



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 AM UTC

PDB ID : 2H7S / pdb_00002h7s
Title : L244A mutant of Cytochrome P450cam
Authors : Verras, A.; Alian, A.; Montellano, P.R.
Deposited on : 2006-06-02
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

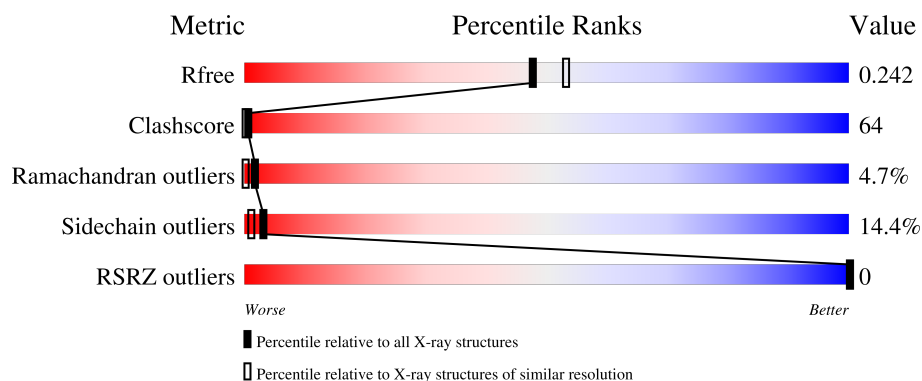
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	414	
1	C	414	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6696 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.

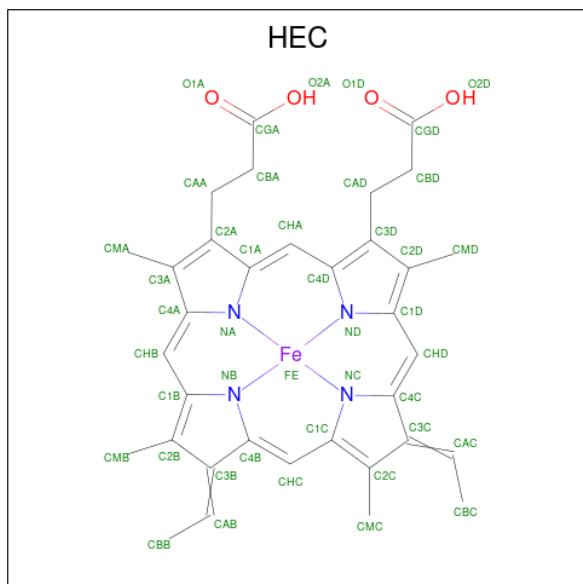
- Molecule 1 is a protein called Cytochrome P450-cam.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3201	2029	560	595	17			
1	C	405	Total	C	N	O	S	0	0	0
			3199	2026	559	597	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ALA	LEU	engineered mutation	UNP P00183
A	334	ALA	CYS	engineered mutation	UNP P00183
C	244	ALA	LEU	engineered mutation	UNP P00183
C	334	ALA	CYS	engineered mutation	UNP P00183

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 3 is water.

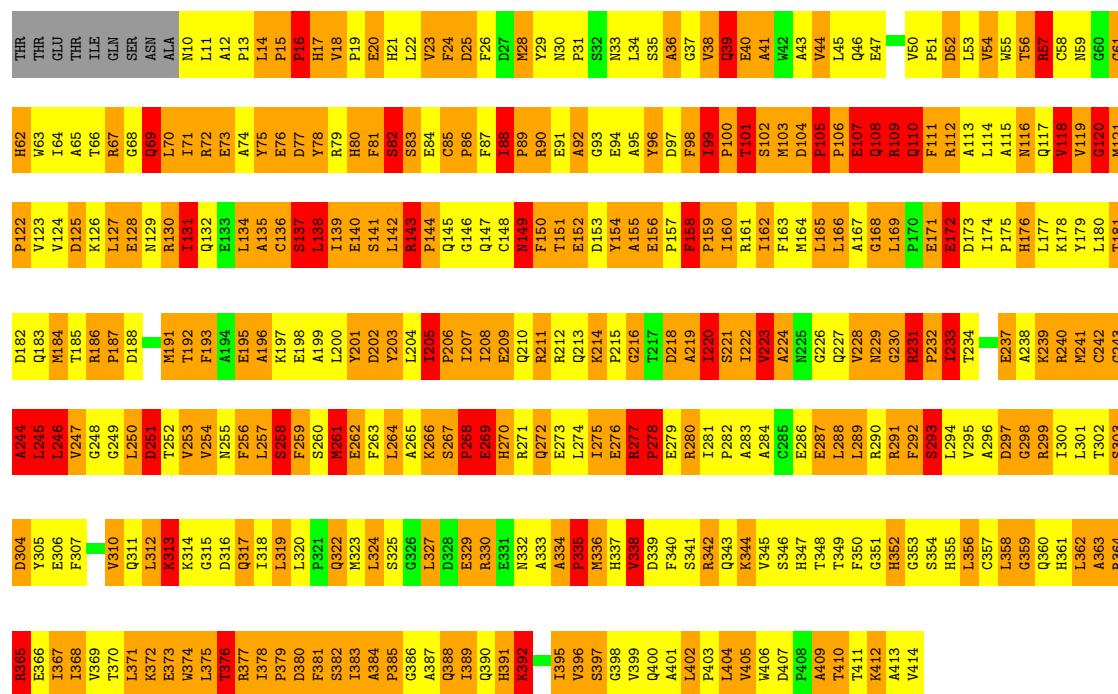
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total 111	O 111	25	0
3	C	99	Total 99	O 99	24	0

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.

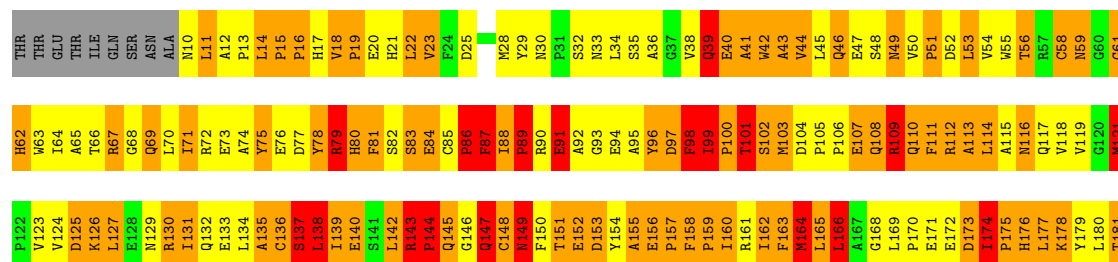
• Molecule 1: Cytochrome P450-cam

Chain A: 



• Molecule 1: Cytochrome P450-cam

Chain C: 



E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414																																																																																																																																																																																								
S303	D304	D304	D305	E306	F307		F310		G311	G312	G313	G314	G315	D316	F317	G318	F319	G320	F321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414																																																																																																																								
D182	E183	E184	E185	E186	E187	E188			E191	E192	E193	E194	E195	E196	E197	E198	E199	L200	L201	D202	F203	L204	L205	P206	L207	L208	E209	L210	L211	L212	L213	L214	L215	G216	G217	G218	L219	L220	L221	L222	L223	L224	L225	G226	G227	L228	L229	G230	G231	L232	L233	L234	S235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.70Å 59.85Å 114.12Å 90.00° 104.69° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 50.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.15) 80.3 (50.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.249 0.236 , 0.242	Depositor DCC
R_{free} test set	3755 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 13.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.407 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.391 for h,-k,-h-l	Depositor
Outliers	1 of 37909 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6696	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 52.41 % 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 4.8801e-05. 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: HEC

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	3.63	485/3280 (14.8%)	2.92	375/4456 (8.4%)
1	C	3.65	475/3278 (14.5%)	2.99	390/4454 (8.8%)
All	All	3.64	960/6558 (14.6%)	2.96	765/8910 (8.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	C	0	9
All	All	0	17

All (960) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	ALA	CA-CB	-21.65	1.19	1.53
1	A	367	ILE	N-CA	20.27	1.70	1.46
1	C	401	ALA	C-O	19.13	1.48	1.24
1	A	88	ILE	CA-C	18.28	1.72	1.52
1	A	96	TYR	CA-C	17.81	1.76	1.52
1	C	369	VAL	CA-CB	17.79	1.78	1.54
1	C	99	ILE	CA-CB	-17.59	1.31	1.54
1	C	113	ALA	CA-CB	-15.99	1.28	1.53
1	C	237	GLU	C-O	15.95	1.44	1.24
1	A	300	ILE	C-O	-15.62	1.07	1.24
1	C	291	ARG	N-CA	-15.59	1.27	1.46
1	A	257	LEU	CA-C	15.41	1.75	1.52
1	A	401	ALA	C-O	-15.07	1.05	1.23
1	A	228	VAL	C-O	-15.02	1.08	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	ARG	C-O	-14.90	1.06	1.24
1	C	403	PRO	CA-C	14.68	1.67	1.52
1	A	24	PHE	CA-C	14.67	1.70	1.52
1	A	118	VAL	C-O	-14.25	1.08	1.24
1	A	231	ARG	N-CA	13.99	1.58	1.45
1	C	185	THR	C-O	-13.83	1.05	1.24
1	C	394	GLY	N-CA	13.79	1.61	1.45
1	A	242	CYS	CA-C	13.77	1.71	1.52
1	C	139	ILE	CA-CB	13.66	1.72	1.54
1	C	79	ARG	CA-C	-13.64	1.33	1.52
1	C	151	THR	C-O	-13.61	1.08	1.24
1	C	112	ARG	N-CA	-13.42	1.28	1.46
1	C	82	SER	C-O	-13.41	1.08	1.23
1	A	231	ARG	CA-C	13.38	1.65	1.52
1	C	389	ILE	N-CA	-13.35	1.30	1.46
1	C	118	VAL	N-CA	13.30	1.62	1.46
1	C	146	GLY	N-CA	13.24	1.65	1.45
1	C	403	PRO	C-O	13.16	1.39	1.23
1	A	409	ALA	CA-CB	13.00	1.75	1.53
1	C	87	PHE	N-CA	12.92	1.62	1.45
1	C	85	CYS	C-O	-12.87	1.09	1.24
1	C	61	GLY	CA-C	-12.76	1.43	1.52
1	C	103	MET	CA-C	-12.72	1.37	1.52
1	C	389	ILE	CA-CB	-12.69	1.38	1.54
1	C	201	TYR	C-O	12.55	1.39	1.24
1	A	125	ASP	CA-C	-12.52	1.38	1.53
1	C	103	MET	CG-SD	-12.47	1.49	1.80
1	C	205	ILE	CA-C	12.47	1.66	1.52
1	A	253	VAL	CA-CB	-12.24	1.37	1.54
1	A	378	ILE	N-CA	11.99	1.61	1.46
1	A	205	ILE	N-CA	11.98	1.61	1.46
1	A	361	HIS	C-O	11.90	1.39	1.24
1	A	80	HIS	CA-CB	-11.75	1.35	1.53
1	A	65	ALA	CA-CB	11.71	1.70	1.53
1	C	158	PHE	C-O	11.56	1.35	1.24
1	C	265	ALA	C-O	11.55	1.38	1.24
1	A	283	ALA	N-CA	11.54	1.60	1.46
1	A	116	ASN	C-O	11.48	1.38	1.24
1	A	50	VAL	CA-CB	-11.48	1.44	1.54
1	A	99	ILE	CA-CB	11.42	1.69	1.54
1	C	86	PRO	CA-C	11.42	1.65	1.52
1	A	228	VAL	CA-C	-11.36	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	ARG	CZ-NH2	11.36	1.48	1.33
1	C	236	ASP	C-O	-11.35	1.10	1.24
1	A	18	VAL	CA-C	11.32	1.62	1.53
1	C	261	MET	N-CA	-11.31	1.31	1.46
1	A	280	ARG	CA-C	11.31	1.68	1.52
1	C	223	VAL	CA-CB	-11.23	1.41	1.54
1	A	254	VAL	N-CA	-11.22	1.32	1.46
1	C	131	ILE	CA-CB	11.18	1.69	1.54
1	C	155	ALA	N-CA	11.15	1.60	1.46
1	C	28	MET	CA-C	11.14	1.68	1.52
1	A	199	ALA	CA-CB	-11.13	1.36	1.53
1	A	43	ALA	C-O	-11.11	1.09	1.24
1	C	130	ARG	CZ-NH1	-11.08	1.17	1.32
1	C	277	ARG	N-CA	-11.06	1.35	1.46
1	C	78	TYR	CA-C	11.00	1.67	1.52
1	C	90	ARG	N-CA	10.98	1.59	1.46
1	C	41	ALA	N-CA	10.94	1.59	1.46
1	C	278	PRO	CA-C	-10.94	1.34	1.52
1	A	338	VAL	C-O	-10.92	1.11	1.24
1	C	354	SER	N-CA	10.90	1.60	1.46
1	C	259	PHE	C-O	10.86	1.36	1.24
1	A	310	VAL	CA-CB	10.83	1.68	1.54
1	A	66	THR	CA-CB	10.82	1.71	1.53
1	A	406	TRP	C-O	10.81	1.37	1.23
1	A	398	GLY	N-CA	10.78	1.56	1.45
1	C	301	LEU	CA-C	10.76	1.66	1.52
1	C	53	LEU	CA-C	-10.76	1.41	1.52
1	C	377	ARG	CA-C	10.74	1.66	1.52
1	A	113	ALA	N-CA	10.72	1.60	1.46
1	C	399	VAL	CB-CG2	10.72	1.88	1.52
1	A	342	ARG	CA-C	-10.70	1.39	1.52
1	C	292	PHE	CA-C	10.63	1.66	1.53
1	C	264	LEU	CA-CB	10.61	1.70	1.53
1	C	150	PHE	C-O	-10.61	1.11	1.24
1	A	284	ALA	CA-CB	-10.57	1.36	1.53
1	A	388	GLN	CA-C	10.56	1.65	1.52
1	C	401	ALA	CA-CB	-10.54	1.35	1.53
1	A	352	HIS	CA-C	10.50	1.65	1.52
1	C	258	SER	N-CA	10.50	1.59	1.46
1	A	103	MET	N-CA	10.48	1.58	1.45
1	A	409	ALA	CA-C	10.44	1.66	1.52
1	C	138	LEU	N-CA	10.36	1.59	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	ASN	C-O	-10.31	1.10	1.24
1	A	59	ASN	C-O	10.31	1.37	1.23
1	C	307	PHE	C-O	-10.30	1.11	1.24
1	C	327	LEU	N-CA	-10.30	1.32	1.46
1	C	402	LEU	CA-C	10.26	1.65	1.52
1	A	227	GLN	CA-C	-10.22	1.40	1.52
1	A	134	LEU	CG-CD1	10.21	1.86	1.52
1	C	182	ASP	C-O	10.19	1.36	1.24
1	C	253	VAL	CA-CB	10.18	1.67	1.54
1	C	154	TYR	C-O	10.14	1.36	1.24
1	C	335	PRO	CB-CG	10.13	2.00	1.49
1	A	380	ASP	N-CA	-10.09	1.34	1.46
1	C	73	GLU	CA-C	10.08	1.65	1.52
1	A	276	GLU	CA-C	-10.07	1.40	1.52
1	C	158	PHE	N-CA	-10.07	1.39	1.46
1	C	159	PRO	C-O	10.07	1.36	1.24
1	C	378	ILE	CA-C	-10.06	1.42	1.52
1	C	97	ASP	C-O	10.00	1.36	1.24
1	A	77	ASP	CA-C	9.94	1.64	1.53
1	A	108	GLN	CA-C	-9.91	1.38	1.52
1	C	42	TRP	CA-C	-9.90	1.39	1.52
1	C	92	ALA	CA-CB	9.90	1.69	1.53
1	A	307	PHE	C-O	-9.90	1.12	1.24
1	A	337	HIS	CA-CB	9.87	1.65	1.53
1	A	18	VAL	CA-CB	9.84	1.64	1.53
1	C	130	ARG	C-O	9.82	1.36	1.24
1	C	84	GLU	CA-C	9.81	1.67	1.52
1	A	333	ALA	N-CA	9.75	1.58	1.46
1	A	80	HIS	C-O	9.73	1.36	1.24
1	A	387	ALA	CA-CB	9.73	1.67	1.53
1	C	338	VAL	N-CA	9.71	1.58	1.46
1	C	265	ALA	CA-CB	-9.70	1.37	1.53
1	A	252	THR	C-O	9.69	1.35	1.23
1	C	68	GLY	C-O	9.69	1.35	1.23
1	C	273	GLU	N-CA	-9.61	1.34	1.46
1	A	389	ILE	CB-CG2	9.60	1.84	1.52
1	A	157	PRO	C-O	-9.58	1.12	1.24
1	A	254	VAL	CA-C	-9.56	1.39	1.52
1	C	225	ASN	C-N	-9.48	1.23	1.33
1	A	385	PRO	C-O	9.48	1.34	1.23
1	A	162	ILE	CA-C	9.44	1.64	1.52
1	C	149	ASN	CA-CB	9.43	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	LEU	N-CA	-9.43	1.36	1.46
1	C	112	ARG	CG-CD	9.42	1.80	1.52
1	C	365	ARG	N-CA	9.40	1.57	1.46
1	C	345	VAL	CA-CB	9.40	1.63	1.53
1	A	188	ASP	C-O	9.39	1.36	1.24
1	C	284	ALA	C-O	9.39	1.35	1.24
1	A	264	LEU	CG-CD2	9.37	1.83	1.52
1	C	277	ARG	C-N	9.33	1.45	1.33
1	A	151	THR	N-CA	9.31	1.58	1.46
1	C	263	PHE	C-O	-9.30	1.13	1.24
1	A	228	VAL	CA-CB	9.28	1.71	1.55
1	C	363	ALA	CA-CB	-9.26	1.37	1.53
1	A	123	VAL	CA-C	9.24	1.65	1.52
1	C	78	TYR	C-O	9.24	1.35	1.24
1	A	118	VAL	N-CA	-9.23	1.34	1.46
1	C	362	LEU	C-N	-9.22	1.20	1.33
1	C	206	PRO	C-O	-9.19	1.12	1.24
1	A	71	ILE	C-O	9.18	1.34	1.24
1	C	196	ALA	CA-CB	-9.16	1.39	1.53
1	C	294	LEU	N-CA	-9.14	1.39	1.47
1	C	97	ASP	CA-C	-9.14	1.42	1.52
1	C	220	ILE	N-CA	9.12	1.57	1.46
1	C	153	ASP	CA-C	9.12	1.65	1.52
1	A	101	THR	CB-CG2	-9.10	1.22	1.52
1	C	389	ILE	CB-CG2	9.10	1.82	1.52
1	A	240	ARG	CG-CD	9.02	1.79	1.52
1	A	266	LYS	N-CA	9.00	1.57	1.46
1	C	16	PRO	CA-C	-9.00	1.39	1.52
1	A	135	ALA	C-O	-8.98	1.13	1.24
1	C	103	MET	N-CA	8.98	1.57	1.45
1	C	242	CYS	CA-C	8.98	1.64	1.52
1	C	174	ILE	CA-CB	8.96	1.65	1.54
1	C	250	LEU	C-O	8.94	1.36	1.24
1	C	182	ASP	CA-C	8.94	1.64	1.52
1	C	373	GLU	CD-OE1	8.88	1.42	1.25
1	A	296	ALA	CA-C	-8.87	1.43	1.52
1	A	81	PHE	N-CA	8.87	1.57	1.46
1	A	357	CYS	C-O	8.86	1.35	1.23
1	C	203	TYR	CA-C	8.85	1.64	1.52
1	A	168	GLY	N-CA	8.84	1.58	1.45
1	A	410	THR	N-CA	8.84	1.56	1.46
1	C	18	VAL	CA-CB	8.84	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	367	ILE	C-O	-8.83	1.13	1.24
1	C	356	LEU	CB-CG	8.82	1.71	1.53
1	C	245	LEU	CA-CB	-8.82	1.38	1.53
1	A	155	ALA	CA-CB	-8.80	1.39	1.53
1	A	77	ASP	CG-OD1	-8.78	1.08	1.25
1	A	402	LEU	CA-CB	8.77	1.67	1.53
1	C	22	LEU	C-O	8.76	1.35	1.24
1	A	277	ARG	CA-C	8.76	1.63	1.52
1	C	119	VAL	CA-CB	-8.74	1.44	1.54
1	A	392	LYS	CA-C	-8.74	1.42	1.52
1	C	80	HIS	CA-CB	8.73	1.67	1.53
1	A	18	VAL	N-CA	8.71	1.52	1.46
1	C	407	ASP	CA-C	8.71	1.63	1.52
1	A	250	LEU	CA-C	8.70	1.64	1.52
1	A	397	SER	CA-CB	8.68	1.67	1.53
1	A	135	ALA	CA-CB	8.68	1.66	1.53
1	A	67	ARG	N-CA	8.68	1.56	1.46
1	A	247	VAL	N-CA	8.67	1.57	1.46
1	C	296	ALA	CA-CB	8.65	1.65	1.52
1	C	234	THR	CA-CB	8.65	1.67	1.53
1	A	346	SER	C-O	-8.64	1.13	1.24
1	A	350	PHE	C-O	8.61	1.35	1.24
1	C	265	ALA	N-CA	8.60	1.57	1.46
1	A	334	ALA	CA-C	8.60	1.63	1.52
1	C	340	PHE	C-O	-8.56	1.13	1.24
1	C	34	LEU	CA-C	8.55	1.64	1.52
1	A	219	ALA	CA-CB	-8.55	1.39	1.53
1	C	387	ALA	CA-CB	-8.52	1.38	1.53
1	C	204	LEU	N-CA	-8.51	1.35	1.46
1	C	245	LEU	CA-C	8.50	1.64	1.52
1	A	143	ARG	C-O	-8.50	1.16	1.24
1	C	86	PRO	N-CA	-8.50	1.38	1.47
1	C	102	SER	CA-C	-8.50	1.40	1.52
1	A	339	ASP	N-CA	8.47	1.56	1.46
1	C	159	PRO	CA-CB	8.45	1.66	1.53
1	A	307	PHE	CA-C	-8.45	1.42	1.52
1	C	401	ALA	N-CA	-8.45	1.35	1.46
1	C	246	LEU	N-CA	8.44	1.57	1.46
1	C	114	LEU	N-CA	8.42	1.56	1.46
1	C	181	THR	CA-CB	-8.42	1.40	1.53
1	C	388	GLN	C-O	-8.41	1.14	1.24
1	A	316	ASP	N-CA	8.39	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	ALA	CA-C	-8.39	1.41	1.52
1	A	104	ASP	C-O	-8.39	1.13	1.24
1	C	205	ILE	N-CA	-8.38	1.36	1.46
1	A	319	LEU	CA-C	8.38	1.64	1.52
1	C	254	VAL	CB-CG1	8.36	1.80	1.52
1	A	387	ALA	C-O	8.32	1.34	1.24
1	A	205	ILE	CB-CG2	8.30	1.79	1.52
1	A	376	THR	CA-C	8.29	1.63	1.52
1	C	342	ARG	CA-C	-8.29	1.41	1.52
1	C	93	GLY	C-O	-8.29	1.14	1.23
1	A	256	PHE	C-O	8.28	1.33	1.24
1	A	296	ALA	C-O	-8.27	1.13	1.23
1	A	389	ILE	N-CA	8.27	1.56	1.46
1	C	129	ASN	N-CA	-8.26	1.36	1.46
1	C	145	GLN	CG-CD	-8.25	1.31	1.52
1	C	132	GLN	C-O	8.24	1.34	1.24
1	A	390	GLN	CA-C	8.22	1.62	1.52
1	A	253	VAL	CA-C	8.22	1.63	1.52
1	C	254	VAL	CA-CB	-8.22	1.45	1.54
1	A	96	TYR	C-O	8.20	1.34	1.24
1	A	204	LEU	CA-C	-8.19	1.41	1.52
1	A	348	THR	N-CA	-8.19	1.36	1.46
1	A	192	THR	N-CA	8.19	1.56	1.45
1	A	358	LEU	N-CA	8.18	1.56	1.46
1	A	405	VAL	CA-CB	8.15	1.66	1.54
1	C	110	GLN	CA-C	8.13	1.64	1.52
1	A	297	ASP	C-O	-8.13	1.14	1.24
1	A	400	GLN	C-O	-8.12	1.14	1.24
1	A	315	GLY	C-O	-8.12	1.12	1.24
1	C	109	ARG	N-CA	-8.11	1.36	1.46
1	C	398	GLY	N-CA	8.10	1.54	1.45
1	A	79	ARG	C-O	-8.09	1.13	1.24
1	A	378	ILE	CA-C	-8.08	1.44	1.52
1	A	239	LYS	CA-C	8.08	1.63	1.52
1	A	318	ILE	C-O	8.07	1.32	1.24
1	C	315	GLY	C-O	-8.05	1.12	1.24
1	A	163	PHE	C-O	-8.05	1.14	1.24
1	A	231	ARG	CZ-NH1	8.05	1.44	1.32
1	C	156	GLU	C-O	8.04	1.34	1.24
1	C	92	ALA	CA-C	8.04	1.62	1.52
1	C	285	CYS	CA-CB	8.04	1.66	1.53
1	A	90	ARG	C-O	-8.04	1.13	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	GLU	C-O	-8.03	1.14	1.24
1	C	183	GLN	C-O	-8.02	1.14	1.24
1	A	92	ALA	C-O	-8.02	1.14	1.24
1	A	124	VAL	CA-CB	8.01	1.64	1.54
1	C	372	LYS	C-O	8.01	1.33	1.24
1	A	111	PHE	N-CA	-8.01	1.35	1.46
1	C	411	THR	CA-CB	8.00	1.65	1.53
1	C	303	SER	CA-C	7.99	1.62	1.52
1	C	175	PRO	CA-C	7.99	1.63	1.52
1	A	165	LEU	CA-C	7.98	1.62	1.52
1	C	383	ILE	C-O	-7.97	1.13	1.24
1	A	262	GLU	N-CA	-7.97	1.35	1.46
1	A	169	LEU	C-O	-7.96	1.13	1.23
1	C	324	LEU	N-CA	7.96	1.56	1.46
1	A	101	THR	C-O	7.95	1.34	1.24
1	C	260	SER	CA-CB	7.95	1.66	1.53
1	A	305	TYR	C-O	7.93	1.34	1.23
1	A	290	ARG	CA-C	7.91	1.62	1.52
1	C	136	CYS	CA-C	-7.91	1.42	1.52
1	C	306	GLU	C-O	-7.90	1.13	1.23
1	C	79	ARG	C-N	7.89	1.45	1.33
1	C	113	ALA	C-O	7.88	1.33	1.24
1	A	389	ILE	C-O	7.83	1.31	1.24
1	C	257	LEU	C-O	7.81	1.33	1.24
1	C	175	PRO	C-O	7.79	1.34	1.24
1	A	264	LEU	C-O	7.78	1.33	1.24
1	C	75	TYR	CA-C	-7.78	1.42	1.52
1	A	385	PRO	CB-CG	7.77	1.88	1.49
1	A	141	SER	C-O	7.76	1.33	1.24
1	A	104	ASP	CA-C	-7.76	1.42	1.53
1	C	19	PRO	N-CA	-7.76	1.38	1.46
1	A	84	GLU	CA-C	7.73	1.63	1.52
1	A	102	SER	CA-C	7.72	1.63	1.52
1	A	298	GLY	C-O	7.72	1.34	1.23
1	C	373	GLU	CB-CG	7.71	1.75	1.52
1	C	131	ILE	CB-CG2	7.71	1.77	1.52
1	A	114	LEU	CA-C	-7.70	1.42	1.52
1	A	40	GLU	CD-OE1	7.68	1.40	1.25
1	A	112	ARG	C-O	7.68	1.33	1.24
1	A	39	GLN	CA-C	7.68	1.63	1.52
1	C	221	SER	CA-C	7.67	1.62	1.52
1	A	269	GLU	C-O	-7.66	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	196	ALA	N-CA	7.65	1.55	1.46
1	A	223	VAL	CA-C	-7.65	1.43	1.52
1	A	263	PHE	CA-C	-7.65	1.42	1.52
1	C	366	GLU	CA-C	7.65	1.63	1.52
1	C	98	PHE	N-CA	7.63	1.56	1.46
1	A	234	THR	CA-C	-7.63	1.42	1.53
1	C	385	PRO	C-O	7.62	1.33	1.24
1	C	339	ASP	CA-C	7.62	1.61	1.52
1	A	98	PHE	C-N	-7.61	1.24	1.33
1	A	65	ALA	C-O	7.61	1.33	1.23
1	C	378	ILE	C-N	7.60	1.41	1.33
1	A	364	ARG	C-O	7.60	1.32	1.24
1	A	244	ALA	C-O	7.59	1.33	1.24
1	A	317	GLN	N-CA	7.59	1.54	1.45
1	C	362	LEU	CA-C	-7.58	1.43	1.52
1	C	124	VAL	CA-C	7.55	1.63	1.52
1	A	413	ALA	CA-C	7.54	1.62	1.52
1	A	150	PHE	N-CA	7.54	1.55	1.46
1	C	264	LEU	CA-C	-7.53	1.42	1.52
1	A	263	PHE	CB-CG	-7.51	1.33	1.50
1	A	38	VAL	CA-CB	-7.50	1.44	1.54
1	C	87	PHE	C-N	7.50	1.41	1.33
1	A	227	GLN	CG-CD	-7.50	1.33	1.52
1	C	76	GLU	N-CA	7.49	1.55	1.46
1	A	229	ASN	N-CA	-7.48	1.36	1.46
1	A	291	ARG	N-CA	-7.48	1.37	1.46
1	A	401	ALA	CA-CB	7.47	1.66	1.53
1	C	104	ASP	N-CA	7.46	1.57	1.45
1	A	336	MET	CG-SD	7.46	1.99	1.80
1	C	200	LEU	N-CA	-7.45	1.36	1.46
1	A	82	SER	C-O	-7.44	1.14	1.23
1	A	243	GLY	N-CA	-7.44	1.34	1.45
1	A	288	LEU	C-O	-7.43	1.15	1.24
1	A	346	SER	CA-C	7.43	1.62	1.52
1	C	355	HIS	CA-C	7.42	1.62	1.52
1	C	397	SER	C-O	7.42	1.33	1.23
1	A	83	SER	N-CA	7.41	1.56	1.46
1	A	391	HIS	N-CA	7.41	1.54	1.45
1	C	79	ARG	CB-CG	-7.41	1.30	1.52
1	A	260	SER	CA-C	-7.40	1.42	1.52
1	C	283	ALA	N-CA	7.40	1.55	1.46
1	C	393	SER	N-CA	7.40	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ARG	C-O	-7.38	1.15	1.24
1	C	185	THR	N-CA	-7.38	1.36	1.46
1	C	23	VAL	CA-C	7.37	1.61	1.52
1	A	180	LEU	N-CA	7.37	1.55	1.46
1	C	135	ALA	CA-CB	7.33	1.65	1.53
1	A	38	VAL	CA-C	7.33	1.62	1.52
1	A	151	THR	CA-C	-7.33	1.43	1.52
1	A	405	VAL	N-CA	7.33	1.54	1.46
1	A	382	SER	CA-C	7.32	1.61	1.52
1	C	227	GLN	C-O	7.32	1.32	1.23
1	A	227	GLN	C-O	7.31	1.33	1.23
1	A	13	PRO	C-O	-7.29	1.15	1.23
1	C	240	ARG	CB-CG	7.29	1.74	1.52
1	A	402	LEU	CB-CG	7.29	1.68	1.53
1	C	285	CYS	C-O	-7.28	1.15	1.24
1	C	116	ASN	C-O	7.28	1.32	1.24
1	A	176	HIS	C-O	7.28	1.32	1.24
1	A	347	HIS	N-CA	7.28	1.54	1.46
1	A	322	GLN	N-CA	7.26	1.55	1.46
1	A	105	PRO	CG-CD	7.26	1.75	1.50
1	A	85	CYS	CA-C	-7.26	1.44	1.52
1	A	356	LEU	N-CA	7.25	1.55	1.46
1	A	404	LEU	CG-CD1	7.23	1.76	1.52
1	C	406	TRP	CB-CG	7.23	1.72	1.50
1	A	244	ALA	CA-CB	-7.23	1.41	1.53
1	A	362	LEU	CA-C	-7.23	1.43	1.52
1	C	88	ILE	CA-C	7.22	1.60	1.52
1	A	110	GLN	C-O	7.21	1.33	1.24
1	C	318	ILE	C-O	7.20	1.32	1.24
1	A	86	PRO	N-CA	7.18	1.55	1.47
1	C	202	ASP	C-O	7.18	1.33	1.24
1	A	14	LEU	CA-C	7.16	1.61	1.52
1	C	188	ASP	C-O	7.16	1.33	1.24
1	A	66	THR	N-CA	-7.15	1.36	1.46
1	A	257	LEU	CG-CD2	-7.15	1.28	1.52
1	C	207	ILE	CA-CB	7.15	1.63	1.54
1	A	297	ASP	CA-CB	7.14	1.63	1.53
1	C	302	THR	C-O	7.14	1.33	1.24
1	C	408	PRO	CA-C	7.14	1.63	1.52
1	A	68	GLY	C-O	7.13	1.33	1.23
1	C	413	ALA	N-CA	-7.12	1.37	1.46
1	C	155	ALA	C-O	7.12	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	39	GLN	C-O	7.12	1.33	1.24
1	C	348	THR	C-O	7.11	1.32	1.24
1	C	319	LEU	CA-C	7.11	1.62	1.52
1	A	207	ILE	CA-CB	7.10	1.64	1.54
1	C	369	VAL	N-CA	7.09	1.55	1.46
1	A	151	THR	CB-CG2	7.09	1.75	1.52
1	C	74	ALA	N-CA	7.08	1.54	1.46
1	C	284	ALA	N-CA	7.08	1.54	1.46
1	A	139	ILE	CB-CG2	7.07	1.75	1.52
1	C	231	ARG	N-CA	7.07	1.56	1.46
1	C	280	ARG	CA-CB	-7.07	1.43	1.54
1	C	301	LEU	C-O	7.06	1.32	1.23
1	A	278	PRO	C-O	-7.06	1.14	1.24
1	A	63	TRP	CA-C	-7.06	1.43	1.53
1	A	34	LEU	CA-C	7.05	1.62	1.52
1	C	43	ALA	CA-CB	-7.05	1.41	1.53
1	A	108	GLN	C-O	-7.03	1.15	1.24
1	A	76	GLU	C-O	7.02	1.32	1.24
1	C	239	LYS	N-CA	7.02	1.54	1.46
1	C	143	ARG	C-O	7.02	1.31	1.24
1	C	197	LYS	N-CA	7.01	1.54	1.46
1	C	248	GLY	N-CA	-7.00	1.35	1.45
1	C	331	GLU	C-O	7.00	1.33	1.24
1	A	79	ARG	CA-C	-7.00	1.42	1.52
1	A	136	CYS	N-CA	7.00	1.54	1.46
1	A	377	ARG	C-O	6.99	1.33	1.24
1	A	259	PHE	CA-CB	-6.98	1.41	1.53
1	C	94	GLU	N-CA	6.97	1.54	1.46
1	A	275	ILE	N-CA	-6.96	1.37	1.46
1	A	88	ILE	CA-CB	6.95	1.63	1.54
1	C	12	ALA	CA-C	6.94	1.61	1.53
1	C	323	MET	CA-C	-6.94	1.43	1.52
1	C	409	ALA	C-O	6.93	1.32	1.24
1	A	231	ARG	C-O	6.91	1.30	1.24
1	A	117	GLN	N-CA	6.91	1.55	1.46
1	C	335	PRO	N-CA	6.91	1.56	1.47
1	A	181	THR	CA-C	6.91	1.62	1.52
1	C	148	CYS	C-O	6.91	1.32	1.23
1	C	290	ARG	CZ-NH2	6.88	1.42	1.33
1	A	84	GLU	N-CA	6.88	1.54	1.46
1	C	322	GLN	N-CA	6.87	1.55	1.46
1	C	337	HIS	CA-CB	6.87	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	LEU	CA-C	6.87	1.61	1.52
1	A	185	THR	CA-CB	-6.86	1.44	1.54
1	C	59	ASN	CA-C	6.86	1.62	1.53
1	C	199	ALA	CA-CB	-6.86	1.41	1.53
1	A	80	HIS	CA-C	-6.84	1.43	1.52
1	A	276	GLU	CA-CB	-6.84	1.42	1.53
1	A	106	PRO	CB-CG	6.84	1.77	1.51
1	A	143	ARG	C-N	-6.83	1.26	1.34
1	A	145	GLN	CD-NE2	6.82	1.47	1.33
1	A	169	LEU	CA-C	6.82	1.61	1.53
1	C	297	ASP	CA-C	6.82	1.61	1.52
1	A	365	ARG	C-O	6.80	1.32	1.24
1	A	143	ARG	CA-C	6.80	1.61	1.52
1	A	110	GLN	CB-CG	6.80	1.72	1.52
1	C	235	SER	CA-C	6.80	1.61	1.52
1	A	36	ALA	CA-C	6.79	1.61	1.52
1	C	212	ARG	CA-C	6.79	1.61	1.52
1	A	406	TRP	CA-C	6.78	1.61	1.52
1	C	356	LEU	CG-CD1	6.78	1.75	1.52
1	C	292	PHE	N-CA	6.78	1.54	1.46
1	A	180	LEU	C-O	-6.77	1.15	1.24
1	C	349	THR	CA-CB	6.77	1.64	1.53
1	A	266	LYS	C-O	6.77	1.33	1.24
1	C	185	THR	CA-CB	-6.76	1.43	1.53
1	A	265	ALA	CA-C	6.75	1.62	1.52
1	A	303	SER	C-O	6.75	1.31	1.23
1	C	206	PRO	N-CA	-6.75	1.38	1.47
1	A	232	PRO	CG-CD	6.73	1.73	1.50
1	A	378	ILE	CA-CB	-6.71	1.45	1.54
1	A	384	ALA	CA-CB	6.69	1.63	1.53
1	C	69	GLN	N-CA	6.69	1.54	1.46
1	A	95	ALA	C-O	6.69	1.31	1.24
1	C	88	ILE	CA-CB	6.68	1.62	1.54
1	A	246	LEU	C-N	6.68	1.39	1.33
1	C	185	THR	CA-C	6.68	1.61	1.52
1	A	121	MET	CA-CB	6.67	1.61	1.53
1	A	204	LEU	N-CA	6.66	1.54	1.46
1	C	184	MET	C-O	-6.66	1.16	1.24
1	A	71	ILE	CA-CB	6.66	1.61	1.54
1	C	282	PRO	C-O	-6.65	1.15	1.24
1	C	361	HIS	C-O	6.63	1.32	1.24
1	A	74	ALA	CA-C	-6.61	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	GLU	CA-C	6.61	1.61	1.52
1	A	109	ARG	CA-CB	6.60	1.64	1.53
1	A	402	LEU	C-O	-6.60	1.15	1.24
1	A	375	LEU	C-O	6.60	1.31	1.24
1	A	101	THR	CB-OG1	-6.59	1.33	1.43
1	A	233	ILE	CA-CB	6.59	1.61	1.54
1	A	110	GLN	N-CA	6.58	1.54	1.46
1	A	343	GLN	C-O	6.57	1.32	1.24
1	C	75	TYR	CG-CD2	6.57	1.53	1.39
1	C	176	HIS	N-CA	6.56	1.54	1.46
1	C	367	ILE	C-N	6.56	1.42	1.34
1	C	261	MET	CA-C	6.55	1.61	1.52
1	A	290	ARG	CA-CB	-6.55	1.43	1.53
1	A	139	ILE	CA-CB	-6.54	1.45	1.54
1	C	276	GLU	CA-CB	-6.52	1.43	1.53
1	C	340	PHE	CA-C	-6.52	1.43	1.52
1	C	107	GLU	C-O	6.52	1.32	1.24
1	A	98	PHE	N-CA	-6.51	1.37	1.46
1	A	263	PHE	N-CA	-6.51	1.38	1.46
1	C	409	ALA	CA-C	6.51	1.62	1.52
1	A	122	PRO	C-N	-6.51	1.25	1.34
1	C	334	ALA	CA-C	6.51	1.61	1.52
1	C	243	GLY	C-O	-6.50	1.15	1.23
1	A	114	LEU	C-O	-6.50	1.15	1.24
1	C	256	PHE	C-O	6.49	1.31	1.24
1	C	142	LEU	CA-CB	6.48	1.63	1.53
1	C	157	PRO	C-O	-6.48	1.16	1.24
1	C	313	LYS	CA-C	-6.48	1.45	1.52
1	A	192	THR	C-O	6.47	1.32	1.23
1	A	62	HIS	C-O	-6.47	1.16	1.23
1	A	218	ASP	N-CA	6.47	1.53	1.45
1	C	97	ASP	N-CA	6.47	1.52	1.46
1	A	175	PRO	CG-CD	6.46	1.72	1.50
1	C	81	PHE	C-O	-6.45	1.16	1.23
1	A	239	LYS	C-O	-6.45	1.16	1.24
1	C	65	ALA	N-CA	6.45	1.54	1.46
1	C	342	ARG	C-O	-6.45	1.15	1.24
1	A	310	VAL	CB-CG2	6.45	1.73	1.52
1	C	168	GLY	N-CA	6.44	1.54	1.45
1	C	149	ASN	C-N	-6.44	1.24	1.33
1	C	304	ASP	N-CA	6.43	1.54	1.46
1	A	375	LEU	N-CA	6.42	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	238	ALA	C-O	6.42	1.31	1.24
1	A	10	ASN	CB-CG	6.40	1.68	1.52
1	C	406	TRP	CA-C	-6.40	1.45	1.52
1	A	365	ARG	N-CA	-6.40	1.38	1.46
1	A	251	ASP	C-N	-6.39	1.26	1.33
1	C	263	PHE	CE2-CZ	6.39	1.57	1.38
1	A	87	PHE	CE1-CZ	6.39	1.57	1.38
1	A	157	PRO	N-CA	6.37	1.55	1.47
1	C	338	VAL	CA-CB	6.37	1.63	1.54
1	A	78	TYR	CA-C	6.36	1.61	1.52
1	C	108	GLN	C-N	-6.36	1.25	1.33
1	C	75	TYR	C-O	-6.35	1.16	1.24
1	C	392	LYS	C-O	-6.34	1.15	1.23
1	C	170	PRO	N-CA	6.34	1.54	1.47
1	C	253	VAL	C-O	6.34	1.31	1.24
1	C	62	HIS	N-CA	-6.34	1.38	1.46
1	A	197	LYS	C-O	-6.33	1.16	1.24
1	A	75	TYR	CG-CD2	-6.33	1.26	1.39
1	C	76	GLU	C-O	-6.31	1.16	1.24
1	A	13	PRO	CA-C	-6.29	1.45	1.52
1	C	34	LEU	CG-CD1	6.29	1.73	1.52
1	C	368	ILE	CB-CG1	-6.29	1.40	1.53
1	A	98	PHE	C-O	-6.29	1.16	1.24
1	C	93	GLY	C-N	6.29	1.42	1.33
1	C	20	GLU	CA-C	-6.28	1.44	1.52
1	C	102	SER	C-N	6.28	1.43	1.33
1	A	96	TYR	CD1-CE1	6.28	1.57	1.38
1	C	311	GLN	CB-CG	6.28	1.71	1.52
1	C	165	LEU	C-O	6.27	1.31	1.24
1	C	389	ILE	C-O	6.27	1.32	1.24
1	A	259	PHE	CG-CD1	6.27	1.52	1.38
1	A	103	MET	C-O	-6.26	1.15	1.23
1	C	242	CYS	N-CA	6.26	1.53	1.46
1	C	359	GLY	N-CA	6.25	1.54	1.45
1	C	365	ARG	CZ-NH2	-6.25	1.25	1.33
1	A	250	LEU	CG-CD1	6.25	1.73	1.52
1	A	64	ILE	CA-C	6.24	1.60	1.52
1	A	332	ASN	N-CA	6.24	1.53	1.46
1	A	388	GLN	CA-CB	-6.24	1.44	1.53
1	C	288	LEU	C-O	6.24	1.31	1.24
1	C	379	PRO	CG-CD	6.23	1.72	1.50
1	A	302	THR	C-O	6.23	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	TYR	N-CA	-6.23	1.38	1.46
1	C	221	SER	N-CA	6.23	1.53	1.46
1	A	89	PRO	CA-C	6.22	1.65	1.52
1	C	402	LEU	C-O	-6.21	1.16	1.24
1	A	343	GLN	CA-CB	6.21	1.63	1.53
1	C	144	PRO	N-CD	-6.21	1.39	1.47
1	C	163	PHE	CA-C	6.20	1.60	1.52
1	C	138	LEU	C-O	6.20	1.31	1.24
1	A	374	TRP	C-O	6.20	1.31	1.24
1	C	110	GLN	C-O	-6.20	1.16	1.24
1	C	370	THR	N-CA	6.20	1.53	1.46
1	C	159	PRO	N-CA	6.19	1.55	1.47
1	A	288	LEU	N-CA	6.18	1.53	1.46
1	A	385	PRO	CA-C	6.17	1.58	1.52
1	C	387	ALA	CA-C	-6.17	1.45	1.52
1	C	116	ASN	CB-CG	6.17	1.67	1.52
1	C	237	GLU	CA-CB	-6.16	1.42	1.53
1	A	151	THR	CA-CB	-6.15	1.43	1.53
1	C	116	ASN	CA-C	-6.15	1.44	1.52
1	C	262	GLU	CD-OE1	6.15	1.37	1.25
1	C	193	PHE	CA-CB	-6.15	1.43	1.53
1	C	390	GLN	C-O	6.14	1.31	1.24
1	C	314	LYS	C-O	-6.14	1.16	1.24
1	C	377	ARG	CG-CD	6.14	1.70	1.52
1	A	92	ALA	C-N	-6.13	1.26	1.33
1	A	82	SER	CA-C	-6.13	1.45	1.52
1	A	62	HIS	CA-C	6.13	1.60	1.52
1	A	161	ARG	CZ-NH2	6.13	1.41	1.33
1	A	343	GLN	N-CA	6.12	1.54	1.46
1	A	146	GLY	C-O	-6.12	1.16	1.24
1	A	41	ALA	N-CA	6.12	1.53	1.46
1	A	359	GLY	N-CA	6.12	1.54	1.45
1	C	99	ILE	N-CA	-6.12	1.39	1.46
1	A	379	PRO	CB-CG	6.12	1.80	1.49
1	C	316	ASP	C-O	-6.11	1.16	1.23
1	A	363	ALA	N-CA	6.10	1.53	1.46
1	A	205	ILE	C-N	-6.10	1.26	1.34
1	C	263	PHE	CB-CG	-6.10	1.36	1.50
1	A	116	ASN	CA-C	6.09	1.60	1.52
1	A	207	ILE	CB-CG1	6.09	1.65	1.53
1	C	294	LEU	CA-C	-6.09	1.47	1.52
1	A	385	PRO	CA-CB	6.08	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	LEU	N-CA	6.08	1.53	1.46
1	C	132	GLN	CD-OE1	6.08	1.35	1.23
1	A	404	LEU	C-N	6.07	1.42	1.33
1	A	57	ARG	CB-CG	6.07	1.70	1.52
1	C	153	ASP	CA-CB	6.06	1.64	1.53
1	C	258	SER	CA-C	6.06	1.60	1.52
1	C	193	PHE	CG-CD1	6.06	1.51	1.38
1	C	12	ALA	N-CA	6.06	1.52	1.45
1	C	43	ALA	CA-C	6.06	1.63	1.52
1	C	337	HIS	CA-C	6.06	1.60	1.52
1	A	67	ARG	CA-C	-6.05	1.45	1.52
1	A	356	LEU	CG-CD1	6.05	1.72	1.52
1	A	40	GLU	N-CA	6.04	1.53	1.46
1	C	164	MET	C-O	-6.04	1.16	1.24
1	C	231	ARG	CZ-NH1	6.04	1.41	1.32
1	C	268	PRO	CA-CB	-6.03	1.45	1.53
1	C	387	ALA	N-CA	6.03	1.53	1.45
1	A	64	ILE	C-O	-6.03	1.17	1.24
1	A	330	ARG	N-CA	6.02	1.53	1.46
1	C	67	ARG	C-O	6.01	1.31	1.23
1	A	344	LYS	N-CA	6.01	1.53	1.46
1	A	372	LYS	CG-CD	6.00	1.70	1.52
1	A	260	SER	N-CA	-6.00	1.38	1.46
1	A	391	HIS	C-O	-6.00	1.16	1.23
1	A	374	TRP	CA-CB	-6.00	1.44	1.53
1	C	325	SER	C-O	-6.00	1.16	1.24
1	C	165	LEU	CG-CD2	5.99	1.72	1.52
1	C	400	GLN	N-CA	5.98	1.53	1.46
1	A	259	PHE	N-CA	-5.98	1.38	1.46
1	A	84	GLU	CD-OE2	5.98	1.36	1.25
1	C	240	ARG	CZ-NH1	-5.98	1.24	1.32
1	C	162	ILE	CB-CG2	-5.97	1.32	1.52
1	A	169	LEU	C-N	5.97	1.40	1.33
1	A	406	TRP	CB-CG	5.96	1.68	1.50
1	A	153	ASP	CA-C	5.95	1.61	1.52
1	A	220	ILE	N-CA	5.94	1.53	1.46
1	A	202	ASP	N-CA	5.94	1.54	1.46
1	A	327	LEU	CA-C	5.94	1.61	1.52
1	C	283	ALA	CA-C	-5.93	1.45	1.52
1	A	98	PHE	CD1-CE1	-5.92	1.20	1.38
1	A	141	SER	CA-C	5.92	1.60	1.52
1	C	238	ALA	N-CA	-5.92	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	PRO	C-O	5.91	1.35	1.23
1	C	62	HIS	CA-CB	-5.91	1.43	1.53
1	A	159	PRO	CA-CB	5.90	1.62	1.53
1	A	214	LYS	CA-CB	5.90	1.60	1.53
1	A	314	LYS	CD-CE	5.90	1.70	1.52
1	A	291	ARG	CA-C	5.89	1.60	1.52
1	C	373	GLU	C-O	5.89	1.31	1.24
1	A	137	SER	CA-C	5.89	1.60	1.52
1	A	208	ILE	C-O	-5.89	1.17	1.24
1	A	221	SER	CA-C	5.88	1.60	1.52
1	A	118	VAL	CA-CB	5.88	1.62	1.54
1	A	85	CYS	C-N	5.88	1.39	1.33
1	C	335	PRO	C-N	5.88	1.41	1.33
1	A	142	LEU	C-O	-5.87	1.17	1.23
1	C	412	LYS	N-CA	5.86	1.53	1.46
1	C	317	GLN	CD-OE1	5.86	1.34	1.23
1	A	228	VAL	N-CA	-5.85	1.39	1.46
1	C	369	VAL	C-O	5.84	1.31	1.24
1	A	247	VAL	C-O	5.84	1.29	1.23
1	C	263	PHE	CA-CB	5.83	1.62	1.53
1	A	254	VAL	CA-CB	5.83	1.62	1.54
1	A	253	VAL	CB-CG1	5.83	1.71	1.52
1	C	274	LEU	CG-CD2	5.82	1.71	1.52
1	A	108	GLN	CB-CG	-5.82	1.35	1.52
1	A	333	ALA	CA-C	5.82	1.59	1.52
1	C	279	GLU	CD-OE2	5.82	1.36	1.25
1	A	297	ASP	N-CA	-5.81	1.37	1.46
1	C	94	GLU	CA-C	-5.81	1.45	1.52
1	C	398	GLY	CA-C	5.80	1.58	1.51
1	A	36	ALA	CA-CB	5.80	1.63	1.53
1	A	258	SER	N-CA	5.80	1.53	1.46
1	A	356	LEU	CA-CB	-5.79	1.44	1.53
1	C	76	GLU	CA-C	-5.79	1.44	1.52
1	A	127	LEU	CG-CD2	5.78	1.71	1.52
1	A	84	GLU	CB-CG	5.78	1.69	1.52
1	C	205	ILE	C-O	-5.78	1.17	1.24
1	C	232	PRO	N-CA	5.77	1.53	1.47
1	A	87	PHE	C-O	5.77	1.31	1.24
1	A	129	ASN	C-O	-5.77	1.16	1.24
1	A	198	GLU	N-CA	5.76	1.53	1.46
1	C	135	ALA	CA-C	5.76	1.60	1.52
1	A	228	VAL	C-N	-5.76	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	188	ASP	CA-CB	-5.76	1.43	1.53
1	A	184	MET	CG-SD	-5.75	1.66	1.80
1	C	147	GLN	CD-OE1	-5.75	1.12	1.23
1	C	169	LEU	CA-C	5.74	1.60	1.53
1	A	84	GLU	C-O	-5.74	1.17	1.24
1	C	208	ILE	CB-CG2	5.73	1.71	1.52
1	C	262	GLU	C-O	-5.73	1.17	1.24
1	A	146	GLY	N-CA	-5.72	1.36	1.45
1	C	61	GLY	C-O	-5.72	1.15	1.23
1	C	163	PHE	CB-CG	-5.72	1.37	1.50
1	A	226	GLY	N-CA	5.71	1.51	1.45
1	A	159	PRO	C-N	-5.71	1.27	1.33
1	A	280	ARG	N-CA	5.71	1.53	1.46
1	A	315	GLY	C-N	-5.70	1.25	1.33
1	C	116	ASN	CA-CB	5.70	1.62	1.53
1	C	112	ARG	CZ-NH1	5.70	1.40	1.32
1	C	118	VAL	CA-CB	5.70	1.61	1.54
1	C	154	TYR	CB-CG	5.69	1.64	1.51
1	A	44	VAL	CA-C	-5.69	1.44	1.52
1	A	23	VAL	N-CA	-5.68	1.40	1.46
1	A	338	VAL	CA-C	5.68	1.59	1.52
1	C	127	LEU	CA-C	5.68	1.60	1.52
1	C	375	LEU	C-O	5.68	1.31	1.24
1	C	181	THR	CB-OG1	-5.67	1.34	1.43
1	C	276	GLU	C-O	5.67	1.31	1.24
1	A	158	PHE	N-CA	-5.66	1.38	1.46
1	C	115	ALA	CA-C	-5.66	1.45	1.52
1	A	152	GLU	CA-C	-5.66	1.44	1.52
1	A	224	ALA	N-CA	5.66	1.53	1.46
1	A	374	TRP	CG-CD1	5.66	1.51	1.36
1	C	286	GLU	C-O	-5.66	1.17	1.24
1	C	20	GLU	N-CA	-5.66	1.38	1.46
1	C	197	LYS	CB-CG	5.66	1.69	1.52
1	C	111	PHE	CD2-CE2	-5.65	1.21	1.38
1	C	346	SER	CB-OG	-5.65	1.30	1.42
1	A	367	ILE	CA-CB	-5.64	1.47	1.54
1	C	90	ARG	CA-CB	5.64	1.62	1.53
1	C	323	MET	N-CA	-5.64	1.39	1.46
1	C	378	ILE	N-CA	5.64	1.53	1.46
1	C	156	GLU	C-N	5.64	1.41	1.33
1	C	333	ALA	N-CA	5.63	1.52	1.46
1	A	54	VAL	CA-CB	5.63	1.63	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	318	ILE	N-CA	5.63	1.53	1.46
1	A	392	LYS	CE-NZ	5.62	1.66	1.49
1	C	132	GLN	N-CA	5.62	1.53	1.46
1	C	78	TYR	N-CA	5.62	1.53	1.46
1	C	50	VAL	CA-C	5.60	1.58	1.52
1	C	180	LEU	N-CA	5.60	1.53	1.46
1	C	206	PRO	C-N	-5.59	1.26	1.33
1	C	343	GLN	N-CA	-5.59	1.39	1.46
1	A	37	GLY	C-N	5.59	1.40	1.33
1	C	287	GLU	CA-C	-5.59	1.44	1.52
1	A	160	ILE	C-O	5.58	1.31	1.24
1	C	211	ARG	CA-C	5.58	1.60	1.52
1	A	186	ARG	CG-CD	5.58	1.69	1.52
1	A	243	GLY	C-O	-5.58	1.16	1.23
1	A	353	GLY	C-O	5.58	1.30	1.23
1	C	366	GLU	N-CA	5.58	1.53	1.46
1	A	314	LYS	CB-CG	5.57	1.69	1.52
1	A	292	PHE	N-CA	5.57	1.52	1.46
1	A	109	ARG	CA-C	5.57	1.60	1.52
1	C	70	LEU	CA-C	-5.56	1.45	1.52
1	A	149	ASN	CG-OD1	5.56	1.34	1.23
1	A	102	SER	CB-OG	5.56	1.53	1.42
1	C	317	GLN	CB-CG	5.55	1.69	1.52
1	C	313	LYS	C-N	5.55	1.41	1.33
1	C	368	ILE	CA-CB	-5.55	1.47	1.54
1	C	135	ALA	C-O	5.54	1.30	1.24
1	C	254	VAL	CA-C	-5.54	1.46	1.52
1	C	147	GLN	CA-CB	5.54	1.62	1.53
1	C	90	ARG	CG-CD	5.54	1.69	1.52
1	A	183	GLN	C-O	-5.54	1.17	1.24
1	C	275	ILE	CA-CB	5.53	1.60	1.54
1	C	291	ARG	CD-NE	5.53	1.53	1.46
1	A	293	SER	C-O	5.53	1.30	1.24
1	A	365	ARG	CA-C	-5.53	1.45	1.52
1	C	208	ILE	N-CA	-5.53	1.39	1.46
1	C	159	PRO	CG-CD	5.52	1.69	1.50
1	C	255	ASN	C-O	5.52	1.31	1.24
1	C	353	GLY	CA-C	-5.52	1.44	1.52
1	C	397	SER	N-CA	5.52	1.52	1.45
1	A	158	PHE	CE2-CZ	-5.51	1.22	1.38
1	A	31	PRO	N-CA	-5.51	1.41	1.46
1	A	227	GLN	CB-CG	-5.51	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	THR	CA-CB	5.51	1.62	1.53
1	A	238	ALA	CA-C	-5.51	1.45	1.52
1	A	160	ILE	CB-CG2	-5.51	1.34	1.52
1	C	73	GLU	N-CA	5.51	1.52	1.46
1	C	374	TRP	CA-C	5.51	1.60	1.52
1	A	183	GLN	CB-CG	5.50	1.69	1.52
1	C	406	TRP	CE3-CZ3	-5.50	1.22	1.38
1	A	110	GLN	CA-C	5.50	1.60	1.52
1	A	369	VAL	C-N	-5.49	1.27	1.33
1	C	89	PRO	N-CA	5.49	1.56	1.47
1	A	131	ILE	CA-C	5.48	1.59	1.52
1	A	356	LEU	CA-C	-5.47	1.46	1.52
1	A	270	HIS	N-CA	-5.47	1.39	1.46
1	A	368	ILE	C-N	-5.47	1.26	1.33
1	C	364	ARG	CZ-NH2	-5.47	1.26	1.33
1	C	384	ALA	CA-C	5.46	1.58	1.53
1	A	252	THR	CA-C	5.46	1.57	1.52
1	A	148	CYS	N-CA	5.46	1.52	1.46
1	C	51	PRO	N-CA	5.46	1.53	1.47
1	C	367	ILE	CB-CG2	5.46	1.70	1.52
1	A	230	GLY	C-N	5.45	1.39	1.33
1	C	391	HIS	CA-C	5.45	1.59	1.52
1	A	178	LYS	N-CA	-5.45	1.39	1.46
1	A	262	GLU	CA-CB	-5.45	1.44	1.53
1	A	289	LEU	CG-CD2	5.45	1.70	1.52
1	C	396	VAL	CA-C	-5.45	1.46	1.52
1	A	214	LYS	CA-C	5.44	1.58	1.52
1	A	63	TRP	CA-CB	-5.43	1.44	1.53
1	A	289	LEU	C-O	-5.43	1.17	1.24
1	A	181	THR	N-CA	5.42	1.53	1.46
1	A	273	GLU	N-CA	-5.42	1.39	1.46
1	A	73	GLU	CA-C	5.42	1.59	1.52
1	A	289	LEU	C-N	5.41	1.40	1.33
1	C	145	GLN	N-CA	-5.41	1.39	1.46
1	A	256	PHE	N-CA	5.41	1.52	1.46
1	C	391	HIS	C-O	-5.41	1.17	1.23
1	C	81	PHE	CA-C	-5.41	1.45	1.53
1	A	174	ILE	C-N	5.40	1.40	1.34
1	C	388	GLN	CB-CG	5.40	1.68	1.52
1	A	35	SER	N-CA	5.40	1.53	1.46
1	C	192	THR	CA-C	5.40	1.60	1.53
1	A	284	ALA	C-O	5.39	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	LYS	CA-C	-5.39	1.46	1.52
1	C	203	TYR	N-CA	5.39	1.53	1.46
1	A	140	GLU	N-CA	5.38	1.52	1.46
1	C	151	THR	CA-C	-5.38	1.46	1.52
1	C	86	PRO	CG-CD	5.38	1.69	1.50
1	C	130	ARG	CA-C	-5.38	1.45	1.52
1	A	238	ALA	N-CA	-5.36	1.39	1.46
1	C	396	VAL	N-CA	-5.36	1.40	1.46
1	C	400	GLN	C-O	5.36	1.30	1.24
1	A	362	LEU	C-N	-5.36	1.27	1.33
1	A	313	LYS	CA-C	5.35	1.59	1.52
1	C	214	LYS	CA-CB	5.35	1.59	1.53
1	C	284	ALA	CA-CB	-5.35	1.45	1.53
1	A	224	ALA	C-O	-5.34	1.17	1.24
1	C	180	LEU	CG-CD1	-5.34	1.34	1.52
1	C	275	ILE	CA-C	5.34	1.59	1.52
1	A	267	SER	CA-CB	5.34	1.59	1.53
1	C	72	ARG	CZ-NH2	-5.34	1.26	1.33
1	A	287	GLU	N-CA	-5.33	1.39	1.46
1	C	58	CYS	CB-SG	-5.33	1.63	1.81
1	A	56	THR	N-CA	5.33	1.52	1.46
1	C	90	ARG	CB-CG	5.32	1.68	1.52
1	C	347	HIS	CA-C	5.32	1.58	1.52
1	C	400	GLN	CA-CB	-5.32	1.44	1.53
1	C	393	SER	CA-C	5.32	1.59	1.52
1	C	302	THR	CB-OG1	-5.31	1.35	1.43
1	A	323	MET	CB-CG	5.31	1.68	1.52
1	A	200	LEU	C-N	-5.30	1.27	1.33
1	C	139	ILE	CA-C	5.30	1.59	1.52
1	A	276	GLU	N-CA	-5.30	1.39	1.46
1	C	364	ARG	CG-CD	5.30	1.68	1.52
1	A	132	GLN	CA-C	5.30	1.59	1.52
1	C	179	TYR	C-O	5.30	1.30	1.24
1	C	177	LEU	C-O	-5.29	1.17	1.24
1	C	204	LEU	C-O	-5.29	1.17	1.24
1	C	228	VAL	CB-CG1	5.29	1.70	1.52
1	C	381	PHE	CA-C	-5.29	1.46	1.52
1	C	228	VAL	CA-C	-5.29	1.46	1.52
1	A	152	GLU	CD-OE1	5.28	1.35	1.25
1	A	249	GLY	C-O	5.28	1.30	1.23
1	C	219	ALA	CA-C	-5.28	1.45	1.52
1	C	251	ASP	CA-C	5.28	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	261	MET	C-O	-5.27	1.16	1.23
1	C	161	ARG	C-O	-5.27	1.17	1.24
1	A	156	GLU	CA-CB	5.27	1.61	1.53
1	A	86	PRO	C-O	5.26	1.30	1.24
1	A	93	GLY	N-CA	5.26	1.52	1.45
1	A	292	PHE	C-O	5.25	1.32	1.24
1	C	272	GLN	CA-CB	-5.25	1.44	1.53
1	C	399	VAL	CA-CB	5.25	1.60	1.54
1	A	238	ALA	C-O	5.25	1.30	1.24
1	C	152	GLU	C-O	5.25	1.30	1.24
1	A	262	GLU	CB-CG	5.24	1.68	1.52
1	A	371	LEU	CG-CD2	-5.24	1.35	1.52
1	A	311	GLN	CG-CD	5.24	1.65	1.52
1	A	240	ARG	CA-CB	-5.23	1.44	1.53
1	A	358	LEU	CA-CB	5.23	1.61	1.53
1	C	75	TYR	CE2-CZ	5.23	1.50	1.38
1	A	83	SER	C-O	-5.23	1.15	1.23
1	C	150	PHE	N-CA	-5.23	1.39	1.46
1	A	28	MET	CA-C	5.22	1.59	1.52
1	C	181	THR	CB-CG2	5.22	1.69	1.52
1	A	269	GLU	CA-CB	5.21	1.63	1.53
1	C	310	VAL	CA-C	-5.21	1.46	1.52
1	C	88	ILE	C-N	5.21	1.44	1.34
1	A	73	GLU	N-CA	-5.21	1.40	1.46
1	C	72	ARG	N-CA	5.20	1.52	1.46
1	C	75	TYR	CA-CB	5.20	1.61	1.53
1	A	311	GLN	CA-C	5.19	1.59	1.52
1	A	405	VAL	CA-C	5.19	1.58	1.52
1	A	81	PHE	CE2-CZ	5.18	1.54	1.38
1	A	395	ILE	C-O	5.18	1.31	1.24
1	A	297	ASP	C-N	5.18	1.41	1.33
1	C	73	GLU	C-O	-5.18	1.18	1.24
1	C	139	ILE	C-O	5.18	1.29	1.24
1	C	368	ILE	CA-C	5.17	1.59	1.52
1	C	277	ARG	CD-NE	5.17	1.53	1.46
1	C	66	THR	CB-CG2	-5.17	1.35	1.52
1	A	250	LEU	N-CA	5.17	1.52	1.46
1	C	40	GLU	CB-CG	5.17	1.68	1.52
1	C	195	GLU	N-CA	5.17	1.52	1.46
1	A	357	CYS	CA-C	5.17	1.59	1.52
1	A	108	GLN	CA-CB	5.16	1.62	1.53
1	A	172	GLU	CG-CD	5.16	1.65	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	ARG	NE-CZ	5.16	1.38	1.33
1	A	301	LEU	N-CA	-5.15	1.39	1.46
1	A	163	PHE	CG-CD2	5.15	1.49	1.38
1	C	91	GLU	N-CA	5.14	1.52	1.46
1	A	269	GLU	CA-C	-5.13	1.45	1.52
1	A	59	ASN	N-CA	5.13	1.54	1.46
1	A	323	MET	CA-CB	5.13	1.61	1.53
1	C	347	HIS	CA-CB	5.13	1.62	1.53
1	C	111	PHE	N-CA	-5.12	1.39	1.46
1	C	241	MET	CA-C	-5.12	1.46	1.52
1	A	313	LYS	CA-CB	5.12	1.61	1.53
1	A	397	SER	CA-C	5.11	1.60	1.53
1	A	230	GLY	C-O	5.11	1.30	1.23
1	A	360	GLN	CB-CG	5.11	1.67	1.52
1	A	322	GLN	CA-CB	5.11	1.61	1.53
1	A	41	ALA	CA-CB	-5.09	1.45	1.53
1	A	72	ARG	CA-C	-5.09	1.46	1.52
1	A	292	PHE	CG-CD1	-5.09	1.28	1.38
1	C	86	PRO	N-CD	5.09	1.54	1.47
1	C	274	LEU	C-O	-5.09	1.18	1.24
1	A	396	VAL	CA-C	-5.09	1.46	1.52
1	C	142	LEU	CB-CG	-5.09	1.43	1.53
1	C	322	GLN	CA-C	5.09	1.59	1.52
1	C	292	PHE	CA-CB	-5.08	1.46	1.53
1	A	30	ASN	CA-C	5.08	1.59	1.52
1	A	376	THR	N-CA	5.08	1.52	1.46
1	C	111	PHE	CA-C	5.08	1.59	1.52
1	C	225	ASN	CA-C	-5.08	1.45	1.52
1	C	373	GLU	CA-C	5.08	1.59	1.52
1	C	321	PRO	CA-C	-5.07	1.45	1.52
1	C	394	GLY	CA-C	5.07	1.57	1.51
1	A	240	ARG	CZ-NH2	5.06	1.40	1.33
1	A	345	VAL	CB-CG1	-5.06	1.35	1.52
1	A	406	TRP	CE2-CZ2	-5.06	1.29	1.39
1	A	26	PHE	CA-CB	5.05	1.61	1.53
1	A	202	ASP	C-O	5.05	1.30	1.24
1	A	335	PRO	N-CA	-5.05	1.40	1.47
1	A	338	VAL	N-CA	-5.05	1.40	1.46
1	C	393	SER	C-N	5.05	1.38	1.33
1	C	73	GLU	CA-CB	-5.05	1.45	1.53
1	A	193	PHE	CG-CD1	-5.04	1.28	1.38
1	C	406	TRP	C-O	5.04	1.29	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	100	PRO	CG-CD	5.04	1.65	1.51
1	A	54	VAL	CB-CG1	5.03	1.69	1.52
1	A	299	ARG	CZ-NH1	5.03	1.39	1.32
1	A	388	GLN	N-CA	-5.03	1.40	1.46
1	C	101	THR	CA-CB	5.03	1.61	1.53
1	C	154	TYR	CD1-CE1	5.03	1.53	1.38
1	A	260	SER	C-O	-5.03	1.17	1.24
1	A	136	CYS	C-O	-5.02	1.18	1.24
1	C	203	TYR	CD2-CE2	-5.02	1.23	1.38
1	C	117	GLN	C-N	5.02	1.40	1.33
1	A	163	PHE	CA-CB	-5.01	1.45	1.53
1	A	70	LEU	CA-C	-5.01	1.46	1.52
1	A	206	PRO	N-CA	-5.01	1.41	1.47
1	C	364	ARG	N-CA	5.01	1.52	1.46
1	C	28	MET	SD-CE	5.01	1.92	1.79
1	A	307	PHE	N-CA	5.01	1.52	1.46
1	A	372	LYS	N-CA	5.00	1.52	1.46
1	C	247	VAL	CA-CB	-5.00	1.47	1.54
1	A	196	ALA	N-CA	5.00	1.52	1.46
1	A	203	TYR	CA-C	5.00	1.59	1.52
1	A	231	ARG	NE-CZ	5.00	1.38	1.33
1	C	94	GLU	CB-CG	5.00	1.67	1.52

All (765) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ILE	CA-C-N	-19.09	100.28	119.56
1	A	174	ILE	C-N-CA	-19.09	100.28	119.56
1	C	264	LEU	N-CA-C	-16.37	89.70	112.45
1	C	143	ARG	CA-C-N	-15.37	103.89	119.87
1	C	143	ARG	C-N-CA	-15.37	103.89	119.87
1	A	265	ALA	N-CA-C	14.92	130.85	111.75
1	C	225	ASN	CA-C-N	-14.45	109.57	122.43
1	C	225	ASN	C-N-CA	-14.45	109.57	122.43
1	A	254	VAL	CB-CA-C	-14.36	93.00	112.24
1	C	14	LEU	CA-C-N	14.16	134.96	120.38
1	C	14	LEU	C-N-CA	14.16	134.96	120.38
1	C	15	PRO	CA-C-N	14.03	133.83	119.24
1	C	15	PRO	C-N-CA	14.03	133.83	119.24
1	A	214	LYS	CA-C-N	13.85	133.60	119.76
1	A	214	LYS	C-N-CA	13.85	133.60	119.76
1	A	373	GLU	N-CA-C	13.64	125.66	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ILE	CA-C-N	13.47	134.10	119.28
1	C	205	ILE	C-N-CA	13.47	134.10	119.28
1	C	290	ARG	NE-CZ-NH1	-13.41	108.09	121.50
1	C	130	ARG	NE-CZ-NH1	-13.13	108.37	121.50
1	A	30	ASN	CA-C-N	-13.07	106.41	120.66
1	A	30	ASN	C-N-CA	-13.07	106.41	120.66
1	A	94	GLU	N-CA-C	-13.07	95.76	112.23
1	C	173	ASP	N-CA-C	12.82	126.69	111.82
1	A	270	HIS	N-CA-C	-12.79	93.62	112.04
1	C	130	ARG	NE-CZ-NH2	12.77	130.70	119.20
1	A	371	LEU	N-CA-C	-12.75	96.17	112.23
1	A	18	VAL	N-CA-C	12.50	120.38	107.76
1	C	112	ARG	N-CA-C	-12.17	96.90	112.23
1	A	142	LEU	CD1-CG-CD2	-12.12	84.15	110.80
1	A	86	PRO	CB-CA-C	-11.91	94.91	110.27
1	C	165	LEU	N-CA-C	-11.90	98.38	111.36
1	A	266	LYS	CA-C-N	-11.72	109.96	122.85
1	A	266	LYS	C-N-CA	-11.72	109.96	122.85
1	A	384	ALA	N-CA-C	-11.64	94.86	109.64
1	C	214	LYS	CA-C-N	11.62	131.74	119.89
1	C	214	LYS	C-N-CA	11.62	131.74	119.89
1	C	368	ILE	N-CA-C	11.61	123.85	110.62
1	C	111	PHE	N-CA-C	-11.59	99.14	113.28
1	A	40	GLU	N-CA-C	11.55	124.97	111.11
1	A	302	THR	N-CA-C	11.54	126.46	112.38
1	A	324	LEU	N-CA-C	11.47	125.21	111.33
1	C	111	PHE	CA-C-N	-11.28	101.51	120.68
1	C	111	PHE	C-N-CA	-11.28	101.51	120.68
1	A	134	LEU	CB-CA-C	-11.20	93.20	110.90
1	C	150	PHE	N-CA-C	-11.15	97.98	111.69
1	A	378	ILE	CA-C-N	11.13	131.52	119.28
1	A	378	ILE	C-N-CA	11.13	131.52	119.28
1	C	143	ARG	CB-CG-CD	-11.06	85.86	111.30
1	C	377	ARG	NE-CZ-NH1	-10.79	110.70	121.50
1	A	151	THR	CA-CB-CG2	-10.71	92.29	110.50
1	C	272	GLN	N-CA-C	10.69	125.70	112.23
1	C	289	LEU	N-CA-C	-10.63	98.83	112.23
1	C	254	VAL	N-CA-CB	10.56	121.71	110.62
1	C	324	LEU	N-CA-C	10.52	123.80	111.71
1	A	184	MET	CG-SD-CE	-10.38	78.06	100.90
1	C	53	LEU	CB-CA-C	-10.28	96.50	110.79
1	C	223	VAL	CB-CA-C	-10.21	98.67	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	PRO	CB-CA-C	-10.17	96.89	113.06
1	C	291	ARG	N-CA-C	10.14	122.41	111.36
1	A	372	LYS	N-CA-C	-9.95	99.26	111.40
1	A	246	LEU	CA-C-N	9.95	134.09	122.35
1	A	246	LEU	C-N-CA	9.95	134.09	122.35
1	C	402	LEU	N-CA-C	9.92	131.73	109.81
1	C	118	VAL	CA-C-N	-9.77	111.30	122.14
1	C	118	VAL	C-N-CA	-9.77	111.30	122.14
1	A	85	CYS	N-CA-CB	-9.76	96.86	111.21
1	C	250	LEU	N-CA-C	9.76	126.38	113.30
1	A	101	THR	N-CA-C	9.74	125.01	112.34
1	A	347	HIS	N-CA-C	9.74	122.82	108.60
1	A	385	PRO	N-CA-C	9.74	129.93	112.01
1	C	90	ARG	CA-C-O	-9.74	110.67	120.70
1	C	403	PRO	CB-CA-C	9.73	122.16	111.56
1	C	260	SER	N-CA-CB	9.64	125.22	110.28
1	A	255	ASN	N-CA-C	9.63	121.37	111.07
1	A	340	PHE	N-CA-C	9.61	122.76	111.71
1	C	130	ARG	N-CA-C	-9.58	100.71	111.82
1	C	96	TYR	CB-CA-C	-9.55	94.61	109.89
1	C	284	ALA	CA-C-N	9.55	133.43	120.54
1	C	284	ALA	C-N-CA	9.55	133.43	120.54
1	C	87	PHE	N-CA-C	9.54	125.49	110.32
1	A	284	ALA	N-CA-C	9.31	126.65	111.37
1	C	335	PRO	N-CA-C	-9.28	100.20	113.47
1	C	113	ALA	CA-C-N	9.23	134.67	120.82
1	C	113	ALA	C-N-CA	9.23	134.67	120.82
1	A	275	ILE	N-CA-C	-9.23	100.43	113.07
1	A	389	ILE	CB-CA-C	-9.21	98.99	111.33
1	C	131	ILE	N-CA-CB	9.20	125.92	110.56
1	A	102	SER	N-CA-C	-9.11	101.13	112.88
1	C	80	HIS	N-CA-CB	9.07	123.94	110.33
1	A	220	ILE	CB-CA-C	-9.04	99.75	112.22
1	C	354	SER	N-CA-C	9.03	123.31	111.75
1	C	188	ASP	N-CA-CB	-9.02	95.70	110.40
1	A	369	VAL	CB-CA-C	-9.01	100.16	112.24
1	A	392	LYS	N-CA-C	-8.99	95.64	109.85
1	A	369	VAL	N-CA-C	-8.95	101.24	111.00
1	A	95	ALA	N-CA-C	8.95	120.73	110.97
1	C	300	ILE	CA-C-N	-8.94	108.18	120.87
1	C	300	ILE	C-N-CA	-8.94	108.18	120.87
1	C	152	GLU	N-CA-C	8.91	123.45	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	LEU	N-CA-C	8.74	121.60	111.11
1	A	209	GLU	N-CA-C	-8.74	101.22	112.23
1	A	181	THR	N-CA-C	-8.69	100.37	112.45
1	C	12	ALA	CA-C-N	8.67	128.74	119.90
1	C	12	ALA	C-N-CA	8.67	128.74	119.90
1	C	254	VAL	CB-CA-C	-8.66	100.61	111.70
1	C	233	ILE	N-CA-C	-8.64	95.84	108.71
1	C	105	PRO	C-N-CD	-8.61	101.67	120.60
1	C	92	ALA	CA-C-N	8.60	129.70	119.99
1	C	92	ALA	C-N-CA	8.60	129.70	119.99
1	A	14	LEU	CA-C-N	-8.55	111.57	120.38
1	A	14	LEU	C-N-CA	-8.55	111.57	120.38
1	C	42	TRP	N-CA-C	-8.54	101.19	111.69
1	C	93	GLY	CA-C-O	-8.52	112.27	121.05
1	A	252	THR	N-CA-C	-8.49	98.69	111.34
1	C	193	PHE	N-CA-C	-8.49	101.25	111.69
1	A	280	ARG	CG-CD-NE	-8.48	93.35	112.00
1	A	79	ARG	N-CA-C	-8.47	102.21	112.54
1	C	211	ARG	CA-CB-CG	8.46	131.01	114.10
1	C	147	GLN	CB-CG-CD	8.45	126.97	112.60
1	C	171	GLU	N-CA-C	8.42	121.39	111.71
1	C	235	SER	CA-C-N	8.39	132.20	120.29
1	C	235	SER	C-N-CA	8.39	132.20	120.29
1	C	182	ASP	N-CA-C	8.38	120.42	111.28
1	A	390	GLN	N-CA-C	8.35	123.31	109.46
1	C	99	ILE	CG1-CB-CG2	8.29	135.56	110.70
1	A	322	GLN	CA-C-N	8.29	131.21	120.44
1	A	322	GLN	C-N-CA	8.29	131.21	120.44
1	A	267	SER	CB-CA-C	8.27	123.42	111.27
1	A	81	PHE	CA-C-N	-8.24	109.59	122.87
1	A	81	PHE	C-N-CA	-8.24	109.59	122.87
1	A	17	HIS	N-CA-C	8.23	123.16	113.20
1	A	121	MET	CA-C-N	8.21	128.68	119.32
1	A	121	MET	C-N-CA	8.21	128.68	119.32
1	C	129	ASN	N-CA-C	-8.21	102.41	111.36
1	A	376	THR	CB-CA-C	8.21	123.59	110.96
1	C	290	ARG	NE-CZ-NH2	8.20	126.58	119.20
1	A	151	THR	N-CA-C	8.19	128.25	110.80
1	A	153	ASP	N-CA-C	8.19	122.53	112.54
1	A	227	GLN	CB-CG-CD	-8.17	98.72	112.60
1	A	77	ASP	CB-CG-OD2	8.13	137.10	118.40
1	C	284	ALA	N-CA-C	8.12	120.13	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	ALA	N-CA-C	-8.12	103.53	113.19
1	A	146	GLY	N-CA-C	-8.11	104.03	115.30
1	A	277	ARG	CA-CB-CG	-8.08	97.94	114.10
1	A	307	PHE	CA-C-O	-8.07	111.58	120.38
1	C	137	SER	CA-CB-OG	-8.07	94.96	111.10
1	C	174	ILE	CA-C-N	-8.06	109.77	119.84
1	C	174	ILE	C-N-CA	-8.06	109.77	119.84
1	C	95	ALA	N-CA-C	8.05	122.06	111.75
1	C	82	SER	N-CA-CB	-8.05	97.51	110.63
1	A	332	ASN	N-CA-C	8.04	121.60	107.61
1	A	179	TYR	N-CA-C	-7.98	102.66	111.36
1	A	367	ILE	CA-C-N	7.97	130.60	120.56
1	A	367	ILE	C-N-CA	7.97	130.60	120.56
1	C	96	TYR	CA-C-N	-7.94	107.94	120.17
1	C	96	TYR	C-N-CA	-7.94	107.94	120.17
1	C	261	MET	CB-CA-C	7.92	121.86	109.03
1	A	112	ARG	N-CA-C	-7.92	102.65	111.28
1	C	99	ILE	CB-CA-C	-7.89	96.99	111.36
1	A	372	LYS	CA-C-N	-7.89	110.19	120.44
1	A	372	LYS	C-N-CA	-7.89	110.19	120.44
1	C	85	CYS	CB-CA-C	-7.87	98.86	111.14
1	C	110	GLN	O-C-N	-7.84	113.26	122.20
1	A	383	ILE	CA-C-N	7.83	131.27	120.39
1	A	383	ILE	C-N-CA	7.83	131.27	120.39
1	C	130	ARG	O-C-N	7.83	131.89	122.27
1	C	204	LEU	CD1-CG-CD2	-7.82	93.59	110.80
1	A	318	ILE	CA-C-N	7.82	131.89	120.95
1	A	318	ILE	C-N-CA	7.82	131.89	120.95
1	A	409	ALA	O-C-N	-7.80	112.21	122.59
1	A	72	ARG	NE-CZ-NH1	-7.79	113.72	121.50
1	C	272	GLN	CA-CB-CG	-7.78	98.54	114.10
1	A	339	ASP	N-CA-C	7.78	121.09	108.34
1	C	147	GLN	CG-CD-NE2	7.78	128.07	116.40
1	C	158	PHE	CA-C-N	-7.76	110.39	118.85
1	C	158	PHE	C-N-CA	-7.76	110.39	118.85
1	C	390	GLN	N-CA-C	7.75	121.55	109.07
1	A	125	ASP	N-CA-C	-7.75	99.71	111.56
1	A	207	ILE	N-CA-CB	-7.75	96.75	110.77
1	C	344	LYS	N-CA-C	-7.74	94.24	108.02
1	C	115	ALA	N-CA-C	-7.74	102.84	111.28
1	A	248	GLY	N-CA-C	-7.74	102.25	113.86
1	A	101	THR	CA-C-O	7.74	128.74	119.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	TYR	O-C-N	-7.66	112.40	122.59
1	C	388	GLN	CA-C-N	-7.63	109.41	121.62
1	C	388	GLN	C-N-CA	-7.63	109.41	121.62
1	A	284	ALA	CA-C-N	7.61	133.29	121.19
1	A	284	ALA	C-N-CA	7.61	133.29	121.19
1	A	275	ILE	CA-C-N	-7.57	110.04	122.08
1	A	275	ILE	C-N-CA	-7.57	110.04	122.08
1	C	240	ARG	CG-CD-NE	-7.54	95.40	112.00
1	C	293	SER	CA-C-N	-7.54	106.68	119.35
1	C	293	SER	C-N-CA	-7.54	106.68	119.35
1	C	102	SER	CA-C-O	-7.54	110.74	119.56
1	C	110	GLN	CA-C-N	-7.52	108.08	122.06
1	C	110	GLN	C-N-CA	-7.52	108.08	122.06
1	A	15	PRO	CA-C-N	7.51	129.23	119.84
1	A	15	PRO	C-N-CA	7.51	129.23	119.84
1	A	396	VAL	CB-CA-C	7.51	119.67	110.73
1	C	50	VAL	CA-C-N	-7.51	112.27	119.85
1	C	50	VAL	C-N-CA	-7.51	112.27	119.85
1	A	278	PRO	CA-C-N	-7.50	106.96	121.58
1	A	278	PRO	C-N-CA	-7.50	106.96	121.58
1	A	141	SER	CA-C-N	7.47	132.09	120.89
1	A	141	SER	C-N-CA	7.47	132.09	120.89
1	C	70	LEU	N-CA-C	-7.46	102.31	111.40
1	A	165	LEU	N-CA-C	-7.42	102.88	110.97
1	C	146	GLY	N-CA-C	-7.42	105.08	115.32
1	A	107	GLU	CA-C-O	7.41	128.49	119.97
1	C	368	ILE	CA-C-N	7.41	135.30	121.97
1	C	368	ILE	C-N-CA	7.41	135.30	121.97
1	C	375	LEU	N-CA-C	-7.40	103.71	112.89
1	A	161	ARG	N-CA-C	-7.39	102.60	111.69
1	C	364	ARG	NE-CZ-NH2	7.39	125.85	119.20
1	A	82	SER	N-CA-C	-7.37	98.23	109.95
1	C	89	PRO	CA-C-N	7.37	130.46	120.44
1	C	89	PRO	C-N-CA	7.37	130.46	120.44
1	C	186	ARG	CB-CG-CD	7.37	128.24	111.30
1	A	383	ILE	N-CA-C	7.35	124.63	109.34
1	C	18	VAL	N-CA-C	7.34	115.18	107.76
1	C	389	ILE	N-CA-C	-7.34	99.42	109.55
1	A	169	LEU	N-CA-C	7.33	120.19	110.08
1	A	108	GLN	N-CA-C	-7.30	103.64	112.54
1	C	364	ARG	CA-C-N	7.29	130.05	120.28
1	C	364	ARG	C-N-CA	7.29	130.05	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	MET	CA-C-O	-7.27	112.61	121.11
1	C	112	ARG	NE-CZ-NH2	-7.18	112.74	119.20
1	A	330	ARG	N-CA-C	7.18	121.87	113.18
1	C	131	ILE	N-CA-C	-7.18	103.17	111.00
1	C	21	HIS	N-CA-C	-7.17	104.51	113.18
1	A	39	GLN	N-CA-C	7.17	120.92	111.75
1	A	118	VAL	N-CA-C	-7.16	104.41	113.22
1	C	335	PRO	O-C-N	7.15	130.25	122.17
1	C	79	ARG	CA-C-O	-7.14	111.25	119.60
1	A	205	ILE	CG1-CB-CG2	7.13	132.10	110.70
1	C	357	CYS	O-C-N	-7.13	113.53	123.01
1	A	61	GLY	N-CA-C	-7.12	96.31	113.18
1	C	107	GLU	N-CA-C	-7.12	103.53	111.71
1	C	239	LYS	CB-CA-C	-7.09	98.79	110.85
1	C	268	PRO	CA-C-N	-7.09	108.89	120.72
1	C	268	PRO	C-N-CA	-7.09	108.89	120.72
1	A	104	ASP	CA-C-N	-7.08	113.09	120.38
1	A	104	ASP	C-N-CA	-7.08	113.09	120.38
1	C	11	LEU	N-CA-C	7.06	120.87	107.75
1	C	102	SER	O-C-N	7.06	130.81	122.34
1	C	413	ALA	N-CA-C	-7.05	98.54	109.76
1	A	37	GLY	CA-C-N	-7.05	111.21	121.65
1	A	37	GLY	C-N-CA	-7.05	111.21	121.65
1	C	205	ILE	N-CA-CB	-7.04	101.36	111.21
1	A	76	GLU	N-CA-C	7.03	118.94	111.28
1	A	371	LEU	CB-CG-CD2	-7.01	89.68	110.70
1	C	112	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	C	315	GLY	CA-C-N	7.00	130.65	120.71
1	C	315	GLY	C-N-CA	7.00	130.65	120.71
1	C	77	ASP	N-CA-CB	-6.99	102.52	110.35
1	A	91	GLU	CB-CA-C	-6.99	99.13	110.74
1	C	287	GLU	N-CA-C	-6.99	103.75	112.90
1	C	337	HIS	CB-CA-C	6.98	121.74	110.29
1	A	346	SER	CB-CA-C	6.97	121.20	109.84
1	A	363	ALA	N-CA-C	-6.96	102.53	111.02
1	A	37	GLY	CA-C-O	-6.95	117.45	122.45
1	C	32	SER	CA-C-N	-6.94	111.53	123.25
1	C	32	SER	C-N-CA	-6.94	111.53	123.25
1	A	111	PHE	N-CA-C	-6.92	104.97	113.41
1	A	90	ARG	CA-C-O	-6.92	110.62	120.51
1	A	323	MET	N-CA-C	6.92	118.47	111.07
1	A	195	GLU	CB-CA-C	-6.92	99.92	110.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	HIS	N-CA-C	6.92	120.82	112.38
1	A	23	VAL	CB-CA-C	-6.91	102.99	111.08
1	C	93	GLY	N-CA-C	-6.91	104.28	112.64
1	C	113	ALA	O-C-N	6.91	129.47	122.08
1	A	410	THR	N-CA-C	6.90	120.59	112.72
1	A	218	ASP	N-CA-C	6.88	120.56	110.59
1	A	84	GLU	CA-C-O	6.85	128.03	120.63
1	C	266	LYS	CB-CG-CD	-6.83	95.60	111.30
1	C	105	PRO	CA-C-N	6.82	143.37	127.00
1	C	105	PRO	C-N-CA	6.82	143.37	127.00
1	C	79	ARG	O-C-N	6.82	132.04	122.36
1	A	345	VAL	CA-C-N	-6.80	111.78	121.50
1	A	345	VAL	C-N-CA	-6.80	111.78	121.50
1	A	105	PRO	N-CD-CG	-6.78	93.03	103.20
1	C	88	ILE	C-N-CD	-6.78	105.69	120.60
1	A	263	PHE	CA-C-O	-6.76	113.67	120.90
1	C	299	ARG	NE-CZ-NH2	-6.75	113.12	119.20
1	A	364	ARG	N-CA-C	6.74	118.32	110.97
1	C	248	GLY	CA-C-N	6.74	128.78	120.22
1	C	248	GLY	C-N-CA	6.74	128.78	120.22
1	C	369	VAL	CG1-CB-CG2	-6.74	95.97	110.80
1	A	257	LEU	CD1-CG-CD2	-6.74	95.97	110.80
1	C	109	ARG	N-CA-C	6.74	118.51	111.03
1	C	180	LEU	N-CA-C	6.73	118.41	111.14
1	C	84	GLU	CA-C-N	6.73	131.29	123.15
1	C	84	GLU	C-N-CA	6.73	131.29	123.15
1	C	252	THR	N-CA-C	-6.73	103.73	112.68
1	C	143	ARG	CG-CD-NE	-6.71	97.23	112.00
1	C	405	VAL	CA-C-N	-6.69	111.00	122.10
1	C	405	VAL	C-N-CA	-6.69	111.00	122.10
1	C	367	ILE	CA-C-N	6.67	129.94	120.53
1	C	367	ILE	C-N-CA	6.67	129.94	120.53
1	A	380	ASP	N-CA-CB	-6.66	100.71	110.84
1	A	222	ILE	CB-CA-C	-6.66	101.31	112.16
1	C	160	ILE	CB-CA-C	-6.65	103.17	112.14
1	A	237	GLU	N-CA-C	6.64	119.53	111.82
1	A	79	ARG	CA-C-N	-6.64	110.21	122.09
1	A	79	ARG	C-N-CA	-6.64	110.21	122.09
1	A	143	ARG	CA-C-N	-6.64	113.32	119.82
1	A	143	ARG	C-N-CA	-6.64	113.32	119.82
1	A	139	ILE	CA-CB-CG1	-6.63	99.13	110.40
1	C	291	ARG	NE-CZ-NH2	6.63	125.17	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	LYS	CA-C-O	-6.63	113.78	121.07
1	C	129	ASN	CA-C-O	-6.62	113.40	120.42
1	C	40	GLU	CB-CA-C	6.59	122.75	110.70
1	C	237	GLU	CA-C-O	6.54	127.40	119.49
1	A	240	ARG	CA-C-O	-6.52	112.47	119.97
1	A	373	GLU	CA-CB-CG	-6.52	101.06	114.10
1	C	71	ILE	CA-C-N	6.52	129.34	120.54
1	C	71	ILE	C-N-CA	6.52	129.34	120.54
1	A	361	HIS	N-CA-C	-6.51	104.27	111.82
1	A	144	PRO	CB-CA-C	-6.51	102.12	111.62
1	C	301	LEU	N-CA-C	6.50	119.89	110.28
1	C	342	ARG	CG-CD-NE	6.50	126.29	112.00
1	A	310	VAL	N-CA-C	-6.50	98.16	107.77
1	C	269	GLU	N-CA-C	-6.48	104.63	112.54
1	C	118	VAL	CG1-CB-CG2	-6.47	96.55	110.80
1	A	135	ALA	N-CA-C	-6.47	104.15	111.07
1	A	320	LEU	N-CA-C	-6.47	97.75	108.75
1	C	299	ARG	CA-C-N	-6.47	112.41	122.69
1	C	299	ARG	C-N-CA	-6.47	112.41	122.69
1	C	130	ARG	N-CA-CB	6.46	120.30	110.28
1	C	278	PRO	CB-CA-C	-6.46	102.13	112.21
1	C	356	LEU	CB-CG-CD1	6.45	130.06	110.70
1	A	278	PRO	O-C-N	-6.44	113.95	122.64
1	A	100	PRO	CA-C-N	6.44	131.00	120.63
1	A	100	PRO	C-N-CA	6.44	131.00	120.63
1	C	275	ILE	CA-C-N	-6.43	112.56	122.60
1	C	275	ILE	C-N-CA	-6.43	112.56	122.60
1	C	338	VAL	CA-CB-CG1	6.43	121.32	110.40
1	A	57	ARG	N-CA-C	-6.42	105.19	113.16
1	A	302	THR	CA-C-N	6.42	133.38	121.62
1	A	302	THR	C-N-CA	6.42	133.38	121.62
1	A	85	CYS	CA-C-N	-6.42	113.12	120.89
1	A	85	CYS	C-N-CA	-6.42	113.12	120.89
1	A	131	ILE	CA-C-N	6.42	128.79	120.44
1	A	131	ILE	C-N-CA	6.42	128.79	120.44
1	C	398	GLY	N-CA-C	6.42	121.08	110.55
1	C	215	PRO	N-CA-C	6.42	121.31	111.11
1	A	384	ALA	CA-C-N	-6.41	112.44	120.51
1	A	384	ALA	C-N-CA	-6.41	112.44	120.51
1	C	240	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	C	40	GLU	N-CA-C	-6.39	103.83	111.69
1	C	334	ALA	CA-C-N	6.39	125.61	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	ALA	C-N-CA	6.39	125.61	118.97
1	A	110	GLN	N-CA-C	6.38	124.38	110.80
1	C	243	GLY	CA-C-N	-6.37	109.38	121.54
1	C	243	GLY	C-N-CA	-6.37	109.38	121.54
1	C	378	ILE	CA-C-N	6.36	127.51	120.45
1	C	378	ILE	C-N-CA	6.36	127.51	120.45
1	A	130	ARG	CA-C-O	-6.36	113.68	120.42
1	C	109	ARG	CA-C-N	-6.36	111.10	120.38
1	C	109	ARG	C-N-CA	-6.36	111.10	120.38
1	A	41	ALA	CA-C-N	-6.35	111.27	120.29
1	A	41	ALA	C-N-CA	-6.35	111.27	120.29
1	A	233	ILE	N-CA-C	-6.35	101.36	109.80
1	C	290	ARG	CA-CB-CG	-6.34	101.41	114.10
1	C	400	GLN	CB-CG-CD	-6.33	101.83	112.60
1	C	83	SER	CA-CB-OG	-6.33	98.45	111.10
1	C	251	ASP	O-C-N	-6.32	114.19	122.59
1	A	329	GLU	N-CA-C	6.30	124.23	110.80
1	C	67	ARG	CA-C-N	6.30	126.97	119.98
1	C	67	ARG	C-N-CA	6.30	126.97	119.98
1	A	291	ARG	CA-C-N	-6.29	112.40	122.66
1	A	291	ARG	C-N-CA	-6.29	112.40	122.66
1	C	15	PRO	N-CA-C	6.29	118.37	110.70
1	A	332	ASN	CB-CA-C	-6.28	102.06	110.79
1	C	352	HIS	N-CA-C	-6.28	98.84	108.76
1	C	286	GLU	N-CA-C	-6.27	104.50	111.71
1	A	63	TRP	N-CA-C	-6.27	101.25	110.52
1	C	394	GLY	CA-C-O	-6.25	115.47	121.41
1	C	412	LYS	N-CA-C	6.25	118.59	108.34
1	A	251	ASP	N-CA-C	6.24	124.10	110.80
1	A	163	PHE	CZ-CE2-CD2	-6.24	108.77	120.00
1	A	250	LEU	CB-CA-C	6.24	122.37	109.95
1	A	370	THR	N-CA-CB	6.24	119.24	109.94
1	A	79	ARG	O-C-N	-6.24	114.08	122.43
1	A	82	SER	CA-C-O	-6.23	114.12	121.16
1	A	96	TYR	CA-C-N	-6.22	111.75	122.14
1	A	96	TYR	C-N-CA	-6.22	111.75	122.14
1	C	238	ALA	N-CA-C	-6.22	104.58	111.36
1	A	375	LEU	CA-C-O	6.22	127.01	120.42
1	A	38	VAL	N-CA-CB	6.21	120.25	110.31
1	C	343	GLN	CA-C-N	-6.21	114.04	122.86
1	C	343	GLN	C-N-CA	-6.21	114.04	122.86
1	C	377	ARG	CD-NE-CZ	-6.21	115.71	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	GLY	N-CA-C	6.20	127.88	113.18
1	A	109	ARG	CB-CA-C	6.19	122.03	110.70
1	A	356	LEU	CB-CA-C	-6.19	101.11	109.71
1	C	121	MET	CA-C-N	-6.19	112.53	118.97
1	C	121	MET	C-N-CA	-6.19	112.53	118.97
1	C	158	PHE	O-C-N	6.19	124.54	120.27
1	C	125	ASP	CA-C-N	-6.19	112.39	120.44
1	C	125	ASP	C-N-CA	-6.19	112.39	120.44
1	A	207	ILE	CA-C-O	6.17	127.14	120.47
1	A	291	ARG	N-CA-C	-6.17	103.87	111.40
1	C	58	CYS	CA-C-N	-6.17	113.46	122.40
1	C	58	CYS	C-N-CA	-6.17	113.46	122.40
1	A	123	VAL	CG1-CB-CG2	-6.16	97.24	110.80
1	A	318	ILE	O-C-N	6.14	128.50	122.97
1	A	333	ALA	N-CA-C	6.14	119.73	110.64
1	A	409	ALA	CA-C-O	6.14	129.29	120.51
1	A	220	ILE	N-CA-CB	6.14	119.79	110.58
1	A	241	MET	CA-C-N	-6.14	110.86	121.66
1	A	241	MET	C-N-CA	-6.14	110.86	121.66
1	C	374	TRP	CA-C-N	-6.14	110.39	121.14
1	C	374	TRP	C-N-CA	-6.14	110.39	121.14
1	C	367	ILE	CA-C-O	-6.14	113.11	120.78
1	A	338	VAL	N-CA-C	6.13	122.09	109.34
1	A	227	GLN	CA-C-N	-6.13	113.51	122.58
1	A	227	GLN	C-N-CA	-6.13	113.51	122.58
1	A	297	ASP	CA-C-O	-6.13	114.09	121.32
1	C	207	ILE	N-CA-C	-6.12	104.88	110.82
1	A	149	ASN	N-CA-C	-6.12	99.18	108.67
1	C	147	GLN	CG-CD-OE1	-6.12	108.57	120.80
1	C	324	LEU	CA-C-N	-6.12	111.47	120.28
1	C	324	LEU	C-N-CA	-6.12	111.47	120.28
1	A	134	LEU	O-C-N	6.11	128.68	122.09
1	A	294	LEU	N-CA-C	6.09	123.55	113.50
1	A	249	GLY	N-CA-C	6.08	120.56	112.77
1	C	409	ALA	CA-C-O	6.08	126.78	119.61
1	C	145	GLN	N-CA-C	6.08	119.89	112.23
1	C	260	SER	CA-CB-OG	-6.07	98.96	111.10
1	A	350	PHE	N-CA-CB	-6.07	100.59	110.42
1	C	383	ILE	CA-C-O	-6.07	113.89	121.11
1	A	377	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	C	242	CYS	CA-C-N	6.05	133.26	121.41
1	C	242	CYS	C-N-CA	6.05	133.26	121.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	VAL	N-CA-C	6.04	121.90	109.34
1	C	231	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	C	405	VAL	CB-CA-C	-6.03	100.32	111.18
1	A	410	THR	OG1-CB-CG2	-6.02	97.25	109.30
1	A	290	ARG	N-CA-CB	-6.01	101.29	110.01
1	C	130	ARG	CB-CA-C	-6.01	99.13	110.67
1	C	192	THR	N-CA-C	6.01	118.08	110.33
1	A	315	GLY	O-C-N	-6.00	116.16	122.52
1	C	20	GLU	N-CA-C	-6.00	105.45	112.89
1	A	250	LEU	N-CA-C	6.00	120.44	113.18
1	A	350	PHE	CB-CA-C	5.99	121.48	110.11
1	A	337	HIS	CB-CA-C	5.97	120.67	110.81
1	C	389	ILE	O-C-N	5.97	129.94	122.59
1	C	44	VAL	N-CA-C	-5.97	105.24	113.00
1	C	251	ASP	N-CA-C	5.97	123.52	110.80
1	A	117	GLN	N-CA-CB	5.97	120.29	110.39
1	A	243	GLY	CA-C-N	-5.97	110.14	121.54
1	A	243	GLY	C-N-CA	-5.97	110.14	121.54
1	C	327	LEU	CB-CG-CD1	-5.96	92.83	110.70
1	A	191	MET	CA-CB-CG	5.95	126.00	114.10
1	C	143	ARG	C-N-CD	5.95	149.39	125.00
1	C	322	GLN	CA-C-N	5.95	128.57	120.54
1	C	322	GLN	C-N-CA	5.95	128.57	120.54
1	A	334	ALA	N-CA-C	5.94	122.94	109.81
1	A	110	GLN	N-CA-CB	-5.94	100.45	110.49
1	C	30	ASN	CA-C-N	-5.93	113.85	120.14
1	C	30	ASN	C-N-CA	-5.93	113.85	120.14
1	A	256	PHE	CB-CA-C	-5.93	100.94	110.79
1	A	283	ALA	CA-C-O	5.93	127.24	120.90
1	A	63	TRP	CA-C-N	5.92	131.76	122.70
1	A	63	TRP	C-N-CA	5.92	131.76	122.70
1	C	266	LYS	N-CA-C	5.92	120.92	111.81
1	C	399	VAL	CA-C-N	-5.92	111.14	120.60
1	C	399	VAL	C-N-CA	-5.92	111.14	120.60
1	C	373	GLU	N-CA-C	5.91	119.75	112.54
1	A	140	GLU	CA-C-N	5.91	129.00	120.38
1	A	140	GLU	C-N-CA	5.91	129.00	120.38
1	A	129	ASN	CA-C-N	5.90	128.67	120.29
1	A	129	ASN	C-N-CA	5.90	128.67	120.29
1	C	255	ASN	N-CA-C	5.90	118.66	111.82
1	C	39	GLN	CB-CG-CD	5.89	122.62	112.60
1	C	159	PRO	CA-C-O	5.88	128.27	119.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ALA	N-CA-C	-5.87	104.96	111.36
1	A	207	ILE	N-CA-C	-5.87	103.75	111.09
1	C	372	LYS	N-CA-CB	5.87	118.74	109.82
1	C	358	LEU	N-CA-C	-5.86	105.62	112.89
1	C	239	LYS	CB-CG-CD	-5.86	97.83	111.30
1	A	93	GLY	N-CA-C	-5.86	105.52	113.37
1	A	126	LYS	CB-CA-C	-5.86	101.02	110.74
1	A	290	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	C	147	GLN	N-CA-C	5.85	117.29	108.46
1	C	188	ASP	CB-CG-OD2	-5.83	104.99	118.40
1	C	382	SER	CA-CB-OG	-5.82	99.46	111.10
1	A	77	ASP	OD1-CG-OD2	-5.82	108.94	122.90
1	C	265	ALA	CA-C-N	-5.82	114.50	123.17
1	C	265	ALA	C-N-CA	-5.82	114.50	123.17
1	A	367	ILE	CB-CA-C	-5.81	104.30	112.14
1	A	401	ALA	CB-CA-C	5.81	120.79	110.16
1	A	312	LEU	N-CA-C	-5.81	100.20	109.96
1	A	395	ILE	CB-CA-C	-5.80	98.60	111.77
1	A	40	GLU	CA-CB-CG	-5.80	102.50	114.10
1	C	62	HIS	N-CA-CB	-5.80	101.83	111.57
1	C	362	LEU	N-CA-CB	5.80	118.38	109.98
1	C	110	GLN	CA-C-O	5.78	126.67	120.20
1	C	392	LYS	CA-C-O	-5.78	114.57	121.56
1	A	292	PHE	CA-CB-CG	-5.78	108.03	113.80
1	C	375	LEU	CA-C-N	-5.76	112.95	120.44
1	C	375	LEU	C-N-CA	-5.76	112.95	120.44
1	A	154	TYR	CA-C-N	-5.76	112.48	120.38
1	A	154	TYR	C-N-CA	-5.76	112.48	120.38
1	C	103	MET	CB-CA-C	-5.76	97.34	109.38
1	C	25	ASP	CB-CA-C	-5.75	103.77	111.88
1	C	364	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	C	164	MET	CB-CG-SD	5.75	129.94	112.70
1	A	201	TYR	N-CA-CB	-5.74	100.43	109.78
1	A	117	GLN	N-CA-C	5.73	119.53	112.54
1	A	223	VAL	CB-CA-C	-5.73	104.53	112.04
1	A	77	ASP	O-C-N	-5.73	115.55	122.71
1	C	206	PRO	N-CA-C	-5.73	105.92	113.65
1	C	371	LEU	N-CA-CB	5.73	118.38	110.07
1	C	156	GLU	CA-C-N	-5.73	112.98	119.28
1	C	156	GLU	C-N-CA	-5.73	112.98	119.28
1	C	221	SER	CB-CA-C	-5.71	101.89	110.90
1	C	112	ARG	CA-C-N	-5.70	112.86	120.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	ARG	C-N-CA	-5.70	112.86	120.79
1	C	259	PHE	O-C-N	5.70	128.16	122.12
1	A	99	ILE	CB-CA-C	-5.70	101.00	111.36
1	C	411	THR	CB-CA-C	-5.69	99.77	109.51
1	A	266	LYS	CA-C-O	5.69	126.22	119.56
1	C	342	ARG	N-CA-C	-5.69	98.69	110.80
1	A	311	GLN	N-CA-C	5.68	117.73	108.63
1	A	404	LEU	CA-C-N	5.68	130.83	122.94
1	A	404	LEU	C-N-CA	5.68	130.83	122.94
1	C	391	HIS	N-CA-C	5.67	119.17	110.20
1	C	181	THR	CA-C-N	5.67	127.88	120.28
1	C	181	THR	C-N-CA	5.67	127.88	120.28
1	C	75	TYR	CA-C-O	-5.67	114.51	120.63
1	C	277	ARG	O-C-N	5.67	125.96	121.20
1	A	70	LEU	CA-CB-CG	5.66	136.12	116.30
1	A	119	VAL	CA-C-N	-5.65	116.67	122.27
1	A	119	VAL	C-N-CA	-5.65	116.67	122.27
1	A	110	GLN	CA-CB-CG	-5.65	102.81	114.10
1	C	85	CYS	N-CA-C	-5.65	99.00	108.94
1	A	70	LEU	CD1-CG-CD2	-5.64	98.39	110.80
1	A	144	PRO	N-CA-C	5.64	121.26	113.98
1	C	257	LEU	CB-CG-CD1	5.64	127.62	110.70
1	A	172	GLU	CA-CB-CG	-5.63	102.83	114.10
1	A	208	ILE	N-CA-C	-5.63	104.01	111.05
1	A	277	ARG	CB-CA-C	5.63	121.27	110.17
1	A	141	SER	CA-C-O	5.62	126.49	120.20
1	C	284	ALA	O-C-N	5.62	128.07	122.12
1	C	299	ARG	N-CA-C	-5.61	101.00	108.74
1	C	111	PHE	CA-C-O	5.61	125.85	119.18
1	C	178	LYS	N-CA-CB	-5.60	101.59	110.28
1	C	411	THR	N-CA-C	5.60	119.23	110.32
1	A	376	THR	CA-CB-OG1	-5.59	101.22	109.60
1	C	86	PRO	CB-CA-C	5.59	117.48	110.27
1	A	201	TYR	N-CA-C	5.57	120.56	111.37
1	A	234	THR	N-CA-C	-5.57	102.22	110.46
1	A	134	LEU	CA-C-N	5.56	127.67	120.44
1	A	134	LEU	C-N-CA	5.56	127.67	120.44
1	C	378	ILE	N-CA-CB	5.56	119.00	111.21
1	A	20	GLU	N-CA-C	-5.55	106.21	112.87
1	C	278	PRO	CA-C-N	-5.55	111.28	122.55
1	C	278	PRO	C-N-CA	-5.55	111.28	122.55
1	C	375	LEU	CA-C-O	5.54	126.18	119.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	LEU	N-CA-C	5.54	122.59	110.80
1	C	56	THR	N-CA-C	5.53	118.65	109.46
1	A	197	LYS	CA-CB-CG	5.53	125.16	114.10
1	A	254	VAL	CA-C-N	-5.53	113.25	120.44
1	A	254	VAL	C-N-CA	-5.53	113.25	120.44
1	C	22	LEU	N-CA-C	5.53	119.65	113.02
1	C	207	ILE	N-CA-CB	-5.52	102.57	110.52
1	A	96	TYR	N-CA-C	5.52	122.56	110.80
1	A	258	SER	N-CA-C	-5.51	105.18	111.14
1	C	332	ASN	N-CA-C	-5.51	99.05	110.80
1	A	357	CYS	CB-CA-C	5.51	117.72	110.06
1	A	399	VAL	CA-C-N	-5.51	113.28	120.44
1	A	399	VAL	C-N-CA	-5.51	113.28	120.44
1	C	116	ASN	N-CA-CB	5.51	118.32	110.06
1	C	321	PRO	CA-C-N	-5.51	111.50	121.14
1	C	321	PRO	C-N-CA	-5.51	111.50	121.14
1	A	295	VAL	CA-C-O	-5.50	115.77	121.93
1	A	346	SER	O-C-N	-5.50	116.61	123.04
1	C	290	ARG	CA-C-O	5.49	126.02	119.60
1	A	381	PHE	CA-C-N	-5.48	113.33	122.21
1	A	381	PHE	C-N-CA	-5.48	113.33	122.21
1	C	280	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	C	310	VAL	N-CA-C	-5.48	100.34	108.45
1	C	39	GLN	N-CA-C	5.48	118.18	111.82
1	C	378	ILE	O-C-N	5.48	127.34	121.10
1	C	38	VAL	N-CA-C	-5.47	105.04	111.00
1	C	264	LEU	N-CA-CB	5.47	118.41	110.26
1	A	221	SER	CB-CA-C	-5.46	101.73	110.79
1	A	337	HIS	CA-C-O	5.46	126.42	120.58
1	A	87	PHE	N-CA-C	5.46	118.52	109.46
1	A	290	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	C	165	LEU	CA-C-O	5.45	126.20	120.42
1	A	376	THR	N-CA-CB	-5.44	101.97	109.91
1	C	94	GLU	N-CA-CB	5.44	118.19	110.13
1	C	260	SER	N-CA-C	-5.44	105.51	111.82
1	A	25	ASP	N-CA-C	5.43	122.38	110.80
1	C	356	LEU	CA-CB-CG	-5.43	97.30	116.30
1	A	304	ASP	N-CA-CB	5.43	117.89	109.48
1	A	342	ARG	CA-C-O	-5.43	115.52	120.95
1	A	64	ILE	O-C-N	-5.42	117.45	123.03
1	A	80	HIS	CA-C-N	-5.41	114.96	123.13
1	A	80	HIS	C-N-CA	-5.41	114.96	123.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ILE	CA-C-O	-5.41	114.40	120.95
1	C	125	ASP	O-C-N	-5.41	116.39	122.12
1	A	378	ILE	CB-CA-C	-5.40	101.53	111.36
1	A	253	VAL	N-CA-C	5.39	120.56	109.34
1	A	39	GLN	CA-CB-CG	-5.39	103.33	114.10
1	C	61	GLY	CA-C-O	-5.39	114.98	121.98
1	C	174	ILE	N-CA-C	5.38	120.51	108.88
1	C	151	THR	N-CA-C	-5.38	105.31	111.07
1	C	270	HIS	N-CA-CB	5.38	117.78	109.98
1	A	333	ALA	O-C-N	-5.38	116.22	122.89
1	A	241	MET	N-CA-CB	5.37	118.49	110.22
1	C	285	CYS	CB-CA-C	-5.37	102.22	110.81
1	C	364	ARG	CG-CD-NE	5.37	123.81	112.00
1	C	402	LEU	CD1-CG-CD2	-5.36	99.01	110.80
1	C	166	LEU	N-CA-C	-5.36	105.48	112.23
1	A	158	PHE	N-CA-C	5.35	121.64	109.81
1	A	171	GLU	N-CA-C	5.35	118.97	112.23
1	A	143	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	349	THR	N-CA-C	5.34	117.80	111.33
1	C	142	LEU	N-CA-C	-5.34	106.89	113.41
1	A	114	LEU	CA-C-O	-5.34	113.48	120.00
1	C	107	GLU	CB-CG-CD	5.34	121.68	112.60
1	A	250	LEU	CA-C-O	5.34	125.94	119.11
1	C	319	LEU	CA-C-N	-5.34	116.59	123.16
1	C	319	LEU	C-N-CA	-5.34	116.59	123.16
1	A	368	ILE	CA-CB-CG1	-5.33	101.33	110.40
1	C	277	ARG	CB-CA-C	5.33	118.77	111.41
1	C	226	GLY	CA-C-N	-5.33	114.10	122.73
1	C	226	GLY	C-N-CA	-5.33	114.10	122.73
1	A	253	VAL	N-CA-CB	5.33	120.02	111.23
1	C	404	LEU	CB-CG-CD2	5.32	126.67	110.70
1	C	238	ALA	CB-CA-C	5.32	119.89	110.85
1	C	19	PRO	CA-C-N	-5.32	111.84	121.14
1	C	19	PRO	C-N-CA	-5.32	111.84	121.14
1	A	375	LEU	CD1-CG-CD2	5.31	122.49	110.80
1	C	61	GLY	CA-C-N	-5.31	112.22	122.09
1	C	61	GLY	C-N-CA	-5.31	112.22	122.09
1	A	69	GLN	CB-CG-CD	5.30	121.61	112.60
1	C	28	MET	CG-SD-CE	-5.30	89.25	100.90
1	A	245	LEU	CA-CB-CG	5.30	134.84	116.30
1	A	246	LEU	CA-C-O	-5.29	112.95	120.51
1	C	109	ARG	N-CA-CB	-5.29	102.31	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	MET	CG-SD-CE	-5.29	89.27	100.90
1	A	130	ARG	N-CA-C	-5.29	105.60	111.36
1	A	286	GLU	N-CA-C	5.28	117.44	111.11
1	C	130	ARG	CG-CD-NE	5.28	123.61	112.00
1	A	62	HIS	O-C-N	-5.27	118.02	123.29
1	A	365	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	C	276	GLU	CA-C-O	5.27	125.80	119.59
1	A	157	PRO	O-C-N	-5.26	115.43	122.22
1	A	306	GLU	CB-CA-C	-5.26	102.12	110.81
1	C	191	MET	CA-CB-CG	5.26	124.63	114.10
1	A	138	LEU	N-CA-C	5.26	122.00	110.80
1	A	80	HIS	N-CA-C	-5.25	107.00	113.41
1	A	200	LEU	O-C-N	-5.25	116.63	122.09
1	C	165	LEU	CB-CG-CD2	5.25	126.46	110.70
1	A	20	GLU	CA-C-N	-5.25	112.84	121.92
1	A	20	GLU	C-N-CA	-5.25	112.84	121.92
1	A	113	ALA	CA-C-O	5.24	125.83	119.49
1	A	210	GLN	N-CA-C	-5.24	105.48	111.14
1	C	82	SER	N-CA-C	5.24	118.61	110.17
1	C	299	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	187	PRO	N-CD-CG	-5.24	95.35	103.20
1	C	158	PHE	N-CA-C	-5.24	105.05	112.17
1	A	202	ASP	CA-C-N	-5.23	112.40	120.88
1	A	202	ASP	C-N-CA	-5.23	112.40	120.88
1	A	221	SER	N-CA-C	5.23	116.98	111.28
1	A	174	ILE	C-N-CD	5.22	146.42	125.00
1	C	142	LEU	CB-CA-C	-5.22	100.10	109.24
1	C	149	ASN	N-CA-C	-5.21	99.29	108.20
1	A	376	THR	CA-CB-CG2	5.20	119.34	110.50
1	C	398	GLY	CA-C-O	-5.20	116.56	121.60
1	A	18	VAL	CA-C-N	-5.19	114.60	119.85
1	A	18	VAL	C-N-CA	-5.19	114.60	119.85
1	A	240	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	C	267	SER	CB-CA-C	5.19	117.59	111.15
1	A	386	GLY	CA-C-N	-5.19	114.88	122.19
1	A	386	GLY	C-N-CA	-5.19	114.88	122.19
1	C	35	SER	N-CA-C	-5.19	106.21	112.54
1	A	290	ARG	CA-C-O	5.18	126.26	120.82
1	A	307	PHE	CB-CA-C	-5.18	100.75	109.72
1	A	399	VAL	CA-CB-CG1	5.18	119.21	110.40
1	A	149	ASN	CA-C-O	-5.18	114.75	120.60
1	A	228	VAL	CA-CB-CG2	-5.18	101.60	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	CG-CD-NE	-5.17	100.62	112.00
1	C	72	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	A	216	GLY	N-CA-C	-5.17	100.92	113.18
1	A	230	GLY	CA-C-N	5.17	132.37	123.11
1	A	230	GLY	C-N-CA	5.17	132.37	123.11
1	C	373	GLU	N-CA-CB	5.17	118.97	110.39
1	C	48	SER	N-CA-C	-5.16	106.14	112.90
1	C	349	THR	CA-C-O	5.16	125.97	120.24
1	A	211	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	C	99	ILE	N-CA-CB	-5.15	103.99	111.21
1	A	121	MET	CB-CG-SD	5.15	128.15	112.70
1	C	402	LEU	CA-CB-CG	5.14	134.28	116.30
1	A	55	TRP	N-CA-CB	-5.13	102.51	110.57
1	C	43	ALA	CA-C-N	-5.13	113.03	121.19
1	C	43	ALA	C-N-CA	-5.13	113.03	121.19
1	A	74	ALA	N-CA-C	-5.13	106.28	112.54
1	C	138	LEU	N-CA-CB	5.13	119.16	110.49
1	A	82	SER	CA-C-N	-5.13	112.66	122.61
1	A	82	SER	C-N-CA	-5.13	112.66	122.61
1	A	151	THR	OG1-CB-CG2	5.12	119.55	109.30
1	A	243	GLY	N-CA-C	-5.12	101.04	113.18
1	A	183	GLN	N-CA-CB	5.12	119.03	110.32
1	C	210	GLN	N-CA-C	-5.11	105.70	111.28
1	C	340	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	313	LYS	N-CA-C	5.11	117.65	110.14
1	C	335	PRO	CA-C-N	5.11	128.77	120.60
1	C	335	PRO	C-N-CA	5.11	128.77	120.60
1	C	88	ILE	CA-C-O	-5.10	113.11	119.95
1	C	263	PHE	O-C-N	-5.10	116.71	122.12
1	C	303	SER	CB-CA-C	5.10	121.42	110.45
1	A	36	ALA	CA-C-N	-5.10	114.63	122.69
1	A	36	ALA	C-N-CA	-5.10	114.63	122.69
1	C	88	ILE	CA-C-N	5.10	139.24	127.00
1	C	88	ILE	C-N-CA	5.10	139.24	127.00
1	C	18	VAL	CA-C-O	5.10	122.16	119.15
1	C	109	ARG	CA-C-O	-5.10	115.65	120.90
1	C	239	LYS	CA-C-N	5.09	127.36	120.38
1	C	239	LYS	C-N-CA	5.09	127.36	120.38
1	C	90	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	391	HIS	CB-CA-C	-5.09	100.55	109.71
1	A	24	PHE	CA-C-O	5.08	125.82	120.33
1	A	75	TYR	CA-C-N	5.08	127.09	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	TYR	C-N-CA	5.08	127.09	120.28
1	A	292	PHE	CA-C-N	-5.07	111.85	121.54
1	A	292	PHE	C-N-CA	-5.07	111.85	121.54
1	A	302	THR	O-C-N	5.07	128.98	122.39
1	C	90	ARG	N-CA-C	5.07	116.61	111.14
1	C	38	VAL	CB-CA-C	5.06	119.03	112.24
1	A	257	LEU	CB-CA-C	5.06	119.14	110.74
1	A	262	GLU	N-CA-CB	5.06	119.04	110.49
1	A	262	GLU	CA-C-N	5.06	127.37	120.54
1	A	262	GLU	C-N-CA	5.06	127.37	120.54
1	C	112	ARG	CD-NE-CZ	5.06	131.48	124.40
1	A	247	VAL	CA-CB-CG1	5.06	119.00	110.40
1	A	401	ALA	CA-C-O	-5.05	115.33	120.89
1	C	371	LEU	CA-CB-CG	5.05	133.98	116.30
1	A	147	GLN	N-CA-C	5.04	116.08	108.46
1	A	28	MET	N-CA-C	5.04	117.67	111.82
1	A	327	LEU	N-CA-CB	-5.04	102.73	110.44
1	C	227	GLN	CA-C-N	-5.04	114.99	122.70
1	C	227	GLN	C-N-CA	-5.04	114.99	122.70
1	C	242	CYS	O-C-N	5.04	127.46	122.12
1	A	69	GLN	CB-CA-C	5.03	120.33	110.67
1	C	187	PRO	CB-CA-C	-5.03	103.25	111.56
1	A	120	GLY	CA-C-O	-5.03	117.25	122.28
1	C	150	PHE	CA-C-O	-5.03	114.66	120.24
1	A	214	LYS	CB-CG-CD	5.02	122.85	111.30
1	A	352	HIS	O-C-N	-5.02	117.45	123.27
1	C	98	PHE	N-CA-C	5.02	121.49	110.80
1	A	405	VAL	N-CA-C	5.02	115.93	108.46
1	A	253	VAL	CB-CA-C	-5.01	103.07	111.29
1	C	304	ASP	CB-CA-C	-5.01	101.69	109.61
1	A	55	TRP	N-CA-C	5.01	117.14	109.07
1	A	139	ILE	N-CA-C	-5.01	104.72	111.44
1	C	377	ARG	NH1-CZ-NH2	5.01	125.81	119.30
1	A	75	TYR	N-CA-CB	5.01	118.04	110.28
1	A	141	SER	N-CA-CB	-5.01	102.23	110.14

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	GLU	Peptide
1	A	108	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	120	GLY	Peptide
1	A	258	SER	Mainchain
1	A	261	MET	Mainchain
1	A	303	SER	Peptide
1	A	382	SER	Peptide
1	A	81	PHE	Peptide
1	C	204	LEU	Peptide
1	C	205	ILE	Mainchain
1	C	238	ALA	Mainchain
1	C	263	PHE	Mainchain
1	C	270	HIS	Peptide
1	C	303	SER	Peptide
1	C	359	GLY	Peptide
1	C	379	PRO	Peptide
1	C	403	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3201	0	3148	431	11
1	C	3199	0	3138	404	12
2	A	43	0	32	18	0
2	C	43	0	32	9	0
3	A	111	0	0	9	0
3	C	99	0	0	9	0
All	All	6696	0	6350	821	23

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 64.

All (821) 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:C:356:LEU:CD1	1:C:356:LEU:CG	1.74	1.61
1:A:404:LEU:CG	1:A:404:LEU:CD1	1.76	1.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:CG2	1:A:151:THR:CB	1.75	1.58
1:C:373:GLU:CG	1:C:373:GLU:CB	1.75	1.58
1:A:257:LEU:C	1:A:257:LEU:CA	1.75	1.57
1:A:96:TYR:C	1:A:96:TYR:CA	1.76	1.56
1:C:131:ILE:CB	1:C:131:ILE:CG2	1.78	1.56
1:C:369:VAL:CB	1:C:369:VAL:CA	1.78	1.56
1:C:389:ILE:CB	1:C:389:ILE:CG2	1.82	1.56
1:A:139:ILE:CG2	1:A:139:ILE:CB	1.75	1.56
1:A:240:ARG:CG	1:A:240:ARG:CD	1.79	1.56
1:A:409:ALA:CA	1:A:409:ALA:CB	1.75	1.55
1:C:254:VAL:CB	1:C:254:VAL:CG1	1.80	1.55
1:A:389:ILE:CB	1:A:389:ILE:CG2	1.84	1.54
1:C:112:ARG:CD	1:C:112:ARG:CG	1.80	1.53
1:C:143:ARG:HH11	1:C:143:ARG:CG	1.22	1.52
1:A:134:LEU:CG	1:A:134:LEU:CD1	1.86	1.52
1:A:205:ILE:CB	1:A:205:ILE:CG2	1.79	1.52
1:A:264:LEU:CG	1:A:264:LEU:CD2	1.83	1.51
1:A:367:ILE:N	1:A:367:ILE:CA	1.70	1.51
1:A:105:PRO:CD	1:A:105:PRO:CG	1.75	1.50
1:C:399:VAL:CB	1:C:399:VAL:CG2	1.87	1.49
1:A:379:PRO:CB	1:A:379:PRO:CG	1.80	1.47
1:A:106:PRO:CG	1:A:106:PRO:CB	1.77	1.44
1:A:20:GLU:CD	1:C:165:LEU:HG	1.39	1.43
1:A:385:PRO:CB	1:A:385:PRO:CG	1.88	1.43
1:C:335:PRO:CB	1:C:335:PRO:CG	2.00	1.39
1:A:277:ARG:NH2	1:A:280:ARG:HH21	1.27	1.28
1:A:247:VAL:HG12	3:A:519:HOH:O	1.29	1.25
1:A:20:GLU:CD	1:C:165:LEU:CG	2.10	1.22
1:C:277:ARG:HE	1:C:280:ARG:NH2	1.42	1.16
1:A:20:GLU:OE2	1:C:165:LEU:HG	1.44	1.14
1:C:143:ARG:NH1	1:C:143:ARG:HG2	1.17	1.14
1:C:205:ILE:CG2	1:C:206:PRO:HD3	1.79	1.11
1:C:56:THR:HG22	1:C:64:ILE:HD11	1.19	1.10
1:C:40:GLU:HG3	1:C:336:MET:CE	1.80	1.10
1:A:277:ARG:NH2	1:A:280:ARG:NH2	1.98	1.10
1:C:99:ILE:HG22	1:C:99:ILE:O	1.45	1.09
1:C:143:ARG:CG	1:C:143:ARG:NH1	1.88	1.08
1:A:39:GLN:H	1:A:39:GLN:NE2	1.50	1.08
1:A:151:THR:CG2	1:A:151:THR:CA	2.31	1.08
2:C:415:HEC:HBB3	2:C:415:HEC:HMB3	1.35	1.08
1:A:151:THR:HG23	1:A:151:THR:H	1.22	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ARG:NH1	1:C:165:LEU:HD21	1.71	1.04
1:C:191:MET:HE2	1:C:196:ALA:HA	1.36	1.04
1:C:277:ARG:NE	1:C:280:ARG:HH21	1.55	1.04
1:A:298:GLY:O	1:A:299:ARG:HD3	1.53	1.04
1:C:160:ILE:HG12	1:C:250:LEU:HG	1.37	1.04
1:C:41:ALA:O	1:C:44:VAL:HG13	1.59	1.02
1:C:228:VAL:O	1:C:231:ARG:HD2	1.59	1.02
1:A:384:ALA:HA	1:A:405:VAL:HG22	1.42	1.01
1:A:277:ARG:CZ	1:A:280:ARG:NH2	2.24	1.00
1:A:237:GLU:HG2	1:A:240:ARG:NH2	1.74	1.00
1:C:40:GLU:HG3	1:C:336:MET:HE2	1.40	1.00
1:A:191:MET:HE2	1:A:196:ALA:HA	1.41	1.00
1:C:205:ILE:HG22	1:C:206:PRO:HD3	1.03	1.00
1:C:414:VAL:CG1	1:C:414:VAL:OXT	2.11	0.98
1:A:277:ARG:HH21	1:A:280:ARG:NH2	1.56	0.98
1:A:277:ARG:HE	1:A:280:ARG:CZ	1.75	0.98
1:A:277:ARG:NE	1:A:280:ARG:NH2	2.12	0.97
1:A:103:MET:HE2	1:A:107:GLU:OE1	1.63	0.97
1:C:166:LEU:HD12	1:C:166:LEU:O	1.64	0.97
1:C:267:SER:HG	1:C:270:HIS:HD1	1.11	0.96
1:A:205:ILE:CG2	1:A:205:ILE:HB	1.94	0.96
1:A:69:GLN:O	1:A:73:GLU:HG3	1.66	0.96
1:A:77:ASP:OD2	1:A:80:HIS:ND1	1.98	0.95
1:C:277:ARG:NE	1:C:280:ARG:NH2	2.11	0.95
1:A:277:ARG:O	1:A:279:GLU:N	2.00	0.95
1:C:143:ARG:HH11	1:C:143:ARG:HG3	1.28	0.94
1:C:205:ILE:HG22	1:C:206:PRO:CD	1.96	0.93
1:C:185:THR:HA	1:C:395:ILE:HD13	1.47	0.92
1:A:96:TYR:OH	1:A:101:THR:OG1	1.86	0.92
1:C:254:VAL:CG1	1:C:254:VAL:C	2.42	0.92
1:A:151:THR:CG2	1:A:151:THR:N	2.33	0.92
1:A:242:CYS:O	1:A:246:LEU:HD23	1.70	0.91
1:A:131:ILE:HD12	1:A:162:ILE:HD12	1.51	0.91
1:C:111:PHE:CE2	1:C:228:VAL:HG21	2.05	0.91
1:A:151:THR:HG23	1:A:151:THR:N	1.86	0.89
1:C:46:GLN:O	1:C:67:ARG:NH2	2.04	0.89
1:A:384:ALA:HA	1:A:405:VAL:CG2	2.02	0.89
1:C:356:LEU:CD1	1:C:356:LEU:HG	2.01	0.89
1:A:39:GLN:H	1:A:39:GLN:HE21	1.19	0.88
1:C:134:LEU:HD11	1:C:138:LEU:HD11	1.56	0.88
1:A:209:GLU:O	1:A:213:GLN:HG3	1.74	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:HH	1:A:101:THR:HG1	1.17	0.87
1:A:237:GLU:HG2	1:A:240:ARG:HH21	1.39	0.87
1:C:322:GLN:HB3	1:C:348:THR:O	1.74	0.87
1:C:205:ILE:N	1:C:206:PRO:CD	2.38	0.86
1:A:181:THR:HA	1:A:184:MET:CE	2.06	0.86
1:A:277:ARG:HE	1:A:280:ARG:NH2	1.70	0.86
1:C:91:GLU:H	1:C:91:GLU:CD	1.84	0.86
1:A:192:THR:OG1	1:A:195:GLU:HG2	1.76	0.85
1:C:56:THR:CG2	1:C:64:ILE:HD11	2.06	0.85
1:C:103:MET:HE2	1:C:107:GLU:OE1	1.77	0.85
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.56	0.84
1:A:103:MET:CE	1:A:107:GLU:OE1	2.25	0.84
1:C:254:VAL:CG1	1:C:254:VAL:CA	2.56	0.84
1:C:277:ARG:HE	1:C:280:ARG:HH21	0.88	0.84
1:C:99:ILE:CG2	1:C:241:MET:HB2	2.06	0.83
1:C:220:ILE:HD13	1:C:242:CYS:SG	2.17	0.83
1:A:138:LEU:HD23	1:A:154:TYR:CD2	2.13	0.83
1:A:378:ILE:N	1:A:379:PRO:HD3	1.92	0.83
1:A:17:HIS:HA	1:C:217:THR:HG23	1.61	0.83
1:C:356:LEU:CD1	1:C:356:LEU:CD2	2.57	0.82
1:A:127:LEU:O	1:A:131:ILE:HD13	1.80	0.82
1:A:121:MET:N	1:A:122:PRO:HD2	1.94	0.82
1:C:131:ILE:HG22	1:C:369:VAL:HG11	1.62	0.82
1:C:191:MET:HE2	1:C:196:ALA:CA	2.10	0.82
1:C:56:THR:HG22	1:C:64:ILE:CD1	2.08	0.81
1:A:20:GLU:OE1	1:C:165:LEU:CA	2.28	0.81
1:A:20:GLU:OE1	1:C:165:LEU:C	2.23	0.81
1:A:274:LEU:HD22	1:A:281:ILE:HD13	1.61	0.81
1:A:277:ARG:O	1:A:280:ARG:N	2.13	0.81
1:C:181:THR:HA	1:C:184:MET:HE3	1.59	0.81
1:C:295:VAL:HG22	1:C:396:VAL:HG22	1.61	0.81
1:C:390:GLN:O	1:C:400:GLN:N	2.13	0.81
1:A:237:GLU:CG	1:A:240:ARG:HH21	1.93	0.81
1:C:395:ILE:H	1:C:395:ILE:HD12	1.44	0.81
1:C:166:LEU:HD12	1:C:166:LEU:C	2.06	0.81
1:A:103:MET:SD	1:A:107:GLU:OE1	2.39	0.80
1:A:276:GLU:C	1:A:277:ARG:HG3	2.06	0.80
1:A:233:ILE:HD13	1:A:237:GLU:HB2	1.62	0.80
1:A:277:ARG:O	1:A:278:PRO:C	2.24	0.79
1:C:414:VAL:OXT	1:C:414:VAL:HG13	1.82	0.79
1:A:191:MET:HE2	1:A:196:ALA:CA	2.13	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ALA:O	1:C:139:ILE:HG12	1.82	0.79
1:C:383:ILE:HD13	1:C:389:ILE:HD11	1.62	0.79
1:A:389:ILE:HD12	1:A:389:ILE:H	1.47	0.79
1:C:400:GLN:O	1:C:401:ALA:HB2	1.81	0.79
1:C:244:ALA:O	1:C:245:LEU:C	2.25	0.78
1:C:40:GLU:HG3	1:C:336:MET:HE3	1.63	0.78
1:A:40:GLU:OE1	1:A:40:GLU:N	2.15	0.78
1:A:177:LEU:HD13	1:A:246:LEU:CD1	2.13	0.78
1:C:192:THR:OG1	1:C:195:GLU:HG2	1.83	0.78
1:C:254:VAL:C	1:C:254:VAL:HG12	2.07	0.78
1:A:21:HIS:HA	1:C:130:ARG:HD3	1.65	0.77
1:A:404:LEU:CD1	1:A:404:LEU:HG	2.10	0.77
1:C:99:ILE:HG22	1:C:241:MET:HB2	1.67	0.77
1:A:253:VAL:HG12	1:A:253:VAL:O	1.85	0.76
1:C:337:HIS:O	1:C:342:ARG:NH2	2.16	0.76
1:A:181:THR:HA	1:A:184:MET:HE3	1.68	0.76
1:A:134:LEU:CD1	1:A:134:LEU:HG	2.10	0.76
1:A:203:TYR:O	1:A:207:ILE:HD13	1.85	0.75
1:C:276:GLU:O	1:C:277:ARG:HG3	1.86	0.75
1:A:139:ILE:CG2	1:A:139:ILE:HB	2.12	0.75
1:A:40:GLU:HG3	1:A:336:MET:CE	2.16	0.75
1:A:389:ILE:CG2	1:A:389:ILE:CA	2.65	0.75
1:C:273:GLU:O	1:C:277:ARG:HB2	1.87	0.75
1:A:98:PHE:CE2	1:A:243:GLY:O	2.39	0.75
1:C:11:LEU:N	1:C:11:LEU:HD12	2.02	0.75
1:A:39:GLN:HE21	1:A:39:GLN:N	1.85	0.75
1:A:96:TYR:C	1:A:96:TYR:HA	2.05	0.74
1:A:209:GLU:O	1:A:213:GLN:NE2	2.21	0.74
1:C:113:ALA:O	1:C:116:ASN:HB3	1.88	0.74
1:A:233:ILE:CD1	1:A:237:GLU:HB2	2.17	0.74
1:C:267:SER:O	1:C:270:HIS:N	2.19	0.74
1:A:86:PRO:O	1:A:298:GLY:N	2.21	0.74
1:A:384:ALA:CA	1:A:405:VAL:HG22	2.18	0.73
1:C:201:TYR:CG	1:C:239:LYS:HD2	2.23	0.73
1:C:205:ILE:H	1:C:206:PRO:CD	2.01	0.73
2:C:415:HEC:HMB3	2:C:415:HEC:CBB	2.00	0.73
1:C:290:ARG:NH2	1:C:335:PRO:O	2.21	0.73
1:A:322:GLN:HG2	1:A:351:GLY:HA2	1.69	0.73
1:A:20:GLU:OE1	1:C:165:LEU:CG	2.36	0.73
1:A:205:ILE:N	1:A:206:PRO:CD	2.52	0.72
1:A:143:ARG:HG3	1:A:411:THR:HB	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:O	1:A:293:SER:C	2.32	0.72
1:A:17:HIS:CD2	1:A:313:LYS:CD	2.72	0.72
1:C:357:CYS:SG	2:C:415:HEC:CHB	2.74	0.72
1:C:39:GLN:H	1:C:39:GLN:HE21	1.37	0.72
1:C:99:ILE:HG23	1:C:100:PRO:N	2.05	0.72
1:A:125:ASP:O	1:A:128:GLU:HB2	1.88	0.72
1:A:139:ILE:HD12	1:A:374:TRP:CZ3	2.25	0.72
1:A:39:GLN:H	1:A:39:GLN:CD	1.96	0.72
1:A:181:THR:HG23	1:A:247:VAL:HG22	1.71	0.71
1:A:205:ILE:HG22	1:A:206:PRO:HD3	1.70	0.71
1:A:257:LEU:C	1:A:257:LEU:HA	2.06	0.71
1:C:278:PRO:O	1:C:281:ILE:HG13	1.90	0.71
1:C:389:ILE:CG2	1:C:389:ILE:CA	2.66	0.71
1:A:139:ILE:CG2	1:A:139:ILE:CA	2.65	0.71
1:A:223:VAL:HG12	1:A:224:ALA:N	2.05	0.71
1:A:98:PHE:CE2	1:A:243:GLY:C	2.69	0.71
1:C:183:GLN:O	1:C:187:PRO:HG3	1.90	0.71
1:C:108:GLN:O	1:C:108:GLN:HG2	1.85	0.70
1:A:395:ILE:O	1:A:395:ILE:HG22	1.90	0.70
1:C:195:GLU:HA	1:C:195:GLU:OE1	1.91	0.70
1:A:298:GLY:O	1:A:299:ARG:NH1	2.18	0.69
1:C:257:LEU:CD2	1:C:367:ILE:HD13	2.22	0.69
1:C:130:ARG:HH11	1:C:165:LEU:HD21	1.56	0.69
1:A:99:ILE:HG12	1:A:103:MET:HE3	1.72	0.69
1:A:39:GLN:NE2	1:A:39:GLN:N	2.33	0.69
1:C:195:GLU:OE1	1:C:195:GLU:CA	2.38	0.69
1:A:12:ALA:O	1:A:57:ARG:HB3	1.92	0.69
1:A:20:GLU:CG	1:C:165:LEU:HG	2.23	0.69
1:A:167:ALA:O	1:A:220:ILE:HD13	1.93	0.69
1:C:228:VAL:O	1:C:231:ARG:CD	2.40	0.69
1:A:115:ALA:HB3	1:A:358:LEU:HD13	1.74	0.69
1:A:136:CYS:O	1:A:137:SER:C	2.35	0.69
1:A:291:ARG:HG3	1:A:292:PHE:CE1	2.28	0.69
1:C:201:TYR:CD2	1:C:239:LYS:HD2	2.28	0.69
1:A:115:ALA:HB3	1:A:358:LEU:CD1	2.23	0.69
1:C:29:TYR:HE2	1:C:89:PRO:HD3	1.56	0.69
1:A:20:GLU:OE1	1:C:165:LEU:CB	2.41	0.69
1:A:277:ARG:NE	1:A:280:ARG:CZ	2.53	0.69
1:C:103:MET:HG2	1:C:107:GLU:OE1	1.92	0.69
1:C:134:LEU:CD1	1:C:138:LEU:CD1	2.71	0.69
1:A:366:GLU:C	1:A:367:ILE:CA	2.64	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASP:HB3	1:A:410:THR:HG23	1.74	0.68
1:A:139:ILE:HD11	1:A:154:TYR:CE2	2.28	0.68
1:A:258:SER:O	1:A:259:PHE:C	2.32	0.68
1:C:56:THR:O	1:C:61:GLY:HA2	1.93	0.68
1:A:139:ILE:O	1:A:142:LEU:HB2	1.94	0.68
1:A:359:GLY:HA3	2:A:415:HEC:C3C	2.23	0.68
1:A:373:GLU:HB3	1:A:377:ARG:NH1	2.09	0.68
1:C:99:ILE:HG21	1:C:241:MET:HB2	1.73	0.68
1:C:209:GLU:O	1:C:213:GLN:HG3	1.94	0.68
1:C:130:ARG:HH12	1:C:165:LEU:HD11	1.58	0.68
1:A:29:TYR:OH	1:A:88:ILE:O	2.06	0.68
1:A:208:ILE:O	1:A:212:ARG:HG3	1.94	0.68
1:C:61:GLY:O	1:C:62:HIS:HB3	1.93	0.68
1:A:378:ILE:HG22	1:A:378:ILE:O	1.93	0.68
1:A:19:PRO:HB2	1:A:21:HIS:ND1	2.10	0.67
1:A:203:TYR:O	1:A:206:PRO:HD2	1.93	0.67
1:A:268:PRO:O	1:A:271:ARG:HB2	1.93	0.67
1:A:414:VAL:CG1	1:A:414:VAL:OXT	2.42	0.67
1:C:158:PHE:O	1:C:162:ILE:HD13	1.94	0.67
1:C:164:MET:HE1	1:C:177:LEU:HD13	1.76	0.67
1:C:191:MET:CE	1:C:196:ALA:HA	2.18	0.67
1:C:287:GLU:OE1	1:C:342:ARG:HD2	1.94	0.67
1:A:19:PRO:HB2	1:A:21:HIS:CE1	2.28	0.67
1:C:205:ILE:N	1:C:206:PRO:HD2	2.08	0.67
1:C:29:TYR:HE2	1:C:89:PRO:CD	2.07	0.67
1:A:14:LEU:O	1:A:15:PRO:C	2.36	0.67
1:A:56:THR:O	1:A:61:GLY:HA2	1.95	0.67
1:A:220:ILE:HG22	1:A:220:ILE:O	1.92	0.67
1:A:377:ARG:HB3	1:A:412:LYS:O	1.95	0.67
1:A:20:GLU:CD	1:C:165:LEU:CB	2.68	0.66
1:A:17:HIS:CD2	1:A:313:LYS:HD3	2.31	0.66
1:A:377:ARG:C	1:A:379:PRO:HD3	2.21	0.66
1:A:191:MET:CE	1:A:196:ALA:HA	2.23	0.66
1:C:78:TYR:CE1	1:C:79:ARG:HD2	2.29	0.66
1:A:277:ARG:HH21	1:A:280:ARG:HH21	0.70	0.66
1:C:257:LEU:HD21	1:C:367:ILE:HD13	1.78	0.66
1:A:17:HIS:CD2	1:A:313:LYS:HD2	2.31	0.65
1:A:112:ARG:NH1	2:A:415:HEC:O1D	2.26	0.65
1:A:365:ARG:HD3	3:A:423:HOH:O	1.95	0.65
1:A:384:ALA:CB	1:A:403:PRO:HB2	2.26	0.65
1:A:363:ALA:HB1	2:A:415:HEC:HBB2	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:SER:O	1:C:268:PRO:C	2.37	0.65
1:A:205:ILE:CG2	1:A:205:ILE:C	2.69	0.65
1:A:277:ARG:HA	3:A:438:HOH:O	1.96	0.65
1:C:290:ARG:NH1	1:C:335:PRO:O	2.30	0.65
1:A:209:GLU:C	1:A:213:GLN:HE21	2.05	0.65
1:A:281:ILE:HG23	1:A:371:LEU:HD12	1.79	0.65
1:C:130:ARG:HG3	1:C:165:LEU:HD21	1.79	0.65
1:C:294:LEU:HD12	1:C:397:SER:O	1.97	0.65
1:C:103:MET:CE	1:C:107:GLU:OE1	2.44	0.65
1:A:139:ILE:HD12	1:A:374:TRP:CE3	2.32	0.65
1:C:88:ILE:HA	1:C:89:PRO:O	1.96	0.65
1:A:151:THR:HG22	1:A:258:SER:OG	1.97	0.64
1:A:269:GLU:HA	1:A:272:GLN:HB2	1.79	0.64
1:C:287:GLU:OE1	1:C:345:VAL:HG13	1.97	0.64
1:C:67:ARG:NH1	3:C:498:HOH:O	2.30	0.64
1:C:100:PRO:HG3	1:C:112:ARG:HA	1.80	0.64
1:C:131:ILE:CG2	1:C:131:ILE:CA	2.74	0.64
1:C:365:ARG:O	1:C:369:VAL:HB	1.97	0.64
1:A:115:ALA:CB	1:A:358:LEU:HD13	2.28	0.64
1:C:111:PHE:O	1:C:112:ARG:C	2.28	0.64
1:C:414:VAL:OXT	1:C:414:VAL:HG12	1.94	0.64
1:C:149:ASN:ND2	1:C:151:THR:OG1	2.31	0.64
2:C:415:HEC:HBB3	2:C:415:HEC:CMB	2.21	0.64
1:C:112:ARG:CZ	1:C:358:LEU:HD21	2.26	0.64
1:A:15:PRO:HG2	1:A:18:VAL:HG23	1.80	0.64
1:A:164:MET:HE3	1:A:169:LEU:CB	2.28	0.64
1:A:177:LEU:HD13	1:A:246:LEU:HD12	1.79	0.64
1:A:138:LEU:O	1:A:142:LEU:HG	1.97	0.64
1:A:237:GLU:O	1:A:241:MET:N	2.31	0.63
1:A:277:ARG:HB3	1:A:280:ARG:HG3	1.78	0.63
1:C:205:ILE:CG2	1:C:206:PRO:CD	2.66	0.63
1:A:71:ILE:HG21	1:A:325:SER:OG	1.97	0.63
1:C:391:HIS:N	1:C:391:HIS:CD2	2.61	0.63
1:C:204:LEU:O	1:C:207:ILE:HB	1.98	0.63
1:C:99:ILE:HD11	1:C:240:ARG:NH2	2.14	0.63
1:C:172:GLU:N	1:C:172:GLU:OE1	2.30	0.63
1:A:33:ASN:HD22	1:A:44:VAL:HG11	1.61	0.63
1:C:103:MET:SD	1:C:107:GLU:OE1	2.57	0.63
1:C:369:VAL:CA	1:C:369:VAL:HB	2.15	0.63
1:A:374:TRP:NE1	1:A:381:PHE:CE1	2.65	0.63
1:A:216:GLY:H	1:A:221:SER:HB3	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:PRO:O	1:C:269:GLU:C	2.36	0.62
1:A:205:ILE:N	1:A:206:PRO:HD2	2.14	0.62
1:C:108:GLN:HE22	1:C:354:SER:HB2	1.64	0.62
1:A:358:LEU:CD1	2:A:415:HEC:HBD2	2.30	0.62
1:A:111:PHE:O	1:A:241:MET:HE1	1.99	0.62
1:C:184:MET:HE1	1:C:200:LEU:HD22	1.82	0.62
1:C:262:GLU:HB2	1:C:402:LEU:HD13	1.81	0.62
1:C:262:GLU:O	1:C:265:ALA:HB3	1.99	0.62
1:C:301:LEU:N	1:C:301:LEU:CD2	2.62	0.62
1:C:144:PRO:HG2	1:C:145:GLN:N	2.15	0.62
1:A:19:PRO:HD2	1:A:22:LEU:HD12	1.82	0.62
1:A:20:GLU:OE1	1:C:165:LEU:O	2.17	0.62
1:C:149:ASN:O	1:C:153:ASP:HB2	2.00	0.62
1:C:193:PHE:CD2	1:C:193:PHE:C	2.78	0.62
1:A:20:GLU:OE1	1:C:165:LEU:HD12	2.00	0.61
1:C:178:LYS:NZ	1:C:250:LEU:O	2.29	0.61
1:C:273:GLU:OE2	1:C:280:ARG:NH1	2.32	0.61
1:C:373:GLU:CB	1:C:373:GLU:CD	2.70	0.61
1:A:118:VAL:HG12	1:A:222:ILE:HD12	1.82	0.61
1:A:253:VAL:O	1:A:253:VAL:CG1	2.47	0.61
1:A:341:SER:O	1:A:342:ARG:C	2.40	0.61
1:C:99:ILE:O	1:C:99:ILE:CG2	2.15	0.61
1:C:277:ARG:HE	1:C:280:ARG:CZ	2.10	0.61
1:A:88:ILE:HD13	1:A:319:LEU:HD13	1.82	0.61
1:C:63:TRP:C	1:C:64:ILE:HD12	2.26	0.61
1:C:242:CYS:O	1:C:246:LEU:HD23	2.01	0.61
1:C:377:ARG:C	1:C:378:ILE:HD12	2.25	0.61
1:A:256:PHE:HZ	1:A:288:LEU:C	2.09	0.61
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.64	0.61
1:A:96:TYR:CZ	1:A:98:PHE:HB2	2.36	0.61
1:C:174:ILE:O	1:C:175:PRO:C	2.41	0.61
1:A:149:ASN:ND2	1:A:151:THR:OG1	2.33	0.61
1:C:173:ASP:HB3	1:C:177:LEU:HD11	1.82	0.61
1:A:205:ILE:HG22	1:A:206:PRO:CD	2.30	0.60
1:C:134:LEU:HD11	1:C:138:LEU:CD1	2.27	0.60
1:C:159:PRO:HG3	1:C:257:LEU:HD12	1.83	0.60
1:C:254:VAL:CG1	1:C:254:VAL:CG2	2.72	0.60
1:C:290:ARG:NH2	1:C:337:HIS:O	2.34	0.60
1:A:206:PRO:HB2	1:A:207:ILE:HD12	1.83	0.60
1:A:374:TRP:CD1	1:A:381:PHE:CE1	2.89	0.60
1:A:404:LEU:CD1	1:A:404:LEU:CD2	2.76	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:O	1:A:396:VAL:HG11	2.02	0.60
1:A:304:ASP:HA	1:A:313:LYS:HA	1.83	0.60
1:A:358:LEU:HG	2:A:415:HEC:HBD2	1.83	0.60
1:A:17:HIS:CG	1:A:313:LYS:HD3	2.37	0.60
1:A:151:THR:CG2	1:A:151:THR:H	1.96	0.60
1:A:240:ARG:CD	1:A:240:ARG:CB	2.77	0.60
1:C:389:ILE:CG2	1:C:389:ILE:HB	2.19	0.60
1:C:281:ILE:HB	1:C:282:PRO:HD3	1.84	0.60
1:C:373:GLU:CG	1:C:373:GLU:CA	2.73	0.60
1:A:277:ARG:N	1:A:278:PRO:CD	2.65	0.59
1:A:110:GLN:HE21	1:A:229:ASN:HA	1.66	0.59
1:A:231:ARG:O	1:A:231:ARG:HD3	2.01	0.59
1:A:272:GLN:CA	1:A:272:GLN:HE21	2.16	0.59
1:C:257:LEU:HD23	1:C:367:ILE:CD1	2.32	0.59
1:C:99:ILE:HD11	1:C:103:MET:HE3	1.82	0.59
1:A:237:GLU:HG2	1:A:240:ARG:HH22	1.63	0.59
1:A:15:PRO:HG2	1:A:18:VAL:CG2	2.31	0.59
1:A:96:TYR:CE1	1:A:102:SER:HB3	2.38	0.59
1:C:177:LEU:HD21	1:C:203:TYR:CE2	2.38	0.59
1:C:39:GLN:H	1:C:39:GLN:NE2	2.00	0.59
1:C:75:TYR:CZ	1:C:320:LEU:HB2	2.38	0.59
1:C:142:LEU:HD22	1:C:148:CYS:HB3	1.84	0.58
1:C:214:LYS:N	1:C:215:PRO:HD3	2.18	0.58
1:C:287:GLU:HA	1:C:345:VAL:HG11	1.85	0.58
1:C:184:MET:HE1	1:C:200:LEU:CD2	2.33	0.58
1:C:395:ILE:H	1:C:395:ILE:CD1	2.16	0.58
1:A:164:MET:HE3	1:A:169:LEU:HB3	1.85	0.58
1:A:277:ARG:N	1:A:278:PRO:HD2	2.18	0.58
1:A:362:LEU:O	1:A:363:ALA:C	2.46	0.58
1:C:11:LEU:N	1:C:11:LEU:CD1	2.66	0.58
1:C:139:ILE:HD12	1:C:374:TRP:CE3	2.38	0.58
1:A:244:ALA:O	1:A:245:LEU:C	2.46	0.58
1:A:85:CYS:SG	1:A:317:GLN:NE2	2.77	0.58
1:A:88:ILE:HD12	1:A:88:ILE:N	2.19	0.58
1:A:88:ILE:HG23	1:A:89:PRO:HA	1.84	0.58
1:A:209:GLU:O	1:A:213:GLN:CG	2.48	0.58
1:A:407:ASP:OD1	1:A:409:ALA:HB3	2.04	0.58
1:A:130:ARG:NH2	1:A:165:LEU:HD11	2.18	0.58
1:C:99:ILE:HG21	1:C:241:MET:HE3	1.86	0.58
1:A:121:MET:N	1:A:122:PRO:CD	2.67	0.57
1:A:277:ARG:CB	1:A:280:ARG:HG3	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ARG:CZ	1:C:335:PRO:O	2.52	0.57
1:C:341:SER:C	1:C:342:ARG:O	2.35	0.57
1:A:201:TYR:CD1	1:A:239:LYS:HG2	2.39	0.57
1:A:201:TYR:OH	1:A:240:ARG:HG2	2.03	0.57
1:A:46:GLN:O	1:A:67:ARG:NH2	2.33	0.57
1:A:143:ARG:HG3	1:A:411:THR:CB	2.33	0.57
1:C:204:LEU:C	1:C:208:ILE:HD13	2.29	0.57
1:A:184:MET:HB3	1:A:193:PHE:HE1	1.70	0.57
1:C:106:PRO:O	1:C:107:GLU:C	2.47	0.57
1:C:205:ILE:H	1:C:206:PRO:HD3	1.67	0.57
1:A:288:LEU:CD2	1:A:292:PHE:HE2	2.18	0.57
1:C:130:ARG:HH11	1:C:130:ARG:HG3	1.70	0.57
1:C:148:CYS:SG	1:C:404:LEU:HD12	2.45	0.57
1:C:99:ILE:CG2	1:C:241:MET:HE3	2.34	0.57
1:A:378:ILE:O	1:A:381:PHE:HD1	1.88	0.56
1:C:96:TYR:HD2	1:C:193:PHE:CZ	2.22	0.56
1:C:266:LYS:HD2	1:C:383:ILE:CD1	2.35	0.56
1:A:207:ILE:HD12	1:A:207:ILE:N	2.20	0.56
1:A:358:LEU:HD12	2:A:415:HEC:HMD2	1.87	0.56
1:A:22:LEU:HD22	1:A:53:LEU:O	2.05	0.56
1:A:237:GLU:CG	1:A:240:ARG:NH2	2.54	0.56
1:A:272:GLN:CA	1:A:272:GLN:NE2	2.68	0.56
1:C:356:LEU:HG	1:C:357:CYS:N	2.20	0.56
1:A:156:GLU:O	1:A:160:ILE:HD12	2.05	0.56
1:A:195:GLU:HA	1:A:195:GLU:OE1	2.06	0.56
1:A:384:ALA:HB2	1:A:403:PRO:HB2	1.88	0.56
1:A:277:ARG:HD2	3:A:495:HOH:O	2.05	0.56
1:A:100:PRO:HB2	2:A:415:HEC:O2D	2.06	0.56
1:A:240:ARG:CG	1:A:240:ARG:NE	2.63	0.56
1:C:99:ILE:CD1	1:C:103:MET:HE3	2.35	0.56
1:A:205:ILE:CG2	1:A:205:ILE:CA	2.76	0.56
1:A:287:GLU:OE1	1:A:342:ARG:HD2	2.06	0.56
1:C:235:SER:O	1:C:238:ALA:HB3	2.06	0.56
1:C:355:HIS:ND1	2:C:415:HEC:O2D	2.39	0.56
1:C:64:ILE:HD12	1:C:64:ILE:N	2.21	0.56
1:C:184:MET:CE	1:C:200:LEU:HD22	2.35	0.56
1:A:75:TYR:OH	1:A:322:GLN:NE2	2.39	0.55
1:A:134:LEU:CD1	1:A:134:LEU:CD2	2.79	0.55
1:A:276:GLU:C	1:A:277:ARG:CG	2.78	0.55
1:C:29:TYR:CE2	1:C:89:PRO:HD3	2.40	0.55
1:A:276:GLU:C	1:A:278:PRO:HD2	2.31	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:O	1:A:56:THR:HB	2.06	0.55
1:A:218:ASP:O	1:A:219:ALA:C	2.48	0.55
1:C:369:VAL:CA	1:C:369:VAL:CG2	2.75	0.55
1:C:100:PRO:CG	1:C:112:ARG:HA	2.36	0.55
1:C:256:PHE:HD2	1:C:367:ILE:CD1	2.18	0.55
1:A:220:ILE:O	1:A:220:ILE:CG2	2.52	0.55
1:C:14:LEU:HD11	1:C:18:VAL:HB	1.88	0.55
1:C:29:TYR:CE2	1:C:89:PRO:CD	2.89	0.55
1:C:289:LEU:HD13	1:C:350:PHE:HE2	1.72	0.55
1:A:228:VAL:O	1:A:231:ARG:CD	2.55	0.55
1:A:20:GLU:OE1	1:C:165:LEU:CD1	2.55	0.55
1:A:216:GLY:H	1:A:221:SER:CB	2.19	0.55
1:C:10:ASN:C	1:C:11:LEU:HD12	2.32	0.55
1:C:131:ILE:HG23	1:C:158:PHE:CZ	2.42	0.55
1:C:305:TYR:N	3:C:505:HOH:O	2.35	0.55
1:A:409:ALA:CB	1:A:409:ALA:N	2.63	0.54
1:A:205:ILE:HD11	1:A:239:LYS:HD2	1.89	0.54
1:C:88:ILE:HD11	1:C:317:GLN:HB3	1.90	0.54
1:A:20:GLU:CG	1:C:165:LEU:CG	2.83	0.54
1:C:87:PHE:CD1	1:C:87:PHE:N	2.76	0.54
1:A:154:TYR:O	1:A:155:ALA:C	2.47	0.54
1:A:372:LYS:O	1:A:376:THR:HB	2.08	0.54
1:C:87:PHE:N	1:C:87:PHE:HD1	2.06	0.54
1:C:147:GLN:HA	1:C:406:TRP:CZ3	2.43	0.54
1:C:164:MET:HE1	1:C:177:LEU:CD1	2.38	0.54
1:C:277:ARG:HB3	1:C:280:ARG:HG3	1.90	0.54
1:A:409:ALA:CB	1:A:409:ALA:HA	2.18	0.54
1:C:63:TRP:CE2	1:C:312:LEU:CD2	2.91	0.54
1:C:407:ASP:O	1:C:410:THR:HG23	2.08	0.54
1:A:184:MET:HB3	1:A:193:PHE:CE1	2.44	0.53
1:A:127:LEU:HB3	1:A:131:ILE:CD1	2.39	0.53
1:A:264:LEU:CD2	1:A:264:LEU:CD1	2.84	0.53
1:A:276:GLU:O	1:A:277:ARG:HG3	2.06	0.53
1:A:358:LEU:HG	2:A:415:HEC:CBD	2.37	0.53
1:A:20:GLU:OE2	1:C:165:LEU:CG	2.32	0.53
1:A:288:LEU:HD23	1:A:292:PHE:CE2	2.43	0.53
1:A:322:GLN:CG	1:A:351:GLY:HA2	2.38	0.53
1:C:96:TYR:HD2	1:C:193:PHE:HZ	1.57	0.53
1:C:166:LEU:C	1:C:166:LEU:CD1	2.80	0.53
1:C:121:MET:HB3	3:C:426:HOH:O	2.08	0.53
1:A:99:ILE:HD11	1:A:240:ARG:NH2	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:O	1:A:138:LEU:HB2	2.08	0.53
1:A:138:LEU:HD22	1:A:158:PHE:HB2	1.90	0.53
1:A:383:ILE:HD11	1:A:402:LEU:HD11	1.90	0.53
1:C:377:ARG:NH1	1:C:377:ARG:HG3	2.23	0.53
1:C:113:ALA:O	1:C:116:ASN:CB	2.56	0.53
1:A:177:LEU:HD13	1:A:246:LEU:HD13	1.90	0.53
1:C:78:TYR:CZ	1:C:79:ARG:NH1	2.76	0.53
1:C:177:LEU:HD21	1:C:203:TYR:CD2	2.43	0.53
1:A:139:ILE:HD11	1:A:154:TYR:CD2	2.44	0.53
1:A:205:ILE:CG2	1:A:206:PRO:HD3	2.38	0.52
1:A:38:VAL:N	1:A:391:HIS:ND1	2.56	0.52
1:A:125:ASP:HA	3:A:497:HOH:O	2.08	0.52
1:A:266:LYS:O	1:A:267:SER:HB2	2.08	0.52
1:A:20:GLU:CD	1:C:165:LEU:CD1	2.83	0.52
1:A:182:ASP:OD2	1:A:186:ARG:NH2	2.42	0.52
1:C:51:PRO:HD2	1:C:54:VAL:HG12	1.91	0.52
1:C:63:TRP:CE2	1:C:312:LEU:HD23	2.44	0.52
1:A:22:LEU:HD11	1:A:310:VAL:HG22	1.90	0.52
1:C:40:GLU:CG	1:C:336:MET:HE2	2.28	0.52
1:C:253:VAL:HG23	2:C:415:HEC:HMC3	1.92	0.52
1:A:267:SER:O	1:A:268:PRO:C	2.53	0.52
1:A:389:ILE:CG2	1:A:389:ILE:CG1	2.78	0.52
1:C:131:ILE:HG23	1:C:158:PHE:CE1	2.45	0.52
1:C:134:LEU:CD1	1:C:138:LEU:HD11	2.26	0.52
1:A:19:PRO:C	1:A:21:HIS:N	2.66	0.52
1:A:119:VAL:HG11	2:A:415:HEC:HBC1	1.92	0.52
1:A:167:ALA:HB1	1:A:220:ILE:HD11	1.92	0.52
1:C:14:LEU:HD12	1:C:15:PRO:HG2	1.91	0.52
1:C:185:THR:CA	1:C:395:ILE:HD13	2.30	0.52
1:C:201:TYR:O	1:C:205:ILE:HB	2.10	0.52
1:C:276:GLU:O	1:C:277:ARG:CG	2.56	0.52
1:A:364:ARG:O	1:A:365:ARG:C	2.53	0.52
1:C:98:PHE:HA	1:C:240:ARG:O	2.10	0.52
1:C:130:ARG:NH1	1:C:165:LEU:CD2	2.60	0.52
1:C:204:LEU:O	1:C:208:ILE:HD13	2.10	0.52
1:C:341:SER:O	1:C:342:ARG:O	2.27	0.52
1:C:273:GLU:O	1:C:277:ARG:CB	2.56	0.51
1:A:272:GLN:O	1:A:276:GLU:HG2	2.10	0.51
1:A:312:LEU:HD23	1:A:312:LEU:N	2.25	0.51
1:C:289:LEU:HD13	1:C:350:PHE:CE2	2.44	0.51
1:A:118:VAL:CG1	1:A:219:ALA:HA	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HD23	1:A:292:PHE:HE2	1.75	0.51
1:A:383:ILE:CD1	1:A:402:LEU:HD11	2.40	0.51
1:C:100:PRO:CG	1:C:112:ARG:HB2	2.41	0.51
1:C:313:LYS:O	1:C:316:ASP:HB2	2.10	0.51
1:C:350:PHE:O	1:C:357:CYS:HB2	2.09	0.51
1:C:88:ILE:C	1:C:89:PRO:O	2.54	0.51
1:C:109:ARG:HD3	3:C:443:HOH:O	2.11	0.51
1:C:13:PRO:O	1:C:15:PRO:HD2	2.11	0.51
1:C:156:GLU:O	1:C:160:ILE:HB	2.11	0.51
1:C:377:ARG:NH1	1:C:377:ARG:CG	2.73	0.51
1:C:83:SER:HB3	1:C:101:THR:O	2.11	0.51
1:C:106:PRO:HA	3:C:443:HOH:O	2.09	0.51
1:A:272:GLN:HE21	1:A:272:GLN:C	2.18	0.51
1:C:87:PHE:CE2	1:C:395:ILE:HG12	2.46	0.51
1:A:211:ARG:HG3	1:A:221:SER:OG	2.11	0.51
1:A:276:GLU:O	1:A:277:ARG:CG	2.59	0.50
1:C:97:ASP:O	1:C:99:ILE:HD13	2.11	0.50
1:C:294:LEU:O	1:C:294:LEU:HG	2.10	0.50
1:A:24:PHE:HB3	1:A:54:VAL:HG21	1.94	0.50
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.76	0.50
1:A:207:ILE:N	1:A:207:ILE:CD1	2.75	0.50
1:A:237:GLU:CB	1:A:240:ARG:HH21	2.23	0.50
1:C:358:LEU:HG	2:C:415:HEC:HBD2	1.93	0.50
1:A:28:MET:HE1	1:A:395:ILE:HD13	1.92	0.50
1:C:186:ARG:O	1:C:187:PRO:C	2.51	0.50
1:C:256:PHE:HZ	1:C:288:LEU:HB3	1.75	0.50
1:A:97:ASP:OD1	1:A:97:ASP:N	2.28	0.50
1:A:98:PHE:CD2	1:A:243:GLY:C	2.90	0.50
1:A:384:ALA:HA	1:A:405:VAL:HG21	1.90	0.50
1:C:97:ASP:OD2	1:C:240:ARG:HD2	2.11	0.50
1:A:23:VAL:HG12	1:A:23:VAL:O	2.11	0.50
1:A:75:TYR:HE1	1:A:299:ARG:CZ	2.24	0.50
1:C:18:VAL:HG11	1:C:55:TRP:CG	2.46	0.50
1:C:88:ILE:CA	1:C:89:PRO:O	2.59	0.50
1:A:96:TYR:CZ	1:A:101:THR:OG1	2.64	0.50
1:C:42:TRP:C	1:C:44:VAL:N	2.68	0.50
1:C:137:SER:O	1:C:139:ILE:N	2.45	0.50
1:A:19:PRO:C	1:A:21:HIS:H	2.18	0.50
1:A:88:ILE:HD12	1:A:88:ILE:H	1.77	0.50
1:A:207:ILE:O	1:A:208:ILE:C	2.50	0.50
1:C:143:ARG:O	1:C:144:PRO:C	2.51	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:OD2	2:A:415:HEC:O2A	2.30	0.50
1:A:384:ALA:HB3	1:A:403:PRO:HB2	1.93	0.50
1:C:134:LEU:CD1	1:C:138:LEU:HD13	2.42	0.50
1:A:39:GLN:N	1:A:39:GLN:CD	2.67	0.49
1:A:72:ARG:HH11	1:A:72:ARG:CG	2.21	0.49
1:C:377:ARG:HB3	1:C:378:ILE:HD12	1.93	0.49
1:A:131:ILE:CD1	1:A:162:ILE:HD12	2.35	0.49
1:C:111:PHE:CD2	1:C:228:VAL:HG21	2.44	0.49
1:A:57:ARG:HA	1:A:61:GLY:HA2	1.94	0.49
1:A:140:GLU:O	1:A:144:PRO:HD2	2.12	0.49
1:C:15:PRO:HG3	1:C:55:TRP:CZ2	2.47	0.49
1:A:99:ILE:CG1	1:A:103:MET:HE3	2.41	0.49
1:C:91:GLU:HG2	3:C:472:HOH:O	2.12	0.49
1:C:249:GLY:C	1:C:250:LEU:HD12	2.37	0.49
1:C:311:GLN:CD	3:C:505:HOH:O	2.55	0.49
1:C:395:ILE:HD12	1:C:395:ILE:N	2.22	0.49
1:A:17:HIS:CG	1:A:313:LYS:CD	2.95	0.49
1:A:164:MET:HE3	1:A:169:LEU:HB2	1.94	0.49
1:C:114:LEU:HD23	1:C:233:ILE:HD12	1.94	0.49
1:C:369:VAL:CB	1:C:369:VAL:C	2.79	0.49
1:C:137:SER:O	1:C:138:LEU:C	2.55	0.49
1:C:251:ASP:O	1:C:255:ASN:ND2	2.45	0.49
1:C:383:ILE:CD1	1:C:389:ILE:HD11	2.38	0.49
1:A:98:PHE:CD2	1:A:244:ALA:N	2.81	0.49
1:A:395:ILE:O	1:A:395:ILE:CG2	2.60	0.49
1:A:228:VAL:O	1:A:231:ARG:HD2	2.13	0.49
1:A:291:ARG:HG3	1:A:292:PHE:CZ	2.48	0.49
1:C:29:TYR:CE2	1:C:89:PRO:HD2	2.48	0.49
1:C:43:ALA:C	1:C:45:LEU:N	2.68	0.49
1:C:134:LEU:HD23	1:C:158:PHE:HA	1.94	0.49
1:C:91:GLU:CD	1:C:91:GLU:N	2.59	0.49
1:C:257:LEU:CD2	1:C:367:ILE:CD1	2.88	0.49
1:A:72:ARG:HD3	1:A:352:HIS:CE1	2.47	0.49
1:A:88:ILE:HD13	1:A:319:LEU:CD1	2.42	0.49
1:C:131:ILE:HG22	1:C:131:ILE:O	2.13	0.49
1:C:152:GLU:O	1:C:157:PRO:HD3	2.12	0.49
1:C:33:ASN:O	1:C:36:ALA:HB3	2.13	0.48
1:A:158:PHE:HD2	1:A:159:PRO:HD3	1.77	0.48
1:C:49:ASN:H	1:C:49:ASN:HD22	1.61	0.48
1:C:130:ARG:HH11	1:C:130:ARG:CG	2.18	0.48
1:A:171:GLU:C	1:A:173:ASP:H	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:O	1:C:113:ALA:C	2.49	0.48
1:C:256:PHE:HD2	1:C:367:ILE:HD11	1.76	0.48
1:C:340:PHE:N	1:C:340:PHE:CD1	2.76	0.48
1:C:389:ILE:CG2	1:C:399:VAL:HG13	2.43	0.48
1:A:149:ASN:C	1:A:149:ASN:HD22	2.22	0.48
1:A:41:ALA:O	1:A:44:VAL:HG22	2.13	0.48
1:A:92:ALA:O	1:A:96:TYR:N	2.34	0.48
1:A:414:VAL:OXT	1:A:414:VAL:HG12	2.13	0.48
1:A:127:LEU:HB3	1:A:131:ILE:HD11	1.95	0.48
1:C:266:LYS:HD2	1:C:383:ILE:HD12	1.95	0.48
1:A:118:VAL:HG23	1:A:119:VAL:HG13	1.96	0.48
1:A:291:ARG:HD2	1:A:291:ARG:O	2.14	0.48
1:A:359:GLY:HA3	2:A:415:HEC:C4C	2.43	0.48
1:C:10:ASN:C	1:C:10:ASN:OD1	2.55	0.48
1:C:99:ILE:HG23	1:C:100:PRO:CD	2.43	0.48
1:C:243:GLY:O	1:C:244:ALA:C	2.49	0.48
1:A:107:GLU:O	1:A:108:GLN:C	2.54	0.48
1:A:143:ARG:HH11	1:A:143:ARG:CG	2.25	0.48
1:C:130:ARG:HG3	1:C:165:LEU:CD2	2.43	0.48
1:C:392:LYS:HD2	1:C:392:LYS:HA	1.50	0.48
1:A:61:GLY:O	1:A:62:HIS:HB3	2.13	0.47
1:C:395:ILE:C	1:C:396:VAL:HG23	2.39	0.47
1:A:100:PRO:HG3	1:A:112:ARG:HA	1.96	0.47
1:A:166:LEU:O	1:A:166:LEU:HD12	2.14	0.47
1:A:389:ILE:CG2	1:A:389:ILE:C	2.87	0.47
1:C:290:ARG:O	1:C:290:ARG:HG2	1.98	0.47
1:A:298:GLY:C	1:A:299:ARG:HD3	2.35	0.47
1:A:383:ILE:HD13	1:A:404:LEU:CD2	2.44	0.47
1:C:99:ILE:HD11	1:C:240:ARG:CZ	2.45	0.47
1:C:100:PRO:O	1:C:355:HIS:HE1	1.97	0.47
1:C:160:ILE:HG23	1:C:250:LEU:HD11	1.96	0.47
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.30	0.47
1:A:338:VAL:O	1:A:338:VAL:HG12	2.13	0.47
1:C:234:THR:OG1	1:C:237:GLU:HG3	2.14	0.47
1:A:167:ALA:HB1	1:A:220:ILE:CD1	2.45	0.47
1:A:186:ARG:O	1:A:187:PRO:C	2.55	0.47
1:A:195:GLU:OE1	1:A:195:GLU:CA	2.60	0.47
1:A:414:VAL:OXT	1:A:414:VAL:HG13	2.15	0.47
1:A:201:TYR:O	1:A:205:ILE:N	2.47	0.47
1:A:228:VAL:C	1:A:230:GLY:H	2.22	0.47
1:C:80:HIS:CD2	1:C:305:TYR:CG	3.03	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:LEU:HD23	1:C:367:ILE:HD12	1.96	0.47
1:A:11:LEU:HD21	1:A:25:ASP:OD2	2.15	0.47
1:A:40:GLU:CG	1:A:336:MET:HE2	2.37	0.47
1:C:100:PRO:O	1:C:355:HIS:CE1	2.68	0.47
1:C:160:ILE:O	1:C:160:ILE:HG22	2.12	0.47
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.97	0.47
1:A:150:PHE:CE1	1:A:261:MET:HG2	2.50	0.47
1:A:313:LYS:HE2	3:A:505:HOH:O	2.13	0.47
2:A:415:HEC:HHD	2:A:415:HEC:HAC	1.62	0.47
1:C:295:VAL:O	1:C:322:GLN:N	2.46	0.47
1:C:324:LEU:O	1:C:325:SER:C	2.55	0.47
1:A:39:GLN:HB3	1:A:327:LEU:HD11	1.97	0.46
1:A:213:GLN:O	1:A:215:PRO:HD3	2.15	0.46
1:C:103:MET:CG	1:C:107:GLU:OE1	2.60	0.46
1:C:265:ALA:HA	1:C:381:PHE:CE2	2.50	0.46
1:A:115:ALA:CB	1:A:358:LEU:CD1	2.88	0.46
1:A:140:GLU:CD	1:A:143:ARG:HE	2.23	0.46
1:A:363:ALA:CB	2:A:415:HEC:HBB2	2.43	0.46
1:C:125:ASP:O	1:C:126:LYS:C	2.52	0.46
1:C:391:HIS:N	1:C:391:HIS:HD2	2.11	0.46
1:C:256:PHE:CD2	1:C:367:ILE:CD1	2.98	0.46
1:A:67:ARG:HD2	1:A:330:ARG:CZ	2.46	0.46
1:A:171:GLU:C	1:A:173:ASP:N	2.72	0.46
1:A:266:LYS:O	1:A:267:SER:CB	2.63	0.46
1:A:378:ILE:O	1:A:381:PHE:CD1	2.68	0.46
1:C:155:ALA:O	1:C:254:VAL:HG22	2.15	0.46
1:A:201:TYR:CG	1:A:239:LYS:HE3	2.51	0.46
1:C:114:LEU:CD2	1:C:233:ILE:HD12	2.45	0.46
1:C:205:ILE:N	1:C:206:PRO:HD3	2.23	0.46
1:C:377:ARG:CG	1:C:377:ARG:HH11	2.24	0.46
1:A:82:SER:HB2	1:A:104:ASP:OD2	2.16	0.46
1:A:99:ILE:HG22	1:A:241:MET:HE2	1.98	0.46
1:A:192:THR:HG1	1:A:195:GLU:HG2	1.80	0.46
1:C:266:LYS:HD2	1:C:383:ILE:HD11	1.96	0.46
1:C:149:ASN:O	1:C:153:ASP:CB	2.63	0.46
1:C:243:GLY:O	1:C:244:ALA:O	2.34	0.46
1:C:131:ILE:CG2	1:C:131:ILE:C	2.89	0.45
1:C:301:LEU:N	1:C:301:LEU:HD23	2.31	0.45
1:A:334:ALA:O	1:A:335:PRO:C	2.53	0.45
1:C:100:PRO:HG2	1:C:112:ARG:HB2	1.98	0.45
1:A:15:PRO:HA	1:A:16:PRO:HD2	1.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:HB3	1:A:377:ARG:HH12	1.80	0.45
1:C:109:ARG:O	1:C:110:GLN:C	2.58	0.45
1:C:294:LEU:N	1:C:294:LEU:HD23	2.30	0.45
1:C:402:LEU:HA	1:C:403:PRO:HD3	1.85	0.45
1:A:38:VAL:HG11	1:A:397:SER:HB3	1.98	0.45
1:A:15:PRO:CG	1:A:18:VAL:HG23	2.47	0.45
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.80	0.45
1:A:270:HIS:O	1:A:271:ARG:C	2.59	0.45
1:A:358:LEU:CG	2:A:415:HEC:HBD2	2.47	0.45
1:A:367:ILE:N	1:A:367:ILE:CB	2.64	0.45
1:C:18:VAL:HA	1:C:19:PRO:HD3	1.57	0.45
1:C:134:LEU:HD12	1:C:138:LEU:CD1	2.47	0.45
1:A:40:GLU:N	1:A:40:GLU:CD	2.74	0.45
1:A:359:GLY:HA3	2:A:415:HEC:C2C	2.46	0.45
1:C:293:SER:HB2	1:C:349:THR:OG1	2.17	0.45
1:C:201:TYR:O	1:C:204:LEU:N	2.40	0.45
1:C:205:ILE:H	1:C:206:PRO:HD2	1.72	0.45
1:C:359:GLY:HA3	2:C:415:HEC:C3C	2.46	0.45
1:A:136:CYS:SG	1:A:377:ARG:NH2	2.90	0.45
1:C:14:LEU:HA	1:C:15:PRO:HD2	1.54	0.45
1:C:233:ILE:O	1:C:233:ILE:HG23	2.17	0.44
1:A:130:ARG:HG3	1:A:165:LEU:HD21	1.99	0.44
1:A:261:MET:HG3	1:A:404:LEU:CD1	2.47	0.44
1:C:114:LEU:HD22	1:C:228:VAL:CG1	2.47	0.44
1:C:245:LEU:O	1:C:247:VAL:N	2.51	0.44
1:C:327:LEU:O	1:C:335:PRO:HB3	2.18	0.44
1:A:19:PRO:CB	1:A:21:HIS:CE1	2.98	0.44
1:C:83:SER:O	1:C:84:GLU:C	2.60	0.44
1:C:98:PHE:CD1	1:C:98:PHE:N	2.85	0.44
1:C:253:VAL:CG2	2:C:415:HEC:HMC3	2.47	0.44
1:C:395:ILE:O	1:C:396:VAL:HG23	2.17	0.44
1:C:19:PRO:HG2	1:C:22:LEU:HD12	2.00	0.44
1:C:75:TYR:CE2	1:C:320:LEU:HB2	2.53	0.44
1:C:99:ILE:HG12	1:C:240:ARG:HH21	1.82	0.44
1:A:187:PRO:HD2	3:A:440:HOH:O	2.17	0.44
1:A:392:LYS:HE3	1:A:392:LYS:HB3	1.87	0.44
1:C:99:ILE:CD1	1:C:240:ARG:NH2	2.79	0.44
1:C:304:ASP:N	1:C:314:LYS:H	2.16	0.44
1:A:256:PHE:CZ	1:A:288:LEU:C	2.94	0.44
1:A:261:MET:HG3	1:A:404:LEU:HD11	1.99	0.44
1:C:83:SER:O	1:C:86:PRO:HD3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:CD1	1:A:131:ILE:N	2.81	0.44
1:A:358:LEU:HD12	2:A:415:HEC:HBD2	1.99	0.44
1:A:354:SER:OG	1:A:355:HIS:CD2	2.71	0.44
1:C:374:TRP:CD1	1:C:374:TRP:C	2.96	0.44
1:C:378:ILE:N	1:C:379:PRO:HD3	2.32	0.44
1:C:365:ARG:O	1:C:369:VAL:CB	2.65	0.43
1:A:121:MET:HB2	1:A:122:PRO:CD	2.48	0.43
1:A:258:SER:O	1:A:262:GLU:HB2	2.18	0.43
1:C:58:CYS:O	1:C:59:ASN:C	2.57	0.43
1:C:204:LEU:O	1:C:208:ILE:CD1	2.65	0.43
1:C:209:GLU:O	1:C:213:GLN:CG	2.64	0.43
1:C:406:TRP:O	1:C:408:PRO:HD3	2.18	0.43
1:A:72:ARG:HG3	1:A:72:ARG:NH1	2.32	0.43
1:A:269:GLU:H	1:A:269:GLU:HG3	1.66	0.43
1:C:143:ARG:C	1:C:145:GLN:N	2.75	0.43
1:C:364:ARG:HG3	1:C:364:ARG:HH11	1.84	0.43
1:A:112:ARG:HD2	2:A:415:HEC:O1D	2.18	0.43
1:A:187:PRO:HB3	3:A:472:HOH:O	2.19	0.43
1:A:205:ILE:O	1:A:209:GLU:HG3	2.19	0.43
1:C:112:ARG:CD	1:C:112:ARG:CB	2.83	0.43
1:C:334:ALA:HA	1:C:335:PRO:HD2	1.89	0.43
1:C:239:LYS:HE3	1:C:239:LYS:HB3	1.70	0.43
1:A:158:PHE:O	1:A:162:ILE:HG12	2.19	0.43
1:A:72:ARG:O	1:A:76:GLU:HG3	2.18	0.43
1:A:149:ASN:HB3	1:A:152:GLU:HG3	2.00	0.43
1:C:99:ILE:O	1:C:241:MET:HA	2.19	0.43
1:C:276:GLU:C	1:C:277:ARG:HG3	2.44	0.43
1:C:389:ILE:H	1:C:389:ILE:HG13	1.49	0.43
1:A:78:TYR:CZ	1:A:105:PRO:HB2	2.53	0.43
1:A:96:TYR:CD1	1:A:102:SER:HB3	2.54	0.43
1:A:108:GLN:HE21	1:A:108:GLN:HB3	1.23	0.43
1:C:143:ARG:HG3	1:C:411:THR:HG21	2.00	0.43
1:C:205:ILE:CB	1:C:206:PRO:HD3	2.42	0.43
1:A:67:ARG:HD2	1:A:330:ARG:NH1	2.34	0.42
1:C:63:TRP:CZ2	1:C:312:LEU:HD23	2.54	0.42
1:C:139:ILE:CD1	1:C:374:TRP:HE3	2.32	0.42
1:A:19:PRO:CD	1:A:22:LEU:HD12	2.47	0.42
1:A:45:LEU:HD12	1:A:324:LEU:HD11	2.01	0.42
1:C:71:ILE:HD13	1:C:321:PRO:O	2.19	0.42
1:C:405:VAL:O	1:C:406:TRP:HB3	2.18	0.42
1:C:407:ASP:OD1	1:C:407:ASP:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD23	1:A:154:TYR:HD2	1.78	0.42
1:C:81:PHE:HB3	1:C:299:ARG:HG3	2.01	0.42
1:A:19:PRO:O	1:A:20:GLU:C	2.59	0.42
1:A:322:GLN:NE2	2:A:415:HEC:HBA2	2.34	0.42
1:A:51:PRO:HD2	1:A:54:VAL:HG12	2.01	0.42
1:A:262:GLU:HA	1:A:402:LEU:HD21	2.01	0.42
1:A:272:GLN:NE2	1:A:272:GLN:HA	2.33	0.42
1:C:163:PHE:CG	1:C:249:GLY:HA3	2.55	0.42
1:C:362:LEU:O	1:C:363:ALA:C	2.58	0.42
1:A:130:ARG:CZ	1:A:165:LEU:HD11	2.50	0.42
1:A:135:ALA:O	1:A:139:ILE:HG12	2.19	0.42
1:A:139:ILE:HG23	1:A:378:ILE:HD12	2.01	0.42
1:A:220:ILE:N	1:A:220:ILE:HD12	2.34	0.42
1:A:172:GLU:H	1:A:172:GLU:CD	2.28	0.42
1:C:275:ILE:CD1	1:C:379:PRO:HB3	2.50	0.42
1:A:254:VAL:O	1:A:254:VAL:HG12	2.18	0.42
1:A:375:LEU:O	1:A:379:PRO:HG3	2.19	0.42
1:C:356:LEU:HG	1:C:357:CYS:H	1.81	0.42
1:A:20:GLU:OE2	1:C:165:LEU:CB	2.65	0.42
1:A:131:ILE:HD12	1:A:162:ILE:CD1	2.36	0.42
1:C:143:ARG:HD2	1:C:411:THR:HB	2.02	0.42
1:C:369:VAL:O	1:C:370:THR:C	2.62	0.42
1:A:56:THR:OG1	1:A:58:CYS:HB2	2.20	0.42
1:A:164:MET:CE	1:A:169:LEU:HB3	2.47	0.42
1:A:363:ALA:O	1:A:367:ILE:HD12	2.19	0.42
1:C:239:LYS:HE2	1:C:239:LYS:HB2	1.84	0.42
1:A:51:PRO:C	1:A:53:LEU:H	2.28	0.41
1:A:330:ARG:H	1:A:330:ARG:HG3	1.63	0.41
1:C:84:GLU:HA	1:C:102:SER:O	2.20	0.41
1:C:134:LEU:HD12	1:C:138:LEU:HD13	2.02	0.41
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.78	0.41
1:C:110:GLN:H	1:C:110:GLN:HG2	1.71	0.41
1:C:112:ARG:HG3	1:C:358:LEU:HD11	2.02	0.41
1:C:134:LEU:O	1:C:138:LEU:HD13	2.20	0.41
1:A:213:GLN:C	1:A:215:PRO:HD3	2.45	0.41
1:C:131:ILE:CG2	1:C:158:PHE:CZ	3.03	0.41
1:C:281:ILE:HB	1:C:282:PRO:CD	2.50	0.41
1:C:285:CYS:SG	1:C:367:ILE:HG21	2.60	0.41
1:C:311:GLN:NE2	3:C:505:HOH:O	2.53	0.41
1:A:364:ARG:O	1:A:368:ILE:HG12	2.19	0.41
1:C:322:GLN:N	1:C:322:GLN:OE1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:O	1:C:134:LEU:HG	2.17	0.41
1:C:173:ASP:HB3	1:C:177:LEU:CD1	2.50	0.41
1:C:399:VAL:CG2	1:C:399:VAL:CA	2.89	0.41
1:C:131:ILE:CG2	1:C:131:ILE:O	2.68	0.41
1:C:136:CYS:O	1:C:137:SER:C	2.63	0.41
1:C:388:GLN:O	1:C:389:ILE:C	2.53	0.41
1:A:256:PHE:HZ	1:A:289:LEU:N	2.18	0.41
1:C:233:ILE:H	1:C:233:ILE:HG22	1.60	0.41
1:C:270:HIS:O	1:C:271:ARG:C	2.64	0.41
1:A:14:LEU:HA	1:A:14:LEU:HD12	1.72	0.41
1:A:78:TYR:CG	1:A:105:PRO:HD2	2.56	0.41
1:A:88:ILE:CG2	1:A:89:PRO:HA	2.50	0.41
1:A:96:TYR:C	1:A:96:TYR:CB	2.79	0.41
1:A:120:GLY:O	1:A:121:MET:C	2.63	0.41
1:A:150:PHE:HB3	1:A:402:LEU:HB3	2.02	0.41
1:A:251:ASP:O	1:A:251:ASP:CG	2.63	0.41
1:C:369:VAL:CA	1:C:369:VAL:CG1	2.83	0.41
1:A:159:PRO:O	1:A:160:ILE:C	2.60	0.41
1:A:254:VAL:HG23	3:A:494:HOH:O	2.21	0.40
1:A:256:PHE:CE1	1:A:292:PHE:HB2	2.56	0.40
1:C:173:ASP:C	1:C:177:LEU:HD12	2.46	0.40
1:C:201:TYR:HB3	1:C:239:LYS:HD2	2.03	0.40
1:C:277:ARG:CZ	1:C:280:ARG:HH21	2.28	0.40
1:C:365:ARG:HE	1:C:369:VAL:HG23	1.86	0.40
1:C:395:ILE:O	1:C:396:VAL:CG2	2.69	0.40
1:A:51:PRO:O	1:A:52:ASP:C	2.63	0.40
1:A:75:TYR:CE1	1:A:299:ARG:CZ	3.04	0.40
1:A:160:ILE:HG23	1:A:250:LEU:HG	2.03	0.40
1:A:191:MET:HE2	1:A:196:ALA:N	2.36	0.40
1:A:407:ASP:HB3	1:A:410:THR:CG2	2.46	0.40
1:C:155:ALA:O	1:C:159:PRO:CD	2.69	0.40
1:C:261:MET:HE3	1:C:261:MET:HB2	1.67	0.40
1:C:262:GLU:HA	1:C:402:LEU:HD11	2.03	0.40
1:C:109:ARG:NH1	3:C:443:HOH:O	2.54	0.40
1:A:130:ARG:HD2	1:A:130:ARG:HA	1.50	0.40
1:A:229:ASN:HA	1:A:229:ASN:HD22	1.47	0.40
1:A:262:GLU:HG3	1:A:402:LEU:HD13	2.04	0.40
1:A:291:ARG:HG3	1:A:292:PHE:CD1	2.56	0.40
1:C:256:PHE:HD2	1:C:367:ILE:HD12	1.87	0.40
1:A:298:GLY:O	1:A:299:ARG:CD	2.46	0.40

All (23) 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:A:109:ARG:NH2	1:A:176:HIS:CB[2_545]	1.02	1.18
1:C:109:ARG:NH2	1:C:176:HIS:CB[2_546]	1.05	1.15
1:C:107:GLU:OE2	1:C:410:THR:CG2[1_455]	1.48	0.72
1:C:110:GLN:OE1	1:C:176:HIS:ND1[2_546]	1.54	0.66
1:A:110:GLN:OE1	1:A:176:HIS:ND1[2_545]	1.59	0.61
1:A:110:GLN:OE1	1:A:176:HIS:CE1[2_545]	1.63	0.57
1:C:110:GLN:OE1	1:C:176:HIS:CE1[2_546]	1.77	0.43
1:A:109:ARG:CZ	1:A:176:HIS:CB[2_545]	1.82	0.38
1:C:109:ARG:CZ	1:C:176:HIS:CB[2_546]	1.82	0.38
1:A:107:GLU:OE2	1:A:410:THR:CG2[1_455]	1.83	0.37
1:C:110:GLN:CD	1:C:176:HIS:ND1[2_546]	1.89	0.31
1:C:172:GLU:OE2	1:C:276:GLU:OE2[2_656]	1.89	0.31
1:C:116:ASN:ND2	1:C:202:ASP:OD2[2_546]	1.93	0.27
1:A:109:ARG:NH2	1:A:176:HIS:CA[2_545]	1.94	0.26
1:C:109:ARG:NH2	1:C:176:HIS:CA[2_546]	1.95	0.25
1:A:172:GLU:OE2	1:A:276:GLU:OE2[2_655]	2.03	0.17
1:A:109:ARG:NH2	1:A:176:HIS:CG[2_545]	2.06	0.14
1:A:116:ASN:ND2	1:A:202:ASP:OD2[2_545]	2.07	0.13
1:C:109:ARG:NE	1:C:176:HIS:CD2[2_546]	2.09	0.11
1:C:109:ARG:CZ	1:C:176:HIS:CG[2_546]	2.12	0.08
1:C:107:GLU:OE2	1:C:410:THR:CB[1_455]	2.13	0.07
1:A:116:ASN:ND2	1:A:202:ASP:OD1[2_545]	2.17	0.03
1:A:209:GLU:OE2	1:A:356:LEU:CD2[2_555]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	403/414 (97%)	345 (86%)	38 (9%)	20 (5%)	1	0
1	C	403/414 (97%)	336 (83%)	49 (12%)	18 (4%)	2	0
All	All	806/828 (97%)	681 (84%)	87 (11%)	38 (5%)	2	0

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	246	LEU
1	A	278	PRO
1	A	282	PRO
1	A	293	SER
1	C	47	GLU
1	C	52	ASP
1	C	98	PHE
1	C	137	SER
1	C	244	ALA
1	C	246	LEU
1	C	271	ARG
1	A	52	ASP
1	A	168	GLY
1	A	329	GLU
1	C	89	PRO
1	C	245	LEU
1	C	314	LYS
1	C	342	ARG
1	A	110	GLN
1	A	137	SER
1	A	172	GLU
1	A	251	ASP
1	A	268	PRO
1	C	138	LEU
1	A	36	ALA
1	A	138	LEU
1	A	244	ALA
1	A	338	VAL
1	A	365	ARG
1	C	229	ASN
1	C	293	SER
1	C	356	LEU
1	A	16	PRO
1	C	363	ALA
1	C	369	VAL
1	A	277	ARG
1	C	174	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/356 (98%)	303 (87%)	44 (13%)	4	1
1	C	347/356 (98%)	291 (84%)	56 (16%)	2	1
All	All	694/712 (98%)	594 (86%)	100 (14%)	3	1

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PRO
1	A	39	GLN
1	A	47	GLU
1	A	57	ARG
1	A	69	GLN
1	A	70	LEU
1	A	82	SER
1	A	83	SER
1	A	88	ILE
1	A	99	ILE
1	A	101	THR
1	A	105	PRO
1	A	108	GLN
1	A	109	ARG
1	A	118	VAL
1	A	128	GLU
1	A	131	ILE
1	A	141	SER
1	A	143	ARG
1	A	149	ASN
1	A	158	PHE
1	A	166	LEU
1	A	205	ILE
1	A	214	LYS
1	A	220	ILE
1	A	223	VAL
1	A	231	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	PRO
1	A	233	ILE
1	A	245	LEU
1	A	261	MET
1	A	268	PRO
1	A	269	GLU
1	A	272	GLN
1	A	275	ILE
1	A	313	LYS
1	A	335	PRO
1	A	344	LYS
1	A	365	ARG
1	A	376	THR
1	A	380	ASP
1	A	388	GLN
1	A	392	LYS
1	A	412	LYS
1	C	16	PRO
1	C	23	VAL
1	C	39	GLN
1	C	46	GLN
1	C	49	ASN
1	C	53	LEU
1	C	69	GLN
1	C	79	ARG
1	C	86	PRO
1	C	87	PHE
1	C	91	GLU
1	C	99	ILE
1	C	101	THR
1	C	109	ARG
1	C	121	MET
1	C	126	LYS
1	C	127	LEU
1	C	133	GLU
1	C	138	LEU
1	C	140	GLU
1	C	143	ARG
1	C	144	PRO
1	C	147	GLN
1	C	149	ASN
1	C	164	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	166	LEU
1	C	182	ASP
1	C	193	PHE
1	C	205	ILE
1	C	211	ARG
1	C	212	ARG
1	C	213	GLN
1	C	220	ILE
1	C	229	ASN
1	C	231	ARG
1	C	232	PRO
1	C	239	LYS
1	C	241	MET
1	C	246	LEU
1	C	261	MET
1	C	264	LEU
1	C	268	PRO
1	C	272	GLN
1	C	276	GLU
1	C	301	LEU
1	C	312	LEU
1	C	323	MET
1	C	325	SER
1	C	344	LYS
1	C	385	PRO
1	C	388	GLN
1	C	392	LYS
1	C	395	ILE
1	C	405	VAL
1	C	410	THR
1	C	414	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	39	GLN
1	A	46	GLN
1	A	59	ASN
1	A	108	GLN
1	A	110	GLN
1	A	149	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	225	ASN
1	A	229	ASN
1	A	272	GLN
1	A	317	GLN
1	A	322	GLN
1	A	343	GLN
1	A	355	HIS
1	A	388	GLN
1	C	30	ASN
1	C	39	GLN
1	C	46	GLN
1	C	49	ASN
1	C	59	ASN
1	C	80	HIS
1	C	108	GLN
1	C	129	ASN
1	C	132	GLN
1	C	149	ASN
1	C	272	GLN
1	C	317	GLN
1	C	343	GLN
1	C	400	GLN

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 ⓘ

2 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	HEC	C	415	3,1	46,50,50	4.19	32 (69%)	58,82,82	3.92	29 (50%)
2	HEC	A	415	3,1	46,50,50	2.77	20 (43%)	58,82,82	3.11	30 (51%)

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	HEC	C	415	3,1	-	5/14/54/54	-
2	HEC	A	415	3,1	-	7/14/54/54	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	415	HEC	C4B-NB	-10.64	1.19	1.39
2	C	415	HEC	C4D-C3D	9.09	1.62	1.44
2	C	415	HEC	CMD-C2D	8.55	1.68	1.50
2	A	415	HEC	CAC-C3C	8.30	1.62	1.35
2	C	415	HEC	CAB-C3B	6.69	1.56	1.35
2	C	415	HEC	C4C-NC	-6.38	1.27	1.39
2	C	415	HEC	CHA-C4D	-6.08	1.25	1.39
2	C	415	HEC	C1B-NB	-5.76	1.28	1.39
2	C	415	HEC	C4A-NA	-5.44	1.29	1.39
2	C	415	HEC	C1D-ND	-5.38	1.29	1.39
2	C	415	HEC	CMC-C2C	5.32	1.61	1.50
2	C	415	HEC	C3D-C2D	5.24	1.52	1.38
2	A	415	HEC	CBB-CAB	-4.75	1.31	1.49
2	C	415	HEC	CHD-C1D	-4.56	1.29	1.39
2	A	415	HEC	CAB-C3B	4.48	1.49	1.35
2	C	415	HEC	CBC-CAC	-4.44	1.33	1.49
2	C	415	HEC	CHB-C1B	-4.36	1.29	1.39
2	C	415	HEC	CHC-C4B	-4.35	1.29	1.38
2	A	415	HEC	C1C-C2C	4.35	1.53	1.43
2	A	415	HEC	C4C-NC	-4.34	1.31	1.39
2	C	415	HEC	C1C-C2C	4.23	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEC	CAA-C2A	4.23	1.62	1.51
2	A	415	HEC	CAD-C3D	4.16	1.62	1.51
2	A	415	HEC	CMD-C2D	4.15	1.59	1.50
2	A	415	HEC	C3D-C2D	4.14	1.49	1.38
2	C	415	HEC	C3B-C2B	-4.08	1.27	1.41
2	C	415	HEC	C1C-NC	-4.07	1.32	1.39
2	C	415	HEC	CMB-C2B	3.97	1.58	1.50
2	C	415	HEC	CBB-CAB	-3.87	1.35	1.49
2	C	415	HEC	CAC-C3C	3.84	1.47	1.35
2	A	415	HEC	O1A-CGA	-3.73	1.09	1.22
2	A	415	HEC	CBC-CAC	-3.69	1.35	1.49
2	A	415	HEC	C3B-C2B	-3.64	1.28	1.41
2	C	415	HEC	CAD-C3D	3.52	1.60	1.51
2	C	415	HEC	C1A-C2A	-3.31	1.39	1.45
2	C	415	HEC	C1D-C2D	3.07	1.50	1.43
2	A	415	HEC	CHD-C1D	-3.01	1.32	1.39
2	A	415	HEC	O2D-CGD	-2.98	1.21	1.30
2	A	415	HEC	CMC-C2C	2.94	1.56	1.50
2	A	415	HEC	CHB-C4A	2.91	1.44	1.38
2	C	415	HEC	C3B-C4B	-2.84	1.41	1.46
2	A	415	HEC	C3B-C4B	2.76	1.50	1.46
2	A	415	HEC	CBD-CAD	2.67	1.61	1.51
2	C	415	HEC	CBD-CGD	2.64	1.56	1.50
2	A	415	HEC	CBD-CGD	2.52	1.56	1.50
2	C	415	HEC	CHB-C4A	-2.50	1.33	1.38
2	C	415	HEC	O2A-CGA	-2.35	1.23	1.30
2	C	415	HEC	CHA-C1A	-2.33	1.33	1.38
2	A	415	HEC	C1A-C2A	2.28	1.49	1.45
2	C	415	HEC	CHD-C4C	-2.18	1.34	1.38
2	C	415	HEC	CHC-C1C	-2.04	1.34	1.39
2	C	415	HEC	C4A-C3A	-2.00	1.41	1.45

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	415	HEC	CMB-C2B-C1B	11.85	143.47	125.42
2	A	415	HEC	CHC-C4B-NB	9.77	135.09	124.45
2	C	415	HEC	CHC-C4B-C3B	-8.75	110.45	125.21
2	C	415	HEC	CAA-C2A-C1A	8.37	141.87	124.85
2	C	415	HEC	CHC-C4B-NB	7.69	132.82	124.45
2	C	415	HEC	CHA-C4D-ND	6.75	136.10	123.86
2	A	415	HEC	C2A-C1A-NA	-6.72	103.84	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	415	HEC	CHD-C1D-ND	6.50	135.65	123.86
2	C	415	HEC	CAA-C2A-C3A	-6.17	116.32	127.87
2	C	415	HEC	CMB-C2B-C3B	-6.16	112.06	126.55
2	C	415	HEC	CHB-C4A-NA	6.10	131.09	124.45
2	A	415	HEC	O2A-CGA-CBA	5.98	132.88	114.00
2	A	415	HEC	CHD-C4C-NC	5.72	130.68	124.45
2	C	415	HEC	O2D-CGD-O1D	-5.55	109.05	123.33
2	A	415	HEC	CHB-C1B-NB	5.44	133.73	123.86
2	A	415	HEC	O1A-CGA-CBA	-5.35	106.11	123.09
2	A	415	HEC	CHD-C4C-C3C	-5.22	116.40	125.21
2	C	415	HEC	C4D-ND-C1D	5.10	114.13	105.82
2	C	415	HEC	O2D-CGD-CBD	5.04	129.94	114.00
2	A	415	HEC	CMA-C3A-C4A	-4.98	115.96	124.73
2	C	415	HEC	CHD-C1D-C2D	-4.82	113.44	127.43
2	C	415	HEC	CHA-C4D-C3D	-4.80	114.78	125.30
2	C	415	HEC	CBB-CAB-C3B	4.58	136.58	127.43
2	C	415	HEC	C4A-C3A-C2A	4.56	113.74	106.97
2	A	415	HEC	CBC-CAC-C3C	-4.44	118.55	127.43
2	C	415	HEC	C4D-C3D-C2D	-4.43	100.00	106.87
2	A	415	HEC	CHB-C4A-NA	4.20	129.02	124.45
2	A	415	HEC	CAD-C3D-C4D	4.18	133.10	124.94
2	C	415	HEC	C1A-C2A-C3A	-4.09	101.73	107.11
2	C	415	HEC	CAD-C3D-C2D	4.06	136.19	127.07
2	A	415	HEC	CMD-C2D-C1D	3.98	131.47	125.42
2	A	415	HEC	C3D-C4D-ND	3.83	114.41	110.15
2	C	415	HEC	C3D-C4D-ND	-3.83	105.90	110.15
2	A	415	HEC	C4D-C3D-C2D	-3.72	101.11	106.87
2	A	415	HEC	CHB-C1B-C2B	-3.57	117.06	127.43
2	C	415	HEC	C4C-NC-C1C	3.52	111.56	105.82
2	C	415	HEC	CHD-C4C-C3C	3.37	130.89	125.21
2	A	415	HEC	CMB-C2B-C1B	3.35	130.53	125.42
2	C	415	HEC	CMC-C2C-C1C	3.05	130.06	125.42
2	C	415	HEC	C4D-CHA-C1A	-3.04	115.27	124.66
2	C	415	HEC	CMC-C2C-C3C	3.02	133.66	126.55
2	C	415	HEC	CBC-CAC-C3C	-3.01	121.42	127.43
2	A	415	HEC	O2D-CGD-O1D	-2.94	115.78	123.33
2	A	415	HEC	CMA-C3A-C2A	2.94	134.09	126.15
2	A	415	HEC	C1B-CHB-C4A	-2.88	115.79	124.66
2	A	415	HEC	C4A-NA-C1A	2.81	110.40	105.82
2	A	415	HEC	CMC-C2C-C3C	2.72	132.95	126.55
2	C	415	HEC	O2A-CGA-O1A	-2.71	116.36	123.33
2	A	415	HEC	CMB-C2B-C3B	-2.59	120.47	126.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	415	HEC	CHA-C1A-C2A	2.51	128.84	124.86
2	A	415	HEC	CBB-CAB-C3B	2.46	132.36	127.43
2	A	415	HEC	C1C-CHC-C4B	-2.39	117.29	124.66
2	C	415	HEC	C2C-C1C-NC	2.21	113.69	110.14
2	A	415	HEC	CMD-C2D-C3D	-2.20	120.95	125.62
2	A	415	HEC	CHC-C4B-C3B	-2.20	121.50	125.21
2	A	415	HEC	CMC-C2C-C1C	-2.18	122.10	125.42
2	C	415	HEC	CMD-C2D-C1D	2.14	128.69	125.42
2	A	415	HEC	CHA-C4D-ND	-2.05	120.13	123.86
2	A	415	HEC	C4B-NB-C1B	2.05	109.16	105.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	415	HEC	C3A-C2A-CAA-CBA
2	A	415	HEC	C4B-C3B-CAB-CBB
2	C	415	HEC	C2B-C3B-CAB-CBB
2	C	415	HEC	C4B-C3B-CAB-CBB
2	C	415	HEC	C2C-C3C-CAC-CBC
2	A	415	HEC	C1A-C2A-CAA-CBA
2	C	415	HEC	C1A-C2A-CAA-CBA
2	C	415	HEC	C3A-C2A-CAA-CBA
2	A	415	HEC	C2B-C3B-CAB-CBB
2	A	415	HEC	CAA-CBA-CGA-O1A
2	A	415	HEC	CAA-CBA-CGA-O2A
2	A	415	HEC	CAD-CBD-CGD-O2D

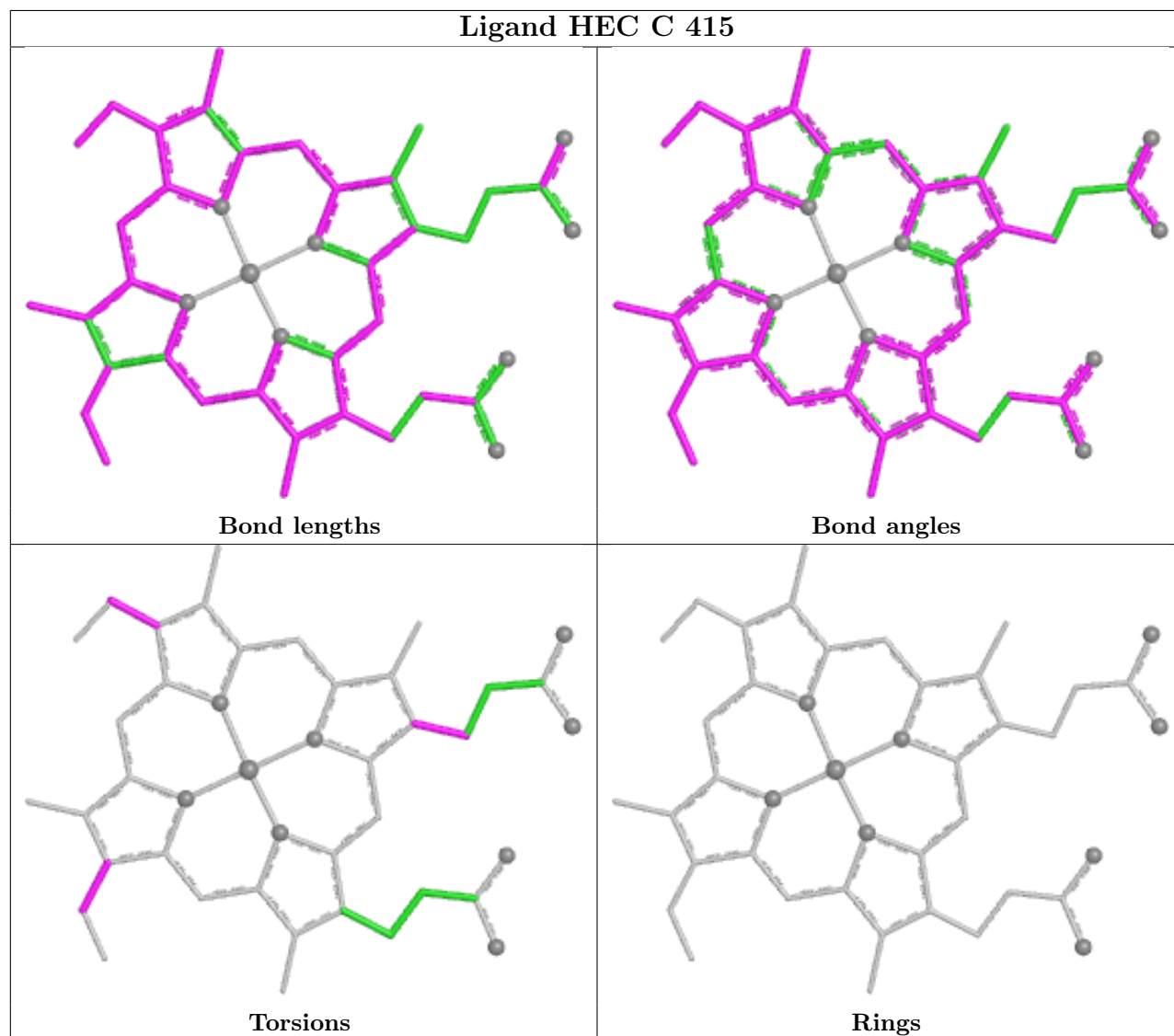
There are no ring outliers.

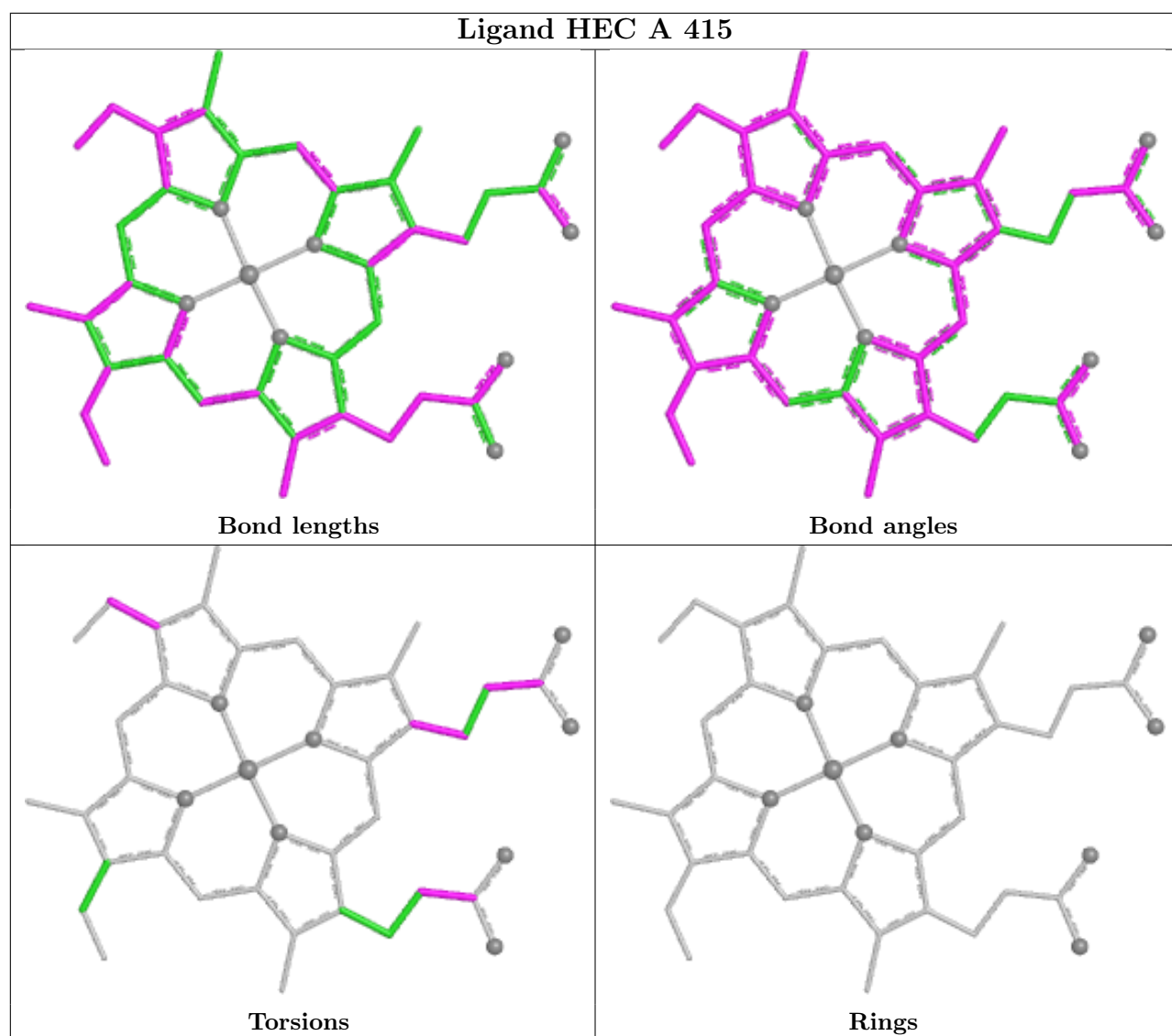
2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	415	HEC	9	0
2	A	415	HEC	18	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	405/414 (97%)	-1.01	0 100 100	8, 24, 36, 49	0
1	C	405/414 (97%)	-1.00	0 100 100	11, 24, 34, 44	0
All	All	810/828 (97%)	-1.00	0 100 100	8, 24, 36, 49	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](#)

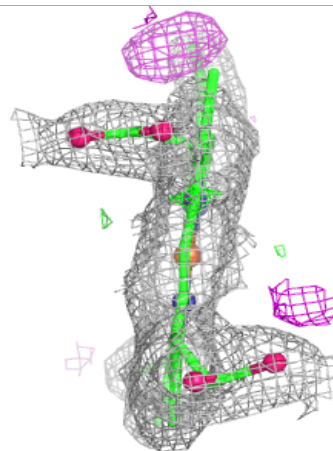
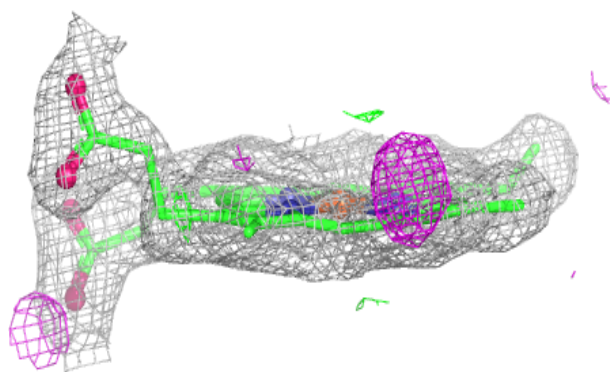
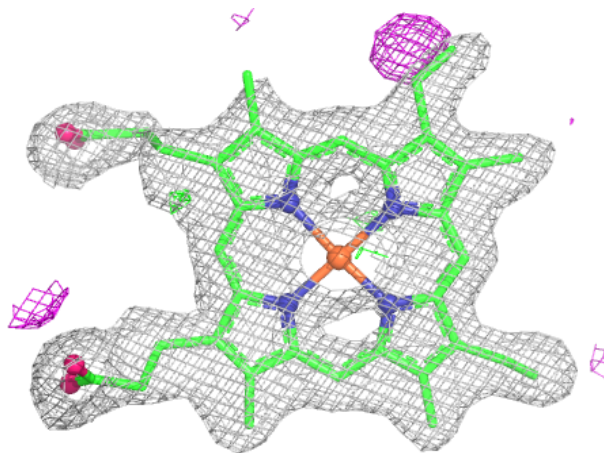
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

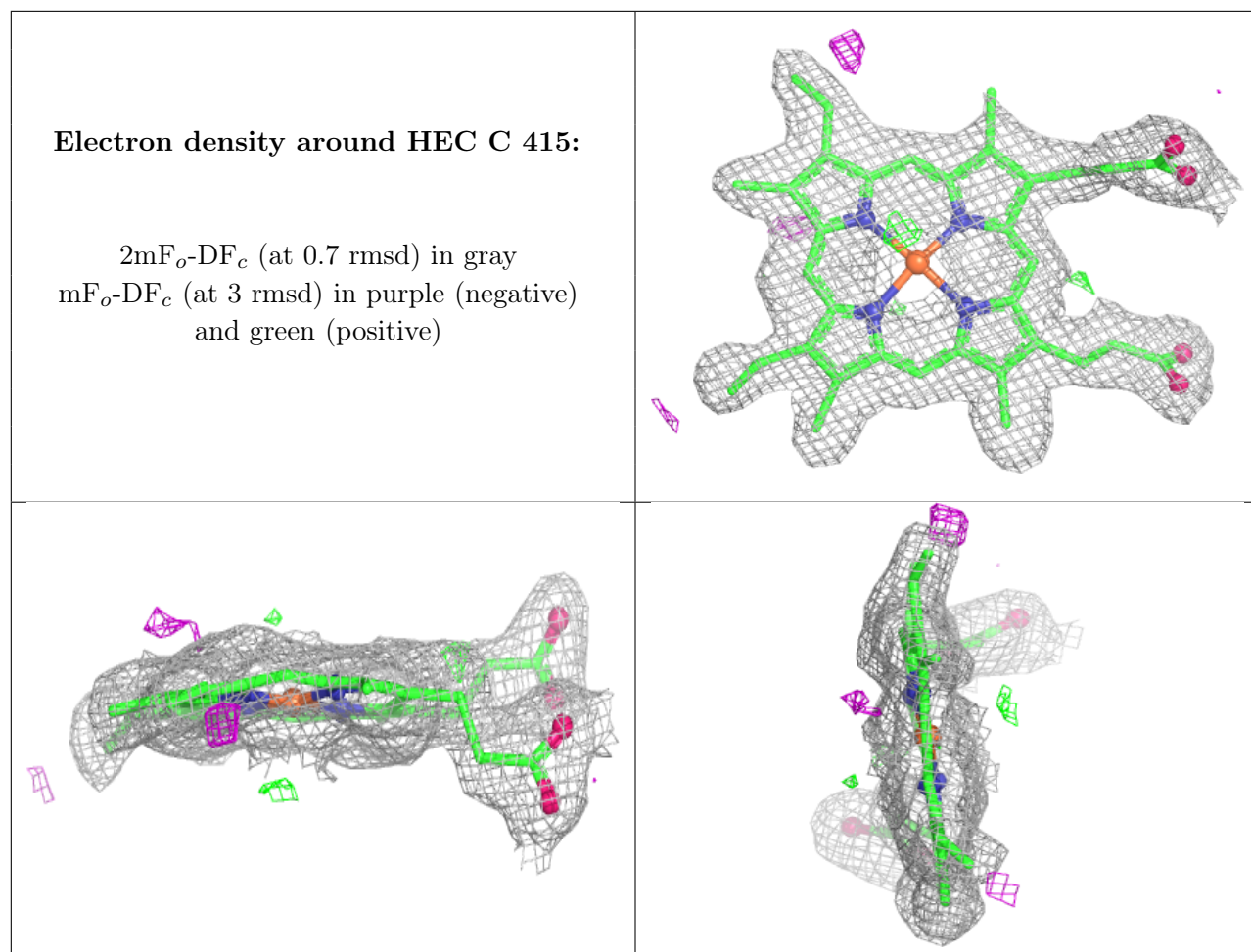
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEC	A	415	43/43	0.99	0.04	13,15,17,18	0
2	HEC	C	415	43/43	0.99	0.04	13,18,20,21	0

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 HEC A 415:

$2mF_o-DF_c$ (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.