Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 03:28 AM EDT

PDB ID	:	1MZZ
Title	:	Crystal Structure of Mutant (M182T)of Nitrite Reductase
Authors	:	Guo, H.; Olesen, K.; Xue, Y.; Shapliegh, J.; Sjolin, L.
Deposited on	:	2002-10-10
Resolution	:	2.00 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 (i) symbol.

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

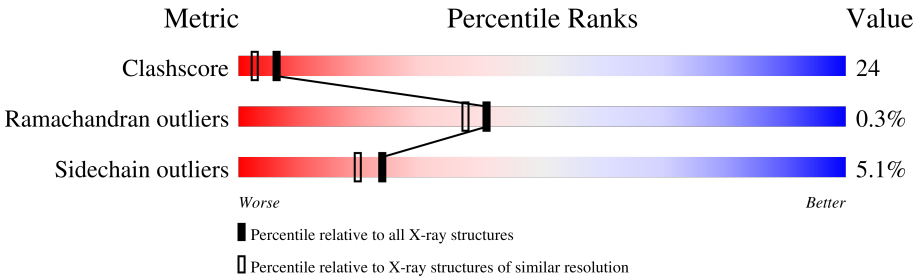
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	334	32% 49% 16% .
1	B	334	34% 48% 15% .
1	C	334	35% 44% 18% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8561 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			
1	B	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			
1	C	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	MET	engineered mutation	UNP Q53239
A	230	ASP	THR	conflict	UNP Q53239
A	281	ASN	LYS	conflict	UNP Q53239
A	351	HIS	SER	conflict	UNP Q53239
A	367	VAL	TRP	conflict	UNP Q53239
A	368	ALA	PRO	conflict	UNP Q53239
A	372	LEU	-	cloning artifact	UNP Q53239
B	1182	THR	MET	engineered mutation	UNP Q53239
B	1230	ASP	THR	conflict	UNP Q53239
B	1281	ASN	LYS	conflict	UNP Q53239
B	1351	HIS	SER	conflict	UNP Q53239
B	1367	VAL	TRP	conflict	UNP Q53239
B	1368	ALA	PRO	conflict	UNP Q53239
B	1372	LEU	-	cloning artifact	UNP Q53239
C	2182	THR	MET	engineered mutation	UNP Q53239
C	2230	ASP	THR	conflict	UNP Q53239
C	2281	ASN	LYS	conflict	UNP Q53239
C	2351	HIS	SER	conflict	UNP Q53239
C	2367	VAL	TRP	conflict	UNP Q53239
C	2368	ALA	PRO	conflict	UNP Q53239
C	2372	LEU	-	cloning artifact	UNP Q53239

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	289	Total O 289 289	0	0
3	B	276	Total O 276 276	0	0
3	C	289	Total O 289 289	0	0

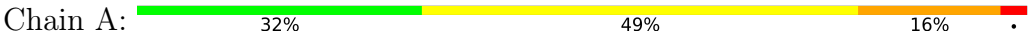
3 Residue-property plots (i)

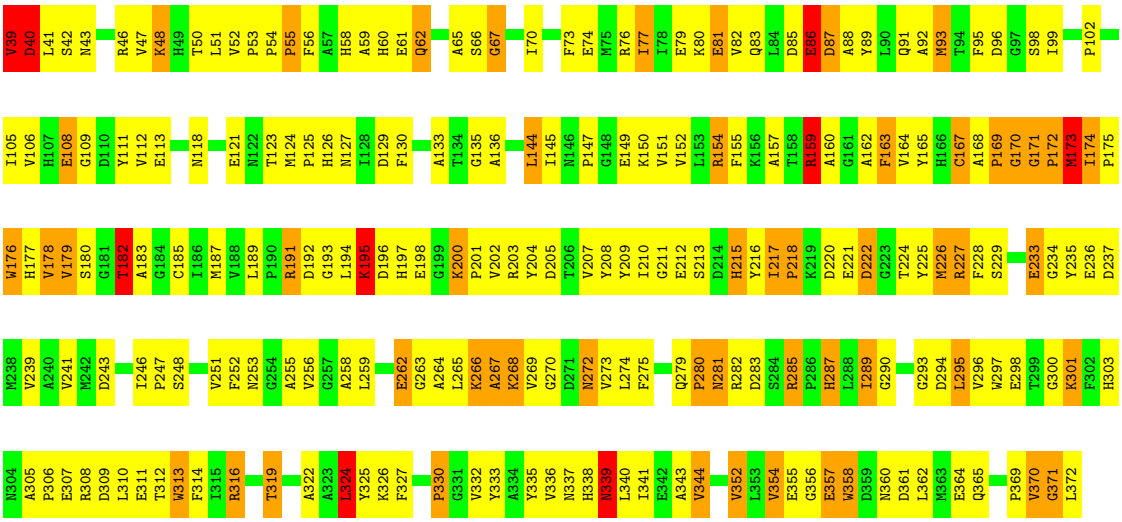
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Copper-containing nitrite reductase

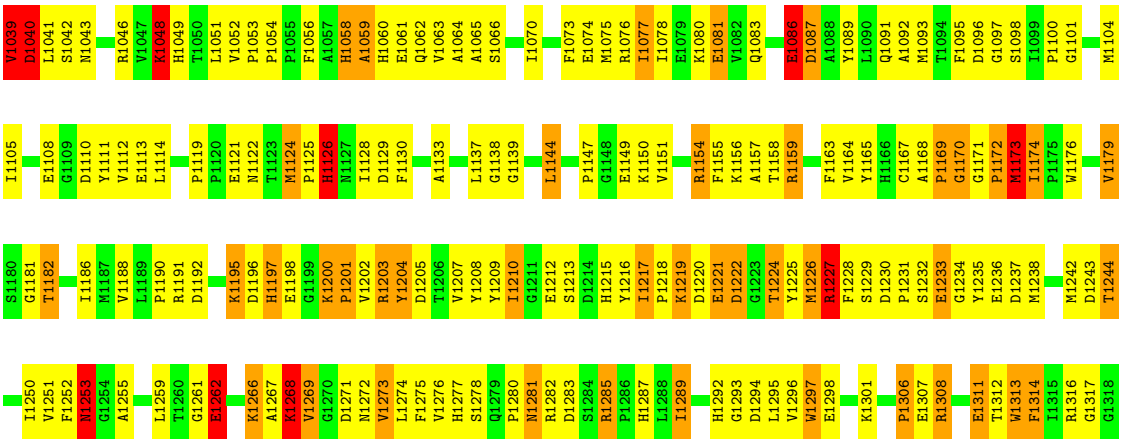
Chain A:

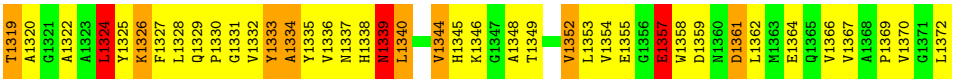




• Molecule 1: Copper-containing nitrite reductase

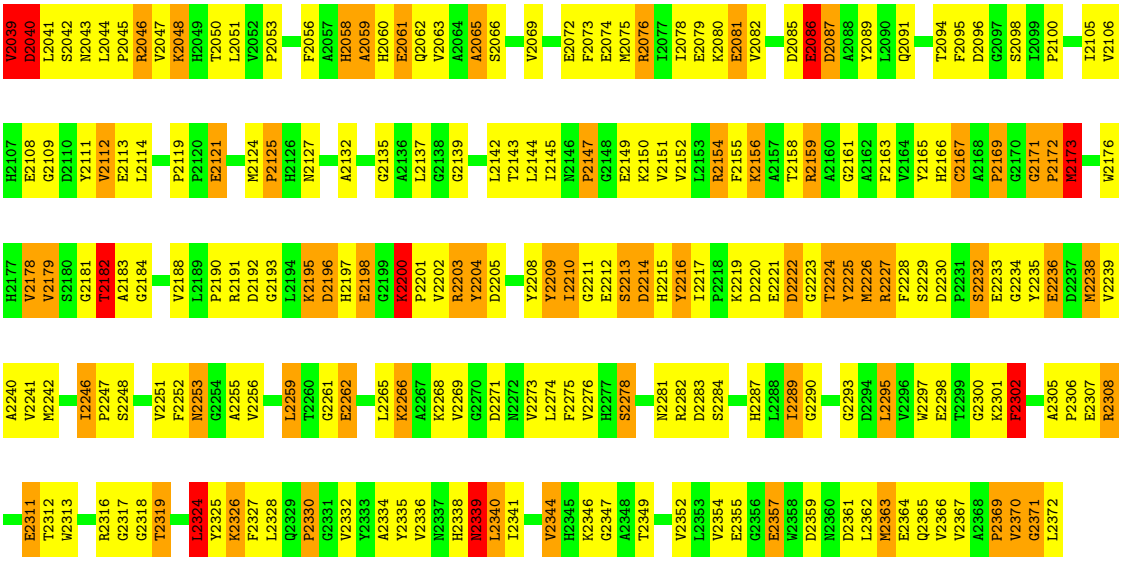
Chain B:





• Molecule 1: Copper-containing nitrite reductase

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.50Å 123.73Å 130.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	91.4 (30.00-2.00)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.170 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8561	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

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: CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	3.64	298/2640 (11.3%)	2.69	149/3599 (4.1%)
1	B	3.59	304/2640 (11.5%)	2.51	157/3599 (4.4%)
1	C	3.67	267/2640 (10.1%)	2.53	155/3599 (4.3%)
All	All	3.63	869/7920 (11.0%)	2.58	461/10797 (4.3%)

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	5
1	B	0	8
1	C	0	7
All	All	0	20

All (869) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ARG	CZ-NH1	44.61	1.91	1.33
1	C	2121	GLU	CD-OE2	30.47	1.59	1.25
1	C	2262	GLU	CD-OE2	28.84	1.57	1.25
1	A	86	GLU	CD-OE1	27.63	1.56	1.25
1	C	2262	GLU	CG-CD	27.51	1.93	1.51
1	C	2232	SER	CB-OG	27.07	1.77	1.42
1	B	1262	GLU	CD-OE2	25.95	1.54	1.25
1	A	86	GLU	CD-OE2	25.87	1.54	1.25
1	C	2086	GLU	CD-OE1	24.77	1.52	1.25
1	C	2061	GLU	CD-OE2	24.50	1.52	1.25
1	C	2061	GLU	CD-OE1	23.33	1.51	1.25
1	B	1086	GLU	CD-OE1	23.17	1.51	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1262	GLU	CG-CD	23.00	1.86	1.51
1	C	2355	GLU	CD-OE2	22.73	1.50	1.25
1	B	1061	GLU	CD-OE1	22.13	1.50	1.25
1	C	2086	GLU	CG-CD	22.12	1.85	1.51
1	B	1121	GLU	CD-OE2	21.62	1.49	1.25
1	C	2355	GLU	CD-OE1	20.70	1.48	1.25
1	B	1061	GLU	CD-OE2	20.44	1.48	1.25
1	C	2167	CYS	CB-SG	-20.42	1.47	1.82
1	B	1355	GLU	CD-OE1	20.35	1.48	1.25
1	B	1086	GLU	CD-OE2	19.69	1.47	1.25
1	A	357	GLU	CD-OE2	19.68	1.47	1.25
1	A	221	GLU	CD-OE1	19.42	1.47	1.25
1	A	86	GLU	CG-CD	19.12	1.80	1.51
1	A	233	GLU	CG-CD	18.65	1.79	1.51
1	B	1262	GLU	CD-OE1	18.64	1.46	1.25
1	C	2266	LYS	CE-NZ	18.47	1.95	1.49
1	C	2203	ARG	CZ-NH2	18.34	1.56	1.33
1	B	1355	GLU	CD-OE2	18.19	1.45	1.25
1	A	357	GLU	CD-OE1	18.06	1.45	1.25
1	A	262	GLU	CD-OE2	17.92	1.45	1.25
1	A	319	THR	CB-CG2	-17.75	0.93	1.52
1	C	2076	ARG	CZ-NH2	17.61	1.55	1.33
1	B	1221	GLU	CD-OE2	17.31	1.44	1.25
1	C	2065	ALA	CA-CB	16.63	1.87	1.52
1	B	1221	GLU	CG-CD	16.49	1.76	1.51
1	A	262	GLU	CG-CD	16.16	1.76	1.51
1	B	1357	GLU	CG-CD	16.16	1.76	1.51
1	B	1087	ASP	CB-CG	16.05	1.85	1.51
1	C	2121	GLU	CB-CG	-15.86	1.22	1.52
1	A	176	TRP	CZ3-CH2	15.82	1.65	1.40
1	C	2076	ARG	CZ-NH1	15.50	1.53	1.33
1	A	355	GLU	CD-OE1	15.48	1.42	1.25
1	C	2203	ARG	CZ-NH1	15.44	1.53	1.33
1	C	2048	LYS	CD-CE	15.10	1.89	1.51
1	C	2236	GLU	CG-CD	15.07	1.74	1.51
1	A	191	ARG	NE-CZ	14.90	1.52	1.33
1	A	200	LYS	CB-CG	-14.86	1.12	1.52
1	A	221	GLU	CD-OE2	14.82	1.42	1.25
1	C	2086	GLU	CD-OE2	14.60	1.41	1.25
1	A	154	ARG	CD-NE	-14.24	1.22	1.46
1	B	1269	VAL	CB-CG2	14.23	1.82	1.52
1	B	1200	LYS	CD-CE	14.21	1.86	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2121	GLU	CG-CD	14.16	1.73	1.51
1	C	2154	ARG	NE-CZ	14.10	1.51	1.33
1	C	2236	GLU	CD-OE2	14.06	1.41	1.25
1	A	235	TYR	CD2-CE2	13.92	1.60	1.39
1	C	2208	TYR	CE2-CZ	13.91	1.56	1.38
1	C	2198	GLU	CD-OE2	13.91	1.41	1.25
1	B	1086	GLU	CG-CD	13.88	1.72	1.51
1	A	209	TYR	CE2-CZ	13.64	1.56	1.38
1	A	87	ASP	CB-CG	13.61	1.80	1.51
1	B	1266	LYS	CE-NZ	13.55	1.82	1.49
1	C	2066	SER	CB-OG	13.54	1.59	1.42
1	A	229	SER	CB-OG	13.54	1.59	1.42
1	B	1208	TYR	CE2-CZ	13.45	1.56	1.38
1	B	1040	ASP	C-O	13.44	1.48	1.23
1	A	48	LYS	CD-CE	13.43	1.84	1.51
1	B	1355	GLU	CG-CD	13.26	1.71	1.51
1	B	1170	GLY	C-O	13.24	1.44	1.23
1	A	195	LYS	CE-NZ	13.22	1.82	1.49
1	C	2221	GLU	CG-CD	13.16	1.71	1.51
1	B	1113	GLU	CB-CG	-13.15	1.27	1.52
1	A	200	LYS	CE-NZ	13.04	1.81	1.49
1	C	2098	SER	CB-OG	12.96	1.59	1.42
1	B	1039	VAL	CA-CB	12.94	1.81	1.54
1	C	2213	SER	CB-OG	12.87	1.58	1.42
1	A	227	ARG	CD-NE	-12.70	1.24	1.46
1	B	1221	GLU	CD-OE1	12.70	1.39	1.25
1	C	2262	GLU	CD-OE1	12.59	1.39	1.25
1	A	76	ARG	CZ-NH2	12.46	1.49	1.33
1	B	1061	GLU	CG-CD	12.46	1.70	1.51
1	B	1236	GLU	CD-OE1	12.40	1.39	1.25
1	C	2357	GLU	CD-OE1	12.37	1.39	1.25
1	B	1113	GLU	CG-CD	12.30	1.70	1.51
1	B	1198	GLU	CD-OE2	12.16	1.39	1.25
1	C	2226	MET	SD-CE	-12.10	1.10	1.77
1	C	2156	LYS	CE-NZ	12.10	1.79	1.49
1	A	111	TYR	CD1-CE1	12.07	1.57	1.39
1	B	1086	GLU	CB-CG	12.07	1.75	1.52
1	A	40	ASP	C-O	12.02	1.46	1.23
1	B	1268	LYS	CD-CE	11.91	1.81	1.51
1	B	1121	GLU	CG-CD	11.90	1.69	1.51
1	B	1357	GLU	CD-OE1	11.90	1.38	1.25
1	B	1167	CYS	CB-SG	-11.88	1.62	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2154	ARG	CZ-NH1	11.87	1.48	1.33
1	B	1191	ARG	CZ-NH2	11.82	1.48	1.33
1	B	1173	MET	CA-CB	11.80	1.79	1.53
1	B	1252	PHE	CE1-CZ	11.78	1.59	1.37
1	B	1191	ARG	CZ-NH1	11.64	1.48	1.33
1	A	221	GLU	CG-CD	11.62	1.69	1.51
1	C	2357	GLU	CD-OE2	11.49	1.38	1.25
1	B	1073	PHE	CD2-CE2	11.41	1.62	1.39
1	A	98	SER	CB-OG	11.39	1.57	1.42
1	B	1195	LYS	CD-CE	11.36	1.79	1.51
1	B	1076	ARG	CZ-NH1	11.35	1.47	1.33
1	A	61	GLU	CD-OE1	11.34	1.38	1.25
1	C	2302	PHE	CE1-CZ	-11.33	1.15	1.37
1	A	76	ARG	CZ-NH1	11.31	1.47	1.33
1	C	2225	TYR	CG-CD2	11.27	1.53	1.39
1	B	1225	TYR	CE2-CZ	11.10	1.52	1.38
1	A	61	GLU	CD-OE2	11.09	1.37	1.25
1	C	2236	GLU	CD-OE1	11.08	1.37	1.25
1	A	266	LYS	CD-CE	11.08	1.78	1.51
1	C	2087	ASP	CB-CG	11.00	1.74	1.51
1	C	2357	GLU	CG-CD	10.99	1.68	1.51
1	A	48	LYS	CG-CD	10.88	1.89	1.52
1	B	1357	GLU	CD-OE2	10.86	1.37	1.25
1	C	2233	GLU	CG-CD	10.83	1.68	1.51
1	A	159	ARG	CB-CG	10.80	1.81	1.52
1	B	1171	GLY	C-O	10.68	1.40	1.23
1	C	2221	GLU	CD-OE2	10.67	1.37	1.25
1	B	1048	LYS	CD-CE	10.66	1.77	1.51
1	A	62	GLN	CG-CD	10.65	1.75	1.51
1	A	178	VAL	CB-CG2	10.57	1.75	1.52
1	C	2087	ASP	CG-OD2	10.56	1.49	1.25
1	C	2039	VAL	CA-CB	10.55	1.76	1.54
1	B	1216	TYR	CD2-CE2	10.54	1.55	1.39
1	A	262	GLU	CB-CG	-10.54	1.32	1.52
1	B	1076	ARG	CZ-NH2	10.50	1.46	1.33
1	A	237	ASP	CB-CG	10.46	1.73	1.51
1	A	86	GLU	CB-CG	10.44	1.72	1.52
1	C	2319	THR	CB-CG2	-10.34	1.18	1.52
1	B	1198	GLU	CD-OE1	10.33	1.37	1.25
1	C	2178	VAL	CB-CG1	10.30	1.74	1.52
1	C	2154	ARG	CD-NE	-10.29	1.28	1.46
1	C	2043	ASN	CG-OD1	10.25	1.46	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	GLU	CD-OE2	10.17	1.36	1.25
1	B	1262	GLU	CB-CG	-10.16	1.32	1.52
1	B	1130	PHE	CD2-CE2	10.12	1.59	1.39
1	C	2325	TYR	CD1-CE1	-10.09	1.24	1.39
1	B	1225	TYR	CG-CD1	10.08	1.52	1.39
1	A	335	TYR	CD2-CE2	10.07	1.54	1.39
1	B	1235	TYR	CD2-CE2	10.07	1.54	1.39
1	A	159	ARG	CZ-NH1	10.03	1.46	1.33
1	A	52	VAL	CB-CG1	10.01	1.73	1.52
1	B	1203	ARG	CB-CG	-10.01	1.25	1.52
1	A	255	ALA	CA-CB	9.95	1.73	1.52
1	C	2056	PHE	CE2-CZ	9.95	1.56	1.37
1	C	2239	VAL	CB-CG1	9.93	1.73	1.52
1	A	333	TYR	CB-CG	-9.93	1.36	1.51
1	B	1203	ARG	CZ-NH1	9.86	1.45	1.33
1	A	262	GLU	CD-OE1	9.86	1.36	1.25
1	A	111	TYR	CE1-CZ	-9.85	1.25	1.38
1	A	364	GLU	CG-CD	9.85	1.66	1.51
1	A	236	GLU	CD-OE2	9.84	1.36	1.25
1	A	305	ALA	CA-CB	9.81	1.73	1.52
1	B	1073	PHE	CG-CD1	9.81	1.53	1.38
1	C	2372	LEU	C-O	9.80	1.42	1.23
1	B	1203	ARG	CZ-NH2	9.79	1.45	1.33
1	A	268	LYS	CE-NZ	9.77	1.73	1.49
1	A	344	VAL	CB-CG2	9.75	1.73	1.52
1	A	208	TYR	CE2-CZ	9.74	1.51	1.38
1	A	109	GLY	CA-C	9.73	1.67	1.51
1	C	2112	VAL	CA-CB	9.73	1.75	1.54
1	A	155	PHE	CD2-CE2	9.72	1.58	1.39
1	B	1319	THR	CB-CG2	-9.69	1.20	1.52
1	A	336	VAL	CB-CG2	9.60	1.73	1.52
1	C	2039	VAL	N-CA	9.59	1.65	1.46
1	B	1048	LYS	CE-NZ	9.58	1.73	1.49
1	A	216	TYR	CD2-CE2	9.57	1.53	1.39
1	B	1308	ARG	NE-CZ	9.51	1.45	1.33
1	A	195	LYS	CD-CE	9.49	1.75	1.51
1	A	355	GLU	CB-CG	-9.48	1.34	1.52
1	A	173	MET	CA-CB	9.44	1.74	1.53
1	C	2043	ASN	CG-ND2	9.43	1.56	1.32
1	B	1364	GLU	CD-OE1	-9.40	1.15	1.25
1	B	1087	ASP	CG-OD2	9.38	1.47	1.25
1	A	173	MET	CB-CG	9.37	1.81	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2228	PHE	CE2-CZ	9.36	1.55	1.37
1	C	2086	GLU	CB-CG	9.34	1.70	1.52
1	C	2227	ARG	CD-NE	-9.31	1.30	1.46
1	B	1066	SER	CB-OG	9.26	1.54	1.42
1	B	1370	VAL	CB-CG1	9.26	1.72	1.52
1	B	1095	PHE	CD1-CE1	9.25	1.57	1.39
1	A	172	PRO	CA-C	-9.25	1.34	1.52
1	A	313	TRP	CE3-CZ3	9.25	1.54	1.38
1	C	2191	ARG	CZ-NH1	9.23	1.45	1.33
1	A	308	ARG	CZ-NH1	9.21	1.45	1.33
1	B	1192	ASP	CB-CG	-9.20	1.32	1.51
1	B	1176	TRP	CE3-CZ3	9.19	1.54	1.38
1	B	1357	GLU	CB-CG	-9.19	1.34	1.52
1	C	2113	GLU	CG-CD	9.14	1.65	1.51
1	C	2173	MET	CG-SD	9.13	2.04	1.81
1	C	2082	VAL	CA-CB	9.12	1.74	1.54
1	C	2357	GLU	CB-CG	-9.11	1.34	1.52
1	A	121	GLU	CD-OE2	9.09	1.35	1.25
1	C	2282	ARG	CZ-NH2	9.06	1.44	1.33
1	C	2039	VAL	C-O	9.05	1.40	1.23
1	A	89	TYR	CE2-CZ	-9.04	1.26	1.38
1	C	2326	LYS	CD-CE	9.04	1.73	1.51
1	C	2048	LYS	CG-CD	9.03	1.83	1.52
1	A	163	PHE	CE2-CZ	9.00	1.54	1.37
1	A	215	HIS	CB-CG	-8.99	1.33	1.50
1	C	2227	ARG	CZ-NH2	8.98	1.44	1.33
1	A	226	MET	SD-CE	8.93	2.27	1.77
1	A	76	ARG	CB-CG	-8.92	1.28	1.52
1	A	40	ASP	CG-OD2	8.91	1.45	1.25
1	B	1229	SER	CB-OG	8.91	1.53	1.42
1	B	1209	TYR	CE2-CZ	8.90	1.50	1.38
1	C	2040	ASP	CG-OD2	8.90	1.45	1.25
1	A	193	GLY	CA-C	8.88	1.66	1.51
1	B	1111	TYR	CG-CD1	-8.84	1.27	1.39
1	A	357	GLU	CG-CD	8.81	1.65	1.51
1	B	1203	ARG	CG-CD	8.81	1.74	1.51
1	B	1191	ARG	CG-CD	8.80	1.74	1.51
1	B	1192	ASP	CG-OD2	8.78	1.45	1.25
1	C	2326	LYS	CE-NZ	8.74	1.71	1.49
1	B	1098	SER	CB-OG	8.74	1.53	1.42
1	C	2056	PHE	CD2-CE2	-8.74	1.21	1.39
1	C	2266	LYS	CD-CE	8.73	1.73	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	ASN	C-O	8.69	1.39	1.23
1	A	74	GLU	CD-OE2	8.69	1.35	1.25
1	C	2335	TYR	CE1-CZ	8.69	1.49	1.38
1	A	333	TYR	CD1-CE1	8.67	1.52	1.39
1	A	222	ASP	CG-OD2	8.66	1.45	1.25
1	C	2172	PRO	CA-C	-8.66	1.35	1.52
1	A	48	LYS	CE-NZ	8.62	1.70	1.49
1	B	1081	GLU	CG-CD	8.62	1.64	1.51
1	B	1111	TYR	CG-CD2	8.61	1.50	1.39
1	A	268	LYS	CD-CE	8.57	1.72	1.51
1	A	216	TYR	CD1-CE1	8.54	1.52	1.39
1	B	1236	GLU	CB-CG	8.54	1.68	1.52
1	B	1313	TRP	CE3-CZ3	8.54	1.52	1.38
1	B	1314	PHE	CD2-CE2	8.54	1.56	1.39
1	C	2355	GLU	CG-CD	8.54	1.64	1.51
1	A	258	ALA	CA-CB	8.53	1.70	1.52
1	A	154	ARG	CZ-NH1	8.49	1.44	1.33
1	B	1252	PHE	CG-CD2	8.46	1.51	1.38
1	A	337	ASN	CB-CG	8.46	1.70	1.51
1	A	343	ALA	CA-CB	8.46	1.70	1.52
1	C	2221	GLU	CD-OE1	8.43	1.34	1.25
1	C	2089	TYR	CD2-CE2	8.42	1.51	1.39
1	C	2082	VAL	CB-CG2	-8.41	1.35	1.52
1	A	272	ASN	CG-OD1	8.40	1.42	1.24
1	C	2229	SER	CB-OG	8.40	1.53	1.42
1	C	2073	PHE	CD2-CE2	8.38	1.56	1.39
1	B	1307	GLU	CD-OE2	-8.38	1.16	1.25
1	A	167	CYS	CB-SG	-8.37	1.68	1.82
1	B	1307	GLU	CG-CD	8.33	1.64	1.51
1	C	2297	TRP	CE3-CZ3	8.32	1.52	1.38
1	C	2298	GLU	CB-CG	8.32	1.68	1.52
1	B	1111	TYR	CE1-CZ	8.31	1.49	1.38
1	B	1202	VAL	CB-CG1	-8.30	1.35	1.52
1	C	2151	VAL	C-O	8.30	1.39	1.23
1	C	2216	TYR	CB-CG	8.29	1.64	1.51
1	A	159	ARG	CG-CD	-8.29	1.31	1.51
1	B	1253	ASN	CG-OD1	8.28	1.42	1.24
1	C	2222	ASP	CG-OD2	8.25	1.44	1.25
1	C	2173	MET	SD-CE	-8.24	1.31	1.77
1	A	130	PHE	CG-CD1	8.20	1.51	1.38
1	A	202	VAL	CB-CG2	-8.17	1.35	1.52
1	C	2155	PHE	CD1-CE1	8.15	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	PHE	C-O	8.10	1.38	1.23
1	A	225	TYR	CE2-CZ	8.08	1.49	1.38
1	B	1040	ASP	CG-OD2	8.06	1.43	1.25
1	A	203	ARG	NE-CZ	-8.06	1.22	1.33
1	C	2308	ARG	NE-CZ	8.06	1.43	1.33
1	B	1227	ARG	CD-NE	-8.06	1.32	1.46
1	A	171	GLY	C-O	8.06	1.36	1.23
1	C	2074	GLU	CB-CG	8.05	1.67	1.52
1	C	2233	GLU	CB-CG	-8.05	1.36	1.52
1	C	2278	SER	CA-CB	8.04	1.65	1.52
1	B	1278	SER	CB-OG	8.02	1.52	1.42
1	B	1367	VAL	CA-CB	8.01	1.71	1.54
1	C	2074	GLU	CG-CD	8.00	1.64	1.51
1	B	1182	THR	C-O	7.96	1.38	1.23
1	C	2200	LYS	CA-CB	-7.94	1.36	1.53
1	A	178	VAL	CB-CG1	7.92	1.69	1.52
1	C	2346	LYS	CD-CE	7.92	1.71	1.51
1	C	2059	ALA	CA-CB	7.92	1.69	1.52
1	A	108	GLU	CD-OE2	-7.90	1.17	1.25
1	B	1203	ARG	NE-CZ	7.90	1.43	1.33
1	A	209	TYR	CD2-CE2	-7.89	1.27	1.39
1	B	1230	ASP	CG-OD1	7.89	1.43	1.25
1	B	1272	ASN	N-CA	7.87	1.62	1.46
1	B	1232	SER	CA-CB	7.87	1.64	1.52
1	A	270	GLY	C-O	-7.85	1.11	1.23
1	C	2091	GLN	CD-OE1	7.83	1.41	1.24
1	C	2224	THR	CB-CG2	7.80	1.78	1.52
1	A	268	LYS	CB-CG	-7.79	1.31	1.52
1	C	2171	GLY	CA-C	-7.78	1.39	1.51
1	C	2152	VAL	CB-CG1	-7.77	1.36	1.52
1	B	1327	PHE	CE2-CZ	7.77	1.52	1.37
1	A	95	PHE	C-O	7.74	1.38	1.23
1	A	165	TYR	CE1-CZ	7.74	1.48	1.38
1	A	333	TYR	CE1-CZ	-7.74	1.28	1.38
1	A	335	TYR	CE2-CZ	7.73	1.48	1.38
1	C	2325	TYR	CE1-CZ	7.72	1.48	1.38
1	B	1216	TYR	CE1-CZ	7.69	1.48	1.38
1	A	333	TYR	CG-CD1	7.69	1.49	1.39
1	A	269	VAL	CA-CB	7.69	1.70	1.54
1	C	2079	GLU	CD-OE2	-7.68	1.17	1.25
1	C	2213	SER	CA-CB	7.65	1.64	1.52
1	B	1266	LYS	CD-CE	7.65	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1364	GLU	CD-OE2	-7.63	1.17	1.25
1	B	1059	ALA	CA-CB	7.63	1.68	1.52
1	A	43	ASN	CG-ND2	7.61	1.51	1.32
1	C	2176	TRP	CZ3-CH2	7.60	1.52	1.40
1	B	1204	TYR	N-CA	-7.58	1.31	1.46
1	C	2154	ARG	CZ-NH2	7.58	1.42	1.33
1	A	354	VAL	CB-CG1	7.55	1.68	1.52
1	A	147	PRO	CA-CB	-7.53	1.38	1.53
1	A	229	SER	CA-CB	7.53	1.64	1.52
1	A	285	ARG	CZ-NH2	7.52	1.42	1.33
1	A	47	VAL	CB-CG2	7.51	1.68	1.52
1	B	1163	PHE	CG-CD2	7.49	1.50	1.38
1	A	325	TYR	CG-CD1	7.48	1.48	1.39
1	A	191	ARG	CB-CG	7.48	1.72	1.52
1	B	1219	LYS	CE-NZ	7.47	1.67	1.49
1	A	335	TYR	CG-CD2	-7.47	1.29	1.39
1	A	62	GLN	CB-CG	-7.46	1.32	1.52
1	B	1089	TYR	CE1-CZ	7.45	1.48	1.38
1	A	81	GLU	N-CA	-7.44	1.31	1.46
1	A	88	ALA	CA-CB	7.44	1.68	1.52
1	A	145	ILE	N-CA	7.43	1.61	1.46
1	C	2307	GLU	CG-CD	7.42	1.63	1.51
1	A	112	VAL	CB-CG2	7.42	1.68	1.52
1	B	1297	TRP	CD1-NE1	7.42	1.50	1.38
1	C	2330	PRO	CG-CD	7.42	1.75	1.50
1	B	1217	ILE	CB-CG2	7.40	1.75	1.52
1	A	372	LEU	C-O	7.40	1.37	1.23
1	B	1325	TYR	CZ-OH	7.40	1.50	1.37
1	C	2371	GLY	C-O	7.39	1.35	1.23
1	B	1352	VAL	CB-CG1	7.38	1.68	1.52
1	C	2154	ARG	CG-CD	7.38	1.70	1.51
1	B	1275	PHE	CA-CB	7.38	1.70	1.53
1	A	121	GLU	CG-CD	7.37	1.63	1.51
1	B	1216	TYR	CG-CD1	7.34	1.48	1.39
1	B	1046	ARG	CD-NE	7.34	1.58	1.46
1	B	1331	GLY	C-O	7.33	1.35	1.23
1	B	1089	TYR	C-O	-7.31	1.09	1.23
1	A	330	PRO	N-CD	7.31	1.58	1.47
1	B	1172	PRO	C-O	-7.31	1.08	1.23
1	C	2349	THR	CA-CB	7.31	1.72	1.53
1	C	2252	PHE	CG-CD1	7.31	1.49	1.38
1	C	2124	MET	SD-CE	-7.30	1.36	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	ILE	CB-CG2	7.30	1.75	1.52
1	C	2169	PRO	C-O	7.30	1.37	1.23
1	A	372	LEU	C-OXT	7.28	1.37	1.23
1	B	1336	VAL	CB-CG1	7.28	1.68	1.52
1	A	163	PHE	CD2-CE2	7.27	1.53	1.39
1	C	2259	LEU	CG-CD1	7.26	1.78	1.51
1	A	267	ALA	CA-CB	7.25	1.67	1.52
1	B	1316	ARG	CG-CD	7.25	1.70	1.51
1	B	1281	ASN	CG-OD1	7.24	1.39	1.24
1	C	2324	LEU	CG-CD2	7.24	1.78	1.51
1	A	248	SER	CA-CB	7.24	1.63	1.52
1	B	1163	PHE	C-O	7.22	1.37	1.23
1	C	2173	MET	CB-CG	7.22	1.74	1.51
1	A	326	LYS	CE-NZ	7.21	1.67	1.49
1	C	2079	GLU	CB-CG	7.21	1.65	1.52
1	B	1306	PRO	CA-C	7.19	1.67	1.52
1	A	263	GLY	CA-C	7.19	1.63	1.51
1	A	301	LYS	CE-NZ	7.16	1.67	1.49
1	A	121	GLU	N-CA	-7.15	1.32	1.46
1	B	1173	MET	N-CA	-7.11	1.32	1.46
1	A	235	TYR	CG-CD1	7.11	1.48	1.39
1	A	183	ALA	N-CA	7.10	1.60	1.46
1	A	191	ARG	CZ-NH2	-7.09	1.23	1.33
1	B	1217	ILE	C-O	7.09	1.36	1.23
1	C	2192	ASP	CG-OD1	7.08	1.41	1.25
1	A	73	PHE	CD2-CE2	7.07	1.53	1.39
1	B	1372	LEU	C-O	7.06	1.36	1.23
1	B	1244	THR	CB-CG2	7.06	1.75	1.52
1	C	2179	VAL	C-O	-7.06	1.09	1.23
1	A	307	GLU	CG-CD	7.05	1.62	1.51
1	B	1210	ILE	N-CA	-7.03	1.32	1.46
1	B	1181	GLY	C-O	7.03	1.34	1.23
1	C	2297	TRP	CG-CD1	7.03	1.46	1.36
1	C	2150	LYS	CD-CE	7.03	1.68	1.51
1	A	338	HIS	CA-CB	7.03	1.69	1.53
1	A	136	ALA	CA-CB	7.00	1.67	1.52
1	B	1275	PHE	C-O	6.99	1.36	1.23
1	B	1348	ALA	CA-CB	6.99	1.67	1.52
1	A	327	PHE	CG-CD1	-6.97	1.28	1.38
1	B	1173	MET	CB-CG	6.96	1.73	1.51
1	C	2318	GLY	N-CA	-6.95	1.35	1.46
1	A	170	GLY	C-O	6.95	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1334	ALA	CA-CB	6.94	1.67	1.52
1	B	1056	PHE	CE2-CZ	6.93	1.50	1.37
1	B	1255	ALA	CA-CB	6.92	1.67	1.52
1	A	191	ARG	CA-CB	6.92	1.69	1.53
1	C	2344	VAL	CB-CG1	6.92	1.67	1.52
1	A	273	VAL	CB-CG1	6.91	1.67	1.52
1	B	1192	ASP	C-O	6.89	1.36	1.23
1	A	79	GLU	CD-OE1	-6.88	1.18	1.25
1	A	333	TYR	CE2-CZ	6.88	1.47	1.38
1	C	2305	ALA	CA-CB	6.88	1.66	1.52
1	B	1104	MET	CG-SD	6.88	1.99	1.81
1	A	252	PHE	CD1-CE1	-6.87	1.25	1.39
1	A	76	ARG	CG-CD	6.86	1.69	1.51
1	A	46	ARG	CZ-NH2	6.86	1.42	1.33
1	B	1095	PHE	CE2-CZ	6.86	1.50	1.37
1	C	2364	GLU	CG-CD	6.84	1.62	1.51
1	A	358	TRP	CE3-CZ3	6.84	1.50	1.38
1	A	235	TYR	CE1-CZ	6.84	1.47	1.38
1	A	358	TRP	CG-CD1	6.83	1.46	1.36
1	B	1208	TYR	CD1-CE1	6.82	1.49	1.39
1	B	1359	ASP	C-O	6.82	1.36	1.23
1	A	130	PHE	CD2-CE2	6.82	1.52	1.39
1	B	1216	TYR	CE2-CZ	-6.81	1.29	1.38
1	A	67	GLY	CA-C	6.81	1.62	1.51
1	C	2076	ARG	CB-CG	-6.80	1.34	1.52
1	A	39	VAL	CA-CB	6.80	1.69	1.54
1	A	113	GLU	CD-OE1	-6.79	1.18	1.25
1	A	152	VAL	CA-CB	-6.79	1.40	1.54
1	A	285	ARG	CD-NE	6.78	1.57	1.46
1	A	209	TYR	CZ-OH	-6.76	1.26	1.37
1	C	2363	MET	CG-SD	6.76	1.98	1.81
1	C	2327	PHE	CG-CD2	-6.76	1.28	1.38
1	C	2326	LYS	CB-CG	6.76	1.70	1.52
1	C	2241	VAL	CB-CG2	6.75	1.67	1.52
1	B	1126	HIS	C-O	6.75	1.36	1.23
1	C	2248	SER	CB-OG	6.74	1.51	1.42
1	A	208	TYR	CD2-CE2	6.72	1.49	1.39
1	B	1332	VAL	CB-CG2	6.72	1.67	1.52
1	B	1200	LYS	CB-CG	-6.72	1.34	1.52
1	B	1207	VAL	CB-CG2	6.71	1.67	1.52
1	A	56	PHE	CG-CD1	6.70	1.48	1.38
1	C	2246	ILE	C-O	6.70	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1173	MET	CG-SD	6.69	1.98	1.81
1	B	1138	GLY	C-O	6.69	1.34	1.23
1	C	2080	LYS	CB-CG	6.69	1.70	1.52
1	A	322	ALA	CA-CB	6.68	1.66	1.52
1	C	2072	GLU	CD-OE2	6.68	1.32	1.25
1	B	1075	MET	CG-SD	6.68	1.98	1.81
1	C	2143	THR	C-O	6.67	1.36	1.23
1	C	2262	GLU	CB-CG	-6.67	1.39	1.52
1	A	168	ALA	CA-CB	6.65	1.66	1.52
1	B	1179	VAL	CB-CG1	6.64	1.66	1.52
1	B	1091	GLN	C-O	6.64	1.35	1.23
1	B	1267	ALA	CA-CB	6.62	1.66	1.52
1	A	65	ALA	CA-CB	6.61	1.66	1.52
1	C	2163	PHE	CG-CD1	-6.60	1.28	1.38
1	A	150	LYS	C-O	6.60	1.35	1.23
1	A	135	GLY	C-O	6.58	1.34	1.23
1	B	1346	LYS	CD-CE	6.58	1.67	1.51
1	B	1111	TYR	CD1-CE1	6.57	1.49	1.39
1	B	1056	PHE	CD1-CE1	6.55	1.52	1.39
1	B	1164	VAL	CB-CG2	6.55	1.66	1.52
1	B	1089	TYR	CE2-CZ	6.54	1.47	1.38
1	B	1294	ASP	CG-OD2	6.54	1.40	1.25
1	C	2362	LEU	N-CA	6.54	1.59	1.46
1	A	74	GLU	C-O	6.53	1.35	1.23
1	A	173	MET	CG-SD	6.53	1.98	1.81
1	A	203	ARG	CD-NE	-6.53	1.35	1.46
1	C	2293	GLY	C-O	6.53	1.34	1.23
1	C	2313	TRP	CE3-CZ3	6.53	1.49	1.38
1	C	2352	VAL	CB-CG2	6.53	1.66	1.52
1	C	2147	PRO	CA-CB	-6.52	1.40	1.53
1	A	215	HIS	C-O	6.52	1.35	1.23
1	B	1070	ILE	C-O	6.52	1.35	1.23
1	A	211	GLY	C-O	6.51	1.34	1.23
1	A	266	LYS	CG-CD	-6.51	1.30	1.52
1	C	2156	LYS	C-O	6.51	1.35	1.23
1	C	2251	VAL	CB-CG2	6.51	1.66	1.52
1	C	2216	TYR	CG-CD2	6.50	1.47	1.39
1	C	2208	TYR	CE1-CZ	-6.50	1.30	1.38
1	A	274	LEU	C-O	6.48	1.35	1.23
1	B	1367	VAL	CB-CG1	6.48	1.66	1.52
1	A	339	ASN	CG-OD1	6.47	1.38	1.24
1	A	352	VAL	CB-CG2	6.47	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2347	GLY	CA-C	-6.47	1.41	1.51
1	B	1083	GLN	CG-CD	6.46	1.66	1.51
1	B	1039	VAL	CA-C	6.46	1.69	1.52
1	C	2364	GLU	CA-CB	6.46	1.68	1.53
1	B	1130	PHE	CG-CD2	6.44	1.48	1.38
1	B	1076	ARG	CG-CD	6.44	1.68	1.51
1	B	1080	LYS	CD-CE	-6.44	1.35	1.51
1	C	2200	LYS	CE-NZ	6.44	1.65	1.49
1	B	1046	ARG	CB-CG	6.43	1.70	1.52
1	A	42	SER	CB-OG	6.43	1.50	1.42
1	A	372	LEU	CG-CD1	-6.43	1.28	1.51
1	B	1225	TYR	CZ-OH	6.43	1.48	1.37
1	A	98	SER	CA-CB	-6.42	1.43	1.52
1	B	1063	VAL	CB-CG1	6.42	1.66	1.52
1	C	2188	VAL	CB-CG1	6.42	1.66	1.52
1	A	298	GLU	CD-OE2	6.42	1.32	1.25
1	B	1052	VAL	C-O	-6.42	1.11	1.23
1	B	1226	MET	SD-CE	-6.41	1.42	1.77
1	A	99	ILE	CA-CB	-6.40	1.40	1.54
1	B	1168	ALA	C-O	-6.40	1.11	1.23
1	B	1163	PHE	CE2-CZ	6.39	1.49	1.37
1	C	2235	TYR	CG-CD1	-6.39	1.30	1.39
1	B	1325	TYR	CG-CD2	6.39	1.47	1.39
1	A	133	ALA	CA-CB	6.38	1.65	1.52
1	C	2111	TYR	CE2-CZ	6.38	1.46	1.38
1	B	1251	VAL	CB-CG2	6.37	1.66	1.52
1	A	55	PRO	N-CD	6.36	1.56	1.47
1	C	2065	ALA	C-O	6.35	1.35	1.23
1	C	2295	LEU	CG-CD1	6.35	1.75	1.51
1	A	164	VAL	N-CA	6.35	1.59	1.46
1	C	2125	PRO	CB-CG	6.35	1.81	1.50
1	C	2169	PRO	C-N	-6.34	1.21	1.33
1	B	1372	LEU	C-OXT	6.34	1.35	1.23
1	C	2239	VAL	CB-CG2	-6.34	1.39	1.52
1	C	2220	ASP	CB-CG	-6.33	1.38	1.51
1	B	1066	SER	C-O	6.33	1.35	1.23
1	C	2191	ARG	NE-CZ	6.33	1.41	1.33
1	B	1163	PHE	CD2-CE2	6.33	1.51	1.39
1	A	151	VAL	C-O	6.32	1.35	1.23
1	A	152	VAL	C-O	6.31	1.35	1.23
1	A	297	TRP	CG-CD1	6.30	1.45	1.36
1	B	1128	ILE	CB-CG2	6.30	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2076	ARG	C-O	6.29	1.35	1.23
1	A	371	GLY	CA-C	-6.28	1.41	1.51
1	A	372	LEU	CA-C	6.28	1.69	1.52
1	B	1301	LYS	N-CA	6.28	1.58	1.46
1	C	2225	TYR	CD2-CE2	6.28	1.48	1.39
1	C	2370	VAL	CA-C	6.28	1.69	1.52
1	C	2256	VAL	CB-CG2	6.28	1.66	1.52
1	C	2142	LEU	CB-CG	6.27	1.70	1.52
1	B	1191	ARG	CB-CG	6.25	1.69	1.52
1	C	2190	PRO	CA-C	6.25	1.65	1.52
1	B	1364	GLU	CA-CB	6.24	1.67	1.53
1	B	1097	GLY	N-CA	-6.23	1.36	1.46
1	B	1236	GLU	CG-CD	6.23	1.61	1.51
1	C	2193	GLY	CA-C	6.23	1.61	1.51
1	A	200	LYS	CA-CB	-6.22	1.40	1.53
1	A	275	PHE	CG-CD1	-6.22	1.29	1.38
1	B	1062	GLN	CG-CD	6.22	1.65	1.51
1	C	2317	GLY	N-CA	6.22	1.55	1.46
1	C	2347	GLY	N-CA	6.21	1.55	1.46
1	B	1238	MET	CB-CG	6.21	1.71	1.51
1	A	47	VAL	CB-CG1	6.20	1.65	1.52
1	C	2275	PHE	CE1-CZ	6.20	1.49	1.37
1	A	256	VAL	CB-CG1	6.19	1.65	1.52
1	B	1144	LEU	CG-CD2	6.19	1.74	1.51
1	B	1149	GLU	C-O	6.16	1.35	1.23
1	A	251	VAL	N-CA	-6.16	1.34	1.46
1	B	1196	ASP	N-CA	-6.16	1.34	1.46
1	B	1261	GLY	CA-C	-6.15	1.42	1.51
1	B	1056	PHE	C-O	6.14	1.35	1.23
1	C	2273	VAL	C-O	6.13	1.35	1.23
1	A	159	ARG	CZ-NH2	6.13	1.41	1.33
1	A	280	PRO	CA-CB	6.12	1.65	1.53
1	B	1154	ARG	CG-CD	6.12	1.67	1.51
1	C	2075	MET	CG-SD	6.11	1.97	1.81
1	B	1222	ASP	CG-OD2	6.11	1.39	1.25
1	B	1125	PRO	CA-C	6.09	1.65	1.52
1	B	1216	TYR	CD1-CE1	6.09	1.48	1.39
1	C	2295	LEU	C-O	6.09	1.34	1.23
1	A	43	ASN	CG-OD1	6.09	1.37	1.24
1	C	2274	LEU	C-O	6.09	1.34	1.23
1	C	2359	ASP	C-O	6.09	1.34	1.23
1	A	272	ASN	C-O	6.08	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1275	PHE	CD1-CE1	6.08	1.51	1.39
1	A	217	ILE	CA-CB	-6.08	1.40	1.54
1	B	1268	LYS	CB-CG	-6.08	1.36	1.52
1	A	165	TYR	C-O	6.07	1.34	1.23
1	A	209	TYR	CB-CG	6.07	1.60	1.51
1	C	2089	TYR	CA-CB	6.07	1.67	1.53
1	C	2354	VAL	CA-C	6.07	1.68	1.52
1	B	1259	LEU	CA-CB	6.06	1.67	1.53
1	A	198	GLU	CD-OE1	-6.06	1.19	1.25
1	B	1216	TYR	CA-CB	6.06	1.67	1.53
1	A	316	ARG	CD-NE	6.05	1.56	1.46
1	B	1092	ALA	C-O	6.04	1.34	1.23
1	B	1268	LYS	CE-NZ	6.04	1.64	1.49
1	B	1236	GLU	CD-OE2	6.04	1.32	1.25
1	B	1171	GLY	CA-C	-6.04	1.42	1.51
1	C	2297	TRP	CB-CG	6.04	1.61	1.50
1	A	293	GLY	CA-C	6.03	1.61	1.51
1	C	2139	GLY	C-O	6.03	1.33	1.23
1	A	203	ARG	C-O	6.02	1.34	1.23
1	C	2155	PHE	CE1-CZ	6.02	1.48	1.37
1	C	2327	PHE	CA-C	6.01	1.68	1.52
1	B	1204	TYR	CE1-CZ	6.00	1.46	1.38
1	B	1220	ASP	CA-C	6.00	1.68	1.52
1	B	1197	HIS	N-CA	6.00	1.58	1.46
1	B	1065	ALA	CA-CB	-6.00	1.39	1.52
1	A	95	PHE	CD2-CE2	5.99	1.51	1.39
1	C	2233	GLU	CD-OE2	-5.98	1.19	1.25
1	C	2366	VAL	CB-CG2	-5.98	1.40	1.52
1	A	252	PHE	CE1-CZ	5.98	1.48	1.37
1	C	2239	VAL	CA-CB	5.98	1.67	1.54
1	B	1112	VAL	CB-CG1	-5.96	1.40	1.52
1	A	332	VAL	C-O	5.96	1.34	1.23
1	C	2198	GLU	CB-CG	-5.96	1.40	1.52
1	C	2311	GLU	C-O	5.96	1.34	1.23
1	A	327	PHE	CD2-CE2	5.96	1.51	1.39
1	B	1369	PRO	C-O	5.96	1.35	1.23
1	C	2289	ILE	CB-CG2	5.95	1.71	1.52
1	C	2154	ARG	CA-CB	5.94	1.67	1.53
1	A	124	MET	N-CA	5.93	1.58	1.46
1	C	2176	TRP	CE3-CZ3	5.93	1.48	1.38
1	A	297	TRP	CE3-CZ3	5.92	1.48	1.38
1	A	85	ASP	CB-CG	5.92	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ALA	C-O	5.92	1.34	1.23
1	A	210	ILE	C-O	5.91	1.34	1.23
1	C	2336	VAL	C-O	5.91	1.34	1.23
1	B	1345	HIS	CB-CG	5.90	1.60	1.50
1	B	1130	PHE	CE2-CZ	5.90	1.48	1.37
1	A	234	GLY	CA-C	5.90	1.61	1.51
1	A	209	TYR	C-O	5.89	1.34	1.23
1	B	1043	ASN	CG-OD1	5.89	1.36	1.24
1	A	228	PHE	CE1-CZ	5.89	1.48	1.37
1	B	1114	LEU	CA-CB	5.89	1.67	1.53
1	B	1227	ARG	CG-CD	5.87	1.66	1.51
1	B	1165	TYR	C-O	5.86	1.34	1.23
1	A	252	PHE	CG-CD2	5.86	1.47	1.38
1	A	282	ARG	CZ-NH2	5.86	1.40	1.33
1	C	2165	TYR	CG-CD1	5.84	1.46	1.39
1	C	2268	LYS	CE-NZ	5.83	1.63	1.49
1	A	154	ARG	NE-CZ	5.83	1.40	1.33
1	B	1110	ASP	CA-CB	5.83	1.66	1.53
1	A	93	MET	CG-SD	5.83	1.96	1.81
1	C	2061	GLU	CB-CG	5.83	1.63	1.52
1	A	106	VAL	CB-CG2	5.82	1.65	1.52
1	A	121	GLU	CB-CG	-5.81	1.41	1.52
1	C	2098	SER	CA-CB	5.81	1.61	1.52
1	B	1333	TYR	CE2-CZ	5.80	1.46	1.38
1	C	2228	PHE	CG-CD1	5.80	1.47	1.38
1	C	2063	VAL	CB-CG2	5.80	1.65	1.52
1	B	1336	VAL	CA-CB	5.79	1.67	1.54
1	C	2365	GLN	C-O	5.79	1.34	1.23
1	A	248	SER	CB-OG	5.79	1.49	1.42
1	C	2098	SER	N-CA	5.79	1.57	1.46
1	A	296	VAL	C-O	5.78	1.34	1.23
1	C	2284	SER	CA-CB	5.78	1.61	1.52
1	B	1157	ALA	N-CA	5.78	1.57	1.46
1	C	2081	GLU	CD-OE1	-5.78	1.19	1.25
1	A	336	VAL	CB-CG1	5.78	1.65	1.52
1	B	1208	TYR	CG-CD2	5.77	1.46	1.39
1	B	1096	ASP	N-CA	5.77	1.57	1.46
1	B	1242	MET	C-O	5.77	1.34	1.23
1	C	2050	THR	CB-CG2	5.77	1.71	1.52
1	C	2265	LEU	CG-CD1	5.76	1.73	1.51
1	B	1198	GLU	CB-CG	-5.76	1.41	1.52
1	B	1333	TYR	CD1-CE1	5.75	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1349	THR	CA-CB	5.75	1.68	1.53
1	C	2204	TYR	CE2-CZ	5.75	1.46	1.38
1	A	220	ASP	CB-CG	-5.75	1.39	1.51
1	C	2268	LYS	CG-CD	5.74	1.72	1.52
1	B	1295	LEU	N-CA	-5.74	1.34	1.46
1	C	2204	TYR	CD1-CE1	5.74	1.48	1.39
1	C	2355	GLU	CA-C	-5.73	1.38	1.52
1	C	2370	VAL	N-CA	-5.73	1.34	1.46
1	A	91	GLN	N-CA	5.73	1.57	1.46
1	B	1158	THR	CB-CG2	5.73	1.71	1.52
1	A	91	GLN	CG-CD	-5.73	1.37	1.51
1	B	1222	ASP	CG-OD1	5.73	1.38	1.25
1	A	187	MET	CA-CB	5.72	1.66	1.53
1	A	236	GLU	CD-OE1	5.71	1.31	1.25
1	C	2316	ARG	CG-CD	5.71	1.66	1.51
1	A	281	ASN	CG-OD1	5.71	1.36	1.24
1	B	1333	TYR	CB-CG	-5.70	1.43	1.51
1	B	1182	THR	CA-CB	5.69	1.68	1.53
1	B	1202	VAL	CA-CB	5.69	1.66	1.54
1	A	213	SER	CB-OG	5.69	1.49	1.42
1	B	1186	ILE	CA-CB	5.68	1.68	1.54
1	A	225	TYR	C-O	5.68	1.34	1.23
1	A	314	PHE	CD1-CE1	-5.68	1.27	1.39
1	B	1292	HIS	N-CA	5.68	1.57	1.46
1	C	2236	GLU	CB-CG	5.67	1.62	1.52
1	B	1311	GLU	CD-OE1	5.67	1.31	1.25
1	C	2184	GLY	C-O	5.66	1.32	1.23
1	B	1089	TYR	CD1-CE1	5.65	1.47	1.39
1	B	1100	PRO	CA-C	5.65	1.64	1.52
1	C	2058	HIS	C-O	5.64	1.34	1.23
1	A	96	ASP	CB-CG	-5.64	1.40	1.51
1	A	169	PRO	CG-CD	5.63	1.69	1.50
1	A	194	LEU	CG-CD2	5.63	1.72	1.51
1	B	1078	ILE	C-O	5.62	1.34	1.23
1	A	309	ASP	CB-CG	5.62	1.63	1.51
1	B	1225	TYR	CD1-CE1	5.62	1.47	1.39
1	B	1274	LEU	CA-CB	5.62	1.66	1.53
1	C	2346	LYS	CB-CG	5.59	1.67	1.52
1	A	95	PHE	CG-CD2	-5.59	1.30	1.38
1	A	258	ALA	C-O	5.59	1.33	1.23
1	B	1307	GLU	CD-OE1	5.59	1.31	1.25
1	A	168	ALA	C-O	-5.59	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2240	ALA	CA-CB	5.58	1.64	1.52
1	C	2058	HIS	CA-CB	-5.58	1.41	1.53
1	B	1149	GLU	CA-CB	-5.58	1.41	1.53
1	A	80	LYS	C-O	5.58	1.33	1.23
1	A	279	GLN	CA-C	5.57	1.67	1.52
1	A	145	ILE	CB-CG1	5.57	1.69	1.54
1	C	2202	VAL	CB-CG2	5.57	1.64	1.52
1	B	1289	ILE	C-N	-5.57	1.23	1.33
1	C	2137	LEU	N-CA	-5.57	1.35	1.46
1	C	2302	PHE	CE2-CZ	5.56	1.48	1.37
1	B	1222	ASP	CB-CG	5.56	1.63	1.51
1	A	335	TYR	CD1-CE1	5.55	1.47	1.39
1	A	297	TRP	CZ3-CH2	5.55	1.49	1.40
1	B	1051	LEU	C-O	5.55	1.33	1.23
1	A	89	TYR	CD2-CE2	5.54	1.47	1.39
1	C	2046	ARG	CZ-NH2	5.54	1.40	1.33
1	B	1361	ASP	CA-C	5.54	1.67	1.52
1	B	1311	GLU	N-CA	-5.53	1.35	1.46
1	C	2155	PHE	CG-CD2	5.53	1.47	1.38
1	A	196	ASP	CB-CG	5.53	1.63	1.51
1	A	211	GLY	CA-C	5.53	1.60	1.51
1	C	2269	VAL	CB-CG2	5.53	1.64	1.52
1	B	1322	ALA	CA-CB	5.52	1.64	1.52
1	B	1237	ASP	C-O	-5.51	1.12	1.23
1	A	360	ASN	CA-C	-5.51	1.38	1.52
1	B	1108	GLU	CD-OE2	-5.51	1.19	1.25
1	C	2132	ALA	CA-C	5.50	1.67	1.52
1	A	196	ASP	C-O	-5.50	1.12	1.23
1	A	151	VAL	CB-CG2	5.50	1.64	1.52
1	A	356	GLY	C-O	5.50	1.32	1.23
1	C	2234	GLY	CA-C	5.49	1.60	1.51
1	C	2371	GLY	CA-C	-5.49	1.43	1.51
1	C	2268	LYS	CD-CE	5.49	1.65	1.51
1	B	1129	ASP	CB-CG	5.48	1.63	1.51
1	C	2195	LYS	CD-CE	5.48	1.65	1.51
1	B	1329	GLN	CA-C	-5.48	1.38	1.52
1	A	266	LYS	CE-NZ	5.48	1.62	1.49
1	C	2209	TYR	CG-CD2	5.47	1.46	1.39
1	C	2301	LYS	CE-NZ	5.47	1.62	1.49
1	B	1101	GLY	C-O	5.46	1.32	1.23
1	A	212	GLU	C-O	5.45	1.33	1.23
1	C	2149	GLU	C-O	5.45	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ALA	N-CA	-5.45	1.35	1.46
1	A	207	VAL	CB-CG1	-5.44	1.41	1.52
1	C	2053	PRO	CA-C	5.44	1.63	1.52
1	B	1042	SER	CA-CB	5.43	1.61	1.52
1	A	198	GLU	CB-CG	-5.43	1.41	1.52
1	B	1282	ARG	C-O	5.43	1.33	1.23
1	B	1355	GLU	CA-C	-5.43	1.38	1.52
1	C	2079	GLU	CD-OE1	-5.42	1.19	1.25
1	A	285	ARG	N-CA	5.42	1.57	1.46
1	B	1243	ASP	CB-CG	5.42	1.63	1.51
1	B	1182	THR	N-CA	5.41	1.57	1.46
1	A	83	GLN	CA-C	5.41	1.67	1.52
1	A	163	PHE	C-O	5.41	1.33	1.23
1	C	2300	GLY	CA-C	5.41	1.60	1.51
1	C	2204	TYR	CG-CD1	5.40	1.46	1.39
1	C	2106	VAL	CB-CG1	5.40	1.64	1.52
1	A	171	GLY	N-CA	-5.39	1.38	1.46
1	B	1212	GLU	C-O	5.39	1.33	1.23
1	B	1226	MET	N-CA	-5.38	1.35	1.46
1	C	2203	ARG	NE-CZ	5.38	1.40	1.33
1	C	2109	GLY	N-CA	-5.38	1.38	1.46
1	C	2276	VAL	CB-CG1	5.37	1.64	1.52
1	A	316	ARG	CG-CD	5.37	1.65	1.51
1	B	1235	TYR	N-CA	5.36	1.57	1.46
1	A	289	ILE	CB-CG1	5.35	1.69	1.54
1	B	1195	LYS	CG-CD	-5.35	1.34	1.52
1	B	1320	ALA	CA-CB	5.35	1.63	1.52
1	C	2078	ILE	C-O	5.34	1.33	1.23
1	A	247	PRO	N-CD	5.34	1.55	1.47
1	A	335	TYR	N-CA	5.33	1.57	1.46
1	A	91	GLN	CA-CB	5.33	1.65	1.53
1	B	1366	VAL	CA-C	5.33	1.66	1.52
1	C	2112	VAL	CB-CG2	-5.33	1.41	1.52
1	B	1267	ALA	C-O	5.33	1.33	1.23
1	A	287	HIS	CA-CB	-5.32	1.42	1.53
1	B	1124	MET	CA-CB	-5.31	1.42	1.53
1	B	1064	ALA	CA-CB	5.31	1.63	1.52
1	A	159	ARG	N-CA	5.31	1.56	1.46
1	A	98	SER	CA-C	5.31	1.66	1.52
1	A	357	GLU	CB-CG	5.30	1.62	1.52
1	C	2332	VAL	CB-CG2	-5.30	1.41	1.52
1	A	218	PRO	CG-CD	5.30	1.68	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1196	ASP	CB-CG	5.29	1.62	1.51
1	C	2042	SER	CA-CB	5.29	1.60	1.52
1	C	2145	ILE	CB-CG2	5.29	1.69	1.52
1	B	1273	VAL	CB-CG2	5.29	1.64	1.52
1	B	1209	TYR	CG-CD1	5.29	1.46	1.39
1	C	2062	GLN	CG-CD	5.28	1.63	1.51
1	C	2232	SER	CA-CB	5.28	1.60	1.52
1	C	2106	VAL	N-CA	-5.27	1.35	1.46
1	B	1056	PHE	CG-CD1	5.27	1.46	1.38
1	C	2253	ASN	CA-CB	5.27	1.66	1.53
1	B	1159	ARG	CZ-NH1	5.27	1.39	1.33
1	B	1330	PRO	C-N	-5.26	1.23	1.33
1	B	1169	PRO	CG-CD	5.26	1.68	1.50
1	A	112	VAL	CB-CG1	5.25	1.63	1.52
1	C	2078	ILE	CB-CG2	5.25	1.69	1.52
1	C	2119	PRO	N-CD	-5.25	1.40	1.47
1	C	2048	LYS	CE-NZ	5.24	1.62	1.49
1	A	325	TYR	CB-CG	5.23	1.59	1.51
1	B	1227	ARG	CZ-NH2	-5.23	1.26	1.33
1	C	2255	ALA	CA-CB	5.23	1.63	1.52
1	A	95	PHE	CD1-CE1	5.23	1.49	1.39
1	B	1155	PHE	CE2-CZ	5.23	1.47	1.37
1	C	2145	ILE	CB-CG1	5.21	1.68	1.54
1	C	2195	LYS	CG-CD	-5.21	1.34	1.52
1	A	48	LYS	C-O	-5.21	1.13	1.23
1	A	179	VAL	C-O	5.21	1.33	1.23
1	B	1040	ASP	CA-C	5.21	1.66	1.52
1	C	2087	ASP	CA-CB	5.21	1.65	1.53
1	C	2247	PRO	CA-C	5.21	1.63	1.52
1	B	1273	VAL	N-CA	-5.20	1.35	1.46
1	B	1372	LEU	CG-CD1	-5.20	1.32	1.51
1	B	1124	MET	CB-CG	-5.20	1.34	1.51
1	A	176	TRP	CG-CD2	-5.20	1.34	1.43
1	B	1074	GLU	CD-OE1	-5.20	1.20	1.25
1	B	1335	TYR	CG-CD1	-5.19	1.32	1.39
1	A	204	TYR	CG-CD2	5.19	1.45	1.39
1	A	91	GLN	CA-C	5.19	1.66	1.52
1	C	2216	TYR	N-CA	5.18	1.56	1.46
1	A	314	PHE	CG-CD2	5.18	1.46	1.38
1	B	1100	PRO	CA-CB	5.18	1.64	1.53
1	A	92	ALA	C-O	5.18	1.33	1.23
1	B	1220	ASP	CG-OD1	5.17	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1295	LEU	CG-CD1	5.17	1.71	1.51
1	A	287	HIS	CB-CG	5.17	1.59	1.50
1	C	2111	TYR	CE1-CZ	5.17	1.45	1.38
1	B	1234	GLY	C-O	-5.17	1.15	1.23
1	B	1358	TRP	CG-CD1	5.16	1.44	1.36
1	C	2242	MET	N-CA	5.16	1.56	1.46
1	A	172	PRO	N-CA	-5.16	1.38	1.47
1	B	1281	ASN	C-O	5.16	1.33	1.23
1	B	1043	ASN	CB-CG	5.16	1.62	1.51
1	A	174	ILE	CB-CG1	5.15	1.68	1.54
1	A	306	PRO	C-O	5.15	1.33	1.23
1	C	2156	LYS	CD-CE	5.15	1.64	1.51
1	B	1208	TYR	CD2-CE2	-5.14	1.31	1.39
1	A	50	THR	CB-CG2	5.14	1.69	1.52
1	A	93	MET	CB-CG	5.14	1.67	1.51
1	B	1298	GLU	CD-OE1	5.14	1.31	1.25
1	A	241	VAL	CB-CG2	5.13	1.63	1.52
1	B	1334	ALA	C-O	5.13	1.33	1.23
1	C	2338	HIS	CA-CB	5.12	1.65	1.53
1	C	2274	LEU	CB-CG	5.12	1.67	1.52
1	B	1172	PRO	CA-C	-5.12	1.42	1.52
1	A	352	VAL	CB-CG1	5.11	1.63	1.52
1	A	209	TYR	CE1-CZ	5.10	1.45	1.38
1	B	1332	VAL	CA-CB	-5.10	1.44	1.54
1	A	123	THR	CB-OG1	5.10	1.53	1.43
1	B	1292	HIS	CG-CD2	5.09	1.44	1.35
1	B	1125	PRO	CG-CD	5.09	1.67	1.50
1	B	1235	TYR	CG-CD2	-5.09	1.32	1.39
1	C	2176	TRP	C-O	5.09	1.33	1.23
1	A	222	ASP	CB-CG	5.09	1.62	1.51
1	C	2349	THR	C-O	5.09	1.33	1.23
1	B	1052	VAL	CB-CG1	5.09	1.63	1.52
1	B	1336	VAL	CB-CG2	5.08	1.63	1.52
1	C	2163	PHE	CG-CD2	5.08	1.46	1.38
1	C	2108	GLU	C-O	5.07	1.32	1.23
1	B	1242	MET	CA-CB	5.07	1.65	1.53
1	A	91	GLN	CB-CG	-5.07	1.38	1.52
1	B	1043	ASN	CG-ND2	5.07	1.45	1.32
1	B	1298	GLU	CD-OE2	-5.07	1.20	1.25
1	B	1137	LEU	CB-CG	5.06	1.67	1.52
1	B	1325	TYR	CE1-CZ	5.06	1.45	1.38
1	A	365	GLN	C-O	-5.06	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1335	TYR	CD1-CE1	5.06	1.47	1.39
1	A	82	VAL	CB-CG1	5.05	1.63	1.52
1	C	2361	ASP	CA-C	5.05	1.66	1.52
1	B	1354	VAL	CB-CG2	5.05	1.63	1.52
1	C	2365	GLN	CA-CB	-5.04	1.42	1.53
1	B	1058	HIS	C-O	5.04	1.32	1.23
1	B	1190	PRO	N-CD	5.04	1.54	1.47
1	A	290	GLY	C-O	5.04	1.31	1.23
1	B	1358	TRP	CE3-CZ3	-5.04	1.29	1.38
1	C	2181	GLY	N-CA	5.03	1.53	1.46
1	C	2308	ARG	CG-CD	5.03	1.64	1.51
1	B	1332	VAL	CB-CG1	5.02	1.63	1.52
1	A	327	PHE	CA-C	5.01	1.66	1.52
1	B	1151	VAL	C-O	5.01	1.32	1.23
1	B	1276	VAL	CB-CG2	5.00	1.63	1.52
1	A	124	MET	CB-CG	-5.00	1.35	1.51
1	C	2346	LYS	N-CA	5.00	1.56	1.46

All (461) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	191	ARG	NE-CZ-NH2	-42.44	99.08	120.30
1	C	2227	ARG	NE-CZ-NH2	-34.08	103.26	120.30
1	A	203	ARG	NE-CZ-NH2	-33.63	103.48	120.30
1	A	227	ARG	NE-CZ-NH1	30.69	135.64	120.30
1	A	124	MET	CG-SD-CE	-29.68	52.72	100.20
1	C	2227	ARG	NE-CZ-NH1	29.59	135.09	120.30
1	A	191	ARG	NE-CZ-NH1	27.35	133.98	120.30
1	B	1227	ARG	NE-CZ-NH1	27.35	133.97	120.30
1	B	1227	ARG	NE-CZ-NH2	-26.91	106.85	120.30
1	A	227	ARG	NE-CZ-NH2	-25.01	107.80	120.30
1	C	2076	ARG	NE-CZ-NH1	-24.58	108.01	120.30
1	B	1124	MET	CG-SD-CE	-24.46	61.06	100.20
1	A	48	LYS	CD-CE-NZ	-19.48	66.90	111.70
1	B	1233	GLU	OE1-CD-OE2	-19.12	100.35	123.30
1	A	76	ARG	NE-CZ-NH1	-17.59	111.50	120.30
1	A	154	ARG	NE-CZ-NH1	-17.52	111.54	120.30
1	C	2048	LYS	CD-CE-NZ	-17.16	72.23	111.70
1	C	2220	ASP	CB-CG-OD2	-16.89	103.09	118.30
1	A	226	MET	CG-SD-CE	16.19	126.11	100.20
1	C	2316	ARG	NE-CZ-NH1	-15.90	112.35	120.30
1	B	1192	ASP	CB-CG-OD2	15.70	132.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1191	ARG	NE-CZ-NH1	15.28	127.94	120.30
1	C	2355	GLU	OE1-CD-OE2	15.27	141.62	123.30
1	B	1040	ASP	CB-CG-OD1	-14.80	104.98	118.30
1	B	1048	LYS	CD-CE-NZ	-14.72	77.84	111.70
1	B	1226	MET	CG-SD-CE	14.57	123.51	100.20
1	C	2283	ASP	CB-CG-OD1	14.43	131.29	118.30
1	B	1076	ARG	NE-CZ-NH2	-14.15	113.22	120.30
1	B	1200	LYS	CD-CE-NZ	-13.84	79.87	111.70
1	B	1222	ASP	CB-CG-OD2	13.66	130.59	118.30
1	B	1236	GLU	OE1-CD-OE2	-13.61	106.96	123.30
1	A	222	ASP	CB-CG-OD2	13.55	130.49	118.30
1	B	1319	THR	CA-CB-CG2	-13.26	93.83	112.40
1	B	1205	ASP	CB-CG-OD2	13.12	130.10	118.30
1	A	203	ARG	NH1-CZ-NH2	13.00	133.70	119.40
1	C	2076	ARG	NH1-CZ-NH2	12.60	133.26	119.40
1	A	220	ASP	CB-CG-OD2	-11.89	107.59	118.30
1	A	40	ASP	CB-CG-OD1	-11.88	107.61	118.30
1	C	2154	ARG	CG-CD-NE	-11.75	87.12	111.80
1	A	154	ARG	NE-CZ-NH2	11.51	126.05	120.30
1	C	2226	MET	CG-SD-CE	11.15	118.03	100.20
1	A	326	LYS	CD-CE-NZ	-10.94	86.55	111.70
1	C	2222	ASP	CB-CG-OD2	10.73	127.95	118.30
1	A	233	GLU	CG-CD-OE2	10.48	139.26	118.30
1	B	1237	ASP	CB-CG-OD1	-10.43	108.91	118.30
1	B	1355	GLU	OE1-CD-OE2	10.40	135.78	123.30
1	C	2326	LYS	CD-CE-NZ	-10.36	87.87	111.70
1	B	1203	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	B	1332	VAL	CG1-CB-CG2	-10.19	94.60	110.90
1	B	1222	ASP	CB-CG-OD1	-10.10	109.21	118.30
1	C	2192	ASP	CB-CG-OD1	10.02	127.32	118.30
1	B	1340	LEU	CB-CG-CD1	-9.95	94.08	111.00
1	A	285	ARG	NE-CZ-NH1	-9.85	115.38	120.30
1	C	2191	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	A	361	ASP	CB-CG-OD2	9.76	127.08	118.30
1	A	233	GLU	OE1-CD-OE2	-9.75	111.60	123.30
1	B	1192	ASP	CB-CG-OD1	-9.66	109.61	118.30
1	A	144	LEU	CB-CG-CD2	-9.46	94.92	111.00
1	C	2096	ASP	CB-CG-OD1	9.46	126.81	118.30
1	A	200	LYS	CB-CG-CD	-9.31	87.40	111.60
1	B	1149	GLU	OE1-CD-OE2	-9.29	112.15	123.30
1	C	2156	LYS	CD-CE-NZ	-9.26	90.41	111.70
1	A	149	GLU	OE1-CD-OE2	-9.24	112.21	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2203	ARG	CB-CA-C	-9.21	91.99	110.40
1	C	2271	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	B	1233	GLU	CG-CD-OE2	9.13	136.56	118.30
1	C	2167	CYS	CA-CB-SG	-9.12	97.58	114.00
1	A	325	TYR	CD1-CE1-CZ	-9.11	111.60	119.80
1	A	283	ASP	CB-CG-OD2	9.10	126.49	118.30
1	C	2262	GLU	CA-CB-CG	9.05	133.30	113.40
1	C	2328	LEU	CB-CG-CD1	8.94	126.20	111.00
1	A	76	ARG	NH1-CZ-NH2	8.90	129.19	119.40
1	A	239	VAL	CA-CB-CG2	-8.83	97.65	110.90
1	B	1204	TYR	CD1-CE1-CZ	-8.80	111.88	119.80
1	A	46	ARG	NE-CZ-NH2	8.74	124.67	120.30
1	A	208	TYR	CG-CD1-CE1	8.74	128.29	121.30
1	A	243	ASP	CB-CG-OD2	-8.65	110.51	118.30
1	B	1326	LYS	CD-CE-NZ	-8.64	91.82	111.70
1	A	307	GLU	OE1-CD-OE2	-8.64	112.93	123.30
1	C	2191	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	A	163	PHE	CZ-CE2-CD2	-8.48	109.92	120.10
1	B	1340	LEU	CB-CG-CD2	8.40	125.28	111.00
1	C	2039	VAL	CG1-CB-CG2	-8.39	97.48	110.90
1	A	173	MET	CB-CA-C	-8.35	93.71	110.40
1	A	326	LYS	CB-CG-CD	-8.33	89.93	111.60
1	C	2046	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	C	2305	ALA	CB-CA-C	-8.31	97.63	110.10
1	B	1149	GLU	CG-CD-OE1	8.29	134.87	118.30
1	B	1192	ASP	CB-CA-C	-8.21	93.97	110.40
1	C	2236	GLU	OE1-CD-OE2	-8.21	113.45	123.30
1	A	129	ASP	CB-CG-OD1	8.20	125.68	118.30
1	B	1155	PHE	CB-CG-CD2	8.20	126.54	120.80
1	C	2233	GLU	CG-CD-OE2	8.19	134.68	118.30
1	A	332	VAL	CG1-CB-CG2	-8.17	97.82	110.90
1	A	324	LEU	CA-CB-CG	8.17	134.09	115.30
1	A	355	GLU	OE1-CD-OE2	8.13	133.06	123.30
1	A	268	LYS	CG-CD-CE	-8.13	87.51	111.90
1	C	2325	TYR	CZ-CE2-CD2	-8.10	112.51	119.80
1	A	192	ASP	CB-CG-OD1	8.09	125.58	118.30
1	B	1089	TYR	CD1-CE1-CZ	-8.07	112.53	119.80
1	C	2339	ASN	N-CA-C	-8.07	89.22	111.00
1	C	2111	TYR	CZ-CE2-CD2	-8.06	112.55	119.80
1	B	1173	MET	CB-CA-C	-8.06	94.29	110.40
1	A	305	ALA	CB-CA-C	-8.05	98.03	110.10
1	B	1228	PHE	CB-CG-CD1	-8.02	115.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	191	ARG	CG-CD-NE	-8.01	94.97	111.80
1	A	171	GLY	CA-C-O	7.98	134.96	120.60
1	C	2212	GLU	OE1-CD-OE2	-7.97	113.74	123.30
1	C	2204	TYR	CZ-CE2-CD2	-7.96	112.63	119.80
1	C	2061	GLU	OE1-CD-OE2	7.93	132.82	123.30
1	B	1124	MET	CB-CA-C	-7.93	94.54	110.40
1	B	1093	MET	CG-SD-CE	7.91	112.86	100.20
1	C	2159	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	B	1167	CYS	CA-CB-SG	-7.79	99.97	114.00
1	A	165	TYR	CG-CD2-CE2	7.76	127.51	121.30
1	B	1275	PHE	CD1-CE1-CZ	-7.71	110.85	120.10
1	B	1340	LEU	CA-CB-CG	-7.67	97.66	115.30
1	C	2204	TYR	CB-CG-CD1	-7.65	116.41	121.00
1	A	111	TYR	CB-CG-CD2	7.62	125.57	121.00
1	B	1129	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	B	1087	ASP	CB-CG-OD1	7.56	125.10	118.30
1	C	2192	ASP	OD1-CG-OD2	-7.52	109.01	123.30
1	A	61	GLU	CA-CB-CG	-7.48	96.94	113.40
1	B	1339	ASN	N-CA-C	-7.48	90.80	111.00
1	B	1316	ARG	CA-CB-CG	-7.48	96.95	113.40
1	B	1268	LYS	CA-CB-CG	-7.47	96.96	113.40
1	B	1158	THR	CA-CB-CG2	-7.46	101.95	112.40
1	B	1319	THR	OG1-CB-CG2	-7.46	92.85	110.00
1	A	169	PRO	CA-C-N	7.45	131.09	116.20
1	C	2308	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	294	ASP	CB-CG-OD1	-7.42	111.62	118.30
1	C	2205	ASP	CB-CG-OD2	7.41	124.97	118.30
1	C	2150	LYS	CD-CE-NZ	-7.36	94.76	111.70
1	B	1352	VAL	CG1-CB-CG2	-7.36	99.13	110.90
1	C	2262	GLU	N-CA-CB	-7.35	97.36	110.60
1	A	362	LEU	CB-CG-CD2	-7.31	98.58	111.00
1	B	1327	PHE	CZ-CE2-CD2	-7.31	111.33	120.10
1	A	61	GLU	CG-CD-OE1	-7.31	103.69	118.30
1	C	2200	LYS	CD-CE-NZ	-7.29	94.93	111.70
1	A	295	LEU	CB-CG-CD1	-7.28	98.63	111.00
1	C	2307	GLU	OE1-CD-OE2	-7.23	114.62	123.30
1	C	2040	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	C	2316	ARG	NH1-CZ-NH2	7.23	127.35	119.40
1	C	2182	THR	OG1-CB-CG2	-7.23	93.38	110.00
1	C	2282	ARG	NE-CZ-NH1	-7.21	116.69	120.30
1	A	227	ARG	CB-CG-CD	-7.19	92.90	111.60
1	B	1319	THR	CB-CA-C	-7.16	92.27	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1268	LYS	CD-CE-NZ	-7.14	95.28	111.70
1	A	112	VAL	CG1-CB-CG2	-7.12	99.50	110.90
1	B	1227	ARG	CD-NE-CZ	7.12	133.56	123.60
1	B	1040	ASP	OD1-CG-OD2	7.11	136.82	123.30
1	A	236	GLU	OE1-CD-OE2	-7.08	114.80	123.30
1	A	370	VAL	CA-CB-CG2	-7.07	100.30	110.90
1	C	2113	GLU	CG-CD-OE1	-7.06	104.17	118.30
1	A	124	MET	CB-CA-C	-7.03	96.34	110.40
1	B	1144	LEU	CB-CG-CD2	-7.03	99.06	111.00
1	C	2203	ARG	CB-CG-CD	-7.02	93.35	111.60
1	C	2366	VAL	CA-CB-CG2	-7.00	100.40	110.90
1	B	1076	ARG	NH1-CZ-NH2	6.99	127.09	119.40
1	B	1191	ARG	NH1-CZ-NH2	-6.99	111.71	119.40
1	C	2355	GLU	CA-CB-CG	-6.99	98.02	113.40
1	C	2155	PHE	CG-CD1-CE1	-6.96	113.14	120.80
1	C	2163	PHE	CZ-CE2-CD2	-6.96	111.75	120.10
1	A	154	ARG	CD-NE-CZ	6.96	133.34	123.60
1	A	335	TYR	CZ-CE2-CD2	-6.93	113.56	119.80
1	C	2238	MET	CG-SD-CE	-6.92	89.12	100.20
1	C	2355	GLU	CG-CD-OE2	-6.90	104.51	118.30
1	B	1200	LYS	N-CA-CB	-6.87	98.23	110.60
1	A	77	ILE	CB-CG1-CD1	-6.85	94.72	113.90
1	A	191	ARG	NH1-CZ-NH2	6.85	126.93	119.40
1	B	1366	VAL	CG1-CB-CG2	-6.84	99.95	110.90
1	C	2236	GLU	CG-CD-OE2	6.82	131.95	118.30
1	B	1173	MET	CA-CB-CG	6.81	124.88	113.30
1	C	2210	ILE	CB-CG1-CD1	-6.81	94.82	113.90
1	B	1237	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	225	TYR	CG-CD2-CE2	-6.78	115.87	121.30
1	B	1208	TYR	CD1-CE1-CZ	6.78	125.90	119.80
1	B	1361	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	332	VAL	CA-CB-CG2	-6.74	100.79	110.90
1	B	1208	TYR	CG-CD1-CE1	-6.72	115.93	121.30
1	B	1156	LYS	CD-CE-NZ	-6.71	96.26	111.70
1	B	1296	VAL	CA-CB-CG2	-6.68	100.87	110.90
1	C	2282	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	2114	LEU	CB-CA-C	-6.67	97.52	110.20
1	A	298	GLU	OE1-CD-OE2	-6.67	115.29	123.30
1	A	39	VAL	N-CA-C	-6.67	93.00	111.00
1	B	1328	LEU	CB-CG-CD1	6.63	122.27	111.00
1	B	1111	TYR	CD1-CE1-CZ	-6.62	113.84	119.80
1	C	2085	ASP	CB-CG-OD2	6.62	124.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1327	PHE	CB-CG-CD2	-6.61	116.17	120.80
1	B	1307	GLU	OE1-CD-OE2	-6.61	115.38	123.30
1	A	252	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	C	2332	VAL	CB-CA-C	-6.59	98.87	111.40
1	A	191	ARG	CD-NE-CZ	-6.58	114.39	123.60
1	A	222	ASP	CB-CG-OD1	-6.56	112.39	118.30
1	A	40	ASP	OD1-CG-OD2	6.56	135.77	123.30
1	C	2256	VAL	CA-CB-CG2	-6.54	101.09	110.90
1	C	2155	PHE	CG-CD2-CE2	6.52	127.98	120.80
1	C	2325	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	B	1227	ARG	CB-CG-CD	-6.49	94.72	111.60
1	C	2169	PRO	C-N-CA	-6.47	108.71	122.30
1	A	96	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	169	PRO	C-N-CA	-6.46	108.74	122.30
1	C	2198	GLU	CG-CD-OE1	-6.44	105.42	118.30
1	C	2319	THR	CA-CB-OG1	6.44	122.52	109.00
1	C	2111	TYR	CG-CD2-CE2	6.43	126.44	121.30
1	A	297	TRP	CE3-CZ3-CH2	-6.42	114.13	121.20
1	B	1357	GLU	N-CA-CB	-6.42	99.04	110.60
1	B	1336	VAL	CB-CA-C	-6.41	99.22	111.40
1	B	1295	LEU	CB-CG-CD1	-6.40	100.11	111.00
1	C	2295	LEU	CB-CG-CD1	-6.40	100.12	111.00
1	B	1283	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	1219	LYS	C-N-CA	-6.38	105.76	121.70
1	C	2204	TYR	CB-CG-CD2	6.37	124.82	121.00
1	C	2268	LYS	CD-CE-NZ	-6.36	97.06	111.70
1	B	1359	ASP	CB-CG-OD1	6.34	124.01	118.30
1	C	2087	ASP	N-CA-CB	-6.32	99.22	110.60
1	C	2370	VAL	CA-CB-CG2	-6.32	101.43	110.90
1	B	1048	LYS	CB-CG-CD	6.31	128.01	111.60
1	C	2359	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	171	GLY	N-CA-C	6.27	128.77	113.10
1	B	1367	VAL	CA-CB-CG1	-6.27	101.50	110.90
1	C	2108	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	B	1121	GLU	OE1-CD-OE2	6.25	130.81	123.30
1	C	2214	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	316	ARG	CD-NE-CZ	-6.23	114.87	123.60
1	A	61	GLU	CG-CD-OE2	6.23	130.76	118.30
1	C	2220	ASP	OD1-CG-OD2	6.23	135.13	123.30
1	A	205	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	113	GLU	OE1-CD-OE2	-6.22	115.84	123.30
1	A	301	LYS	CD-CE-NZ	-6.22	97.40	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	THR	OG1-CB-CG2	-6.21	95.70	110.00
1	C	2165	TYR	CD1-CE1-CZ	6.21	125.39	119.80
1	C	2152	VAL	CG1-CB-CG2	-6.19	100.99	110.90
1	B	1353	LEU	CA-CB-CG	-6.19	101.06	115.30
1	A	169	PRO	O-C-N	-6.19	112.68	123.20
1	C	2302	PHE	CZ-CE2-CD2	-6.16	112.70	120.10
1	B	1130	PHE	CD1-CE1-CZ	6.14	127.47	120.10
1	A	355	GLU	CG-CD-OE2	-6.14	106.02	118.30
1	C	2325	TYR	CG-CD1-CE1	6.13	126.20	121.30
1	C	2297	TRP	CG-CD1-NE1	-6.11	103.99	110.10
1	B	1335	TYR	N-CA-C	-6.11	94.51	111.00
1	A	196	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	A	372	LEU	CB-CG-CD2	-6.10	100.62	111.00
1	C	2196	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	200	LYS	N-CA-CB	-6.10	99.62	110.60
1	C	2225	TYR	CD1-CE1-CZ	6.10	125.29	119.80
1	B	1262	GLU	CB-CA-C	6.09	122.59	110.40
1	C	2293	GLY	N-CA-C	-6.09	97.88	113.10
1	A	170	GLY	N-CA-C	-6.08	97.91	113.10
1	B	1370	VAL	CA-CB-CG1	6.08	120.02	110.90
1	C	2047	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	B	1039	VAL	N-CA-C	-6.06	94.63	111.00
1	B	1077	ILE	CB-CG1-CD1	-6.06	96.93	113.90
1	B	1326	LYS	CB-CG-CD	-6.05	95.88	111.60
1	C	2087	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	189	LEU	CB-CA-C	-6.02	98.76	110.20
1	B	1188	VAL	CA-CB-CG2	-6.02	101.87	110.90
1	C	2336	VAL	CB-CA-C	-6.02	99.97	111.40
1	A	113	GLU	CG-CD-OE2	6.01	130.32	118.30
1	A	296	VAL	CG1-CB-CG2	6.01	120.51	110.90
1	A	268	LYS	CB-CA-C	-6.01	98.39	110.40
1	B	1204	TYR	CG-CD1-CE1	6.00	126.10	121.30
1	C	2302	PHE	CG-CD1-CE1	-6.00	114.20	120.80
1	B	1198	GLU	CA-CB-CG	-5.99	100.23	113.40
1	A	262	GLU	N-CA-CB	-5.98	99.84	110.60
1	B	1048	LYS	CG-CD-CE	5.97	129.83	111.90
1	B	1203	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	56	PHE	CZ-CE2-CD2	-5.97	112.93	120.10
1	B	1104	MET	CA-CB-CG	-5.97	103.16	113.30
1	A	95	PHE	CG-CD2-CE2	5.96	127.36	120.80
1	B	1210	ILE	CB-CG1-CD1	-5.96	97.21	113.90
1	A	218	PRO	O-C-N	5.96	132.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1324	LEU	CB-CG-CD1	5.96	121.12	111.00
1	C	2357	GLU	CB-CG-CD	-5.95	98.14	114.20
1	C	2336	VAL	CG1-CB-CG2	-5.95	101.39	110.90
1	A	124	MET	CA-CB-CG	5.93	123.39	113.30
1	B	1191	ARG	CG-CD-NE	-5.93	99.36	111.80
1	B	1203	ARG	CB-CA-C	-5.92	98.56	110.40
1	C	2319	THR	CB-CA-C	-5.92	95.63	111.60
1	C	2225	TYR	CG-CD2-CE2	-5.91	116.57	121.30
1	C	2274	LEU	CB-CG-CD1	5.90	121.03	111.00
1	C	2233	GLU	CG-CD-OE1	-5.88	106.54	118.30
1	A	355	GLU	CB-CA-C	-5.86	98.69	110.40
1	A	212	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	C	2302	PHE	CD1-CE1-CZ	5.84	127.11	120.10
1	A	125	PRO	N-CD-CG	-5.83	94.46	103.20
1	A	192	ASP	OD1-CG-OD2	-5.82	112.24	123.30
1	B	1200	LYS	CA-CB-CG	-5.82	100.60	113.40
1	C	2204	TYR	CG-CD2-CE2	5.80	125.94	121.30
1	B	1195	LYS	CB-CA-C	-5.78	98.83	110.40
1	C	2364	GLU	CA-CB-CG	-5.77	100.70	113.40
1	B	1228	PHE	CZ-CE2-CD2	-5.76	113.19	120.10
1	B	1362	LEU	CA-CB-CG	-5.74	102.09	115.30
1	B	1087	ASP	N-CA-CB	-5.73	100.28	110.60
1	C	2282	ARG	NH1-CZ-NH2	5.73	125.70	119.40
1	A	258	ALA	N-CA-CB	5.72	118.11	110.10
1	A	327	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	B	1125	PRO	CB-CA-C	-5.71	97.72	112.00
1	C	2063	VAL	CG1-CB-CG2	5.69	120.01	110.90
1	A	241	VAL	CB-CA-C	-5.69	100.59	111.40
1	B	1295	LEU	N-CA-C	-5.69	95.65	111.00
1	A	209	TYR	CG-CD2-CE2	5.68	125.85	121.30
1	C	2061	GLU	CA-CB-CG	-5.68	100.90	113.40
1	A	171	GLY	CA-C-N	-5.68	101.20	117.10
1	B	1092	ALA	N-CA-CB	-5.68	102.15	110.10
1	B	1201	PRO	CA-CB-CG	-5.67	93.22	104.00
1	A	51	LEU	CA-CB-CG	-5.66	102.28	115.30
1	B	1173	MET	CG-SD-CE	-5.65	91.16	100.20
1	B	1295	LEU	CB-CG-CD2	5.65	120.61	111.00
1	A	282	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	C	2076	ARG	CB-CA-C	-5.63	99.15	110.40
1	A	42	SER	O-C-N	-5.62	113.70	122.70
1	A	310	LEU	CA-CB-CG	-5.62	102.38	115.30
1	C	2319	THR	OG1-CB-CG2	-5.62	97.08	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225	TYR	CD1-CE1-CZ	-5.61	114.75	119.80
1	C	2050	THR	CA-CB-OG1	-5.60	97.25	109.00
1	B	1228	PHE	CG-CD1-CE1	-5.59	114.65	120.80
1	C	2132	ALA	CB-CA-C	-5.58	101.73	110.10
1	A	176	TRP	CD1-CG-CD2	5.57	110.76	106.30
1	C	2163	PHE	CD1-CE1-CZ	-5.56	113.43	120.10
1	C	2155	PHE	CB-CG-CD1	-5.55	116.91	120.80
1	B	1225	TYR	CB-CG-CD1	5.55	124.33	121.00
1	C	2095	PHE	CZ-CE2-CD2	5.54	126.75	120.10
1	B	1205	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	357	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	C	2265	LEU	CB-CG-CD1	-5.52	101.61	111.00
1	B	1108	GLU	CG-CD-OE1	5.52	129.34	118.30
1	C	2340	LEU	CD1-CG-CD2	-5.52	93.95	110.50
1	A	339	ASN	N-CA-C	-5.50	96.14	111.00
1	C	2063	VAL	N-CA-C	-5.50	96.14	111.00
1	C	2290	GLY	CA-C-N	5.50	127.20	116.20
1	A	235	TYR	CZ-CE2-CD2	-5.49	114.86	119.80
1	C	2198	GLU	CA-CB-CG	-5.49	101.32	113.40
1	A	173	MET	CB-CG-SD	5.48	128.85	112.40
1	A	265	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	A	167	CYS	CA-CB-SG	-5.48	104.14	114.00
1	C	2173	MET	CB-CA-C	-5.47	99.46	110.40
1	B	1224	THR	OG1-CB-CG2	-5.46	97.44	110.00
1	A	93	MET	N-CA-C	-5.45	96.28	111.00
1	B	1250	ILE	N-CA-C	-5.45	96.29	111.00
1	C	2200	LYS	N-CA-CB	-5.45	100.79	110.60
1	A	274	LEU	CB-CG-CD2	-5.44	101.75	111.00
1	B	1200	LYS	CB-CG-CD	5.44	125.75	111.60
1	C	2266	LYS	CA-CB-CG	5.44	125.37	113.40
1	B	1344	VAL	C-N-CA	-5.44	108.10	121.70
1	C	2195	LYS	CD-CE-NZ	-5.44	99.19	111.70
1	C	2158	THR	CA-C-O	-5.44	108.68	120.10
1	B	1076	ARG	CB-CA-C	-5.43	99.54	110.40
1	A	174	ILE	CA-CB-CG1	-5.43	100.68	111.00
1	C	2094	THR	OG1-CB-CG2	-5.42	97.52	110.00
1	C	2227	ARG	CB-CG-CD	-5.42	97.50	111.60
1	B	1285	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	1276	VAL	CG1-CB-CG2	5.42	119.57	110.90
1	C	2040	ASP	OD1-CG-OD2	5.42	133.59	123.30
1	C	2283	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	C	2069	VAL	CA-CB-CG2	5.42	119.02	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1281	ASN	CB-CA-C	-5.41	99.58	110.40
1	A	354	VAL	CG1-CB-CG2	-5.41	102.25	110.90
1	B	1139	GLY	N-CA-C	-5.41	99.58	113.10
1	C	2216	TYR	CZ-CE2-CD2	-5.41	114.94	119.80
1	C	2370	VAL	CG1-CB-CG2	-5.41	102.25	110.90
1	C	2095	PHE	CE1-CZ-CE2	-5.40	110.28	120.00
1	C	2221	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	A	208	TYR	CG-CD2-CE2	-5.39	116.99	121.30
1	C	2241	VAL	CA-CB-CG2	-5.39	102.82	110.90
1	B	1174	ILE	CA-CB-CG1	-5.39	100.76	111.00
1	A	352	VAL	CA-CB-CG1	-5.38	102.83	110.90
1	B	1367	VAL	CG1-CB-CG2	5.38	119.50	110.90
1	B	1171	GLY	CA-C-O	5.37	130.27	120.60
1	A	282	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	364	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	C	2235	TYR	CD1-CE1-CZ	5.34	124.61	119.80
1	C	2274	LEU	CA-CB-CG	-5.34	103.03	115.30
1	A	77	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	A	89	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	B	1308	ARG	CG-CD-NE	-5.32	100.62	111.80
1	A	155	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	B	1076	ARG	CG-CD-NE	-5.31	100.66	111.80
1	B	1111	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	B	1325	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	1208	TYR	CG-CD2-CE2	5.30	125.54	121.30
1	A	180	SER	CA-CB-OG	-5.29	96.91	111.20
1	C	2192	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	2223	GLY	O-C-N	-5.28	114.25	122.70
1	B	1046	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	C	2076	ARG	CG-CD-NE	-5.28	100.71	111.80
1	A	70	ILE	N-CA-C	-5.27	96.76	111.00
1	C	2065	ALA	CA-C-O	-5.27	109.03	120.10
1	B	1337	ASN	N-CA-CB	-5.27	101.11	110.60
1	B	1112	VAL	CA-CB-CG2	-5.27	103.00	110.90
1	B	1130	PHE	CB-CG-CD1	-5.27	117.11	120.80
1	C	2073	PHE	CZ-CE2-CD2	-5.27	113.78	120.10
1	B	1319	THR	CA-CB-OG1	5.26	120.05	109.00
1	C	2232	SER	CA-CB-OG	-5.25	97.01	111.20
1	A	118	ASN	N-CA-C	-5.25	96.82	111.00
1	A	93	MET	CB-CG-SD	-5.24	96.67	112.40
1	C	2061	GLU	CG-CD-OE1	-5.24	107.82	118.30
1	B	1335	TYR	CD1-CE1-CZ	-5.24	115.09	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1328	LEU	CB-CG-CD2	-5.24	102.10	111.00
1	A	316	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	361	ASP	OD1-CG-OD2	-5.22	113.37	123.30
1	B	1293	GLY	N-CA-C	-5.21	100.06	113.10
1	C	2224	THR	OG1-CB-CG2	-5.20	98.03	110.00
1	B	1061	GLU	CG-CD-OE1	-5.20	107.90	118.30
1	C	2276	VAL	CG1-CB-CG2	5.20	119.21	110.90
1	B	1259	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	B	1046	ARG	CA-CB-CG	-5.19	101.98	113.40
1	B	1108	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	B	1078	ILE	CB-CA-C	-5.18	101.23	111.60
1	A	73	PHE	CB-CA-C	-5.18	100.04	110.40
1	B	1087	ASP	OD1-CG-OD2	-5.17	113.47	123.30
1	B	1182	THR	OG1-CB-CG2	-5.17	98.11	110.00
1	A	178	VAL	CA-CB-CG1	-5.17	103.15	110.90
1	B	1232	SER	CA-CB-OG	-5.16	97.27	111.20
1	B	1181	GLY	C-N-CA	-5.15	108.83	121.70
1	A	216	TYR	N-CA-CB	-5.15	101.34	110.60
1	A	259	LEU	CB-CG-CD2	-5.14	102.25	111.00
1	A	337	ASN	N-CA-C	-5.14	97.12	111.00
1	B	1173	MET	CB-CG-SD	5.14	127.82	112.40
1	B	1325	TYR	CG-CD2-CE2	-5.14	117.19	121.30
1	C	2082	VAL	CG1-CB-CG2	5.13	119.11	110.90
1	C	2204	TYR	CG-CD1-CE1	-5.13	117.19	121.30
1	B	1062	GLN	CA-CB-CG	-5.12	102.12	113.40
1	C	2255	ALA	CB-CA-C	-5.12	102.42	110.10
1	A	160	ALA	C-N-CA	-5.12	111.55	122.30
1	A	327	PHE	CD1-CG-CD2	5.12	124.95	118.30
1	B	1040	ASP	O-C-N	5.12	130.89	122.70
1	A	241	VAL	CA-CB-CG2	-5.11	103.24	110.90
1	A	225	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	B	1164	VAL	CA-CB-CG2	-5.10	103.25	110.90
1	A	283	ASP	OD1-CG-OD2	-5.10	113.61	123.30
1	C	2205	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	B	1081	GLU	CA-CB-CG	-5.09	102.20	113.40
1	C	2152	VAL	CB-CA-C	-5.09	101.73	111.40
1	C	2334	ALA	N-CA-C	-5.09	97.27	111.00
1	B	1196	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	2367	VAL	CG1-CB-CG2	5.08	119.03	110.90
1	C	2179	VAL	CA-CB-CG1	-5.08	103.28	110.90
1	A	262	GLU	CG-CD-OE1	-5.08	108.14	118.30
1	C	2219	LYS	CD-CE-NZ	-5.08	100.02	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2275	PHE	CD1-CE1-CZ	-5.08	114.01	120.10
1	C	2046	ARG	O-C-N	-5.07	114.59	122.70
1	A	319	THR	CB-CA-C	-5.07	97.92	111.60
1	C	2135	GLY	O-C-N	5.06	130.80	122.70
1	C	2308	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	A	157	ALA	O-C-N	5.06	130.79	122.70
1	B	1073	PHE	CD1-CE1-CZ	5.04	126.15	120.10
1	B	1186	ILE	CA-C-O	5.04	130.68	120.10
1	B	1308	ARG	CA-CB-CG	-5.04	102.32	113.40
1	A	187	MET	CA-CB-CG	-5.04	104.74	113.30
1	A	102	PRO	CA-N-CD	5.03	118.74	111.70
1	C	2216	TYR	N-CA-CB	-5.03	101.55	110.60
1	B	1324	LEU	N-CA-CB	-5.03	100.35	110.40
1	C	2261	GLY	CA-C-O	5.02	129.64	120.60
1	A	203	ARG	CB-CG-CD	-5.02	98.54	111.60
1	B	1212	GLU	OE1-CD-OE2	-5.02	117.27	123.30
1	B	1364	GLU	CA-CB-CG	-5.02	102.36	113.40
1	A	203	ARG	CA-C-O	-5.01	109.57	120.10
1	C	2051	LEU	CA-CB-CG	-5.01	103.78	115.30
1	A	62	GLN	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	GLU	Mainchain
1	A	159	ARG	Sidechain
1	A	173	MET	Mainchain
1	A	272	ASN	Mainchain
1	A	352	VAL	Mainchain
1	B	1126	HIS	Mainchain
1	B	1159	ARG	Sidechain
1	B	1169	PRO	Mainchain
1	B	1170	GLY	Mainchain
1	B	1173	MET	Mainchain
1	B	1233	GLU	Sidechain
1	B	1268	LYS	Mainchain
1	B	1317	GLY	Mainchain
1	C	2046	ARG	Mainchain
1	C	2159	ARG	Sidechain
1	C	2169	PRO	Mainchain
1	C	2209	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	2225	TYR	Sidechain
1	C	2278	SER	Mainchain
1	C	2302	PHE	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	2567	0	2477	139	0
1	B	2567	0	2476	116	0
1	C	2567	0	2477	137	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	289	0	0	11	0
3	B	276	0	0	7	0
3	C	289	0	0	9	0
All	All	8561	0	7430	367	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (367) 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:2178:VAL:CB	1:C:2178:VAL:CG1	1.74	1.65
1:A:173:MET:CB	1:A:173:MET:CA	1.74	1.64
1:B:1086:GLU:CB	1:B:1086:GLU:CG	1.75	1.63
1:C:2295:LEU:CG	1:C:2295:LEU:CD1	1.75	1.62
1:A:289:ILE:CB	1:A:289:ILE:CG2	1.75	1.62
1:B:1217:ILE:CG2	1:B:1217:ILE:CB	1.75	1.61
1:C:2039:VAL:CA	1:C:2039:VAL:CB	1.76	1.61
1:B:1244:THR:CG2	1:B:1244:THR:CB	1.75	1.60
1:A:246:ILE:CD1	1:A:246:ILE:CG1	1.77	1.60
1:B:1144:LEU:CD2	1:B:1144:LEU:CG	1.74	1.60
1:B:1048:LYS:CD	1:B:1048:LYS:CE	1.77	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2324:LEU:CD2	1:C:2324:LEU:CG	1.78	1.60
1:C:2259:LEU:CG	1:C:2259:LEU:CD1	1.78	1.59
1:B:1173:MET:CB	1:B:1173:MET:CA	1.79	1.59
1:C:2112:VAL:CA	1:C:2112:VAL:CB	1.75	1.59
1:C:2224:THR:CB	1:C:2224:THR:CG2	1.78	1.58
1:A:173:MET:CB	1:A:173:MET:CG	1.81	1.58
1:B:1174:ILE:CD1	1:B:1174:ILE:CG1	1.81	1.57
1:B:1269:VAL:CG2	1:B:1269:VAL:CB	1.82	1.57
1:C:2048:LYS:CD	1:C:2048:LYS:CG	1.83	1.57
1:A:178:VAL:CG2	1:A:178:VAL:CB	1.75	1.56
1:A:266:LYS:CE	1:A:266:LYS:CD	1.78	1.56
1:A:195:LYS:CE	1:A:195:LYS:CD	1.75	1.56
1:C:2246:ILE:CG1	1:C:2246:ILE:CD1	1.83	1.56
1:B:1195:LYS:CE	1:B:1195:LYS:CD	1.79	1.55
1:B:1039:VAL:CA	1:B:1039:VAL:CB	1.81	1.55
1:A:159:ARG:CG	1:A:159:ARG:CB	1.81	1.55
1:C:2217:ILE:CG1	1:C:2217:ILE:CD1	1.80	1.55
1:A:62:GLN:CD	1:A:62:GLN:CG	1.75	1.54
1:B:1219:LYS:CE	1:B:1219:LYS:NZ	1.67	1.54
1:C:2236:GLU:CD	1:C:2236:GLU:CG	1.74	1.53
1:B:1221:GLU:CD	1:B:1221:GLU:CG	1.76	1.53
1:B:1268:LYS:CD	1:B:1268:LYS:CE	1.81	1.53
1:A:48:LYS:CE	1:A:48:LYS:NZ	1.70	1.53
1:C:2326:LYS:CE	1:C:2326:LYS:NZ	1.70	1.53
1:C:2087:ASP:CG	1:C:2087:ASP:CB	1.74	1.52
1:A:262:GLU:CD	1:A:262:GLU:CG	1.76	1.52
1:B:1357:GLU:CD	1:B:1357:GLU:CG	1.76	1.52
1:A:48:LYS:CE	1:A:48:LYS:CD	1.84	1.51
1:B:1200:LYS:CE	1:B:1200:LYS:CD	1.86	1.51
1:C:2125:PRO:CG	1:C:2125:PRO:CB	1.81	1.50
1:A:87:ASP:CG	1:A:87:ASP:CB	1.80	1.50
1:A:233:GLU:CD	1:A:233:GLU:CG	1.79	1.50
1:C:2065:ALA:CB	1:C:2065:ALA:CA	1.87	1.50
1:B:1048:LYS:CE	1:B:1048:LYS:NZ	1.73	1.50
1:C:2330:PRO:CD	1:C:2330:PRO:CG	1.75	1.49
1:A:268:LYS:CE	1:A:268:LYS:NZ	1.73	1.49
1:C:2048:LYS:CD	1:C:2048:LYS:CE	1.89	1.48
1:A:48:LYS:CD	1:A:48:LYS:CG	1.89	1.48
1:A:86:GLU:CD	1:A:86:GLU:CG	1.80	1.48
1:C:2173:MET:CG	1:C:2173:MET:SD	2.04	1.45
1:C:2156:LYS:CE	1:C:2156:LYS:NZ	1.79	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1262:GLU:CD	1:B:1262:GLU:CG	1.86	1.44
1:A:195:LYS:CE	1:A:195:LYS:NZ	1.82	1.43
1:B:1087:ASP:CG	1:B:1087:ASP:CB	1.85	1.43
1:C:2086:GLU:CG	1:C:2086:GLU:CD	1.85	1.42
1:A:200:LYS:NZ	1:A:200:LYS:CE	1.81	1.42
1:B:1266:LYS:NZ	1:B:1266:LYS:CE	1.82	1.41
1:C:2262:GLU:CD	1:C:2262:GLU:CG	1.93	1.37
1:A:191:ARG:CZ	1:A:191:ARG:NH1	1.91	1.34
1:A:319:THR:CG2	1:A:319:THR:CA	2.06	1.33
1:C:2232:SER:CB	1:C:2232:SER:OG	1.77	1.31
1:C:2266:LYS:NZ	1:C:2266:LYS:CE	1.95	1.30
1:A:48:LYS:NZ	1:A:48:LYS:CD	1.96	1.27
1:A:226:MET:SD	1:A:226:MET:CE	2.27	1.21
1:C:2226:MET:CE	1:C:2226:MET:SD	1.10	1.19
1:A:319:THR:CG2	1:A:319:THR:OG1	1.94	1.15
1:C:2048:LYS:CD	1:C:2048:LYS:NZ	2.08	1.14
1:A:319:THR:CG2	1:A:319:THR:HB	1.59	1.10
1:A:39:VAL:O	1:A:40:ASP:HB3	1.48	1.09
1:C:2226:MET:SD	1:C:2226:MET:HE1	1.69	1.08
1:A:173:MET:HG2	3:A:3773:HOH:O	1.54	1.07
1:C:2226:MET:SD	1:C:2226:MET:HE2	1.69	1.07
1:A:319:THR:CB	1:A:319:THR:HG21	1.55	1.06
1:C:2226:MET:SD	1:C:2226:MET:HE3	1.69	1.06
1:A:319:THR:CB	1:A:319:THR:HG23	1.55	1.05
1:B:1048:LYS:CD	1:B:1048:LYS:NZ	2.20	1.05
1:B:1173:MET:HG3	3:B:3638:HOH:O	1.54	1.04
1:A:319:THR:CB	1:A:319:THR:HG22	1.55	1.02
1:B:1200:LYS:CD	1:B:1200:LYS:NZ	2.22	1.02
1:B:1039:VAL:O	1:B:1040:ASP:HB3	1.59	1.01
1:B:1222:ASP:OD1	1:B:1224:THR:HG23	1.64	0.96
1:C:2039:VAL:O	1:C:2040:ASP:HB3	1.62	0.95
1:B:1040:ASP:OD1	1:B:1041:LEU:N	2.00	0.94
1:A:319:THR:CG2	1:A:319:THR:CB	0.93	0.93
1:A:173:MET:CB	1:A:173:MET:C	2.37	0.92
1:A:48:LYS:CD	1:A:48:LYS:HZ2	1.77	0.92
1:B:1058:HIS:HE1	1:B:1105:ILE:H	1.16	0.92
1:B:1173:MET:CB	1:B:1173:MET:C	2.39	0.89
1:B:1144:LEU:CD2	1:B:1144:LEU:CB	2.51	0.89
3:A:3467:HOH:O	1:C:2039:VAL:HG11	1.72	0.88
1:A:40:ASP:OD1	1:A:41:LEU:N	2.06	0.88
1:C:2295:LEU:CD1	1:C:2295:LEU:CB	2.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2121:GLU:OE1	3:C:3785:HOH:O	1.92	0.86
1:B:1357:GLU:CD	1:B:1357:GLU:CB	2.44	0.85
1:C:2324:LEU:CD2	1:C:2324:LEU:CB	2.55	0.85
1:C:2326:LYS:NZ	1:C:2326:LYS:CD	2.39	0.85
1:B:1144:LEU:CD2	1:B:1144:LEU:CD1	2.54	0.84
1:C:2178:VAL:CG1	1:C:2178:VAL:CG2	2.55	0.84
1:C:2295:LEU:CD1	1:C:2295:LEU:CD2	2.55	0.84
1:A:340:LEU:H	1:C:2281:ASN:ND2	1.74	0.84
1:A:62:GLN:CD	1:A:62:GLN:CB	2.47	0.82
1:B:1040:ASP:CG	1:B:1041:LEU:N	2.32	0.82
1:A:48:LYS:NZ	1:A:48:LYS:HD3	1.94	0.81
1:B:1039:VAL:N	3:B:3809:HOH:O	2.14	0.81
1:C:2226:MET:CE	1:C:2226:MET:CG	2.59	0.81
1:B:1058:HIS:CE1	1:B:1105:ILE:H	1.98	0.80
1:C:2156:LYS:NZ	1:C:2156:LYS:CD	2.43	0.80
1:C:2040:ASP:CG	1:C:2041:LEU:H	1.81	0.79
1:A:173:MET:HE2	1:A:173:MET:HA	1.64	0.79
1:A:40:ASP:CG	1:A:41:LEU:H	1.81	0.79
1:A:39:VAL:O	1:A:40:ASP:CB	2.27	0.79
1:C:2112:VAL:CA	1:C:2112:VAL:CG2	2.59	0.79
1:A:222:ASP:OD1	1:A:224:THR:HG23	1.83	0.78
1:A:262:GLU:OE2	3:A:3715:HOH:O	2.00	0.78
1:B:1195:LYS:CE	1:B:1195:LYS:CG	2.60	0.78
1:C:2048:LYS:NZ	1:C:2048:LYS:HD3	1.98	0.78
1:A:48:LYS:HZ2	1:A:48:LYS:HD2	1.45	0.78
1:A:266:LYS:CE	1:A:266:LYS:CG	2.59	0.78
1:C:2259:LEU:CD1	1:C:2259:LEU:CB	2.62	0.78
1:B:1053:PRO:HD2	3:B:3442:HOH:O	1.83	0.77
1:C:2040:ASP:CG	1:C:2041:LEU:N	2.34	0.77
1:B:1077:ILE:N	1:B:1077:ILE:HD12	1.98	0.77
1:C:2039:VAL:CA	1:C:2039:VAL:CG1	2.63	0.77
1:C:2112:VAL:CA	1:C:2112:VAL:CG1	2.62	0.76
1:C:2048:LYS:CD	1:C:2048:LYS:HZ2	1.99	0.76
1:A:40:ASP:CG	1:A:41:LEU:N	2.34	0.75
1:B:1269:VAL:CG2	1:B:1269:VAL:CG1	2.65	0.75
1:C:2222:ASP:OD1	1:C:2224:THR:HG23	1.86	0.74
1:C:2324:LEU:CD2	1:C:2324:LEU:CD1	2.64	0.74
1:B:1048:LYS:NZ	1:B:1048:LYS:HD3	2.03	0.74
1:C:2058:HIS:HE1	1:C:2105:ILE:H	1.36	0.74
1:C:2112:VAL:CB	1:C:2112:VAL:C	2.56	0.74
1:B:1200:LYS:HE3	3:B:3789:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1040:ASP:CG	1:B:1041:LEU:H	1.82	0.72
1:A:40:ASP:OD2	3:A:3685:HOH:O	2.06	0.72
1:A:191:ARG:NE	3:A:3798:HOH:O	1.77	0.72
1:A:262:GLU:CD	1:A:262:GLU:CB	2.53	0.72
1:C:2178:VAL:CG1	1:C:2178:VAL:CA	2.67	0.72
1:C:2236:GLU:HG3	3:C:3679:HOH:O	1.90	0.71
1:B:1268:LYS:CD	1:B:1268:LYS:NZ	2.55	0.70
1:A:178:VAL:CG2	1:A:178:VAL:CA	2.69	0.70
1:B:1289:ILE:HD12	1:B:1334:ALA:HB3	1.73	0.70
1:C:2224:THR:CG2	1:C:2224:THR:OG1	2.38	0.70
1:C:2040:ASP:OD1	1:C:2041:LEU:N	2.20	0.70
1:B:1217:ILE:CG2	1:B:1217:ILE:CG1	2.69	0.69
1:A:58:HIS:HE1	1:A:105:ILE:H	1.39	0.69
1:A:246:ILE:CD1	1:A:246:ILE:CB	2.68	0.69
1:A:58:HIS:CE1	1:A:105:ILE:H	2.11	0.68
1:C:2266:LYS:NZ	1:C:2266:LYS:HG3	2.08	0.68
1:C:2039:VAL:O	1:C:2040:ASP:CB	2.40	0.68
1:C:2167:CYS:HB2	1:C:2182:THR:HB	1.74	0.68
1:A:289:ILE:CG2	1:A:289:ILE:CA	2.71	0.68
1:A:344:VAL:HG11	1:C:2172:PRO:HA	1.75	0.68
1:C:2217:ILE:CD1	1:C:2217:ILE:CB	2.71	0.67
1:A:312:THR:HB	1:C:2319:THR:CG2	2.25	0.67
1:B:1281:ASN:O	1:C:2339:ASN:HA	1.94	0.67
1:A:159:ARG:CG	1:A:159:ARG:CA	2.72	0.66
1:C:2266:LYS:NZ	1:C:2266:LYS:CG	2.58	0.66
1:C:2197:HIS:CE1	1:C:2308:ARG:HD3	2.30	0.66
1:A:173:MET:HA	1:A:173:MET:CE	2.25	0.66
1:C:2173:MET:CG	1:C:2173:MET:CE	2.68	0.66
1:B:1200:LYS:CD	1:B:1200:LYS:HZ2	2.06	0.66
1:B:1219:LYS:NZ	1:B:1219:LYS:CD	2.57	0.66
1:B:1269:VAL:CG2	1:B:1269:VAL:CA	2.73	0.66
1:B:1173:MET:CB	1:B:1173:MET:N	2.56	0.65
1:C:2058:HIS:O	1:C:2060:HIS:HD2	1.77	0.65
1:B:1203:ARG:NE	3:B:3401:HOH:O	2.03	0.65
1:B:1174:ILE:CD1	1:B:1174:ILE:CB	2.73	0.65
1:A:281:ASN:ND2	1:B:1340:LEU:H	1.95	0.65
1:C:2200:LYS:HE3	3:C:3589:HOH:O	1.94	0.65
1:B:1200:LYS:NZ	1:B:1200:LYS:HD3	2.10	0.64
1:B:1281:ASN:ND2	1:C:2340:LEU:H	1.96	0.64
1:A:159:ARG:CB	1:A:159:ARG:CD	2.68	0.63
1:A:289:ILE:CG2	1:A:289:ILE:CG1	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1244:THR:CG2	1:B:1244:THR:CA	2.74	0.63
1:B:1339:ASN:C	1:B:1339:ASN:HD22	2.02	0.63
1:A:340:LEU:H	1:C:2281:ASN:HD21	1.47	0.63
1:C:2048:LYS:HD3	1:C:2048:LYS:HZ3	1.63	0.63
1:B:1268:LYS:CE	1:B:1268:LYS:CG	2.75	0.62
1:C:2039:VAL:CA	1:C:2039:VAL:CG2	2.75	0.62
1:A:179:VAL:O	1:A:215:HIS:HD2	1.82	0.62
1:C:2058:HIS:CE1	1:C:2105:ILE:H	2.17	0.62
1:A:266:LYS:HG3	1:A:266:LYS:NZ	2.14	0.62
1:A:319:THR:CG2	1:A:319:THR:N	2.61	0.62
1:A:127:ASN:HB3	1:A:144:LEU:HA	1.80	0.61
1:A:319:THR:HG23	1:A:319:THR:N	2.15	0.61
1:A:62:GLN:CG	1:A:62:GLN:NE2	2.58	0.60
1:B:1319:THR:CG2	1:C:2312:THR:HB	2.31	0.60
1:B:1060:HIS:HE1	1:B:1204:TYR:OH	1.84	0.60
1:B:1039:VAL:HG21	3:C:3695:HOH:O	2.01	0.60
1:B:1213:SER:OG	1:B:1215:HIS:HE1	1.84	0.60
1:A:339:ASN:HD22	1:A:341:ILE:H	1.49	0.59
1:A:58:HIS:HD2	1:A:59:ALA:O	1.85	0.59
1:B:1048:LYS:CD	1:B:1048:LYS:HZ2	2.13	0.59
1:C:2324:LEU:CD2	1:C:2324:LEU:HB2	2.32	0.59
1:B:1218:PRO:HB2	1:B:1226:MET:CE	2.33	0.59
1:C:2339:ASN:C	1:C:2339:ASN:HD22	2.06	0.59
1:A:266:LYS:CD	1:A:266:LYS:NZ	2.65	0.59
1:C:2040:ASP:OD2	3:C:3269:HOH:O	2.17	0.58
1:A:233:GLU:CG	1:A:233:GLU:OE1	2.46	0.58
1:B:1039:VAL:CA	1:B:1039:VAL:CG2	2.77	0.58
1:B:1086:GLU:CG	1:B:1086:GLU:CA	2.77	0.57
1:A:178:VAL:CG2	1:A:178:VAL:CG1	2.78	0.57
1:A:266:LYS:CG	1:A:266:LYS:NZ	2.68	0.57
1:A:370:VAL:HG22	1:A:371:GLY:N	2.20	0.57
1:B:1058:HIS:HE1	1:B:1105:ILE:N	1.97	0.57
1:B:1217:ILE:CG2	1:B:1217:ILE:CA	2.78	0.56
1:A:154:ARG:HD2	3:A:3611:HOH:O	2.05	0.56
1:A:339:ASN:HD22	1:A:339:ASN:C	2.09	0.56
1:B:1213:SER:OG	1:B:1215:HIS:CE1	2.58	0.56
1:A:281:ASN:O	1:B:1339:ASN:HA	2.06	0.56
1:C:2326:LYS:NZ	1:C:2326:LYS:HG3	2.21	0.56
1:B:1154:ARG:NH1	3:B:3808:HOH:O	2.39	0.56
1:B:1039:VAL:O	1:B:1040:ASP:CB	2.37	0.55
1:A:233:GLU:CD	1:A:233:GLU:CB	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2266:LYS:HG3	1:C:2266:LYS:HZ3	1.71	0.55
1:A:287:HIS:HD2	1:A:289:ILE:HG12	1.70	0.55
1:B:1060:HIS:CE1	1:B:1204:TYR:OH	2.60	0.55
1:A:173:MET:CA	1:A:173:MET:CE	2.85	0.55
1:B:1173:MET:HE2	1:B:1173:MET:HA	1.88	0.55
1:A:167:CYS:HB2	1:A:182:THR:HB	1.88	0.54
1:A:339:ASN:ND2	1:A:341:ILE:H	2.05	0.54
1:B:1297:TRP:CE2	1:B:1306:PRO:HB3	2.42	0.54
1:C:2197:HIS:HA	1:C:2306:PRO:HD2	1.89	0.54
1:A:173:MET:CG	3:A:3773:HOH:O	2.31	0.54
1:A:319:THR:HG22	1:B:1311:GLU:CG	2.37	0.54
1:C:2326:LYS:NZ	1:C:2326:LYS:CG	2.70	0.54
1:A:173:MET:C	1:A:173:MET:HB3	2.25	0.54
1:B:1218:PRO:HB2	1:B:1226:MET:HE3	1.90	0.54
1:C:2173:MET:CG	1:C:2173:MET:HE2	2.38	0.53
1:A:66:SER:O	1:A:191:ARG:NH2	2.42	0.53
1:C:2167:CYS:HB2	1:C:2182:THR:CB	2.39	0.53
1:C:2171:GLY:O	1:C:2173:MET:N	2.41	0.53
1:C:2246:ILE:CD1	1:C:2246:ILE:CB	2.81	0.52
1:B:1172:PRO:HA	1:C:2344:VAL:HG11	1.92	0.52
1:C:2061:GLU:OE1	1:C:2065:ALA:HB2	2.10	0.52
1:A:268:LYS:NZ	1:A:268:LYS:CD	2.70	0.52
1:A:339:ASN:HA	1:C:2281:ASN:O	2.10	0.52
1:C:2179:VAL:O	1:C:2215:HIS:HD2	1.92	0.52
1:A:267:ALA:O	1:A:354:VAL:HA	2.10	0.51
1:A:262:GLU:CG	1:A:262:GLU:OE1	2.54	0.51
1:A:287:HIS:CD2	1:A:289:ILE:HG12	2.46	0.51
1:C:2232:SER:OG	1:C:2232:SER:CA	2.53	0.51
1:A:218:PRO:HB2	1:A:226:MET:CE	2.41	0.51
1:A:54:PRO:HB2	1:A:253:ASN:HD21	1.76	0.51
1:A:319:THR:HG22	1:B:1311:GLU:HG3	1.91	0.50
1:B:1173:MET:C	1:B:1173:MET:HB3	2.29	0.50
1:C:2048:LYS:HZ2	1:C:2048:LYS:HD2	1.76	0.50
1:C:2224:THR:CG2	1:C:2224:THR:CA	2.82	0.50
1:A:48:LYS:HD3	1:A:48:LYS:HZ3	1.71	0.50
1:C:2171:GLY:O	1:C:2172:PRO:C	2.47	0.50
1:C:2213:SER:OG	1:C:2215:HIS:CE1	2.64	0.50
1:B:1179:VAL:O	1:B:1215:HIS:HD2	1.94	0.50
1:C:2127:ASN:HB3	1:C:2144:LEU:HA	1.94	0.50
1:B:1119:PRO:HD2	1:B:1122:ASN:ND2	2.27	0.49
1:C:2112:VAL:CB	1:C:2112:VAL:N	2.68	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1048:LYS:HD2	1:B:1049:HIS:N	2.27	0.49
1:C:2370:VAL:HG22	1:C:2371:GLY:N	2.27	0.49
1:A:344:VAL:CG1	1:C:2172:PRO:HA	2.42	0.49
1:A:163:PHE:O	1:A:185:CYS:HA	2.13	0.49
1:A:285:ARG:HA	1:A:313:TRP:O	2.13	0.49
1:B:1319:THR:HG21	1:C:2312:THR:HB	1.94	0.49
1:C:2060:HIS:HE1	1:C:2204:TYR:OH	1.95	0.49
1:B:1222:ASP:OD1	1:B:1222:ASP:C	2.51	0.49
1:A:173:MET:CA	1:A:173:MET:HE3	2.43	0.48
1:A:340:LEU:N	1:C:2281:ASN:HD21	2.11	0.48
1:C:2287:HIS:CD2	1:C:2289:ILE:HG12	2.47	0.48
1:C:2154:ARG:HD2	3:C:3248:HOH:O	2.14	0.48
1:B:1195:LYS:CD	1:B:1195:LYS:NZ	2.66	0.48
1:C:2326:LYS:CD	1:C:2326:LYS:HZ3	2.24	0.48
1:A:173:MET:CB	1:A:173:MET:N	2.62	0.48
1:A:339:ASN:HD22	1:A:341:ILE:N	2.10	0.48
1:C:2210:ILE:HD12	1:C:2210:ILE:HG23	1.65	0.48
1:B:1197:HIS:CE1	1:B:1308:ARG:HD3	2.49	0.47
1:C:2195:LYS:HE2	1:C:2201:PRO:HG3	1.96	0.47
1:C:2224:THR:CG2	1:C:2224:THR:HG1	2.25	0.47
1:A:174:ILE:N	1:A:175:PRO:HD2	2.29	0.47
1:C:2259:LEU:CD1	1:C:2259:LEU:CD2	2.83	0.47
1:A:93:MET:HE1	1:A:176:TRP:CZ3	2.49	0.47
1:B:1287:HIS:CD2	1:B:1338:HIS:HD2	2.33	0.47
1:A:170:GLY:H	1:A:174:ILE:HG13	1.79	0.47
1:A:174:ILE:HB	1:A:175:PRO:HD3	1.96	0.47
1:B:1319:THR:HG22	1:C:2311:GLU:HG3	1.97	0.47
1:A:172:PRO:HA	1:B:1344:VAL:HG11	1.96	0.47
1:C:2217:ILE:CD1	1:C:2217:ILE:CA	2.94	0.47
1:B:1262:GLU:CD	1:B:1262:GLU:CB	2.69	0.46
1:A:311:GLU:HG3	1:C:2319:THR:HG22	1.98	0.46
1:C:2039:VAL:CB	1:C:2039:VAL:C	2.77	0.46
1:C:2287:HIS:HD2	1:C:2289:ILE:HG12	1.80	0.46
1:B:1222:ASP:OD1	1:B:1224:THR:CG2	2.52	0.46
1:A:312:THR:HB	1:C:2319:THR:HG22	1.98	0.46
1:A:319:THR:CA	1:A:319:THR:HG22	2.18	0.46
1:B:1048:LYS:HD3	1:B:1048:LYS:HZ3	1.80	0.45
1:A:58:HIS:O	1:A:60:HIS:HD2	1.99	0.45
1:A:197:HIS:ND1	1:A:197:HIS:N	2.64	0.45
1:A:319:THR:CG2	1:B:1312:THR:HB	2.47	0.45
1:A:330:PRO:HD2	1:A:358:TRP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1218:PRO:HB2	1:B:1226:MET:HE2	1.98	0.45
1:A:53:PRO:HD2	3:A:3632:HOH:O	2.17	0.45
1:C:2161:GLY:HA2	1:C:2302:PHE:CD2	2.52	0.45
1:B:1173:MET:HA	1:B:1173:MET:CE	2.47	0.45
1:A:233:GLU:O	1:A:233:GLU:HG2	2.16	0.44
1:C:2326:LYS:HG3	1:C:2326:LYS:HZ2	1.82	0.44
1:A:87:ASP:CG	1:A:87:ASP:CA	2.75	0.44
1:A:169:PRO:HG2	1:A:177:HIS:CE1	2.52	0.44
1:B:1058:HIS:HD2	1:B:1059:ALA:O	2.00	0.44
1:C:2213:SER:OG	1:C:2215:HIS:HE1	2.00	0.44
1:A:295:LEU:HD12	1:A:324:LEU:HD23	2.00	0.44
1:B:1361:ASP:HA	3:B:3287:HOH:O	2.17	0.43
1:B:1173:MET:CA	1:B:1173:MET:CE	2.96	0.43
1:B:1150:LYS:O	1:C:2369:PRO:HA	2.17	0.43
1:A:175:PRO:HG3	1:B:1344:VAL:HB	2.01	0.43
1:A:300:GLY:O	1:A:301:LYS:HD3	2.19	0.43
1:C:2044:LEU:HA	1:C:2045:PRO:HD3	1.84	0.43
1:A:163:PHE:CE2	1:A:301:LYS:HE3	2.54	0.43
1:B:1271:ASP:O	1:B:1326:LYS:HA	2.18	0.43
1:B:1285:ARG:HA	1:B:1313:TRP:O	2.18	0.43
1:A:195:LYS:HG2	3:A:3554:HOH:O	2.19	0.43
1:C:2216:TYR:O	1:C:2238:MET:HG3	2.19	0.43
1:A:54:PRO:HB2	1:A:253:ASN:ND2	2.34	0.43
1:A:66:SER:HB2	1:A:67:GLY:H	1.70	0.43
1:A:218:PRO:HB2	1:A:226:MET:HE3	2.00	0.43
1:A:81:GLU:OE2	1:A:227:ARG:HD3	2.19	0.42
1:C:2236:GLU:CB	3:C:3679:HOH:O	2.67	0.42
1:B:1081:GLU:OE2	1:B:1227:ARG:HD3	2.18	0.42
1:B:1210:ILE:O	1:B:1277:HIS:HA	2.19	0.42
1:A:171:GLY:O	1:A:172:PRO:C	2.58	0.42
1:C:2081:GLU:OE2	1:C:2227:ARG:HD3	2.18	0.42
1:A:370:VAL:HG22	1:A:371:GLY:H	1.85	0.42
1:A:303:HIS:HD2	3:A:3377:HOH:O	2.01	0.42
1:C:2039:VAL:CB	1:C:2039:VAL:HA	2.19	0.42
1:A:39:VAL:O	3:A:3511:HOH:O	2.22	0.42
1:A:316:ARG:HG2	1:B:1314:PHE:HB2	2.01	0.42
1:B:1048:LYS:HD2	1:B:1049:HIS:H	1.85	0.42
1:C:2166:HIS:HA	1:C:2183:ALA:HA	2.01	0.41
1:B:1273:VAL:O	1:B:1324:LEU:HA	2.20	0.41
1:A:77:ILE:HD12	1:A:77:ILE:N	2.35	0.41
1:A:93:MET:HE1	1:A:176:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1058:HIS:O	1:B:1060:HIS:HD2	2.03	0.41
1:B:1200:LYS:HA	1:B:1201:PRO:HD3	1.81	0.41
1:C:2076:ARG:HH11	1:C:2076:ARG:HD2	1.56	0.41
1:C:2200:LYS:HA	1:C:2201:PRO:HD3	2.00	0.41
1:B:1058:HIS:CE1	1:B:1105:ILE:N	2.77	0.41
1:A:319:THR:CG2	1:A:319:THR:HG1	2.25	0.41
1:B:1133:ALA:HB1	1:C:2363:MET:CE	2.51	0.41
1:C:2173:MET:CE	1:C:2173:MET:CA	2.99	0.41
1:C:2203:ARG:HH11	1:C:2203:ARG:HD2	1.81	0.41
1:C:2216:TYR:CD1	1:C:2216:TYR:N	2.88	0.41
1:C:2339:ASN:ND2	1:C:2341:ILE:H	2.18	0.41
1:B:1333:TYR:HB2	1:B:1352:VAL:HB	2.03	0.41
1:B:1039:VAL:HA	3:C:3512:HOH:O	2.21	0.41
1:A:174:ILE:HB	1:A:175:PRO:CD	2.50	0.41
1:A:217:ILE:N	1:A:217:ILE:HD13	2.36	0.41
1:B:1077:ILE:HG21	1:B:1126:HIS:CD2	2.56	0.41
1:B:1287:HIS:CD2	1:B:1289:ILE:HG12	2.56	0.41
1:C:2173:MET:SD	1:C:2173:MET:CB	3.04	0.41
1:C:2196:ASP:OD1	1:C:2198:GLU:N	2.50	0.41
1:B:1054:PRO:HB2	1:B:1253:ASN:ND2	2.36	0.41
1:B:1173:MET:CA	1:B:1173:MET:HE3	2.51	0.40
1:C:2058:HIS:HD2	1:C:2059:ALA:O	2.04	0.40
1:C:2266:LYS:NZ	1:C:2266:LYS:CD	2.82	0.40
1:C:2173:MET:HE2	1:C:2173:MET:CB	2.51	0.40
1:A:77:ILE:HG21	1:A:126:HIS:CD2	2.56	0.40
1:C:2203:ARG:NE	3:C:3331:HOH:O	2.30	0.40
1:A:200:LYS:HA	1:A:201:PRO:HD3	1.98	0.40
1:C:2100:PRO:HG3	1:C:2211:GLY:HA3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	332/334 (99%)	321 (97%)	10 (3%)	1 (0%)	41	37
1	B	332/334 (99%)	319 (96%)	12 (4%)	1 (0%)	41	37
1	C	332/334 (99%)	316 (95%)	15 (4%)	1 (0%)	41	37
All	All	996/1002 (99%)	956 (96%)	37 (4%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	B	1040	ASP
1	C	2040	ASP

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	270/270 (100%)	258 (96%)	12 (4%)	28	25
1	B	270/270 (100%)	254 (94%)	16 (6%)	19	15
1	C	270/270 (100%)	257 (95%)	13 (5%)	25	22
All	All	810/810 (100%)	769 (95%)	41 (5%)	24	19

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	40	ASP
1	A	55	PRO
1	A	86	GLU
1	A	173	MET
1	A	182	THR
1	A	195	LYS
1	A	280	PRO
1	A	324	LEU
1	A	339	ASN

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Mol	Chain	Res	Type
1	A	357	GLU
1	A	369	PRO
1	B	1039	VAL
1	B	1040	ASP
1	B	1048	LYS
1	B	1086	GLU
1	B	1124	MET
1	B	1147	PRO
1	B	1173	MET
1	B	1182	THR
1	B	1227	ARG
1	B	1231	PRO
1	B	1253	ASN
1	B	1262	GLU
1	B	1280	PRO
1	B	1324	LEU
1	B	1339	ASN
1	B	1357	GLU
1	C	2039	VAL
1	C	2086	GLU
1	C	2147	PRO
1	C	2173	MET
1	C	2182	THR
1	C	2200	LYS
1	C	2214	ASP
1	C	2230	ASP
1	C	2253	ASN
1	C	2324	LEU
1	C	2339	ASN
1	C	2357	GLU
1	C	2369	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	60	HIS
1	A	215	HIS
1	A	253	ASN
1	A	281	ASN
1	A	339	ASN
1	B	1058	HIS

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Mol	Chain	Res	Type
1	B	1060	HIS
1	B	1215	HIS
1	B	1253	ASN
1	B	1281	ASN
1	B	1339	ASN
1	C	2058	HIS
1	C	2060	HIS
1	C	2215	HIS
1	C	2253	ASN
1	C	2281	ASN
1	C	2339	ASN

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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.