS:HB3	2.07	0.55
1:F:136:PHE:CD1	1:F:392:LEU:HD11	2.42	0.55
1:F:106:ALA:HB1	1:F:108:ARG:NH2	2.21	0.55
1:B:374:ASP:CG	1:B:374:ASP:O	2.49	0.55
1:C:163:LEU:HD22	1:C:193:PHE:HZ	1.72	0.55
1:F:16:ILE:C	1:F:16:ILE:HD12	2.32	0.55
4:B:439:HOH:O	1:D:5:HIS:HD2	1.90	0.54
1:C:295:GLY:O	1:C:296:VAL:CG1	2.55	0.54
1:D:66:ARG:HH11	1:E:395:ARG:HD2	1.72	0.54
1:E:28:ALA:O	1:E:32:THR:HG23	2.06	0.54
1:A:117:VAL:HG13	1:A:148:ILE:HG12	1.88	0.54
1:F:108:ARG:HH11	1:F:108:ARG:HB3	1.72	0.54
1:B:248:LEU:HD11	1:B:252:ARG:NH1	2.23	0.54
1:E:87:LEU:H	1:E:230:ASN:HD21	1.53	0.54
1:F:209:ILE:O	1:F:212:GLU:HB2	2.08	0.54
1:C:118:GLN:HA	1:C:357:VAL:HG13	1.88	0.54
1:F:72:LEU:HD22	1:F:88:GLN:NE2	2.23	0.54
1:D:207:SER:O	1:D:208:ARG:C	2.49	0.54
1:F:124:LEU:HD21	1:F:143:ILE:CG2	2.37	0.54
1:C:263:ARG:HD3	1:C:265:ASP:OD1	2.08	0.54
1:E:263:ARG:HD3	1:E:266:LEU:HD23	1.89	0.54
1:E:113:LEU:HD13	1:E:152:LEU:HD22	1.90	0.54
1:F:273:GLU:CD	1:F:276:ARG:HH21	2.15	0.54
1:A:2:ILE:HD13	1:A:2:ILE:N	2.23	0.53
1:D:178:THR:HG22	1:D:181:GLN:CD	2.33	0.53
1:D:362:TRP:O	1:D:366:MET:HB2	2.08	0.53
1:D:85:ILE:HD11	1:D:226:ARG:CZ	2.38	0.53
1:E:161:PRO:O	1:E:165:GLN:HG3	2.08	0.53
1:F:124:LEU:HA	1:F:127:SER:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:O	1:B:54:GLY:C	2.51	0.53
1:D:82:MET:HE1	1:D:182:LEU:HD23	1.91	0.53
2:D:417:HEM:HMB1	2:D:417:HEM:CBB	2.38	0.53
1:C:163:LEU:HD22	1:C:193:PHE:CZ	2.44	0.53
1:B:144:LEU:HB3	1:B:145:PRO:HD3	1.90	0.53
1:F:255:GLU:OE1	1:F:255:GLU:N	2.28	0.53
1:B:27:PHE:O	1:B:31:LYS:HG3	2.08	0.53
1:E:94:HIS:HE1	2:E:417:HEM:O2D	1.91	0.53
1:A:172:ARG:CZ	1:A:237:ASP:HB3	2.35	0.53
1:C:153:ILE:C	1:C:197:ARG:HH12	2.14	0.53
1:D:239:VAL:O	1:D:243:ILE:HG12	2.09	0.52
1:B:82:MET:CE	1:B:182:LEU:HD23	2.39	0.52
1:C:172:ARG:HH22	1:C:237:ASP:CB	1.97	0.52
1:C:242:MET:HB2	4:C:431:HOH:O	2.10	0.52
1:D:12:VAL:O	1:D:42:SER:HA	2.08	0.52
1:A:277:ARG:NH2	1:A:322:GLU:HG2	2.25	0.52
1:E:53:ARG:HD2	1:E:55:ASP:OD1	2.08	0.52
1:E:52:ALA:HA	1:E:310:LEU:HD23	1.90	0.52
1:E:149:PHE:HZ	1:E:190:LEU:HD21	1.75	0.52
1:E:243:ILE:HG22	1:E:244:GLY:N	2.25	0.52
1:E:277:ARG:O	1:E:313:LEU:HD21	2.09	0.52
1:B:13:ASP:OD2	1:B:13:ASP:N	2.43	0.52
1:C:61:TRP:CG	1:C:340:VAL:HG13	2.45	0.52
1:C:272:ASP:OD1	1:C:352:ARG:NE	2.39	0.52
1:E:133:SER:HB2	1:E:393:VAL:HG12	1.92	0.52
1:B:61:TRP:CG	1:B:340:VAL:HG13	2.45	0.52
1:B:197:ARG:HG2	1:B:207:SER:OG	2.10	0.52
1:C:85:ILE:C	1:C:230:ASN:HD22	2.18	0.52
1:F:190:LEU:HB3	1:F:194:ILE:HD11	1.92	0.52
1:A:170:LEU:C	1:A:172:ARG:HA	2.35	0.51
1:B:309:VAL:HG23	1:B:313:LEU:CD1	2.39	0.51
1:E:151:THR:HA	1:E:160:ARG:HH22	1.75	0.51
1:B:61:TRP:CB	1:B:340:VAL:HG13	2.39	0.51
1:E:98:ARG:HH12	1:E:346:VAL:HG12	1.70	0.51
1:B:58:ARG:HD2	1:B:340:VAL:HG21	1.93	0.51
1:B:164:ARG:O	1:B:168:VAL:HG23	2.10	0.51
1:E:197:ARG:HG2	1:E:207:SER:OG	2.10	0.51
1:E:257:GLN:HE22	1:E:369:PHE:H	1.57	0.51
1:A:338:MET:HE3	1:A:345:CYS:CB	2.40	0.51
1:D:78:LEU:HA	1:D:179:VAL:HG21	1.93	0.51
1:E:323:GLU:OE1	1:E:325:ARG:HD3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:MET:HE1	2:F:417:HEM:C3B	2.44	0.51
1:A:85:ILE:O	1:A:227:MET:HA	2.10	0.51
1:D:87:LEU:H	1:D:230:ASN:ND2	2.08	0.51
1:D:248:LEU:HD13	1:D:377:VAL:HG11	1.92	0.51
1:B:309:VAL:HG13	1:B:310:LEU:HD13	1.93	0.51
1:D:144:LEU:HG	1:D:148:ILE:HD12	1.93	0.51
1:F:24:GLN:CD	1:F:24:GLN:N	2.68	0.51
1:A:289:ALA:HB2	1:F:95:LYS:HE2	1.93	0.51
1:E:98:ARG:NH2	1:E:344:ARG:O	2.42	0.51
1:F:186:ALA:O	1:F:190:LEU:HG	2.10	0.51
1:A:82:MET:O	1:A:229:ARG:NH1	2.44	0.51
1:A:262:GLU:C	1:A:264:PRO:HD3	2.36	0.51
1:D:58:ARG:HD2	1:D:340:VAL:HG11	1.93	0.51
1:B:320:ALA:N	1:B:321:PRO:HD3	2.25	0.51
1:C:153:ILE:HG13	1:C:155:VAL:HG13	1.93	0.51
1:C:248:LEU:HD13	1:C:390:LEU:CD1	2.41	0.51
1:E:140:PHE:CE2	1:E:144:LEU:HD22	2.45	0.51
1:F:33:LEU:C	1:F:35:ASP:N	2.64	0.51
1:B:277:ARG:HG3	1:B:278:TYR:CE2	2.46	0.50
1:D:53:ARG:NH1	1:D:55:ASP:OD2	2.44	0.50
1:F:120:VAL:HG11	1:F:147:ASN:HB3	1.93	0.50
1:A:268:PRO:HA	1:A:356:ILE:HD11	1.92	0.50
1:E:374:ASP:OD2	1:E:374:ASP:N	2.42	0.50
1:F:210:LEU:HA	1:F:219:TRP:CD1	2.47	0.50
1:B:257:GLN:O	1:B:261:ARG:HG3	2.12	0.50
1:B:102:MET:HG2	4:B:425:HOH:O	2.10	0.50
1:F:94:HIS:HE1	2:F:417:HEM:O2D	1.95	0.50
1:B:279:PRO:HB3	1:B:337:THR:OG1	2.12	0.50
1:E:136:PHE:HE2	1:E:243:ILE:HG22	1.77	0.50
1:B:102:MET:HG3	4:B:425:HOH:O	2.12	0.50
1:A:52:ALA:HA	1:A:310:LEU:HD23	1.93	0.50
1:A:295:GLY:O	1:A:296:VAL:HG13	2.12	0.50
1:B:248:LEU:O	1:B:249:HIS:C	2.52	0.50
1:A:227:MET:HE3	1:A:228:CYS:SG	2.51	0.49
1:C:71:CYS:HB2	4:C:450:HOH:O	2.10	0.49
1:A:239:VAL:HA	2:A:417:HEM:HBB1	1.94	0.49
1:E:111:VAL:O	1:E:114:GLU:HB3	2.12	0.49
1:F:53:ARG:O	1:F:54:GLY:C	2.55	0.49
1:E:375:LYS:HB2	1:E:391:PRO:HG3	1.94	0.49
1:A:109:PHE:CZ	1:A:113:LEU:HD21	2.48	0.49
1:C:16:ILE:HD12	1:C:305:TYR:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LYS:HZ3	1:B:197:ARG:HH21	1.60	0.49
1:B:239:VAL:O	1:B:243:ILE:HG12	2.13	0.49
1:E:30:TRP:O	1:E:310:LEU:HD11	2.13	0.49
1:D:245:MET:HE3	1:D:245:MET:CA	2.33	0.49
1:F:97:PHE:CZ	1:F:223:GLU:HG2	2.48	0.49
1:C:135:ASP:HB3	4:C:399:HOH:O	2.12	0.49
1:D:343:HIS:O	2:D:417:HEM:HAA2	2.12	0.49
1:E:292:ASP:OD1	1:E:297:THR:HG23	2.13	0.49
1:D:21:GLY:O	1:D:22:VAL:C	2.54	0.49
1:E:246:VAL:HG13	1:E:274:LEU:HD13	1.94	0.49
1:A:206:PHE:O	1:A:207:SER:C	2.51	0.49
1:A:309:VAL:HG13	1:A:310:LEU:HD13	1.95	0.49
1:E:241:ALA:O	1:E:245:MET:HG2	2.12	0.49
1:C:234:GLY:HA2	3:C:397:ID3:H18B	1.94	0.48
1:A:257:GLN:HG2	1:A:261:ARG:NH2	2.28	0.48
1:A:257:GLN:HE22	1:A:369:PHE:H	1.60	0.48
1:F:106:ALA:O	1:F:110:VAL:HG23	2.13	0.48
1:D:52:ALA:O	4:D:433:HOH:O	2.20	0.48
1:C:132:GLY:HA2	1:C:394:TRP:NE1	2.29	0.48
1:C:137:VAL:HA	1:C:141:ALA:HB3	1.95	0.48
1:C:257:GLN:HE22	1:C:369:PHE:H	1.60	0.48
1:D:261:ARG:HD3	1:D:363:LEU:O	2.14	0.48
1:D:255:GLU:HG2	1:D:256:ASP:N	2.29	0.48
1:E:362:TRP:NE1	1:E:369:PHE:CZ	2.80	0.48
1:E:1:MET:N	1:E:1:MET:SD	2.87	0.48
1:A:118:GLN:HA	1:A:357:VAL:HG11	1.96	0.48
1:A:144:LEU:HG	1:A:148:ILE:CD1	2.44	0.48
1:B:87:LEU:H	1:B:230:ASN:HD21	1.61	0.48
1:B:309:VAL:HG22	1:B:313:LEU:HD12	1.94	0.48
1:D:82:MET:CE	1:D:182:LEU:HD23	2.43	0.48
1:C:84:PHE:CB	1:C:88:GLN:HE21	2.26	0.48
1:C:183:LYS:HG3	1:C:184:GLN:N	2.27	0.48
1:E:150:LEU:HD12	1:E:155:VAL:HG11	1.95	0.48
1:F:86:PRO:HG2	2:F:417:HEM:CGD	2.44	0.48
1:F:136:PHE:HE2	1:F:243:ILE:HG22	1.79	0.48
1:D:336:THR:O	1:D:337:THR:C	2.56	0.48
1:B:31:LYS:O	1:B:34:LEU:HB2	2.14	0.47
1:C:239:VAL:HA	2:C:417:HEM:HBB1	1.96	0.47
1:F:198:MET:HE1	1:F:221:VAL:HG22	1.96	0.47
1:E:343:HIS:O	2:E:417:HEM:HAA2	2.13	0.47
1:F:336:THR:HG23	1:F:340:VAL:HG12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:ALA:N	1:E:321:PRO:CD	2.76	0.47
1:C:85:ILE:HG12	1:C:89:GLN:CD	2.40	0.47
1:C:144:LEU:HB3	1:C:145:PRO:HD3	1.96	0.47
1:F:190:LEU:HB3	1:F:194:ILE:CD1	2.43	0.47
1:B:344:ARG:O	1:B:345:CYS:C	2.57	0.47
1:C:2:ILE:HD13	1:C:2:ILE:N	2.29	0.47
1:F:87:LEU:HD13	2:F:417:HEM:HAD2	1.97	0.47
1:F:118:GLN:HG2	1:F:361:GLU:OE1	2.14	0.47
1:A:318:PHE:O	1:A:321:PRO:HG3	2.15	0.47
1:C:82:MET:HG3	1:C:84:PHE:CZ	2.49	0.47
1:E:259:LEU:O	1:E:263:ARG:HB2	2.14	0.47
1:F:52:ALA:O	1:F:53:ARG:HB2	2.13	0.47
1:F:184:GLN:O	1:F:185:ALA:C	2.55	0.47
1:F:309:VAL:HG13	1:F:310:LEU:N	2.29	0.47
1:B:383:ASN:CB	3:B:397:ID3:H17B	2.44	0.47
1:C:239:VAL:HA	2:C:417:HEM:CBB	2.45	0.47
1:D:241:ALA:O	1:D:245:MET:HG2	2.15	0.47
1:E:3:PRO:O	1:E:5:HIS:N	2.47	0.47
1:B:159:ASP:OD1	1:B:162:ARG:NH2	2.42	0.47
1:C:248:LEU:HB3	4:C:410:HOH:O	2.15	0.47
1:F:179:VAL:O	1:F:182:LEU:HB3	2.14	0.47
1:D:168:VAL:H	1:D:169:GLN:NE2	2.13	0.47
1:D:178:THR:HG23	1:D:181:GLN:HB2	1.97	0.47
1:A:10:ARG:HD2	1:A:39:LEU:O	2.15	0.47
1:B:55:ASP:O	1:B:59:GLU:HG2	2.15	0.47
1:B:207:SER:O	1:B:208:ARG:C	2.58	0.47
1:C:205:LEU:HD21	1:C:231:LEU:HD13	1.97	0.47
1:F:84:PHE:CE1	1:F:229:ARG:HG2	2.49	0.47
1:A:118:GLN:HG3	1:A:357:VAL:HG13	1.97	0.46
1:A:257:GLN:HE22	1:A:369:PHE:N	2.13	0.46
1:D:236:LEU:HD23	1:D:236:LEU:HA	1.72	0.46
1:E:12:VAL:HG12	1:E:13:ASP:H	1.80	0.46
1:E:366:MET:HE3	1:E:367:PRO:HD2	1.97	0.46
1:C:53:ARG:NH1	1:C:55:ASP:OD2	2.49	0.46
1:C:144:LEU:HG	1:C:148:ILE:HD12	1.97	0.46
1:A:87:LEU:O	1:A:87:LEU:HG	2.10	0.46
1:B:148:ILE:O	1:B:149:PHE:C	2.58	0.46
1:D:141:ALA:O	1:D:145:PRO:HD3	2.15	0.46
1:E:30:TRP:HB3	1:E:310:LEU:CD1	2.45	0.46
1:E:125:MET:SD	1:E:125:MET:C	2.99	0.46
1:F:61:TRP:CG	1:F:340:VAL:HG13	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:LEU:O	1:D:372:ALA:C	2.57	0.46
1:F:40:VAL:HG22	1:F:50:ILE:HB	1.97	0.46
1:C:85:ILE:O	1:C:227:MET:HA	2.15	0.46
1:D:190:LEU:O	1:D:191:TRP:C	2.59	0.46
1:E:149:PHE:C	1:E:149:PHE:CD2	2.93	0.46
1:A:144:LEU:HG	1:A:148:ILE:HD12	1.97	0.46
1:D:325:ARG:NH2	1:D:327:ASP:OD1	2.47	0.46
1:E:2:ILE:HG22	1:E:3:PRO:HD2	1.97	0.46
1:F:263:ARG:HB3	1:F:266:LEU:HD22	1.97	0.46
1:F:279:PRO:HG2	1:F:309:VAL:HA	1.97	0.46
1:A:248:LEU:O	1:A:249:HIS:C	2.57	0.46
1:E:149:PHE:CZ	1:E:190:LEU:HD21	2.51	0.46
1:F:38:GLY:HA3	1:F:53:ARG:NH2	2.31	0.46
1:A:299:ARG:O	1:A:300:LYS:C	2.59	0.46
1:E:217:ARG:NH1	1:E:223:GLU:OE1	2.43	0.46
1:A:31:LYS:HE2	1:A:313:LEU:HB3	1.98	0.45
1:D:148:ILE:HD13	1:D:354:GLU:HG2	1.97	0.45
1:B:172:ARG:HB2	1:B:174:ASP:OD1	2.16	0.45
1:E:11:VAL:HA	1:E:41:TRP:O	2.16	0.45
1:E:106:ALA:O	1:E:110:VAL:HG23	2.16	0.45
1:B:82:MET:HE1	1:B:182:LEU:HD23	1.97	0.45
1:C:313:LEU:HD23	1:C:313:LEU:N	2.31	0.45
1:D:16:ILE:HD11	1:D:74:VAL:HG21	1.97	0.45
1:D:155:VAL:O	1:D:155:VAL:HG23	2.15	0.45
1:A:5:HIS:HE1	1:A:302:ASP:OD1	1.99	0.45
1:A:198:MET:HG3	1:A:210:LEU:HD13	1.98	0.45
1:D:53:ARG:O	1:D:54:GLY:C	2.59	0.45
1:E:191:TRP:O	1:E:192:PRO:C	2.57	0.45
1:A:310:LEU:O	1:A:314:ASP:HB2	2.17	0.45
1:C:383:ASN:HB3	3:C:397:ID3:H17B	1.99	0.45
1:A:141:ALA:O	1:A:145:PRO:CD	2.64	0.45
1:D:103:LYS:HE2	1:D:212:GLU:OE1	2.16	0.45
1:D:135:ASP:HB3	4:D:405:HOH:O	2.16	0.45
1:F:56:VAL:CG1	1:F:60:LEU:HD22	2.46	0.45
1:B:77:GLY:O	1:B:81:VAL:HG23	2.17	0.45
1:B:258:ARG:NH1	1:B:368:GLU:OE2	2.49	0.45
1:E:338:MET:HE3	1:E:345:CYS:CB	2.47	0.45
1:F:149:PHE:CD2	1:F:149:PHE:C	2.94	0.45
1:B:53:ARG:HH11	1:B:55:ASP:CG	2.25	0.45
1:C:170:LEU:C	1:C:172:ARG:HG3	2.42	0.45
1:D:166:LEU:O	1:D:169:GLN:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:VAL:CG2	1:D:313:LEU:HD12	2.47	0.45
1:E:131:ARG:NH2	1:E:134:CYS:HA	2.31	0.45
1:E:225:ARG:O	1:E:229:ARG:HB2	2.17	0.45
1:F:336:THR:HG22	1:F:336:THR:O	2.17	0.45
1:B:85:ILE:O	1:B:227:MET:HA	2.16	0.45
1:B:125:MET:HG2	1:B:366:MET:SD	2.57	0.45
1:C:191:TRP:HA	1:C:191:TRP:CE3	2.52	0.45
1:D:42:SER:O	1:D:47:GLY:HA2	2.17	0.45
1:E:124:LEU:HD21	1:E:143:ILE:HB	1.99	0.45
1:E:189:TYR:O	1:E:192:PRO:HD2	2.17	0.45
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.73	0.45
1:B:140:PHE:CE2	1:B:144:LEU:HD22	2.52	0.45
1:D:194:ILE:O	1:D:198:MET:HG3	2.16	0.45
1:C:53:ARG:O	1:C:57:VAL:HG23	2.18	0.44
1:B:83:GLN:HB3	1:B:226:ARG:HE	1.82	0.44
1:B:118:GLN:HA	1:B:357:VAL:HG11	1.99	0.44
1:C:25:ASP:OD1	1:C:25:ASP:C	2.61	0.44
1:D:67:LEU:HD21	1:D:291:VAL:HG21	1.98	0.44
1:D:148:ILE:O	1:D:149:PHE:C	2.58	0.44
1:F:3:PRO:O	1:F:4:ALA:C	2.60	0.44
1:F:339:GLY:C	1:F:340:VAL:HG12	2.42	0.44
1:B:114:GLU:N	1:B:115:PRO:CD	2.79	0.44
1:B:257:GLN:NE2	1:B:261:ARG:NH2	2.58	0.44
1:E:98:ARG:HH11	1:E:98:ARG:CG	2.30	0.44
1:F:344:ARG:HD2	4:F:421:HOH:O	2.16	0.44
1:B:257:GLN:HE22	1:B:369:PHE:H	1.66	0.44
1:D:257:GLN:HE22	1:D:369:PHE:H	1.65	0.44
1:E:1:MET:N	1:E:1:MET:CE	2.72	0.44
1:E:155:VAL:HG21	1:E:160:ARG:HG2	1.99	0.44
1:A:72:LEU:HD22	1:A:88:GLN:NE2	2.33	0.44
1:C:148:ILE:O	1:C:149:PHE:C	2.60	0.44
1:D:34:LEU:HD13	1:D:310:LEU:HG	2.00	0.44
1:F:392:LEU:CB	1:F:394:TRP:HZ3	2.30	0.44
1:E:54:GLY:HA2	1:E:311:HIS:HA	2.00	0.44
1:A:166:LEU:HD12	1:A:166:LEU:HA	1.82	0.44
1:E:330:LEU:O	1:E:331:ALA:C	2.61	0.44
3:A:397:ID3:H4A	3:A:397:ID3:H17A	2.00	0.44
1:C:113:LEU:HD13	1:C:152:LEU:HD22	1.98	0.44
1:E:168:VAL:C	1:E:170:LEU:H	2.25	0.44
1:E:168:VAL:C	1:E:170:LEU:N	2.76	0.44
1:A:214:VAL:O	1:A:217:ARG:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LYS:HD3	1:C:388:THR:CG2	2.47	0.44
1:D:82:MET:O	1:D:229:ARG:NH1	2.46	0.44
1:D:94:HIS:HE1	2:D:417:HEM:O2D	2.00	0.44
1:F:2:ILE:HG22	1:F:3:PRO:HD2	2.00	0.44
1:F:77:GLY:O	1:F:81:VAL:HG23	2.18	0.44
1:A:263:ARG:HD3	1:A:265:ASP:OD1	2.18	0.43
1:B:209:ILE:O	1:B:212:GLU:HB2	2.17	0.43
1:B:261:ARG:HD3	1:B:363:LEU:O	2.18	0.43
1:F:136:PHE:HD1	1:F:392:LEU:CD1	2.31	0.43
1:A:6:VAL:O	1:A:6:VAL:HG12	2.13	0.43
1:A:53:ARG:O	1:A:57:VAL:HG23	2.18	0.43
1:A:165:GLN:HE21	1:A:165:GLN:HA	1.83	0.43
1:D:203:ASP:OD1	1:D:203:ASP:N	2.51	0.43
1:E:57:VAL:O	1:E:61:TRP:HB2	2.18	0.43
1:C:55:ASP:OD1	1:C:55:ASP:N	2.51	0.43
1:D:68:SER:OG	1:D:90:ASP:OD2	2.31	0.43
1:D:79:GLY:O	1:D:80:LYS:C	2.61	0.43
1:F:352:ARG:O	1:F:356:ILE:HG13	2.18	0.43
1:A:159:ASP:OD1	1:A:159:ASP:N	2.52	0.43
1:B:120:VAL:HG11	1:B:147:ASN:HB3	2.00	0.43
1:B:260:LEU:HB2	1:B:363:LEU:HD13	2.00	0.43
1:C:145:PRO:HG2	1:C:240:ALA:HB2	2.00	0.43
1:E:142:GLU:OE1	4:E:435:HOH:O	2.21	0.43
1:F:150:LEU:HD12	1:F:150:LEU:HA	1.87	0.43
1:A:174:ASP:HB2	1:A:175:GLY:HA2	2.01	0.43
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.77	0.43
1:C:78:LEU:HG	1:C:179:VAL:HG21	2.01	0.43
1:D:53:ARG:NH1	1:D:55:ASP:OD1	2.51	0.43
1:E:196:LYS:HE2	1:E:200:GLN:HG3	2.01	0.43
1:B:149:PHE:C	1:B:151:THR:N	2.77	0.43
1:B:212:GLU:OE2	1:B:213:PRO:HD2	2.18	0.43
1:B:384:VAL:HG23	3:B:397:ID3:H17A	2.00	0.43
1:D:309:VAL:HG23	1:D:313:LEU:CD1	2.48	0.43
1:E:152:LEU:HD13	1:E:205:LEU:HD22	2.00	0.43
3:A:397:ID3:H17A	3:A:397:ID3:C4	2.49	0.43
1:B:136:PHE:HE2	1:B:243:ILE:HG22	1.82	0.43
1:C:206:PHE:HE1	1:C:231:LEU:HD12	1.83	0.43
1:C:380:LYS:HD3	1:C:388:THR:HG22	2.01	0.43
1:D:249:HIS:ND1	1:D:278:TYR:OH	2.44	0.43
1:E:336:THR:HG23	1:E:340:VAL:HG12	2.00	0.43
1:E:343:HIS:ND1	2:E:417:HEM:O1D	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:HIS:HD2	1:A:49:TRP:O	2.01	0.43
1:C:98:ARG:NH2	1:C:344:ARG:O	2.41	0.43
1:C:114:GLU:HB3	1:C:115:PRO:CD	2.46	0.43
1:E:26:TYR:CD2	1:E:26:TYR:C	2.96	0.43
1:E:87:LEU:HA	1:E:87:LEU:HD12	1.54	0.43
1:E:95:LYS:NZ	1:E:95:LYS:CB	2.82	0.43
1:F:349:GLY:O	1:F:352:ARG:HB3	2.18	0.43
1:C:319:GLU:O	1:C:320:ALA:C	2.62	0.43
1:D:19:PRO:HA	1:D:20:PRO:HD3	1.71	0.43
1:B:343:HIS:O	2:B:417:HEM:HAA2	2.19	0.43
3:B:397:ID3:H7	3:B:397:ID3:H18	1.80	0.43
1:C:350:LEU:HA	1:C:350:LEU:HD12	1.80	0.43
1:F:372:ALA:HA	1:F:373:PRO:HD2	1.72	0.43
1:B:89:GLN:O	1:B:343:HIS:HE1	2.01	0.42
1:B:325:ARG:NE	1:B:327:ASP:OD2	2.47	0.42
1:E:217:ARG:HD2	1:E:217:ARG:C	2.44	0.42
1:F:40:VAL:HG22	1:F:50:ILE:O	2.18	0.42
1:F:40:VAL:CG2	1:F:50:ILE:HB	2.48	0.42
1:F:49:TRP:CD1	1:F:302:ASP:HB3	2.54	0.42
1:A:65:GLU:OE2	1:F:91:GLY:HA2	2.18	0.42
1:A:86:PRO:HD2	2:A:417:HEM:HMD2	2.01	0.42
1:B:16:ILE:CD1	1:B:305:TYR:CZ	3.03	0.42
1:C:263:ARG:O	1:C:265:ASP:N	2.52	0.42
1:D:31:LYS:O	1:D:34:LEU:HB2	2.19	0.42
1:D:53:ARG:HD2	1:D:53:ARG:HH11	1.65	0.42
1:D:155:VAL:O	1:D:155:VAL:CG2	2.67	0.42
1:C:125:MET:CE	1:C:365:GLY:HA3	2.49	0.42
1:D:49:TRP:CD1	1:D:298:ILE:HG23	2.55	0.42
1:E:6:VAL:CG1	1:E:41:TRP:HB3	2.47	0.42
1:F:198:MET:HE2	1:F:198:MET:HB2	1.74	0.42
1:A:348:ALA:O	1:A:349:GLY:C	2.62	0.42
1:B:5:HIS:CD2	1:B:5:HIS:H	2.37	0.42
1:B:141:ALA:O	1:B:145:PRO:HD3	2.16	0.42
1:C:336:THR:HG22	1:C:336:THR:O	2.19	0.42
1:B:149:PHE:C	1:B:151:THR:H	2.28	0.42
1:C:128:LEU:O	1:C:131:ARG:HB2	2.19	0.42
1:F:281:VAL:HG21	2:F:417:HEM:HHB	2.01	0.42
1:A:25:ASP:C	1:A:25:ASP:OD1	2.62	0.42
1:A:97:PHE:CZ	1:A:214:VAL:HG11	2.55	0.42
1:A:320:ALA:N	1:A:321:PRO:HD3	2.34	0.42
1:B:87:LEU:HD12	1:B:87:LEU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ALA:C	1:E:10:ARG:H	2.26	0.42
1:E:160:ARG:O	1:E:164:ARG:HB2	2.20	0.42
1:F:242:MET:HE2	1:F:242:MET:HB2	1.84	0.42
1:A:222:ASP:O	1:A:225:ARG:HB2	2.20	0.42
1:C:171:THR:O	1:C:171:THR:HG23	2.17	0.42
1:C:295:GLY:O	1:C:296:VAL:HG12	2.19	0.42
1:D:263:ARG:O	1:D:264:PRO:C	2.62	0.42
1:E:8:ALA:O	1:E:10:ARG:N	2.51	0.42
1:A:205:LEU:CD2	1:A:231:LEU:HD13	2.49	0.42
1:C:113:LEU:HD23	1:C:113:LEU:HA	1.63	0.42
1:F:353:MET:O	1:F:354:GLU:C	2.62	0.42
1:A:82:MET:O	1:A:83:GLN:C	2.63	0.42
1:C:52:ALA:HA	1:C:310:LEU:HD23	2.00	0.42
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.64	0.42
1:F:227:MET:HE3	1:F:227:MET:HB3	1.91	0.42
1:B:16:ILE:HD12	1:B:305:TYR:CZ	2.55	0.42
1:B:166:LEU:O	1:B:169:GLN:HB2	2.20	0.42
1:B:170:LEU:HD13	1:B:232:LEU:HD21	2.01	0.42
1:C:333:ILE:HG13	1:C:344:ARG:CZ	2.50	0.42
1:E:160:ARG:H	1:E:160:ARG:HG3	1.60	0.42
1:F:129:ARG:HB3	1:F:130:PRO:CD	2.50	0.42
1:C:263:ARG:C	1:C:265:ASP:N	2.75	0.41
1:D:118:GLN:HA	1:D:357:VAL:CG1	2.50	0.41
1:D:168:VAL:HA	1:D:171:THR:HG23	2.02	0.41
1:F:133:SER:HA	1:F:392:LEU:O	2.20	0.41
1:F:156:PRO:O	1:F:159:ASP:HB2	2.19	0.41
1:B:172:ARG:HE	1:B:172:ARG:HB3	1.60	0.41
1:C:307:PRO:HG3	1:C:310:LEU:HD22	2.01	0.41
1:C:338:MET:HE3	1:C:345:CYS:CB	2.50	0.41
1:C:348:ALA:O	1:C:349:GLY:C	2.63	0.41
1:E:87:LEU:H	1:E:230:ASN:ND2	2.17	0.41
1:E:90:ASP:N	4:E:421:HOH:O	2.36	0.41
1:E:380:LYS:HE2	1:E:380:LYS:HB3	1.29	0.41
1:F:68:SER:OG	1:F:90:ASP:OD2	2.31	0.41
1:F:155:VAL:HG23	1:F:156:PRO:O	2.20	0.41
1:C:122:ARG:HB2	1:C:361:GLU:OE2	2.21	0.41
1:C:362:TRP:O	1:C:366:MET:CB	2.68	0.41
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.68	0.41
1:D:178:THR:O	1:D:179:VAL:C	2.63	0.41
1:E:27:PHE:O	1:E:28:ALA:C	2.64	0.41
1:B:21:GLY:O	1:B:22:VAL:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PRO:CG	1:B:310:LEU:HD22	2.49	0.41
1:C:40:VAL:O	1:C:49:TRP:HA	2.20	0.41
1:E:125:MET:HE3	1:E:126:GLU:HG3	2.01	0.41
1:A:13:ASP:O	1:A:14:PHE:C	2.60	0.41
1:A:239:VAL:HA	2:A:417:HEM:CBB	2.50	0.41
1:B:375:LYS:HB2	1:B:391:PRO:HG3	2.03	0.41
1:C:158:GLU:O	1:C:161:PRO:HD2	2.21	0.41
1:D:87:LEU:HD12	1:D:87:LEU:O	2.20	0.41
1:E:8:ALA:O	1:E:11:VAL:HG23	2.20	0.41
1:D:107:SER:C	1:D:109:PHE:N	2.78	0.41
1:E:263:ARG:HD3	1:E:266:LEU:HD21	2.01	0.41
1:F:57:VAL:HG12	1:F:311:HIS:HB2	2.02	0.41
1:F:249:HIS:HD2	1:F:250:LEU:HD23	1.86	0.41
1:B:89:GLN:O	1:B:343:HIS:CE1	2.73	0.41
1:D:66:ARG:NH1	1:E:395:ARG:HD2	2.35	0.41
1:E:70:GLN:NE2	4:E:421:HOH:O	2.51	0.41
1:E:227:MET:O	1:E:228:CYS:C	2.63	0.41
1:E:380:LYS:HG2	1:E:381:GLY:N	2.35	0.41
1:A:58:ARG:HH11	1:A:311:HIS:CD2	2.39	0.41
1:D:129:ARG:HB3	1:D:129:ARG:HE	1.60	0.41
1:E:48:HIS:HD2	1:E:49:TRP:O	2.04	0.41
1:F:61:TRP:CD1	1:F:340:VAL:HG13	2.56	0.41
1:F:191:TRP:O	1:F:192:PRO:C	2.64	0.41
1:A:49:TRP:CD1	1:A:298:ILE:HG23	2.56	0.41
1:B:50:ILE:HG22	1:B:51:ALA:O	2.21	0.41
1:B:117:VAL:HG13	1:B:148:ILE:HG12	2.03	0.41
1:C:27:PHE:CZ	1:C:278:TYR:HD1	2.39	0.41
1:C:61:TRP:HB3	1:C:340:VAL:HG13	2.03	0.41
1:C:257:GLN:NE2	1:C:368:GLU:HG3	2.36	0.41
1:C:279:PRO:HG2	1:C:309:VAL:HA	2.03	0.41
1:D:107:SER:O	1:D:111:VAL:HG23	2.21	0.41
1:E:125:MET:CE	1:E:126:GLU:HG3	2.50	0.41
1:E:136:PHE:CD1	1:E:392:LEU:HD12	2.56	0.41
1:E:353:MET:O	1:E:354:GLU:C	2.64	0.41
1:F:54:GLY:N	1:F:314:ASP:OD2	2.50	0.41
1:F:54:GLY:HA3	1:F:317:SER:OG	2.21	0.41
1:F:136:PHE:HD1	1:F:392:LEU:HD11	1.85	0.41
1:F:151:THR:O	1:F:152:LEU:C	2.64	0.41
1:F:258:ARG:HH11	1:F:258:ARG:HG3	1.86	0.41
1:F:350:LEU:O	1:F:353:MET:HB3	2.20	0.41
1:B:109:PHE:HD1	1:B:109:PHE:HA	1.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:MET:HE1	2:B:417:HEM:C3B	2.56	0.41
1:D:178:THR:CG2	1:D:181:GLN:CD	2.94	0.41
1:E:101:VAL:HA	1:E:209:ILE:HG12	2.03	0.41
1:F:136:PHE:HB3	1:F:390:LEU:HB3	2.02	0.41
1:A:260:LEU:HB3	1:A:363:LEU:HD13	2.02	0.40
1:A:263:ARG:NH1	1:A:265:ASP:OD2	2.54	0.40
1:A:352:ARG:HH21	1:A:352:ARG:HD3	1.77	0.40
4:B:439:HOH:O	1:D:5:HIS:CD2	2.69	0.40
1:C:132:GLY:HA3	4:C:447:HOH:O	2.21	0.40
1:E:212:GLU:HA	1:E:213:PRO:HD2	1.86	0.40
1:D:262:GLU:O	1:D:264:PRO:HD2	2.21	0.40
1:B:141:ALA:O	1:B:145:PRO:HD2	2.21	0.40
1:D:55:ASP:O	1:D:59:GLU:HG2	2.21	0.40
1:F:159:ASP:HA	4:F:425:HOH:O	2.20	0.40
1:B:14:PHE:CZ	1:B:19:PRO:HB3	2.56	0.40
1:C:336:THR:HG23	1:C:340:VAL:HG12	2.03	0.40
1:E:32:THR:O	1:E:35:ASP:HB2	2.21	0.40
1:E:344:ARG:O	1:E:345:CYS:C	2.64	0.40
1:A:78:LEU:HA	1:A:179:VAL:HG21	2.02	0.40
1:D:154:ASP:O	1:D:154:ASP:CG	2.62	0.40
1:D:168:VAL:N	1:D:169:GLN:NE2	2.70	0.40
1:F:361:GLU:O	1:F:362:TRP:C	2.64	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)
1:B:80:LYS:NZ	1:D:200:GLN:OE1[1_455]	2.19	0.01

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	394/396 (100%)	355 (90%)	34 (9%)	5 (1%)	9	31
1	B	394/396 (100%)	365 (93%)	25 (6%)	4 (1%)	12	38
1	C	394/396 (100%)	360 (91%)	30 (8%)	4 (1%)	12	38
1	D	390/396 (98%)	351 (90%)	38 (10%)	1 (0%)	36	66
1	E	386/396 (98%)	331 (86%)	42 (11%)	13 (3%)	3	11
1	F	386/396 (98%)	321 (83%)	52 (14%)	13 (3%)	3	11
All	All	2344/2376 (99%)	2083 (89%)	221 (9%)	40 (2%)	7	25

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	LEU
1	A	172	ARG
1	B	172	ARG
1	B	173	PRO
1	B	174	ASP
1	C	172	ARG
1	C	173	PRO
1	E	9	ASP
1	F	4	ALA
1	A	173	PRO
1	E	152	LEU
1	E	195	GLU
1	C	72	LEU
1	C	169	GLN
1	E	194	ILE
1	E	307	PRO
1	E	345	CYS
1	F	3	PRO
1	F	53	ARG
1	F	152	LEU
1	F	168	VAL
1	A	175	GLY
1	E	3	PRO
1	E	158	GLU
1	E	169	GLN
1	F	7	PRO
1	F	133	SER
1	F	362	TRP
1	A	174	ASP
1	B	14	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	33	LEU
1	E	157	LEU
1	E	367	PRO
1	F	130	PRO
1	F	194	ILE
1	E	7	PRO
1	E	346	VAL
1	F	47	GLY
1	F	156	PRO
1	F	54	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/321 (100%)	286 (89%)	35 (11%)	6	21
1	B	321/321 (100%)	285 (89%)	36 (11%)	6	19
1	C	321/321 (100%)	290 (90%)	31 (10%)	8	25
1	D	319/321 (99%)	291 (91%)	28 (9%)	9	29
1	E	316/321 (98%)	270 (85%)	46 (15%)	3	11
1	F	316/321 (98%)	276 (87%)	40 (13%)	4	15
All	All	1914/1926 (99%)	1698 (89%)	216 (11%)	5	19

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ILE
1	A	18	ASN
1	A	23	GLU
1	A	31	LYS
1	A	34	LEU
1	A	60	LEU
1	A	78	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	123	LYS
1	A	131	ARG
1	A	143	ILE
1	A	150	LEU
1	A	157	LEU
1	A	159	ASP
1	A	165	GLN
1	A	166	LEU
1	A	170	LEU
1	A	172	ARG
1	A	174	ASP
1	A	196	LYS
1	A	197	ARG
1	A	208	ARG
1	A	217	ARG
1	A	237	ASP
1	A	266	LEU
1	A	268	PRO
1	A	300	LYS
1	A	303	LEU
1	A	310	LEU
1	A	319	GLU
1	A	340	VAL
1	A	356	ILE
1	A	366	MET
1	A	380	LYS
1	A	395	ARG
1	B	1	MET
1	B	18	ASN
1	B	24	GLN
1	B	34	LEU
1	B	60	LEU
1	B	75	THR
1	B	78	LEU
1	B	116	LYS
1	B	138	SER
1	B	143	ILE
1	B	146	LEU
1	B	150	LEU
1	B	151	THR
1	B	157	LEU
1	B	171	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	172	ARG
1	B	173	PRO
1	B	174	ASP
1	B	176	SER
1	B	181	GLN
1	B	183	LYS
1	B	196	LYS
1	B	197	ARG
1	B	221	VAL
1	B	237	ASP
1	B	238	THR
1	B	266	LEU
1	B	303	LEU
1	B	310	LEU
1	B	319	GLU
1	B	330	LEU
1	B	340	VAL
1	B	366	MET
1	B	378	THR
1	B	380	LYS
1	B	395	ARG
1	C	1	MET
1	C	11	VAL
1	C	18	ASN
1	C	24	GLN
1	C	34	LEU
1	C	35	ASP
1	C	60	LEU
1	C	69	SER
1	C	78	LEU
1	C	108	ARG
1	C	116	LYS
1	C	150	LEU
1	C	157	LEU
1	C	166	LEU
1	C	168	VAL
1	C	170	LEU
1	C	171	THR
1	C	172	ARG
1	C	178	THR
1	C	221	VAL
1	C	231	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	236	LEU
1	C	243	ILE
1	C	266	LEU
1	C	268	PRO
1	C	300	LYS
1	C	303	LEU
1	C	310	LEU
1	C	313	LEU
1	C	319	GLU
1	C	340	VAL
1	D	9	ASP
1	D	34	LEU
1	D	60	LEU
1	D	70	GLN
1	D	75	THR
1	D	78	LEU
1	D	103	LYS
1	D	107	SER
1	D	116	LYS
1	D	138	SER
1	D	151	THR
1	D	157	LEU
1	D	169	GLN
1	D	170	LEU
1	D	171	THR
1	D	172	ARG
1	D	177	MET
1	D	178	THR
1	D	183	LYS
1	D	221	VAL
1	D	236	LEU
1	D	266	LEU
1	D	310	LEU
1	D	332	PRO
1	D	340	VAL
1	D	357	VAL
1	D	366	MET
1	D	380	LYS
1	E	1	MET
1	E	2	ILE
1	E	11	VAL
1	E	12	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	23	GLU
1	E	34	LEU
1	E	70	GLN
1	E	74	VAL
1	E	75	THR
1	E	78	LEU
1	E	80	LYS
1	E	82	MET
1	E	85	ILE
1	E	95	LYS
1	E	102	MET
1	E	103	LYS
1	E	107	SER
1	E	108	ARG
1	E	114	GLU
1	E	120	VAL
1	E	124	LEU
1	E	138	SER
1	E	150	LEU
1	E	157	LEU
1	E	158	GLU
1	E	166	LEU
1	E	168	VAL
1	E	177	MET
1	E	183	LYS
1	E	196	LYS
1	E	243	ILE
1	E	250	LEU
1	E	262	GLU
1	E	263	ARG
1	E	300	LYS
1	E	303	LEU
1	E	304	VAL
1	E	317	SER
1	E	330	LEU
1	E	340	VAL
1	E	357	VAL
1	E	363	LEU
1	E	377	VAL
1	E	380	LYS
1	E	390	LEU
1	E	395	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	2	ILE
1	F	11	VAL
1	F	12	VAL
1	F	22	VAL
1	F	23	GLU
1	F	24	GLN
1	F	32	THR
1	F	34	LEU
1	F	57	VAL
1	F	74	VAL
1	F	78	LEU
1	F	80	LYS
1	F	103	LYS
1	F	107	SER
1	F	108	ARG
1	F	120	VAL
1	F	123	LYS
1	F	144	LEU
1	F	150	LEU
1	F	155	VAL
1	F	158	GLU
1	F	160	ARG
1	F	166	LEU
1	F	169	GLN
1	F	177	MET
1	F	179	VAL
1	F	181	GLN
1	F	182	LEU
1	F	183	LYS
1	F	198	MET
1	F	237	ASP
1	F	238	THR
1	F	248	LEU
1	F	250	LEU
1	F	303	LEU
1	F	330	LEU
1	F	340	VAL
1	F	357	VAL
1	F	374	ASP
1	F	380	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	88	GLN
1	A	94	HIS
1	A	165	GLN
1	A	169	GLN
1	A	181	GLN
1	A	184	GLN
1	A	230	ASN
1	A	257	GLN
1	A	286	ASN
1	A	311	HIS
1	B	5	HIS
1	B	24	GLN
1	B	48	HIS
1	B	88	GLN
1	B	94	HIS
1	B	118	GLN
1	B	184	GLN
1	B	230	ASN
1	B	253	HIS
1	B	257	GLN
1	B	311	HIS
1	B	343	HIS
1	B	383	ASN
1	C	5	HIS
1	C	18	ASN
1	C	48	HIS
1	C	88	GLN
1	C	94	HIS
1	C	169	GLN
1	C	200	GLN
1	C	230	ASN
1	C	257	GLN
1	C	311	HIS
1	D	5	HIS
1	D	48	HIS
1	D	88	GLN
1	D	94	HIS
1	D	169	GLN
1	D	184	GLN
1	D	200	GLN
1	D	230	ASN
1	D	257	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	311	HIS
1	E	5	HIS
1	E	48	HIS
1	E	88	GLN
1	E	89	GLN
1	E	94	HIS
1	E	165	GLN
1	E	181	GLN
1	E	184	GLN
1	E	230	ASN
1	E	257	GLN
1	E	286	ASN
1	E	311	HIS
1	E	383	ASN
1	F	5	HIS
1	F	18	ASN
1	F	48	HIS
1	F	70	GLN
1	F	83	GLN
1	F	88	GLN
1	F	94	HIS
1	F	118	GLN
1	F	169	GLN
1	F	181	GLN
1	F	230	ASN
1	F	257	GLN
1	F	286	ASN
1	F	311	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	E	417	1	50,50,50	2.48	15 (30%)	67,82,82	1.80	14 (20%)
2	HEM	C	417	1	50,50,50	2.09	13 (26%)	67,82,82	1.71	16 (23%)
2	HEM	F	417	1	50,50,50	2.46	16 (32%)	67,82,82	1.58	13 (19%)
3	ID3	A	397	-	14,14,14	2.04	7 (50%)	20,20,20	2.22	6 (30%)
3	ID3	B	397	-	14,14,14	1.88	6 (42%)	20,20,20	3.12	8 (40%)
2	HEM	D	417	1	50,50,50	2.09	14 (28%)	67,82,82	1.67	16 (23%)
2	HEM	A	417	1	50,50,50	2.44	17 (34%)	67,82,82	2.00	23 (34%)
3	ID3	C	397	-	14,14,14	2.32	7 (50%)	20,20,20	2.72	7 (35%)
2	HEM	B	417	1	50,50,50	2.21	15 (30%)	67,82,82	1.53	14 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	E	417	1	-	2/14/54/54	-
2	HEM	C	417	1	-	5/14/54/54	-
2	HEM	F	417	1	-	4/14/54/54	-
3	ID3	A	397	-	-	2/5/22/22	0/1/1/1
3	ID3	B	397	-	-	4/5/22/22	0/1/1/1
2	HEM	D	417	1	-	2/14/54/54	-
2	HEM	A	417	1	-	3/14/54/54	-
3	ID3	C	397	-	-	4/5/22/22	0/1/1/1
2	HEM	B	417	1	-	2/14/54/54	-

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	HEM	C3D-C2D	9.16	1.56	1.36
2	F	417	HEM	FE-NB	9.01	2.22	1.94
2	F	417	HEM	C3D-C2D	8.46	1.55	1.36
2	E	417	HEM	C3D-C2D	7.96	1.53	1.36
2	B	417	HEM	C3D-C2D	7.02	1.51	1.36
2	E	417	HEM	FE-NB	7.00	2.16	1.94
2	C	417	HEM	C3D-C2D	6.95	1.51	1.36
2	D	417	HEM	C3D-C2D	6.78	1.51	1.36
2	E	417	HEM	FE-ND	5.41	2.11	1.94
2	C	417	HEM	CHA-C1A	-5.08	1.28	1.39
2	B	417	HEM	CAC-C3C	4.89	1.60	1.47
2	D	417	HEM	CMA-C3A	4.78	1.60	1.50
2	B	417	HEM	O1A-CGA	4.64	1.37	1.22
2	A	417	HEM	FE-NC	4.60	2.10	1.95
2	E	417	HEM	CMB-C2B	4.39	1.59	1.50
2	E	417	HEM	CAC-C3C	4.35	1.59	1.47
2	F	417	HEM	CAC-C3C	4.32	1.58	1.47
2	D	417	HEM	O1A-CGA	4.19	1.35	1.22
2	A	417	HEM	CAC-C3C	4.13	1.58	1.47
2	D	417	HEM	CHC-C1C	-4.11	1.30	1.38
2	B	417	HEM	CBD-CGD	4.10	1.60	1.50
2	E	417	HEM	CMA-C3A	4.06	1.59	1.50
3	C	397	ID3	C4-C5	4.03	1.58	1.51
2	A	417	HEM	CBD-CGD	3.90	1.59	1.50
2	D	417	HEM	O1D-CGD	3.90	1.34	1.22
2	F	417	HEM	FE-NC	3.89	2.08	1.95
2	D	417	HEM	CAC-C3C	3.79	1.57	1.47
2	C	417	HEM	CMB-C2B	3.75	1.58	1.50
2	C	417	HEM	C1A-NA	-3.70	1.32	1.39
2	C	417	HEM	CAC-C3C	3.61	1.57	1.47
2	B	417	HEM	CHC-C1C	-3.57	1.31	1.38
2	B	417	HEM	CHA-C4D	-3.53	1.31	1.38
3	C	397	ID3	C8-C9	3.50	1.55	1.47
2	C	417	HEM	CBD-CGD	3.50	1.58	1.50
3	C	397	ID3	C1-C6	3.44	1.58	1.53
2	B	417	HEM	CMB-C2B	3.43	1.57	1.50
2	D	417	HEM	CBD-CGD	3.40	1.58	1.50
2	B	417	HEM	CMA-C3A	3.37	1.57	1.50
2	A	417	HEM	CHA-C4D	-3.34	1.31	1.38
2	A	417	HEM	CMC-C2C	3.33	1.57	1.50
2	A	417	HEM	C1D-ND	3.30	1.45	1.38
2	E	417	HEM	C1A-NA	-3.29	1.33	1.39
3	A	397	ID3	C4-C5	3.29	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	397	ID3	C8-C9	3.28	1.55	1.47
2	F	417	HEM	CMA-C3A	3.19	1.57	1.50
3	C	397	ID3	C7-C6	3.18	1.56	1.45
2	E	417	HEM	CHD-C4C	3.11	1.44	1.38
3	A	397	ID3	C7-C6	3.10	1.55	1.45
2	B	417	HEM	CMC-C2C	3.08	1.57	1.50
2	C	417	HEM	C4D-ND	-3.08	1.34	1.40
2	D	417	HEM	CMB-C2B	3.04	1.57	1.50
2	E	417	HEM	CMD-C2D	3.04	1.57	1.50
3	B	397	ID3	C1-C6	3.04	1.57	1.53
3	B	397	ID3	C2-C1	3.03	1.61	1.54
2	E	417	HEM	FE-NC	3.03	2.05	1.95
2	F	417	HEM	FE-ND	3.02	2.04	1.94
2	A	417	HEM	CMD-C2D	2.96	1.56	1.50
3	A	397	ID3	C1-C6	2.92	1.57	1.53
2	A	417	HEM	CMA-C3A	2.91	1.56	1.50
2	E	417	HEM	CMC-C2C	2.90	1.56	1.50
2	F	417	HEM	C1A-NA	-2.89	1.34	1.39
2	A	417	HEM	C1A-NA	-2.80	1.34	1.39
3	C	397	ID3	C5-C6	2.78	1.39	1.34
2	A	417	HEM	C1D-C2D	2.76	1.50	1.44
2	F	417	HEM	C3B-C2B	-2.74	1.31	1.37
3	B	397	ID3	C2-C3	2.67	1.58	1.52
3	B	397	ID3	C7-C6	2.67	1.54	1.45
2	A	417	HEM	CHA-C1A	-2.67	1.33	1.39
2	A	417	HEM	FE-ND	2.61	2.02	1.94
2	D	417	HEM	CBA-CGA	2.60	1.56	1.50
2	B	417	HEM	C3B-C2B	-2.56	1.32	1.37
2	C	417	HEM	C4D-C3D	2.55	1.49	1.45
3	B	397	ID3	C8-C7	2.51	1.40	1.33
2	E	417	HEM	CAB-C3B	2.51	1.54	1.47
2	D	417	HEM	C3C-C4C	2.48	1.50	1.46
2	D	417	HEM	CHA-C1A	-2.48	1.33	1.39
2	A	417	HEM	O1A-CGA	2.47	1.30	1.22
2	A	417	HEM	C1C-NC	-2.46	1.35	1.39
2	A	417	HEM	CAB-C3B	2.46	1.53	1.47
2	C	417	HEM	C4B-NB	-2.45	1.34	1.38
2	F	417	HEM	CMD-C2D	2.45	1.55	1.50
2	D	417	HEM	CMC-C2C	2.41	1.55	1.50
2	C	417	HEM	CAB-C3B	2.40	1.53	1.47
2	B	417	HEM	CHA-C1A	-2.39	1.34	1.39
2	E	417	HEM	C1B-C2B	2.38	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	397	ID3	C8-C7	2.36	1.40	1.33
2	D	417	HEM	CHA-C4D	-2.34	1.33	1.38
2	B	417	HEM	C1B-NB	-2.32	1.36	1.40
2	D	417	HEM	C3B-C2B	-2.30	1.32	1.37
3	B	397	ID3	C4-C5	2.29	1.55	1.51
3	C	397	ID3	C2-C1	2.27	1.59	1.54
2	F	417	HEM	FE-NA	2.24	2.02	1.95
2	E	417	HEM	C3B-C4B	-2.24	1.40	1.44
2	F	417	HEM	CMC-C2C	2.23	1.55	1.50
2	A	417	HEM	C1A-C2A	2.23	1.49	1.44
3	A	397	ID3	C5-C6	2.22	1.38	1.34
2	B	417	HEM	O1D-CGD	2.21	1.29	1.22
3	A	397	ID3	C2-C3	2.18	1.57	1.52
2	F	417	HEM	C1D-C2D	2.15	1.48	1.44
2	B	417	HEM	CAB-C3B	2.14	1.53	1.47
3	A	397	ID3	C8-C7	2.13	1.39	1.33
2	C	417	HEM	C4C-NC	2.12	1.43	1.39
2	C	417	HEM	O2D-CGD	-2.11	1.23	1.30
2	F	417	HEM	CAD-C3D	2.09	1.56	1.51
2	F	417	HEM	CAB-C3B	2.09	1.53	1.47
2	F	417	HEM	CAA-C2A	2.09	1.56	1.51
2	B	417	HEM	C4A-C3A	2.06	1.48	1.43
2	F	417	HEM	CMB-C2B	2.05	1.55	1.50
2	C	417	HEM	FE-NC	2.03	2.01	1.95
2	E	417	HEM	O1D-CGD	2.01	1.28	1.22

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	397	ID3	C18-C5-C6	-7.75	116.03	124.48
3	A	397	ID3	C1-C6-C5	-6.65	113.55	122.64
3	C	397	ID3	C1-C6-C5	-5.89	114.59	122.64
3	C	397	ID3	C18-C5-C6	-5.70	118.27	124.48
2	E	417	HEM	CMD-C2D-C1D	5.42	133.50	125.03
3	B	397	ID3	C1-C6-C5	-5.35	115.32	122.64
3	C	397	ID3	C2-C1-C6	5.30	118.14	110.44
2	A	417	HEM	C4D-ND-C1D	5.21	111.38	105.21
2	F	417	HEM	C4C-C3C-C2C	5.14	111.27	106.81
2	E	417	HEM	C4D-ND-C1D	5.08	111.22	105.21
3	B	397	ID3	C17-C1-C6	-4.71	102.85	110.24
3	B	397	ID3	C18-C5-C4	4.70	123.61	113.60
3	B	397	ID3	C2-C1-C6	4.54	117.03	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	C4C-C3C-C2C	4.51	110.72	106.81
2	B	417	HEM	C4D-ND-C1D	4.43	110.46	105.21
2	D	417	HEM	C4D-ND-C1D	4.37	110.39	105.21
2	A	417	HEM	C3B-C2B-C1B	-4.33	103.16	106.41
2	C	417	HEM	O2D-CGD-O1D	-4.25	112.40	123.33
2	A	417	HEM	CMD-C2D-C1D	4.11	131.45	125.03
2	F	417	HEM	C4D-ND-C1D	3.93	109.86	105.21
3	B	397	ID3	O1-C9-C19	3.92	125.47	119.32
3	C	397	ID3	C7-C8-C9	3.90	131.80	124.56
3	A	397	ID3	C18-C5-C6	-3.85	120.28	124.48
2	C	417	HEM	C4D-ND-C1D	3.74	109.63	105.21
2	E	417	HEM	C4C-C3C-C2C	3.63	109.97	106.81
2	E	417	HEM	O1A-CGA-CBA	-3.63	111.58	123.09
2	D	417	HEM	CAD-C3D-C4D	3.61	131.00	124.70
2	D	417	HEM	CBA-CAA-C2A	-3.60	102.57	112.53
2	E	417	HEM	C1D-C2D-C3D	-3.60	103.19	106.98
2	A	417	HEM	CHC-C4B-NB	3.60	128.29	124.42
2	E	417	HEM	CAD-C3D-C4D	3.47	130.75	124.70
2	A	417	HEM	C3C-C2C-C1C	-3.47	103.77	107.05
2	C	417	HEM	CAA-C2A-C1A	3.44	131.66	124.94
2	E	417	HEM	C2B-C1B-NB	-3.42	105.91	109.84
2	A	417	HEM	O2D-CGD-O1D	-3.42	114.53	123.33
2	C	417	HEM	C3B-C2B-C1B	-3.37	103.88	106.41
2	D	417	HEM	C4D-C3D-C2D	-3.30	102.09	106.89
2	C	417	HEM	CAD-C3D-C4D	3.29	130.44	124.70
2	C	417	HEM	CBA-CAA-C2A	-3.29	103.44	112.53
2	A	417	HEM	C4B-C3B-C2B	3.26	110.27	107.28
3	C	397	ID3	C17-C1-C6	-3.24	105.16	110.24
2	A	417	HEM	CBA-CAA-C2A	-3.22	103.63	112.53
2	D	417	HEM	CHD-C1D-ND	3.18	127.85	124.42
2	F	417	HEM	C2B-C1B-NB	-3.17	106.20	109.84
2	D	417	HEM	CHC-C4B-NB	3.12	127.79	124.42
2	E	417	HEM	CHB-C4A-NA	3.12	129.52	123.86
3	B	397	ID3	C1-C6-C7	3.08	124.01	115.65
2	E	417	HEM	CHD-C4C-NC	3.07	127.79	124.45
2	D	417	HEM	C4C-C3C-C2C	3.07	109.47	106.81
2	B	417	HEM	C2D-C1D-ND	-3.04	106.39	109.90
2	B	417	HEM	CBA-CAA-C2A	-3.02	104.19	112.53
2	A	417	HEM	CHD-C4C-NC	3.01	127.73	124.45
2	B	417	HEM	CAD-C3D-C4D	3.00	129.93	124.70
2	F	417	HEM	C1D-C2D-C3D	-3.00	103.83	106.98
2	D	417	HEM	C3C-C2C-C1C	-2.98	104.23	107.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	O2A-CGA-CBA	2.98	123.40	114.00
2	A	417	HEM	CAD-C3D-C4D	2.96	129.86	124.70
2	E	417	HEM	C3A-C4A-NA	-2.94	105.43	110.14
2	F	417	HEM	CMD-C2D-C1D	2.93	129.61	125.03
2	B	417	HEM	CMD-C2D-C1D	2.92	129.59	125.03
2	A	417	HEM	C4C-CHD-C1D	-2.82	120.02	126.02
2	B	417	HEM	O1A-CGA-CBA	-2.82	114.14	123.09
2	D	417	HEM	CMA-C3A-C2A	2.81	131.59	125.62
2	E	417	HEM	CAD-C3D-C2D	-2.67	122.86	127.87
2	C	417	HEM	CHC-C1C-NC	-2.66	121.55	124.45
2	C	417	HEM	C4B-C3B-C2B	2.64	109.71	107.28
2	D	417	HEM	C2D-C1D-ND	-2.64	106.85	109.90
2	D	417	HEM	CBB-CAB-C3B	-2.64	114.35	127.53
2	E	417	HEM	C4A-NA-C1A	2.61	110.08	105.82
2	A	417	HEM	CAC-C3C-C4C	-2.61	118.59	124.82
2	B	417	HEM	O2A-CGA-O1A	2.61	130.04	123.33
2	D	417	HEM	CMD-C2D-C1D	2.56	129.03	125.03
3	A	397	ID3	C2-C1-C6	2.56	114.15	110.44
2	E	417	HEM	C1B-NB-C4B	2.56	108.23	105.21
2	C	417	HEM	C4D-C3D-C2D	-2.55	103.18	106.89
2	B	417	HEM	C3B-C2B-C1B	-2.55	104.50	106.41
2	C	417	HEM	CMD-C2D-C1D	2.55	129.01	125.03
3	A	397	ID3	C7-C8-C9	2.54	129.28	124.56
2	A	417	HEM	C2D-C1D-ND	-2.53	106.98	109.90
2	E	417	HEM	O2A-CGA-CBA	2.49	121.87	114.00
2	B	417	HEM	CBB-CAB-C3B	-2.48	115.14	127.53
2	D	417	HEM	C4B-C3B-C2B	2.44	109.52	107.28
3	C	397	ID3	C16-C1-C6	-2.43	106.43	110.24
2	C	417	HEM	CAC-C3C-C4C	-2.37	119.16	124.82
2	A	417	HEM	O2A-CGA-O1A	-2.37	117.24	123.33
2	F	417	HEM	C1B-NB-C4B	2.37	108.01	105.21
2	C	417	HEM	O2A-CGA-CBA	2.34	121.38	114.00
2	F	417	HEM	C3A-C4A-NA	-2.31	106.44	110.14
2	A	417	HEM	C3B-C4B-NB	-2.29	107.82	109.47
2	B	417	HEM	C4D-C3D-C2D	-2.28	103.57	106.89
2	B	417	HEM	O2D-CGD-O1D	-2.25	117.54	123.33
3	A	397	ID3	O1-C9-C19	-2.23	115.82	119.32
2	F	417	HEM	O2A-CGA-CBA	2.23	121.03	114.00
2	A	417	HEM	C4A-CHB-C1B	-2.22	121.03	126.25
2	D	417	HEM	CMA-C3A-C4A	-2.18	122.10	125.42
2	F	417	HEM	CHB-C4A-NA	2.18	127.81	123.86
2	C	417	HEM	C4A-CHB-C1B	-2.18	121.13	126.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	417	HEM	C4C-NC-C1C	2.18	109.37	105.82
2	A	417	HEM	CAD-CBD-CGD	2.17	119.43	113.67
2	A	417	HEM	CBB-CAB-C3B	-2.17	116.69	127.53
2	A	417	HEM	CHD-C1D-ND	2.16	126.75	124.42
3	C	397	ID3	C1-C6-C7	2.15	121.49	115.65
3	A	397	ID3	C16-C1-C6	-2.13	106.90	110.24
2	F	417	HEM	O2D-CGD-CBD	2.10	120.63	114.00
2	F	417	HEM	CAA-CBA-CGA	2.09	119.22	113.67
2	F	417	HEM	CHD-C4C-C3C	2.09	128.74	125.21
2	C	417	HEM	O2A-CGA-O1A	-2.09	117.97	123.33
2	D	417	HEM	C3D-C4D-ND	2.07	112.45	110.17
3	B	397	ID3	C17-C1-C16	-2.07	102.72	108.63
2	A	417	HEM	C2B-C1B-NB	2.06	112.21	109.84
2	C	417	HEM	C4C-C3C-C2C	2.05	108.59	106.81
2	B	417	HEM	CAC-C3C-C4C	2.05	129.72	124.82
2	A	417	HEM	C4D-C3D-C2D	-2.04	103.92	106.89
2	D	417	HEM	CHA-C4D-C3D	-2.04	121.46	125.23
2	B	417	HEM	CHD-C1D-ND	2.03	126.61	124.42
2	B	417	HEM	CHA-C4D-C3D	-2.02	121.50	125.23
2	C	417	HEM	CHC-C4B-NB	2.01	126.59	124.42

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	417	HEM	C2C-C3C-CAC-CBC
2	D	417	HEM	C4C-C3C-CAC-CBC
2	E	417	HEM	C2C-C3C-CAC-CBC
2	E	417	HEM	C4C-C3C-CAC-CBC
2	F	417	HEM	C2C-C3C-CAC-CBC
3	A	397	ID3	C7-C8-C9-O1
3	A	397	ID3	C7-C8-C9-C19
3	B	397	ID3	C7-C8-C9-O1
3	B	397	ID3	C7-C8-C9-C19
3	C	397	ID3	C7-C8-C9-O1
3	C	397	ID3	C7-C8-C9-C19
3	B	397	ID3	C1-C6-C7-C8
3	B	397	ID3	C5-C6-C7-C8
3	C	397	ID3	C1-C6-C7-C8
3	C	397	ID3	C5-C6-C7-C8
2	F	417	HEM	C2B-C3B-CAB-CBB
2	F	417	HEM	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

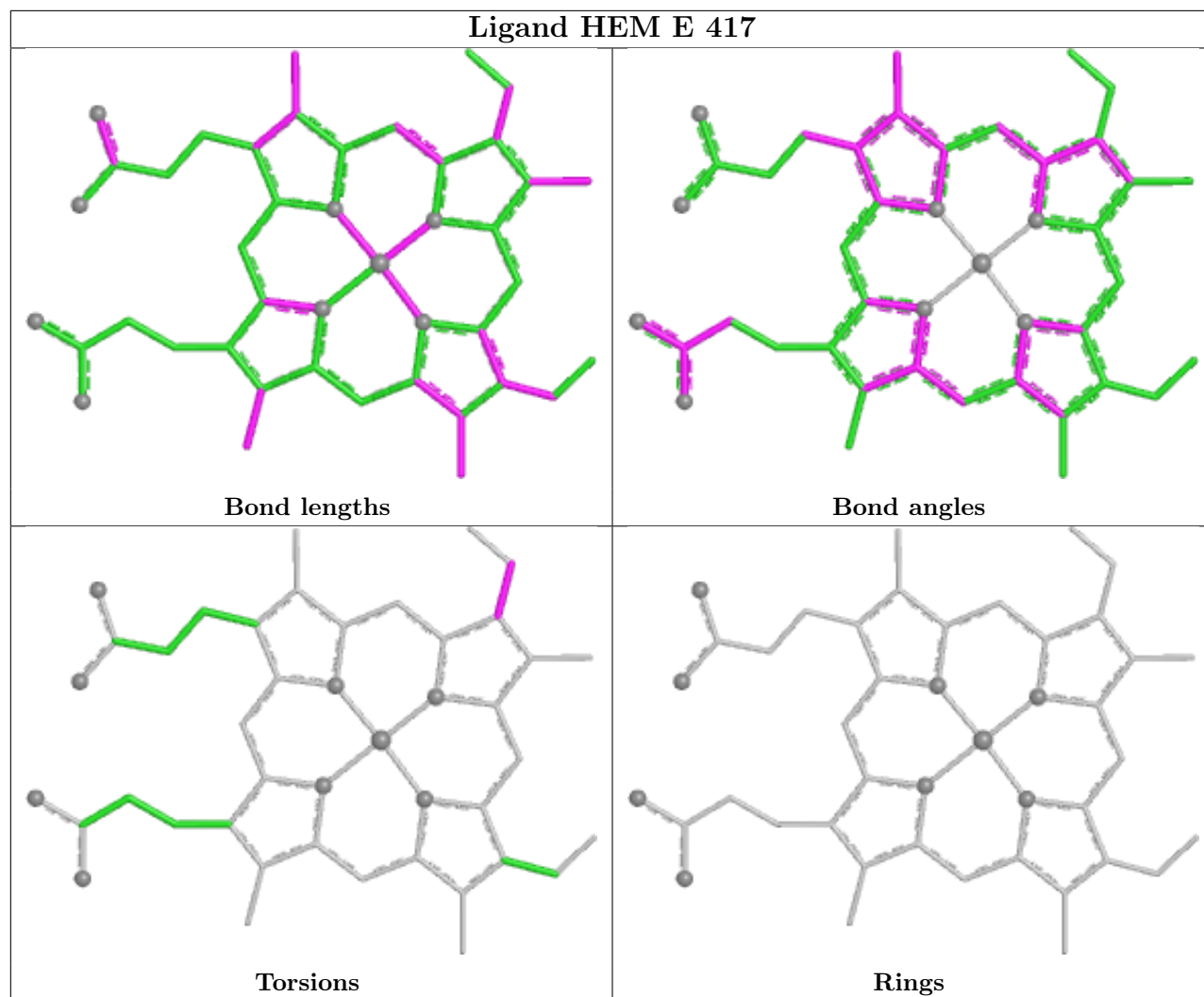
Mol	Chain	Res	Type	Atoms
2	F	417	HEM	C4C-C3C-CAC-CBC
2	C	417	HEM	C2C-C3C-CAC-CBC
2	B	417	HEM	C4C-C3C-CAC-CBC
2	B	417	HEM	C2C-C3C-CAC-CBC
2	C	417	HEM	CAA-CBA-CGA-O1A
2	A	417	HEM	C4B-C3B-CAB-CBB
2	C	417	HEM	C4B-C3B-CAB-CBB
2	C	417	HEM	C4C-C3C-CAC-CBC
2	C	417	HEM	CAA-CBA-CGA-O2A
2	A	417	HEM	CAA-CBA-CGA-O2A
2	A	417	HEM	C2B-C3B-CAB-CBB

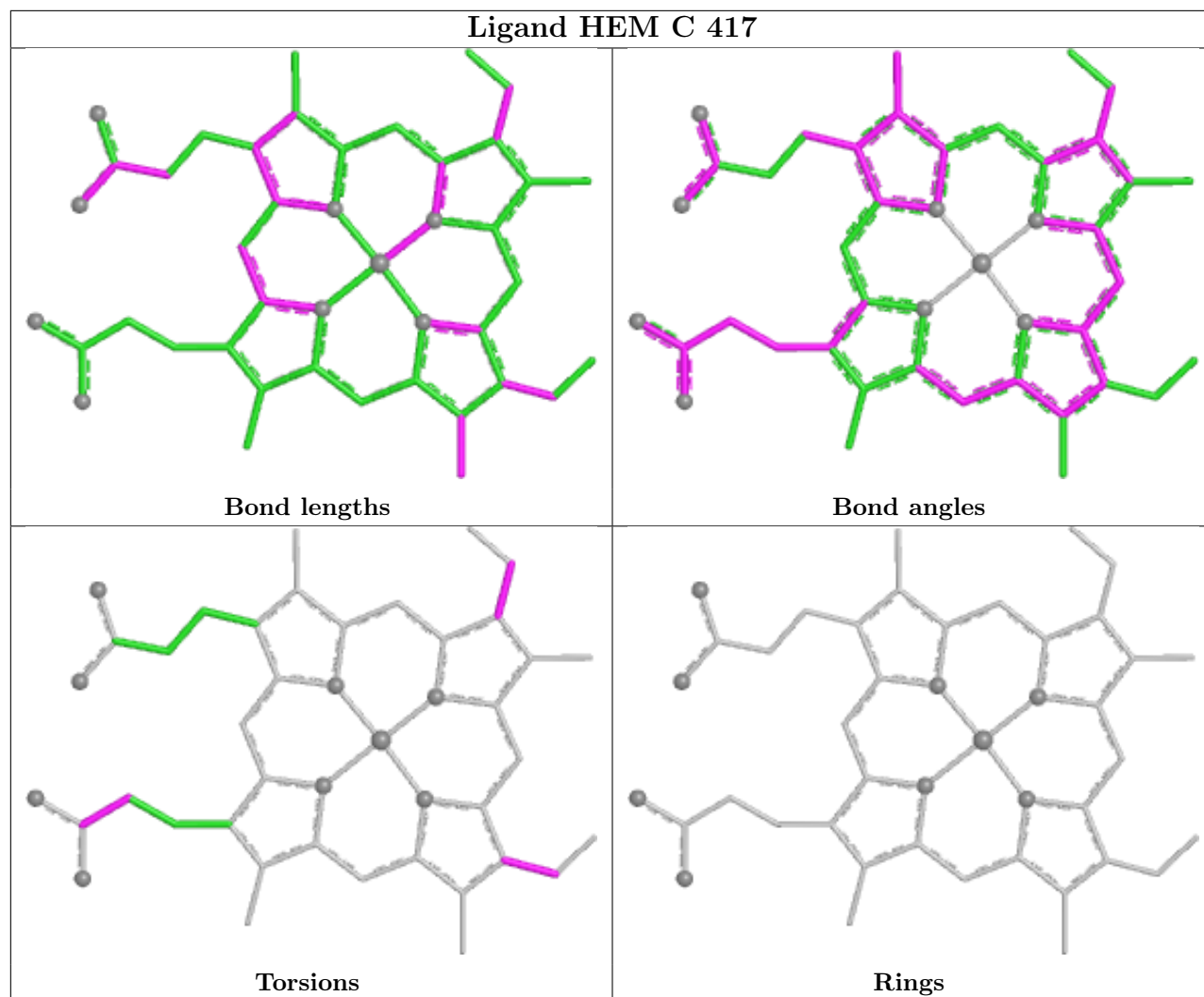
There are no ring outliers.

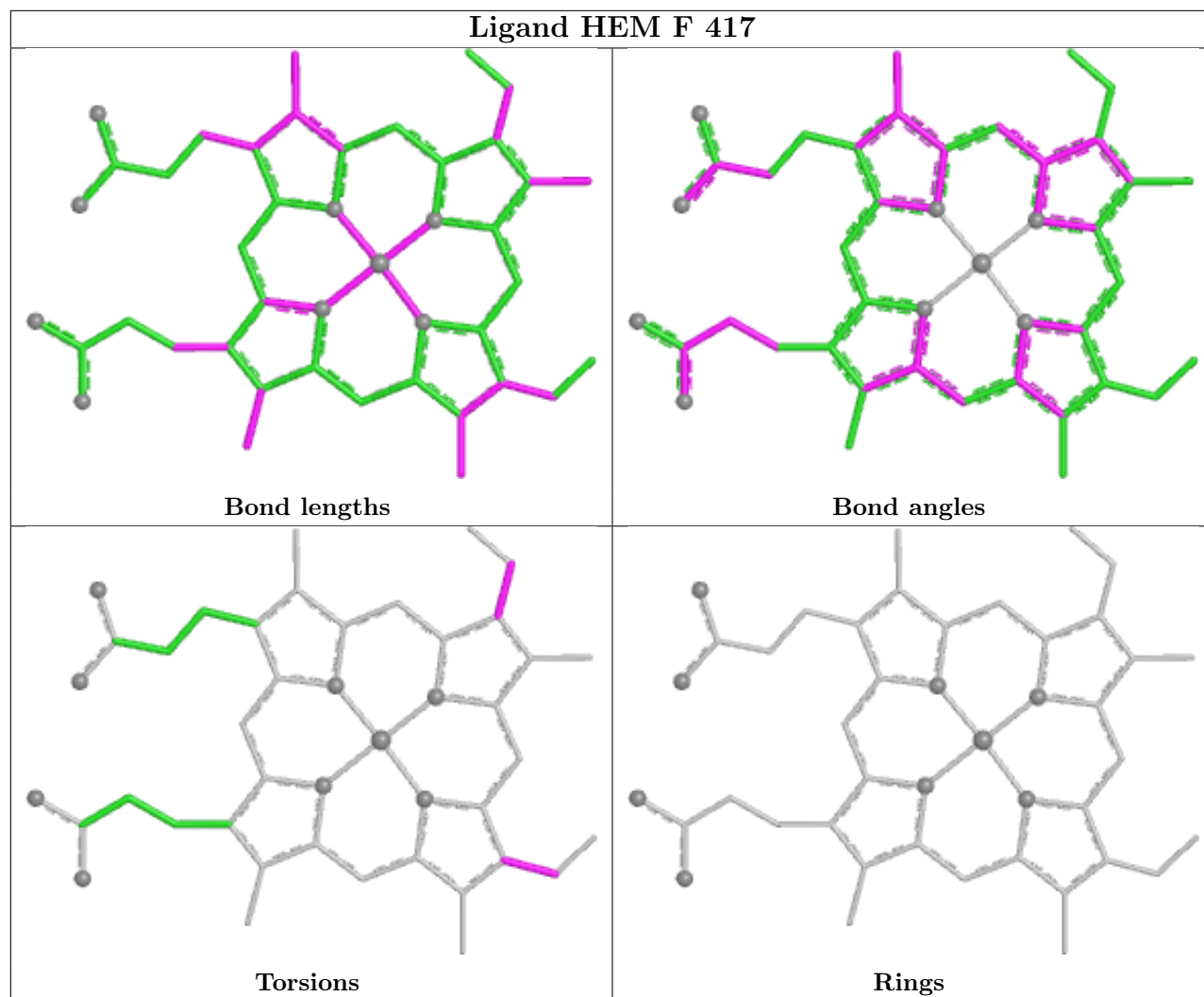
9 monomers are involved in 31 short contacts:

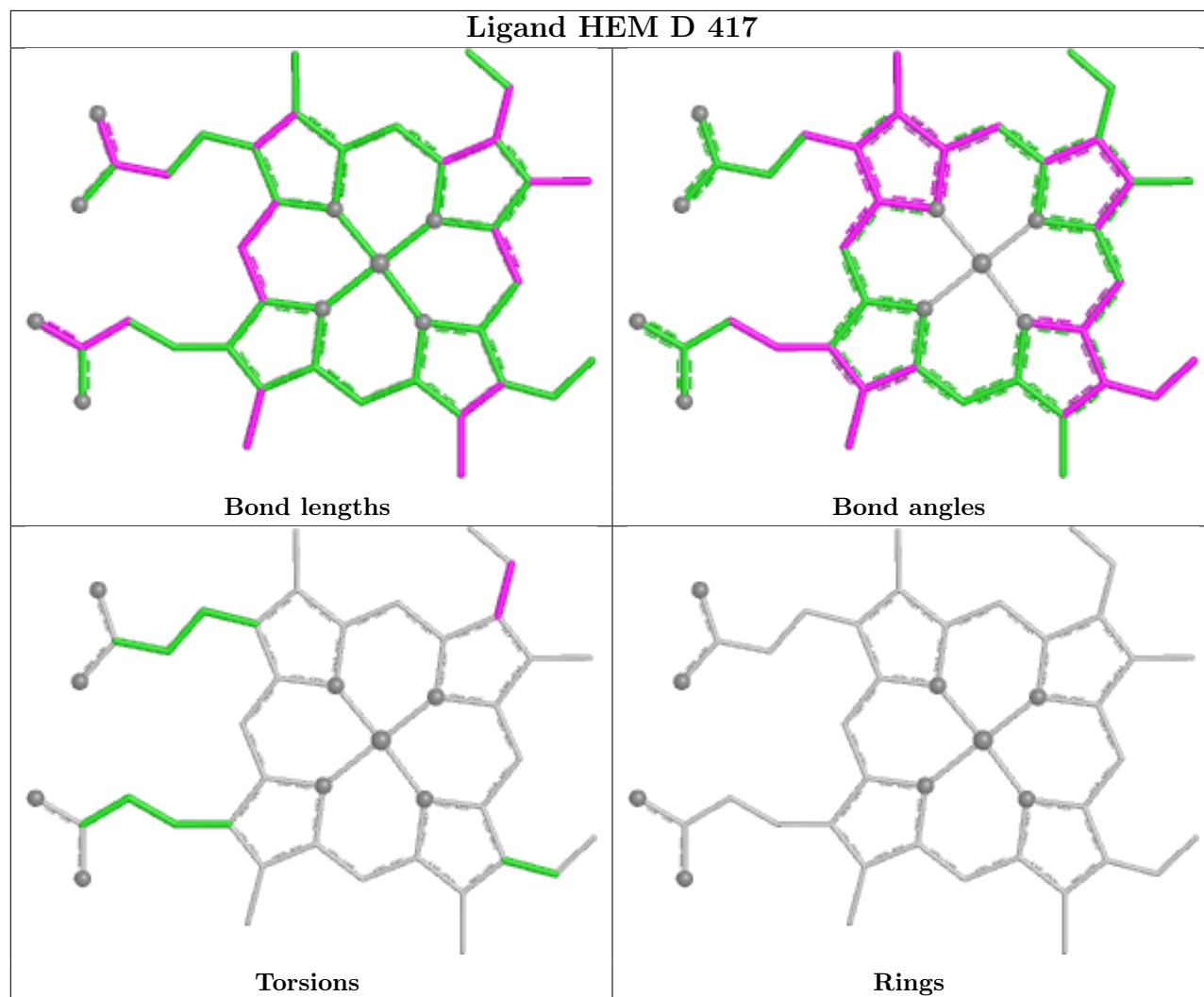
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	417	HEM	3	0
2	C	417	HEM	2	0
2	F	417	HEM	6	0
3	A	397	ID3	2	0
3	B	397	ID3	5	0
2	D	417	HEM	5	0
2	A	417	HEM	4	0
3	C	397	ID3	2	0
2	B	417	HEM	2	0

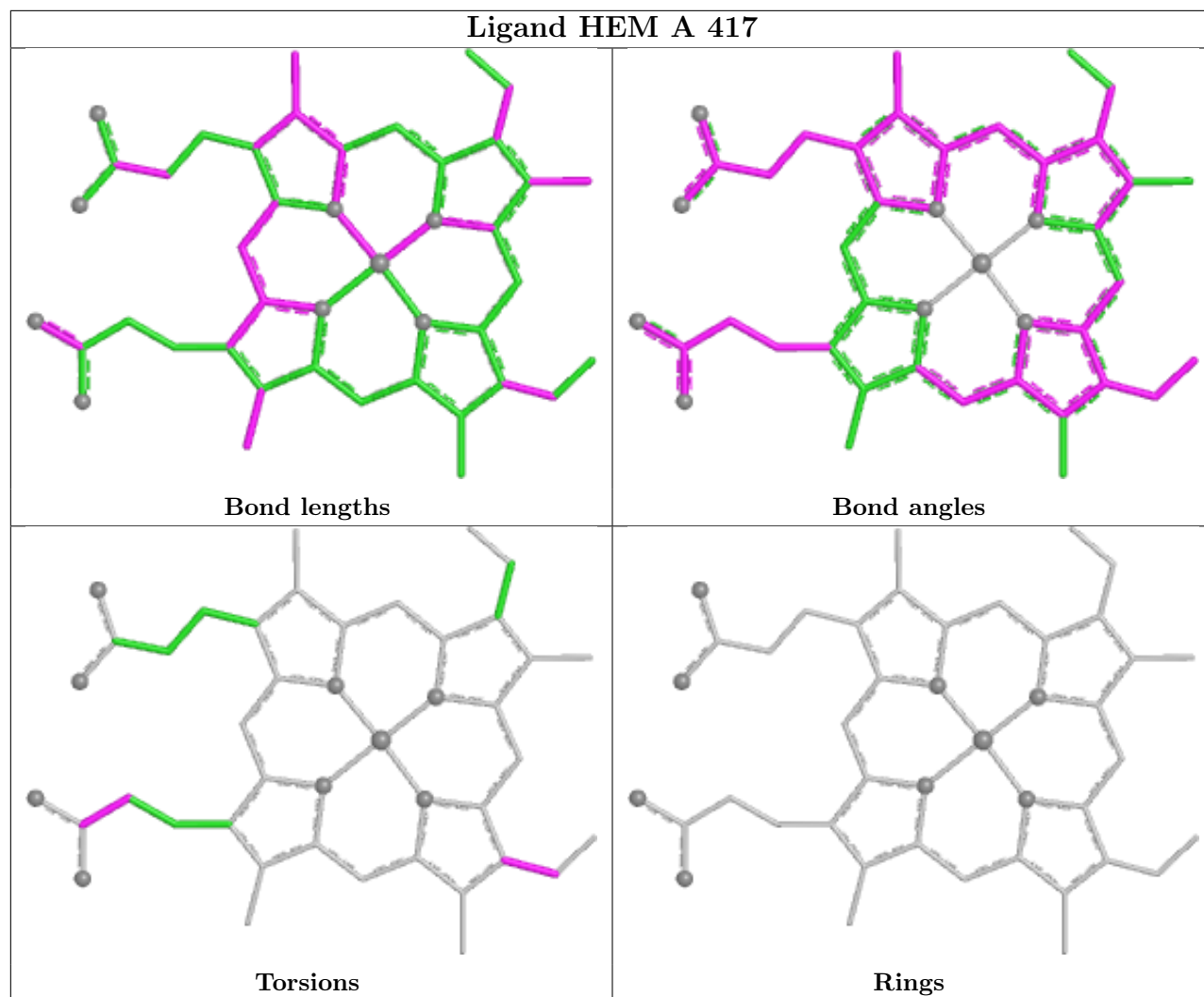
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

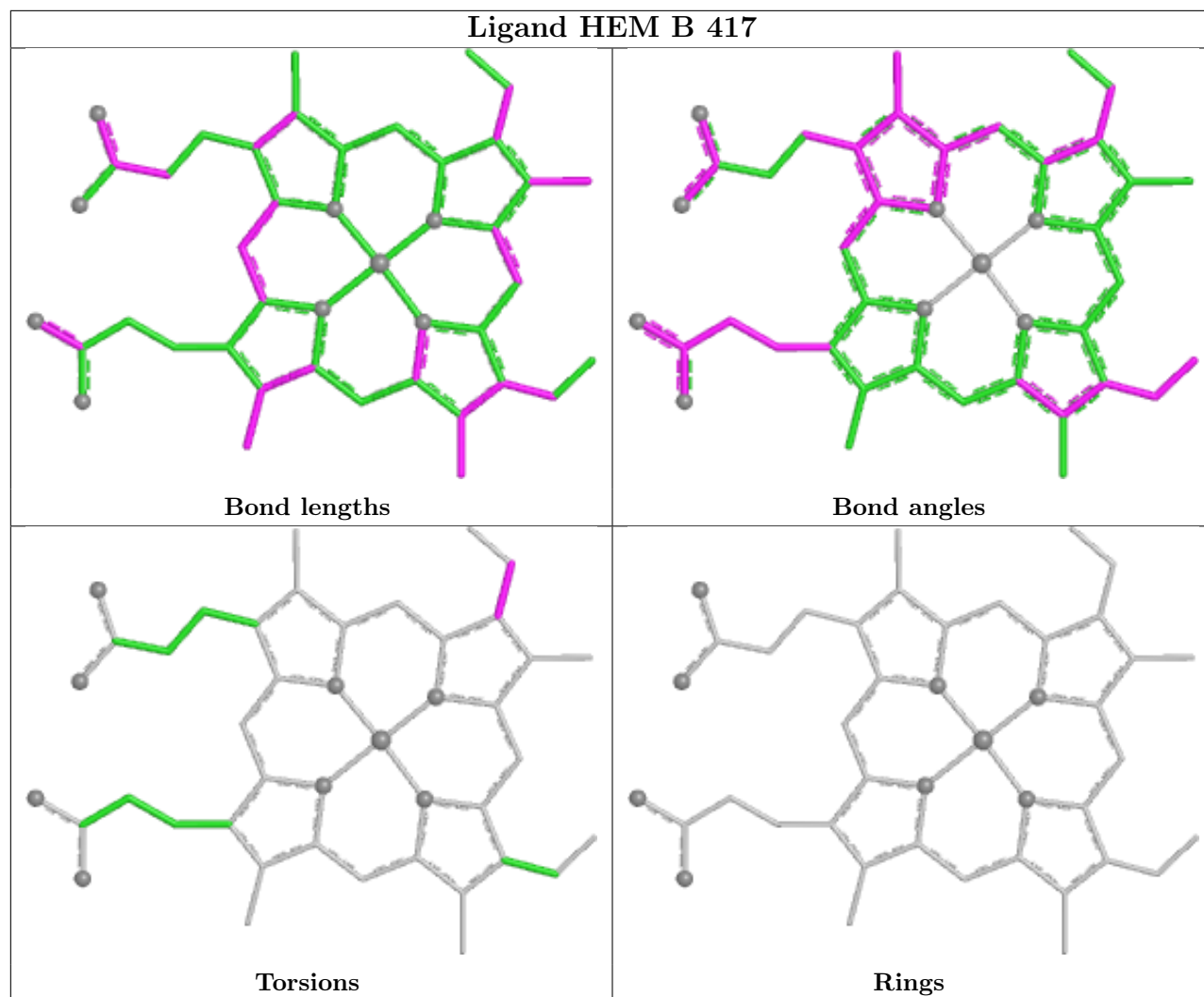












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/396 (100%)	-1.71	0 100 100	5, 17, 39, 75	0
1	B	396/396 (100%)	-1.70	0 100 100	6, 19, 44, 71	0
1	C	396/396 (100%)	-1.71	0 100 100	5, 18, 37, 80	0
1	D	394/396 (99%)	-1.69	0 100 100	7, 19, 43, 64	0
1	E	390/396 (98%)	-1.45	0 100 100	19, 38, 70, 78	0
1	F	390/396 (98%)	-1.46	0 100 100	22, 38, 67, 77	0
All	All	2362/2376 (99%)	-1.62	0 100 100	5, 23, 60, 80	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ID3	B	397	14/14	0.98	0.06	28,44,50,52	0

Continued on next page...

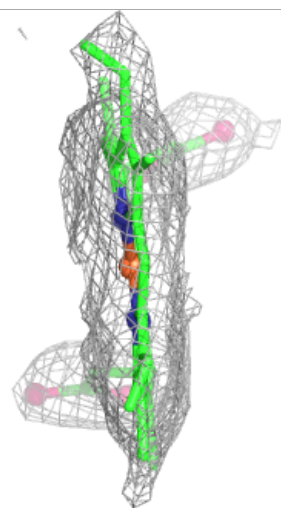
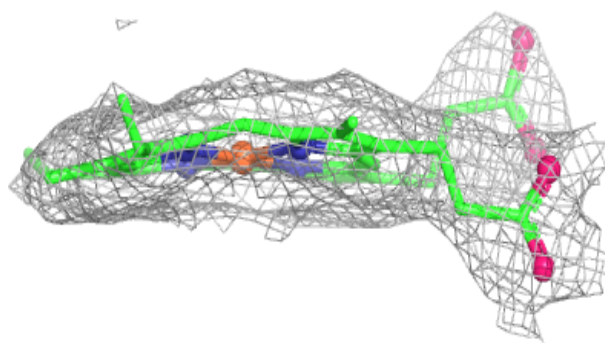
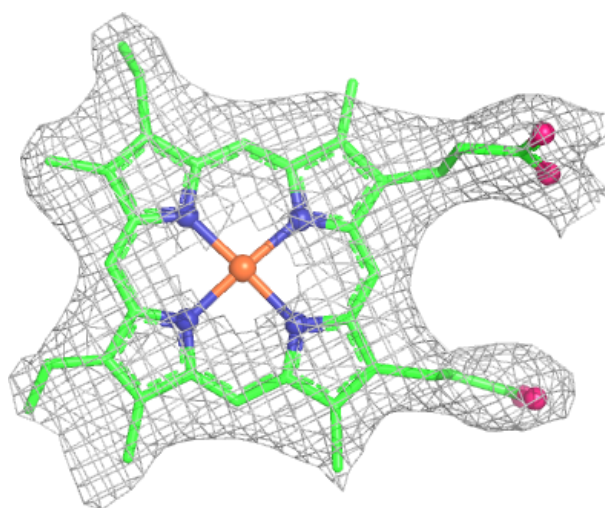
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ID3	C	397	14/14	0.98	0.08	54,59,63,65	14
3	ID3	A	397	14/14	0.99	0.05	31,41,43,43	0
2	HEM	D	417	43/43	1.00	0.02	3,12,18,27	0
2	HEM	E	417	43/43	1.00	0.03	17,24,29,32	0
2	HEM	F	417	43/43	1.00	0.03	13,22,27,32	0
2	HEM	A	417	43/43	1.00	0.03	2,7,14,17	0
2	HEM	B	417	43/43	1.00	0.02	3,10,16,22	0
2	HEM	C	417	43/43	1.00	0.03	2,10,16,21	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.

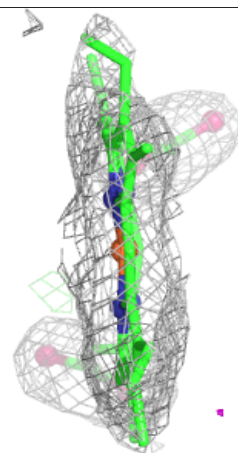
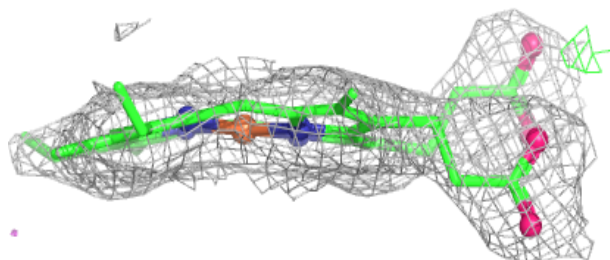
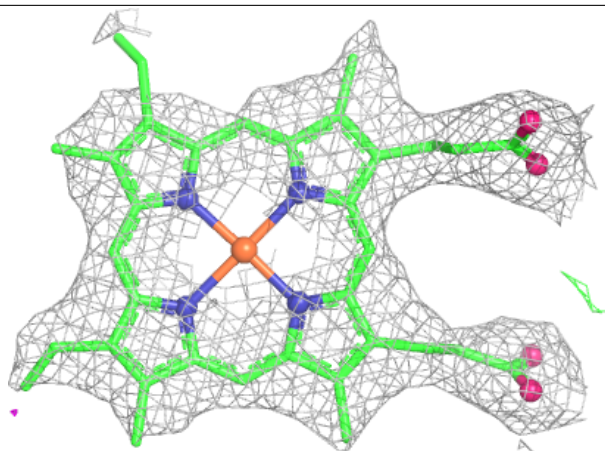
Electron density around HEM D 417:

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



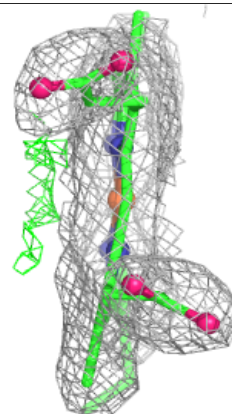
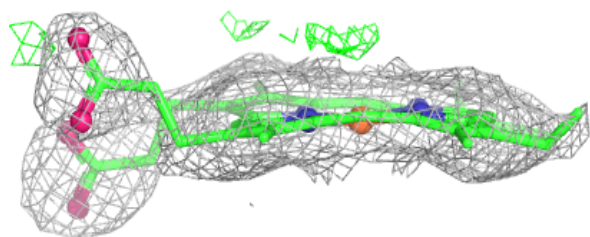
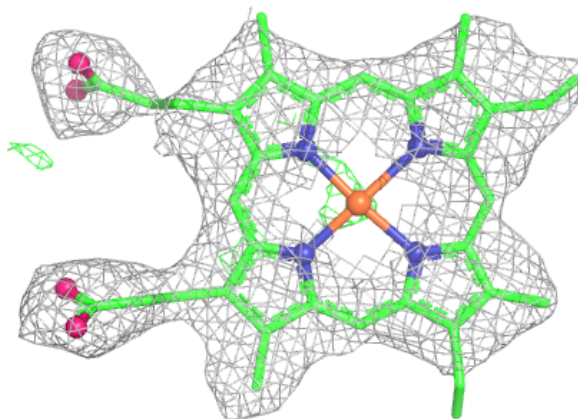
Electron density around HEM E 417:

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



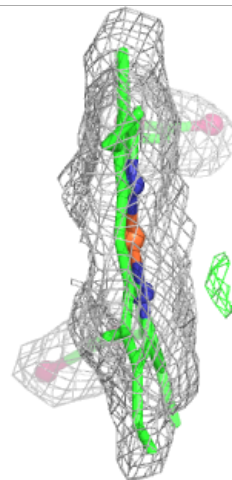
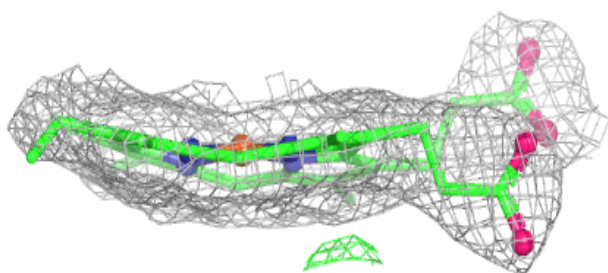
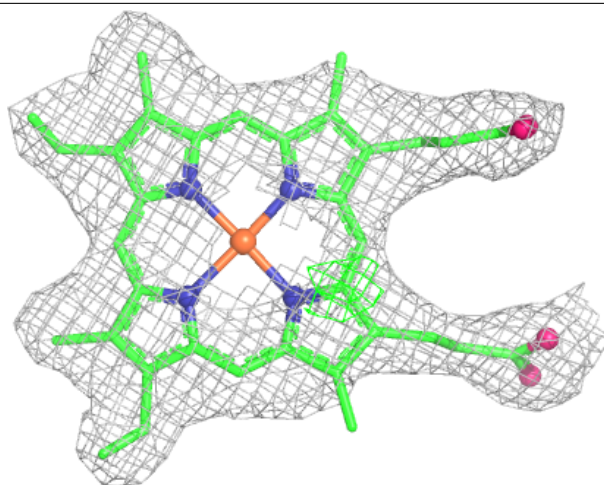
Electron density around HEM F 417:

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



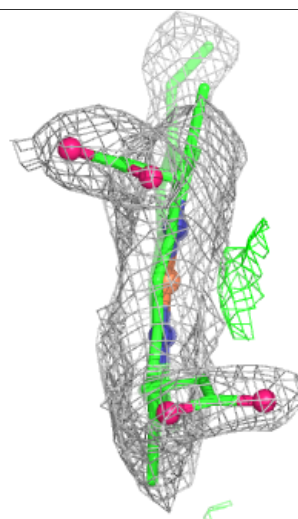
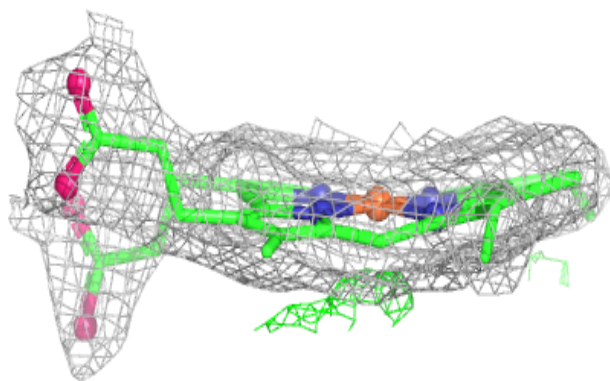
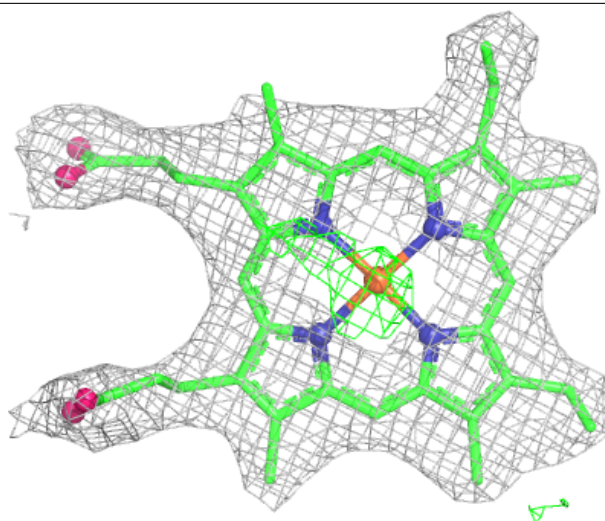
Electron density around HEM A 417:

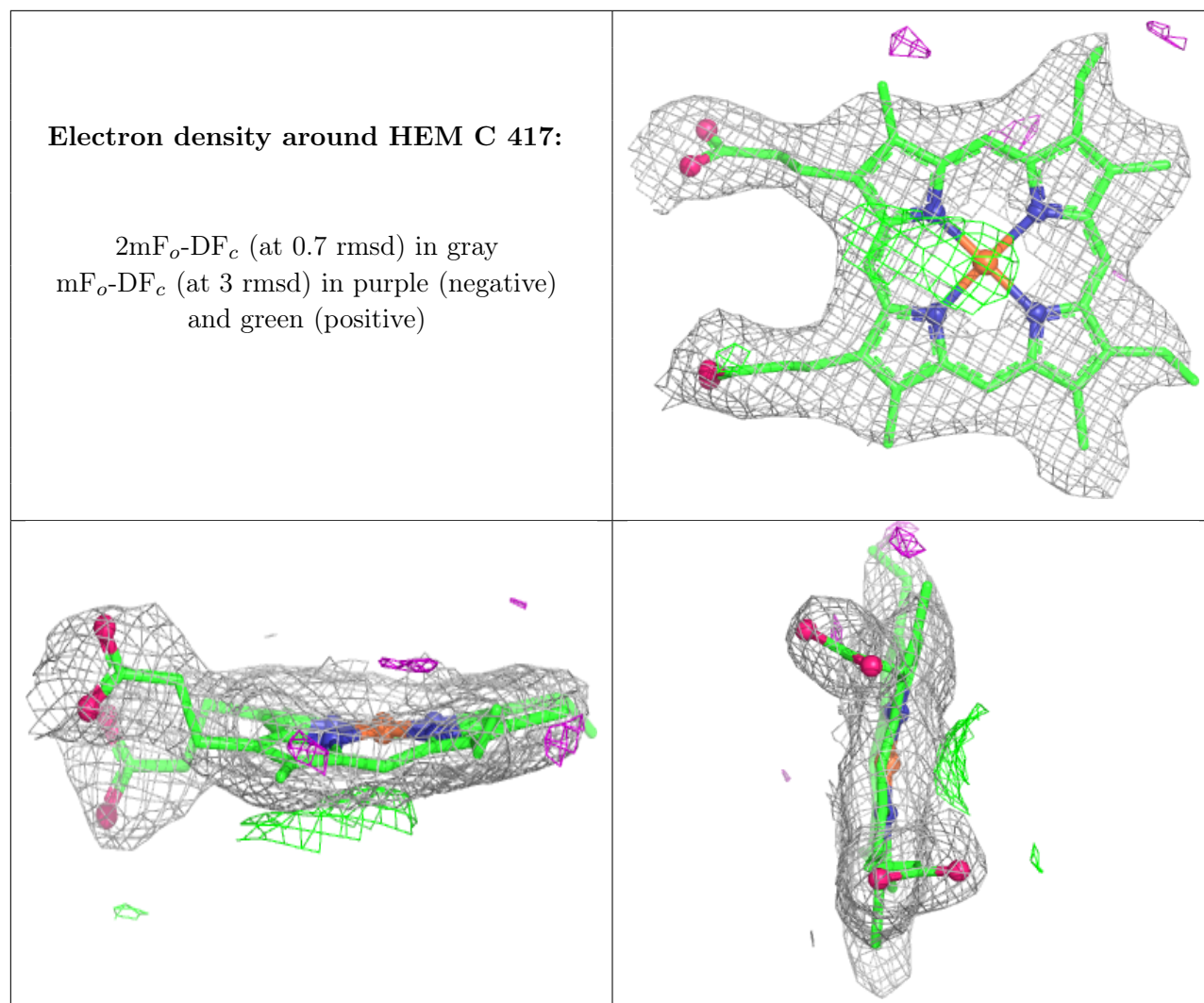
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 417:

$2mF_o-DF_c$ (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.