Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:32 PM GMT

PDB ID	:	1U5I
Title	:	Crystal Structure analysis of rat m-calpain mutant Lys10 Thr
Authors	:	Hosfield, C.M.; Pal, G.P.; Elce, J.S.; Jia, Z.
Deposited on	:	2004-07-27
Resolution	:	2.86 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
http://wwpdb.org/validation/2016/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:

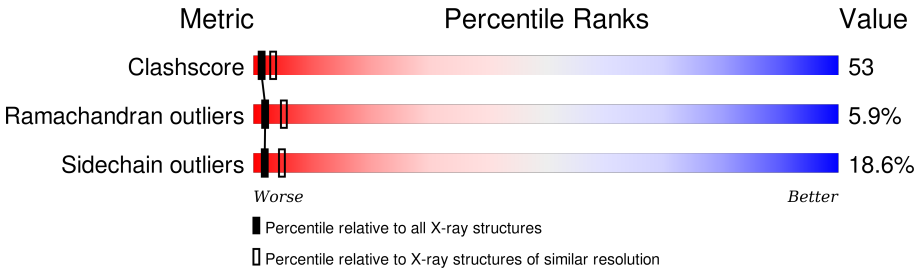
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.86 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	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	700	12% 37% 29% 10% 11%
2	B	184	20% 34% 33% 10% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6706 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 Calpain 2, large [catalytic] subunit precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			4980	3176	836	945	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	THR	LYS	ENGINEERED	UNP Q07009
A	105	SER	CYS	ENGINEERED	UNP Q07009

- Molecule 2 is a protein called Calpain small subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1427	897	246	274	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP Q64537

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		
3	B	52	Total	O	0	0
			52	52		

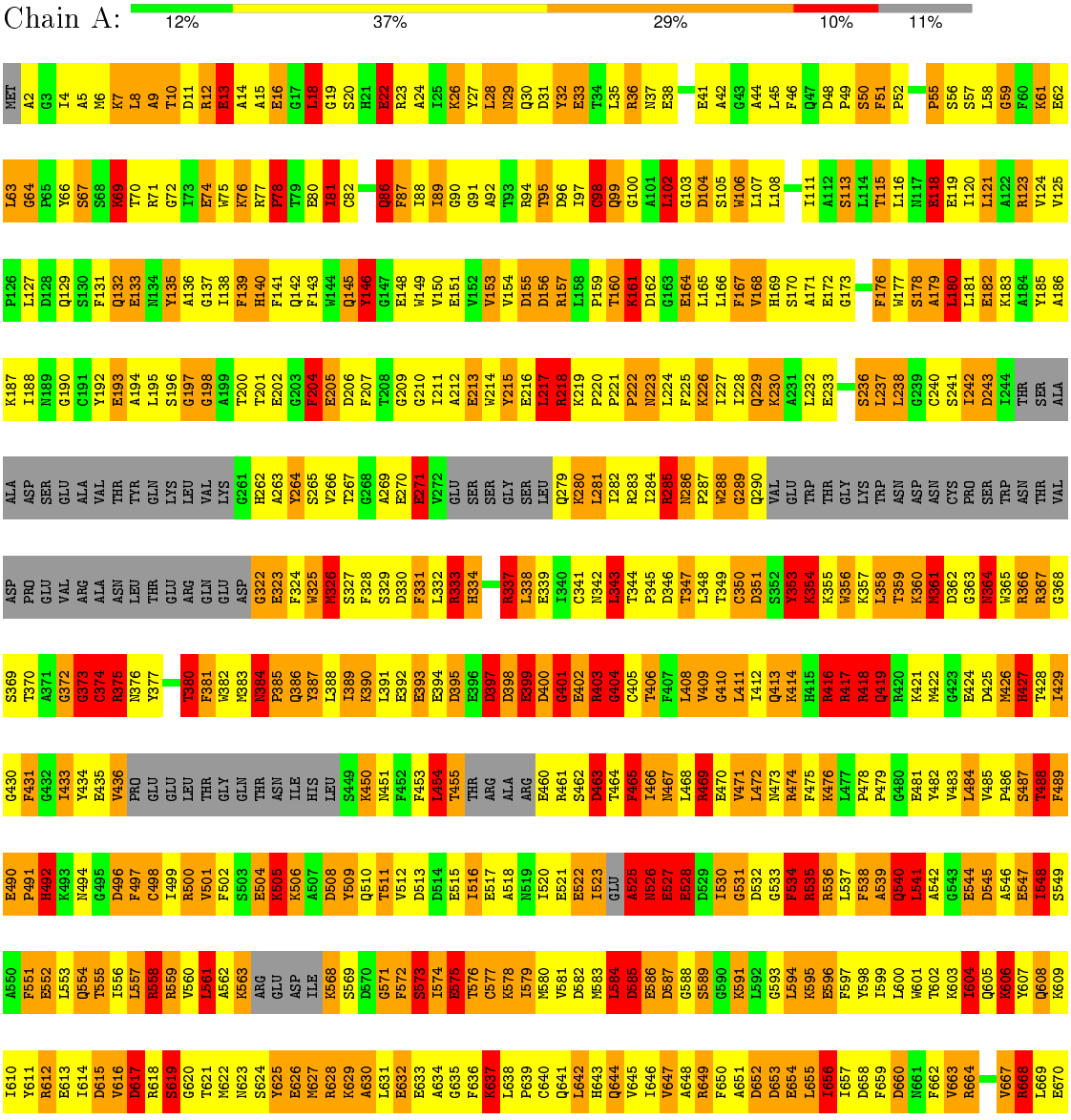
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

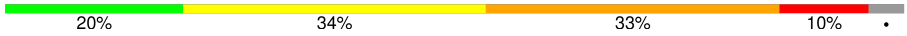
- Molecule 1: Calpain 2, large [catalytic] subunit precursor

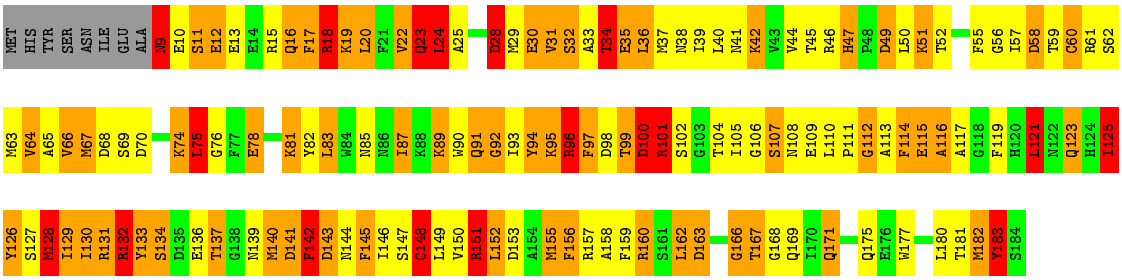
Chain A:



- Molecule 2: Calpain small subunit 1

Chain B:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.66Å 156.52Å 64.23Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	25.00 – 2.86	Depositor
% Data completeness (in resolution range)	90.1 (25.00-2.86)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.191 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6706	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	3.07	491/5083 (9.7%)	2.24	221/6854 (3.2%)
2	B	2.76	104/1454 (7.2%)	2.06	43/1955 (2.2%)
All	All	3.01	595/6537 (9.1%)	2.20	264/8809 (3.0%)

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	19
2	B	0	2
All	All	0	21

All (595) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	ASP	C-N	31.66	1.90	1.33
1	A	402	GLU	C-N	23.12	1.87	1.34
2	B	133	TYR	CD2-CE2	15.60	1.62	1.39
1	A	417	ARG	CG-CD	14.55	1.88	1.51
1	A	628	ARG	CZ-NH2	14.16	1.51	1.33
1	A	205	GLU	CD-OE2	-14.00	1.10	1.25
1	A	7	LYS	CD-CE	13.91	1.86	1.51
1	A	527	GLU	C-N	-13.60	1.02	1.34
1	A	699	VAL	CA-CB	13.28	1.82	1.54
1	A	521	GLU	C-N	13.26	1.64	1.34
1	A	218	ARG	CG-CD	13.21	1.84	1.51
1	A	374	CYS	CB-SG	-13.01	1.60	1.82
1	A	226	LYS	CD-CE	12.89	1.83	1.51
1	A	74	GLU	CD-OE2	12.68	1.39	1.25
1	A	356	TRP	CZ3-CH2	-12.61	1.19	1.40
2	B	177	TRP	CE3-CZ3	12.30	1.59	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	156	PHE	CG-CD2	11.97	1.56	1.38
1	A	7	LYS	CE-NZ	11.87	1.78	1.49
1	A	153	VAL	CB-CG2	-11.86	1.27	1.52
1	A	676	PHE	CE2-CZ	11.78	1.59	1.37
1	A	699	VAL	CB-CG1	11.76	1.77	1.52
1	A	27	TYR	CE2-CZ	-11.75	1.23	1.38
1	A	540	GLN	CB-CG	11.74	1.84	1.52
1	A	375	ARG	CG-CD	11.71	1.81	1.51
1	A	146	TYR	CE2-CZ	-11.43	1.23	1.38
1	A	527	GLU	C-O	11.33	1.44	1.23
1	A	409	VAL	CB-CG1	11.26	1.76	1.52
2	B	137	THR	CA-CB	11.21	1.82	1.53
1	A	148	GLU	CD-OE1	11.01	1.37	1.25
2	B	133	TYR	CE1-CZ	10.99	1.52	1.38
1	A	685	GLY	C-O	-10.91	1.06	1.23
1	A	161	LYS	CB-CG	10.85	1.81	1.52
1	A	674	LYS	CE-NZ	10.72	1.75	1.49
1	A	522	GLU	C-N	10.67	1.58	1.34
1	A	668	ARG	NE-CZ	10.52	1.46	1.33
2	B	58	ASP	CB-CG	10.49	1.73	1.51
1	A	105	SER	CA-CB	10.35	1.68	1.52
1	A	422	MET	CG-SD	-10.24	1.54	1.81
1	A	118	GLU	CG-CD	10.23	1.67	1.51
1	A	27	TYR	CD1-CE1	-10.20	1.24	1.39
1	A	192	TYR	CE1-CZ	-10.16	1.25	1.38
1	A	403	ARG	C-N	10.02	1.51	1.33
1	A	628	ARG	CG-CD	9.99	1.76	1.51
1	A	654	GLU	CD-OE2	9.88	1.36	1.25
1	A	226	LYS	CE-NZ	9.72	1.73	1.49
1	A	365	TRP	CG-CD1	-9.70	1.23	1.36
1	A	434	TYR	CB-CG	-9.61	1.37	1.51
1	A	674	LYS	CD-CE	9.57	1.75	1.51
1	A	435	GLU	CD-OE1	9.54	1.36	1.25
1	A	431	PHE	CG-CD2	-9.53	1.24	1.38
1	A	422	MET	C-O	9.49	1.41	1.23
1	A	142	GLN	C-O	9.39	1.41	1.23
1	A	322	GLY	C-O	9.32	1.38	1.23
1	A	118	GLU	CB-CG	9.28	1.69	1.52
1	A	141	PHE	CG-CD2	9.22	1.52	1.38
1	A	632	GLU	CG-CD	9.16	1.65	1.51
1	A	46	PHE	CE1-CZ	9.12	1.54	1.37
1	A	387	TYR	CE2-CZ	9.11	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	MET	CG-SD	9.10	2.04	1.81
1	A	382	TRP	C-O	9.06	1.40	1.23
1	A	364	ASN	CB-CG	-9.03	1.30	1.51
1	A	410	GLY	C-O	8.92	1.38	1.23
1	A	490	GLU	CD-OE2	8.92	1.35	1.25
1	A	151	GLU	CD-OE2	8.88	1.35	1.25
1	A	660	ASP	C-O	-8.80	1.06	1.23
1	A	148	GLU	C-O	8.80	1.40	1.23
1	A	364	ASN	N-CA	-8.79	1.28	1.46
2	B	160	ARG	CG-CD	8.79	1.74	1.51
1	A	548	ILE	CA-CB	-8.69	1.34	1.54
2	B	177	TRP	CD2-CE3	-8.66	1.27	1.40
1	A	431	PHE	CD2-CE2	-8.65	1.22	1.39
1	A	213	GLU	CD-OE1	8.62	1.35	1.25
1	A	44	ALA	CA-CB	-8.59	1.34	1.52
2	B	156	PHE	CD1-CE1	8.59	1.56	1.39
2	B	70	ASP	CB-CG	-8.58	1.33	1.51
1	A	455	THR	CB-CG2	8.52	1.80	1.52
1	A	24	ALA	CA-CB	8.46	1.70	1.52
1	A	627	MET	SD-CE	-8.45	1.30	1.77
2	B	69	SER	CB-OG	-8.44	1.31	1.42
1	A	135	TYR	CG-CD1	-8.43	1.28	1.39
2	B	155	MET	CG-SD	8.41	2.03	1.81
2	B	175	GLN	CG-CD	8.39	1.70	1.51
1	A	125	VAL	CB-CG2	8.38	1.70	1.52
1	A	608	GLN	C-O	-8.38	1.07	1.23
1	A	233	GLU	CD-OE1	8.37	1.34	1.25
1	A	606	LYS	CG-CD	8.36	1.80	1.52
1	A	474	ARG	CG-CD	8.35	1.72	1.51
1	A	334	HIS	N-CA	8.32	1.62	1.46
1	A	197	GLY	C-O	8.30	1.36	1.23
1	A	414	LYS	C-O	-8.30	1.07	1.23
2	B	115	GLU	CG-CD	8.30	1.64	1.51
1	A	677	LYS	CD-CE	8.27	1.72	1.51
1	A	218	ARG	CB-CG	8.26	1.74	1.52
1	A	46	PHE	CB-CG	8.26	1.65	1.51
1	A	578	LYS	C-O	8.25	1.39	1.23
1	A	401	GLY	C-N	-8.22	1.15	1.34
1	A	98	CYS	CB-SG	8.20	1.96	1.82
1	A	361	MET	CG-SD	8.16	2.02	1.81
2	B	83	LEU	C-O	-8.12	1.07	1.23
2	B	148	CYS	CB-SG	-8.10	1.68	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	512	VAL	CA-CB	8.10	1.71	1.54
2	B	82	TYR	CG-CD1	-8.10	1.28	1.39
1	A	681	PRO	CA-C	-8.09	1.36	1.52
2	B	129	ILE	C-O	8.09	1.38	1.23
1	A	575	GLU	CD-OE2	8.07	1.34	1.25
1	A	634	ALA	CA-CB	-8.06	1.35	1.52
2	B	128	MET	CG-SD	8.06	2.02	1.81
1	A	539	ALA	CA-CB	8.02	1.69	1.52
1	A	204	PHE	CD2-CE2	-7.97	1.23	1.39
1	A	637	LYS	CD-CE	7.97	1.71	1.51
1	A	125	VAL	C-O	-7.95	1.08	1.23
1	A	233	GLU	CG-CD	7.93	1.63	1.51
1	A	625	TYR	CD2-CE2	-7.93	1.27	1.39
1	A	578	LYS	CE-NZ	7.92	1.68	1.49
1	A	181	LEU	CG-CD2	-7.91	1.22	1.51
1	A	22	GLU	CG-CD	7.89	1.63	1.51
1	A	595	LYS	CE-NZ	7.88	1.68	1.49
1	A	186	ALA	CA-CB	7.88	1.69	1.52
1	A	123	ARG	NE-CZ	7.86	1.43	1.33
2	B	133	TYR	CD1-CE1	7.86	1.51	1.39
1	A	27	TYR	CZ-OH	-7.85	1.24	1.37
1	A	16	GLU	CD-OE2	7.85	1.34	1.25
1	A	673	PHE	CE1-CZ	-7.80	1.22	1.37
1	A	141	PHE	CD2-CE2	-7.79	1.23	1.39
1	A	23	ARG	CB-CG	-7.79	1.31	1.52
1	A	534	PHE	CD2-CE2	-7.79	1.23	1.39
1	A	140	HIS	C-O	-7.79	1.08	1.23
1	A	510	GLN	CD-NE2	7.78	1.52	1.32
1	A	157	ARG	CZ-NH1	-7.76	1.23	1.33
1	A	506	LYS	CB-CG	7.75	1.73	1.52
1	A	288	TRP	CB-CG	-7.74	1.36	1.50
2	B	151	ARG	CA-C	-7.74	1.32	1.52
1	A	365	TRP	CD2-CE2	-7.72	1.32	1.41
1	A	135	TYR	CG-CD2	7.71	1.49	1.39
1	A	146	TYR	N-CA	-7.71	1.30	1.46
1	A	469	ARG	CZ-NH1	7.69	1.43	1.33
1	A	33	GLU	CG-CD	-7.66	1.40	1.51
2	B	62	SER	C-O	7.66	1.38	1.23
2	B	159	PHE	CG-CD2	-7.65	1.27	1.38
1	A	167	PHE	CB-CG	7.64	1.64	1.51
1	A	215	TYR	CD2-CE2	7.63	1.50	1.39
1	A	629	LYS	CB-CG	7.63	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	597	PHE	CD1-CE1	7.62	1.54	1.39
1	A	675	ILE	C-O	-7.61	1.08	1.23
1	A	373	GLY	C-O	-7.58	1.11	1.23
1	A	71	ARG	CZ-NH1	7.58	1.43	1.33
1	A	659	PHE	CE1-CZ	-7.56	1.23	1.37
1	A	390	LYS	CG-CD	7.55	1.78	1.52
1	A	497	PHE	CB-CG	-7.53	1.38	1.51
1	A	518	ALA	C-O	-7.51	1.09	1.23
1	A	489	PHE	C-O	7.50	1.37	1.23
1	A	289	GLY	CA-C	7.50	1.63	1.51
1	A	577	CYS	CB-SG	7.49	1.95	1.82
1	A	663	VAL	CA-CB	7.49	1.70	1.54
1	A	673	PHE	CG-CD2	-7.49	1.27	1.38
1	A	662	PHE	CD2-CE2	7.48	1.54	1.39
1	A	146	TYR	CG-CD1	-7.48	1.29	1.39
1	A	377	TYR	CE1-CZ	7.46	1.48	1.38
1	A	27	TYR	CG-CD1	-7.43	1.29	1.39
1	A	154	VAL	CB-CG1	-7.42	1.37	1.52
1	A	237	LEU	C-O	-7.37	1.09	1.23
2	B	81	LYS	CB-CG	7.35	1.72	1.52
1	A	645	VAL	CB-CG2	-7.34	1.37	1.52
1	A	33	GLU	CD-OE2	7.33	1.33	1.25
1	A	182	GLU	CD-OE1	-7.33	1.17	1.25
1	A	87	PHE	CG-CD1	-7.32	1.27	1.38
2	B	74	LYS	CE-NZ	7.32	1.67	1.49
1	A	450	LYS	CE-NZ	7.31	1.67	1.49
1	A	540	GLN	CG-CD	7.30	1.67	1.51
1	A	270	GLU	CD-OE2	7.29	1.33	1.25
1	A	597	PHE	CE2-CZ	7.29	1.51	1.37
1	A	155	ASP	C-O	7.29	1.37	1.23
1	A	674	LYS	CB-CG	7.28	1.72	1.52
1	A	176	PHE	CD2-CE2	-7.25	1.24	1.39
1	A	670	GLU	CA-CB	-7.24	1.38	1.53
1	A	179	ALA	CA-CB	7.23	1.67	1.52
1	A	131	PHE	CG-CD1	-7.22	1.27	1.38
2	B	156	PHE	CE1-CZ	7.21	1.51	1.37
1	A	455	THR	CA-CB	7.18	1.72	1.53
1	A	476	LYS	CG-CD	7.16	1.76	1.52
2	B	132	ARG	CG-CD	7.14	1.69	1.51
1	A	13	GLU	CA-C	7.14	1.71	1.52
2	B	145	PHE	CD2-CE2	7.14	1.53	1.39
2	B	97	PHE	C-O	7.12	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	TYR	CA-CB	-7.11	1.38	1.53
1	A	236	SER	CB-OG	7.10	1.51	1.42
1	A	431	PHE	CE2-CZ	-7.09	1.23	1.37
1	A	386	GLN	CD-NE2	7.09	1.50	1.32
2	B	159	PHE	CD1-CE1	-7.08	1.25	1.39
1	A	362	ASP	CB-CG	-7.08	1.36	1.51
1	A	663	VAL	CB-CG2	-7.07	1.38	1.52
1	A	106	TRP	CD2-CE3	7.05	1.50	1.40
1	A	356	TRP	CE2-CZ2	-7.05	1.27	1.39
1	A	475	PHE	CD1-CE1	-7.04	1.25	1.39
1	A	489	PHE	CD1-CE1	7.01	1.53	1.39
1	A	156	ASP	CG-OD1	7.00	1.41	1.25
1	A	390	LYS	CD-CE	6.97	1.68	1.51
1	A	183	LYS	CE-NZ	-6.97	1.31	1.49
1	A	483	VAL	CB-CG1	-6.96	1.38	1.52
1	A	75	TRP	CG-CD1	-6.94	1.27	1.36
1	A	417	ARG	CB-CG	6.94	1.71	1.52
2	B	183	TYR	CE2-CZ	6.93	1.47	1.38
1	A	453	PHE	C-O	6.93	1.36	1.23
2	B	18	ARG	CA-C	6.91	1.71	1.52
1	A	434	TYR	CG-CD2	-6.89	1.30	1.39
1	A	465	PHE	N-CA	-6.89	1.32	1.46
1	A	406	THR	C-O	6.89	1.36	1.23
1	A	498	CYS	CB-SG	6.88	1.94	1.82
1	A	465	PHE	CD2-CE2	-6.87	1.25	1.39
1	A	18	LEU	CG-CD1	-6.86	1.26	1.51
1	A	96	ASP	CB-CG	-6.86	1.37	1.51
1	A	161	LYS	CG-CD	6.85	1.75	1.52
1	A	325	TRP	CE2-CZ2	6.85	1.51	1.39
1	A	66	TYR	CE1-CZ	6.84	1.47	1.38
1	A	598	TYR	CG-CD1	6.83	1.48	1.39
1	A	271	GLU	CD-OE1	6.82	1.33	1.25
2	B	74	LYS	C-O	6.82	1.36	1.23
1	A	190	GLY	C-O	-6.82	1.12	1.23
1	A	551	PHE	CG-CD2	-6.81	1.28	1.38
2	B	156	PHE	CE2-CZ	6.81	1.50	1.37
2	B	95	LYS	CE-NZ	6.81	1.66	1.49
1	A	215	TYR	CE1-CZ	6.80	1.47	1.38
1	A	325	TRP	CE3-CZ3	6.80	1.50	1.38
1	A	161	LYS	CE-NZ	6.79	1.66	1.49
1	A	482	TYR	CD2-CE2	6.78	1.49	1.39
2	B	67	MET	CG-SD	-6.78	1.63	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	552	GLU	CG-CD	6.77	1.62	1.51
2	B	35	GLU	CD-OE1	6.77	1.33	1.25
1	A	131	PHE	N-CA	6.76	1.59	1.46
1	A	611	TYR	CD2-CE2	6.75	1.49	1.39
1	A	552	GLU	CB-CG	6.74	1.65	1.52
2	B	95	LYS	CD-CE	6.74	1.68	1.51
1	A	95	THR	C-O	-6.73	1.10	1.23
1	A	89	ILE	CA-CB	6.72	1.70	1.54
1	A	46	PHE	CG-CD2	6.72	1.48	1.38
1	A	227	ILE	C-O	6.71	1.36	1.23
1	A	392	GLU	CD-OE1	6.71	1.33	1.25
1	A	18	LEU	CA-CB	-6.70	1.38	1.53
1	A	326	MET	SD-CE	6.70	2.15	1.77
1	A	510	GLN	CG-CD	6.69	1.66	1.51
1	A	534	PHE	CG-CD2	-6.68	1.28	1.38
1	A	417	ARG	NE-CZ	6.68	1.41	1.33
1	A	142	GLN	CB-CG	-6.66	1.34	1.52
1	A	431	PHE	CE1-CZ	-6.66	1.24	1.37
1	A	325	TRP	CB-CG	-6.65	1.38	1.50
1	A	357	LYS	CD-CE	6.65	1.67	1.51
1	A	98	CYS	CA-C	-6.64	1.35	1.52
2	B	94	TYR	CD1-CE1	6.64	1.49	1.39
2	B	115	GLU	CB-CG	6.63	1.64	1.52
1	A	640	CYS	CA-C	6.63	1.70	1.52
1	A	682	GLU	CD-OE2	6.62	1.32	1.25
1	A	356	TRP	CD2-CE2	-6.62	1.33	1.41
2	B	133	TYR	CB-CG	6.61	1.61	1.51
1	A	139	PHE	CD2-CE2	-6.61	1.26	1.39
1	A	506	LYS	CG-CD	6.60	1.74	1.52
1	A	629	LYS	N-CA	-6.59	1.33	1.46
1	A	160	THR	N-CA	6.57	1.59	1.46
1	A	133	GLU	C-O	6.57	1.35	1.23
1	A	374	CYS	N-CA	-6.56	1.33	1.46
1	A	391	LEU	C-O	6.55	1.35	1.23
1	A	618	ARG	NE-CZ	6.55	1.41	1.33
1	A	433	ILE	CA-CB	-6.55	1.39	1.54
2	B	160	ARG	CB-CG	6.54	1.70	1.52
1	A	408	LEU	C-O	6.53	1.35	1.23
1	A	465	PHE	CD1-CE1	-6.52	1.26	1.39
1	A	14	ALA	CA-CB	-6.51	1.38	1.52
1	A	668	ARG	CB-CG	6.51	1.70	1.52
1	A	331	PHE	C-O	6.51	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	642	LEU	C-O	6.50	1.35	1.23
1	A	673	PHE	CE2-CZ	6.49	1.49	1.37
1	A	573	SER	CB-OG	6.48	1.50	1.42
1	A	27	TYR	CD2-CE2	6.46	1.49	1.39
1	A	544	GLU	CG-CD	6.46	1.61	1.51
1	A	604	ILE	CA-CB	-6.45	1.40	1.54
1	A	31	ASP	N-CA	-6.44	1.33	1.46
1	A	143	PHE	CE1-CZ	-6.44	1.25	1.37
2	B	168	GLY	N-CA	6.43	1.55	1.46
1	A	192	TYR	CG-CD2	-6.43	1.30	1.39
1	A	558	ARG	NE-CZ	6.42	1.41	1.33
1	A	46	PHE	CD1-CE1	6.42	1.52	1.39
1	A	689	LEU	N-CA	-6.42	1.33	1.46
1	A	52	PRO	C-O	6.41	1.36	1.23
2	B	90	TRP	CZ3-CH2	-6.41	1.29	1.40
2	B	66	VAL	CA-CB	-6.40	1.41	1.54
1	A	157	ARG	CZ-NH2	-6.40	1.24	1.33
1	A	454	LEU	C-O	6.40	1.35	1.23
1	A	289	GLY	C-O	6.39	1.33	1.23
1	A	692	ILE	CG1-CD1	6.39	1.94	1.50
1	A	670	GLU	CG-CD	6.38	1.61	1.51
1	A	467	ASN	C-O	6.38	1.35	1.23
1	A	641	GLN	C-O	6.38	1.35	1.23
1	A	99	GLN	C-O	-6.37	1.11	1.23
1	A	515	GLU	CD-OE2	6.36	1.32	1.25
1	A	489	PHE	CG-CD2	6.36	1.48	1.38
1	A	87	PHE	CG-CD2	-6.35	1.29	1.38
1	A	137	GLY	C-O	-6.35	1.13	1.23
2	B	145	PHE	CD1-CE1	6.35	1.51	1.39
1	A	202	GLU	CG-CD	-6.34	1.42	1.51
2	B	61	ARG	CZ-NH2	6.34	1.41	1.33
1	A	14	ALA	C-O	6.33	1.35	1.23
2	B	112	GLY	C-O	6.33	1.33	1.23
1	A	87	PHE	C-O	6.33	1.35	1.23
1	A	469	ARG	CD-NE	-6.32	1.35	1.46
2	B	157	ARG	C-O	6.32	1.35	1.23
1	A	69	LYS	C-O	6.31	1.35	1.23
2	B	133	TYR	CG-CD1	6.31	1.47	1.39
1	A	605	GLN	CB-CG	6.30	1.69	1.52
1	A	511	THR	C-O	-6.29	1.11	1.23
1	A	555	THR	C-O	6.28	1.35	1.23
1	A	409	VAL	CB-CG2	-6.27	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	23	GLN	CG-CD	6.27	1.65	1.51
1	A	669	LEU	CA-CB	-6.26	1.39	1.53
1	A	568	LYS	CD-CE	6.25	1.66	1.51
2	B	78	GLU	CD-OE2	6.25	1.32	1.25
1	A	150	VAL	C-O	-6.24	1.11	1.23
1	A	198	GLY	C-O	-6.24	1.13	1.23
1	A	604	ILE	C-O	-6.24	1.11	1.23
1	A	349	THR	CB-CG2	6.24	1.73	1.52
1	A	637	LYS	CE-NZ	6.22	1.64	1.49
1	A	591	LYS	CB-CG	6.22	1.69	1.52
1	A	325	TRP	CG-CD1	-6.21	1.28	1.36
1	A	681	PRO	C-O	-6.21	1.10	1.23
1	A	182	GLU	CD-OE2	6.19	1.32	1.25
1	A	488	THR	CB-CG2	-6.19	1.31	1.52
1	A	682	GLU	CD-OE1	6.19	1.32	1.25
1	A	636	PHE	C-O	6.18	1.35	1.23
1	A	369	SER	C-O	-6.17	1.11	1.23
2	B	94	TYR	CE2-CZ	6.17	1.46	1.38
1	A	581	VAL	CB-CG2	-6.17	1.40	1.52
1	A	635	GLY	N-CA	6.17	1.55	1.46
1	A	14	ALA	N-CA	-6.16	1.34	1.46
1	A	474	ARG	CA-CB	-6.15	1.40	1.53
2	B	32	SER	CA-CB	-6.14	1.43	1.52
2	B	158	ALA	C-O	-6.14	1.11	1.23
1	A	571	GLY	CA-C	6.13	1.61	1.51
1	A	143	PHE	CG-CD1	-6.13	1.29	1.38
1	A	230	LYS	CD-CE	6.13	1.66	1.51
2	B	94	TYR	CG-CD1	6.12	1.47	1.39
1	A	8	LEU	C-O	-6.12	1.11	1.23
1	A	697	PHE	CD2-CE2	6.12	1.51	1.39
1	A	662	PHE	CE1-CZ	6.11	1.49	1.37
2	B	129	ILE	CA-CB	-6.09	1.40	1.54
1	A	123	ARG	CG-CD	-6.09	1.36	1.51
2	B	153	ASP	CA-CB	6.08	1.67	1.53
1	A	351	ASP	CB-CG	6.08	1.64	1.51
1	A	214	TRP	C-O	-6.07	1.11	1.23
1	A	669	LEU	CG-CD2	6.07	1.74	1.51
2	B	131	ARG	NE-CZ	6.06	1.41	1.33
1	A	577	CYS	CA-C	-6.05	1.37	1.52
1	A	359	THR	CB-CG2	-6.01	1.32	1.52
1	A	271	GLU	CD-OE2	6.01	1.32	1.25
1	A	697	PHE	CB-CG	-6.00	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	LYS	CE-NZ	6.00	1.64	1.49
1	A	606	LYS	CA-C	6.00	1.68	1.52
2	B	9	ASN	C-O	6.00	1.34	1.23
1	A	10	THR	C-O	6.00	1.34	1.23
1	A	241	SER	CB-OG	6.00	1.50	1.42
1	A	219	LYS	CB-CG	6.00	1.68	1.52
1	A	172	GLU	CD-OE2	5.99	1.32	1.25
1	A	686	THR	CA-CB	-5.99	1.37	1.53
1	A	656	ILE	CA-CB	5.98	1.68	1.54
1	A	489	PHE	CE1-CZ	5.98	1.48	1.37
1	A	74	GLU	CD-OE1	5.98	1.32	1.25
1	A	491	PRO	CG-CD	-5.96	1.30	1.50
1	A	497	PHE	C-O	-5.96	1.12	1.23
1	A	124	VAL	CB-CG2	-5.96	1.40	1.52
1	A	612	ARG	CZ-NH1	5.96	1.40	1.33
1	A	146	TYR	CD2-CE2	-5.95	1.30	1.39
1	A	377	TYR	CE2-CZ	5.95	1.46	1.38
1	A	601	TRP	CG-CD1	5.94	1.45	1.36
1	A	148	GLU	CG-CD	5.93	1.60	1.51
1	A	469	ARG	CZ-NH2	5.93	1.40	1.33
1	A	15	ALA	CA-CB	-5.93	1.40	1.52
2	B	61	ARG	CZ-NH1	5.92	1.40	1.33
1	A	159	PRO	N-CD	-5.92	1.39	1.47
1	A	280	LYS	CE-NZ	-5.91	1.34	1.49
1	A	466	ILE	CG1-CD1	5.91	1.91	1.50
2	B	130	ILE	CA-CB	5.91	1.68	1.54
1	A	285	ARG	CG-CD	-5.90	1.37	1.51
1	A	360	LYS	N-CA	-5.89	1.34	1.46
1	A	538	PHE	CE2-CZ	-5.88	1.26	1.37
1	A	695	LEU	C-O	-5.87	1.12	1.23
1	A	475	PHE	CE1-CZ	5.86	1.48	1.37
1	A	692	ILE	CA-CB	5.86	1.68	1.54
1	A	696	SER	CB-OG	5.86	1.49	1.42
1	A	232	LEU	C-O	-5.85	1.12	1.23
1	A	574	ILE	N-CA	-5.85	1.34	1.46
1	A	644	GLN	C-O	5.84	1.34	1.23
1	A	76	LYS	N-CA	-5.83	1.34	1.46
1	A	651	ALA	C-O	5.83	1.34	1.23
1	A	497	PHE	CE2-CZ	5.83	1.48	1.37
2	B	162	LEU	CA-C	5.82	1.68	1.52
1	A	649	ARG	CD-NE	5.82	1.56	1.46
1	A	419	GLN	CG-CD	-5.81	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	SER	CA-CB	-5.80	1.44	1.52
1	A	215	TYR	CE2-CZ	-5.79	1.31	1.38
1	A	604	ILE	CB-CG2	-5.79	1.34	1.52
2	B	96	ARG	C-O	5.79	1.34	1.23
2	B	12	GLU	CD-OE2	5.78	1.32	1.25
1	A	605	GLN	CA-C	-5.78	1.38	1.52
1	A	613	GLU	CD-OE2	5.78	1.32	1.25
1	A	547	GLU	CG-CD	5.76	1.60	1.51
1	A	668	ARG	CG-CD	5.76	1.66	1.51
1	A	28	LEU	N-CA	5.74	1.57	1.46
1	A	366	ARG	CG-CD	5.74	1.66	1.51
1	A	197	GLY	N-CA	5.73	1.54	1.46
1	A	428	THR	CA-C	-5.73	1.38	1.52
2	B	51	LYS	CB-CG	5.73	1.68	1.52
1	A	607	TYR	CD1-CE1	-5.72	1.30	1.39
2	B	87	ILE	CB-CG2	5.72	1.70	1.52
1	A	263	ALA	CA-CB	5.72	1.64	1.52
1	A	150	VAL	CA-CB	5.71	1.66	1.54
2	B	25	ALA	CA-CB	5.70	1.64	1.52
1	A	673	PHE	CG-CD1	-5.70	1.30	1.38
1	A	435	GLU	CG-CD	5.70	1.60	1.51
1	A	145	GLN	CA-CB	-5.70	1.41	1.53
1	A	337	ARG	CG-CD	5.68	1.66	1.51
1	A	644	GLN	CD-OE1	5.68	1.36	1.24
1	A	118	GLU	CA-CB	5.67	1.66	1.53
1	A	185	TYR	CZ-OH	5.67	1.47	1.37
1	A	601	TRP	CG-CD2	-5.67	1.34	1.43
1	A	469	ARG	NE-CZ	5.67	1.40	1.33
1	A	107	LEU	CA-C	-5.66	1.38	1.52
1	A	331	PHE	CE2-CZ	-5.66	1.26	1.37
1	A	513	ASP	CG-OD1	5.66	1.38	1.25
2	B	19	LYS	CB-CG	5.66	1.67	1.52
2	B	181	THR	CB-CG2	-5.66	1.33	1.52
1	A	688	GLN	CA-CB	-5.65	1.41	1.53
1	A	150	VAL	CB-CG1	-5.64	1.41	1.52
1	A	358	LEU	C-O	-5.63	1.12	1.23
2	B	134	SER	CA-CB	-5.63	1.44	1.52
1	A	9	ALA	CA-CB	-5.63	1.40	1.52
1	A	607	TYR	CB-CG	5.62	1.60	1.51
1	A	6	MET	CG-SD	5.62	1.95	1.81
1	A	582	ASP	CB-CG	5.62	1.63	1.51
1	A	347	THR	C-O	-5.61	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	GLU	C-O	5.60	1.33	1.23
1	A	629	LYS	C-O	5.60	1.33	1.23
2	B	140	MET	N-CA	-5.60	1.35	1.46
2	B	159	PHE	CE1-CZ	5.60	1.48	1.37
1	A	138	ILE	N-CA	-5.59	1.35	1.46
1	A	192	TYR	CG-CD1	-5.59	1.31	1.39
1	A	559	ARG	NE-CZ	5.59	1.40	1.33
1	A	131	PHE	CE1-CZ	-5.58	1.26	1.37
1	A	35	LEU	CA-CB	-5.58	1.41	1.53
2	B	125	ILE	CA-CB	-5.58	1.42	1.54
1	A	12	ARG	C-O	-5.58	1.12	1.23
1	A	285	ARG	C-O	-5.58	1.12	1.23
2	B	68	ASP	CG-OD1	5.57	1.38	1.25
1	A	640	CYS	CB-SG	-5.57	1.72	1.81
1	A	470	GLU	CD-OE2	-5.56	1.19	1.25
1	A	579	ILE	C-O	5.56	1.33	1.23
1	A	2	ALA	C-O	-5.56	1.12	1.23
1	A	176	PHE	CB-CG	-5.56	1.41	1.51
1	A	237	LEU	CG-CD2	-5.56	1.31	1.51
1	A	505	LYS	CD-CE	5.56	1.65	1.51
1	A	19	GLY	CA-C	5.55	1.60	1.51
1	A	650	PHE	CB-CG	5.54	1.60	1.51
1	A	426	MET	CB-CG	-5.52	1.33	1.51
1	A	652	ASP	CB-CG	5.51	1.63	1.51
1	A	646	ILE	CB-CG2	-5.51	1.35	1.52
1	A	188	ILE	C-O	-5.50	1.12	1.23
2	B	151	ARG	CZ-NH1	5.50	1.40	1.33
1	A	55	PRO	CG-CD	5.50	1.68	1.50
1	A	233	GLU	CB-CG	5.50	1.62	1.52
1	A	512	VAL	CB-CG2	5.50	1.64	1.52
1	A	149	TRP	CZ3-CH2	5.48	1.48	1.40
1	A	579	ILE	CB-CG1	-5.47	1.38	1.54
1	A	222	PRO	CB-CG	5.47	1.77	1.50
1	A	64	GLY	CA-C	5.47	1.60	1.51
1	A	667	VAL	C-O	5.46	1.33	1.23
1	A	20	SER	CB-OG	-5.46	1.35	1.42
1	A	557	LEU	CG-CD2	5.46	1.72	1.51
1	A	383	MET	C-O	-5.46	1.12	1.23
2	B	90	TRP	CB-CG	-5.46	1.40	1.50
1	A	49	PRO	N-CA	5.45	1.56	1.47
1	A	207	PHE	CD2-CE2	-5.45	1.28	1.39
1	A	425	ASP	N-CA	5.43	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	429	ILE	N-CA	-5.43	1.35	1.46
1	A	390	LYS	CB-CG	5.43	1.67	1.52
2	B	167	THR	CA-C	-5.43	1.38	1.52
1	A	393	GLU	CG-CD	5.43	1.60	1.51
1	A	78	PRO	CG-CD	5.42	1.68	1.50
1	A	504	GLU	CD-OE2	5.42	1.31	1.25
1	A	626	GLU	CD-OE2	5.42	1.31	1.25
1	A	500	ARG	C-N	-5.41	1.21	1.34
1	A	475	PHE	CE2-CZ	-5.41	1.27	1.37
1	A	132	GLN	CG-CD	5.39	1.63	1.51
1	A	399	GLU	N-CA	5.38	1.57	1.46
2	B	177	TRP	CZ3-CH2	-5.38	1.31	1.40
1	A	370	THR	C-O	5.38	1.33	1.23
1	A	409	VAL	N-CA	-5.37	1.35	1.46
1	A	211	ILE	CA-C	-5.37	1.39	1.52
2	B	18	ARG	C-O	5.36	1.33	1.23
1	A	151	GLU	N-CA	-5.36	1.35	1.46
1	A	139	PHE	CB-CG	-5.36	1.42	1.51
1	A	515	GLU	CA-C	5.36	1.66	1.52
1	A	686	THR	CB-CG2	-5.35	1.34	1.52
1	A	75	TRP	CE2-CZ2	-5.35	1.30	1.39
1	A	161	LYS	CD-CE	5.34	1.64	1.51
1	A	185	TYR	CG-CD2	-5.33	1.32	1.39
2	B	116	ALA	CA-CB	5.32	1.63	1.52
1	A	136	ALA	CA-C	-5.31	1.39	1.52
1	A	72	GLY	N-CA	-5.30	1.38	1.46
2	B	65	ALA	C-O	5.30	1.33	1.23
2	B	183	TYR	CA-C	5.30	1.66	1.52
1	A	631	LEU	N-CA	-5.30	1.35	1.46
1	A	28	LEU	C-O	-5.28	1.13	1.23
1	A	29	ASN	CG-ND2	5.28	1.46	1.32
1	A	450	LYS	CB-CG	-5.28	1.38	1.52
1	A	572	PHE	CG-CD1	-5.28	1.30	1.38
1	A	36	ARG	CB-CG	-5.28	1.38	1.52
1	A	142	GLN	CA-CB	5.28	1.65	1.53
1	A	497	PHE	CG-CD1	5.28	1.46	1.38
1	A	9	ALA	C-O	-5.27	1.13	1.23
1	A	611	TYR	CG-CD1	5.27	1.46	1.39
1	A	539	ALA	C-O	5.27	1.33	1.23
2	B	126	TYR	CB-CG	-5.26	1.43	1.51
2	B	182	MET	SD-CE	-5.26	1.48	1.77
1	A	667	VAL	CA-CB	5.26	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	SER	CB-OG	5.25	1.49	1.42
1	A	143	PHE	CB-CG	-5.24	1.42	1.51
1	A	541	LEU	CG-CD2	5.24	1.71	1.51
1	A	372	GLY	C-O	-5.24	1.15	1.23
2	B	168	GLY	C-O	-5.24	1.15	1.23
1	A	469	ARG	CA-C	-5.24	1.39	1.52
1	A	225	PHE	CA-C	-5.23	1.39	1.52
1	A	692	ILE	CB-CG2	5.23	1.69	1.52
1	A	80	GLU	CD-OE2	5.22	1.31	1.25
1	A	397	ASP	N-CA	5.22	1.56	1.46
1	A	574	ILE	CA-CB	5.22	1.66	1.54
2	B	126	TYR	CE2-CZ	-5.22	1.31	1.38
1	A	614	ILE	C-O	-5.21	1.13	1.23
1	A	634	ALA	CA-C	-5.20	1.39	1.52
1	A	431	PHE	CD1-CE1	-5.19	1.28	1.39
2	B	49	ASP	CB-CG	5.19	1.62	1.51
1	A	284	ILE	CB-CG2	5.19	1.69	1.52
1	A	76	LYS	C-O	-5.18	1.13	1.23
1	A	598	TYR	CD1-CE1	5.18	1.47	1.39
1	A	658	ASP	CG-OD1	5.18	1.37	1.25
2	B	108	ASN	CB-CG	5.18	1.62	1.51
1	A	41	GLU	CD-OE1	5.18	1.31	1.25
1	A	613	GLU	CG-CD	-5.18	1.44	1.51
1	A	354	LYS	CG-CD	5.18	1.70	1.52
1	A	512	VAL	CB-CG1	-5.17	1.42	1.52
1	A	384	ASN	C-O	-5.17	1.13	1.23
1	A	668	ARG	CD-NE	5.17	1.55	1.46
1	A	180	LEU	CG-CD1	-5.16	1.32	1.51
1	A	591	LYS	CD-CE	5.16	1.64	1.51
2	B	159	PHE	N-CA	-5.16	1.36	1.46
1	A	697	PHE	CD1-CE1	-5.16	1.28	1.39
1	A	61	LYS	N-CA	5.15	1.56	1.46
2	B	119	PHE	C-O	5.15	1.33	1.23
1	A	198	GLY	CA-C	-5.14	1.43	1.51
2	B	75	LEU	C-N	-5.14	1.23	1.33
1	A	492	HIS	CA-CB	-5.13	1.42	1.53
1	A	657	ILE	C-O	5.13	1.33	1.23
1	A	87	PHE	CD2-CE2	-5.13	1.28	1.39
1	A	625	TYR	CD1-CE1	-5.13	1.31	1.39
1	A	353	TYR	CB-CG	5.12	1.59	1.51
1	A	153	VAL	C-O	5.12	1.33	1.23
2	B	30	GLU	CD-OE2	5.12	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	GLN	CD-OE1	5.12	1.35	1.24
1	A	534	PHE	CE1-CZ	-5.11	1.27	1.37
2	B	144	ASN	CB-CG	5.11	1.62	1.51
1	A	74	GLU	CG-CD	5.10	1.59	1.51
2	B	171	GLN	CG-CD	5.08	1.62	1.51
1	A	193	GLU	CD-OE1	-5.08	1.20	1.25
1	A	8	LEU	CG-CD2	5.08	1.70	1.51
1	A	607	TYR	CD2-CE2	-5.08	1.31	1.39
1	A	229	GLN	N-CA	-5.08	1.36	1.46
2	B	82	TYR	CE2-CZ	-5.08	1.31	1.38
1	A	411	LEU	CG-CD1	5.07	1.70	1.51
2	B	70	ASP	N-CA	-5.06	1.36	1.46
1	A	202	GLU	N-CA	-5.06	1.36	1.46
2	B	142	PHE	CD1-CE1	5.06	1.49	1.39
1	A	664	ARG	CZ-NH1	5.06	1.39	1.33
1	A	151	GLU	CG-CD	5.06	1.59	1.51
2	B	20	LEU	C-O	5.05	1.32	1.23
2	B	29	MET	CG-SD	5.04	1.94	1.81
1	A	139	PHE	CG-CD2	-5.04	1.31	1.38
2	B	31	VAL	CB-CG1	-5.04	1.42	1.52
1	A	123	ARG	CZ-NH2	5.04	1.39	1.33
1	A	433	ILE	CB-CG1	-5.04	1.40	1.54
1	A	356	TRP	C-O	-5.04	1.13	1.23
2	B	33	ALA	CA-C	-5.03	1.39	1.52
1	A	74	GLU	CB-CG	5.03	1.61	1.52
1	A	434	TYR	CE1-CZ	-5.02	1.32	1.38
1	A	243	ASP	CA-C	5.02	1.66	1.52
1	A	399	GLU	C-N	-5.01	1.22	1.34
1	A	98	CYS	C-O	-5.01	1.13	1.23
1	A	563	LYS	CB-CG	5.01	1.66	1.52
1	A	576	THR	CB-CG2	-5.01	1.35	1.52
2	B	85	ASN	C-O	-5.01	1.13	1.23
1	A	164	GLU	CB-CG	5.00	1.61	1.52

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	400	ASP	C-N-CA	-23.66	72.61	122.30
1	A	23	ARG	NE-CZ-NH1	22.54	131.57	120.30
1	A	402	GLU	CA-C-N	-20.02	73.17	117.20
1	A	403	ARG	CA-C-N	-19.27	77.66	116.20
1	A	23	ARG	NE-CZ-NH2	-18.54	111.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	628	ARG	NE-CZ-NH1	-16.63	111.98	120.30
1	A	523	ILE	CA-C-O	15.46	152.56	120.10
1	A	400	ASP	CA-C-N	-15.08	86.03	116.20
1	A	400	ASP	O-C-N	14.04	147.06	123.20
1	A	399	GLU	C-N-CA	13.77	156.13	121.70
2	B	152	LEU	CB-CG-CD2	-13.68	87.75	111.00
2	B	28	ASP	CB-CG-OD2	13.56	130.50	118.30
1	A	104	ASP	CB-CG-OD2	13.11	130.10	118.30
1	A	525	ALA	O-C-N	-12.62	102.50	122.70
1	A	547	GLU	OE1-CD-OE2	-12.39	108.43	123.30
1	A	525	ALA	CA-C-N	-12.21	90.33	117.20
1	A	361	MET	CG-SD-CE	11.93	119.29	100.20
1	A	628	ARG	NE-CZ-NH2	11.83	126.22	120.30
1	A	71	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	A	367	ARG	NE-CZ-NH2	11.56	126.08	120.30
2	B	151	ARG	NE-CZ-NH2	-11.18	114.71	120.30
2	B	100	ASP	CB-CG-OD2	10.27	127.54	118.30
1	A	69	LYS	CD-CE-NZ	-10.22	88.18	111.70
1	A	118	GLU	OE1-CD-OE2	-10.07	111.22	123.30
1	A	618	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	A	157	ARG	NE-CZ-NH2	9.71	125.15	120.30
1	A	526	ASN	C-N-CA	9.56	145.60	121.70
1	A	582	ASP	CB-CG-OD2	9.47	126.82	118.30
1	A	649	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	A	632	GLU	OE1-CD-OE2	-9.30	112.14	123.30
1	A	612	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	404	GLY	C-N-CA	-9.23	98.62	121.70
1	A	496	ASP	CB-CG-OD1	9.23	126.61	118.30
2	B	30	GLU	OE1-CD-OE2	9.22	134.37	123.30
1	A	552	GLU	OE1-CD-OE2	-9.12	112.35	123.30
2	B	89	LYS	CD-CE-NZ	-9.08	90.81	111.70
1	A	652	ASP	CB-CG-OD2	9.07	126.46	118.30
1	A	161	LYS	CD-CE-NZ	8.98	132.35	111.70
1	A	629	LYS	CD-CE-NZ	-8.94	91.13	111.70
1	A	94	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	A	545	ASP	CB-CG-OD2	8.63	126.07	118.30
1	A	417	ARG	NE-CZ-NH2	8.62	124.61	120.30
1	A	700	LEU	CA-CB-CG	8.50	134.84	115.30
1	A	12	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	A	96	ASP	CB-CG-OD1	-8.37	110.77	118.30
1	A	36	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	B	132	ARG	NE-CZ-NH2	8.28	124.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	617	ASP	CB-CG-OD2	8.27	125.75	118.30
1	A	526	ASN	O-C-N	-8.25	109.50	122.70
1	A	116	LEU	CB-CG-CD2	8.24	125.01	111.00
1	A	96	ASP	CB-CG-OD2	8.23	125.71	118.30
1	A	508	ASP	CB-CG-OD2	8.19	125.67	118.30
1	A	455	THR	OG1-CB-CG2	-8.12	91.31	110.00
2	B	68	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	A	613	GLU	OE1-CD-OE2	7.96	132.85	123.30
1	A	399	GLU	O-C-N	-7.94	109.99	122.70
2	B	61	ARG	NE-CZ-NH2	-7.93	116.34	120.30
2	B	24	LEU	CB-CG-CD2	7.91	124.44	111.00
1	A	196	SER	C-N-CA	-7.89	105.72	122.30
1	A	359	THR	OG1-CB-CG2	-7.85	91.94	110.00
1	A	22	GLU	OE1-CD-OE2	-7.80	113.94	123.30
1	A	381	PHE	CB-CG-CD2	7.78	126.25	120.80
1	A	433	ILE	CG1-CB-CG2	-7.65	94.58	111.40
2	B	152	LEU	CA-CB-CG	7.62	132.82	115.30
1	A	669	LEU	CB-CG-CD1	-7.53	98.20	111.00
1	A	500	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	525	ALA	C-N-CA	7.49	140.41	121.70
2	B	70	ASP	CB-CG-OD2	7.45	125.00	118.30
1	A	585	ASP	CB-CG-OD2	7.42	124.98	118.30
1	A	337	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	668	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	A	522	GLU	C-N-CA	-7.30	103.46	121.70
1	A	375	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	A	627	MET	CG-SD-CE	7.16	111.66	100.20
1	A	385	PRO	N-CD-CG	-7.09	92.57	103.20
1	A	403	ARG	CA-C-O	7.05	134.92	120.10
1	A	425	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	419	GLN	N-CA-C	-6.98	92.15	111.00
1	A	380	THR	OG1-CB-CG2	-6.94	94.04	110.00
1	A	653	ASP	CB-CG-OD2	6.94	124.55	118.30
2	B	61	ARG	NE-CZ-NH1	-6.94	116.83	120.30
2	B	115	GLU	OE1-CD-OE2	-6.87	115.06	123.30
1	A	401	GLY	CA-C-N	-6.84	102.16	117.20
1	A	647	VAL	CG1-CB-CG2	-6.83	99.97	110.90
1	A	522	GLU	CA-C-N	-6.82	102.19	117.20
1	A	667	VAL	CG1-CB-CG2	-6.81	100.00	110.90
1	A	474	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	61	LYS	CA-CB-CG	6.77	128.30	113.40
1	A	402	GLU	O-C-N	-6.75	111.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	528	GLU	CB-CA-C	6.73	123.86	110.40
2	B	61	ARG	NH1-CZ-NH2	6.72	126.79	119.40
1	A	157	ARG	NH1-CZ-NH2	-6.72	112.01	119.40
1	A	381	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	A	156	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	A	226	LYS	CD-CE-NZ	6.62	126.93	111.70
1	A	162	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	33	GLU	CG-CD-OE1	-6.60	105.10	118.30
2	B	163	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	A	124	VAL	CG1-CB-CG2	-6.53	100.44	110.90
1	A	630	ALA	N-CA-CB	-6.53	100.95	110.10
1	A	100	GLY	N-CA-C	-6.53	96.77	113.10
1	A	515	GLU	CA-CB-CG	6.53	127.77	113.40
1	A	699	VAL	CA-CB-CG1	6.50	120.65	110.90
1	A	26	LYS	CD-CE-NZ	-6.48	96.80	111.70
1	A	469	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	403	ARG	CB-CA-C	-6.43	97.53	110.40
1	A	535	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	A	107	LEU	CA-CB-CG	-6.43	100.51	115.30
1	A	391	LEU	CB-CG-CD1	6.41	121.89	111.00
1	A	465	PHE	N-CA-C	-6.39	93.75	111.00
1	A	227	ILE	CG1-CB-CG2	-6.38	97.37	111.40
1	A	403	ARG	O-C-N	6.38	134.04	123.20
1	A	58	LEU	CB-CG-CD2	6.37	121.82	111.00
1	A	474	ARG	CG-CD-NE	-6.34	98.48	111.80
1	A	374	CYS	CA-CB-SG	-6.32	102.63	114.00
2	B	151	ARG	CA-CB-CG	-6.32	99.50	113.40
1	A	700	LEU	CB-CG-CD2	6.31	121.73	111.00
1	A	150	VAL	CG1-CB-CG2	6.29	120.96	110.90
1	A	36	ARG	CG-CD-NE	-6.28	98.61	111.80
1	A	48	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	406	THR	OG1-CB-CG2	-6.27	95.58	110.00
1	A	520	ILE	CA-C-N	-6.26	103.43	117.20
2	B	162	LEU	CB-CG-CD2	6.25	121.62	111.00
1	A	33	GLU	CA-CB-CG	6.24	127.12	113.40
1	A	113	SER	N-CA-CB	6.23	119.84	110.50
1	A	618	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	B	18	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	367	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	A	680	ASP	CB-CG-OD1	6.18	123.86	118.30
2	B	101	ARG	NE-CZ-NH2	-6.18	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	29	MET	CG-SD-CE	-6.16	90.34	100.20
1	A	680	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	695	LEU	CB-CG-CD1	6.12	121.41	111.00
2	B	58	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	690	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	16	GLU	OE1-CD-OE2	6.10	130.62	123.30
1	A	520	ILE	O-C-N	6.09	132.45	122.70
1	A	619	SER	N-CA-C	6.09	127.43	111.00
1	A	669	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	468	LEU	CB-CG-CD1	-6.07	100.67	111.00
1	A	322	GLY	N-CA-C	-6.06	97.94	113.10
1	A	133	GLU	OE1-CD-OE2	6.06	130.57	123.30
1	A	485	VAL	CB-CA-C	-6.05	99.90	111.40
1	A	283	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	660	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	375	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	A	520	ILE	C-N-CA	-5.95	106.83	121.70
1	A	222	PRO	N-CA-C	-5.94	96.65	112.10
1	A	664	ARG	CG-CD-NE	5.94	124.27	111.80
1	A	416	ARG	CG-CD-NE	-5.94	99.33	111.80
1	A	516	ILE	CB-CA-C	-5.91	99.78	111.60
1	A	27	TYR	CZ-CE2-CD2	-5.90	114.49	119.80
2	B	66	VAL	CG1-CB-CG2	-5.90	101.45	110.90
2	B	125	ILE	CG1-CB-CG2	5.89	124.35	111.40
2	B	10	GLU	OE1-CD-OE2	5.88	130.36	123.30
1	A	487	SER	CB-CA-C	-5.88	98.93	110.10
1	A	361	MET	CA-CB-CG	5.85	123.24	113.30
1	A	455	THR	N-CA-C	-5.82	95.29	111.00
1	A	528	GLU	N-CA-C	-5.82	95.29	111.00
1	A	680	ASP	OD1-CG-OD2	-5.80	112.28	123.30
1	A	45	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	A	102	LEU	C-N-CA	-5.78	110.16	122.30
1	A	676	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	A	551	PHE	N-CA-CB	-5.76	100.23	110.60
1	A	652	ASP	OD1-CG-OD2	-5.74	112.40	123.30
1	A	395	ASP	CB-CA-C	-5.73	98.94	110.40
1	A	463	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	626	GLU	OE1-CD-OE2	5.71	130.16	123.30
1	A	416	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	201	THR	OG1-CB-CG2	-5.68	96.93	110.00
1	A	166	LEU	CB-CG-CD2	-5.67	101.35	111.00
1	A	654	GLU	OE1-CD-OE2	5.67	130.11	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	657	ILE	CG1-CB-CG2	-5.65	98.97	111.40
1	A	6	MET	CA-CB-CG	5.64	122.88	113.30
1	A	333	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	12	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	59	GLY	CA-C-O	5.61	130.69	120.60
1	A	610	ILE	C-N-CA	-5.60	107.71	121.70
2	B	47	HIS	CB-CA-C	5.59	121.57	110.40
1	A	42	ALA	O-C-N	-5.58	113.72	123.20
1	A	86	GLN	N-CA-CB	-5.58	100.56	110.60
1	A	27	TYR	CD1-CE1-CZ	5.57	124.82	119.80
1	A	337	ARG	CG-CD-NE	-5.57	100.10	111.80
1	A	351	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	501	VAL	CA-CB-CG1	-5.56	102.56	110.90
1	A	488	THR	N-CA-CB	-5.55	99.75	110.30
1	A	615	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	404	GLY	O-C-N	-5.54	113.84	122.70
1	A	49	PRO	N-CD-CG	-5.51	94.94	103.20
1	A	104	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	29	ASN	N-CA-C	5.47	125.78	111.00
1	A	373	GLY	N-CA-C	5.47	126.79	113.10
1	A	63	LEU	CA-CB-CG	-5.47	102.71	115.30
1	A	561	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	418	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	695	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	A	501	VAL	CB-CA-C	-5.42	101.09	111.40
2	B	81	LYS	CB-CG-CD	-5.42	97.50	111.60
2	B	121	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	360	LYS	N-CA-CB	-5.42	100.85	110.60
1	A	548	ILE	CB-CA-C	-5.40	100.80	111.60
1	A	346	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	496	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	B	168	GLY	C-N-CA	5.38	135.15	121.70
1	A	102	LEU	O-C-N	-5.38	114.05	123.20
1	A	18	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	584	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	450	LYS	CD-CE-NZ	5.36	124.02	111.70
1	A	453	PHE	N-CA-CB	5.35	120.23	110.60
2	B	107	SER	N-CA-CB	-5.35	102.48	110.50
2	B	159	PHE	CG-CD1-CE1	5.34	126.68	120.80
2	B	34	THR	OG1-CB-CG2	-5.32	97.76	110.00
2	B	18	ARG	CA-CB-CG	-5.31	101.72	113.40
1	A	681	PRO	N-CD-CG	-5.31	95.24	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	33	ALA	CB-CA-C	-5.31	102.14	110.10
1	A	679	LEU	N-CA-CB	5.30	121.00	110.40
2	B	60	CYS	CA-CB-SG	-5.30	104.47	114.00
1	A	527	GLU	CB-CA-C	5.29	120.99	110.40
1	A	521	GLU	CB-CA-C	5.29	120.98	110.40
1	A	264	TYR	N-CA-C	-5.29	96.72	111.00
1	A	682	GLU	CG-CD-OE2	5.29	128.87	118.30
1	A	377	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	156	ASP	O-C-N	-5.27	114.26	122.70
1	A	389	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	A	638	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	A	195	LEU	CB-CG-CD2	-5.21	102.15	111.00
1	A	559	ARG	N-CA-C	5.21	125.06	111.00
2	B	94	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
2	B	28	ASP	OD1-CG-OD2	-5.20	113.42	123.30
1	A	526	ASN	CA-C-N	5.20	128.63	117.20
2	B	33	ALA	N-CA-CB	5.19	117.37	110.10
2	B	95	LYS	CD-CE-NZ	5.17	123.59	111.70
1	A	121	LEU	CB-CG-CD2	5.17	119.78	111.00
1	A	217	LEU	CB-CG-CD1	5.16	119.78	111.00
1	A	206	ASP	OD1-CG-OD2	-5.16	113.50	123.30
1	A	89	ILE	CB-CA-C	-5.15	101.30	111.60
1	A	179	ALA	CB-CA-C	-5.14	102.38	110.10
1	A	74	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	155	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	23	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	455	THR	CA-CB-CG2	5.13	119.58	112.40
1	A	118	GLU	CA-CB-CG	5.12	124.65	113.40
1	A	656	ILE	CA-CB-CG1	-5.11	101.28	111.00
1	A	70	THR	OG1-CB-CG2	-5.11	98.24	110.00
1	A	322	GLY	O-C-N	5.11	130.87	122.70
1	A	555	THR	OG1-CB-CG2	-5.11	98.26	110.00
2	B	131	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	A	343	LEU	CB-CG-CD1	5.08	119.64	111.00
1	A	375	ARG	CB-CG-CD	5.08	124.81	111.60
1	A	198	GLY	CA-C-O	-5.08	111.46	120.60
1	A	337	ARG	CB-CG-CD	5.07	124.79	111.60
1	A	606	LYS	CB-CG-CD	5.07	124.78	111.60
2	B	85	ASN	CB-CA-C	5.07	120.53	110.40
1	A	243	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	612	ARG	NE-CZ-NH1	5.05	122.82	120.30
2	B	60	CYS	CB-CA-C	5.04	120.48	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	681	PRO	CB-CA-C	-5.04	99.41	112.00
1	A	50	SER	N-CA-CB	-5.02	102.97	110.50
1	A	649	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	B	58	ASP	OD1-CG-OD2	-5.02	113.77	123.30
1	A	576	THR	C-N-CA	5.01	134.23	121.70
1	A	435	GLU	CG-CD-OE2	-5.01	108.29	118.30
1	A	11	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	TYR	Sidechain
1	A	18	LEU	Mainchain
1	A	197	GLY	Peptide
1	A	373	GLY	Mainchain
1	A	384	ASN	Mainchain
1	A	399	GLU	Mainchain,Peptide
1	A	401	GLY	Mainchain,Peptide
1	A	403	ARG	Mainchain,Peptide
1	A	404	GLY	Mainchain
1	A	427	HIS	Sidechain,Mainchain
1	A	525	ALA	Mainchain,Peptide
1	A	527	GLU	Mainchain
1	A	9	ALA	Mainchain
1	A	98	CYS	Mainchain
2	B	142	PHE	Peptide
2	B	64	VAL	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	4980	0	4809	519	10
2	B	1427	0	1375	156	9
3	A	247	0	0	67	0
3	B	52	0	0	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6706	0	6184	668	10

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 53.

All (668) 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:A:218:ARG:CG	1:A:218:ARG:CB	1.74	1.66
1:A:409:VAL:CG1	1:A:409:VAL:CB	1.76	1.64
1:A:628:ARG:CG	1:A:628:ARG:CD	1.76	1.63
1:A:699:VAL:CG1	1:A:699:VAL:CB	1.77	1.62
1:A:455:THR:CG2	1:A:455:THR:CB	1.80	1.60
1:A:161:LYS:CB	1:A:161:LYS:CG	1.81	1.58
1:A:674:LYS:CE	1:A:674:LYS:CD	1.75	1.58
1:A:699:VAL:CA	1:A:699:VAL:CB	1.82	1.57
1:A:390:LYS:CD	1:A:390:LYS:CG	1.78	1.57
1:A:161:LYS:CG	1:A:161:LYS:CD	1.75	1.57
1:A:375:ARG:CD	1:A:375:ARG:CG	1.81	1.55
1:A:476:LYS:CD	1:A:476:LYS:CG	1.76	1.55
1:A:506:LYS:CG	1:A:506:LYS:CD	1.74	1.55
1:A:540:GLN:CB	1:A:540:GLN:CG	1.84	1.53
1:A:606:LYS:CG	1:A:606:LYS:CD	1.80	1.53
2:B:137:THR:CA	2:B:137:THR:CB	1.82	1.53
1:A:226:LYS:CE	1:A:226:LYS:CD	1.83	1.52
1:A:578:LYS:NZ	1:A:578:LYS:CE	1.68	1.52
1:A:7:LYS:CE	1:A:7:LYS:CD	1.86	1.51
1:A:595:LYS:CE	1:A:595:LYS:NZ	1.68	1.51
1:A:218:ARG:CG	1:A:218:ARG:CD	1.85	1.49
1:A:417:ARG:CG	1:A:417:ARG:CD	1.88	1.48
1:A:674:LYS:CE	1:A:674:LYS:NZ	1.75	1.48
1:A:226:LYS:CE	1:A:226:LYS:NZ	1.73	1.48
1:A:466:ILE:CD1	1:A:466:ILE:CG1	1.91	1.48
2:B:128:MET:SD	2:B:128:MET:CG	2.02	1.47
2:B:155:MET:SD	2:B:155:MET:CG	2.03	1.47
1:A:361:MET:SD	1:A:361:MET:CG	2.02	1.47
1:A:326:MET:SD	1:A:326:MET:CG	2.04	1.45
1:A:692:ILE:CD1	1:A:692:ILE:CG1	1.94	1.45
1:A:7:LYS:CE	1:A:7:LYS:NZ	1.78	1.44
1:A:222:PRO:CB	1:A:222:PRO:CG	1.77	1.42
1:A:326:MET:SD	1:A:326:MET:CE	2.15	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASP:C	1:A:401:GLY:CA	2.01	1.28
1:A:69:LYS:HB3	1:A:69:LYS:NZ	1.28	1.26
1:A:400:ASP:C	1:A:401:GLY:N	1.90	1.25
1:A:402:GLU:C	1:A:403:ARG:N	1.87	1.25
1:A:402:GLU:CA	1:A:403:ARG:N	2.04	1.21
1:A:402:GLU:HA	1:A:403:ARG:N	1.56	1.21
2:B:106:GLY:HA2	2:B:139:ASN:ND2	1.55	1.19
1:A:400:ASP:C	1:A:401:GLY:HA2	1.58	1.16
1:A:238:LEU:HD12	1:A:238:LEU:N	1.61	1.15
1:A:699:VAL:O	1:A:700:LEU:HD23	1.46	1.12
2:B:20:LEU:O	2:B:24:LEU:HG	1.47	1.10
1:A:69:LYS:NZ	1:A:69:LYS:CB	1.99	1.09
2:B:106:GLY:HA2	2:B:139:ASN:HD22	0.98	1.09
1:A:290:GLN:N	1:A:322:GLY:N	2.03	1.06
1:A:653:ASP:O	1:A:654:GLU:HG2	1.53	1.06
2:B:47:HIS:HB3	2:B:49:ASP:OD1	1.57	1.02
1:A:462:SER:CB	3:A:809:HOH:O	2.07	1.02
1:A:69:LYS:HZ2	1:A:69:LYS:CB	1.62	1.02
1:A:33:GLU:OE1	3:A:812:HOH:O	1.76	1.02
1:A:115:THR:HG21	3:A:759:HOH:O	1.59	1.00
1:A:220:PRO:HG3	3:A:870:HOH:O	1.62	0.99
1:A:226:LYS:O	1:A:230:LYS:HG3	1.61	0.98
1:A:530:ILE:HB	1:A:535:ARG:NH1	1.80	0.97
1:A:534:PHE:O	1:A:537:LEU:HB3	1.66	0.96
1:A:416:ARG:HG3	1:A:416:ARG:NH1	1.79	0.95
1:A:286:ASN:HD22	1:A:286:ASN:C	1.68	0.95
2:B:9:ASN:N	2:B:9:ASN:HD22	1.64	0.94
2:B:45:THR:O	3:B:218:HOH:O	1.86	0.94
1:A:69:LYS:HZ3	1:A:69:LYS:HB3	1.21	0.93
1:A:629:LYS:HG3	3:A:827:HOH:O	1.65	0.93
1:A:530:ILE:HB	1:A:535:ARG:HH12	1.31	0.92
1:A:517:GLU:OE1	1:A:637:LYS:NZ	2.00	0.92
1:A:224:LEU:HD21	1:A:228:ILE:HD11	1.52	0.91
1:A:373:GLY:H	1:A:384:ASN:HD21	0.99	0.90
1:A:238:LEU:H	1:A:238:LEU:HD12	1.27	0.90
1:A:226:LYS:NZ	3:A:712:HOH:O	2.04	0.89
1:A:168:VAL:HG12	1:A:179:ALA:HA	1.53	0.89
1:A:400:ASP:CA	1:A:401:GLY:N	2.35	0.88
1:A:212:ALA:O	3:A:791:HOH:O	1.91	0.88
1:A:561:LEU:HD12	1:A:571:GLY:HA2	1.53	0.88
1:A:398:ASP:OD1	1:A:398:ASP:N	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:ND2	1:A:288:TRP:H	1.69	0.88
1:A:36:ARG:HH21	1:A:37:ASN:HD21	1.23	0.86
1:A:694:TRP:O	1:A:698:SER:OG	1.92	0.86
2:B:106:GLY:CA	2:B:139:ASN:HD22	1.87	0.86
1:A:558:ARG:HB3	1:A:558:ARG:HH11	1.38	0.86
2:B:146:ILE:O	2:B:150:VAL:HG23	1.76	0.85
1:A:406:THR:OG1	1:A:476:LYS:HG3	1.76	0.85
1:A:281:LEU:HD22	1:A:325:TRP:HE3	1.41	0.85
1:A:409:VAL:CG2	1:A:409:VAL:CG1	2.54	0.84
1:A:243:ASP:HB2	3:A:724:HOH:O	1.75	0.84
1:A:286:ASN:HD21	1:A:288:TRP:H	1.21	0.84
1:A:466:ILE:HG22	1:A:467:ASN:N	1.92	0.84
1:A:668:ARG:HD2	3:A:749:HOH:O	1.76	0.84
1:A:398:ASP:HB3	3:A:805:HOH:O	1.78	0.84
1:A:361:MET:HG2	1:A:509:TYR:CE1	2.13	0.83
1:A:544:GLU:OE2	3:A:845:HOH:O	1.95	0.83
1:A:523:ILE:C	1:A:525:ALA:HB2	1.98	0.83
1:A:216:GLU:HG3	3:A:941:HOH:O	1.77	0.83
1:A:193:GLU:HG3	1:A:193:GLU:O	1.78	0.83
2:B:107:SER:HB2	3:B:201:HOH:O	1.76	0.83
1:A:653:ASP:O	1:A:654:GLU:CG	2.26	0.83
1:A:238:LEU:CD1	1:A:238:LEU:N	2.36	0.83
1:A:522:GLU:CG	1:A:522:GLU:CA	2.56	0.83
2:B:19:LYS:O	3:B:209:HOH:O	1.96	0.82
1:A:403:ARG:O	1:A:478:PRO:HA	1.80	0.82
1:A:4:ILE:HD13	2:B:180:LEU:HD23	1.60	0.82
1:A:416:ARG:HH11	1:A:416:ARG:HG3	1.40	0.81
2:B:100:ASP:OD2	2:B:102:SER:OG	1.98	0.81
1:A:545:ASP:OD1	1:A:591:LYS:NZ	2.13	0.81
1:A:69:LYS:HZ2	1:A:69:LYS:HB3	1.01	0.81
2:B:20:LEU:O	2:B:24:LEU:CG	2.28	0.81
1:A:350:CYS:HB3	1:A:353:TYR:HB2	1.62	0.81
1:A:523:ILE:O	1:A:525:ALA:CB	2.29	0.80
2:B:56:GLY:HA3	3:B:195:HOH:O	1.81	0.80
1:A:561:LEU:HD12	1:A:571:GLY:CA	2.11	0.79
1:A:699:VAL:O	1:A:700:LEU:CD2	2.30	0.79
2:B:132:ARG:HH11	2:B:132:ARG:CG	1.96	0.79
1:A:69:LYS:HZ3	1:A:69:LYS:CB	1.66	0.79
1:A:286:ASN:ND2	1:A:286:ASN:C	2.32	0.79
2:B:81:LYS:NZ	3:B:219:HOH:O	2.11	0.79
1:A:373:GLY:N	1:A:384:ASN:HD21	1.79	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASP:HB3	1:A:401:GLY:N	1.99	0.78
1:A:286:ASN:HD22	1:A:287:PRO:N	1.82	0.78
2:B:18:ARG:O	2:B:22:VAL:HG23	1.84	0.78
1:A:530:ILE:O	1:A:531:GLY:C	2.21	0.78
1:A:530:ILE:O	1:A:531:GLY:O	2.02	0.78
1:A:395:ASP:OD2	1:A:476:LYS:HE3	1.83	0.78
1:A:587:ASP:OD2	1:A:589:SER:OG	2.01	0.78
2:B:145:PHE:CZ	2:B:149:LEU:HD11	2.20	0.77
1:A:455:THR:CG2	1:A:455:THR:OG1	2.32	0.77
1:A:290:GLN:O	3:A:730:HOH:O	2.02	0.77
1:A:286:ASN:ND2	1:A:288:TRP:N	2.31	0.77
1:A:271:GLU:HA	1:A:279:GLN:O	1.84	0.77
2:B:156:PHE:CZ	2:B:160:ARG:HD3	2.20	0.77
2:B:151:ARG:HB3	2:B:151:ARG:HH11	1.49	0.76
1:A:523:ILE:C	1:A:525:ALA:CB	2.54	0.76
1:A:104:ASP:HB2	3:A:879:HOH:O	1.86	0.75
1:A:573:SER:HG	1:A:576:THR:HG1	1.31	0.75
1:A:89:ILE:HG22	1:A:90:GLY:O	1.86	0.75
1:A:281:LEU:HD23	1:A:326:MET:O	1.86	0.75
1:A:236:SER:O	1:A:238:LEU:HD11	1.87	0.75
1:A:218:ARG:CG	1:A:218:ARG:CA	2.64	0.75
1:A:668:ARG:NH2	2:B:182:MET:O	2.19	0.74
1:A:129:GLN:HE22	1:A:140:HIS:H	1.35	0.74
2:B:132:ARG:NH1	2:B:132:ARG:HG3	2.01	0.74
2:B:148:CYS:O	2:B:152:LEU:HD23	1.87	0.74
1:A:523:ILE:O	1:A:525:ALA:HB3	1.88	0.74
1:A:558:ARG:HB3	1:A:558:ARG:NH1	2.03	0.74
1:A:30:GLN:HE22	1:A:187:LYS:HZ1	1.36	0.74
1:A:386:GLN:HE22	1:A:451:ASN:H	1.35	0.74
2:B:137:THR:HB	2:B:137:THR:CA	2.15	0.73
1:A:408:LEU:HD22	1:A:472:LEU:HD21	1.70	0.73
1:A:554:GLN:HG3	1:A:574:ILE:HD13	1.70	0.73
1:A:476:LYS:CB	1:A:476:LYS:CD	2.64	0.73
2:B:134:SER:HB2	3:B:206:HOH:O	1.87	0.73
1:A:409:VAL:CG1	1:A:409:VAL:CA	2.66	0.72
1:A:30:GLN:HE22	1:A:187:LYS:NZ	1.87	0.72
1:A:375:ARG:HD3	1:A:376:ASN:HD22	1.54	0.72
2:B:113:ALA:O	2:B:116:ALA:HB3	1.89	0.72
1:A:373:GLY:H	1:A:384:ASN:ND2	1.82	0.71
1:A:226:LYS:HZ2	1:A:400:ASP:CG	1.93	0.71
2:B:132:ARG:HH11	2:B:132:ARG:HG3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:ARG:CB	1:A:628:ARG:CD	2.69	0.71
2:B:17:PHE:O	2:B:19:LYS:N	2.24	0.71
1:A:398:ASP:CB	3:A:805:HOH:O	2.37	0.71
1:A:226:LYS:NZ	1:A:400:ASP:OD2	2.21	0.71
2:B:20:LEU:HD11	3:B:194:HOH:O	1.90	0.71
1:A:281:LEU:HD21	1:A:326:MET:H	1.56	0.71
1:A:506:LYS:HG3	3:A:831:HOH:O	1.91	0.70
1:A:539:ALA:CB	3:A:893:HOH:O	2.38	0.70
1:A:476:LYS:CE	1:A:476:LYS:CG	2.69	0.70
2:B:142:PHE:O	2:B:143:ASP:C	2.28	0.70
1:A:286:ASN:HD21	1:A:288:TRP:N	1.87	0.70
1:A:213:GLU:OE1	1:A:474:ARG:HD2	1.91	0.70
1:A:400:ASP:CB	1:A:401:GLY:N	2.56	0.69
1:A:585:ASP:O	1:A:586:GLU:HB2	1.91	0.69
1:A:686:THR:HG23	1:A:686:THR:O	1.93	0.69
1:A:216:GLU:CG	3:A:941:HOH:O	2.37	0.69
1:A:617:ASP:OD1	1:A:619:SER:HB2	1.91	0.69
1:A:576:THR:HA	1:A:664:ARG:HD3	1.75	0.69
1:A:585:ASP:OD1	1:A:587:ASP:OD1	2.11	0.69
1:A:410:GLY:O	1:A:499:ILE:HA	1.94	0.68
1:A:500:ARG:HD3	3:A:945:HOH:O	1.93	0.68
2:B:105:ILE:HG22	2:B:110:LEU:HD12	1.76	0.68
2:B:163:ASP:OD1	2:B:167:THR:O	2.11	0.68
1:A:290:GLN:C	1:A:322:GLY:CA	2.62	0.68
1:A:678:GLN:O	1:A:681:PRO:HD3	1.94	0.68
1:A:342:ASN:HD22	1:A:356:TRP:HE1	1.39	0.68
1:A:466:ILE:HG22	1:A:467:ASN:H	1.59	0.68
1:A:403:ARG:HD2	1:A:478:PRO:HB3	1.76	0.68
1:A:554:GLN:HE21	1:A:554:GLN:C	1.97	0.67
1:A:64:GLY:O	1:A:67:SER:HB3	1.93	0.67
1:A:285:ARG:HD3	1:A:286:ASN:N	2.10	0.67
1:A:523:ILE:HD13	1:A:602:THR:HG21	1.75	0.67
2:B:93:ILE:CD1	2:B:117:ALA:HA	2.24	0.67
1:A:364:ASN:ND2	1:A:644:GLN:HE22	1.93	0.67
1:A:223:ASN:HD22	1:A:226:LYS:HE2	1.60	0.67
1:A:56:SER:OG	3:A:804:HOH:O	2.13	0.66
1:A:418:ARG:NH1	3:A:731:HOH:O	2.28	0.66
1:A:562:ALA:HA	1:A:569:SER:O	1.95	0.66
2:B:20:LEU:HD13	2:B:39:ILE:HG23	1.78	0.66
1:A:699:VAL:HB	1:A:699:VAL:CA	2.18	0.66
1:A:652:ASP:OD2	1:A:656:ILE:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD21	1:A:228:ILE:CD1	2.25	0.66
1:A:541:LEU:HG	1:A:556:ILE:CD1	2.26	0.66
1:A:548:ILE:HG22	1:A:552:GLU:CB	2.26	0.66
1:A:164:GLU:OE1	3:A:903:HOH:O	2.14	0.66
1:A:539:ALA:HB1	3:A:893:HOH:O	1.96	0.65
1:A:653:ASP:C	1:A:654:GLU:HG2	2.17	0.65
1:A:472:LEU:HG	3:A:791:HOH:O	1.96	0.65
2:B:137:THR:CB	2:B:137:THR:HA	2.13	0.65
1:A:517:GLU:OE1	1:A:637:LYS:CE	2.44	0.65
1:A:523:ILE:C	1:A:525:ALA:N	2.49	0.65
1:A:688:GLN:HB2	3:A:928:HOH:O	1.95	0.65
1:A:226:LYS:NZ	1:A:400:ASP:CG	2.50	0.65
1:A:387:TYR:OH	3:A:741:HOH:O	2.14	0.65
1:A:578:LYS:NZ	1:A:578:LYS:CD	2.58	0.65
1:A:343:LEU:HG	1:A:347:THR:HG21	1.79	0.65
1:A:374:CYS:HB2	1:A:489:PHE:O	1.96	0.64
1:A:699:VAL:CG2	1:A:699:VAL:CG1	2.74	0.64
1:A:527:GLU:OE2	1:A:527:GLU:HA	1.97	0.64
1:A:328:PHE:O	1:A:332:LEU:HD13	1.98	0.64
1:A:668:ARG:CG	3:A:848:HOH:O	2.45	0.64
2:B:38:ASN:O	2:B:42:LYS:HG3	1.98	0.64
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.62	0.64
2:B:31:VAL:HG12	2:B:32:SER:O	1.98	0.64
1:A:216:GLU:CD	3:A:941:HOH:O	2.35	0.63
1:A:469:ARG:HD2	3:A:946:HOH:O	1.98	0.63
1:A:424:GLU:HB2	3:A:782:HOH:O	1.97	0.63
1:A:64:GLY:C	3:A:795:HOH:O	2.37	0.63
1:A:364:ASN:HD21	1:A:644:GLN:HE22	1.46	0.63
1:A:463:ASP:O	1:A:464:THR:OG1	2.17	0.63
1:A:536:ARG:CG	1:A:536:ARG:HH11	2.11	0.63
1:A:500:ARG:CD	3:A:945:HOH:O	2.45	0.63
1:A:680:ASP:N	1:A:681:PRO:HD2	2.13	0.63
1:A:281:LEU:HD23	1:A:282:ILE:N	2.13	0.62
1:A:429:ILE:CD1	1:A:471:VAL:HG22	2.29	0.62
2:B:34:THR:HB	3:B:222:HOH:O	1.99	0.62
2:B:96:ARG:NH1	2:B:97:PHE:CZ	2.68	0.62
1:A:679:LEU:C	1:A:681:PRO:HD2	2.19	0.62
2:B:34:THR:O	2:B:37:MET:HB3	1.98	0.62
2:B:18:ARG:O	2:B:18:ARG:HG3	1.99	0.62
1:A:344:THR:HB	1:A:345:PRO:HD2	1.79	0.62
1:A:488:THR:HG22	1:A:490:GLU:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLY:HA3	1:A:487:SER:HB2	1.80	0.62
1:A:472:LEU:HD13	1:A:473:ASN:N	2.14	0.62
2:B:32:SER:HB3	2:B:35:GLU:HG3	1.80	0.62
2:B:105:ILE:CG2	2:B:110:LEU:HD12	2.30	0.62
1:A:523:ILE:O	1:A:525:ALA:HB2	1.96	0.61
1:A:368:GLY:O	1:A:624:SER:HB3	2.00	0.61
2:B:63:MET:HG2	2:B:83:LEU:HD11	1.81	0.61
1:A:525:ALA:HB1	1:A:526:ASN:CA	2.24	0.61
2:B:162:LEU:HD11	2:B:180:LEU:HD11	1.80	0.61
2:B:110:LEU:HD22	2:B:130:ILE:HD12	1.83	0.61
1:A:609:LYS:O	1:A:612:ARG:CB	2.49	0.61
1:A:86:GLN:OE1	1:A:132:GLN:NE2	2.33	0.61
1:A:167:PHE:HB3	1:A:182:GLU:OE1	2.00	0.61
1:A:99:GLN:HE21	1:A:168:VAL:HG23	1.66	0.60
2:B:9:ASN:ND2	2:B:9:ASN:N	2.39	0.60
1:A:404:GLY:CA	1:A:476:LYS:HG2	2.32	0.60
1:A:361:MET:CG	1:A:509:TYR:CE1	2.84	0.60
1:A:680:ASP:N	1:A:681:PRO:CD	2.64	0.60
2:B:50:LEU:HD12	2:B:52:THR:HG22	1.83	0.60
2:B:132:ARG:NH1	2:B:132:ARG:CG	2.60	0.60
1:A:375:ARG:HD3	1:A:376:ASN:ND2	2.15	0.60
1:A:216:GLU:OE2	3:A:941:HOH:O	2.15	0.60
1:A:557:LEU:HD23	1:A:572:PHE:HD2	1.66	0.60
1:A:217:LEU:O	1:A:220:PRO:HD3	2.02	0.60
1:A:269:ALA:CB	1:A:282:ILE:HG22	2.32	0.59
1:A:463:ASP:C	1:A:464:THR:OG1	2.41	0.59
1:A:411:LEU:HB3	1:A:471:VAL:HG23	1.84	0.59
1:A:541:LEU:HG	1:A:556:ILE:HD13	1.84	0.59
2:B:121:LEU:HA	3:B:192:HOH:O	2.02	0.59
1:A:63:LEU:HD12	1:A:63:LEU:N	2.17	0.59
1:A:13:GLU:HA	1:A:13:GLU:OE2	2.02	0.59
1:A:606:LYS:CE	1:A:606:LYS:CG	2.76	0.59
2:B:106:GLY:HA3	3:B:199:HOH:O	2.03	0.59
1:A:89:ILE:HB	3:A:798:HOH:O	2.01	0.59
2:B:75:LEU:C	2:B:75:LEU:HD12	2.23	0.59
1:A:395:ASP:N	1:A:404:GLY:O	2.36	0.59
1:A:281:LEU:HD21	1:A:325:TRP:HB3	1.84	0.59
1:A:472:LEU:HD13	1:A:472:LEU:C	2.23	0.59
2:B:50:LEU:HD12	2:B:52:THR:CG2	2.33	0.59
2:B:40:LEU:O	2:B:44:VAL:HG22	2.03	0.59
1:A:620:GLY:O	1:A:621:THR:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:HB3	1:A:385:PRO:CD	2.33	0.58
1:A:77:ARG:NH1	1:A:156:ASP:OD2	2.36	0.58
1:A:548:ILE:HG22	1:A:552:GLU:HB2	1.85	0.58
1:A:363:GLY:HA3	1:A:497:PHE:CZ	2.38	0.58
1:A:558:ARG:HH12	1:A:559:ARG:HH11	1.50	0.58
2:B:36:LEU:HD22	2:B:75:LEU:HD23	1.85	0.58
1:A:516:ILE:HG12	1:A:639:PRO:HD3	1.85	0.58
1:A:538:PHE:CZ	1:A:594:LEU:N	2.71	0.58
1:A:525:ALA:HB1	1:A:526:ASN:HA	1.86	0.57
1:A:289:GLY:C	1:A:322:GLY:N	2.58	0.57
2:B:123:GLN:HB3	3:B:204:HOH:O	2.04	0.57
1:A:145:GLN:O	1:A:146:TYR:C	2.43	0.57
1:A:373:GLY:O	1:A:374:CYS:CB	2.51	0.57
1:A:95:THR:OG1	1:A:97:ILE:HG12	2.05	0.57
2:B:17:PHE:O	2:B:20:LEU:HB2	2.04	0.57
1:A:289:GLY:HA3	3:A:926:HOH:O	2.04	0.57
2:B:47:HIS:CB	2:B:49:ASP:OD1	2.45	0.57
1:A:402:GLU:HA	1:A:403:ARG:CA	2.33	0.57
1:A:629:LYS:HB3	3:A:721:HOH:O	2.05	0.57
1:A:694:TRP:C	1:A:698:SER:HG	2.01	0.57
1:A:404:GLY:HA3	1:A:476:LYS:HE2	1.86	0.57
1:A:394:GLU:OE1	1:A:403:ARG:HB2	2.05	0.57
2:B:58:ASP:O	2:B:59:THR:C	2.41	0.57
1:A:417:ARG:HG3	3:B:191:HOH:O	2.04	0.57
1:A:404:GLY:HA2	1:A:476:LYS:HG2	1.86	0.57
1:A:361:MET:HE3	1:A:387:TYR:HB3	1.86	0.57
1:A:394:GLU:HA	1:A:405:CYS:SG	2.44	0.57
1:A:290:GLN:H	1:A:322:GLY:N	1.96	0.57
1:A:193:GLU:O	1:A:193:GLU:CG	2.52	0.57
1:A:367:ARG:CZ	1:A:655:LEU:HD21	2.35	0.57
1:A:676:PHE:CD1	1:A:687:ILE:HD13	2.39	0.57
1:A:331:PHE:C	1:A:333:ARG:H	2.07	0.56
1:A:200:THR:O	1:A:204:PHE:HB2	2.06	0.56
2:B:96:ARG:NH1	2:B:97:PHE:CE1	2.74	0.56
2:B:110:LEU:HB3	2:B:130:ILE:HD11	1.87	0.56
1:A:224:LEU:C	1:A:224:LEU:HD23	2.25	0.56
1:A:535:ARG:O	1:A:536:ARG:C	2.44	0.56
1:A:353:TYR:O	1:A:353:TYR:HD1	1.89	0.56
1:A:460:GLU:N	3:A:770:HOH:O	2.38	0.56
2:B:169:GLN:NE2	3:B:207:HOH:O	2.38	0.56
1:A:600:LEU:HD11	1:A:604:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:SER:OG	1:A:551:PHE:HB2	2.06	0.56
1:A:596:GLU:HG3	3:A:764:HOH:O	2.05	0.56
1:A:690:ASP:OD1	1:A:693:SER:OG	2.18	0.56
2:B:87:ILE:HG22	2:B:87:ILE:O	2.05	0.56
1:A:88:ILE:O	1:A:88:ILE:CG2	2.54	0.56
2:B:105:ILE:CG2	2:B:109:GLU:HB2	2.36	0.55
1:A:686:THR:CG2	1:A:686:THR:O	2.50	0.55
1:A:639:PRO:HD2	1:A:642:LEU:HD12	1.88	0.55
1:A:236:SER:O	1:A:238:LEU:CD1	2.54	0.55
1:A:530:ILE:CB	1:A:535:ARG:HH12	2.13	0.55
1:A:56:SER:HB2	3:A:703:HOH:O	2.05	0.55
1:A:551:PHE:O	1:A:552:GLU:C	2.45	0.55
1:A:269:ALA:HA	1:A:282:ILE:HG22	1.88	0.55
2:B:39:ILE:CD1	3:B:235:HOH:O	2.55	0.55
1:A:367:ARG:H	1:A:494:ASN:HD21	1.55	0.55
1:A:542:ALA:HB1	1:A:547:GLU:N	2.21	0.55
2:B:63:MET:HG2	2:B:83:LEU:CD1	2.36	0.55
1:A:533:GLY:O	1:A:537:LEU:HB2	2.07	0.55
1:A:36:ARG:HH21	1:A:37:ASN:ND2	2.00	0.55
1:A:575:GLU:N	3:A:786:HOH:O	2.29	0.55
1:A:414:LYS:HZ1	1:A:498:CYS:HB2	1.72	0.55
1:A:568:LYS:NZ	1:A:608:GLN:HG2	2.21	0.54
1:A:394:GLU:HG2	1:A:479:PRO:HD3	1.89	0.54
1:A:558:ARG:CD	3:A:927:HOH:O	2.54	0.54
1:A:98:CYS:SG	1:A:169:HIS:CE1	3.00	0.54
1:A:237:LEU:C	1:A:238:LEU:HD12	2.26	0.54
1:A:399:GLU:HG2	1:A:399:GLU:O	2.08	0.54
1:A:226:LYS:HG2	1:A:230:LYS:HG3	1.89	0.54
1:A:699:VAL:HG23	1:A:700:LEU:CD2	2.38	0.54
1:A:538:PHE:CD2	1:A:594:LEU:HD23	2.43	0.54
2:B:99:THR:O	2:B:101:ARG:N	2.40	0.54
1:A:492:HIS:HD2	1:A:625:TYR:OH	1.91	0.54
1:A:338:LEU:HD22	1:A:339:GLU:N	2.23	0.54
1:A:285:ARG:HD3	1:A:286:ASN:C	2.28	0.54
2:B:23:GLN:N	3:B:209:HOH:O	2.41	0.54
1:A:386:GLN:NE2	1:A:451:ASN:H	2.04	0.54
2:B:41:ASN:O	2:B:45:THR:HG21	2.07	0.53
1:A:350:CYS:CB	1:A:353:TYR:HB2	2.34	0.53
1:A:554:GLN:CG	1:A:574:ILE:HD13	2.37	0.53
1:A:584:LEU:HD23	1:A:600:LEU:HB2	1.90	0.53
1:A:337:ARG:HG2	1:A:337:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:CD2	1:A:472:LEU:HD21	2.38	0.53
1:A:548:ILE:HG22	1:A:552:GLU:HB3	1.90	0.53
2:B:110:LEU:O	2:B:114:PHE:N	2.41	0.53
2:B:93:ILE:HD13	2:B:117:ALA:HA	1.91	0.53
1:A:367:ARG:H	1:A:494:ASN:ND2	2.06	0.53
2:B:107:SER:CB	3:B:201:HOH:O	2.47	0.53
2:B:92:GLY:O	2:B:96:ARG:HB3	2.08	0.53
1:A:290:GLN:CA	1:A:322:GLY:N	2.72	0.53
1:A:119:GLU:HB2	1:A:348:LEU:HD23	1.91	0.53
1:A:394:GLU:CD	1:A:403:ARG:HB2	2.29	0.53
2:B:16:GLN:O	2:B:17:PHE:C	2.47	0.53
1:A:620:GLY:O	1:A:621:THR:CG2	2.56	0.53
1:A:281:LEU:HD23	1:A:282:ILE:H	1.72	0.53
1:A:81:ILE:O	1:A:82:CYS:HB2	2.08	0.53
1:A:390:LYS:HB2	1:A:481:GLU:HG2	1.90	0.52
1:A:427:HIS:CD2	3:A:725:HOH:O	2.61	0.52
1:A:337:ARG:NH1	1:A:339:GLU:OE2	2.43	0.52
1:A:99:GLN:NE2	1:A:168:VAL:HG23	2.23	0.52
1:A:358:LEU:HD13	1:A:502:PHE:CZ	2.44	0.52
1:A:281:LEU:CD2	1:A:326:MET:O	2.56	0.52
1:A:603:LYS:O	1:A:604:ILE:C	2.46	0.52
1:A:583:MET:HG2	1:A:584:LEU:HD13	1.90	0.52
1:A:242:ILE:HG12	1:A:334:HIS:O	2.10	0.52
2:B:16:GLN:O	2:B:19:LYS:HB3	2.09	0.52
1:A:414:LYS:NZ	1:A:498:CYS:HB2	2.24	0.52
1:A:224:LEU:CD2	1:A:228:ILE:CD1	2.88	0.52
1:A:676:PHE:CE1	1:A:687:ILE:HG23	2.45	0.52
2:B:95:LYS:O	2:B:97:PHE:N	2.42	0.52
2:B:32:SER:CB	2:B:35:GLU:HG3	2.40	0.52
2:B:123:GLN:CB	3:B:204:HOH:O	2.58	0.52
1:A:217:LEU:HD22	1:A:337:ARG:N	2.25	0.51
2:B:126:TYR:O	2:B:128:MET:N	2.43	0.51
1:A:281:LEU:CD2	1:A:282:ILE:N	2.73	0.51
1:A:615:ASP:O	1:A:616:VAL:C	2.48	0.51
2:B:83:LEU:O	2:B:87:ILE:HG13	2.10	0.51
1:A:599:ILE:O	1:A:600:LEU:C	2.40	0.51
1:A:106:TRP:CD1	1:A:198:GLY:HA3	2.45	0.51
1:A:267:THR:CG2	1:A:285:ARG:HB2	2.40	0.51
2:B:75:LEU:HD12	2:B:76:GLY:N	2.26	0.51
1:A:609:LYS:O	1:A:612:ARG:N	2.42	0.51
1:A:393:GLU:HB3	1:A:505:LYS:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:TYR:CD2	1:A:286:ASN:HB2	2.46	0.51
2:B:126:TYR:C	2:B:128:MET:H	2.15	0.51
1:A:290:GLN:C	1:A:322:GLY:N	2.65	0.51
1:A:366:ARG:HA	1:A:494:ASN:ND2	2.26	0.51
1:A:129:GLN:NE2	1:A:139:PHE:HA	2.26	0.51
1:A:209:GLY:O	1:A:500:ARG:NH2	2.44	0.51
1:A:81:ILE:HD12	1:A:165:LEU:CD2	2.41	0.51
1:A:412:ILE:HD11	1:A:469:ARG:HD3	1.92	0.50
2:B:98:ASP:OD2	2:B:104:THR:O	2.28	0.50
1:A:402:GLU:CA	1:A:403:ARG:CA	2.88	0.50
2:B:96:ARG:HG2	2:B:97:PHE:CE1	2.45	0.50
2:B:96:ARG:HH11	2:B:96:ARG:HG2	1.77	0.50
1:A:354:LYS:NZ	3:A:844:HOH:O	2.37	0.50
1:A:204:PHE:HZ	1:A:237:LEU:HD12	1.77	0.50
2:B:41:ASN:HD21	2:B:55:PHE:N	2.08	0.50
1:A:463:ASP:O	1:A:464:THR:C	2.50	0.50
1:A:216:GLU:OE1	1:A:337:ARG:HG3	2.12	0.50
1:A:262:HIS:CE1	3:A:740:HOH:O	2.64	0.50
1:A:168:VAL:CG1	1:A:179:ALA:HA	2.34	0.50
2:B:50:LEU:HD21	2:B:94:TYR:CD2	2.47	0.50
1:A:400:ASP:O	1:A:401:GLY:HA2	2.08	0.50
1:A:119:GLU:HB2	1:A:348:LEU:CD2	2.42	0.50
1:A:409:VAL:HG11	1:A:484:LEU:HD21	1.93	0.50
1:A:395:ASP:OD1	1:A:504:GLU:HG3	2.12	0.50
1:A:285:ARG:HA	1:A:323:GLU:HA	1.94	0.50
1:A:281:LEU:HD21	1:A:326:MET:N	2.23	0.49
1:A:12:ARG:O	1:A:16:GLU:HG3	2.12	0.49
1:A:699:VAL:HG23	1:A:700:LEU:HD23	1.94	0.49
1:A:332:LEU:HD23	3:A:870:HOH:O	2.11	0.49
1:A:337:ARG:HD2	3:A:724:HOH:O	2.11	0.49
1:A:416:ARG:CG	1:A:416:ARG:HH11	2.18	0.49
1:A:97:ILE:HA	1:A:170:SER:HA	1.92	0.49
1:A:427:HIS:HD2	3:A:725:HOH:O	1.96	0.49
2:B:60:CYS:O	2:B:64:VAL:HG23	2.12	0.49
2:B:123:GLN:N	2:B:123:GLN:HE21	2.10	0.49
1:A:331:PHE:C	1:A:333:ARG:N	2.63	0.49
1:A:240:CYS:HA	1:A:337:ARG:O	2.12	0.49
2:B:151:ARG:HB3	2:B:151:ARG:NH1	2.23	0.49
1:A:557:LEU:HD23	1:A:572:PHE:CD2	2.46	0.49
1:A:373:GLY:O	1:A:374:CYS:HB2	2.12	0.49
2:B:28:ASP:OD1	2:B:28:ASP:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:O	1:A:177:TRP:HD1	1.96	0.49
2:B:96:ARG:O	2:B:96:ARG:HG3	2.13	0.49
1:A:344:THR:CB	1:A:345:PRO:HD2	2.40	0.49
2:B:42:LYS:HD3	3:B:194:HOH:O	2.12	0.48
2:B:78:GLU:HA	2:B:81:LYS:HE2	1.95	0.48
1:A:467:ASN:O	1:A:467:ASN:CG	2.52	0.48
1:A:228:ILE:HD12	1:A:328:PHE:HE1	1.78	0.48
1:A:4:ILE:CD1	2:B:180:LEU:HD23	2.35	0.48
2:B:87:ILE:O	2:B:87:ILE:CG2	2.60	0.48
1:A:88:ILE:CD1	1:A:121:LEU:HD21	2.43	0.48
1:A:269:ALA:HB2	1:A:282:ILE:HG22	1.95	0.48
1:A:532:ASP:OD1	1:A:536:ARG:NH2	2.46	0.48
1:A:88:ILE:HD11	1:A:121:LEU:HD21	1.94	0.48
1:A:647:VAL:HG13	1:A:648:ALA:N	2.27	0.48
1:A:387:TYR:CD1	1:A:387:TYR:N	2.82	0.48
1:A:573:SER:OG	1:A:576:THR:OG1	2.07	0.48
1:A:541:LEU:HG	1:A:556:ILE:HD11	1.96	0.48
1:A:542:ALA:CB	1:A:546:ALA:HA	2.43	0.48
1:A:63:LEU:CD1	1:A:63:LEU:N	2.76	0.48
1:A:673:PHE:O	1:A:677:LYS:HG3	2.14	0.48
2:B:99:THR:C	2:B:101:ARG:H	2.16	0.48
1:A:372:GLY:O	1:A:491:PRO:HB3	2.14	0.48
1:A:402:GLU:C	1:A:403:ARG:CA	2.80	0.47
2:B:39:ILE:HD11	3:B:235:HOH:O	2.14	0.47
2:B:59:THR:O	2:B:63:MET:HE3	2.14	0.47
2:B:17:PHE:O	2:B:20:LEU:N	2.47	0.47
2:B:148:CYS:O	2:B:152:LEU:CD2	2.59	0.47
1:A:331:PHE:O	1:A:333:ARG:N	2.47	0.47
1:A:558:ARG:HD2	3:A:927:HOH:O	2.12	0.47
1:A:678:GLN:NE2	3:A:807:HOH:O	2.47	0.47
1:A:609:LYS:O	1:A:612:ARG:HB3	2.14	0.47
1:A:536:ARG:HG3	1:A:536:ARG:HH11	1.79	0.47
1:A:285:ARG:NH1	1:A:285:ARG:HG3	2.28	0.47
1:A:7:LYS:HD2	3:A:854:HOH:O	2.14	0.47
1:A:238:LEU:CD1	1:A:238:LEU:H	2.09	0.47
1:A:413:GLN:OE1	1:A:426:MET:HG3	2.14	0.47
1:A:421:LYS:HB3	1:A:424:GLU:HG3	1.96	0.47
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.62	0.47
1:A:674:LYS:CE	1:A:674:LYS:CG	2.83	0.47
1:A:99:GLN:OE1	1:A:103:GLY:HA3	2.15	0.47
1:A:127:LEU:O	1:A:129:GLN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:GLN:N	2:B:123:GLN:NE2	2.63	0.47
1:A:596:GLU:CG	3:A:764:HOH:O	2.62	0.47
1:A:120:ILE:O	1:A:121:LEU:C	2.50	0.47
1:A:327:SER:HB3	1:A:330:ASP:OD2	2.14	0.47
2:B:11:SER:O	2:B:13:GLU:N	2.48	0.47
2:B:166:GLY:O	2:B:167:THR:C	2.53	0.47
1:A:419:GLN:NE2	1:A:424:GLU:O	2.48	0.47
1:A:88:ILE:HG23	1:A:88:ILE:O	2.14	0.47
1:A:436:VAL:C	3:A:944:HOH:O	2.53	0.47
1:A:699:VAL:CG2	1:A:699:VAL:CA	2.83	0.47
1:A:417:ARG:CG	3:B:191:HOH:O	2.63	0.47
1:A:361:MET:HE3	1:A:387:TYR:CB	2.44	0.47
1:A:561:LEU:C	1:A:563:LYS:N	2.68	0.47
1:A:262:HIS:HE2	1:A:288:TRP:HE3	1.62	0.46
1:A:374:CYS:CB	1:A:489:PHE:O	2.63	0.46
1:A:373:GLY:HA3	1:A:487:SER:CB	2.45	0.46
1:A:359:THR:O	1:A:501:VAL:N	2.36	0.46
2:B:41:ASN:O	2:B:45:THR:CG2	2.63	0.46
2:B:93:ILE:HD13	2:B:117:ALA:CA	2.45	0.46
1:A:506:LYS:CG	1:A:506:LYS:CE	2.83	0.46
1:A:573:SER:OG	1:A:660:ASP:OD2	2.24	0.46
1:A:28:LEU:HD23	1:A:50:SER:HB2	1.97	0.46
2:B:59:THR:HG23	2:B:147:SER:HB2	1.97	0.46
2:B:110:LEU:HD22	2:B:130:ILE:CD1	2.45	0.46
1:A:429:ILE:HD12	1:A:471:VAL:HG22	1.97	0.46
1:A:497:PHE:CD2	1:A:497:PHE:C	2.89	0.46
1:A:177:TRP:CG	1:A:178:SER:N	2.84	0.46
1:A:430:GLY:HA3	1:A:465:PHE:CZ	2.51	0.46
1:A:380:THR:O	1:A:381:PHE:C	2.53	0.46
1:A:692:ILE:O	1:A:696:SER:OG	2.34	0.46
1:A:81:ILE:O	1:A:82:CYS:CB	2.59	0.46
1:A:155:ASP:C	1:A:155:ASP:OD2	2.54	0.46
1:A:433:ILE:HG12	1:A:484:LEU:HD22	1.98	0.46
2:B:20:LEU:CD1	3:B:194:HOH:O	2.57	0.46
1:A:269:ALA:CA	1:A:282:ILE:HG22	2.46	0.46
2:B:109:GLU:C	2:B:111:PRO:HD2	2.37	0.46
2:B:50:LEU:CD1	2:B:52:THR:HG22	2.46	0.46
1:A:106:TRP:NE1	1:A:198:GLY:HA3	2.31	0.46
1:A:486:PRO:HG2	1:A:486:PRO:O	2.15	0.46
1:A:74:GLU:O	1:A:160:THR:OG1	2.27	0.45
1:A:62:GLU:C	1:A:63:LEU:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:LEU:CD1	2:B:39:ILE:HG23	2.46	0.45
1:A:4:ILE:CD1	2:B:180:LEU:HA	2.47	0.45
1:A:412:ILE:HG12	1:A:413:GLN:N	2.31	0.45
1:A:626:GLU:HA	3:A:827:HOH:O	2.16	0.45
1:A:527:GLU:CA	1:A:527:GLU:OE2	2.63	0.45
1:A:78:PRO:HG3	1:A:176:PHE:CD2	2.51	0.45
1:A:530:ILE:HD12	1:A:535:ARG:HH12	1.80	0.45
1:A:323:GLU:O	1:A:324:PHE:HB3	2.16	0.45
2:B:133:TYR:HB2	2:B:140:MET:CE	2.47	0.45
1:A:537:LEU:O	1:A:541:LEU:HB2	2.17	0.45
2:B:55:PHE:HA	2:B:143:ASP:OD2	2.17	0.45
1:A:527:GLU:C	1:A:528:GLU:O	2.50	0.45
2:B:57:ILE:HG23	2:B:58:ASP:N	2.32	0.45
1:A:118:GLU:OE1	1:A:119:GLU:HA	2.17	0.45
1:A:30:GLN:NE2	1:A:187:LYS:NZ	2.62	0.45
1:A:173:GLY:HA2	3:A:915:HOH:O	2.16	0.45
2:B:145:PHE:CZ	2:B:149:LEU:CD1	2.97	0.45
2:B:22:VAL:O	2:B:23:GLN:C	2.53	0.44
1:A:551:PHE:HA	1:A:554:GLN:HB2	1.99	0.44
1:A:699:VAL:HB	1:A:699:VAL:CG1	2.19	0.44
2:B:24:LEU:HD11	2:B:39:ILE:HD11	1.99	0.44
1:A:115:THR:CG2	3:A:759:HOH:O	2.38	0.44
1:A:403:ARG:O	1:A:478:PRO:CA	2.59	0.44
1:A:37:ASN:O	1:A:38:GLU:C	2.53	0.44
2:B:112:GLY:O	2:B:116:ALA:HB2	2.18	0.44
1:A:628:ARG:HA	1:A:643:HIS:HE1	1.83	0.44
1:A:113:SER:HB3	1:A:237:LEU:HD13	1.99	0.44
1:A:557:LEU:O	1:A:561:LEU:HB2	2.17	0.44
1:A:649:ARG:HB2	2:B:183:TYR:HD1	1.80	0.44
1:A:649:ARG:NH2	1:A:668:ARG:HH12	2.14	0.44
1:A:584:LEU:O	1:A:585:ASP:O	2.35	0.44
2:B:151:ARG:CB	2:B:151:ARG:HH11	2.23	0.44
1:A:361:MET:HG2	1:A:509:TYR:HE1	1.79	0.44
1:A:210:GLY:C	1:A:500:ARG:HH22	2.20	0.44
1:A:22:GLU:H	1:A:22:GLU:CD	2.21	0.44
2:B:47:HIS:CD2	2:B:47:HIS:N	2.86	0.44
1:A:51:PHE:CE1	1:A:57:SER:HB3	2.53	0.44
1:A:213:GLU:HG2	1:A:215:TYR:CE1	2.53	0.44
1:A:221:PRO:HB2	1:A:222:PRO:O	2.18	0.43
1:A:649:ARG:HB2	2:B:183:TYR:CD1	2.53	0.43
1:A:538:PHE:O	1:A:542:ALA:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:PRO:HB3	1:A:356:TRP:O	2.17	0.43
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.70	0.43
1:A:398:ASP:CG	3:A:805:HOH:O	2.52	0.43
1:A:632:GLU:O	1:A:633:GLU:C	2.56	0.43
1:A:628:ARG:CG	1:A:628:ARG:NE	2.67	0.43
1:A:290:GLN:O	1:A:322:GLY:HA2	2.18	0.43
1:A:668:ARG:HG2	3:A:848:HOH:O	2.14	0.43
1:A:604:ILE:O	1:A:604:ILE:HG22	2.07	0.43
1:A:51:PHE:HB2	1:A:187:LYS:HE3	1.99	0.43
2:B:105:ILE:HG23	2:B:109:GLU:HB2	2.00	0.43
1:A:221:PRO:C	1:A:222:PRO:O	2.56	0.43
1:A:402:GLU:C	1:A:403:ARG:HG2	2.38	0.43
1:A:238:LEU:HB2	1:A:266:VAL:HB	2.01	0.43
1:A:668:ARG:CD	3:A:848:HOH:O	2.66	0.43
1:A:194:ALA:HA	1:A:421:LYS:HG3	2.01	0.43
2:B:50:LEU:CD1	2:B:52:THR:CG2	2.96	0.43
1:A:620:GLY:C	1:A:621:THR:HG23	2.38	0.43
1:A:171:ALA:HB2	3:A:826:HOH:O	2.19	0.43
1:A:628:ARG:HA	1:A:643:HIS:CE1	2.54	0.43
2:B:125:ILE:O	2:B:128:MET:N	2.51	0.43
1:A:267:THR:HG23	1:A:285:ARG:HB2	2.01	0.43
1:A:8:LEU:O	1:A:12:ARG:HG3	2.19	0.43
1:A:629:LYS:O	1:A:630:ALA:C	2.55	0.43
2:B:125:ILE:O	2:B:128:MET:HB2	2.18	0.43
2:B:30:GLU:HB3	2:B:74:LYS:HB3	2.00	0.43
1:A:224:LEU:HD22	1:A:328:PHE:CZ	2.53	0.43
1:A:364:ASN:ND2	1:A:644:GLN:NE2	2.64	0.43
1:A:419:GLN:HE21	1:A:419:GLN:HA	1.83	0.43
1:A:102:LEU:CD1	1:A:102:LEU:N	2.81	0.43
1:A:59:GLY:HA3	1:A:63:LEU:O	2.19	0.43
2:B:110:LEU:HB3	2:B:130:ILE:CD1	2.47	0.43
1:A:431:PHE:N	1:A:431:PHE:CD1	2.87	0.43
2:B:100:ASP:C	2:B:102:SER:N	2.72	0.42
1:A:617:ASP:CG	1:A:619:SER:HB2	2.39	0.42
1:A:120:ILE:O	1:A:123:ARG:N	2.49	0.42
2:B:129:ILE:HD13	2:B:129:ILE:HG21	1.62	0.42
1:A:700:LEU:HD13	2:B:128:MET:HB3	2.01	0.42
1:A:541:LEU:CD1	1:A:556:ILE:HD11	2.49	0.42
2:B:111:PRO:O	2:B:115:GLU:HG3	2.19	0.42
2:B:31:VAL:HG11	2:B:36:LEU:HB2	2.02	0.42
1:A:488:THR:CG2	1:A:490:GLU:O	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:PHE:HD2	2:B:143:ASP:OD2	2.02	0.42
1:A:579:ILE:HG13	1:A:580:MET:N	2.33	0.42
1:A:397:ASP:C	1:A:398:ASP:OD1	2.58	0.42
2:B:31:VAL:HG13	2:B:35:GLU:HB2	2.01	0.42
3:A:883:HOH:O	2:B:171:GLN:HG2	2.19	0.42
1:A:545:ASP:O	1:A:546:ALA:HB3	2.20	0.42
1:A:210:GLY:O	1:A:500:ARG:NH2	2.38	0.42
1:A:156:ASP:O	1:A:157:ARG:C	2.52	0.42
1:A:56:SER:CB	3:A:703:HOH:O	2.66	0.42
2:B:41:ASN:C	2:B:45:THR:HG22	2.40	0.42
1:A:4:ILE:HD12	1:A:5:ALA:N	2.35	0.42
1:A:421:LYS:NZ	3:A:796:HOH:O	2.33	0.42
2:B:89:LYS:C	2:B:91:GLN:N	2.68	0.42
1:A:236:SER:HB3	1:A:341:CYS:O	2.20	0.42
2:B:24:LEU:CD1	3:B:235:HOH:O	2.67	0.42
1:A:62:GLU:HB3	1:A:193:GLU:OE1	2.20	0.42
1:A:412:ILE:HG13	1:A:469:ARG:O	2.19	0.42
2:B:41:ASN:C	2:B:45:THR:CG2	2.89	0.41
2:B:110:LEU:N	2:B:111:PRO:CD	2.83	0.41
1:A:496:ASP:HB3	3:A:739:HOH:O	2.19	0.41
1:A:223:ASN:ND2	1:A:226:LYS:HE2	2.32	0.41
1:A:652:ASP:C	1:A:653:ASP:O	2.53	0.41
1:A:654:GLU:O	1:A:655:LEU:HB2	2.21	0.41
1:A:264:TYR:CE2	1:A:286:ASN:HB2	2.55	0.41
1:A:553:LEU:O	1:A:557:LEU:HD13	2.21	0.41
1:A:364:ASN:HB3	1:A:496:ASP:OD2	2.20	0.41
2:B:11:SER:C	2:B:13:GLU:N	2.73	0.41
1:A:426:MET:O	1:A:427:HIS:C	2.58	0.41
1:A:622:MET:HG2	1:A:623:ASN:N	2.35	0.41
1:A:265:SER:HB3	3:A:887:HOH:O	2.20	0.41
1:A:561:LEU:O	1:A:562:ALA:C	2.59	0.41
1:A:492:HIS:CD2	1:A:625:TYR:OH	2.71	0.41
2:B:66:VAL:HG23	2:B:67:MET:HG2	2.02	0.41
1:A:429:ILE:HD12	1:A:471:VAL:CG2	2.50	0.41
1:A:91:GLY:O	1:A:92:ALA:C	2.56	0.41
1:A:454:LEU:O	3:A:787:HOH:O	2.22	0.41
1:A:558:ARG:NH1	1:A:559:ARG:HH11	2.18	0.41
1:A:583:MET:SD	1:A:667:VAL:HG13	2.61	0.41
1:A:491:PRO:HB2	1:A:492:HIS:CD2	2.55	0.41
1:A:327:SER:OG	1:A:330:ASP:N	2.51	0.41
2:B:126:TYR:C	2:B:128:MET:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:O	2:B:23:GLN:N	2.42	0.41
2:B:39:ILE:HG13	3:B:235:HOH:O	2.20	0.41
1:A:32:TYR:O	1:A:33:GLU:C	2.59	0.41
1:A:586:GLU:C	1:A:588:GLY:H	2.24	0.41
2:B:60:CYS:HA	2:B:63:MET:HE3	2.03	0.41
2:B:17:PHE:C	2:B:19:LYS:H	2.23	0.41
1:A:629:LYS:NZ	3:A:755:HOH:O	2.45	0.41
1:A:627:MET:O	1:A:630:ALA:HB3	2.21	0.41
1:A:593:GLY:O	1:A:594:LEU:C	2.59	0.41
2:B:96:ARG:CG	2:B:96:ARG:O	2.69	0.41
1:A:229:GLN:CD	3:A:846:HOH:O	2.59	0.41
1:A:129:GLN:HE22	1:A:140:HIS:N	2.11	0.40
1:A:393:GLU:HB3	1:A:505:LYS:CG	2.51	0.40
1:A:695:LEU:HD23	1:A:695:LEU:HA	1.92	0.40
1:A:63:LEU:HB2	1:A:193:GLU:HB2	2.03	0.40
1:A:386:GLN:HE22	1:A:451:ASN:N	2.11	0.40
2:B:110:LEU:CD2	2:B:140:MET:HE3	2.51	0.40
1:A:224:LEU:HD22	1:A:328:PHE:HZ	1.87	0.40
2:B:97:PHE:CG	2:B:113:ALA:HB2	2.56	0.40
1:A:523:ILE:HD13	1:A:602:THR:CG2	2.46	0.40

All (10) 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:527:GLU:OE1	2:B:19:LYS:CE[1_554]	0.67	1.53
1:A:527:GLU:CD	2:B:19:LYS:CE[1_554]	0.84	1.36
1:A:527:GLU:CD	2:B:19:LYS:NZ[1_554]	1.15	1.05
1:A:527:GLU:OE1	2:B:19:LYS:CD[1_554]	1.29	0.91
1:A:527:GLU:OE2	2:B:19:LYS:NZ[1_554]	1.33	0.87
1:A:527:GLU:OE2	2:B:19:LYS:CE[1_554]	1.59	0.61
1:A:527:GLU:OE1	2:B:19:LYS:NZ[1_554]	1.75	0.45
1:A:527:GLU:OE1	2:B:19:LYS:CG[1_554]	2.10	0.10
1:A:38:GLU:OE2	1:A:490:GLU:OE2[1_455]	2.17	0.03
1:A:527:GLU:CG	2:B:19:LYS:NZ[1_554]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	609/700 (87%)	506 (83%)	70 (12%)	33 (5%)	2 6
2	B	174/184 (95%)	130 (75%)	31 (18%)	13 (8%)	1 3
All	All	783/884 (89%)	636 (81%)	101 (13%)	46 (6%)	2 5

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	351	ASP
1	A	354	LYS
1	A	373	GLY
1	A	399	GLU
1	A	403	ARG
1	A	427	HIS
1	A	461	ARG
1	A	526	ASN
1	A	527	GLU
1	A	585	ASP
2	B	18	ARG
2	B	96	ARG
2	B	127	SER
2	B	143	ASP
1	A	81	ILE
1	A	375	ARG
1	A	454	LEU
1	A	528	GLU
1	A	531	GLY
1	A	573	SER
1	A	587	ASP
1	A	616	VAL
1	A	617	ASP
2	B	100	ASP

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Mol	Chain	Res	Type
2	B	101	ARG
2	B	141	ASP
1	A	135	TYR
1	A	218	ARG
1	A	350	CYS
1	A	463	ASP
1	A	492	HIS
2	B	99	THR
1	A	398	ASP
1	A	534	PHE
1	A	586	GLU
2	B	17	PHE
2	B	166	GLY
1	A	530	ILE
1	A	535	ARG
1	A	577	CYS
2	B	28	ASP
1	A	374	CYS
2	B	42	LYS
2	B	92	GLY
1	A	51	PHE

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	522/603 (87%)	424 (81%)	98 (19%)	2 5
2	B	155/162 (96%)	127 (82%)	28 (18%)	2 5
All	All	677/765 (88%)	551 (81%)	126 (19%)	2 5

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	13	GLU

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Mol	Chain	Res	Type
1	A	18	LEU
1	A	22	GLU
1	A	26	LYS
1	A	29	ASN
1	A	55	PRO
1	A	61	LYS
1	A	67	SER
1	A	69	LYS
1	A	76	LYS
1	A	78	PRO
1	A	81	ILE
1	A	86	GLN
1	A	102	LEU
1	A	108	LEU
1	A	111	ILE
1	A	115	THR
1	A	118	GLU
1	A	153	VAL
1	A	161	LYS
1	A	168	VAL
1	A	180	LEU
1	A	204	PHE
1	A	205	GLU
1	A	217	LEU
1	A	223	ASN
1	A	238	LEU
1	A	242	ILE
1	A	271	GLU
1	A	280	LYS
1	A	281	LEU
1	A	285	ARG
1	A	286	ASN
1	A	323	GLU
1	A	326	MET
1	A	329	SER
1	A	333	ARG
1	A	337	ARG
1	A	338	LEU
1	A	343	LEU
1	A	353	TYR
1	A	355	LYS
1	A	360	LYS

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Mol	Chain	Res	Type
1	A	361	MET
1	A	364	ASN
1	A	375	ARG
1	A	380	THR
1	A	388	LEU
1	A	397	ASP
1	A	399	GLU
1	A	403	ARG
1	A	413	GLN
1	A	416	ARG
1	A	417	ARG
1	A	418	ARG
1	A	419	GLN
1	A	436	VAL
1	A	450	LYS
1	A	465	PHE
1	A	469	ARG
1	A	471	VAL
1	A	472	LEU
1	A	484	LEU
1	A	488	THR
1	A	505	LYS
1	A	508	ASP
1	A	509	TYR
1	A	511	THR
1	A	527	GLU
1	A	535	ARG
1	A	536	ARG
1	A	540	GLN
1	A	541	LEU
1	A	548	ILE
1	A	554	GLN
1	A	555	THR
1	A	558	ARG
1	A	560	VAL
1	A	561	LEU
1	A	575	GLU
1	A	584	LEU
1	A	589	SER
1	A	594	LEU
1	A	596	GLU
1	A	604	ILE

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Mol	Chain	Res	Type
1	A	606	LYS
1	A	619	SER
1	A	637	LYS
1	A	655	LEU
1	A	656	ILE
1	A	663	VAL
1	A	668	ARG
1	A	672	LEU
1	A	683	ASN
1	A	690	ASP
1	A	696	SER
1	A	698	SER
2	B	9	ASN
2	B	11	SER
2	B	12	GLU
2	B	15	ARG
2	B	16	GLN
2	B	18	ARG
2	B	22	VAL
2	B	23	GLN
2	B	24	LEU
2	B	28	ASP
2	B	34	THR
2	B	36	LEU
2	B	46	ARG
2	B	51	LYS
2	B	75	LEU
2	B	91	GLN
2	B	114	PHE
2	B	121	LEU
2	B	123	GLN
2	B	125	ILE
2	B	128	MET
2	B	131	ARG
2	B	132	ARG
2	B	136	GLU
2	B	141	ASP
2	B	148	CYS
2	B	151	ARG
2	B	183	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	37	ASN
1	A	129	GLN
1	A	169	HIS
1	A	189	ASN
1	A	223	ASN
1	A	286	ASN
1	A	342	ASN
1	A	364	ASN
1	A	376	ASN
1	A	379	ASN
1	A	384	ASN
1	A	386	GLN
1	A	413	GLN
1	A	419	GLN
1	A	427	HIS
1	A	492	HIS
1	A	494	ASN
1	A	540	GLN
1	A	554	GLN
1	A	608	GLN
2	B	23	GLN
2	B	47	HIS
2	B	123	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.