Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 03:19 AM EDT

PDB ID	:	2H7S
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:

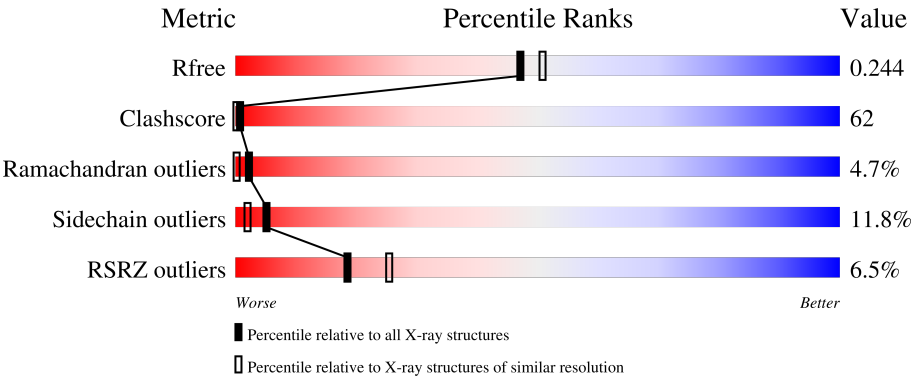
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 <=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	7%, 16%, 39%, 35%, 8%
1	C	414	6%, 19%, 33%, 38%, 8%

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.

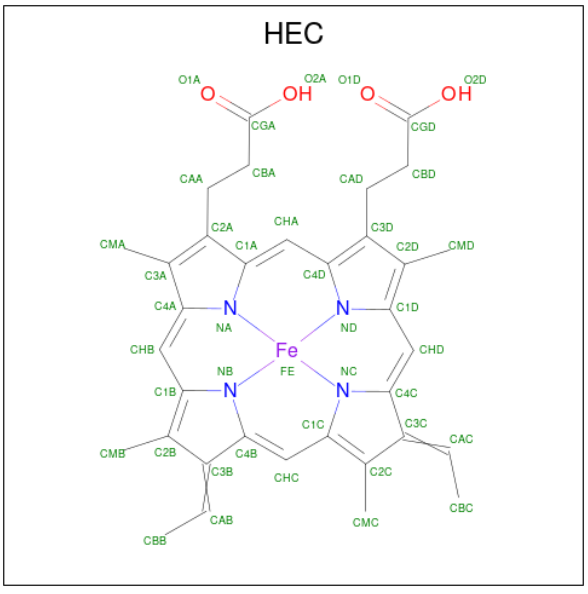
- Molecule 1 is a protein called Cytochrome P450-cam.

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 (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 3 is water.

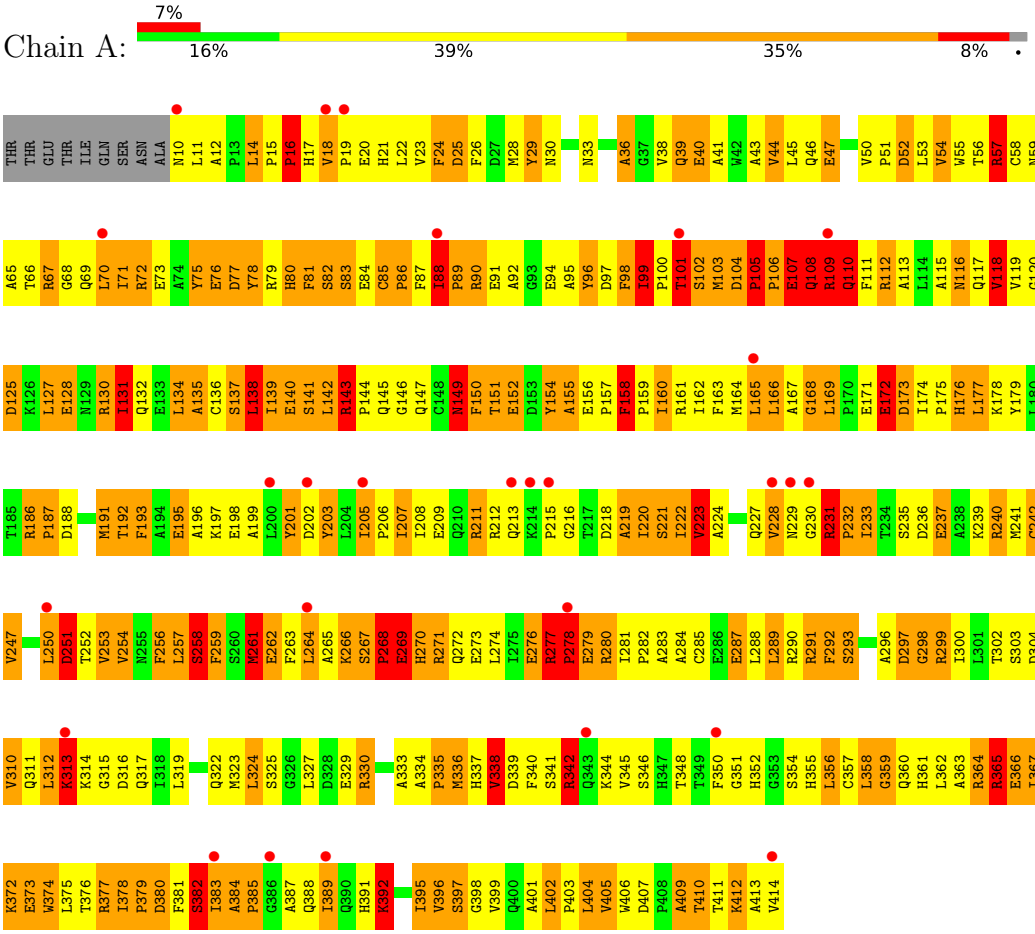
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	25	0
			111	111		
3	C	99	Total	O	24	0
			99	99		

3 Residue-property plots (i)

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.

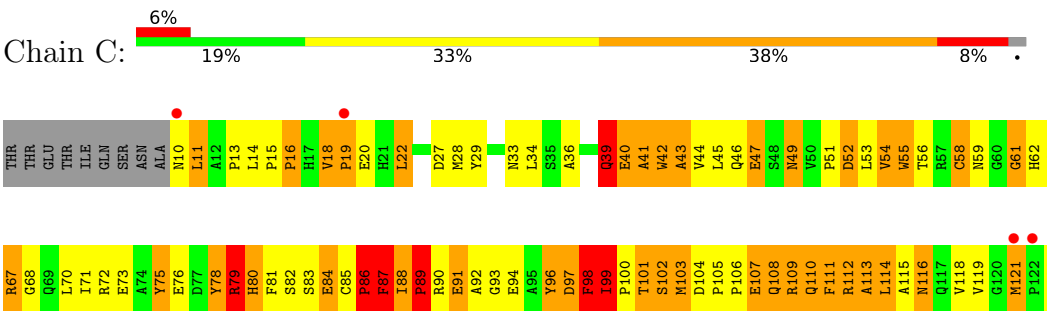
• Molecule 1: Cytochrome P450-cam

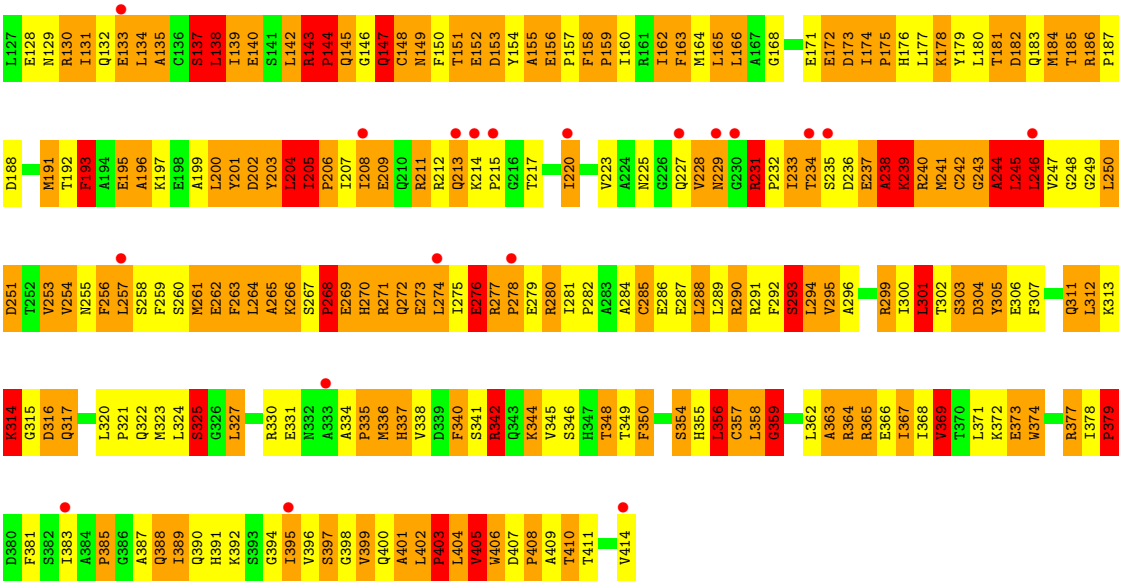
Chain A:



• Molecule 1: Cytochrome P450-cam

Chain C:




L127 E128 N129 R130 I131 Q132 E133 L134 A135 C136 S137 L138 I139 E140 S141 L142 R143 P144 Q145 G146 Q147 C148 N149 F150 T151 E152 D153 Y154 A155 E156 P157 F158 P159 I160 R161 I162 F163 M164 L165 L166 A167 G168 E171 E172 D173 I174 P175 H176 L177 K178 Y179 L180 T181 D182 Q183 M184 T185 R186 P187
D188 M191 T192 F193 A194 E195 A196 K197 E198 A199 L200 Y201 D202 Y203 L204 I205 P206 I207 I208 E209 Q210 R211 R212 Q213 K214 P215 G216 T217 I220 V223 A224 N225 G226 Q227 V228 M229 G230 R231 P232 I233 T234 S235 D236 E237 A238 K239 R240 M241 C242 G243 A244 L245 L246 V247 G248 G249 L250
D251 T252 V253 V254 N255 F256 L257 S258 F259 S260 M261 E262 F263 L264 A265 K266 S267 P268 E269 H270 R271 Q272 E273 L274 I275 E276 R277 P278 E279 R280 I281 P282 A283 A284 C285 E286 E287 L288 L289 R290 R291 F292 S293 L294 V295 A296 R299 I300 L301 T302 S303 D304 Y305 E306 F307 Q311 L312 K313
K314 G315 D316 Q317 L320 P321 Q322 M323 L324 S325 G326 L327 R330 E331 N332 A333 A334 P335 M336 H337 V338 D339 F340 S341 R342 Q343 K344 V345 S346 H347 T348 T349 F350 S354 H355 L356 C357 L358 G359 L362 A363 R364 R365 E366 I367 I368 V369 T370 L371 K372 E373 W374 R377 I378 R379
D380 F381 S382 I383 A384 P385 G386 A387 Q388 I389 Q390 H391 K392 S393 G394 I395 V396 S397 G398 V399 Q400 A401 L402 P403 L404 V405 W406 D407 P408 A409 T410 T411 V414

4 Data and refinement statistics (i)

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 45.43 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.15) 80.3 (45.43-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.77 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.249 0.237 , 0.244	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)	0.35 , 14.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	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	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.85	278/3280 (8.5%)	2.29	173/4456 (3.9%)
1	C	2.87	289/3278 (8.8%)	2.43	180/4454 (4.0%)
All	All	2.86	567/6558 (8.6%)	2.36	353/8910 (4.0%)

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 (567) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	399	VAL	CB-CG2	16.70	1.88	1.52
1	A	95	ALA	CA-CB	-15.72	1.19	1.52
1	C	373	GLU	CD-OE1	15.07	1.42	1.25
1	C	401	ALA	C-O	13.02	1.48	1.23
1	A	40	GLU	CD-OE1	13.00	1.40	1.25
1	C	254	VAL	CB-CG1	13.00	1.80	1.52
1	C	146	GLY	N-CA	12.60	1.65	1.46
1	C	406	TRP	CB-CG	12.46	1.72	1.50
1	C	373	GLU	CB-CG	12.34	1.75	1.52
1	C	130	ARG	CZ-NH1	-12.17	1.17	1.33
1	C	103	MET	CG-SD	-12.15	1.49	1.81
1	A	367	ILE	N-CA	12.14	1.70	1.46
1	A	96	TYR	CD1-CE1	12.09	1.57	1.39
1	A	231	ARG	CZ-NH2	11.67	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	ALA	CA-CB	-11.54	1.28	1.52
1	C	112	ARG	CG-CD	11.50	1.80	1.51
1	C	369	VAL	CA-CB	11.38	1.78	1.54
1	C	237	GLU	C-O	11.11	1.44	1.23
1	A	240	ARG	CG-CD	11.03	1.79	1.51
1	A	409	ALA	CA-CB	10.95	1.75	1.52
1	C	58	CYS	CB-SG	-10.94	1.63	1.82
1	C	263	PHE	CE2-CZ	10.77	1.57	1.37
1	A	87	PHE	CE1-CZ	10.77	1.57	1.37
1	C	75	TYR	CG-CD2	10.76	1.53	1.39
1	A	263	PHE	CB-CG	-10.57	1.33	1.51
1	C	203	TYR	CD2-CE2	-10.51	1.23	1.39
1	C	262	GLU	CD-OE1	10.35	1.37	1.25
1	C	394	GLY	N-CA	10.35	1.61	1.46
1	A	406	TRP	CB-CG	10.26	1.68	1.50
1	A	374	TRP	CG-CD1	10.25	1.51	1.36
1	C	99	ILE	CA-CB	-10.16	1.31	1.54
1	A	389	ILE	CB-CG2	10.12	1.84	1.52
1	C	335	PRO	CB-CG	10.07	2.00	1.50
1	A	75	TYR	CG-CD2	-10.07	1.26	1.39
1	A	84	GLU	CD-OE2	10.05	1.36	1.25
1	A	310	VAL	CB-CG2	9.99	1.73	1.52
1	C	279	GLU	CD-OE2	9.77	1.36	1.25
1	C	154	TYR	CD1-CE1	9.59	1.53	1.39
1	C	406	TRP	CE3-CZ3	-9.59	1.22	1.38
1	C	389	ILE	CB-CG2	9.59	1.82	1.52
1	A	397	SER	CA-CB	9.58	1.67	1.52
1	A	401	ALA	C-O	-9.58	1.05	1.23
1	C	291	ARG	N-CA	-9.58	1.27	1.46
1	C	75	TYR	CE2-CZ	9.42	1.50	1.38
1	A	134	LEU	CG-CD1	9.30	1.86	1.51
1	A	84	GLU	CB-CG	9.28	1.69	1.52
1	C	185	THR	C-O	-9.20	1.05	1.23
1	C	278	PRO	CA-C	-9.19	1.34	1.52
1	A	98	PHE	CD1-CE1	-9.18	1.20	1.39
1	A	96	TYR	CA-C	9.11	1.76	1.52
1	A	101	THR	CB-CG2	-9.04	1.22	1.52
1	C	260	SER	CA-CB	9.03	1.66	1.52
1	A	253	VAL	CB-CG1	9.02	1.71	1.52
1	A	81	PHE	CE2-CZ	8.87	1.54	1.37
1	A	152	GLU	CD-OE1	8.85	1.35	1.25
1	A	259	PHE	CG-CD1	8.84	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	PHE	CD2-CE2	-8.78	1.21	1.39
1	C	112	ARG	N-CA	-8.78	1.28	1.46
1	C	346	SER	CB-OG	-8.77	1.30	1.42
1	A	205	ILE	CB-CG2	8.74	1.79	1.52
1	A	65	ALA	CA-CB	8.71	1.70	1.52
1	C	90	ARG	C-O	-8.70	1.06	1.23
1	C	263	PHE	CB-CG	-8.66	1.36	1.51
1	A	172	GLU	CG-CD	8.66	1.65	1.51
1	C	193	PHE	CG-CD1	8.55	1.51	1.38
1	C	154	TYR	CD2-CE2	8.55	1.52	1.39
1	A	264	LEU	CG-CD2	8.55	1.83	1.51
1	C	350	PHE	CE2-CZ	8.54	1.53	1.37
1	C	145	GLN	CG-CD	-8.53	1.31	1.51
1	A	257	LEU	CA-C	8.49	1.75	1.52
1	A	102	SER	CB-OG	8.47	1.53	1.42
1	A	231	ARG	CZ-NH1	8.43	1.44	1.33
1	A	262	GLU	CB-CG	8.43	1.68	1.52
1	C	154	TYR	CB-CG	8.35	1.64	1.51
1	C	40	GLU	CB-CG	8.32	1.68	1.52
1	A	242	CYS	CB-SG	-8.31	1.68	1.82
1	A	300	ILE	C-O	-8.29	1.07	1.23
1	A	80	HIS	CA-CB	-8.29	1.35	1.53
1	A	361	HIS	C-O	8.28	1.39	1.23
1	C	79	ARG	CB-CG	-8.27	1.30	1.52
1	C	201	TYR	C-O	8.19	1.39	1.23
1	C	228	VAL	CB-CG1	8.18	1.70	1.52
1	C	163	PHE	CB-CG	-8.15	1.37	1.51
1	C	20	GLU	CG-CD	-8.13	1.39	1.51
1	C	131	ILE	CB-CG2	8.11	1.77	1.52
1	A	345	VAL	CB-CG1	-8.10	1.35	1.52
1	A	168	GLY	N-CA	8.09	1.58	1.46
1	C	118	VAL	N-CA	8.07	1.62	1.46
1	A	253	VAL	CA-CB	-8.07	1.37	1.54
1	C	240	ARG	CB-CG	8.06	1.74	1.52
1	A	150	PHE	CE1-CZ	8.05	1.52	1.37
1	C	94	GLU	CB-CG	8.05	1.67	1.52
1	A	158	PHE	CE2-CZ	-8.02	1.22	1.37
1	C	273	GLU	CD-OE1	8.02	1.34	1.25
1	C	82	SER	C-O	-8.01	1.08	1.23
1	A	116	ASN	C-O	8.00	1.38	1.23
1	C	401	ALA	CA-CB	-8.00	1.35	1.52
1	C	87	PHE	N-CA	7.97	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	ALA	C-O	7.93	1.38	1.23
1	C	285	CYS	CB-SG	7.90	1.95	1.82
1	C	403	PRO	C-O	7.88	1.39	1.23
1	C	92	ALA	CA-CB	7.87	1.69	1.52
1	A	228	VAL	CA-CB	7.87	1.71	1.54
1	C	389	ILE	N-CA	-7.86	1.30	1.46
1	C	151	THR	C-O	-7.84	1.08	1.23
1	A	118	VAL	C-O	-7.79	1.08	1.23
1	A	199	ALA	CA-CB	-7.79	1.36	1.52
1	A	198	GLU	CG-CD	7.78	1.63	1.51
1	A	94	GLU	CD-OE1	7.77	1.34	1.25
1	A	54	VAL	CB-CG1	7.77	1.69	1.52
1	A	228	VAL	C-O	-7.76	1.08	1.23
1	A	227	GLN	CG-CD	-7.71	1.33	1.51
1	A	385	PRO	CB-CG	7.71	1.88	1.50
1	C	172	GLU	CG-CD	7.70	1.63	1.51
1	A	254	VAL	CB-CG2	7.70	1.69	1.52
1	A	243	GLY	N-CA	-7.65	1.34	1.46
1	A	287	GLU	CB-CG	-7.63	1.37	1.52
1	C	377	ARG	CG-CD	7.56	1.70	1.51
1	A	314	LYS	CD-CE	7.56	1.70	1.51
1	C	139	ILE	CA-CB	7.55	1.72	1.54
1	A	346	SER	CB-OG	-7.54	1.32	1.42
1	A	110	GLN	CB-CG	7.51	1.72	1.52
1	A	105	PRO	CG-CD	7.51	1.75	1.50
1	C	85	CYS	C-O	-7.50	1.09	1.23
1	C	305	TYR	CD2-CE2	-7.50	1.28	1.39
1	A	378	ILE	N-CA	7.48	1.61	1.46
1	A	205	ILE	N-CA	7.48	1.61	1.46
1	C	79	ARG	CA-C	-7.48	1.33	1.52
1	C	273	GLU	CD-OE2	7.46	1.33	1.25
1	A	139	ILE	CB-CG2	7.43	1.75	1.52
1	A	366	GLU	CD-OE2	-7.41	1.17	1.25
1	A	10	ASN	CB-CG	7.39	1.68	1.51
1	A	140	GLU	CD-OE1	7.38	1.33	1.25
1	C	261	MET	N-CA	-7.38	1.31	1.46
1	A	284	ALA	CA-CB	-7.38	1.36	1.52
1	A	88	ILE	CA-C	7.36	1.72	1.52
1	C	68	GLY	C-O	7.36	1.35	1.23
1	C	265	ALA	CA-CB	-7.35	1.37	1.52
1	C	98	PHE	CE2-CZ	7.34	1.51	1.37
1	A	140	GLU	CG-CD	7.34	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	PHE	CE1-CZ	7.33	1.51	1.37
1	C	374	TRP	CE3-CZ3	7.31	1.50	1.38
1	A	237	GLU	CD-OE1	-7.31	1.17	1.25
1	A	406	TRP	C-O	7.31	1.37	1.23
1	C	325	SER	CB-OG	7.29	1.51	1.42
1	A	357	CYS	CB-SG	-7.29	1.69	1.82
1	A	163	PHE	CG-CD2	7.27	1.49	1.38
1	A	59	ASN	C-O	7.26	1.37	1.23
1	A	77	ASP	CG-OD1	-7.25	1.08	1.25
1	C	264	LEU	CA-CB	7.24	1.70	1.53
1	A	40	GLU	CG-CD	-7.23	1.41	1.51
1	C	248	GLY	N-CA	-7.22	1.35	1.46
1	C	290	ARG	CZ-NH2	7.19	1.42	1.33
1	A	398	GLY	N-CA	7.15	1.56	1.46
1	C	403	PRO	CA-C	7.15	1.67	1.52
1	A	151	THR	CB-CG2	7.15	1.75	1.52
1	A	315	GLY	C-O	-7.15	1.12	1.23
1	C	116	ASN	CB-CG	7.14	1.67	1.51
1	A	242	CYS	CA-C	7.12	1.71	1.52
1	A	43	ALA	C-O	-7.10	1.09	1.23
1	C	259	PHE	C-O	7.09	1.36	1.23
1	C	315	GLY	C-O	-7.09	1.12	1.23
1	A	387	ALA	CA-CB	7.07	1.67	1.52
1	A	292	PHE	CG-CD1	-7.06	1.28	1.38
1	C	154	TYR	C-O	7.06	1.36	1.23
1	A	128	GLU	CG-CD	7.05	1.62	1.51
1	A	118	VAL	CB-CG1	7.05	1.67	1.52
1	A	80	HIS	C-O	7.04	1.36	1.23
1	C	389	ILE	CA-CB	-7.04	1.38	1.54
1	C	269	GLU	CD-OE1	7.02	1.33	1.25
1	A	336	MET	CG-SD	7.02	1.99	1.81
1	A	193	PHE	CG-CD1	-6.99	1.28	1.38
1	C	363	ALA	CA-CB	-6.97	1.37	1.52
1	A	232	PRO	CG-CD	6.96	1.73	1.50
1	C	107	GLU	CG-CD	6.94	1.62	1.51
1	A	179	TYR	CG-CD2	-6.94	1.30	1.39
1	C	311	GLN	CB-CG	6.94	1.71	1.52
1	A	283	ALA	N-CA	6.93	1.60	1.46
1	C	366	GLU	CG-CD	6.93	1.62	1.51
1	A	128	GLU	CD-OE1	-6.93	1.18	1.25
1	C	327	LEU	N-CA	-6.92	1.32	1.46
1	A	113	ALA	N-CA	6.90	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	VAL	CB-CG2	6.90	1.67	1.52
1	C	130	ARG	C-O	6.89	1.36	1.23
1	A	186	ARG	CG-CD	6.89	1.69	1.51
1	C	250	LEU	C-O	6.89	1.36	1.23
1	C	228	VAL	CB-CG2	-6.89	1.38	1.52
1	C	354	SER	N-CA	6.89	1.60	1.46
1	A	254	VAL	N-CA	-6.89	1.32	1.46
1	A	203	TYR	CE2-CZ	-6.88	1.29	1.38
1	A	392	LYS	CE-NZ	6.87	1.66	1.49
1	A	258	SER	CB-OG	6.87	1.51	1.42
1	C	155	ALA	N-CA	6.86	1.60	1.46
1	C	90	ARG	CG-CD	6.85	1.69	1.51
1	A	350	PHE	CG-CD1	6.84	1.49	1.38
1	A	135	ALA	CA-CB	6.83	1.66	1.52
1	C	16	PRO	CA-C	-6.82	1.39	1.52
1	A	66	THR	CA-CB	6.81	1.71	1.53
1	A	223	VAL	CB-CG2	6.79	1.67	1.52
1	C	292	PHE	CG-CD1	6.77	1.49	1.38
1	A	276	GLU	CG-CD	-6.75	1.41	1.51
1	A	140	GLU	CB-CG	-6.74	1.39	1.52
1	A	107	GLU	CB-CG	6.72	1.65	1.52
1	A	369	VAL	CB-CG1	-6.72	1.38	1.52
1	C	236	ASP	C-O	-6.71	1.10	1.23
1	A	57	ARG	CB-CG	6.71	1.70	1.52
1	C	41	ALA	N-CA	6.70	1.59	1.46
1	A	188	ASP	C-O	6.70	1.36	1.23
1	C	258	SER	N-CA	6.69	1.59	1.46
1	C	40	GLU	CD-OE2	6.69	1.33	1.25
1	A	175	PRO	CG-CD	6.68	1.72	1.50
1	A	298	GLY	C-O	6.68	1.34	1.23
1	C	182	ASP	C-O	6.68	1.36	1.23
1	A	276	GLU	CB-CG	-6.67	1.39	1.52
1	C	97	ASP	C-O	6.67	1.36	1.23
1	C	240	ARG	CZ-NH1	-6.67	1.24	1.33
1	A	252	THR	C-O	6.65	1.35	1.23
1	A	404	LEU	CG-CD1	6.64	1.76	1.51
1	C	138	LEU	N-CA	6.60	1.59	1.46
1	C	245	LEU	CA-CB	-6.60	1.38	1.53
1	C	90	ARG	N-CA	6.60	1.59	1.46
1	C	225	ASN	C-O	-6.60	1.10	1.23
1	C	223	VAL	CA-CB	-6.58	1.41	1.54
1	C	276	GLU	CD-OE1	6.56	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	364	ARG	CG-CD	6.56	1.68	1.51
1	A	24	PHE	CA-C	6.56	1.70	1.52
1	A	179	TYR	CD2-CE2	6.53	1.49	1.39
1	A	401	ALA	CA-CB	6.53	1.66	1.52
1	C	159	PRO	C-O	6.51	1.36	1.23
1	A	108	GLN	CB-CG	-6.50	1.35	1.52
1	A	310	VAL	CA-CB	6.49	1.68	1.54
1	C	387	ALA	CA-CB	-6.48	1.38	1.52
1	A	350	PHE	C-O	6.47	1.35	1.23
1	C	22	LEU	C-O	6.47	1.35	1.23
1	C	131	ILE	CA-CB	6.46	1.69	1.54
1	C	179	TYR	CE1-CZ	6.46	1.47	1.38
1	A	338	VAL	C-O	-6.46	1.11	1.23
1	A	163	PHE	CE1-CZ	6.46	1.49	1.37
1	C	78	TYR	C-O	6.46	1.35	1.23
1	C	162	ILE	CB-CG2	-6.46	1.32	1.52
1	C	171	GLU	CD-OE2	6.45	1.32	1.25
1	C	379	PRO	CG-CD	6.45	1.72	1.50
1	C	150	PHE	C-O	-6.44	1.11	1.23
1	A	161	ARG	CZ-NH2	6.43	1.41	1.33
1	C	196	ALA	CA-CB	-6.42	1.39	1.52
1	C	140	GLU	CD-OE2	6.41	1.32	1.25
1	C	356	LEU	CB-CG	6.40	1.71	1.52
1	A	219	ALA	CA-CB	-6.39	1.39	1.52
1	A	256	PHE	CG-CD2	6.39	1.48	1.38
1	A	263	PHE	CE2-CZ	6.39	1.49	1.37
1	C	73	GLU	CG-CD	6.39	1.61	1.51
1	A	146	GLY	N-CA	-6.32	1.36	1.46
1	C	158	PHE	C-O	6.32	1.35	1.23
1	C	197	LYS	CD-CE	6.32	1.67	1.51
1	C	40	GLU	CG-CD	6.30	1.61	1.51
1	A	350	PHE	CE2-CZ	6.29	1.49	1.37
1	C	148	CYS	CB-SG	-6.29	1.71	1.82
1	C	144	PRO	N-CD	-6.28	1.39	1.47
1	C	231	ARG	CZ-NH1	6.27	1.41	1.33
1	C	197	LYS	CB-CG	6.25	1.69	1.52
1	C	307	PHE	C-O	-6.25	1.11	1.23
1	C	263	PHE	CG-CD1	6.24	1.48	1.38
1	C	159	PRO	CA-CB	6.24	1.66	1.53
1	C	356	LEU	CG-CD1	6.23	1.75	1.51
1	C	296	ALA	CA-CB	6.23	1.65	1.52
1	C	209	GLU	CD-OE1	6.22	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	PRO	CA-C	6.22	1.65	1.52
1	C	18	VAL	CB-CG2	6.20	1.65	1.52
1	A	406	TRP	CE2-CZ2	-6.19	1.29	1.39
1	A	257	LEU	CG-CD2	-6.19	1.28	1.51
1	C	284	ALA	C-O	6.19	1.35	1.23
1	A	68	GLY	C-O	6.18	1.33	1.23
1	A	155	ALA	CA-CB	-6.18	1.39	1.52
1	C	273	GLU	N-CA	-6.17	1.34	1.46
1	A	357	CYS	C-O	6.17	1.35	1.23
1	A	273	GLU	CB-CG	6.16	1.63	1.52
1	A	227	GLN	CB-CG	-6.16	1.35	1.52
1	A	314	LYS	CB-CG	6.16	1.69	1.52
1	A	231	ARG	N-CA	6.15	1.58	1.46
1	C	128	GLU	CG-CD	6.15	1.61	1.51
1	C	55	TRP	CZ3-CH2	-6.14	1.30	1.40
1	A	84	GLU	CG-CD	6.14	1.61	1.51
1	C	158	PHE	CD2-CE2	6.14	1.51	1.39
1	C	317	GLN	CB-CG	6.13	1.69	1.52
1	A	305	TYR	CD2-CE2	-6.13	1.30	1.39
1	A	311	GLN	CG-CD	6.12	1.65	1.51
1	A	372	LYS	CE-NZ	6.12	1.64	1.49
1	C	86	PRO	CA-C	6.11	1.65	1.52
1	A	99	ILE	CA-CB	6.11	1.69	1.54
1	A	154	TYR	CB-CG	6.11	1.60	1.51
1	C	277	ARG	C-N	6.11	1.45	1.34
1	C	253	VAL	CA-CB	6.09	1.67	1.54
1	A	183	GLN	CB-CG	6.08	1.69	1.52
1	C	338	VAL	N-CA	6.07	1.58	1.46
1	A	379	PRO	CB-CG	6.06	1.80	1.50
1	C	103	MET	CA-C	-6.05	1.37	1.52
1	A	263	PHE	CD1-CE1	6.05	1.51	1.39
1	A	256	PHE	CE2-CZ	-6.04	1.25	1.37
1	C	80	HIS	CA-CB	6.01	1.67	1.53
1	A	251	ASP	CB-CG	6.01	1.64	1.51
1	C	208	ILE	CB-CG2	6.01	1.71	1.52
1	C	93	GLY	C-O	-5.99	1.14	1.23
1	C	163	PHE	CE2-CZ	-5.99	1.25	1.37
1	A	75	TYR	CD1-CE1	5.98	1.48	1.39
1	C	307	PHE	CG-CD2	5.98	1.47	1.38
1	C	388	GLN	CB-CG	5.97	1.68	1.52
1	A	160	ILE	CB-CG2	-5.96	1.34	1.52
1	A	87	PHE	CG-CD2	5.96	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	305	TYR	CG-CD1	5.95	1.46	1.39
1	A	307	PHE	C-O	-5.95	1.12	1.23
1	C	253	VAL	CB-CG1	5.95	1.65	1.52
1	C	135	ALA	CA-CB	5.95	1.65	1.52
1	C	365	ARG	CZ-NH2	-5.95	1.25	1.33
1	A	118	VAL	N-CA	-5.94	1.34	1.46
1	C	98	PHE	CE1-CZ	5.94	1.48	1.37
1	A	151	THR	N-CA	5.92	1.58	1.46
1	C	279	GLU	CG-CD	5.92	1.60	1.51
1	A	71	ILE	C-O	5.92	1.34	1.23
1	C	203	TYR	CD1-CE1	-5.91	1.30	1.39
1	A	106	PRO	C-O	5.91	1.35	1.23
1	C	286	GLU	CB-CG	5.91	1.63	1.52
1	A	333	ALA	N-CA	5.91	1.58	1.46
1	C	112	ARG	CZ-NH1	5.91	1.40	1.33
1	A	145	GLN	CD-NE2	5.89	1.47	1.32
1	A	402	LEU	CA-CB	5.88	1.67	1.53
1	C	156	GLU	C-O	5.88	1.34	1.23
1	C	90	ARG	CB-CG	5.88	1.68	1.52
1	C	102	SER	CB-OG	5.86	1.49	1.42
1	C	132	GLN	C-O	5.85	1.34	1.23
1	A	103	MET	N-CA	5.85	1.58	1.46
1	A	380	ASP	N-CA	-5.85	1.34	1.46
1	A	47	GLU	CG-CD	5.84	1.60	1.51
1	A	81	PHE	N-CA	5.82	1.57	1.46
1	C	104	ASP	N-CA	5.81	1.57	1.46
1	A	76	GLU	CD-OE1	5.81	1.32	1.25
1	C	34	LEU	CG-CD1	5.80	1.73	1.51
1	A	203	TYR	CD2-CE2	-5.79	1.30	1.39
1	C	104	ASP	CB-CG	5.79	1.64	1.51
1	C	28	MET	CA-C	5.78	1.68	1.52
1	A	29	TYR	CD2-CE2	5.77	1.48	1.39
1	A	96	TYR	C-O	5.77	1.34	1.23
1	C	168	GLY	N-CA	5.77	1.54	1.46
1	C	362	LEU	C-N	-5.77	1.20	1.34
1	A	250	LEU	CG-CD1	5.76	1.73	1.51
1	A	280	ARG	CA-C	5.76	1.68	1.52
1	A	125	ASP	CA-C	-5.76	1.38	1.52
1	A	163	PHE	CB-CG	-5.75	1.41	1.51
1	A	101	THR	C-O	5.74	1.34	1.23
1	A	178	LYS	CE-NZ	5.74	1.63	1.49
1	C	239	LYS	CE-NZ	5.74	1.63	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	TRP	CE3-CZ3	-5.73	1.28	1.38
1	A	307	PHE	CE2-CZ	5.73	1.48	1.37
1	A	83	SER	CB-OG	5.72	1.49	1.42
1	C	159	PRO	CG-CD	5.72	1.69	1.50
1	A	178	LYS	CD-CE	5.71	1.65	1.51
1	A	55	TRP	CE3-CZ3	-5.71	1.28	1.38
1	C	367	ILE	CB-CG2	5.71	1.70	1.52
1	C	365	ARG	N-CA	5.70	1.57	1.46
1	A	184	MET	CG-SD	-5.68	1.66	1.81
1	C	133	GLU	CG-CD	5.68	1.60	1.51
1	A	387	ALA	C-O	5.67	1.34	1.23
1	C	335	PRO	N-CA	5.67	1.56	1.47
1	A	305	TYR	C-O	5.66	1.34	1.23
1	A	149	ASN	CB-CG	5.65	1.64	1.51
1	C	366	GLU	CD-OE2	5.64	1.31	1.25
1	A	360	GLN	CB-CG	5.64	1.67	1.52
1	C	359	GLY	N-CA	5.64	1.54	1.46
1	C	314	LYS	CD-CE	5.63	1.65	1.51
1	A	111	PHE	CB-CG	5.62	1.60	1.51
1	C	179	TYR	CD2-CE2	-5.62	1.30	1.39
1	C	179	TYR	CG-CD1	5.61	1.46	1.39
1	A	107	GLU	CG-CD	-5.61	1.43	1.51
1	A	340	PHE	CB-CG	5.60	1.60	1.51
1	C	150	PHE	CD1-CE1	5.60	1.50	1.39
1	C	342	ARG	CG-CD	5.60	1.66	1.51
1	C	78	TYR	CA-C	5.60	1.67	1.52
1	A	373	GLU	CB-CG	-5.59	1.41	1.52
1	C	204	LEU	N-CA	-5.59	1.35	1.46
1	A	356	LEU	CG-CD1	5.59	1.72	1.51
1	C	79	ARG	CG-CD	5.58	1.66	1.51
1	A	259	PHE	CA-CB	-5.58	1.41	1.53
1	C	86	PRO	CG-CD	5.57	1.69	1.50
1	A	235	SER	CB-OG	5.56	1.49	1.42
1	A	405	VAL	CA-CB	5.56	1.66	1.54
1	A	106	PRO	CB-CG	5.55	1.77	1.50
1	C	165	LEU	CG-CD2	5.53	1.72	1.51
1	C	401	ALA	N-CA	-5.53	1.35	1.46
1	C	256	PHE	CD2-CE2	5.52	1.50	1.39
1	C	186	ARG	CG-CD	-5.51	1.38	1.51
1	A	247	VAL	N-CA	5.50	1.57	1.46
1	A	256	PHE	C-O	5.50	1.33	1.23
1	A	266	LYS	N-CA	5.50	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	86	PRO	N-CA	-5.49	1.38	1.47
1	A	193	PHE	CB-CG	-5.49	1.42	1.51
1	C	89	PRO	N-CA	5.49	1.56	1.47
1	C	153	ASP	CB-CG	5.48	1.63	1.51
1	C	202	ASP	CB-CG	5.48	1.63	1.51
1	C	103	MET	N-CA	5.47	1.57	1.46
1	C	279	GLU	CB-CG	5.47	1.62	1.52
1	A	157	PRO	C-O	-5.46	1.12	1.23
1	A	195	GLU	CD-OE1	5.46	1.31	1.25
1	A	237	GLU	CG-CD	-5.46	1.43	1.51
1	A	359	GLY	N-CA	5.46	1.54	1.46
1	A	141	SER	C-O	5.46	1.33	1.23
1	C	285	CYS	CA-CB	5.46	1.66	1.53
1	A	392	LYS	CD-CE	5.45	1.64	1.51
1	C	175	PRO	CA-C	5.44	1.63	1.52
1	C	19	PRO	N-CA	-5.44	1.38	1.47
1	A	154	TYR	CE1-CZ	5.44	1.45	1.38
1	A	108	GLN	CA-C	-5.43	1.38	1.52
1	C	350	PHE	CE1-CZ	5.43	1.47	1.37
1	C	265	ALA	N-CA	5.43	1.57	1.46
1	C	277	ARG	N-CA	-5.43	1.35	1.46
1	A	172	GLU	CD-OE1	5.43	1.31	1.25
1	C	398	GLY	N-CA	5.42	1.54	1.46
1	C	175	PRO	C-O	5.42	1.34	1.23
1	A	18	VAL	CB-CG2	5.42	1.64	1.52
1	A	40	GLU	CD-OE2	5.41	1.31	1.25
1	C	304	ASP	CB-CG	-5.40	1.40	1.51
1	A	279	GLU	CG-CD	-5.40	1.43	1.51
1	C	225	ASN	C-N	-5.39	1.23	1.33
1	A	269	GLU	CD-OE1	5.39	1.31	1.25
1	C	340	PHE	C-O	-5.39	1.13	1.23
1	A	72	ARG	CB-CG	5.39	1.67	1.52
1	C	61	GLY	CA-C	-5.39	1.43	1.51
1	C	84	GLU	CA-C	5.39	1.67	1.52
1	C	263	PHE	C-O	-5.38	1.13	1.23
1	A	385	PRO	C-O	5.38	1.34	1.23
1	C	274	LEU	CG-CD2	5.38	1.71	1.51
1	C	108	GLN	CB-CG	-5.38	1.38	1.52
1	C	84	GLU	CB-CG	5.38	1.62	1.52
1	A	240	ARG	CZ-NH2	5.37	1.40	1.33
1	A	244	ALA	C-O	5.37	1.33	1.23
1	C	246	LEU	N-CA	5.37	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	397	SER	C-O	5.36	1.33	1.23
1	C	220	ILE	N-CA	5.36	1.57	1.46
1	A	228	VAL	CA-C	-5.35	1.39	1.52
1	A	26	PHE	CE2-CZ	5.35	1.47	1.37
1	A	124	VAL	CB-CG2	-5.35	1.41	1.52
1	A	127	LEU	CG-CD2	5.35	1.71	1.51
1	A	132	GLN	CB-CG	5.35	1.67	1.52
1	C	47	GLU	CD-OE1	5.35	1.31	1.25
1	C	133	GLU	CD-OE1	5.34	1.31	1.25
1	A	150	PHE	CD2-CE2	5.34	1.50	1.39
1	A	382	SER	CA-CB	5.34	1.60	1.52
1	C	61	GLY	C-O	-5.34	1.15	1.23
1	A	402	LEU	CB-CG	5.33	1.68	1.52
1	A	244	ALA	CA-CB	-5.33	1.41	1.52
1	C	188	ASP	C-O	5.33	1.33	1.23
1	A	147	GLN	CB-CG	-5.33	1.38	1.52
1	C	301	LEU	CA-C	5.33	1.66	1.52
1	A	227	GLN	CA-CB	-5.33	1.42	1.53
1	A	313	LYS	CB-CG	5.32	1.67	1.52
1	C	302	THR	C-O	5.32	1.33	1.23
1	A	323	MET	CB-CG	5.32	1.68	1.51
1	C	234	THR	CA-CB	5.32	1.67	1.53
1	A	337	HIS	CA-CB	5.32	1.65	1.53
1	C	243	GLY	C-O	-5.32	1.15	1.23
1	A	221	SER	CB-OG	-5.31	1.35	1.42
1	C	42	TRP	CG-CD1	-5.31	1.29	1.36
1	A	409	ALA	CA-C	5.31	1.66	1.52
1	C	147	GLN	CG-CD	5.31	1.63	1.51
1	C	286	GLU	CG-CD	5.31	1.59	1.51
1	C	385	PRO	C-O	5.31	1.33	1.23
1	C	143	ARG	CG-CD	5.30	1.65	1.51
1	A	372	LYS	CG-CD	5.30	1.70	1.52
1	A	316	ASP	CB-CG	-5.29	1.40	1.51
1	C	20	GLU	CD-OE1	5.28	1.31	1.25
1	A	98	PHE	CE1-CZ	5.28	1.47	1.37
1	C	181	THR	CB-CG2	5.28	1.69	1.52
1	C	27	ASP	CB-CG	5.27	1.62	1.51
1	C	75	TYR	CD1-CE1	-5.27	1.31	1.39
1	C	47	GLU	CG-CD	5.27	1.59	1.51
1	A	78	TYR	CE1-CZ	5.26	1.45	1.38
1	C	372	LYS	C-O	5.26	1.33	1.23
1	C	295	VAL	CB-CG2	5.25	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	ARG	C-O	5.25	1.33	1.23
1	C	237	GLU	CA-CB	-5.24	1.42	1.53
1	C	269	GLU	CB-CG	-5.23	1.42	1.52
1	C	331	GLU	C-O	5.23	1.33	1.23
1	A	67	ARG	N-CA	5.23	1.56	1.46
1	C	206	PRO	C-O	-5.22	1.12	1.23
1	A	262	GLU	N-CA	-5.22	1.35	1.46
1	A	81	PHE	CG-CD2	5.22	1.46	1.38
1	C	43	ALA	CA-CB	-5.22	1.41	1.52
1	C	84	GLU	CD-OE1	-5.21	1.20	1.25
1	C	292	PHE	CE1-CZ	5.21	1.47	1.37
1	C	88	ILE	C-N	5.21	1.44	1.34
1	C	292	PHE	CA-C	5.20	1.66	1.52
1	A	264	LEU	C-O	5.19	1.33	1.23
1	C	237	GLU	CG-CD	-5.19	1.44	1.51
1	A	111	PHE	N-CA	-5.19	1.35	1.46
1	A	299	ARG	CZ-NH1	5.19	1.39	1.33
1	A	316	ASP	N-CA	5.19	1.56	1.46
1	A	346	SER	C-O	-5.18	1.13	1.23
1	A	296	ALA	C-O	-5.18	1.13	1.23
1	C	124	VAL	CB-CG2	5.18	1.63	1.52
1	C	150	PHE	CD2-CE2	5.18	1.49	1.39
1	C	54	VAL	CB-CG2	-5.17	1.42	1.52
1	C	113	ALA	C-O	5.17	1.33	1.23
1	A	65	ALA	C-O	5.17	1.33	1.23
1	A	311	GLN	CB-CG	5.17	1.66	1.52
1	C	98	PHE	CG-CD1	5.17	1.46	1.38
1	A	25	ASP	CB-CG	5.16	1.62	1.51
1	A	254	VAL	CA-C	-5.16	1.39	1.52
1	C	119	VAL	CB-CG1	5.16	1.63	1.52
1	A	192	THR	N-CA	5.16	1.56	1.46
1	C	364	ARG	CZ-NH2	-5.16	1.26	1.33
1	A	276	GLU	CA-CB	-5.16	1.42	1.53
1	C	114	LEU	N-CA	5.16	1.56	1.46
1	A	36	ALA	CA-CB	5.15	1.63	1.52
1	A	342	ARG	CA-C	-5.15	1.39	1.52
1	C	367	ILE	C-O	-5.15	1.13	1.23
1	C	147	GLN	CD-OE1	-5.14	1.12	1.24
1	A	79	ARG	C-O	-5.14	1.13	1.23
1	C	202	ASP	C-O	5.14	1.33	1.23
1	A	112	ARG	C-O	5.14	1.33	1.23
1	C	257	LEU	C-O	5.12	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	GLN	C-O	5.12	1.33	1.23
1	A	110	GLN	C-O	5.11	1.33	1.23
1	A	384	ALA	CA-CB	5.11	1.63	1.52
1	C	66	THR	CB-CG2	-5.11	1.35	1.52
1	A	157	PRO	N-CA	5.11	1.55	1.47
1	C	259	PHE	CG-CD2	-5.11	1.31	1.38
1	C	181	THR	CA-CB	-5.11	1.40	1.53
1	A	377	ARG	CZ-NH2	5.10	1.39	1.33
1	C	39	GLN	C-O	5.10	1.33	1.23
1	C	408	PRO	CA-C	5.10	1.63	1.52
1	C	73	GLU	CB-CG	5.09	1.61	1.52
1	A	266	LYS	C-O	5.09	1.33	1.23
1	C	179	TYR	CG-CD2	5.08	1.45	1.39
1	C	206	PRO	N-CA	-5.08	1.38	1.47
1	C	377	ARG	CA-C	5.08	1.66	1.52
1	A	201	TYR	CB-CG	5.07	1.59	1.51
1	C	129	ASN	N-CA	-5.07	1.36	1.46
1	C	42	TRP	CA-C	-5.07	1.39	1.52
1	C	132	GLN	CD-OE1	5.07	1.35	1.24
1	A	67	ARG	CZ-NH1	5.07	1.39	1.33
1	C	199	ALA	CA-CB	-5.06	1.41	1.52
1	A	169	LEU	C-O	-5.06	1.13	1.23
1	A	410	THR	N-CA	5.05	1.56	1.46
1	C	409	ALA	C-O	5.05	1.32	1.23
1	A	348	THR	N-CA	-5.05	1.36	1.46
1	C	152	GLU	CD-OE2	5.05	1.31	1.25
1	C	348	THR	C-O	5.05	1.32	1.23
1	A	289	LEU	CG-CD2	5.05	1.70	1.51
1	A	176	HIS	C-O	5.04	1.32	1.23
1	A	50	VAL	CB-CG2	5.04	1.63	1.52
1	C	205	ILE	N-CA	-5.04	1.36	1.46
1	C	290	ARG	CZ-NH1	5.04	1.39	1.33
1	A	135	ALA	C-O	-5.04	1.13	1.23
1	A	192	THR	C-O	5.04	1.32	1.23
1	A	195	GLU	CG-CD	-5.04	1.44	1.51
1	A	50	VAL	CA-CB	-5.04	1.44	1.54
1	C	72	ARG	CZ-NH2	-5.03	1.26	1.33
1	A	81	PHE	CD1-CE1	5.03	1.49	1.39
1	A	262	GLU	CD-OE1	-5.03	1.20	1.25
1	C	76	GLU	CG-CD	5.03	1.59	1.51
1	A	83	SER	N-CA	5.02	1.56	1.46
1	A	101	THR	CB-OG1	-5.02	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ASP	C-O	-5.02	1.13	1.23
1	C	109	ARG	CZ-NH2	5.02	1.39	1.33
1	C	86	PRO	N-CD	5.02	1.54	1.47
1	C	110	GLN	CG-CD	5.02	1.62	1.51
1	C	205	ILE	CA-C	5.01	1.66	1.52
1	C	306	GLU	C-O	-5.01	1.13	1.23
1	C	227	GLN	C-O	5.00	1.32	1.23

All (353) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	290	ARG	NE-CZ-NH1	-24.41	108.09	120.30
1	C	130	ARG	NE-CZ-NH1	-23.85	108.37	120.30
1	A	77	ASP	CB-CG-OD2	20.89	137.10	118.30
1	C	130	ARG	NE-CZ-NH2	20.79	130.70	120.30
1	C	377	ARG	NE-CZ-NH1	-19.19	110.70	120.30
1	C	112	ARG	NE-CZ-NH1	16.40	128.50	120.30
1	C	112	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	C	188	ASP	CB-CG-OD2	-14.79	104.99	118.30
1	A	151	THR	CA-CB-CG2	-14.36	92.29	112.40
1	C	299	ARG	NE-CZ-NH2	-14.35	113.12	120.30
1	A	184	MET	CG-SD-CE	-13.84	78.06	100.20
1	A	72	ARG	NE-CZ-NH1	-13.17	113.72	120.30
1	C	231	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	C	299	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	C	290	ARG	NE-CZ-NH2	12.56	126.58	120.30
1	A	371	LEU	CB-CG-CD2	-12.54	89.68	111.00
1	C	280	ARG	NE-CZ-NH2	-12.07	114.27	120.30
1	C	304	ASP	CB-CG-OD1	-12.01	107.49	118.30
1	C	231	ARG	NE-CZ-NH1	11.91	126.26	120.30
1	C	72	ARG	NE-CZ-NH2	-11.51	114.55	120.30
1	C	356	LEU	CB-CG-CD1	11.21	130.06	111.00
1	C	364	ARG	NE-CZ-NH2	11.10	125.85	120.30
1	C	99	ILE	CG1-CB-CG2	10.98	135.56	111.40
1	A	299	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	C	327	LEU	CB-CG-CD1	-10.69	92.83	111.00
1	C	240	ARG	NE-CZ-NH1	-10.40	115.10	120.30
1	C	316	ASP	CB-CG-OD2	-10.32	109.01	118.30
1	A	67	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	C	143	ARG	C-N-CD	9.99	149.39	128.40
1	C	143	ARG	CB-CG-CD	-9.90	85.86	111.60
1	C	260	SER	N-CA-CB	9.81	125.22	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	257	LEU	CB-CG-CD1	9.77	127.62	111.00
1	C	291	ARG	NE-CZ-NH2	9.73	125.17	120.30
1	A	377	ARG	NE-CZ-NH1	-9.73	115.44	120.30
1	C	304	ASP	CB-CG-OD2	9.71	127.03	118.30
1	A	254	VAL	CB-CA-C	-9.68	93.00	111.40
1	A	163	PHE	CZ-CE2-CD2	-9.44	108.77	120.10
1	A	205	ILE	CG1-CB-CG2	9.41	132.10	111.40
1	A	90	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	C	369	VAL	CG1-CB-CG2	-9.33	95.97	110.90
1	C	404	LEU	CB-CG-CD2	9.22	126.67	111.00
1	A	339	ASP	CB-CG-OD2	-9.21	110.01	118.30
1	C	67	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	C	364	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	C	165	LEU	CB-CG-CD2	9.09	126.46	111.00
1	A	70	LEU	CA-CB-CG	9.05	136.12	115.30
1	C	118	VAL	CG1-CB-CG2	-8.97	96.55	110.90
1	A	134	LEU	CB-CA-C	-8.95	93.20	110.20
1	C	11	LEU	CB-CG-CD1	-8.95	95.79	111.00
1	A	236	ASP	CB-CG-OD1	-8.81	110.37	118.30
1	A	142	LEU	CD1-CG-CD2	-8.78	84.15	110.50
1	A	280	ARG	CG-CD-NE	-8.78	93.35	111.80
1	A	52	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	C	82	SER	N-CA-CB	-8.66	97.51	110.50
1	A	297	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	C	280	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	C	105	PRO	C-N-CD	-8.61	101.67	120.60
1	A	174	ILE	C-N-CD	8.58	146.42	128.40
1	A	134	LEU	CB-CG-CD1	8.56	125.55	111.00
1	A	123	VAL	CG1-CB-CG2	-8.54	97.24	110.90
1	A	245	LEU	CA-CB-CG	8.49	134.84	115.30
1	A	251	ASP	CB-CG-OD2	8.45	125.91	118.30
1	A	312	LEU	CB-CG-CD2	-8.43	96.67	111.00
1	A	316	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	C	188	ASP	N-CA-CB	-8.28	95.70	110.60
1	C	330	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	C	402	LEU	CA-CB-CG	8.25	134.28	115.30
1	A	67	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	177	LEU	CB-CG-CD1	-8.19	97.07	111.00
1	A	365	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	C	371	LEU	CA-CB-CG	8.12	133.98	115.30
1	C	111	PHE	C-N-CA	-8.08	101.51	121.70
1	C	200	LEU	CB-CG-CD2	-8.07	97.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	211	ARG	CA-CB-CG	8.01	131.01	113.40
1	A	240	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	C	142	LEU	CB-CG-CD1	7.94	124.50	111.00
1	A	211	ARG	NE-CZ-NH1	-7.91	116.34	120.30
1	C	96	TYR	CB-CA-C	-7.90	94.61	110.40
1	C	264	LEU	N-CA-C	-7.89	89.70	111.00
1	A	138	LEU	CA-CB-CG	7.88	133.44	115.30
1	C	263	PHE	CB-CG-CD1	-7.88	115.29	120.80
1	C	264	LEU	CB-CG-CD2	7.83	124.32	111.00
1	C	356	LEU	CA-CB-CG	-7.83	97.30	115.30
1	C	240	ARG	CG-CD-NE	-7.81	95.40	111.80
1	A	154	TYR	CZ-CE2-CD2	-7.79	112.79	119.80
1	A	257	LEU	CB-CG-CD2	7.68	124.06	111.00
1	C	402	LEU	N-CA-C	7.68	131.73	111.00
1	A	246	LEU	CA-CB-CG	7.64	132.88	115.30
1	A	85	CYS	N-CA-CB	-7.63	96.86	110.60
1	A	290	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	A	77	ASP	OD1-CG-OD2	-7.55	108.94	123.30
1	C	90	ARG	NE-CZ-NH1	-7.55	116.52	120.30
1	A	402	LEU	CB-CG-CD2	7.53	123.80	111.00
1	C	188	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	191	MET	CA-CB-CG	7.47	126.00	113.30
1	C	165	LEU	CA-CB-CG	7.45	132.44	115.30
1	A	112	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	A	143	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	C	80	HIS	N-CA-CB	7.41	123.94	110.60
1	A	70	LEU	CB-CG-CD2	7.41	123.59	111.00
1	A	173	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	265	ALA	N-CA-C	7.35	130.85	111.00
1	C	75	TYR	CB-CG-CD2	7.33	125.40	121.00
1	A	130	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	C	99	ILE	CB-CA-C	-7.30	96.99	111.60
1	C	75	TYR	CB-CG-CD1	-7.30	116.62	121.00
1	C	358	LEU	CB-CG-CD2	-7.25	98.67	111.00
1	A	70	LEU	CB-CG-CD1	7.22	123.27	111.00
1	C	53	LEU	CB-CA-C	-7.21	96.50	110.20
1	A	401	ALA	CB-CA-C	7.13	120.79	110.10
1	C	251	ASP	CB-CG-OD2	7.12	124.70	118.30
1	C	404	LEU	CB-CG-CD1	-7.11	98.91	111.00
1	C	186	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	A	356	LEU	CB-CG-CD2	7.03	122.95	111.00
1	A	277	ARG	CA-CB-CG	-7.03	97.94	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	267	SER	CB-CA-C	7.01	123.42	110.10
1	C	294	LEU	CB-CG-CD1	7.01	122.91	111.00
1	C	90	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	C	338	VAL	CA-CB-CG1	6.95	121.32	110.90
1	A	231	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	C	340	PHE	CB-CG-CD2	6.94	125.66	120.80
1	C	143	ARG	CG-CD-NE	-6.94	97.23	111.80
1	C	342	ARG	CG-CD-NE	6.90	126.29	111.80
1	A	161	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	251	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	A	385	PRO	N-CA-C	6.86	129.93	112.10
1	C	28	MET	CG-SD-CE	-6.85	89.25	100.20
1	A	86	PRO	CB-CA-C	-6.84	94.91	112.00
1	C	184	MET	CG-SD-CE	-6.83	89.27	100.20
1	C	123	VAL	CG1-CB-CG2	-6.83	99.98	110.90
1	A	364	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	250	LEU	CB-CG-CD1	6.80	122.56	111.00
1	A	142	LEU	CB-CG-CD1	6.80	122.56	111.00
1	C	114	LEU	CB-CG-CD2	6.79	122.54	111.00
1	C	97	ASP	CB-CG-OD2	-6.79	112.19	118.30
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	C	272	GLN	CA-CB-CG	-6.76	98.54	113.40
1	A	61	GLY	N-CA-C	-6.71	96.31	113.10
1	C	223	VAL	CB-CA-C	-6.70	98.67	111.40
1	A	161	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	C	191	MET	CA-CB-CG	6.66	124.63	113.30
1	C	134	LEU	CB-CG-CD1	6.66	122.31	111.00
1	A	246	LEU	CB-CG-CD1	6.65	122.31	111.00
1	A	358	LEU	CB-CG-CD1	6.61	122.24	111.00
1	C	131	ILE	N-CA-CB	6.58	125.92	110.80
1	A	290	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	A	409	ALA	O-C-N	-6.56	112.21	122.70
1	C	103	MET	CB-CA-C	-6.53	97.34	110.40
1	C	238	ALA	CB-CA-C	6.53	119.89	110.10
1	C	147	GLN	CG-CD-OE1	-6.52	108.57	121.60
1	A	395	ILE	CB-CA-C	-6.50	98.60	111.60
1	A	247	VAL	CG1-CB-CG2	-6.45	100.58	110.90
1	A	96	TYR	O-C-N	-6.44	112.40	122.70
1	A	270	HIS	N-CA-C	-6.44	93.62	111.00
1	A	402	LEU	CB-CG-CD1	6.41	121.90	111.00
1	A	250	LEU	CB-CA-C	6.40	122.37	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	186	ARG	CB-CG-CD	6.40	128.24	111.60
1	A	151	THR	N-CA-C	6.39	128.25	111.00
1	C	356	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	A	404	LEU	CB-CG-CD1	6.38	121.85	111.00
1	C	377	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	C	244	ALA	N-CA-CB	6.31	118.93	110.10
1	A	389	ILE	CB-CA-C	-6.30	98.99	111.60
1	A	127	LEU	CB-CG-CD1	-6.28	100.33	111.00
1	C	61	GLY	N-CA-C	-6.28	97.41	113.10
1	A	14	LEU	CB-CG-CD1	-6.26	100.36	111.00
1	A	163	PHE	CG-CD1-CE1	-6.25	113.92	120.80
1	A	139	ILE	CA-CB-CG1	-6.25	99.13	111.00
1	C	344	LYS	N-CA-C	-6.21	94.24	111.00
1	A	228	VAL	CA-CB-CG2	-6.20	101.60	110.90
1	A	271	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	C	40	GLU	CB-CA-C	6.18	122.75	110.40
1	C	266	LYS	CB-CG-CD	-6.15	95.60	111.60
1	A	28	MET	CG-SD-CE	-6.14	90.37	100.20
1	C	288	LEU	CA-CB-CG	-6.14	101.18	115.30
1	A	207	ILE	N-CA-CB	-6.11	96.75	110.80
1	A	323	MET	CG-SD-CE	6.10	109.96	100.20
1	C	399	VAL	CG1-CB-CG2	6.09	120.64	110.90
1	C	301	LEU	CB-CG-CD2	6.07	121.32	111.00
1	C	225	ASN	C-N-CA	-6.06	109.57	122.30
1	A	143	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	C	52	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	C	335	PRO	CB-CA-C	-6.04	96.89	112.00
1	A	339	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	409	ALA	CB-CA-C	6.02	119.13	110.10
1	C	137	SER	CA-CB-OG	-6.01	94.96	111.20
1	C	293	SER	C-N-CA	-6.01	106.68	121.70
1	A	365	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	271	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	263	PHE	CB-CG-CD1	-5.99	116.60	120.80
1	A	276	GLU	OE1-CD-OE2	5.99	130.49	123.30
1	A	134	LEU	CB-CG-CD2	-5.99	100.81	111.00
1	C	138	LEU	CB-CG-CD2	5.98	121.17	111.00
1	A	384	ALA	N-CA-C	-5.98	94.86	111.00
1	A	14	LEU	CB-CG-CD2	5.97	121.16	111.00
1	C	303	SER	CB-CA-C	5.96	121.42	110.10
1	C	365	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	220	ILE	CB-CA-C	-5.93	99.75	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	27	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	188	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	305	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	369	VAL	CB-CA-C	-5.92	100.16	111.40
1	A	298	GLY	N-CA-C	5.91	127.88	113.10
1	C	147	GLN	CB-CG-CD	5.91	126.97	111.60
1	C	110	GLN	O-C-N	-5.90	113.26	122.70
1	A	278	PRO	C-N-CA	-5.89	106.96	121.70
1	A	285	CYS	CA-CB-SG	-5.89	103.40	114.00
1	C	164	MET	CB-CG-SD	5.85	129.94	112.40
1	A	346	SER	CB-CA-C	5.84	121.20	110.10
1	C	202	ASP	CB-CG-OD1	5.84	123.55	118.30
1	C	79	ARG	O-C-N	5.84	132.04	122.70
1	C	405	VAL	CB-CA-C	-5.83	100.32	111.40
1	C	377	ARG	NH1-CZ-NH2	5.83	125.81	119.40
1	A	342	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	36	ALA	CB-CA-C	5.82	118.82	110.10
1	A	109	ARG	CB-CA-C	5.82	122.03	110.40
1	C	173	ASP	N-CA-C	5.81	126.69	111.00
1	A	87	PHE	CB-CG-CD1	-5.81	116.73	120.80
1	C	239	LYS	CB-CA-C	-5.80	98.79	110.40
1	A	96	TYR	CB-CG-CD1	5.80	124.48	121.00
1	A	284	ALA	N-CA-C	5.79	126.65	111.00
1	A	195	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	C	261	MET	CG-SD-CE	-5.77	90.97	100.20
1	C	85	CYS	CB-CA-C	-5.77	98.86	110.40
1	C	195	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	C	130	ARG	O-C-N	5.75	131.89	122.70
1	C	357	CYS	O-C-N	-5.73	113.53	122.70
1	C	261	MET	CB-CA-C	5.73	121.86	110.40
1	A	302	THR	N-CA-C	5.72	126.46	111.00
1	C	364	ARG	CG-CD-NE	5.72	123.81	111.80
1	C	250	LEU	N-CA-C	5.70	126.38	111.00
1	C	22	LEU	CB-CG-CD2	5.69	120.68	111.00
1	A	392	LYS	N-CA-C	-5.69	95.64	111.00
1	A	380	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	254	VAL	CB-CA-C	-5.68	100.61	111.40
1	C	337	HIS	CB-CA-C	5.67	121.74	110.40
1	A	173	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	201	TYR	N-CA-CB	-5.65	100.43	110.60
1	C	340	PHE	CB-CG-CD1	-5.65	116.85	120.80
1	A	94	GLU	N-CA-C	-5.64	95.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	271	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	110	GLN	N-CA-CB	-5.64	100.45	110.60
1	C	204	LEU	CD1-CG-CD2	-5.64	93.59	110.50
1	C	377	ARG	CD-NE-CZ	-5.64	115.71	123.60
1	C	130	ARG	CB-CA-C	-5.63	99.13	110.40
1	A	91	GLU	CB-CA-C	-5.63	99.13	110.40
1	C	112	ARG	CD-NE-CZ	5.63	131.48	123.60
1	C	130	ARG	CG-CD-NE	5.62	123.61	111.80
1	C	75	TYR	CE1-CZ-OH	-5.62	104.92	120.10
1	C	266	LYS	CD-CE-NZ	5.62	124.63	111.70
1	C	165	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	C	233	ILE	N-CA-C	-5.62	95.84	111.00
1	A	373	GLU	CA-CB-CG	-5.61	101.06	113.40
1	C	203	TYR	CD1-CE1-CZ	-5.60	114.76	119.80
1	C	245	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	A	142	LEU	CB-CG-CD2	5.59	120.51	111.00
1	A	236	ASP	CB-CG-OD2	5.59	123.34	118.30
1	A	90	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	350	PHE	N-CA-CB	-5.56	100.59	110.60
1	C	79	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	350	PHE	CB-CA-C	5.54	121.48	110.40
1	A	399	VAL	CA-CB-CG1	5.54	119.21	110.90
1	A	410	THR	OG1-CB-CG2	-5.54	97.25	110.00
1	A	79	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	125	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	141	SER	N-CA-CB	-5.51	102.23	110.50
1	C	96	TYR	C-N-CA	-5.50	107.94	121.70
1	C	372	LYS	CD-CE-NZ	5.50	124.36	111.70
1	A	261	MET	CA-CB-CG	5.50	122.65	113.30
1	A	30	ASN	C-N-CD	5.49	139.94	128.40
1	A	371	LEU	N-CA-C	-5.49	96.17	111.00
1	A	380	ASP	N-CA-CB	-5.49	100.71	110.60
1	A	371	LEU	CB-CG-CD1	5.48	120.31	111.00
1	C	288	LEU	CB-CG-CD2	5.48	120.31	111.00
1	A	278	PRO	O-C-N	-5.47	113.95	122.70
1	C	197	LYS	CD-CE-NZ	-5.46	99.15	111.70
1	C	180	LEU	CB-CG-CD1	-5.45	101.73	111.00
1	C	110	GLN	C-N-CA	-5.45	108.08	121.70
1	C	290	ARG	CA-CB-CG	-5.45	101.41	113.40
1	C	272	GLN	N-CA-C	5.45	125.70	111.00
1	C	368	ILE	C-N-CA	5.44	135.30	121.70
1	A	277	ARG	CB-CA-C	5.43	121.27	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	373	GLU	N-CA-C	5.43	125.66	111.00
1	A	251	ASP	OD1-CG-OD2	-5.42	113.00	123.30
1	A	382	SER	CB-CA-C	5.42	120.40	110.10
1	C	300	ILE	C-N-CA	-5.41	108.18	121.70
1	A	247	VAL	CA-CB-CG1	5.40	119.00	110.90
1	A	299	ARG	NH1-CZ-NH2	5.39	125.33	119.40
1	A	79	ARG	O-C-N	-5.39	114.08	122.70
1	C	237	GLU	CA-C-N	-5.39	105.34	117.20
1	C	130	ARG	N-CA-CB	5.39	120.30	110.60
1	A	117	GLN	N-CA-CB	5.38	120.29	110.60
1	A	367	ILE	CG1-CB-CG2	-5.38	99.55	111.40
1	C	371	LEU	CB-CG-CD2	5.37	120.13	111.00
1	C	87	PHE	N-CA-C	5.37	125.49	111.00
1	C	290	ARG	NH1-CZ-NH2	5.36	125.29	119.40
1	A	25	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	197	LYS	CA-CB-CG	5.35	125.16	113.40
1	A	330	ARG	CG-CD-NE	-5.32	100.62	111.80
1	C	251	ASP	O-C-N	-5.32	114.19	122.70
1	C	119	VAL	CG1-CB-CG2	5.32	119.41	110.90
1	C	142	LEU	CB-CA-C	-5.32	100.10	110.20
1	A	57	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	A	99	ILE	CB-CA-C	-5.30	101.00	111.60
1	C	239	LYS	CB-CG-CD	-5.30	97.83	111.60
1	C	124	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	A	290	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	A	324	LEU	N-CA-C	5.26	125.21	111.00
1	A	207	ILE	CG1-CB-CG2	5.26	122.97	111.40
1	C	362	LEU	CB-CG-CD1	5.25	119.93	111.00
1	A	121	MET	CB-CG-SD	5.25	128.15	112.40
1	C	305	TYR	OH-CZ-CE2	-5.24	105.95	120.10
1	A	195	GLU	CB-CA-C	-5.24	99.92	110.40
1	A	187	PRO	N-CD-CG	-5.24	95.35	103.20
1	C	342	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	179	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	C	112	ARG	N-CA-C	-5.22	96.90	111.00
1	C	242	CYS	C-N-CA	5.22	133.26	122.30
1	C	11	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	C	113	ALA	C-N-CA	5.19	134.67	121.70
1	A	101	THR	N-CA-C	5.19	125.01	111.00
1	A	330	ARG	CB-CA-C	-5.19	100.03	110.40
1	A	40	GLU	N-CA-C	5.17	124.97	111.00
1	A	174	ILE	C-N-CA	-5.17	100.28	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	ARG	N-CA-CB	-5.17	101.29	110.60
1	C	211	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	131	ILE	CG1-CB-CG2	-5.16	100.06	111.40
1	A	165	LEU	CA-CB-CG	5.15	127.15	115.30
1	C	97	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	222	ILE	CB-CA-C	-5.15	101.31	111.60
1	C	271	ARG	CG-CD-NE	-5.14	101.01	111.80
1	A	337	HIS	CB-CA-C	5.13	120.67	110.40
1	C	336	MET	CA-CB-CG	5.13	122.02	113.30
1	C	268	PRO	C-N-CA	-5.13	108.89	121.70
1	A	78	TYR	CG-CD2-CE2	5.10	125.38	121.30
1	A	413	ALA	CB-CA-C	5.09	117.74	110.10
1	A	186	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	368	ILE	CA-CB-CG1	-5.09	101.33	111.00
1	C	105	PRO	C-N-CA	5.09	143.37	122.00
1	C	257	LEU	CA-CB-CG	5.09	127.00	115.30
1	C	102	SER	O-C-N	5.07	130.81	122.70
1	A	127	LEU	CB-CG-CD2	5.06	119.61	111.00
1	C	254	VAL	CA-CB-CG1	-5.06	103.31	110.90
1	A	383	ILE	N-CA-C	5.05	124.63	111.00
1	A	396	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	A	387	ALA	CB-CA-C	5.04	117.65	110.10
1	A	378	ILE	CB-CA-C	-5.03	101.53	111.60
1	C	70	LEU	CB-CG-CD2	5.02	119.54	111.00
1	A	50	VAL	CG1-CB-CG2	5.02	118.93	110.90
1	A	72	ARG	NH1-CZ-NH2	5.02	124.92	119.40
1	C	142	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	C	178	LYS	N-CA-CB	-5.00	101.59	110.60

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
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

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Mol	Chain	Res	Type	Group
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3201	0	3148	418	11
1	C	3199	0	3137	392	12
2	A	43	0	32	19	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	6349	797	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 62.

All (797) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:96:TYR:C	1:A:96:TYR:CA	1.76	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:257:LEU:C	1:A:257:LEU:CA	1.75	1.51
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: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:20:GLU:CD	1:C:165:LEU:HG	1.39	1.38
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	1.18
1:C:277:ARG:HE	1:C:280:ARG:NH2	1.42	1.16
2:C:415:HEC:HBB3	2:C:415:HEC:HMB1	1.26	1.15
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
1:A:151:THR:HG23	1:A:151:THR:H	1.22	1.04
1:C:130:ARG:NH1	1:C:165:LEU:HD21	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:ILE:HG22	1:C:206:PRO:HD3	1.03	1.00
1:C:40:GLU:HG3	1:C:336:MET:HE2	1.42	0.99
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: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: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
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:254:VAL:CG1	1:C:254:VAL:C	2.42	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:91:GLU:H	1:C:91:GLU:CD	1.84	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:C:40:GLU:HG3	1:C:336:MET:HE3	1.61	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:A:103:MET:SD	1:A:107:GLU:OE1	2.39	0.80
1:A:233:ILE:HD13	1:A:237:GLU:HB2	1.62	0.80
1:C:414:VAL:OXT	1:C:414:VAL:HG13	1.82	0.79
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: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:A:21:HIS:HA	1:C:130:ARG:HD3	1.65	0.77
1:A:40:GLU:HG3	1:A:336:MET:HE1	1.66	0.77
1:A:404:LEU:CD1	1:A:404:LEU:HG	2.10	0.77
1:A:20:GLU:OE1	1:C:165:LEU:C	2.23	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:276:GLU:C	1:A:277:ARG:HG3	2.06	0.76
1:C:166:LEU:HD12	1:C:166:LEU:C	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:277:ARG:O	1:A:278:PRO:C	2.24	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: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:103:MET:HE1	1:A:107:GLU:OE1	1.86	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:C:244:ALA:O	1:C:245:LEU:C	2.25	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
1:C:254:VAL:C	1:C:254:VAL:HG12	2.07	0.73
1:C:191:MET:CE	1:C:196:ALA:HA	2.18	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
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: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:C:183:GLN:O	1:C:187:PRO:HG3	1.90	0.71
1:A:96:TYR:C	1:A:96:TYR:HA	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:O	1:A:395:ILE:HG22	1.90	0.70
1:C:108:GLN:O	1:C:108:GLN:HG2	1.85	0.70
1:A:20:GLU:OE2	1:C:165:LEU:CG	2.32	0.70
1:C:184:MET:HE2	1:C:200:LEU:HD22	1.74	0.70
1:C:195:GLU:HA	1:C:195:GLU:OE1	1.91	0.70
1:C:191:MET:HE1	1:C:196:ALA:HA	1.73	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: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:A:191:MET:HE1	1:A:196:ALA:HA	1.73	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: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: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: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:A:191:MET:CE	1:A:196:ALA:HA	2.23	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:292:PHE:O	1:A:293:SER:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ILE:HG13	1:C:103:MET:HE1	1.76	0.67
1:C:158:PHE:O	1:C:162:ILE:HD13	1.94	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
2:C:415:HEC:HMB1	2:C:415:HEC:CBB	1.89	0.67
1:A:39:GLN:H	1:A:39:GLN:CD	1.96	0.67
1:C:29:TYR:HE2	1:C:89:PRO:CD	2.07	0.67
1:A:258:SER:O	1:A:259:PHE:C	2.32	0.67
1:A:56:THR:O	1:A:61:GLY:HA2	1.95	0.67
1:A:181:THR:HA	1:A:184:MET:HE3	1.77	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:17:HIS:CD2	1:A:313:LYS:HD3	2.31	0.66
1:A:98:PHE:CE2	1:A:243:GLY:C	2.69	0.66
1:C:78:TYR:CE1	1:C:79:ARG:HD2	2.29	0.66
1:C:103:MET:CE	1:C:107:GLU:OE1	2.44	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ALA:CB	1:A:358:LEU:HD13	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
1:C:112:ARG:CZ	1:C:358:LEU:HD21	2.26	0.64
1:A:136:CYS:O	1:A:137:SER:C	2.35	0.64
1:A:15:PRO:HG2	1:A:18:VAL:HG23	1.80	0.64
1:A:177:LEU:HD13	1:A:246:LEU:HD12	1.79	0.64
1:C:103:MET:HE2	1:C:107:GLU:OE1	1.98	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:191:MET:HE2	1:A:196:ALA:N	2.14	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
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:14:LEU:O	1:A:15:PRO:C	2.36	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:A:20:GLU:CD	1:C:165:LEU:CB	2.68	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: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:A:118:VAL:HG12	1:A:222:ILE:HD12	1.82	0.61
1:A:377:ARG:C	1:A:379:PRO:HD3	2.21	0.61
1:A:253:VAL:O	1:A:253:VAL:CG1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:CYS:O	1:C:246:LEU:HD23	2.01	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:181:THR:HA	1:C:184:MET:HE3	1.82	0.61
1:C:341:SER:C	1:C:342:ARG:O	2.35	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:267:SER:O	1:C:268:PRO:C	2.37	0.60
1:C:290:ARG:NH2	1:C:337:HIS:O	2.34	0.60
1:A:205:ILE:CG2	1:A:205:ILE:C	2.69	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
1:A:209:GLU:C	1:A:213:GLN:HE21	2.05	0.60
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:C:111:PHE:O	1:C:112:ARG:C	2.28	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:268:PRO:O	1:C:269:GLU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:395:ILE:H	1:C:395:ILE:CD1	2.16	0.58
1:A:277:ARG:N	1:A:278:PRO:HD2	2.18	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:99:ILE:HG12	1:A:103:MET:HE3	1.85	0.58
1:A:220:ILE:O	1:A:220:ILE:CG2	2.52	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: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
1:C:290:ARG:CZ	1:C:335:PRO:O	2.52	0.57
1:A:181:THR:HA	1:A:184:MET:HE1	1.86	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:A:184:MET:HB3	1:A:193:PHE:HE1	1.70	0.57
1:C:193:PHE:CD2	1:C:193:PHE:C	2.78	0.57
1:C:205:ILE:H	1:C:206:PRO:HD3	1.67	0.57
1:C:373:GLU:CB	1:C:373:GLU:CD	2.70	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:A:341:SER:O	1:A:342:ARG:C	2.40	0.56
1:A:378:ILE:O	1:A:381:PHE:HD1	1.88	0.56
1:C:63:TRP:C	1:C:64:ILE:HD12	2.26	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: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:256:PHE:HZ	1:A:288:LEU:C	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:174:ILE:O	1:C:175:PRO:C	2.41	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:A:205:ILE:CG2	1:A:205:ILE:CA	2.76	0.56
1:C:377:ARG:C	1:C:378:ILE:HD12	2.25	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:C:29:TYR:CE2	1:C:89:PRO:HD3	2.40	0.55
1:A:24:PHE:O	1:A:56:THR:HB	2.06	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: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:191:MET:HE2	1:C:196:ALA:HA	1.88	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: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: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:277:ARG:HB3	1:C:280:ARG:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:O	1:A:363:ALA:C	2.46	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:244:ALA:O	1:A:245:LEU:C	2.46	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: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: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
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:A:366:GLU:C	1:A:367:ILE:CA	2.64	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:103:MET:HE1	1:A:107:GLU:CD	2.30	0.52
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:C:106:PRO:O	1:C:107:GLU:C	2.47	0.52
1:C:115:ALA:HB2	1:C:241:MET:HE1	1.92	0.52
1:A:266:LYS:O	1:A:267:SER:HB2	2.08	0.52
1:C:204:LEU:C	1:C:208:ILE:HD13	2.29	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:253:VAL:HG23	2:C:415:HEC:HMC3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:191:MET:HE2	1:C:196:ALA:CA	2.40	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:276:GLU:C	1:A:278:PRO:HD2	2.31	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:218:ASP:O	1:A:219:ALA:C	2.48	0.51
1:A:276:GLU:O	1:A:277:ARG:CG	2.59	0.50
1:C:40:GLU:CG	1:C:336:MET:HE2	2.30	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:276:GLU:C	1:A:277:ARG:CG	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:112:ARG:O	1:C:113:ALA:C	2.49	0.50
1:A:96:TYR:CZ	1:A:101:THR:OG1	2.64	0.50
1:C:10:ASN:C	1:C:11:LEU:HD12	2.32	0.50
1:C:137:SER:O	1:C:139:ILE:N	2.45	0.50
1:C:191:MET:HE2	1:C:196:ALA:N	2.26	0.50
1:A:88:ILE:HD12	1:A:88:ILE:H	1.77	0.50
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: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:C:91:GLU:HG2	3:C:472:HOH:O	2.12	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:154:TYR:O	1:A:155:ALA:C	2.47	0.49
1:C:114:LEU:HD23	1:C:233:ILE:HD12	1.94	0.49
1:C:160:ILE:HG22	1:C:160:ILE:O	2.12	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:134:LEU:HD23	1:C:158:PHE:HA	1.94	0.49
2:A:415:HEC:HMB1	2:A:415:HEC:HBB3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:362:LEU:HD23	2:A:415:HEC:HMC1	1.94	0.48
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:19:PRO:C	1:A:21:HIS:N	2.66	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: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:A:195:GLU:OE1	1:A:195:GLU:CA	2.60	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:91:GLU:CD	1:C:91:GLU:N	2.59	0.48
1:C:99:ILE:HG23	1:C:100:PRO:CD	2.43	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: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:191:MET:HE2	1:A:196:ALA:CA	2.44	0.47
1:C:290:ARG:O	1:C:290:ARG:HG2	1.98	0.47
1:A:20:GLU:CD	1:C:165:LEU:CD1	2.83	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:HG12	1:A:338:VAL:O	2.13	0.47
1:C:234:THR:OG1	1:C:237:GLU:HG3	2.14	0.47
1:A:267:SER:O	1:A:268:PRO:C	2.53	0.47
1:A:167:ALA:HB1	1:A:220:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:364:ARG:O	1:A:365:ARG:C	2.53	0.47
1:C:80:HIS:CD2	1:C:305:TYR:CG	3.03	0.47
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:C:100:PRO:O	1:C:355:HIS:CE1	2.68	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: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:164:MET:HE1	1:A:169:LEU:HB3	1.97	0.46
1:C:261:MET:HB2	1:C:261:MET:HE3	1.58	0.46
1:A:363:ALA:CB	2:A:415:HEC:HBB2	2.43	0.46
1:C:391:HIS:N	1:C:391:HIS:HD2	2.11	0.46
1:A:334:ALA:O	1:A:335:PRO:C	2.53	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:266:LYS:O	1:A:267:SER:CB	2.63	0.46
1:A:272:GLN:HE21	1:A:272:GLN:C	2.18	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:42:TRP:C	1:C:44:VAL:N	2.68	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:19:PRO:C	1:A:21:HIS:H	2.18	0.46
1:C:186:ARG:O	1:C:187:PRO:C	2.51	0.46
1:A:82:SER:HB2	1:A:104:ASP:OD2	2.16	0.46
1:A:257:LEU:CA	1:A:258:SER:N	2.64	0.46
1:C:88:ILE:C	1:C:89:PRO:O	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LEU:N	1:C:301:LEU:HD23	2.31	0.45
1:A:98:PHE:CD2	1:A:243:GLY:C	2.90	0.45
1:A:207:ILE:O	1:A:208:ILE:C	2.50	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
1:A:373:GLU:HB3	1:A:377:ARG:HH12	1.80	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:39:GLN:N	1:A:39:GLN:CD	2.67	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: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:10:ASN:C	1:C:10:ASN:OD1	2.55	0.45
1:C:18:VAL:HA	1:C:19:PRO:HD3	1.57	0.45
1:C:249:GLY:C	1:C:250:LEU:HD12	2.37	0.45
1:C:134:LEU:HD12	1:C:138:LEU:CD1	2.47	0.45
1:C:143:ARG:O	1:C:144:PRO:C	2.51	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:311:GLN:CD	3:C:505:HOH:O	2.55	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:A:20:GLU:OE2	1:C:165:LEU:CB	2.65	0.44
1:C:134:LEU:O	1:C:134:LEU:HG	2.17	0.44
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:43:ALA:C	1:C:45:LEU:N	2.68	0.44
1:C:137:SER:O	1:C:138:LEU:C	2.55	0.44
1:A:71:ILE:HG21	1:A:325:SER:HG	1.81	0.44
1:A:164:MET:CE	1:A:169:LEU:HB3	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:98:PHE:CD1	1:C:98:PHE:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:99:ILE:HG12	1:A:103:MET:CE	2.48	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: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
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:171:GLU:C	1:A:173:ASP:H	2.21	0.44
1:A:191:MET:HE2	1:A:196:ALA:HA	1.96	0.44
1:A:354:SER:OG	1:A:355:HIS:CD2	2.71	0.44
1:C:243:GLY:O	1:C:244:ALA:C	2.49	0.44
1:C:378:ILE:N	1:C:379:PRO:HD3	2.32	0.44
1:A:149:ASN:C	1:A:149:ASN:HD22	2.22	0.43
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: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: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:A:107:GLU:O	1:A:108:GLN:C	2.54	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:C:395:ILE:C	1:C:396:VAL:HG23	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:298:GLY:C	1:A:299:ARG:HD3	2.35	0.43
1:A:389:ILE:CG2	1:A:389:ILE:C	2.87	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:A:228:VAL:C	1:A:230:GLY:H	2.22	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:A:138:LEU:HD23	1:A:154:TYR:HD2	1.78	0.42
1:A:186:ARG:O	1:A:187:PRO:C	2.55	0.42
1:C:81:PHE:HB3	1:C:299:ARG:HG3	2.01	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:58:CYS:O	1:C:59:ASN:C	2.57	0.42
1:C:125:ASP:O	1:C:126:LYS:C	2.52	0.42
1:C:163:PHE:CG	1:C:249:GLY:HA3	2.55	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: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:254:VAL:CG1	1:C:254:VAL:O	2.68	0.42
1:C:324:LEU:O	1:C:325:SER:C	2.55	0.42
1:C:356:LEU:HG	1:C:357:CYS:H	1.81	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:A:56:THR:OG1	1:A:58:CYS:HB2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:CD	1:A:143:ARG:HE	2.23	0.41
1:A:171:GLU:C	1:A:173:ASP:N	2.72	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:C:131:ILE:CG2	1:C:158:PHE:CZ	3.03	0.41
1:C:166:LEU:C	1:C:166:LEU:CD1	2.80	0.41
1:C:181:THR:HA	1:C:184:MET:CE	2.48	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
1:C:109:ARG:O	1:C:110:GLN:C	2.58	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: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: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:150:PHE:HB3	1:A:402:LEU:HB3	2.02	0.41
1:C:99:ILE:HG21	1:C:241:MET:HE3	2.02	0.41
1:C:131:ILE:CG2	1:C:131:ILE:C	2.89	0.41
1:C:369:VAL:CA	1:C:369:VAL:CG1	2.83	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: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: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:270:HIS:O	1:A:271:ARG:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:415:HEC:HHB	2:C:415:HEC:HMA1	1.86	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/414 (97%)	345 (86%)	38 (9%)	20 (5%)	2	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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	347/356 (98%)	309 (89%)	38 (11%)	6 3
1	C	347/356 (98%)	303 (87%)	44 (13%)	4 1
All	All	694/712 (98%)	612 (88%)	82 (12%)	5 2

All (82) 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	70	LEU
1	A	82	SER
1	A	83	SER
1	A	88	ILE
1	A	99	ILE
1	A	101	THR

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Mol	Chain	Res	Type
1	A	105	PRO
1	A	108	GLN
1	A	109	ARG
1	A	118	VAL
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	223	VAL
1	A	231	ARG
1	A	232	PRO
1	A	233	ILE
1	A	261	MET
1	A	268	PRO
1	A	269	GLU
1	A	291	ARG
1	A	313	LYS
1	A	335	PRO
1	A	342	ARG
1	A	344	LYS
1	A	365	ARG
1	A	380	ASP
1	A	382	SER
1	A	388	GLN
1	A	392	LYS
1	A	412	LYS
1	C	16	PRO
1	C	39	GLN
1	C	49	ASN
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	121	MET
1	C	126	LYS
1	C	133	GLU
1	C	138	LEU
1	C	140	GLU

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Mol	Chain	Res	Type
1	C	143	ARG
1	C	144	PRO
1	C	147	GLN
1	C	149	ASN
1	C	166	LEU
1	C	182	ASP
1	C	193	PHE
1	C	211	ARG
1	C	212	ARG
1	C	213	GLN
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	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	395	ILE
1	C	405	VAL
1	C	410	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	33	ASN
1	A	39	GLN
1	A	46	GLN
1	A	108	GLN
1	A	110	GLN
1	A	149	ASN
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	272	GLN
1	A	317	GLN
1	A	343	GLN
1	A	355	HIS
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	149	ASN
1	C	272	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 monosaccharides 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	32,50,50	3.89	19 (59%)	24,82,82	4.24	12 (50%)
2	HEC	A	415	3,1	32,50,50	3.46	16 (50%)	24,82,82	3.00	10 (41%)

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	-	2/10/54/54	-
2	HEC	A	415	3,1	-	6/10/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	415	HEC	C2B-C3B	-12.78	1.27	1.40
2	A	415	HEC	C2B-C3B	-11.37	1.28	1.40
2	C	415	HEC	CMD-C2D	8.01	1.68	1.51
2	A	415	HEC	CAD-C3D	6.81	1.62	1.52
2	A	415	HEC	CAA-C2A	5.69	1.62	1.52
2	C	415	HEC	CAD-C3D	5.68	1.60	1.52
2	C	415	HEC	C4D-CHA	-5.47	1.25	1.41
2	C	415	HEC	C3D-C2D	5.03	1.52	1.37
2	A	415	HEC	CBB-CAB	-4.68	1.31	1.49
2	C	415	HEC	CBC-CAC	-4.37	1.33	1.49
2	A	415	HEC	C4B-C3B	4.28	1.50	1.43
2	C	415	HEC	C1D-CHD	-4.25	1.29	1.41
2	C	415	HEC	CMC-C2C	4.24	1.61	1.51
2	C	415	HEC	C1B-CHB	-4.09	1.29	1.41
2	A	415	HEC	C3D-C2D	4.06	1.49	1.37
2	C	415	HEC	CBB-CAB	-3.81	1.35	1.49
2	A	415	HEC	O1A-CGA	-3.70	1.09	1.22
2	A	415	HEC	CMD-C2D	3.67	1.59	1.51
2	A	415	HEC	CBC-CAC	-3.64	1.35	1.49
2	C	415	HEC	C1B-NB	-3.59	1.28	1.36
2	A	415	HEC	C3C-C2C	-3.50	1.37	1.40
2	C	415	HEC	C1D-ND	-3.24	1.29	1.36
2	C	415	HEC	CMB-C2B	3.09	1.58	1.51
2	A	415	HEC	C1D-CHD	-2.99	1.32	1.41
2	A	415	HEC	C2A-C1A	2.93	1.49	1.42
2	A	415	HEC	O2D-CGD	-2.91	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEC	C1C-NC	2.78	1.41	1.36
2	C	415	HEC	CBD-CGD	2.62	1.56	1.50
2	A	415	HEC	CBD-CGD	2.51	1.56	1.50
2	C	415	HEC	C3C-C4C	2.43	1.47	1.43
2	C	415	HEC	C4D-ND	2.38	1.41	1.36
2	C	415	HEC	O2A-CGA	-2.29	1.23	1.30
2	C	415	HEC	C1C-CHC	-2.21	1.34	1.41
2	A	415	HEC	CMC-C2C	2.20	1.56	1.51
2	C	415	HEC	C1C-NC	-2.04	1.32	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	415	HEC	CMB-C2B-C3B	-11.70	112.06	125.82
2	C	415	HEC	CMB-C2B-C1B	9.76	143.47	128.46
2	C	415	HEC	CMC-C2C-C3C	6.67	133.66	125.82
2	A	415	HEC	CMC-C2C-C3C	6.06	132.95	125.82
2	A	415	HEC	O2A-CGA-CBA	5.87	132.88	114.03
2	C	415	HEC	C4C-C3C-C2C	5.86	112.68	106.35
2	C	415	HEC	O2D-CGD-O1D	-5.72	109.05	123.30
2	A	415	HEC	O1A-CGA-CBA	-5.28	106.11	123.08
2	C	415	HEC	O2D-CGD-CBD	4.95	129.94	114.03
2	A	415	HEC	CMA-C3A-C2A	4.85	134.09	124.94
2	A	415	HEC	CMB-C2B-C3B	-4.55	120.47	125.82
2	A	415	HEC	CMC-C2C-C1C	-4.14	122.10	128.46
2	A	415	HEC	C3B-C4B-NB	-4.06	103.28	110.94
2	C	415	HEC	CAA-C2A-C3A	-3.80	116.32	127.25
2	C	415	HEC	CAD-C3D-C2D	3.11	136.19	127.25
2	A	415	HEC	O2D-CGD-O1D	-3.02	115.78	123.30
2	A	415	HEC	C2B-C3B-C4B	2.92	109.50	106.35
2	C	415	HEC	O2A-CGA-O1A	-2.78	116.36	123.30
2	C	415	HEC	C3B-C4B-NB	2.69	116.02	110.94
2	C	415	HEC	C3C-C4C-NC	-2.66	105.93	110.94
2	C	415	HEC	CBA-CAA-C2A	-2.53	108.33	112.60
2	A	415	HEC	CMD-C2D-C3D	-2.12	120.95	124.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	415	HEC	C1A-C2A-CAA-CBA
2	A	415	HEC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	C	415	HEC	C1A-C2A-CAA-CBA
2	C	415	HEC	C3A-C2A-CAA-CBA
2	A	415	HEC	CAA-CBA-CGA-O1A
2	A	415	HEC	CAA-CBA-CGA-O2A
2	A	415	HEC	CAD-CBD-CGD-O2D
2	A	415	HEC	CAD-CBD-CGD-O1D

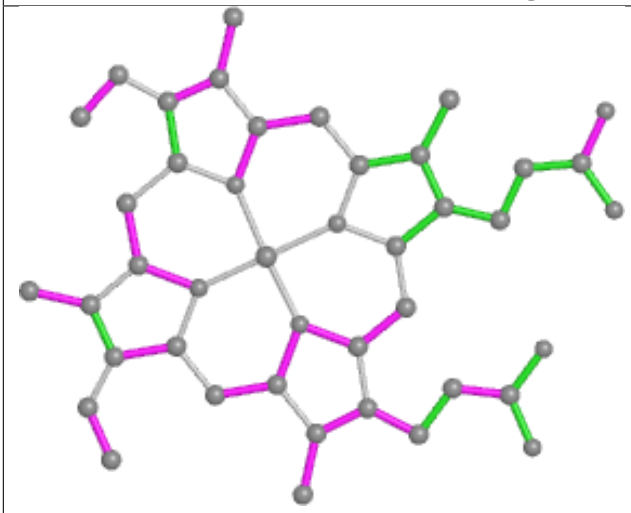
There are no ring outliers.

2 monomers are involved in 28 short contacts:

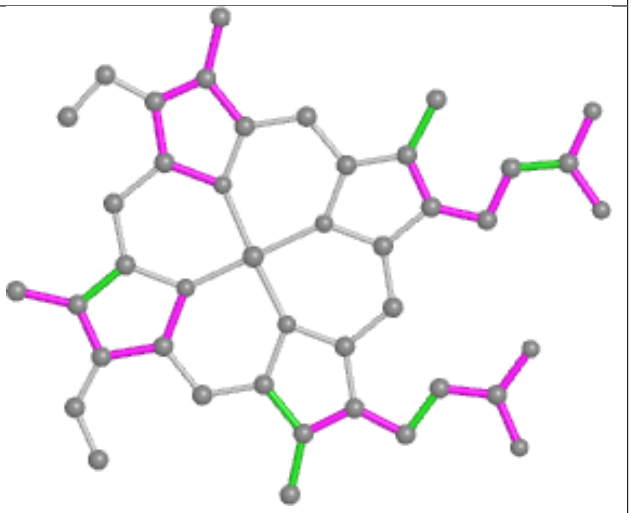
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	415	HEC	9	0
2	A	415	HEC	19	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

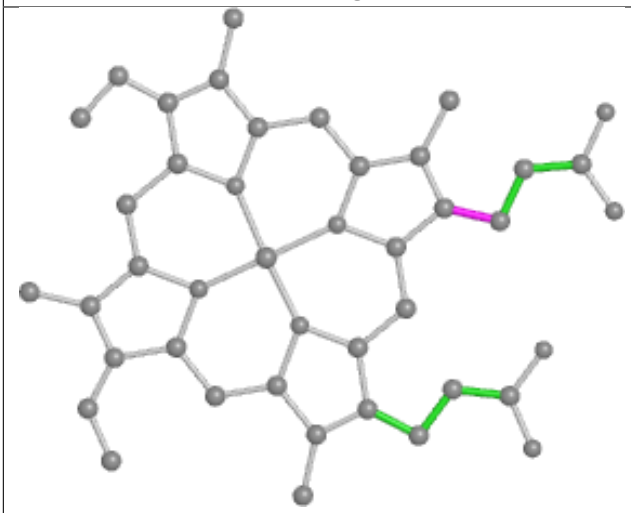
Ligand HEC C 415



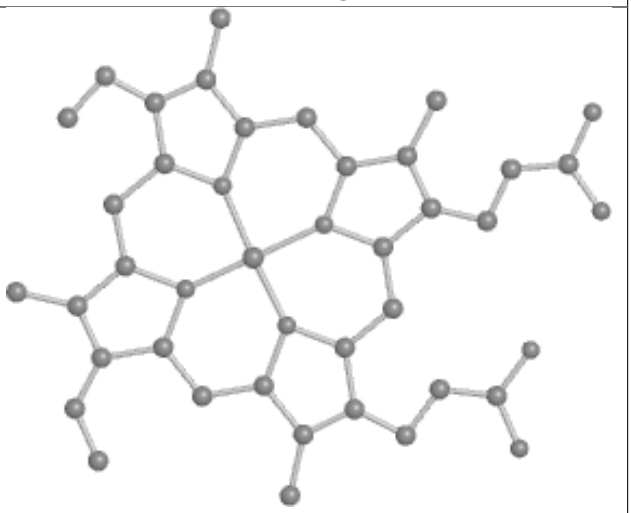
Bond lengths



Bond angles

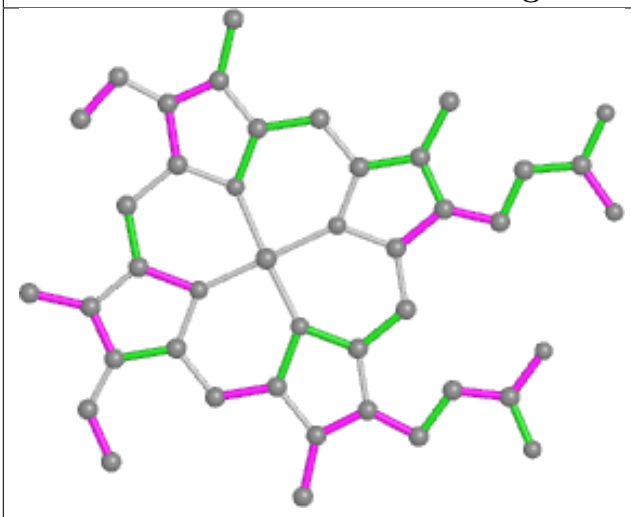


Torsions

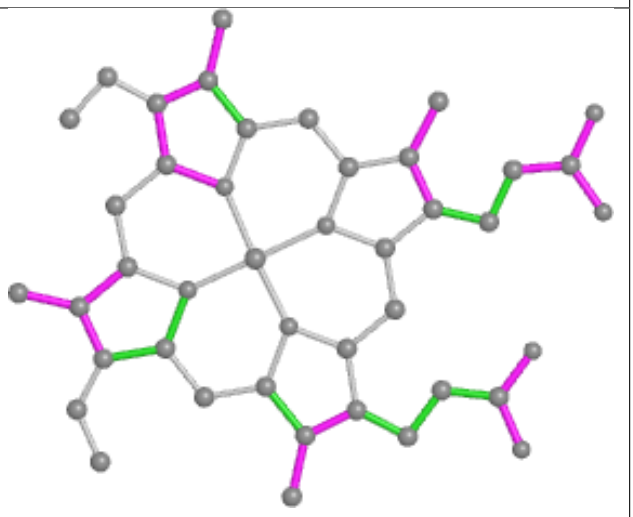


Rings

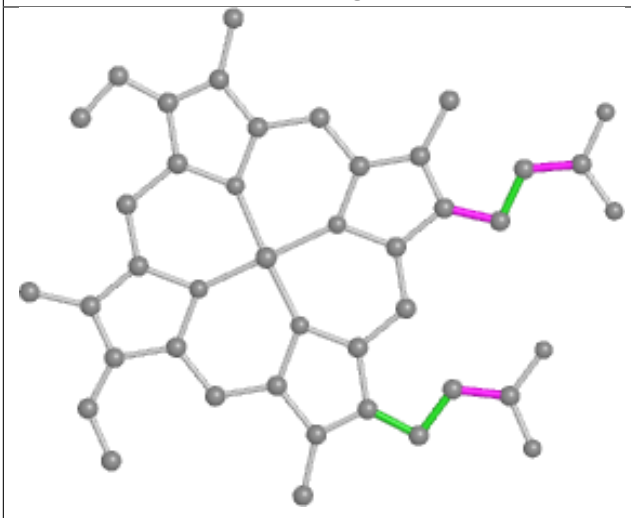
Ligand HEC A 415



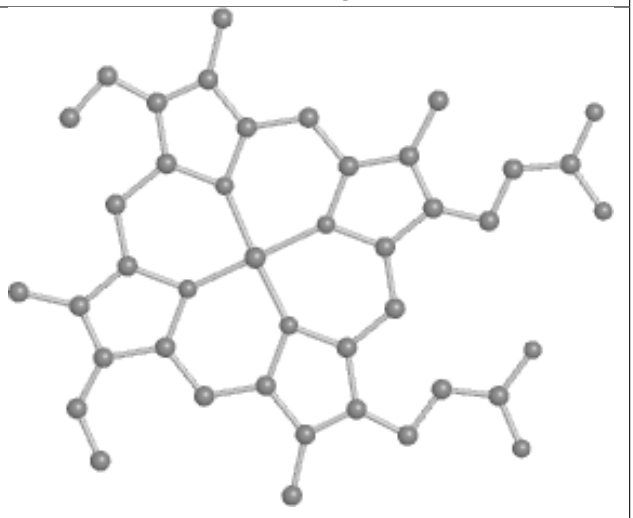
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.77	30 (7%)	14	20	8, 24, 36, 49	0
1	C	405/414 (97%)	0.73	23 (5%)	23	32	11, 24, 34, 44	0
All	All	810/828 (97%)	0.75	53 (6%)	18	25	8, 24, 36, 49	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	7.6
1	A	214	LYS	6.0
1	C	246	LEU	5.9
1	C	229	ASN	5.8
1	C	19	PRO	4.4
1	A	229	ASN	4.3
1	A	246	LEU	4.1
1	A	230	GLY	4.1
1	A	389	ILE	4.1
1	C	414	VAL	3.8
1	A	215	PRO	3.7
1	A	278	PRO	3.5
1	A	121	MET	3.4
1	A	213	GLN	3.3
1	A	228	VAL	3.2
1	C	121	MET	3.2
1	A	19	PRO	3.2
1	C	214	LYS	3.2
1	C	220	ILE	3.2
1	A	10	ASN	3.1
1	A	264	LEU	3.0
1	A	383	ILE	2.9
1	A	313	LYS	2.9
1	A	88	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	2.9
1	C	10	ASN	2.7
1	C	122	PRO	2.6
1	A	343	GLN	2.6
1	C	230	GLY	2.6
1	C	274	LEU	2.5
1	A	165	LEU	2.4
1	C	133	GLU	2.4
1	A	18	VAL	2.4
1	A	101	THR	2.3
1	A	205	ILE	2.3
1	C	395	ILE	2.3
1	A	200	LEU	2.3
1	C	213	GLN	2.3
1	C	234	THR	2.2
1	A	109	ARG	2.2
1	A	350	PHE	2.2
1	A	244	ALA	2.2
1	A	386	GLY	2.2
1	C	215	PRO	2.2
1	C	278	PRO	2.2
1	A	250	LEU	2.1
1	C	227	GLN	2.1
1	C	383	ILE	2.1
1	C	208	ILE	2.1
1	C	257	LEU	2.1
1	C	333	ALA	2.1
1	A	202	ASP	2.0
1	C	235	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

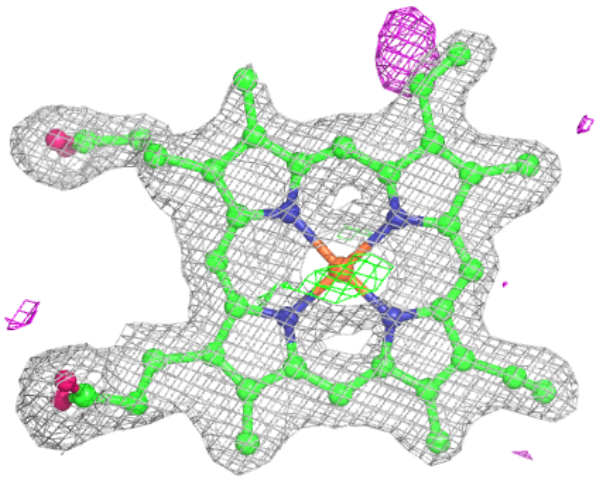
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

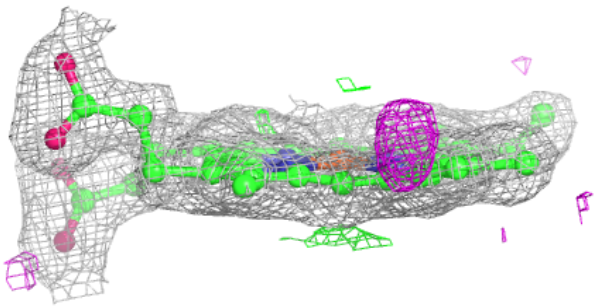
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	A	415	43/43	0.94	0.16	13,15,17,18	0
2	HEC	C	415	43/43	0.94	0.14	13,18,20,21	0

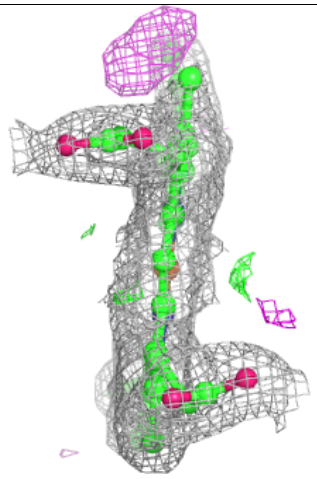
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

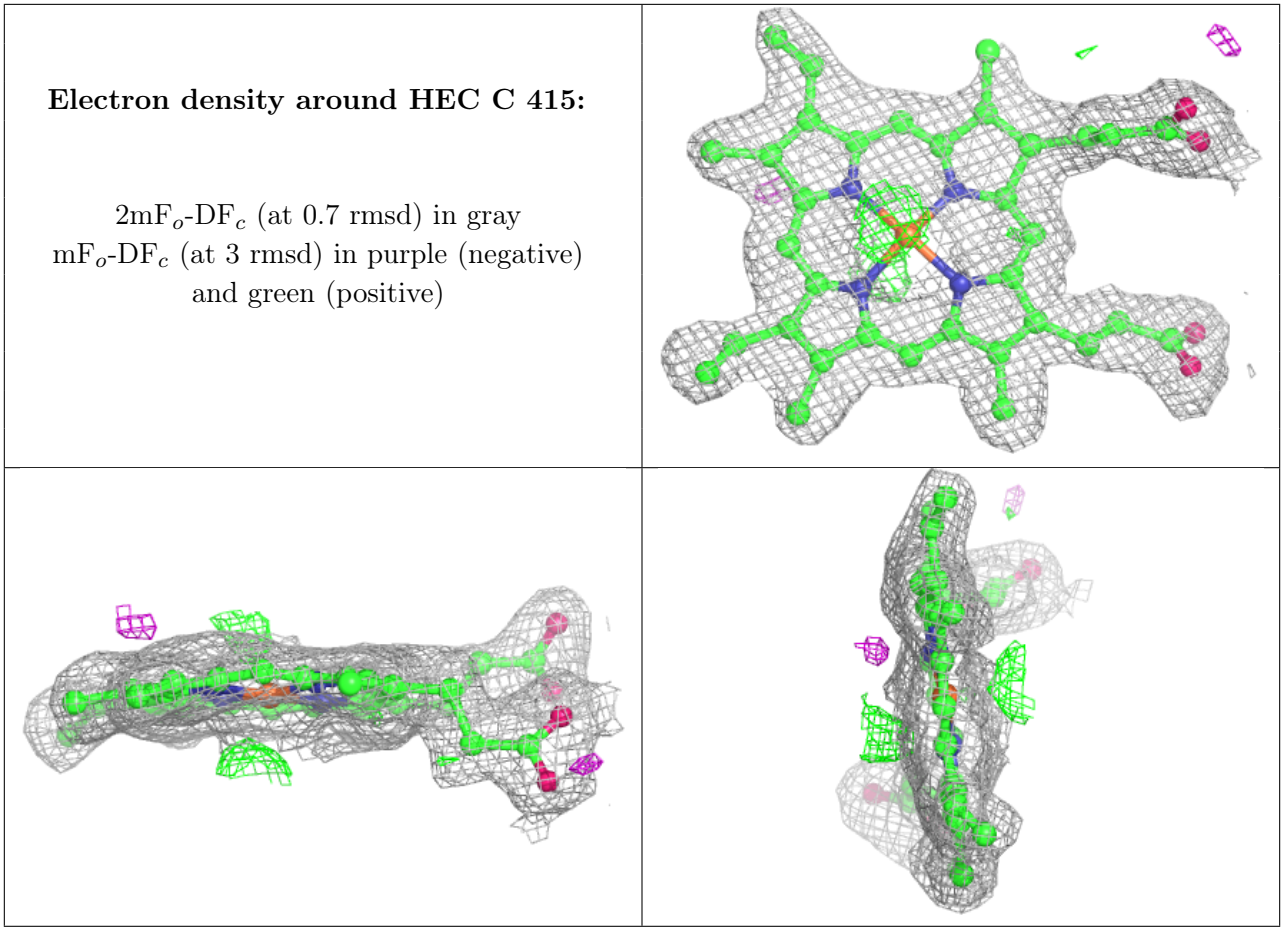






Electron density around HEC C 415:

$2mF_o$-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

There are no such residues in this entry.