



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:23 PM UTC

PDB ID : 1YMH / pdb_00001ymh
Title : anti-HCV Fab 19D9D6 complexed with protein L (PpL) mutant A66W
Authors : Granata, V.; Housden, N.G.; Harrison, S.; Jolivet-Reynaud, C.; Gore, M.G.; Stura, E.A.
Deposited on : 2005-01-21
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

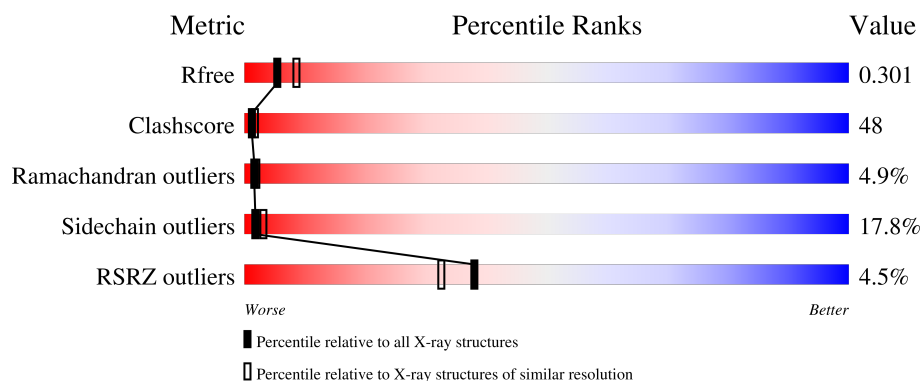
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	220	7% 35% 45% 17%
1	C	220	2% 9% 38% 43% 10%
2	B	218	4% 8% 44% 38% 11%
2	D	218	5% 9% 42% 42% 7%
3	E	65	2% 8% 45% 37% 11%

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Mol	Chain	Length	Quality of chain
3	F	65	9% 6% 29% 43% 22%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7884 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 Fab 16D9D6, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
1	C	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			

- Molecule 2 is a protein called Fab 16D9D6, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
2	D	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			

- Molecule 3 is a protein called Protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	65	Total	C	N	O	S	0	0	0
			516	329	83	103	1			
3	F	65	Total	C	N	O	S	0	0	0
			516	329	83	103	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	31	Total	O	0	0
			31	31		
4	E	6	Total	O	0	0
			6	6		
4	C	20	Total	O	0	0
			20	20		

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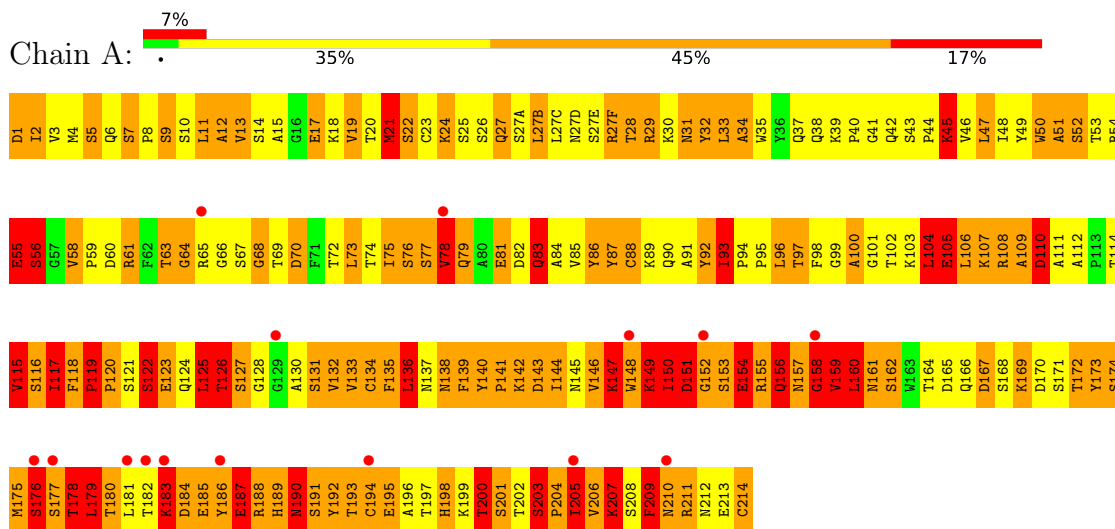
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	26	Total	O	0	0
			26	26		
4	F	3	Total	O	0	0
			3	3		

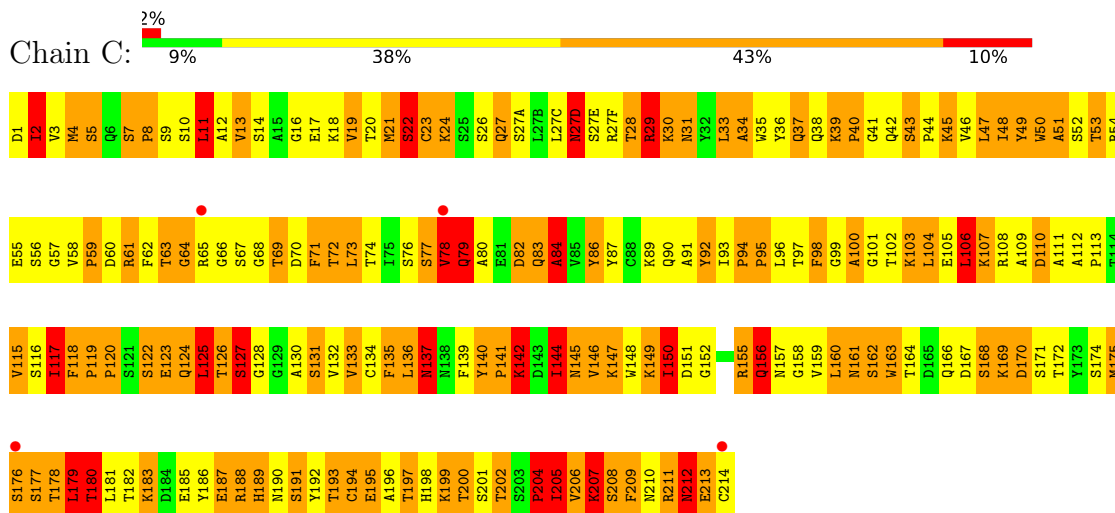
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fab 16D9D6, light chain

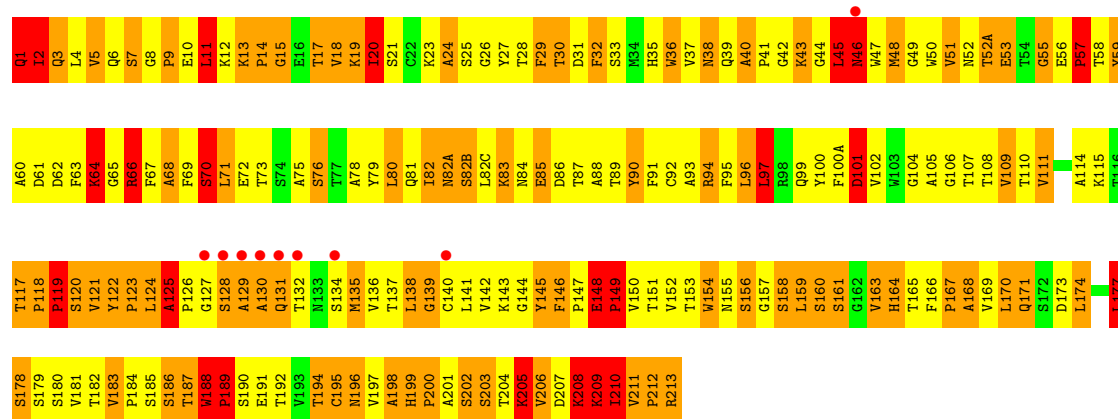


- Molecule 1: Fab 16D9D6, light chain

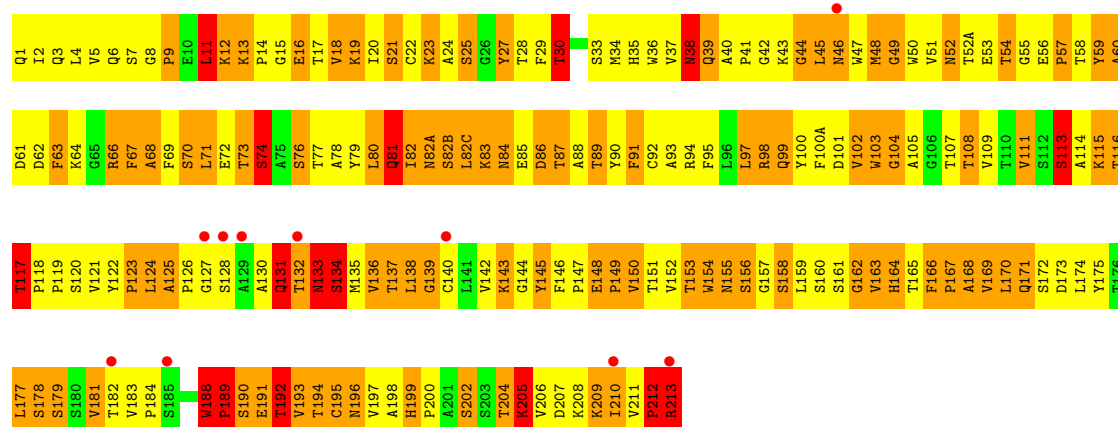


- Molecule 2: Fab 16D9D6, heavy chain

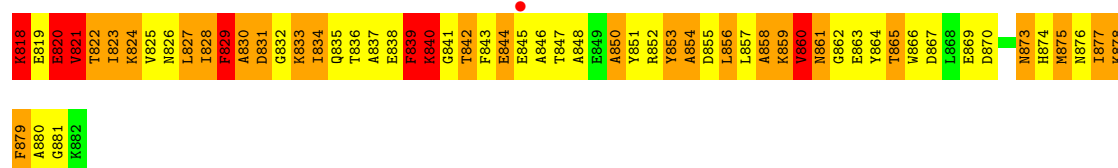




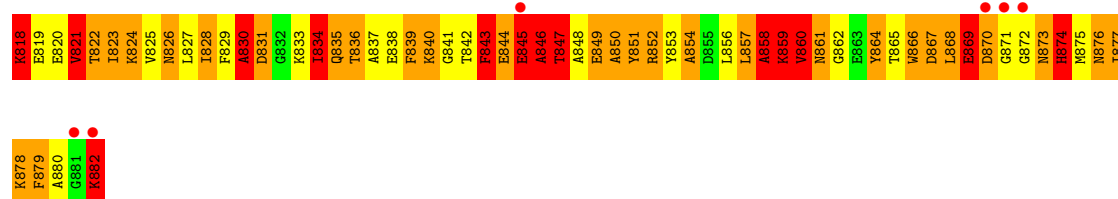
• Molecule 2: Fab 16D9D6, heavy chain



• Molecule 3: Protein L



• Molecule 3: Protein L



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.14Å 111.47Å 148.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.60 87.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (87.71-2.60) 97.5 (87.71-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.68 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.224 , 0.302 0.230 , 0.301	Depositor DCC
R_{free} test set	2008 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7884	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	3.86	316/1745 (18.1%)	2.77	172/2366 (7.3%)
1	C	3.68	266/1745 (15.2%)	2.44	114/2366 (4.8%)
2	B	3.66	256/1707 (15.0%)	2.86	196/2335 (8.4%)
2	D	3.59	250/1707 (14.6%)	2.64	145/2335 (6.2%)
3	E	4.06	100/525 (19.0%)	2.79	35/704 (5.0%)
3	F	3.30	60/525 (11.4%)	2.77	50/704 (7.1%)
All	All	3.70	1248/7954 (15.7%)	2.69	712/10810 (6.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	19
1	C	0	4
2	B	1	14
2	D	3	13
3	E	2	4
3	F	1	3
All	All	8	57

All (1248) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	94	PRO	CA-C	-18.46	1.41	1.51
1	A	46	VAL	CA-CB	-18.16	1.31	1.54
1	C	166	GLN	C-O	-17.81	1.01	1.24
2	B	50	TRP	C-O	-16.99	1.05	1.23
2	D	33	SER	C-O	-16.21	1.04	1.24
2	B	2	ILE	C-O	-15.97	1.05	1.24
3	E	855	ASP	CA-C	-15.96	1.32	1.52
2	D	81	GLN	CA-C	-15.83	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	33	SER	CA-C	-15.55	1.34	1.52
2	B	197	VAL	CA-C	-14.83	1.34	1.52
3	E	840	LYS	CA-C	-14.75	1.32	1.52
3	E	839	PHE	C-O	-14.70	1.06	1.24
2	B	142	VAL	CA-C	-14.56	1.36	1.52
3	E	864	TYR	C-O	-14.51	1.04	1.23
2	D	83	LYS	CA-C	14.36	1.69	1.52
2	B	40	ALA	CA-CB	13.89	1.74	1.53
2	D	95	PHE	C-O	-13.84	1.06	1.24
1	C	93	ILE	CA-CB	13.68	1.71	1.54
1	C	51	ALA	CA-CB	-13.67	1.30	1.53
1	C	100	ALA	CA-CB	13.60	1.75	1.53
1	C	73	LEU	C-O	-13.55	1.07	1.24
1	A	86	TYR	CA-C	13.55	1.69	1.52
3	E	853	TYR	C-O	13.54	1.39	1.24
2	B	197	VAL	CA-CB	13.50	1.74	1.54
3	E	826	ASN	C-O	-13.35	1.07	1.24
2	D	100	TYR	C-O	-13.33	1.07	1.23
1	A	13	VAL	CA-CB	-12.95	1.35	1.54
3	F	841	GLY	CA-C	12.92	1.66	1.52
2	B	149	PRO	N-CD	12.86	1.65	1.47
3	F	870	ASP	CA-C	12.86	1.70	1.52
1	A	93	ILE	N-CA	-12.83	1.30	1.46
2	B	37	VAL	N-CA	-12.79	1.31	1.46
2	B	28	THR	CA-CB	-12.78	1.37	1.52
1	C	127	SER	CA-C	12.77	1.69	1.52
1	A	6	GLN	CA-C	-12.70	1.37	1.52
2	B	10	GLU	CA-C	12.70	1.69	1.52
1	A	92	TYR	C-O	-12.69	1.08	1.24
1	C	3	VAL	CA-CB	-12.64	1.38	1.54
1	A	114	THR	CA-C	-12.62	1.40	1.53
1	A	45	LYS	N-CA	12.59	1.61	1.46
1	A	148	TRP	CA-C	12.45	1.67	1.52
2	D	2	ILE	CA-CB	-12.44	1.39	1.54
2	B	69	PHE	N-CA	-12.41	1.31	1.46
1	A	190	ASN	CA-C	12.40	1.69	1.52
2	D	212	PRO	C-O	12.37	1.40	1.24
2	B	11	LEU	C-O	-12.37	1.09	1.23
2	D	79	TYR	C-O	12.35	1.39	1.23
1	A	90	GLN	CA-C	-12.34	1.38	1.52
2	B	19	LYS	N-CA	12.30	1.60	1.46
3	E	867	ASP	C-O	-12.26	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	103	LYS	CD-CE	12.23	1.89	1.52
1	A	119	PRO	CA-C	-12.15	1.40	1.52
3	E	847	THR	CA-CB	-12.10	1.32	1.53
1	A	1	ASP	N-CA	12.04	1.69	1.46
1	A	9	SER	C-O	12.01	1.39	1.24
1	A	58	VAL	CA-CB	11.94	1.69	1.54
3	F	825	VAL	CA-CB	-11.88	1.40	1.54
3	F	860	VAL	CA-CB	11.88	1.70	1.54
2	B	48	MET	SD-CE	-11.84	1.50	1.79
1	C	93	ILE	C-N	-11.82	1.23	1.33
1	A	143	ASP	C-O	11.78	1.38	1.23
1	A	177	SER	CA-C	11.77	1.66	1.52
2	D	189	PRO	N-CD	11.70	1.64	1.47
1	C	119	PRO	CA-C	-11.65	1.41	1.52
1	C	31	ASN	CA-C	11.62	1.68	1.52
2	D	43	LYS	N-CA	11.62	1.60	1.45
1	A	4	MET	SD-CE	-11.62	1.50	1.79
1	C	146	VAL	C-O	11.60	1.37	1.24
3	E	851	TYR	CA-C	-11.53	1.36	1.52
2	B	57	PRO	CA-C	11.51	1.68	1.52
2	B	5	VAL	N-CA	-11.39	1.32	1.46
1	C	164	THR	C-O	-11.39	1.09	1.23
1	C	91	ALA	CA-CB	11.35	1.70	1.53
1	A	27	GLN	C-O	-11.34	1.13	1.24
2	D	82(A)	ASN	CA-C	-11.30	1.39	1.52
1	A	175	MET	N-CA	11.29	1.60	1.45
2	B	15	GLY	C-O	11.26	1.40	1.24
2	D	77	THR	C-O	-11.20	1.10	1.23
1	C	87	TYR	CA-CB	-11.17	1.34	1.53
3	E	846	ALA	CA-CB	11.16	1.71	1.53
1	C	150	ILE	CA-C	11.13	1.66	1.52
2	B	169	VAL	CA-CB	-11.10	1.38	1.54
1	C	84	ALA	N-CA	11.09	1.60	1.46
1	A	176	SER	CA-C	-11.07	1.39	1.52
1	A	186	TYR	CA-CB	11.07	1.70	1.53
1	A	164	THR	N-CA	-11.05	1.32	1.45
1	C	18	LYS	C-O	-11.04	1.10	1.23
1	C	196	ALA	CA-CB	-11.01	1.38	1.53
1	A	205	ILE	CA-CB	10.98	1.67	1.53
2	B	20	ILE	CA-C	-10.97	1.39	1.52
2	D	3	GLN	CA-CB	10.93	1.70	1.53
2	B	17	THR	CA-C	10.92	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	100	ALA	C-O	-10.89	1.10	1.24
1	A	15	ALA	CA-CB	-10.86	1.35	1.53
2	B	18	VAL	CA-CB	-10.82	1.39	1.54
2	D	89	THR	CA-CB	10.80	1.68	1.53
1	C	52	SER	C-O	10.74	1.37	1.24
2	D	158	SER	CA-C	10.72	1.68	1.52
3	E	840	LYS	CD-CE	10.72	1.84	1.52
3	F	823	ILE	C-O	-10.71	1.11	1.24
2	D	54	THR	C-O	10.70	1.34	1.24
1	A	60	ASP	CA-CB	10.70	1.73	1.53
2	B	51	VAL	N-CA	-10.64	1.33	1.46
2	B	7	SER	CA-CB	10.63	1.70	1.53
2	D	24	ALA	CA-CB	-10.63	1.37	1.53
3	E	848	ALA	CA-CB	10.57	1.70	1.53
1	A	82	ASP	CA-CB	-10.54	1.37	1.53
1	A	27(B)	LEU	CA-C	-10.53	1.39	1.52
2	D	140	CYS	CA-C	-10.50	1.39	1.52
1	A	176	SER	N-CA	-10.49	1.33	1.46
2	B	166	PHE	CA-C	-10.49	1.40	1.52
1	C	131	SER	CA-C	-10.46	1.40	1.52
2	D	211	VAL	CA-CB	10.45	1.67	1.54
1	C	180	THR	CA-CB	-10.44	1.34	1.53
1	A	94	PRO	C-O	-10.43	1.12	1.24
1	C	5	SER	CA-C	10.43	1.65	1.52
2	D	41	PRO	C-O	10.41	1.36	1.23
3	E	837	ALA	CA-C	-10.41	1.39	1.52
1	A	93	ILE	CA-CB	10.35	1.67	1.54
2	B	58	THR	CA-C	-10.28	1.40	1.52
2	D	93	ALA	N-CA	-10.27	1.33	1.46
2	B	48	MET	C-O	-10.26	1.08	1.23
1	A	78	VAL	CA-CB	-10.23	1.44	1.54
1	A	49	TYR	CD2-CE2	10.21	1.69	1.38
2	B	91	PHE	CA-C	-10.20	1.40	1.52
2	D	49	GLY	C-O	-10.20	1.13	1.24
2	B	87	THR	C-O	-10.18	1.11	1.24
2	B	211	VAL	CA-C	-10.15	1.44	1.52
2	B	75	ALA	C-O	-10.13	1.10	1.24
2	D	153	THR	CA-C	10.11	1.65	1.52
2	D	77	THR	CA-CB	-10.10	1.36	1.53
2	B	1	GLN	CD-NE2	10.10	1.54	1.33
1	A	137	ASN	N-CA	-10.09	1.33	1.45
1	A	26	SER	C-O	-10.08	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	53	GLU	CA-C	10.08	1.67	1.52
1	C	27	GLN	CD-OE1	10.06	1.42	1.23
1	C	150	ILE	C-O	10.04	1.36	1.24
2	D	210	ILE	CA-CB	10.04	1.66	1.53
2	B	47	TRP	CA-CB	-10.02	1.37	1.53
2	D	107	THR	CA-CB	-10.01	1.39	1.53
2	D	148	GLU	C-O	10.00	1.37	1.24
1	A	42	GLN	CA-CB	9.98	1.68	1.53
2	D	56	GLU	CA-C	9.97	1.65	1.52
2	D	40	ALA	CA-CB	9.97	1.69	1.53
1	A	172	THR	CA-C	-9.95	1.39	1.52
2	D	157	GLY	C-O	9.95	1.38	1.24
2	D	168	ALA	C-O	-9.94	1.12	1.23
2	D	5	VAL	CA-CB	9.93	1.66	1.53
1	A	2	ILE	CA-CB	-9.91	1.41	1.53
1	C	48	ILE	CA-C	-9.89	1.40	1.52
1	C	108	ARG	CA-C	9.88	1.64	1.52
1	C	45	LYS	CG-CD	9.87	1.82	1.52
1	C	77	SER	N-CA	-9.85	1.33	1.46
1	C	30	LYS	C-O	9.85	1.35	1.24
1	A	110	ASP	C-O	9.83	1.37	1.23
2	D	199	HIS	C-O	-9.83	1.13	1.24
1	C	196	ALA	N-CA	-9.82	1.33	1.46
1	A	51	ALA	CA-CB	-9.82	1.36	1.53
2	B	93	ALA	CA-CB	-9.81	1.37	1.53
1	A	108	ARG	C-O	9.80	1.35	1.23
1	A	43	SER	CB-OG	-9.79	1.22	1.42
1	C	30	LYS	CE-NZ	9.75	1.78	1.49
1	C	78	VAL	N-CA	-9.74	1.34	1.46
2	B	33	SER	N-CA	-9.72	1.34	1.45
1	A	68	GLY	C-O	9.72	1.37	1.23
1	C	47	LEU	N-CA	9.72	1.57	1.46
2	B	199	HIS	CA-C	-9.70	1.41	1.52
3	F	852	ARG	CA-C	9.69	1.65	1.52
3	E	839	PHE	CA-CB	-9.69	1.35	1.53
2	D	111	VAL	CA-C	9.66	1.64	1.52
1	A	100	ALA	CA-C	9.64	1.67	1.52
2	D	82(A)	ASN	N-CA	9.64	1.57	1.46
3	E	852	ARG	N-CA	9.59	1.58	1.46
1	C	31	ASN	CA-CB	-9.56	1.38	1.53
1	C	94	PRO	C-O	-9.55	1.16	1.25
2	D	98	ARG	NE-CZ	-9.55	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	68	ALA	CA-C	9.50	1.64	1.52
3	E	824	LYS	C-O	-9.49	1.12	1.24
1	A	186	TYR	CA-C	9.47	1.65	1.52
2	B	156	SER	N-CA	-9.45	1.35	1.46
1	A	102	THR	CA-C	9.44	1.65	1.52
1	C	90	GLN	CA-C	-9.43	1.41	1.52
1	C	150	ILE	N-CA	9.43	1.58	1.46
2	D	67	PHE	CA-C	-9.42	1.41	1.52
2	D	7	SER	CA-CB	-9.42	1.38	1.53
2	B	46	ASN	CG-ND2	9.41	1.53	1.33
2	D	210	ILE	CA-C	9.41	1.62	1.53
2	D	195	CYS	C-O	9.40	1.35	1.23
1	C	77	SER	CA-C	9.40	1.65	1.52
1	A	27	GLN	CD-OE1	9.39	1.41	1.23
2	D	144	GLY	C-O	9.38	1.36	1.23
2	B	78	ALA	C-O	9.38	1.35	1.23
2	D	169	VAL	CA-CB	-9.35	1.42	1.54
2	B	91	PHE	C-O	-9.32	1.12	1.24
1	A	65	ARG	N-CA	-9.31	1.34	1.45
2	B	195	CYS	CA-C	-9.30	1.41	1.52
3	E	861	ASN	C-O	9.28	1.36	1.24
2	D	178	SER	C-O	9.28	1.35	1.23
2	D	101	ASP	C-O	-9.27	1.11	1.24
1	C	45	LYS	CB-CG	-9.26	1.24	1.52
1	C	21	MET	CA-C	-9.26	1.41	1.52
1	A	56	SER	CA-C	9.25	1.64	1.52
2	B	23	LYS	C-O	-9.23	1.13	1.24
2	D	38	ASN	CA-C	-9.22	1.41	1.52
1	A	104	LEU	CA-CB	-9.20	1.41	1.53
2	B	142	VAL	CA-CB	9.18	1.65	1.53
2	D	46	ASN	CA-C	-9.18	1.41	1.52
1	A	168	SER	C-O	9.14	1.36	1.24
2	B	66	ARG	CA-C	9.14	1.65	1.52
2	B	30	THR	C-O	-9.13	1.12	1.24
3	E	837	ALA	CA-CB	-9.13	1.35	1.53
1	A	78	VAL	CB-CG1	-9.12	1.22	1.52
2	D	150	VAL	CA-CB	-9.12	1.42	1.54
1	C	176	SER	CA-C	-9.12	1.41	1.52
1	C	83	GLN	CD-OE1	9.10	1.40	1.23
2	B	17	THR	CA-CB	-9.08	1.37	1.53
2	B	197	VAL	N-CA	-9.08	1.35	1.46
2	D	58	THR	CA-CB	-9.06	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	192	THR	C-O	9.06	1.34	1.23
2	D	125	ALA	C-N	9.05	1.44	1.33
1	A	78	VAL	N-CA	-9.03	1.34	1.46
1	C	3	VAL	C-O	9.02	1.33	1.24
2	B	97	LEU	CG-CD2	9.02	1.82	1.52
3	E	828	ILE	CA-CB	-9.00	1.42	1.53
2	B	203	SER	C-O	-8.99	1.12	1.23
2	D	74	SER	C-O	-8.99	1.13	1.24
2	B	198	ALA	N-CA	8.97	1.57	1.45
1	A	125	LEU	CA-C	8.97	1.64	1.52
2	B	58	THR	CA-CB	-8.96	1.41	1.53
2	B	60	ALA	C-O	8.95	1.34	1.23
2	D	192	THR	CA-C	8.95	1.64	1.53
1	C	11	LEU	C-O	8.94	1.34	1.23
1	A	168	SER	CA-C	-8.92	1.40	1.52
1	C	58	VAL	CA-CB	8.92	1.65	1.54
2	D	113	SER	N-CA	8.88	1.58	1.46
1	A	99	GLY	CA-C	-8.84	1.41	1.52
2	D	57	PRO	C-O	-8.81	1.12	1.23
1	C	24	LYS	CD-CE	8.81	1.78	1.52
3	E	824	LYS	CB-CG	8.81	1.78	1.52
2	B	119	PRO	C-O	-8.79	1.12	1.24
1	A	48	ILE	N-CA	-8.78	1.35	1.46
2	D	59	TYR	C-O	-8.76	1.11	1.23
2	D	117	THR	CA-CB	8.76	1.67	1.53
3	E	819	GLU	CA-C	8.75	1.63	1.53
1	C	69	THR	C-O	8.75	1.34	1.23
1	C	95	PRO	C-O	8.74	1.40	1.23
1	C	35	TRP	N-CA	8.72	1.56	1.46
2	B	178	SER	C-O	8.72	1.34	1.23
3	F	874	HIS	C-O	-8.71	1.13	1.24
3	F	849	GLU	CD-OE2	8.71	1.41	1.25
2	B	20	ILE	N-CA	8.70	1.56	1.46
1	A	119	PRO	C-O	-8.69	1.14	1.24
1	C	56	SER	CA-CB	-8.68	1.39	1.53
1	A	39	LYS	CA-CB	-8.68	1.39	1.53
2	B	45	LEU	CA-CB	8.68	1.65	1.53
2	D	188	TRP	C-O	8.67	1.34	1.23
3	E	823	ILE	N-CA	-8.67	1.35	1.46
2	B	37	VAL	CA-C	-8.66	1.42	1.52
1	A	50	TRP	CE3-CZ3	8.65	1.64	1.38
1	C	83	GLN	CA-C	-8.64	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	177	LEU	CA-C	-8.64	1.41	1.52
1	A	12	ALA	N-CA	8.63	1.56	1.46
1	C	149	LYS	C-O	8.62	1.34	1.23
2	D	7	SER	CA-C	-8.62	1.41	1.53
1	C	34	ALA	CA-CB	-8.61	1.32	1.53
1	A	45	LYS	CA-CB	-8.61	1.39	1.53
3	E	881	GLY	C-O	-8.59	1.12	1.23
1	A	94	PRO	CA-C	-8.57	1.44	1.52
1	A	188	ARG	NE-CZ	8.57	1.42	1.33
1	C	4	MET	CB-CG	8.56	1.78	1.52
1	A	27(C)	LEU	C-O	8.55	1.34	1.23
3	F	873	ASN	N-CA	8.54	1.55	1.46
2	D	66	ARG	CA-C	8.53	1.64	1.52
1	A	105	GLU	CD-OE2	8.52	1.41	1.25
2	B	81	GLN	N-CA	8.49	1.56	1.46
2	B	109	VAL	CA-CB	-8.48	1.44	1.53
2	D	154	TRP	C-O	8.45	1.33	1.24
1	A	4	MET	CG-SD	-8.43	1.59	1.80
1	C	91	ALA	C-O	8.43	1.36	1.24
1	A	162	SER	CA-C	-8.41	1.42	1.52
2	B	1	GLN	N-CA	8.39	1.62	1.46
2	B	31	ASP	C-O	-8.37	1.12	1.24
2	B	81	GLN	C-O	-8.38	1.14	1.24
1	A	161	ASN	C-O	8.37	1.34	1.23
2	B	140	CYS	CA-C	-8.36	1.42	1.52
1	C	212	ASN	N-CA	8.36	1.56	1.46
2	D	25	SER	CB-OG	-8.36	1.25	1.42
2	D	54	THR	CA-CB	8.35	1.68	1.53
1	C	109	ALA	CA-CB	8.35	1.67	1.53
1	C	101	GLY	N-CA	-8.35	1.37	1.45
2	B	178	SER	CA-C	8.33	1.62	1.52
3	E	824	LYS	N-CA	8.31	1.56	1.46
3	F	865	THR	CA-C	-8.31	1.43	1.52
1	A	17	GLU	CD-OE1	8.30	1.41	1.25
1	C	176	SER	CA-CB	-8.30	1.40	1.53
1	C	205	ILE	CG1-CD1	8.27	1.83	1.51
1	A	133	VAL	N-CA	-8.27	1.36	1.46
1	C	105	GLU	CD-OE1	8.26	1.41	1.25
2	D	205	LYS	CG-CD	8.26	1.77	1.52
1	A	76	SER	N-CA	8.24	1.57	1.46
2	D	81	GLN	N-CA	8.24	1.55	1.46
1	A	118	PHE	CA-CB	8.22	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	27(F)	ARG	C-O	8.22	1.33	1.24
1	C	130	ALA	C-O	8.21	1.33	1.23
2	B	181	VAL	C-O	-8.20	1.15	1.24
3	E	838	GLU	C-N	8.19	1.44	1.33
1	A	90	GLN	CD-NE2	-8.19	1.16	1.33
3	E	828	ILE	C-O	-8.18	1.15	1.24
1	A	169	LYS	CA-C	-8.18	1.43	1.52
2	B	45	LEU	C-O	8.18	1.33	1.24
3	E	850	ALA	N-CA	8.17	1.56	1.46
2	D	69	PHE	CA-CB	8.16	1.63	1.53
1	A	75	ILE	C-O	8.16	1.33	1.24
1	C	206	VAL	CA-C	8.16	1.61	1.52
1	A	10	SER	CA-C	-8.15	1.42	1.52
1	C	17	GLU	C-O	8.14	1.34	1.23
2	B	63	PHE	CA-CB	8.12	1.64	1.53
1	A	142	LYS	CA-C	-8.12	1.41	1.52
2	B	107	THR	CA-CB	-8.11	1.41	1.53
2	D	124	LEU	N-CA	-8.11	1.36	1.46
2	B	122	TYR	CA-C	-8.10	1.45	1.52
2	B	10	GLU	CD-OE2	8.06	1.40	1.25
2	D	210	ILE	C-O	8.06	1.35	1.23
1	C	106	LEU	N-CA	8.05	1.56	1.46
2	B	163	VAL	CA-CB	-8.04	1.43	1.54
1	A	27(E)	SER	N-CA	8.04	1.55	1.46
1	A	182	THR	CA-C	8.04	1.62	1.52
1	C	191	SER	CA-C	8.04	1.63	1.52
3	F	870	ASP	C-O	8.01	1.34	1.24
2	B	195	CYS	C-O	-7.98	1.13	1.23
1	A	29	ARG	NE-CZ	7.98	1.41	1.33
1	C	177	SER	C-O	-7.98	1.14	1.24
1	A	43	SER	C-N	-7.97	1.23	1.33
1	A	61	ARG	CZ-NH2	7.97	1.43	1.33
2	D	155	ASN	C-O	7.97	1.34	1.24
3	E	857	LEU	C-O	7.96	1.33	1.24
1	C	142	LYS	CG-CD	7.95	1.76	1.52
3	F	839	PHE	C-O	-7.95	1.14	1.24
2	B	49	GLY	C-O	-7.93	1.13	1.23
1	A	34	ALA	C-O	7.93	1.33	1.23
1	A	73	LEU	C-O	7.93	1.33	1.24
1	A	184	ASP	CA-C	7.90	1.63	1.52
3	F	833	LYS	C-O	7.90	1.33	1.23
1	C	119	PRO	C-O	-7.89	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	81	GLN	CD-OE1	7.89	1.38	1.23
3	F	840	LYS	CA-C	7.89	1.62	1.52
3	E	840	LYS	C-O	7.88	1.33	1.24
1	C	214	CYS	CA-CB	7.87	1.69	1.53
2	B	43	LYS	CG-CD	7.86	1.76	1.52
2	D	164	HIS	CA-C	-7.85	1.43	1.52
3	E	834	ILE	CG1-CD1	7.85	1.82	1.51
2	B	151	THR	CA-C	-7.84	1.42	1.52
2	B	89	THR	CA-C	-7.83	1.43	1.52
1	C	64	GLY	C-O	7.82	1.33	1.23
1	A	180	THR	CB-CG2	7.82	1.78	1.52
2	B	20	ILE	CG1-CD1	-7.81	1.21	1.51
2	D	50	TRP	N-CA	-7.80	1.34	1.46
3	E	853	TYR	CA-CB	7.80	1.65	1.53
1	C	10	SER	CA-CB	-7.80	1.40	1.53
1	A	109	ALA	CA-C	7.79	1.62	1.52
2	D	196	ASN	C-O	7.79	1.32	1.24
1	A	27(C)	LEU	CA-C	7.78	1.63	1.52
1	C	104	LEU	C-O	-7.77	1.15	1.23
3	E	878	LYS	CA-C	-7.77	1.43	1.52
2	B	100(A)	PHE	N-CA	-7.76	1.36	1.46
1	C	186	TYR	C-O	7.76	1.33	1.24
1	A	146	VAL	C-O	7.75	1.33	1.24
3	F	869	GLU	CA-CB	7.75	1.65	1.53
1	A	52	SER	CB-OG	7.74	1.57	1.42
2	B	90	TYR	CA-C	7.73	1.61	1.52
1	C	42	GLN	CD-OE1	7.73	1.38	1.23
1	C	140	TYR	CA-C	7.73	1.61	1.52
2	D	181	VAL	C-O	-7.71	1.16	1.23
1	C	111	ALA	CA-C	-7.71	1.42	1.52
2	D	69	PHE	CE2-CZ	-7.70	1.15	1.38
1	A	40	PRO	C-O	7.70	1.33	1.24
1	A	101	GLY	CA-C	-7.70	1.41	1.51
2	B	211	VAL	CA-CB	-7.69	1.45	1.54
1	C	117	ILE	CG1-CD1	-7.69	1.21	1.51
1	C	27	GLN	C-O	-7.68	1.15	1.23
1	A	77	SER	C-N	-7.68	1.25	1.33
2	D	42	GLY	C-O	7.68	1.34	1.23
1	A	116	SER	CA-C	-7.67	1.42	1.52
1	A	174	SER	C-N	7.67	1.43	1.33
1	C	112	ALA	CA-CB	7.67	1.64	1.53
2	B	59	TYR	C-O	7.67	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	80	LEU	C-O	7.66	1.32	1.24
2	B	52(A)	THR	CA-C	-7.66	1.42	1.52
2	B	75	ALA	CA-CB	7.64	1.66	1.53
3	F	823	ILE	N-CA	-7.64	1.36	1.46
1	A	61	ARG	NE-CZ	-7.63	1.24	1.33
2	B	91	PHE	N-CA	-7.63	1.36	1.46
2	B	82(A)	ASN	N-CA	7.62	1.55	1.46
2	D	24	ALA	N-CA	-7.62	1.36	1.46
1	A	186	TYR	CZ-OH	7.61	1.54	1.38
1	C	34	ALA	CA-C	-7.61	1.43	1.52
2	B	70	SER	N-CA	7.60	1.57	1.45
2	D	165	THR	CA-CB	-7.59	1.43	1.53
1	A	86	TYR	CG-CD1	-7.59	1.23	1.39
1	C	147	LYS	CG-CD	7.58	1.75	1.52
3	F	822	THR	C-O	-7.58	1.15	1.23
2	D	198	ALA	C-O	7.57	1.32	1.24
2	D	155	ASN	N-CA	7.57	1.55	1.46
1	C	79	GLN	CB-CG	7.57	1.75	1.52
1	C	145	ASN	CB-CG	7.56	1.71	1.52
2	B	45	LEU	CA-C	7.55	1.62	1.52
1	A	90	GLN	CA-CB	-7.55	1.40	1.53
2	D	179	SER	CA-C	-7.55	1.43	1.52
3	E	880	ALA	CA-CB	7.55	1.66	1.53
1	C	98	PHE	N-CA	-7.54	1.36	1.45
2	D	100(A)	PHE	C-N	-7.54	1.22	1.33
3	E	835	GLN	CA-C	-7.54	1.43	1.52
2	D	118	PRO	CA-CB	-7.54	1.43	1.54
1	C	193	THR	CA-C	7.53	1.61	1.52
1	A	152	GLY	C-O	7.53	1.34	1.23
1	A	45	LYS	CG-CD	7.52	1.75	1.52
1	C	52	SER	CA-C	7.52	1.62	1.52
1	A	210	ASN	CA-C	7.50	1.62	1.52
1	A	46	VAL	CA-C	-7.49	1.44	1.52
1	C	116	SER	CA-C	-7.47	1.43	1.52
3	F	864	TYR	CA-C	7.47	1.61	1.52
1	C	27	GLN	CD-NE2	7.46	1.49	1.33
1	C	86	TYR	CA-C	7.45	1.61	1.52
2	B	3	GLN	CA-C	7.45	1.61	1.52
1	C	38	GLN	CG-CD	7.44	1.70	1.52
2	D	116	THR	C-O	-7.44	1.14	1.23
1	C	26	SER	N-CA	-7.44	1.36	1.46
1	C	91	ALA	CA-C	7.44	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	MET	CA-C	-7.43	1.43	1.52
3	E	821	VAL	C-O	7.42	1.32	1.23
1	A	144	ILE	N-CA	-7.42	1.37	1.46
3	E	840	LYS	CG-CD	7.42	1.74	1.52
1	A	91	ALA	N-CA	-7.41	1.36	1.46
2	D	212	PRO	C-N	-7.41	1.23	1.33
2	D	183	VAL	C-N	7.41	1.43	1.33
2	B	14	PRO	CA-CB	-7.40	1.43	1.53
2	D	114	ALA	CA-CB	-7.40	1.41	1.53
1	A	38	GLN	CA-C	7.39	1.61	1.52
1	A	173	TYR	C-O	7.39	1.33	1.23
1	A	146	VAL	CA-CB	7.39	1.64	1.54
2	B	210	ILE	CA-C	-7.39	1.43	1.52
3	E	831	ASP	CA-CB	-7.39	1.44	1.53
2	D	78	ALA	CA-C	7.38	1.61	1.52
2	B	25	SER	N-CA	7.38	1.54	1.46
1	A	126	THR	CA-C	7.37	1.62	1.52
1	C	29	ARG	CA-C	7.37	1.62	1.53
2	D	27	TYR	C-O	-7.36	1.14	1.23
1	A	70	ASP	C-O	7.35	1.32	1.24
2	D	28	THR	CA-CB	7.35	1.62	1.53
1	A	31	ASN	C-O	7.35	1.32	1.24
1	A	110	ASP	CG-OD1	7.35	1.39	1.25
2	B	125	ALA	C-N	7.34	1.51	1.33
2	B	68	ALA	N-CA	7.34	1.54	1.45
1	A	32	TYR	C-O	7.34	1.33	1.23
3	E	866	TRP	N-CA	-7.33	1.37	1.46
2	D	109	VAL	C-O	-7.33	1.16	1.24
1	C	112	ALA	CA-C	-7.32	1.45	1.53
3	E	835	GLN	CA-CB	-7.32	1.42	1.53
1	C	179	LEU	CA-C	-7.32	1.43	1.52
3	E	854	ALA	N-CA	7.31	1.55	1.46
1	A	54	ARG	C-O	-7.31	1.15	1.23
1	C	99	GLY	C-O	-7.30	1.12	1.23
3	E	866	TRP	CB-CG	7.30	1.72	1.50
1	A	68	GLY	CA-C	-7.29	1.41	1.51
2	B	201	ALA	N-CA	7.29	1.55	1.46
3	E	835	GLN	CG-CD	-7.29	1.33	1.52
1	A	184	ASP	CB-CG	7.29	1.70	1.52
2	B	168	ALA	CA-C	-7.29	1.43	1.53
2	B	7	SER	C-O	-7.27	1.14	1.23
2	B	18	VAL	CA-C	-7.26	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	HIS	N-CA	-7.25	1.35	1.46
1	C	147	LYS	CD-CE	7.25	1.74	1.52
1	C	117	ILE	CA-CB	-7.24	1.44	1.54
1	A	173	TYR	CA-CB	7.23	1.66	1.53
3	F	830	ALA	CA-C	7.23	1.62	1.52
1	A	89	LYS	CE-NZ	-7.23	1.27	1.49
2	B	123	PRO	CA-C	-7.22	1.44	1.52
2	D	157	GLY	CA-C	7.22	1.61	1.51
2	B	190	SER	CA-CB	7.22	1.65	1.53
1	C	21	MET	SD-CE	-7.22	1.61	1.79
2	D	74	SER	CA-CB	7.22	1.64	1.53
1	A	2	ILE	CG1-CD1	-7.21	1.23	1.51
2	B	111	VAL	CA-CB	7.21	1.62	1.53
2	B	124	LEU	N-CA	-7.21	1.38	1.46
2	D	46	ASN	C-O	-7.20	1.15	1.24
1	C	111	ALA	CA-CB	7.19	1.65	1.53
1	C	209	PHE	CD1-CE1	7.19	1.60	1.38
3	E	865	THR	C-O	-7.18	1.15	1.23
1	C	59	PRO	CA-C	-7.18	1.44	1.52
1	C	46	VAL	CA-CB	-7.18	1.46	1.54
1	C	55	GLU	CA-C	7.17	1.62	1.52
1	A	174	SER	C-O	7.17	1.33	1.23
2	B	58	THR	CB-CG2	-7.16	1.28	1.52
2	B	187	THR	CA-C	-7.16	1.43	1.52
1	C	162	SER	CA-C	-7.16	1.43	1.52
2	D	70	SER	CA-C	7.15	1.63	1.53
1	A	210	ASN	C-O	7.15	1.32	1.24
3	E	826	ASN	N-CA	-7.15	1.37	1.46
1	C	12	ALA	CA-C	-7.14	1.44	1.52
2	D	136	VAL	CA-C	7.14	1.61	1.52
3	E	860	VAL	C-O	-7.14	1.15	1.23
1	A	24	LYS	N-CA	7.13	1.54	1.46
2	D	91	PHE	CA-C	-7.13	1.43	1.52
2	B	152	VAL	C-O	7.12	1.31	1.24
1	A	63	THR	C-O	7.11	1.32	1.23
1	C	212	ASN	C-O	-7.09	1.15	1.24
1	A	82	ASP	CG-OD2	7.07	1.38	1.25
1	C	48	ILE	C-O	7.06	1.31	1.23
3	F	858	ALA	C-O	7.06	1.32	1.24
2	D	54	THR	CA-C	7.06	1.61	1.52
2	B	72	GLU	C-O	7.06	1.32	1.24
3	F	882	LYS	CD-CE	7.06	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	SER	CA-C	-7.05	1.43	1.52
2	B	170	LEU	CA-C	7.05	1.62	1.53
1	A	65	ARG	NE-CZ	-7.04	1.25	1.33
1	C	43	SER	C-N	-7.04	1.24	1.33
3	F	822	THR	C-N	-7.04	1.23	1.33
1	C	96	LEU	N-CA	7.03	1.54	1.46
3	F	823	ILE	CA-CB	-7.03	1.46	1.54
2	B	203	SER	CA-C	-7.02	1.44	1.53
2	B	178	SER	N-CA	-7.01	1.37	1.46
1	C	43	SER	CA-C	-7.01	1.45	1.53
2	D	6	GLN	N-CA	7.01	1.54	1.45
1	C	2	ILE	C-O	7.00	1.32	1.24
1	A	12	ALA	CA-C	-6.99	1.44	1.52
2	D	82(B)	SER	CA-C	6.98	1.60	1.53
1	A	140	TYR	CA-C	6.98	1.61	1.52
1	C	130	ALA	CA-CB	-6.98	1.42	1.53
3	F	849	GLU	CD-OE1	6.98	1.38	1.25
1	C	4	MET	CA-C	-6.97	1.44	1.52
2	B	165	THR	C-O	-6.97	1.15	1.23
1	C	39	LYS	C-N	-6.96	1.25	1.33
1	C	192	TYR	CA-C	-6.95	1.44	1.52
2	D	6	GLN	C-O	6.95	1.32	1.23
1	A	23	CYS	C-O	6.95	1.31	1.23
1	A	105	GLU	CA-C	-6.95	1.44	1.52
1	C	73	LEU	CG-CD2	-6.94	1.29	1.52
1	A	207	LYS	C-O	6.94	1.32	1.23
2	B	56	GLU	CD-OE1	6.94	1.38	1.25
1	A	193	THR	CA-CB	6.94	1.67	1.53
1	A	39	LYS	CA-C	-6.93	1.43	1.52
2	D	58	THR	C-O	-6.93	1.14	1.23
1	C	135	PHE	N-CA	-6.93	1.37	1.45
1	C	83	GLN	C-N	-6.92	1.24	1.33
1	A	169	LYS	C-O	6.92	1.33	1.23
1	C	64	GLY	CA-C	6.92	1.58	1.52
1	A	205	ILE	CA-C	6.91	1.60	1.52
1	A	44	PRO	CA-C	-6.91	1.43	1.52
1	A	136	LEU	N-CA	-6.90	1.37	1.46
1	C	60	ASP	CG-OD2	6.90	1.38	1.25
1	C	5	SER	C-O	6.90	1.32	1.24
2	D	52(A)	THR	CA-CB	6.90	1.64	1.53
2	B	73	THR	N-CA	-6.89	1.37	1.46
2	D	153	THR	C-O	6.89	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	52	ASN	C-O	6.89	1.32	1.24
1	A	150	ILE	C-O	6.88	1.32	1.24
2	D	62	ASP	C-O	-6.87	1.14	1.24
1	A	65	ARG	CA-C	-6.87	1.44	1.52
1	C	42	GLN	CA-CB	6.87	1.64	1.53
2	B	4	LEU	CB-CG	-6.86	1.39	1.53
2	B	24	ALA	C-N	-6.86	1.24	1.33
2	D	137	THR	N-CA	-6.85	1.38	1.46
1	A	13	VAL	C-O	6.85	1.31	1.23
1	C	106	LEU	CG-CD1	6.85	1.75	1.52
1	A	5	SER	C-O	6.84	1.32	1.24
2	B	1	GLN	CG-CD	6.84	1.69	1.52
2	B	25	SER	CA-CB	-6.84	1.42	1.53
2	B	104	GLY	N-CA	6.84	1.54	1.45
1	C	101	GLY	C-O	-6.83	1.15	1.23
1	A	50	TRP	N-CA	6.83	1.56	1.46
2	D	97	LEU	CG-CD2	6.83	1.75	1.52
2	B	5	VAL	CB-CG1	6.82	1.75	1.52
2	D	148	GLU	CA-C	6.82	1.61	1.52
1	A	190	ASN	CB-CG	6.82	1.69	1.52
3	E	840	LYS	CB-CG	6.81	1.72	1.52
3	E	877	ILE	CA-CB	6.81	1.63	1.54
2	D	33	SER	N-CA	-6.81	1.37	1.46
2	B	33	SER	CA-C	-6.80	1.43	1.53
1	A	76	SER	CA-CB	-6.80	1.41	1.53
1	A	205	ILE	N-CA	6.80	1.54	1.46
1	A	44	PRO	N-CA	-6.78	1.39	1.47
2	B	76	SER	CB-OG	-6.78	1.28	1.42
1	A	42	GLN	C-O	-6.78	1.13	1.23
1	A	12	ALA	CA-CB	-6.78	1.43	1.53
3	E	856	LEU	N-CA	6.78	1.54	1.46
1	A	117	ILE	CA-C	-6.77	1.44	1.52
1	C	49	TYR	CD1-CE1	6.76	1.58	1.38
2	D	35	HIS	C-O	-6.76	1.14	1.23
1	C	168	SER	N-CA	-6.76	1.37	1.46
2	B	4	LEU	N-CA	-6.75	1.38	1.46
3	E	834	ILE	C-O	-6.75	1.17	1.24
2	D	13	LYS	C-O	6.75	1.32	1.23
2	D	29	PHE	CA-C	-6.74	1.43	1.52
3	F	861	ASN	CA-C	6.74	1.60	1.52
1	A	33	LEU	CG-CD2	-6.74	1.30	1.52
1	C	117	ILE	CA-C	-6.74	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	190	SER	N-CA	6.74	1.54	1.46
1	C	160	LEU	CG-CD2	6.73	1.74	1.52
1	A	56	SER	N-CA	6.73	1.54	1.46
1	C	183	LYS	N-CA	6.73	1.54	1.46
1	C	135	PHE	C-O	-6.73	1.15	1.23
1	C	61	ARG	NE-CZ	-6.72	1.25	1.33
2	D	64	LYS	CD-CE	6.72	1.72	1.52
2	D	41	PRO	CA-C	6.72	1.60	1.52
1	A	86	TYR	CA-CB	-6.71	1.43	1.53
1	A	21	MET	SD-CE	-6.70	1.62	1.79
1	A	175	MET	SD-CE	6.70	1.96	1.79
2	B	35	HIS	CG-ND1	6.70	1.45	1.38
1	C	157	ASN	CA-C	6.70	1.62	1.53
2	D	122	TYR	CA-C	-6.69	1.45	1.52
2	D	43	LYS	CG-CD	6.69	1.72	1.52
3	E	847	THR	C-O	-6.69	1.15	1.24
1	A	4	MET	C-O	-6.68	1.16	1.24
2	B	76	SER	N-CA	-6.68	1.37	1.46
2	D	99	GLN	CA-CB	6.68	1.63	1.53
1	C	4	MET	C-O	-6.68	1.16	1.24
2	B	90	TYR	CA-CB	6.67	1.63	1.53
2	D	25	SER	N-CA	6.67	1.54	1.46
1	A	13	VAL	N-CA	-6.67	1.38	1.46
1	A	114	THR	C-O	-6.67	1.15	1.23
3	E	875	MET	C-O	-6.66	1.15	1.23
2	D	22	CYS	CA-C	-6.66	1.45	1.53
1	A	98	PHE	CA-CB	6.65	1.64	1.53
1	A	122	SER	N-CA	-6.65	1.37	1.46
2	D	72	GLU	CD-OE2	6.64	1.38	1.25
2	B	79	TYR	C-O	6.63	1.32	1.23
2	B	192	THR	CA-C	-6.63	1.44	1.52
1	C	53	THR	C-N	-6.63	1.24	1.33
2	D	58	THR	CA-C	-6.63	1.45	1.53
1	A	171	SER	C-O	6.62	1.32	1.23
1	A	190	ASN	CA-CB	6.62	1.64	1.53
1	C	122	SER	CA-C	6.62	1.61	1.52
2	B	35	HIS	CD2-NE2	6.62	1.45	1.37
3	F	846	ALA	CA-CB	6.62	1.64	1.53
2	D	13	LYS	N-CA	6.62	1.54	1.45
3	F	851	TYR	CA-CB	6.62	1.63	1.53
2	B	44	GLY	N-CA	6.61	1.51	1.44
2	D	51	VAL	CB-CG2	6.61	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	877	ILE	C-O	-6.60	1.17	1.24
1	A	60	ASP	N-CA	6.60	1.54	1.46
1	A	178	THR	N-CA	-6.60	1.38	1.46
1	C	28	THR	C-O	-6.59	1.15	1.24
1	A	46	VAL	CB-CG2	-6.58	1.30	1.52
3	E	877	ILE	N-CA	-6.58	1.38	1.46
3	E	865	THR	N-CA	-6.58	1.37	1.46
2	D	206	VAL	CA-CB	6.58	1.63	1.54
1	A	49	TYR	CA-C	6.58	1.60	1.52
1	C	156	GLN	C-O	-6.57	1.15	1.24
2	D	115	LYS	CG-CD	6.57	1.72	1.52
2	D	163	VAL	CA-CB	-6.56	1.45	1.54
1	A	169	LYS	CD-CE	6.56	1.72	1.52
2	B	17	THR	N-CA	-6.56	1.38	1.45
2	D	63	PHE	CA-CB	6.56	1.60	1.52
3	F	854	ALA	CA-CB	-6.56	1.42	1.53
1	C	63	THR	CA-C	-6.55	1.44	1.52
2	B	200	PRO	C-O	-6.55	1.15	1.24
1	A	51	ALA	C-O	6.54	1.32	1.24
1	A	150	ILE	CA-CB	6.54	1.63	1.54
2	D	205	LYS	CD-CE	6.54	1.72	1.52
2	D	34	MET	CA-C	-6.53	1.44	1.52
1	A	171	SER	N-CA	-6.53	1.37	1.46
1	A	18	LYS	CA-CB	-6.53	1.44	1.53
3	F	878	LYS	CA-C	-6.53	1.44	1.52
1	C	54	ARG	C-N	-6.53	1.24	1.33
2	D	142	VAL	CB-CG1	-6.53	1.31	1.52
2	D	170	LEU	N-CA	6.51	1.54	1.46
2	B	62	ASP	N-CA	6.51	1.54	1.46
2	B	63	PHE	CD1-CE1	6.50	1.58	1.38
3	E	880	ALA	CA-C	-6.50	1.44	1.52
1	A	137	ASN	CA-C	6.50	1.61	1.52
2	D	9	PRO	C-O	-6.50	1.16	1.23
1	A	81	GLU	CG-CD	6.49	1.68	1.52
2	D	52(A)	THR	CA-C	-6.49	1.43	1.52
2	D	145	TYR	CA-C	-6.49	1.45	1.52
2	D	12	LYS	N-CA	6.47	1.53	1.46
1	C	145	ASN	CA-C	6.46	1.60	1.52
3	E	875	MET	CG-SD	6.46	1.96	1.80
2	B	121	VAL	CA-CB	6.45	1.63	1.54
1	A	25	SER	CB-OG	-6.43	1.29	1.42
2	B	53	GLU	CA-C	6.43	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	66	ARG	C-O	6.43	1.32	1.24
2	B	114	ALA	CA-CB	6.42	1.64	1.53
1	C	33	LEU	N-CA	6.42	1.54	1.46
2	B	184	PRO	C-O	6.42	1.31	1.23
2	B	50	TRP	N-CA	-6.41	1.38	1.46
1	A	79	GLN	CG-CD	6.41	1.68	1.52
3	E	855	ASP	CA-CB	6.40	1.63	1.53
1	C	78	VAL	C-O	-6.40	1.16	1.24
1	C	144	ILE	N-CA	-6.40	1.39	1.46
1	A	167	ASP	C-O	-6.39	1.16	1.24
2	B	209	LYS	CB-CG	6.39	1.71	1.52
2	D	210	ILE	N-CA	6.39	1.55	1.46
1	A	30	LYS	CA-C	6.38	1.60	1.52
2	B	21	SER	C-O	6.38	1.32	1.23
1	C	42	GLN	CA-C	-6.38	1.45	1.52
2	B	182	THR	CA-C	6.38	1.60	1.52
1	C	202	THR	CA-CB	6.38	1.64	1.53
1	C	107	LYS	CD-CE	6.38	1.71	1.52
1	A	37	GLN	C-N	-6.37	1.25	1.33
1	C	187	GLU	CA-C	6.37	1.61	1.52
3	E	880	ALA	C-N	-6.37	1.24	1.33
2	B	58	THR	C-O	-6.36	1.16	1.24
1	A	27(F)	ARG	NE-CZ	6.36	1.40	1.33
1	A	112	ALA	C-O	-6.36	1.15	1.23
1	A	197	THR	CA-CB	6.36	1.61	1.53
1	A	74	THR	CA-C	-6.35	1.44	1.52
2	B	38	ASN	CA-C	-6.35	1.44	1.53
2	B	169	VAL	CA-C	-6.34	1.44	1.52
1	C	78	VAL	CB-CG1	-6.34	1.31	1.52
2	D	82	ILE	N-CA	6.34	1.53	1.46
2	D	101	ASP	CG-OD1	6.33	1.37	1.25
2	D	151	THR	CA-CB	-6.33	1.43	1.53
2	B	95	PHE	CA-C	6.33	1.60	1.52
2	D	69	PHE	CA-C	6.33	1.61	1.52
1	A	58	VAL	N-CA	6.33	1.54	1.46
2	D	205	LYS	CB-CG	6.33	1.71	1.52
1	C	122	SER	N-CA	6.33	1.54	1.46
1	C	131	SER	C-O	-6.33	1.15	1.23
1	A	206	VAL	CA-CB	6.32	1.62	1.54
2	D	81	GLN	CB-CG	6.32	1.71	1.52
1	A	54	ARG	NE-CZ	6.31	1.40	1.33
1	C	10	SER	CA-C	-6.31	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	GLY	N-CA	6.31	1.54	1.45
1	A	87	TYR	C-N	6.31	1.42	1.33
1	C	55	GLU	C-O	6.31	1.31	1.23
2	D	177	LEU	N-CA	-6.31	1.37	1.45
3	E	865	THR	CA-C	-6.30	1.45	1.52
2	B	182	THR	CA-CB	6.30	1.62	1.53
2	D	40	ALA	CA-C	6.29	1.60	1.52
2	B	13	LYS	C-O	6.28	1.31	1.24
1	C	211	ARG	CB-CG	6.28	1.71	1.52
1	C	59	PRO	C-O	-6.27	1.16	1.23
2	B	104	GLY	CA-C	-6.26	1.42	1.52
3	F	843	PHE	C-O	6.26	1.31	1.24
2	B	85	GLU	CA-C	-6.26	1.44	1.52
2	B	155	ASN	CA-CB	-6.25	1.43	1.53
1	C	80	ALA	CA-CB	-6.25	1.43	1.53
1	C	56	SER	C-O	-6.25	1.16	1.23
2	D	2	ILE	CB-CG1	-6.25	1.41	1.53
1	A	133	VAL	CB-CG1	6.24	1.73	1.52
2	B	124	LEU	CA-C	-6.24	1.45	1.52
1	C	133	VAL	C-O	-6.23	1.17	1.24
1	A	81	GLU	C-O	6.23	1.33	1.24
1	A	145	ASN	CA-CB	6.23	1.62	1.53
1	C	19	VAL	CA-C	-6.22	1.45	1.52
2	B	156	SER	CA-C	-6.22	1.43	1.52
1	C	82	ASP	C-O	6.22	1.32	1.24
3	F	876	ASN	CB-CG	6.22	1.67	1.52
2	B	27	TYR	CG-CD2	-6.22	1.26	1.39
1	A	78	VAL	C-O	-6.21	1.16	1.24
1	C	191	SER	N-CA	6.21	1.54	1.45
1	C	61	ARG	CZ-NH1	6.21	1.41	1.32
2	B	96	LEU	CA-C	6.21	1.60	1.52
1	A	10	SER	C-N	-6.20	1.25	1.33
1	C	3	VAL	CA-C	-6.20	1.45	1.52
1	A	210	ASN	N-CA	6.19	1.54	1.46
3	E	819	GLU	CA-CB	6.19	1.61	1.52
3	E	863	GLU	C-O	-6.19	1.16	1.23
2	B	4	LEU	C-N	6.19	1.41	1.33
1	A	83	GLN	CA-C	-6.18	1.44	1.52
1	A	166	GLN	C-O	-6.17	1.16	1.24
2	D	18	VAL	CA-CB	-6.16	1.46	1.54
1	C	2	ILE	CA-C	6.16	1.60	1.52
2	B	6	GLN	CD-OE1	6.15	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	TYR	CA-C	6.15	1.60	1.52
2	D	8	GLY	N-CA	6.15	1.51	1.43
1	A	24	LYS	CD-CE	6.14	1.70	1.52
2	B	151	THR	C-N	-6.14	1.25	1.33
3	E	834	ILE	CA-C	6.13	1.60	1.52
1	A	165	ASP	CA-C	-6.13	1.44	1.53
2	D	1	GLN	N-CA	6.13	1.57	1.46
2	B	79	TYR	CA-C	-6.13	1.45	1.52
3	E	867	ASP	CG-OD2	6.12	1.36	1.25
2	B	39	GLN	N-CA	-6.12	1.38	1.46
1	A	96	LEU	CG-CD2	6.11	1.72	1.52
1	A	93	ILE	C-O	6.11	1.32	1.24
1	C	16	GLY	C-O	6.10	1.32	1.24
1	C	211	ARG	NE-CZ	6.10	1.39	1.33
2	D	123	PRO	N-CA	6.10	1.54	1.47
2	B	42	GLY	CA-C	6.10	1.59	1.51
2	D	108	THR	CA-CB	-6.09	1.45	1.53
1	C	163	TRP	C-O	-6.08	1.16	1.23
1	A	176	SER	C-O	-6.08	1.16	1.24
3	E	834	ILE	C-N	6.08	1.41	1.33
3	F	859	LYS	CA-C	6.08	1.60	1.52
1	C	39	LYS	CG-CD	6.08	1.70	1.52
1	A	11	LEU	C-O	-6.07	1.16	1.23
1	A	82	ASP	N-CA	-6.07	1.38	1.46
2	B	32	PHE	CA-CB	6.06	1.63	1.53
2	D	169	VAL	CA-C	6.06	1.59	1.52
1	A	143	ASP	CA-C	6.06	1.60	1.52
1	C	209	PHE	C-O	6.05	1.30	1.23
1	A	182	THR	CA-CB	6.05	1.64	1.53
3	F	839	PHE	CA-CB	-6.04	1.42	1.53
1	A	59	PRO	C-O	-6.04	1.16	1.23
1	C	137	ASN	N-CA	-6.04	1.38	1.46
2	D	70	SER	N-CA	-6.04	1.35	1.45
1	A	110	ASP	CB-CG	6.03	1.67	1.52
1	C	170	ASP	C-O	-6.03	1.16	1.24
2	D	193	VAL	CA-CB	-6.03	1.46	1.54
1	C	76	SER	C-O	6.02	1.32	1.24
2	B	91	PHE	CA-CB	6.02	1.64	1.53
1	A	66	GLY	C-O	-6.01	1.17	1.23
2	D	198	ALA	CA-C	6.01	1.59	1.52
2	B	35	HIS	ND1-CE1	6.00	1.38	1.32
1	A	169	LYS	N-CA	-6.00	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	THR	C-O	6.00	1.31	1.24
3	F	873	ASN	CA-C	6.00	1.61	1.52
2	D	76	SER	N-CA	-5.99	1.37	1.46
3	F	840	LYS	C-O	5.99	1.31	1.23
3	E	860	VAL	CA-CB	5.99	1.63	1.54
1	C	40	PRO	CA-CB	5.99	1.61	1.53
1	A	188	ARG	CA-CB	5.99	1.63	1.53
2	B	53	GLU	C-O	-5.99	1.16	1.24
1	C	65	ARG	CB-CG	-5.98	1.34	1.52
1	C	141	PRO	CA-C	-5.98	1.40	1.52
1	C	97	THR	CA-C	-5.98	1.45	1.52
1	C	24	LYS	N-CA	-5.97	1.39	1.46
1	C	45	LYS	CA-C	-5.97	1.45	1.52
1	C	142	LYS	N-CA	-5.97	1.38	1.46
2	D	88	ALA	CA-C	-5.96	1.45	1.52
1	A	173	TYR	CA-C	5.96	1.60	1.52
2	B	10	GLU	CA-CB	-5.96	1.44	1.53
1	A	88	CYS	CA-C	-5.96	1.45	1.52
1	C	120	PRO	CG-CD	5.96	1.71	1.50
2	B	160	SER	C-O	-5.96	1.16	1.24
1	C	193	THR	C-O	5.95	1.31	1.23
2	D	73	THR	C-N	-5.95	1.26	1.33
3	F	856	LEU	N-CA	-5.95	1.39	1.46
3	F	882	LYS	CG-CD	5.94	1.70	1.52
3	F	847	THR	CA-C	5.94	1.60	1.52
2	B	94	ARG	CD-NE	-5.94	1.38	1.46
3	E	825	VAL	CB-CG2	5.94	1.72	1.52
1	A	107	LYS	CE-NZ	5.94	1.67	1.49
3	E	818	LYS	CB-CG	5.94	1.70	1.52
1	C	24	LYS	C-O	-5.93	1.17	1.23
1	C	57	GLY	C-O	5.93	1.32	1.24
3	F	845	GLU	CA-C	5.93	1.60	1.52
2	D	38	ASN	CG-OD1	5.92	1.34	1.23
2	B	71	LEU	C-O	-5.92	1.16	1.23
3	E	861	ASN	C-N	5.92	1.42	1.33
2	B	122	TYR	CD2-CE2	5.91	1.56	1.38
1	C	167	ASP	CG-OD2	5.91	1.36	1.25
2	D	2	ILE	C-O	-5.91	1.17	1.24
1	A	19	VAL	C-O	5.90	1.31	1.24
2	B	64	LYS	C-O	5.90	1.30	1.24
1	A	175	MET	C-O	5.90	1.31	1.23
1	A	47	LEU	C-O	-5.89	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	64	LYS	CA-CB	5.89	1.61	1.53
2	B	181	VAL	N-CA	-5.89	1.39	1.46
2	D	115	LYS	CB-CG	5.89	1.70	1.52
1	A	18	LYS	CG-CD	5.89	1.70	1.52
1	C	105	GLU	CA-C	-5.89	1.45	1.52
2	B	11	LEU	CA-CB	-5.88	1.44	1.53
1	C	149	LYS	CD-CE	5.88	1.70	1.52
3	E	863	GLU	CA-C	-5.88	1.45	1.52
3	E	870	ASP	CA-CB	5.88	1.62	1.53
2	D	107	THR	C-O	-5.88	1.17	1.24
2	D	87	THR	N-CA	-5.88	1.38	1.46
2	D	192	THR	CA-CB	5.88	1.60	1.53
2	D	102	VAL	C-O	5.87	1.29	1.24
2	B	68	ALA	CA-C	5.87	1.59	1.52
1	A	19	VAL	CA-CB	-5.87	1.47	1.54
1	A	61	ARG	CZ-NH1	5.86	1.41	1.32
1	C	3	VAL	C-N	5.86	1.41	1.33
1	A	13	VAL	CA-C	5.86	1.59	1.52
1	C	71	PHE	CD1-CE1	5.86	1.56	1.38
3	F	826	ASN	CA-C	-5.85	1.45	1.52
3	F	826	ASN	C-O	-5.85	1.16	1.23
2	B	120	SER	CA-C	-5.85	1.45	1.52
3	E	834	ILE	CA-CB	-5.84	1.47	1.54
1	A	206	VAL	CB-CG2	5.84	1.71	1.52
1	C	13	VAL	CA-CB	-5.84	1.44	1.55
2	D	118	PRO	CA-C	-5.84	1.46	1.52
2	B	8	GLY	C-N	-5.84	1.26	1.33
1	C	52	SER	CA-CB	5.84	1.63	1.54
2	B	2	ILE	CA-C	-5.83	1.45	1.52
1	A	20	THR	C-O	5.83	1.30	1.24
1	A	125	LEU	CG-CD1	5.83	1.71	1.52
2	D	197	VAL	N-CA	-5.83	1.39	1.46
2	D	48	MET	SD-CE	-5.83	1.65	1.79
1	C	145	ASN	N-CA	5.83	1.53	1.46
1	A	45	LYS	CE-NZ	5.83	1.66	1.49
1	A	106	LEU	CG-CD1	-5.83	1.33	1.52
1	A	56	SER	C-O	-5.82	1.17	1.23
2	B	95	PHE	C-N	-5.82	1.25	1.33
2	B	2	ILE	CB-CG2	5.82	1.71	1.52
1	A	187	GLU	N-CA	5.81	1.53	1.46
2	B	36	TRP	CG-CD1	-5.81	1.22	1.36
2	B	43	LYS	CA-CB	5.81	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	847	THR	C-O	5.80	1.31	1.24
1	A	190	ASN	CG-OD1	5.80	1.34	1.23
1	A	168	SER	N-CA	5.80	1.53	1.46
2	D	90	TYR	CB-CG	5.80	1.64	1.51
1	A	106	LEU	CA-CB	-5.79	1.44	1.53
1	A	210	ASN	CG-OD1	5.79	1.34	1.23
1	C	106	LEU	CA-C	-5.79	1.45	1.52
1	C	27(E)	SER	C-O	5.78	1.30	1.24
1	A	28	THR	C-O	5.78	1.31	1.24
2	B	51	VAL	CA-C	-5.78	1.45	1.52
1	A	170	ASP	CB-CG	-5.78	1.37	1.52
3	F	839	PHE	CD2-CE2	5.78	1.55	1.38
2	D	211	VAL	CA-C	5.77	1.58	1.52
2	B	32	PHE	N-CA	-5.77	1.39	1.46
2	D	1	GLN	CG-CD	5.77	1.66	1.52
3	E	846	ALA	C-O	5.76	1.30	1.24
1	A	88	CYS	C-N	-5.76	1.25	1.33
2	D	193	VAL	CB-CG2	5.76	1.71	1.52
1	A	9	SER	CA-C	5.76	1.60	1.52
2	D	152	VAL	CB-CG2	-5.76	1.33	1.52
2	B	111	VAL	CB-CG2	-5.75	1.33	1.52
3	E	880	ALA	C-O	-5.75	1.16	1.24
1	A	186	TYR	C-O	5.75	1.30	1.24
2	D	100	TYR	CD1-CE1	-5.75	1.21	1.38
1	C	27(A)	SER	N-CA	-5.74	1.38	1.46
2	B	167	PRO	CG-CD	5.74	1.70	1.50
2	D	21	SER	CA-C	5.74	1.60	1.52
1	A	135	PHE	CB-CG	5.73	1.63	1.50
2	D	160	SER	C-O	5.73	1.31	1.24
1	C	178	THR	N-CA	-5.73	1.39	1.46
1	C	29	ARG	N-CA	5.72	1.55	1.46
2	D	143	LYS	CG-CD	5.72	1.69	1.52
2	D	93	ALA	CA-CB	-5.72	1.44	1.53
2	D	51	VAL	C-O	5.72	1.30	1.24
2	B	189	PRO	CA-C	5.71	1.60	1.52
1	C	144	ILE	C-O	5.71	1.30	1.23
2	B	197	VAL	C-N	-5.70	1.25	1.33
2	B	62	ASP	CA-C	5.70	1.60	1.52
3	F	867	ASP	CA-C	5.70	1.59	1.52
3	F	824	LYS	C-N	-5.70	1.26	1.33
3	E	839	PHE	C-N	-5.69	1.25	1.33
2	D	90	TYR	CA-CB	5.69	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLY	C-O	5.69	1.31	1.23
1	A	82	ASP	CA-C	5.68	1.60	1.52
1	A	138	ASN	CG-OD1	5.68	1.34	1.23
1	C	62	PHE	CD2-CE2	-5.67	1.21	1.38
2	B	198	ALA	CA-CB	5.67	1.65	1.54
1	C	80	ALA	CA-C	5.67	1.60	1.52
2	D	16	GLU	CA-C	-5.67	1.45	1.53
2	D	8	GLY	C-O	5.67	1.33	1.24
1	A	32	TYR	CD1-CE1	5.66	1.55	1.38
1	A	178	THR	C-O	5.66	1.30	1.23
1	A	61	ARG	CB-CG	-5.66	1.35	1.52
3	E	844	GLU	CA-CB	5.66	1.62	1.53
3	E	846	ALA	CA-C	5.66	1.59	1.52
2	B	64	LYS	N-CA	5.65	1.53	1.46
1	C	169	LYS	CD-CE	5.65	1.69	1.52
2	D	77	THR	CB-CG2	5.65	1.71	1.52
1	C	92	TYR	CE2-CZ	5.65	1.51	1.38
2	D	57	PRO	CG-CD	5.65	1.70	1.50
1	C	76	SER	CA-CB	-5.64	1.43	1.53
1	C	92	TYR	CD1-CE1	5.64	1.55	1.38
3	E	866	TRP	CG-CD1	5.64	1.51	1.36
1	C	17	GLU	CA-CB	5.64	1.62	1.53
1	C	171	SER	CA-C	5.63	1.60	1.52
3	F	873	ASN	C-O	5.62	1.31	1.24
1	A	67	SER	CA-CB	-5.62	1.45	1.53
1	C	29	ARG	CD-NE	5.62	1.54	1.46
2	D	121	VAL	CA-CB	-5.62	1.47	1.54
1	C	9	SER	CA-C	-5.62	1.45	1.52
1	C	49	TYR	CD2-CE2	5.61	1.55	1.38
1	A	55	GLU	C-O	5.61	1.30	1.23
3	F	835	GLN	C-O	-5.61	1.17	1.23
2	B	5	VAL	CA-CB	-5.60	1.47	1.54
2	D	195	CYS	CB-SG	5.60	1.99	1.81
1	C	115	VAL	CB-CG2	5.60	1.71	1.52
2	D	91	PHE	C-O	-5.60	1.17	1.23
2	D	209	LYS	CA-C	5.59	1.60	1.52
2	D	212	PRO	CB-CG	5.59	1.77	1.49
1	A	209	PHE	CD2-CE2	5.59	1.55	1.38
3	F	828	ILE	C-O	-5.58	1.17	1.24
3	E	831	ASP	CB-CG	5.58	1.66	1.52
2	B	213	ARG	CB-CG	5.58	1.69	1.52
1	C	43	SER	C-O	-5.58	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	PRO	CB-CG	5.58	1.77	1.49
2	D	166	PHE	C-N	-5.58	1.26	1.33
1	A	91	ALA	CA-C	5.57	1.60	1.52
1	A	212	ASN	N-CA	5.57	1.53	1.46
3	E	828	ILE	CG1-CD1	-5.57	1.30	1.51
2	D	213	ARG	CB-CG	5.57	1.69	1.52
2	B	81	GLN	C-N	-5.56	1.25	1.33
2	B	63	PHE	N-CA	5.56	1.52	1.46
3	F	860	VAL	CB-CG2	5.56	1.71	1.52
2	B	82	ILE	N-CA	-5.56	1.39	1.46
1	C	123	GLU	C-O	5.55	1.31	1.24
1	A	22	SER	CB-OG	5.55	1.53	1.42
1	C	95	PRO	CA-CB	-5.55	1.43	1.53
1	A	142	LYS	CG-CD	5.54	1.69	1.52
1	A	98	PHE	CD1-CE1	5.54	1.55	1.38
1	C	202	THR	CB-CG2	5.54	1.70	1.52
2	D	50	TRP	CA-CB	-5.54	1.45	1.53
2	B	109	VAL	CB-CG1	-5.53	1.34	1.52
1	C	37	GLN	N-CA	5.53	1.52	1.46
1	C	69	THR	N-CA	5.53	1.54	1.46
2	D	104	GLY	C-O	5.53	1.30	1.23
2	B	62	ASP	C-O	5.53	1.30	1.24
2	D	53	GLU	CA-CB	5.52	1.63	1.53
2	D	17	THR	CA-C	5.52	1.59	1.52
2	D	161	SER	C-O	5.52	1.30	1.23
3	E	858	ALA	CA-CB	-5.51	1.44	1.53
2	B	45	LEU	N-CA	-5.51	1.39	1.46
2	B	135	MET	C-N	-5.51	1.25	1.33
1	A	135	PHE	CE2-CZ	-5.51	1.22	1.38
2	B	27	TYR	CD1-CE1	-5.51	1.22	1.38
1	C	13	VAL	C-N	-5.51	1.25	1.33
3	E	863	GLU	CD-OE1	5.50	1.35	1.25
2	D	133	ASN	C-N	5.49	1.41	1.33
1	A	95	PRO	CA-CB	5.49	1.63	1.53
2	B	47	TRP	N-CA	5.49	1.52	1.46
2	B	122	TYR	N-CA	-5.49	1.37	1.45
2	B	168	ALA	CA-CB	5.49	1.62	1.53
1	C	127	SER	N-CA	5.48	1.53	1.46
2	D	35	HIS	CA-C	5.48	1.59	1.52
2	D	79	TYR	CD1-CE1	-5.48	1.22	1.38
2	D	38	ASN	CA-CB	-5.48	1.40	1.54
1	A	105	GLU	N-CA	-5.47	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	GLN	CA-C	-5.47	1.45	1.53
3	F	843	PHE	CE2-CZ	5.47	1.55	1.38
2	B	100	TYR	C-O	-5.47	1.17	1.23
1	C	56	SER	CA-C	-5.47	1.46	1.52
1	C	103	LYS	CG-CD	5.46	1.68	1.52
1	A	50	TRP	CZ2-CH2	5.46	1.47	1.37
1	A	102	THR	C-O	5.46	1.30	1.24
2	B	55	GLY	N-CA	5.46	1.53	1.45
2	D	36	TRP	C-O	-5.46	1.17	1.23
2	B	183	VAL	CA-CB	-5.46	1.50	1.54
2	D	72	GLU	CD-OE1	5.45	1.35	1.25
1	A	20	THR	N-CA	5.45	1.52	1.46
2	B	69	PHE	CE1-CZ	5.44	1.54	1.38
2	D	60	ALA	CA-C	-5.44	1.46	1.52
1	A	33	LEU	CA-CB	5.44	1.64	1.53
1	A	8	PRO	C-O	-5.44	1.12	1.23
3	F	862	GLY	C-O	5.44	1.31	1.23
1	C	36	TYR	N-CA	-5.44	1.39	1.46
1	A	195	GLU	CA-C	5.43	1.59	1.52
2	B	67	PHE	CE2-CZ	5.43	1.54	1.38
2	B	120	SER	N-CA	-5.43	1.39	1.45
1	A	194	CYS	C-O	5.43	1.30	1.24
3	E	878	LYS	CG-CD	5.43	1.68	1.52
1	A	151	ASP	N-CA	5.43	1.53	1.46
1	A	183	LYS	N-CA	5.43	1.52	1.46
2	B	39	GLN	CA-C	5.43	1.60	1.52
2	B	80	LEU	CA-CB	5.42	1.64	1.53
2	D	210	ILE	CG1-CD1	5.42	1.72	1.51
1	C	185	GLU	CD-OE1	5.42	1.35	1.25
1	A	67	SER	CA-C	-5.42	1.45	1.52
1	C	72	THR	CB-CG2	5.41	1.70	1.52
2	B	143	LYS	CA-C	-5.41	1.46	1.52
2	B	82	ILE	CA-C	5.41	1.59	1.52
1	A	117	ILE	CA-CB	5.40	1.62	1.54
2	B	67	PHE	CA-CB	5.40	1.61	1.53
1	C	105	GLU	CD-OE2	5.40	1.35	1.25
2	B	117	THR	CA-CB	5.40	1.62	1.54
2	D	156	SER	CA-CB	-5.40	1.44	1.53
1	A	141	PRO	CA-C	-5.40	1.45	1.52
2	D	177	LEU	CA-CB	-5.40	1.43	1.54
1	A	143	ASP	N-CA	5.40	1.52	1.45
2	B	57	PRO	C-O	5.40	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	GLY	C-O	5.40	1.31	1.24
2	B	159	LEU	CG-CD1	5.39	1.70	1.52
1	C	60	ASP	N-CA	5.39	1.53	1.46
3	E	852	ARG	CD-NE	5.39	1.53	1.46
2	D	88	ALA	N-CA	5.38	1.52	1.46
2	D	87	THR	CB-OG1	5.38	1.52	1.43
2	B	154	TRP	CA-C	-5.37	1.46	1.52
2	D	169	VAL	C-O	5.37	1.30	1.24
1	A	58	VAL	C-N	-5.37	1.26	1.33
1	C	13	VAL	CA-C	-5.37	1.46	1.52
1	C	205	ILE	N-CA	5.37	1.53	1.46
1	A	177	SER	CB-OG	5.37	1.52	1.42
1	A	187	GLU	C-O	-5.36	1.17	1.24
2	B	73	THR	CA-CB	5.36	1.61	1.53
1	C	58	VAL	N-CA	5.36	1.53	1.46
1	C	16	GLY	N-CA	5.36	1.52	1.45
1	A	178	THR	CA-CB	-5.36	1.45	1.52
3	F	844	GLU	CA-C	5.35	1.59	1.52
1	A	28	THR	CB-CG2	5.35	1.70	1.52
1	A	53	THR	CA-CB	-5.35	1.45	1.53
1	A	162	SER	CB-OG	5.35	1.52	1.42
1	A	79	GLN	CD-OE1	5.35	1.33	1.23
1	A	166	GLN	N-CA	-5.35	1.39	1.46
2	B	145	TYR	N-CA	5.35	1.52	1.45
2	B	206	VAL	CA-CB	-5.35	1.47	1.54
1	C	51	ALA	CA-C	-5.35	1.45	1.52
2	D	9	PRO	CA-C	5.35	1.58	1.52
1	A	214	CYS	CA-CB	5.34	1.64	1.53
2	B	202	SER	C-O	-5.34	1.16	1.24
1	A	98	PHE	CE1-CZ	5.34	1.54	1.38
3	E	829	PHE	CD1-CE1	-5.34	1.22	1.38
1	A	21	MET	C-O	5.33	1.30	1.24
1	A	145	ASN	N-CA	5.33	1.53	1.46
2	D	44	GLY	CA-C	-5.33	1.44	1.51
1	A	22	SER	CA-C	-5.33	1.46	1.52
2	D	167	PRO	C-N	-5.33	1.26	1.33
3	F	872	GLY	CA-C	5.33	1.58	1.51
3	E	833	LYS	CD-CE	5.32	1.68	1.52
1	C	209	PHE	CA-C	5.32	1.58	1.52
1	C	23	CYS	C-O	5.32	1.29	1.23
2	D	212	PRO	CA-CB	5.32	1.61	1.53
1	C	50	TRP	N-CA	5.31	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	84	ASN	C-O	-5.31	1.18	1.24
1	A	179	LEU	CA-C	5.31	1.59	1.52
2	B	82	ILE	CA-CB	-5.31	1.47	1.53
2	B	104	GLY	C-N	-5.31	1.26	1.33
2	B	177	LEU	C-N	-5.30	1.26	1.33
1	A	18	LYS	N-CA	5.30	1.52	1.46
1	C	43	SER	CA-CB	-5.30	1.42	1.53
3	E	840	LYS	CA-CB	5.30	1.60	1.53
1	C	137	ASN	C-O	-5.29	1.17	1.23
2	D	83	LYS	C-O	5.29	1.30	1.23
1	A	27	GLN	CG-CD	5.29	1.65	1.52
2	B	57	PRO	CG-CD	5.29	1.68	1.50
3	F	841	GLY	N-CA	5.29	1.53	1.45
1	A	29	ARG	CA-C	5.29	1.60	1.53
1	C	180	THR	CA-C	-5.28	1.46	1.52
2	D	134	SER	C-O	5.28	1.30	1.24
1	A	104	LEU	CA-C	5.27	1.59	1.52
1	C	159	VAL	CB-CG2	-5.27	1.35	1.52
3	E	840	LYS	N-CA	-5.27	1.39	1.46
3	E	839	PHE	N-CA	5.26	1.52	1.46
1	C	106	LEU	CG-CD2	-5.26	1.35	1.52
1	C	40	PRO	N-CD	5.26	1.55	1.47
2	B	196	ASN	C-O	-5.26	1.17	1.24
2	B	67	PHE	CD1-CE1	5.26	1.54	1.38
3	E	828	ILE	CA-C	-5.26	1.45	1.52
2	D	154	TRP	CA-C	5.26	1.58	1.52
2	B	76	SER	CA-C	5.25	1.59	1.52
1	C	118	PHE	CD1-CE1	-5.25	1.22	1.38
2	D	152	VAL	CA-C	5.25	1.59	1.52
1	A	211	ARG	C-O	-5.25	1.17	1.24
2	B	71	LEU	N-CA	-5.25	1.39	1.45
1	A	192	TYR	CZ-OH	5.24	1.49	1.38
3	E	851	TYR	CG-CD2	-5.24	1.28	1.39
2	D	89	THR	CB-OG1	-5.24	1.35	1.43
2	B	192	THR	C-O	5.24	1.30	1.23
3	E	826	ASN	CB-CG	5.24	1.65	1.52
3	E	864	TYR	CA-CB	5.24	1.61	1.53
3	E	858	ALA	CA-C	-5.23	1.45	1.52
2	D	103	TRP	CA-C	-5.23	1.46	1.52
2	D	70	SER	C-O	-5.23	1.16	1.24
2	D	17	THR	CA-CB	-5.22	1.41	1.53
1	C	90	GLN	CD-NE2	5.22	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	VAL	CA-CB	5.22	1.62	1.54
1	C	159	VAL	CA-CB	-5.22	1.48	1.54
1	A	138	ASN	N-CA	-5.22	1.39	1.46
2	D	12	LYS	CA-C	5.22	1.58	1.52
2	D	209	LYS	CG-CD	5.22	1.68	1.52
3	E	874	HIS	C-O	-5.21	1.17	1.23
2	B	212	PRO	C-O	5.21	1.30	1.24
2	B	35	HIS	CE1-NE2	5.21	1.37	1.32
1	C	1	ASP	C-O	5.20	1.33	1.23
1	C	207	LYS	N-CA	-5.20	1.39	1.46
1	A	177	SER	CA-CB	5.20	1.61	1.53
1	A	123	GLU	C-O	5.19	1.30	1.24
2	B	145	TYR	CZ-OH	5.19	1.49	1.38
1	A	92	TYR	C-N	-5.19	1.27	1.33
2	D	152	VAL	CB-CG1	-5.19	1.35	1.52
2	B	59	TYR	N-CA	-5.18	1.40	1.45
3	E	824	LYS	CA-C	-5.18	1.46	1.52
2	D	71	LEU	CG-CD2	-5.18	1.35	1.52
1	A	134	CYS	N-CA	-5.18	1.39	1.45
2	B	187	THR	C-O	-5.18	1.17	1.24
1	C	188	ARG	CD-NE	5.18	1.53	1.46
2	D	25	SER	CA-CB	-5.18	1.44	1.53
2	D	59	TYR	C-N	-5.18	1.26	1.33
2	D	64	LYS	CE-NZ	5.18	1.64	1.49
2	B	149	PRO	CA-C	-5.17	1.46	1.52
1	A	154	GLU	CA-C	5.17	1.59	1.52
3	E	870	ASP	CB-CG	5.17	1.65	1.52
1	C	135	PHE	CD2-CE2	5.17	1.54	1.38
1	A	158	GLY	C-N	-5.16	1.26	1.33
1	A	3	VAL	N-CA	5.16	1.52	1.46
2	B	93	ALA	C-N	-5.16	1.26	1.33
1	A	139	PHE	CA-C	-5.16	1.46	1.52
2	B	61	ASP	CG-OD1	5.16	1.35	1.25
2	B	100(A)	PHE	C-O	-5.16	1.17	1.24
1	C	113	PRO	CA-CB	-5.16	1.46	1.53
2	B	117	THR	CA-C	5.16	1.58	1.52
1	A	104	LEU	CG-CD1	-5.15	1.35	1.52
3	E	823	ILE	CG1-CD1	-5.15	1.31	1.51
2	D	140	CYS	C-O	-5.15	1.17	1.24
2	B	80	LEU	CG-CD1	-5.15	1.35	1.52
1	C	124	GLN	CA-C	5.15	1.59	1.52
2	D	30	THR	CB-CG2	5.15	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	159	LEU	CA-C	-5.15	1.46	1.52
2	B	12	LYS	C-O	5.14	1.30	1.23
1	A	147	LYS	CA-C	5.14	1.59	1.52
1	A	165	ASP	CG-OD1	5.13	1.35	1.25
1	A	27(B)	LEU	CG-CD1	5.13	1.69	1.52
2	D	196	ASN	CG-ND2	5.13	1.44	1.33
2	B	1	GLN	CD-OE1	5.12	1.33	1.23
2	B	46	ASN	CA-C	-5.12	1.46	1.52
2	B	62	ASP	CG-OD2	5.12	1.35	1.25
1	C	115	VAL	CB-CG1	5.12	1.69	1.52
1	A	149	LYS	CE-NZ	5.11	1.64	1.49
1	A	27(D)	ASN	C-O	5.11	1.30	1.24
2	B	210	ILE	C-N	5.11	1.37	1.32
2	D	94	ARG	C-O	-5.11	1.17	1.23
1	A	137	ASN	CG-OD1	5.11	1.33	1.23
2	D	23	LYS	C-O	-5.10	1.17	1.24
1	A	117	ILE	CB-CG2	5.10	1.69	1.52
2	B	96	LEU	N-CA	-5.10	1.39	1.45
3	F	872	GLY	N-CA	5.10	1.52	1.45
1	A	87	TYR	CA-C	5.09	1.58	1.52
2	D	171	GLN	CA-CB	-5.09	1.44	1.53
1	C	62	PHE	N-CA	5.09	1.52	1.46
1	C	212	ASN	CG-ND2	5.09	1.44	1.33
1	A	142	LYS	N-CA	-5.08	1.39	1.46
1	C	79	GLN	C-O	5.08	1.30	1.23
2	B	182	THR	N-CA	-5.08	1.40	1.46
3	F	836	THR	N-CA	-5.08	1.39	1.46
1	C	30	LYS	N-CA	-5.08	1.40	1.46
3	F	834	ILE	CA-C	-5.08	1.46	1.53
2	B	11	LEU	CB-CG	5.08	1.63	1.53
2	D	54	THR	N-CA	-5.08	1.40	1.46
1	A	74	THR	C-N	-5.08	1.27	1.33
1	A	141	PRO	CG-CD	5.08	1.68	1.50
3	F	879	PHE	CE2-CZ	5.08	1.53	1.38
1	C	108	ARG	CA-CB	5.07	1.62	1.53
3	E	855	ASP	N-CA	-5.07	1.40	1.46
1	C	65	ARG	N-CA	-5.07	1.39	1.45
2	D	90	TYR	CG-CD2	-5.07	1.28	1.39
1	A	110	ASP	CA-CB	5.07	1.61	1.53
2	D	43	LYS	CA-CB	5.06	1.61	1.53
2	D	152	VAL	CA-CB	-5.06	1.48	1.54
2	B	89	THR	N-CA	-5.06	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	25	SER	C-N	-5.06	1.26	1.33
2	B	43	LYS	CA-C	-5.05	1.46	1.53
1	C	7	SER	CA-C	5.05	1.58	1.52
1	A	30	LYS	CB-CG	5.05	1.67	1.52
1	A	105	GLU	CD-OE1	5.05	1.34	1.25
3	E	866	TRP	C-O	-5.05	1.18	1.23
2	D	173	ASP	CB-CG	5.04	1.64	1.52
1	A	148	TRP	C-O	5.04	1.30	1.24
1	A	41	GLY	C-O	-5.04	1.17	1.24
3	F	844	GLU	C-O	-5.04	1.18	1.24
2	B	11	LEU	N-CA	5.03	1.53	1.46
2	D	86	ASP	C-O	5.03	1.30	1.24
1	A	161	ASN	CG-OD1	5.03	1.33	1.23
2	B	95	PHE	N-CA	5.03	1.52	1.46
2	D	3	GLN	CD-OE1	5.03	1.33	1.23
2	D	3	GLN	CB-CG	-5.03	1.37	1.52
3	E	859	LYS	CG-CD	5.01	1.67	1.52
2	D	137	THR	CA-CB	5.01	1.62	1.53
2	B	161	SER	N-CA	-5.01	1.39	1.46
2	D	21	SER	C-N	5.01	1.40	1.33
1	A	169	LYS	CA-CB	-5.01	1.45	1.53
3	F	878	LYS	CB-CG	5.00	1.67	1.52

All (712) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	PHE	O-C-N	-19.94	107.89	121.85
3	E	820	GLU	N-CA-C	15.33	127.99	111.28
2	D	188	TRP	O-C-N	-14.34	104.54	121.31
2	B	149	PRO	CA-N-CD	-13.65	92.89	112.00
2	D	189	PRO	CA-N-CD	-13.49	93.12	112.00
2	D	125	ALA	CA-C-N	-12.93	106.32	119.90
2	D	125	ALA	C-N-CA	-12.93	106.32	119.90
1	A	158	GLY	CA-C-N	12.80	145.00	121.97
1	A	158	GLY	C-N-CA	12.80	145.00	121.97
1	C	26	SER	N-CA-C	-12.71	97.80	113.18
3	E	840	LYS	CB-CA-C	-12.59	91.38	110.26
1	A	157	ASN	OD1-CG-ND2	-12.27	110.33	122.60
1	A	212	ASN	N-CA-C	12.15	127.55	112.23
1	A	115	VAL	CB-CA-C	-11.93	94.67	111.38
2	D	183	VAL	CA-C-N	-11.74	107.67	119.76
2	D	183	VAL	C-N-CA	-11.74	107.67	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	869	GLU	N-CA-C	-11.65	93.11	110.24
2	B	2	ILE	O-C-N	-11.63	108.03	122.57
2	D	133	ASN	OD1-CG-ND2	-11.53	111.07	122.60
1	A	27(B)	LEU	N-CA-C	-11.47	95.07	113.19
3	E	839	PHE	CA-C-N	11.41	137.68	121.24
3	E	839	PHE	C-N-CA	11.41	137.68	121.24
2	B	108	THR	OG1-CB-CG2	-11.13	87.04	109.30
2	B	201	ALA	N-CA-C	10.98	124.61	111.33
1	C	94	PRO	CA-C-O	-10.93	113.03	120.90
2	D	104	GLY	N-CA-C	-10.63	95.44	112.66
1	A	95	PRO	N-CD-CG	10.61	116.54	103.80
2	D	188	TRP	CA-C-O	-10.51	108.61	121.01
2	B	181	VAL	N-CA-C	10.50	123.99	108.45
2	B	2	ILE	CB-CA-C	10.42	128.38	111.29
1	A	211	ARG	CA-C-N	10.37	138.30	120.68
1	A	211	ARG	C-N-CA	10.37	138.30	120.68
2	B	48	MET	N-CA-C	-10.28	100.59	113.55
3	F	856	LEU	N-CA-C	-10.25	100.07	111.14
1	A	114	THR	N-CA-C	-10.21	90.17	107.23
1	A	93	ILE	CA-CB-CG2	10.11	127.68	110.50
1	C	130	ALA	CA-C-N	-10.02	106.99	122.62
1	C	130	ALA	C-N-CA	-10.02	106.99	122.62
2	D	125	ALA	O-C-N	9.99	131.51	121.72
2	B	111	VAL	N-CA-C	9.98	121.02	106.55
3	F	818	LYS	CA-C-N	9.86	140.36	121.54
3	F	818	LYS	C-N-CA	9.86	140.36	121.54
3	F	833	LYS	CA-C-N	-9.82	111.39	122.48
3	F	833	LYS	C-N-CA	-9.82	111.39	122.48
1	C	137	ASN	N-CA-C	9.81	124.80	110.28
3	E	869	GLU	O-C-N	-9.69	112.20	123.25
3	F	851	TYR	N-CA-C	-9.69	101.59	113.41
3	F	821	VAL	CA-C-N	9.65	136.68	122.39
3	F	821	VAL	C-N-CA	9.65	136.68	122.39
3	F	869	GLU	N-CA-CB	9.59	124.35	109.48
3	E	819	GLU	N-CA-C	9.58	125.23	108.56
2	D	108	THR	OG1-CB-CG2	-9.57	90.16	109.30
3	F	868	LEU	CA-C-O	-9.56	110.04	120.36
2	D	83	LYS	N-CA-C	9.51	124.88	110.14
2	B	148	GLU	O-C-N	-9.50	110.40	121.32
2	B	91	PHE	N-CA-C	9.46	124.82	109.59
1	C	76	SER	N-CA-C	9.45	124.43	113.19
1	A	63	THR	CA-C-N	-9.43	113.47	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	THR	C-N-CA	-9.43	113.47	121.58
1	C	197	THR	N-CA-C	9.39	123.53	108.41
1	A	205	ILE	N-CA-CB	9.39	121.24	110.82
2	B	189	PRO	N-CD-CG	-9.34	89.19	103.20
2	B	111	VAL	N-CA-CB	9.28	121.06	112.06
2	D	131	GLN	CA-C-N	9.25	136.15	120.71
2	D	131	GLN	C-N-CA	9.25	136.15	120.71
1	C	177	SER	N-CA-C	9.19	124.25	107.99
2	D	133	ASN	CA-CB-CG	9.19	121.78	112.60
3	E	828	ILE	CA-CB-CG1	9.15	125.95	110.40
1	A	85	VAL	O-C-N	-9.14	112.88	123.03
1	C	72	THR	N-CA-C	9.14	123.94	109.50
2	D	139	GLY	N-CA-C	9.14	123.69	110.80
3	E	876	ASN	CA-C-O	-9.11	110.86	120.70
2	B	129	ALA	O-C-N	-9.09	108.91	122.28
1	C	16	GLY	CA-C-O	9.06	128.43	119.37
2	B	121	VAL	O-C-N	-9.03	113.43	123.18
1	A	114	THR	OG1-CB-CG2	-8.94	91.42	109.30
2	B	149	PRO	CB-CA-C	8.88	123.32	110.63
2	D	130	ALA	CA-C-N	8.82	138.39	121.54
2	D	130	ALA	C-N-CA	8.82	138.39	121.54
2	B	56	GLU	CB-CG-CD	-8.81	97.63	112.60
1	C	94	PRO	O-C-N	8.73	125.33	121.31
2	B	192	THR	N-CA-C	-8.69	95.77	109.50
2	D	210	ILE	N-CA-C	8.69	120.31	106.32
1	C	5	SER	CA-CB-OG	-8.65	93.80	111.10
1	A	195	GLU	CA-C-O	8.63	129.65	120.33
2	B	109	VAL	N-CA-C	8.59	120.94	107.98
2	D	189	PRO	CB-CA-C	8.59	125.73	111.56
1	C	178	THR	N-CA-C	8.56	122.47	108.52
1	A	61	ARG	NE-CZ-NH1	-8.55	112.95	121.50
1	C	31	ASN	N-CA-C	8.53	122.75	109.96
1	A	190	ASN	N-CA-C	8.53	128.96	110.80
2	D	132	THR	N-CA-C	8.52	121.79	111.40
1	A	150	ILE	CA-C-N	8.49	137.75	121.54
1	A	150	ILE	C-N-CA	8.49	137.75	121.54
1	C	156	GLN	N-CA-C	-8.49	103.78	114.56
1	A	89	LYS	CA-C-N	-8.46	110.66	122.93
1	A	89	LYS	C-N-CA	-8.46	110.66	122.93
1	C	123	GLU	N-CA-C	8.45	123.32	112.34
2	B	76	SER	CB-CA-C	8.43	127.20	110.42
3	F	850	ALA	CA-C-O	-8.39	110.80	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	THR	N-CA-C	8.39	122.80	112.23
2	D	44	GLY	N-CA-C	8.38	133.04	113.18
1	C	27(F)	ARG	O-C-N	8.37	130.74	122.03
1	A	148	TRP	N-CA-C	8.33	122.47	109.07
1	A	157	ASN	CA-CB-CG	8.31	120.91	112.60
1	C	47	LEU	N-CA-C	-8.30	102.10	112.72
1	A	78	VAL	CB-CA-C	8.26	123.22	111.08
3	E	828	ILE	O-C-N	-8.26	114.16	122.99
1	A	63	THR	CA-CB-CG2	-8.20	96.56	110.50
3	F	844	GLU	N-CA-C	-8.19	101.94	111.03
2	D	184	PRO	CA-N-CD	-8.17	100.56	112.00
1	A	111	ALA	N-CA-C	8.16	121.80	108.99
1	A	104	LEU	CB-CA-C	-8.16	96.97	110.19
3	F	823	ILE	O-C-N	-8.10	114.04	123.03
2	B	118	PRO	CA-C-O	8.09	132.29	120.56
2	D	81	GLN	CB-CA-C	-8.08	94.83	109.38
1	A	140	TYR	CA-C-N	-8.07	111.69	119.76
1	A	140	TYR	C-N-CA	-8.07	111.69	119.76
2	B	82(A)	ASN	CA-C-O	8.05	130.04	121.19
1	A	83	GLN	N-CA-CB	8.04	124.08	110.49
2	D	116	THR	CA-C-O	8.04	128.99	120.95
2	D	153	THR	CA-C-O	8.03	130.90	121.58
1	C	59	PRO	CA-C-O	-8.02	112.65	121.23
3	E	840	LYS	CB-CG-CD	-7.98	92.94	111.30
2	D	56	GLU	N-CA-C	7.98	127.44	109.81
2	B	138	LEU	CA-C-N	7.96	129.55	121.35
2	B	138	LEU	C-N-CA	7.96	129.55	121.35
3	F	824	LYS	CA-C-N	-7.91	113.38	123.19
3	F	824	LYS	C-N-CA	-7.91	113.38	123.19
3	E	880	ALA	N-CA-C	-7.90	103.66	113.38
3	F	822	THR	O-C-N	-7.89	113.18	123.28
1	A	177	SER	N-CA-C	7.87	121.74	109.07
2	D	118	PRO	N-CD-CG	-7.87	91.39	103.20
1	A	156	GLN	OE1-CD-NE2	-7.84	114.76	122.60
2	B	60	ALA	N-CA-C	-7.81	96.95	109.76
2	B	161	SER	N-CA-C	7.80	121.89	112.38
3	E	853	TYR	N-CA-C	-7.77	102.50	110.97
2	B	3	GLN	N-CA-C	7.75	119.92	108.60
2	B	125	ALA	CB-CA-C	7.75	120.88	108.87
1	A	156	GLN	CG-CD-NE2	-7.73	104.80	116.40
2	D	188	TRP	N-CA-CB	7.72	120.31	110.04
2	B	66	ARG	N-CA-C	7.68	127.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	150	VAL	N-CA-C	7.66	119.87	108.46
2	B	148	GLU	CA-C-N	7.66	128.26	120.14
2	B	148	GLU	C-N-CA	7.66	128.26	120.14
2	B	92	CYS	CA-CB-SG	7.65	132.00	114.40
2	B	125	ALA	CA-C-O	7.65	129.10	120.46
2	B	120	SER	CA-C-N	-7.64	112.51	123.06
2	B	120	SER	C-N-CA	-7.64	112.51	123.06
1	A	131	SER	CB-CA-C	7.63	123.49	109.46
1	C	132	VAL	CB-CA-C	-7.62	99.26	110.62
1	A	157	ASN	N-CA-CB	7.57	121.43	110.37
1	A	112	ALA	CA-C-O	-7.57	112.85	120.64
2	B	152	VAL	N-CA-C	7.53	118.96	108.12
1	A	64	GLY	N-CA-C	7.50	122.74	111.18
2	B	62	ASP	CA-C-O	7.47	128.57	120.20
3	F	819	GLU	CB-CG-CD	7.45	125.27	112.60
2	B	73	THR	N-CA-C	7.44	120.33	111.33
2	D	105	ALA	N-CA-C	-7.42	104.25	113.38
2	B	209	LYS	CA-C-N	-7.39	113.51	123.12
2	B	209	LYS	C-N-CA	-7.39	113.51	123.12
1	A	151	ASP	N-CA-C	7.38	126.53	110.80
1	A	77	SER	CA-C-N	-7.38	110.10	120.35
1	A	77	SER	C-N-CA	-7.38	110.10	120.35
2	B	123	PRO	CA-C-N	-7.38	112.39	122.86
2	B	123	PRO	C-N-CA	-7.38	112.39	122.86
1	A	100	ALA	N-CA-C	-7.36	104.19	113.02
2	B	139	GLY	O-C-N	-7.35	116.73	123.57
2	B	201	ALA	CA-C-N	7.33	135.65	122.38
2	B	201	ALA	C-N-CA	7.33	135.65	122.38
3	E	820	GLU	N-CA-CB	7.30	120.85	110.12
1	C	93	ILE	CA-C-O	7.29	129.72	119.95
2	D	33	SER	CA-C-O	-7.28	113.00	120.71
3	F	824	LYS	O-C-N	-7.27	114.77	123.13
2	B	211	VAL	CA-C-O	-7.25	114.48	119.19
1	A	109	ALA	O-C-N	-7.24	113.96	122.87
3	F	866	TRP	N-CA-C	7.22	119.44	109.54
1	C	141	PRO	CB-CG-CD	-7.22	88.80	105.40
2	D	94	ARG	NE-CZ-NH2	-7.22	112.71	119.20
1	A	130	ALA	CA-C-N	-7.21	109.41	121.39
1	A	130	ALA	C-N-CA	-7.21	109.41	121.39
1	C	176	SER	CB-CA-C	-7.20	97.27	109.72
1	A	76	SER	CA-C-N	-7.19	110.34	122.92
1	A	76	SER	C-N-CA	-7.19	110.34	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	148	GLU	N-CA-CB	7.18	123.16	110.37
2	B	169	VAL	CB-CA-C	-7.18	102.23	110.41
3	F	876	ASN	CA-C-N	-7.18	110.93	120.91
3	F	876	ASN	C-N-CA	-7.18	110.93	120.91
2	B	102	VAL	O-C-N	7.18	130.64	123.18
3	E	840	LYS	N-CA-CB	-7.18	98.66	109.71
2	D	134	SER	CA-C-N	7.17	135.24	121.54
2	D	134	SER	C-N-CA	7.17	135.24	121.54
1	A	138	ASN	N-CA-C	7.16	121.40	111.74
2	D	184	PRO	CB-CA-C	7.14	120.67	111.46
2	B	42	GLY	N-CA-C	-7.13	106.59	115.08
1	A	147	LYS	CA-C-O	7.13	128.73	120.89
3	F	865	THR	CA-C-N	-7.13	112.61	122.87
3	F	865	THR	C-N-CA	-7.13	112.61	122.87
3	F	851	TYR	N-CA-CB	7.12	120.87	110.47
2	D	105	ALA	CA-C-N	-7.12	107.46	121.41
2	D	105	ALA	C-N-CA	-7.12	107.46	121.41
1	C	189	HIS	O-C-N	-7.10	116.19	123.29
2	D	74	SER	CA-C-O	-7.04	113.36	120.90
2	D	86	ASP	N-CA-C	7.04	121.50	112.34
2	D	122	TYR	CA-C-N	7.04	127.59	119.99
2	D	122	TYR	C-N-CA	7.04	127.59	119.99
1	A	175	MET	CA-C-N	-7.04	112.39	122.94
1	A	175	MET	C-N-CA	-7.04	112.39	122.94
1	C	188	ARG	CA-CB-CG	7.04	128.17	114.10
1	A	148	TRP	CA-C-O	7.01	128.03	120.38
1	C	130	ALA	N-CA-C	7.01	119.90	108.26
1	A	4	MET	CG-SD-CE	7.00	116.31	100.90
1	C	161	ASN	CA-C-O	-6.99	113.15	121.60
1	C	27(D)	ASN	N-CA-C	6.98	120.28	108.90
2	B	120	SER	N-CA-C	-6.96	98.06	108.99
2	D	121	VAL	N-CA-C	6.96	117.91	108.17
2	B	170	LEU	N-CA-C	-6.94	101.37	110.53
1	C	5	SER	CA-C-N	-6.94	111.92	122.81
1	C	5	SER	C-N-CA	-6.94	111.92	122.81
2	B	78	ALA	CA-C-N	-6.93	111.17	122.82
2	B	78	ALA	C-N-CA	-6.93	111.17	122.82
2	B	183	VAL	CA-C-N	-6.93	112.64	119.78
2	B	183	VAL	C-N-CA	-6.93	112.64	119.78
1	A	72	THR	N-CA-C	6.93	119.70	109.24
1	C	5	SER	N-CA-C	6.93	120.02	108.73
1	C	63	THR	CA-C-N	-6.92	117.40	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	THR	C-N-CA	-6.92	117.40	122.18
1	A	155	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	A	200	THR	CA-CB-CG2	6.90	122.23	110.50
1	A	90	GLN	O-C-N	6.89	131.96	123.21
2	D	188	TRP	CB-CA-C	6.88	124.48	110.31
1	A	188	ARG	CA-C-N	-6.86	110.58	123.27
1	A	188	ARG	C-N-CA	-6.86	110.58	123.27
1	A	159	VAL	CA-CB-CG2	6.85	122.04	110.40
2	D	71	LEU	N-CA-C	6.85	119.17	108.96
1	A	162	SER	CA-CB-OG	6.84	124.78	111.10
2	B	81	GLN	CA-C-N	-6.84	113.81	123.11
2	B	81	GLN	C-N-CA	-6.84	113.81	123.11
2	B	105	ALA	N-CA-C	6.83	121.20	113.01
2	B	188	TRP	CA-C-N	-6.83	111.31	119.84
2	B	188	TRP	C-N-CA	-6.83	111.31	119.84
2	B	118	PRO	N-CA-C	6.82	119.02	110.70
1	A	132	VAL	CB-CA-C	-6.81	100.33	110.82
2	B	4	LEU	CA-C-N	-6.81	114.75	123.19
2	B	4	LEU	C-N-CA	-6.81	114.75	123.19
2	B	189	PRO	CA-C-N	6.78	134.49	121.54
2	B	189	PRO	C-N-CA	6.78	134.49	121.54
1	A	159	VAL	N-CA-CB	6.73	122.34	111.23
3	E	864	TYR	N-CA-C	6.70	118.69	109.18
1	A	81	GLU	CB-CG-CD	6.67	123.94	112.60
2	D	123	PRO	CB-CA-C	-6.67	101.44	110.85
1	C	189	HIS	CA-C-N	-6.67	108.80	121.54
1	C	189	HIS	C-N-CA	-6.67	108.80	121.54
2	B	117	THR	CA-C-N	-6.65	113.53	120.38
2	B	117	THR	C-N-CA	-6.65	113.53	120.38
3	F	821	VAL	CA-CB-CG1	6.65	121.70	110.40
2	B	67	PHE	CA-C-N	-6.64	111.65	122.81
2	B	67	PHE	C-N-CA	-6.64	111.65	122.81
2	B	15	GLY	N-CA-C	6.62	124.01	114.67
2	B	121	VAL	CA-C-N	-6.62	106.34	122.36
2	B	121	VAL	C-N-CA	-6.62	106.34	122.36
1	C	39	LYS	CA-C-O	6.62	127.48	120.66
1	C	175	MET	O-C-N	-6.62	115.20	123.27
2	B	184	PRO	CB-CA-C	6.61	119.69	111.23
2	B	128	SER	CA-C-O	6.60	129.17	120.98
1	A	109	ALA	CB-CA-C	6.60	120.68	109.72
1	A	77	SER	N-CA-CB	-6.60	100.89	111.58
2	B	163	VAL	CB-CA-C	-6.59	100.48	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ALA	N-CA-C	-6.59	100.62	110.24
1	A	99	GLY	CA-C-O	-6.58	113.49	122.31
2	D	132	THR	N-CA-CB	6.58	119.87	110.13
2	B	27	TYR	N-CA-C	6.58	119.42	109.23
2	D	116	THR	O-C-N	-6.58	115.75	123.11
2	B	12	LYS	N-CA-C	6.55	120.30	110.14
1	C	108	ARG	CA-C-N	6.55	130.13	120.90
1	C	108	ARG	C-N-CA	6.55	130.13	120.90
1	A	195	GLU	N-CA-C	6.53	119.65	108.02
2	D	183	VAL	C-N-CD	6.53	151.78	125.00
1	C	71	PHE	N-CA-C	6.53	119.82	109.50
1	C	193	THR	N-CA-CB	-6.53	100.33	111.69
1	C	182	THR	N-CA-C	-6.53	100.86	110.52
2	B	46	ASN	CB-CG-ND2	6.51	126.16	116.40
1	C	102	THR	CA-C-O	-6.50	111.48	120.52
1	C	65	ARG	N-CA-C	-6.50	99.45	109.52
3	E	842	THR	OG1-CB-CG2	-6.48	96.34	109.30
2	B	157	GLY	N-CA-C	6.47	121.36	113.79
1	C	94	PRO	CB-CA-C	-6.47	105.30	111.39
2	B	124	LEU	CB-CG-CD1	-6.47	91.30	110.70
2	B	55	GLY	CA-C-O	6.46	126.19	119.02
2	B	201	ALA	O-C-N	6.46	128.97	122.12
2	D	184	PRO	N-CA-CB	6.46	109.06	103.31
2	D	140	CYS	CA-CB-SG	-6.46	99.55	114.40
2	B	129	ALA	CA-C-N	-6.45	112.11	122.24
2	B	129	ALA	C-N-CA	-6.45	112.11	122.24
2	D	116	THR	N-CA-C	6.45	119.84	110.42
2	B	136	VAL	O-C-N	6.42	129.97	123.10
2	B	178	SER	CA-C-N	-6.42	112.52	122.59
2	B	178	SER	C-N-CA	-6.42	112.52	122.59
2	B	14	PRO	N-CA-CB	-6.41	97.42	103.19
2	D	156	SER	N-CA-C	6.40	124.44	110.80
2	D	196	ASN	CA-C-O	6.39	127.23	120.33
1	A	5	SER	CA-C-N	-6.38	113.37	122.94
1	A	5	SER	C-N-CA	-6.38	113.37	122.94
1	C	18	LYS	O-C-N	-6.38	115.73	123.19
1	A	25	SER	N-CA-C	6.37	119.89	109.76
1	C	78	VAL	CG1-CB-CG2	-6.37	96.78	110.80
1	A	50	TRP	N-CA-C	-6.37	103.14	111.74
1	A	3	VAL	CB-CA-C	-6.36	101.36	110.83
1	C	42	GLN	N-CA-C	6.36	119.49	110.14
3	F	868	LEU	N-CA-C	-6.34	98.56	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	849	GLU	N-CA-C	-6.33	103.67	111.40
2	B	211	VAL	O-C-N	6.33	127.37	121.61
2	B	70	SER	CB-CA-C	-6.32	103.19	113.37
2	B	164	HIS	N-CA-CB	6.32	121.17	110.49
1	C	119	PRO	N-CD-CG	-6.31	93.74	103.20
2	B	9	PRO	N-CA-CB	6.30	108.94	103.27
2	B	82(A)	ASN	N-CA-C	6.30	119.37	110.23
2	B	97	LEU	N-CA-C	6.29	118.66	111.11
1	A	21	MET	CA-C-N	-6.29	112.94	122.81
1	A	21	MET	C-N-CA	-6.29	112.94	122.81
2	D	49	GLY	N-CA-C	6.29	119.78	110.60
1	A	181	LEU	CA-C-N	6.28	132.62	121.75
1	A	181	LEU	C-N-CA	6.28	132.62	121.75
2	D	39	GLN	CA-C-O	6.28	128.68	120.21
1	A	144	ILE	O-C-N	-6.27	114.73	122.57
2	B	9	PRO	CB-CA-C	-6.27	103.74	111.64
2	D	163	VAL	CA-C-N	-6.26	113.37	122.44
2	D	163	VAL	C-N-CA	-6.26	113.37	122.44
2	B	73	THR	OG1-CB-CG2	-6.24	96.81	109.30
1	A	205	ILE	N-CA-C	6.23	117.07	108.84
1	A	207	LYS	N-CA-C	-6.23	97.41	108.13
2	D	90	TYR	CA-C-O	6.23	127.17	120.32
2	B	43	LYS	CA-C-N	6.21	127.96	122.43
2	B	43	LYS	C-N-CA	6.21	127.96	122.43
3	F	872	GLY	N-CA-C	6.21	123.93	115.30
3	E	825	VAL	CB-CA-C	-6.19	101.30	110.33
2	B	93	ALA	N-CA-C	6.18	119.61	108.48
2	B	117	THR	CA-CB-CG2	6.18	121.01	110.50
2	D	36	TRP	N-CA-CB	6.18	120.84	110.77
2	D	163	VAL	O-C-N	-6.18	116.56	122.98
1	A	82	ASP	N-CA-C	-6.17	104.92	112.88
1	A	200	THR	CB-CA-C	6.17	121.77	110.36
1	A	152	GLY	O-C-N	6.16	130.70	122.70
3	E	831	ASP	N-CA-C	-6.16	104.83	113.20
2	B	160	SER	CA-C-N	6.13	130.41	120.60
2	B	160	SER	C-N-CA	6.13	130.41	120.60
1	A	139	PHE	CA-C-O	-6.12	113.70	120.38
2	B	13	LYS	CA-C-O	6.12	128.06	120.54
2	D	134	SER	N-CA-C	6.12	123.83	110.80
1	A	110	ASP	N-CA-C	-6.11	102.43	110.43
1	A	174	SER	CA-C-O	-6.09	113.93	120.75
2	B	78	ALA	CA-C-O	-6.08	114.29	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	ASP	CA-C-O	-6.07	115.07	121.99
1	A	119	PRO	CA-C-N	-6.07	112.25	119.84
1	A	119	PRO	C-N-CA	-6.07	112.25	119.84
2	B	96	LEU	CA-C-N	6.06	128.72	120.54
2	B	96	LEU	C-N-CA	6.06	128.72	120.54
2	D	150	VAL	CB-CA-C	-6.06	101.17	110.50
1	C	11	LEU	CB-CA-C	-6.05	99.36	110.62
2	D	23	LYS	CA-CB-CG	6.04	126.19	114.10
1	C	208	SER	O-C-N	6.04	129.88	123.42
2	B	15	GLY	CA-C-O	6.04	126.29	119.59
1	C	125	LEU	N-CA-C	-6.03	104.62	111.07
2	D	59	TYR	N-CA-C	6.03	118.33	110.43
2	B	169	VAL	CA-C-O	-6.02	114.86	120.22
2	B	177	LEU	N-CA-C	6.02	119.47	109.96
1	A	178	THR	CA-C-O	6.01	128.59	120.47
2	B	169	VAL	N-CA-C	6.01	117.57	107.18
3	F	861	ASN	O-C-N	-6.00	115.95	123.27
1	C	61	ARG	CD-NE-CZ	-5.99	116.01	124.40
2	D	133	ASN	CA-C-O	5.98	126.74	119.38
2	B	33	SER	N-CA-CB	-5.98	101.19	110.46
1	A	102	THR	CB-CA-C	-5.97	101.22	110.78
2	B	29	PHE	CA-C-O	5.97	126.88	120.55
1	A	56	SER	CA-C-N	5.97	131.69	122.20
1	A	56	SER	C-N-CA	5.97	131.69	122.20
1	A	176	SER	N-CA-C	-5.97	99.67	109.40
2	B	19	LYS	CB-CA-C	-5.96	100.60	110.14
3	F	819	GLU	OE1-CD-OE2	-5.96	108.59	122.90
3	F	872	GLY	CA-C-N	5.96	132.00	122.83
3	F	872	GLY	C-N-CA	5.96	132.00	122.83
1	C	22	SER	N-CA-C	5.96	118.75	109.52
1	A	200	THR	N-CA-C	5.95	120.23	113.15
1	A	27(C)	LEU	CD1-CG-CD2	-5.95	97.71	110.80
1	A	203	SER	N-CA-C	-5.95	102.28	109.72
2	D	9	PRO	CB-CA-C	5.95	118.07	111.11
2	B	66	ARG	CG-CD-NE	-5.95	98.92	112.00
1	C	30	LYS	CA-C-N	-5.94	112.63	120.95
1	C	30	LYS	C-N-CA	-5.94	112.63	120.95
3	E	876	ASN	N-CA-C	-5.94	99.72	109.40
1	A	103	LYS	N-CA-C	5.93	118.31	109.59
1	A	185	GLU	CB-CA-C	-5.93	100.64	110.37
1	C	166	GLN	CA-C-N	5.93	130.15	121.31
1	C	166	GLN	C-N-CA	5.93	130.15	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	864	TYR	N-CA-CB	-5.92	101.77	111.66
3	E	826	ASN	N-CA-C	5.92	117.95	108.41
1	A	66	GLY	CA-C-O	-5.92	117.31	122.16
1	A	18	LYS	CB-CG-CD	5.92	124.91	111.30
3	E	865	THR	CA-C-O	-5.91	115.10	121.36
2	B	89	THR	CA-C-N	5.90	131.15	123.00
2	B	89	THR	C-N-CA	5.90	131.15	123.00
2	D	196	ASN	CB-CA-C	-5.90	101.72	110.62
1	C	82	ASP	CA-C-O	5.89	126.65	119.11
2	B	148	GLU	CA-C-O	-5.89	112.09	120.16
2	D	83	LYS	O-C-N	-5.88	115.51	123.10
2	B	130	ALA	O-C-N	-5.88	115.87	122.34
3	F	864	TYR	N-CA-C	5.88	118.00	109.07
2	B	183	VAL	N-CA-CB	-5.88	106.14	112.37
2	B	86	ASP	N-CA-C	5.87	120.17	113.19
1	C	194	CYS	CA-C-N	-5.87	114.71	122.99
1	C	194	CYS	C-N-CA	-5.87	114.71	122.99
2	D	113	SER	N-CA-C	5.86	119.69	112.54
1	C	112	ALA	CB-CA-C	-5.85	99.86	109.46
1	A	189	HIS	CA-C-N	5.85	132.72	121.54
1	A	189	HIS	C-N-CA	5.85	132.72	121.54
2	B	205	LYS	CA-C-N	-5.85	112.97	122.33
2	B	205	LYS	C-N-CA	-5.85	112.97	122.33
1	A	115	VAL	N-CA-C	5.85	118.17	109.17
2	D	3	GLN	CA-C-N	5.84	130.59	121.76
2	D	3	GLN	C-N-CA	5.84	130.59	121.76
2	B	19	LYS	CA-C-O	-5.84	114.05	120.24
1	A	90	GLN	CA-C-O	-5.84	114.52	120.71
2	B	101	ASP	CA-CB-CG	5.83	118.43	112.60
2	B	30	THR	CA-CB-OG1	-5.80	100.90	109.60
2	B	66	ARG	N-CA-CB	-5.80	100.69	110.49
1	A	91	ALA	N-CA-C	5.80	119.59	111.30
1	C	84	ALA	CB-CA-C	-5.79	98.89	110.42
2	B	149	PRO	N-CA-C	5.79	121.35	111.68
2	D	122	TYR	N-CA-C	-5.79	100.14	109.40
1	A	2	ILE	O-C-N	-5.79	116.00	122.66
2	D	191	GLU	O-C-N	5.79	130.28	122.59
2	D	8	GLY	N-CA-C	5.78	118.94	112.00
2	D	121	VAL	CB-CA-C	-5.78	102.22	110.83
3	E	826	ASN	O-C-N	-5.77	116.00	122.93
1	A	92	TYR	CA-C-O	-5.77	114.38	120.55
2	B	48	MET	O-C-N	-5.77	113.48	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	SER	N-CA-C	-5.76	103.44	111.39
1	A	203	SER	CA-C-N	-5.75	113.85	119.78
1	A	203	SER	C-N-CA	-5.75	113.85	119.78
2	B	23	LYS	N-CA-C	5.75	118.03	108.20
3	E	833	LYS	CA-C-O	-5.75	115.23	121.44
2	B	203	SER	CA-C-N	-5.74	115.07	123.00
2	B	203	SER	C-N-CA	-5.74	115.07	123.00
3	E	862	GLY	CA-C-N	5.74	130.93	121.39
3	E	862	GLY	C-N-CA	5.74	130.93	121.39
2	B	106	GLY	CA-C-O	-5.74	110.59	120.57
3	E	839	PHE	N-CA-C	5.74	118.25	108.90
2	D	18	VAL	CG1-CB-CG2	5.74	123.42	110.80
1	A	29	ARG	N-CA-C	5.73	119.57	112.58
2	D	88	ALA	N-CA-C	5.73	116.12	108.38
2	D	148	GLU	CA-C-N	-5.73	112.68	119.84
2	D	148	GLU	C-N-CA	-5.73	112.68	119.84
2	D	190	SER	CA-C-N	5.72	132.47	121.54
2	D	190	SER	C-N-CA	5.72	132.47	121.54
2	B	125	ALA	N-CA-C	5.72	118.91	109.58
2	B	13	LYS	N-CA-C	-5.72	102.22	110.40
3	E	835	GLN	N-CA-C	-5.71	101.07	109.81
2	D	3	GLN	N-CA-C	5.71	116.09	108.38
3	F	866	TRP	CA-CB-CG	5.71	124.45	113.60
2	B	206	VAL	CA-C-O	-5.69	114.55	120.64
2	B	71	LEU	CA-C-O	5.69	127.54	121.45
2	B	163	VAL	CA-C-N	5.68	132.40	121.54
2	B	163	VAL	C-N-CA	5.68	132.40	121.54
2	D	57	PRO	N-CA-C	5.67	120.13	111.11
2	B	23	LYS	CB-CA-C	-5.67	101.71	110.78
3	F	857	LEU	N-CA-CB	5.66	118.22	110.01
1	A	77	SER	N-CA-C	5.66	119.60	107.67
1	A	84	ALA	N-CA-CB	-5.65	102.71	111.35
3	E	826	ASN	CB-CG-ND2	5.65	124.88	116.40
1	A	53	THR	OG1-CB-CG2	-5.65	98.00	109.30
1	C	43	SER	N-CA-CB	-5.65	102.18	110.14
1	C	178	THR	CB-CA-C	-5.65	100.93	110.19
2	D	182	THR	CA-CB-OG1	5.65	118.07	109.60
1	A	200	THR	O-C-N	-5.65	113.33	122.42
2	D	19	LYS	CA-CB-CG	-5.64	102.81	114.10
2	D	183	VAL	CA-C-O	5.64	127.51	119.95
1	C	30	LYS	CG-CD-CE	5.64	124.27	111.30
1	A	153	SER	CA-C-N	5.64	132.31	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	SER	C-N-CA	5.64	132.31	121.54
1	A	171	SER	CA-C-N	-5.63	110.79	121.54
1	A	171	SER	C-N-CA	-5.63	110.79	121.54
3	F	845	GLU	CA-C-O	5.63	127.26	121.07
2	B	97	LEU	CB-CA-C	-5.61	101.83	110.81
3	E	838	GLU	N-CA-C	5.61	118.87	109.95
1	C	72	THR	CA-C-N	-5.61	115.27	123.00
1	C	72	THR	C-N-CA	-5.61	115.27	123.00
2	D	175	TYR	CA-CB-CG	5.60	123.98	113.90
1	C	73	LEU	O-C-N	-5.59	116.69	123.29
1	C	116	SER	CA-CB-OG	-5.59	99.91	111.10
2	B	30	THR	CA-CB-CG2	5.59	120.00	110.50
2	B	94	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	A	204	PRO	CA-C-N	5.58	129.55	121.18
1	A	204	PRO	C-N-CA	5.58	129.55	121.18
2	B	71	LEU	N-CA-C	5.58	117.28	108.96
1	C	63	THR	CB-CA-C	-5.58	98.63	109.68
2	B	121	VAL	CA-CB-CG1	5.57	119.87	110.40
2	B	122	TYR	CA-C-N	-5.56	115.02	120.52
2	B	122	TYR	C-N-CA	-5.56	115.02	120.52
3	E	846	ALA	N-CA-C	5.56	117.03	110.97
1	C	127	SER	CB-CA-C	5.56	119.56	110.17
1	C	45	LYS	O-C-N	-5.55	116.61	123.44
2	B	104	GLY	N-CA-C	-5.55	104.02	112.51
1	C	10	SER	CA-CB-OG	-5.54	100.02	111.10
1	C	164	THR	CA-C-O	-5.54	114.90	121.66
1	C	195	GLU	N-CA-C	5.54	117.93	108.90
2	D	204	THR	CB-CA-C	-5.54	102.64	111.17
2	B	118	PRO	CA-C-N	-5.53	112.93	119.84
2	B	118	PRO	C-N-CA	-5.53	112.93	119.84
2	B	124	LEU	CB-CG-CD2	5.53	127.29	110.70
1	A	175	MET	CB-CA-C	-5.53	97.91	110.07
3	E	873	ASN	O-C-N	5.53	128.97	122.34
2	B	187	THR	N-CA-C	5.52	121.89	113.61
1	C	39	LYS	CA-C-N	-5.52	114.03	119.93
1	C	39	LYS	C-N-CA	-5.52	114.03	119.93
2	D	200	PRO	CA-C-N	-5.52	110.25	121.18
2	D	200	PRO	C-N-CA	-5.52	110.25	121.18
2	B	132	THR	CA-CB-CG2	5.51	119.87	110.50
2	B	177	LEU	N-CA-CB	5.51	119.62	110.14
2	D	142	VAL	CA-C-N	-5.51	114.68	122.94
2	D	142	VAL	C-N-CA	-5.51	114.68	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	GLY	O-C-N	5.51	129.86	122.70
2	D	53	GLU	N-CA-C	5.50	119.49	112.34
2	D	158	SER	CA-C-O	5.49	127.07	120.92
1	A	17	GLU	N-CA-C	5.49	118.24	110.50
2	B	124	LEU	CA-C-N	-5.49	109.35	122.74
2	B	124	LEU	C-N-CA	-5.49	109.35	122.74
2	B	99	GLN	CB-CG-CD	5.48	121.92	112.60
1	A	201	SER	O-C-N	-5.48	116.70	123.44
1	C	54	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	32	TYR	O-C-N	5.48	128.74	122.55
2	B	122	TYR	CB-CA-C	5.47	117.91	109.15
2	D	153	THR	CA-C-N	-5.47	115.28	123.00
2	D	153	THR	C-N-CA	-5.47	115.28	123.00
1	A	108	ARG	O-C-N	5.47	129.32	122.92
2	B	140	CYS	N-CA-C	-5.47	100.75	109.23
1	A	107	LYS	N-CA-C	-5.47	101.37	110.17
1	C	113	PRO	N-CD-CG	-5.46	95.00	103.20
1	A	54	ARG	N-CA-C	-5.46	100.81	109.76
2	B	156	SER	CA-C-O	-5.46	113.94	119.78
2	D	118	PRO	N-CA-C	5.45	117.35	110.70
2	D	184	PRO	CA-C-N	5.45	129.82	120.72
2	D	184	PRO	C-N-CA	5.45	129.82	120.72
3	F	822	THR	CA-C-O	5.45	126.85	120.20
1	A	116	SER	O-C-N	5.45	129.84	122.59
1	A	141	PRO	N-CA-C	-5.44	102.64	111.19
1	A	157	ASN	CA-C-N	-5.44	113.24	121.51
1	A	157	ASN	C-N-CA	-5.44	113.24	121.51
2	D	131	GLN	OE1-CD-NE2	-5.44	117.16	122.60
2	B	158	SER	CA-C-O	-5.43	115.09	120.90
1	C	62	PHE	N-CA-C	-5.43	100.85	109.59
1	A	130	ALA	N-CA-C	5.42	119.08	108.18
2	D	15	GLY	N-CA-C	5.42	126.03	113.18
2	D	82(C)	LEU	N-CA-C	5.42	117.89	110.24
2	D	152	VAL	CA-C-N	-5.42	113.71	122.82
2	D	152	VAL	C-N-CA	-5.42	113.71	122.82
2	B	110	THR	CA-C-N	5.42	128.45	122.22
2	B	110	THR	C-N-CA	5.42	128.45	122.22
1	C	187	GLU	CB-CA-C	5.42	120.65	110.63
2	D	50	TRP	N-CA-C	5.42	116.50	108.86
1	A	70	ASP	CA-C-N	-5.41	114.09	122.59
1	A	70	ASP	C-N-CA	-5.41	114.09	122.59
2	D	131	GLN	CB-CG-CD	5.41	121.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	16	GLU	O-C-N	5.41	129.61	122.36
1	C	124	GLN	CA-C-N	5.41	127.47	120.44
1	C	124	GLN	C-N-CA	5.41	127.47	120.44
1	A	58	VAL	CA-C-N	5.40	125.32	119.76
1	A	58	VAL	C-N-CA	5.40	125.32	119.76
1	C	186	TYR	N-CA-C	-5.39	105.04	111.03
1	A	97	THR	N-CA-C	5.39	118.24	109.24
2	B	33	SER	CA-C-O	-5.39	115.05	121.89
2	D	202	SER	N-CA-CB	-5.38	102.10	110.98
1	A	28	THR	N-CA-CB	-5.38	102.02	110.30
2	B	83	LYS	CA-CB-CG	5.38	124.86	114.10
2	D	100(A)	PHE	N-CA-CB	-5.37	101.62	109.95
2	D	190	SER	N-CA-C	5.37	118.17	111.24
2	B	95	PHE	CA-C-O	5.37	126.40	120.71
1	A	164	THR	CA-C-O	-5.36	115.08	121.56
3	F	839	PHE	CA-C-O	-5.35	114.58	120.36
2	B	158	SER	CA-CB-OG	5.35	121.79	111.10
2	D	205	LYS	CG-CD-CE	5.34	123.58	111.30
2	D	212	PRO	CB-CA-C	5.34	120.37	111.56
2	B	173	ASP	CA-C-N	5.33	131.38	121.62
2	B	173	ASP	C-N-CA	5.33	131.38	121.62
2	D	156	SER	N-CA-CB	-5.33	101.47	110.49
1	C	27(E)	SER	O-C-N	5.33	131.23	122.70
1	A	7	SER	CB-CA-C	-5.33	101.21	109.20
3	E	844	GLU	CA-C-O	-5.33	113.50	120.00
1	C	27(F)	ARG	CA-C-O	-5.33	115.41	121.00
3	F	877	ILE	N-CA-C	5.33	116.45	109.58
2	D	195	CYS	O-C-N	5.31	129.03	123.03
2	D	13	LYS	N-CA-C	5.31	117.41	110.08
1	C	110	ASP	N-CA-C	-5.30	103.89	110.41
1	A	175	MET	CA-C-O	-5.29	115.43	121.40
2	B	131	GLN	CA-C-N	5.28	130.22	122.77
2	B	131	GLN	C-N-CA	5.28	130.22	122.77
1	C	118	PHE	CB-CA-C	-5.28	101.26	109.55
2	D	40	ALA	CB-CA-C	5.28	117.76	109.37
1	A	211	ARG	N-CA-CB	-5.28	102.82	110.47
2	B	182	THR	CA-CB-CG2	5.27	119.46	110.50
1	C	60	ASP	CB-CG-OD1	-5.27	106.27	118.40
2	D	156	SER	CA-CB-OG	-5.27	100.56	111.10
2	B	166	PHE	CA-C-N	-5.27	114.33	119.76
2	B	166	PHE	C-N-CA	-5.27	114.33	119.76
2	D	40	ALA	N-CA-CB	-5.27	103.63	109.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	166	PHE	N-CA-CB	5.27	116.41	110.03
2	B	109	VAL	N-CA-CB	5.27	117.50	111.39
2	D	92	CYS	N-CA-C	5.27	118.69	110.32
2	B	110	THR	OG1-CB-CG2	-5.26	98.78	109.30
3	F	839	PHE	N-CA-C	5.26	117.47	108.90
1	C	17	GLU	CA-C-N	-5.25	114.82	122.65
1	C	17	GLU	C-N-CA	-5.25	114.82	122.65
2	D	177	LEU	CA-C-N	-5.25	112.67	121.75
2	D	177	LEU	C-N-CA	-5.25	112.67	121.75
2	D	192	THR	N-CA-C	5.25	117.51	107.75
2	B	76	SER	CA-C-N	5.24	130.80	122.94
2	B	76	SER	C-N-CA	5.24	130.80	122.94
3	E	840	LYS	O-C-N	5.24	129.56	122.96
2	B	36	TRP	N-CA-C	5.23	117.70	108.75
2	D	68	ALA	CA-C-N	5.23	129.64	122.84
2	D	68	ALA	C-N-CA	5.23	129.64	122.84
2	B	26	GLY	CA-C-O	5.23	124.92	119.06
2	D	79	TYR	CA-C-O	5.23	127.31	121.40
2	D	89	THR	O-C-N	-5.22	117.37	123.27
1	A	168	SER	N-CA-C	5.22	119.51	113.20
2	B	190	SER	CA-CB-OG	5.21	121.52	111.10
2	D	59	TYR	O-C-N	-5.21	116.66	122.75
1	C	167	ASP	CA-C-O	5.21	126.69	121.07
1	A	27(B)	LEU	CB-CG-CD1	5.20	126.31	110.70
1	C	29	ARG	CA-C-N	5.20	130.32	122.99
1	C	29	ARG	C-N-CA	5.20	130.32	122.99
1	A	52	SER	CB-CA-C	-5.20	100.81	109.75
1	C	201	SER	N-CA-C	-5.20	100.84	108.79
1	A	155	ARG	CD-NE-CZ	5.19	131.67	124.40
1	A	78	VAL	N-CA-C	-5.19	101.58	109.78
1	C	147	LYS	CG-CD-CE	5.18	123.23	111.30
2	D	64	LYS	N-CA-C	-5.18	100.63	108.46
1	A	55	GLU	CA-C-N	-5.18	113.35	120.71
1	A	55	GLU	C-N-CA	-5.18	113.35	120.71
1	C	69	THR	CA-CB-OG1	-5.18	101.83	109.60
2	D	89	THR	N-CA-C	5.18	117.68	109.24
1	A	183	LYS	N-CA-C	5.17	116.72	111.14
2	D	11	LEU	CA-C-O	5.17	125.92	120.54
1	A	194	CYS	CA-CB-SG	5.17	126.28	114.40
2	B	121	VAL	N-CA-C	5.16	115.92	108.48
2	B	82	ILE	N-CA-CB	-5.16	105.17	111.67
3	F	871	GLY	CA-C-O	-5.16	111.59	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	GLN	CG-CD-OE1	-5.15	110.49	120.80
1	A	61	ARG	NH1-CZ-NH2	5.15	126.00	119.30
2	D	80	LEU	CD1-CG-CD2	-5.15	99.47	110.80
1	A	43	SER	CA-CB-OG	-5.15	100.81	111.10
2	D	58	THR	CA-C-O	-5.14	113.77	122.20
3	F	847	THR	CA-C-N	-5.14	112.50	120.31
3	F	847	THR	C-N-CA	-5.14	112.50	120.31
3	F	841	GLY	O-C-N	-5.14	117.97	122.85
2	D	84	ASN	N-CA-C	-5.14	105.68	111.28
1	C	3	VAL	O-C-N	5.14	128.75	123.20
1	C	204	PRO	CA-C-O	-5.14	111.25	120.60
1	A	205	ILE	CA-C-O	5.13	127.16	120.95
1	C	127	SER	CA-C-O	5.13	125.42	119.32
3	E	827	LEU	N-CA-C	5.12	117.08	109.25
2	D	182	THR	CA-CB-CG2	5.11	119.19	110.50
3	F	871	GLY	N-CA-C	-5.11	101.07	113.18
1	C	74	THR	OG1-CB-CG2	-5.11	99.08	109.30
2	B	57	PRO	CB-CA-C	-5.11	103.13	111.56
1	A	88	CYS	CA-C-O	5.10	127.30	121.28
2	D	12	LYS	N-CA-C	5.10	117.72	109.40
1	C	60	ASP	CB-CG-OD2	5.10	130.12	118.40
2	D	66	ARG	N-CA-C	5.09	118.75	112.54
2	B	95	PHE	CA-CB-CG	5.09	118.89	113.80
2	B	18	VAL	CA-CB-CG2	-5.09	101.75	110.40
2	B	91	PHE	CA-C-N	5.08	130.30	122.93
2	B	91	PHE	C-N-CA	5.08	130.30	122.93
1	A	141	PRO	CB-CA-C	5.08	117.97	111.21
2	B	56	GLU	N-CA-CB	-5.08	99.88	109.37
2	B	210	ILE	CA-C-N	-5.08	118.37	123.04
2	B	210	ILE	C-N-CA	-5.08	118.37	123.04
1	A	174	SER	CB-CA-C	-5.07	101.82	109.99
1	A	37	GLN	N-CA-CB	-5.07	102.41	111.08
3	E	823	ILE	N-CA-CB	-5.06	105.08	111.41
1	C	8	PRO	N-CD-CG	-5.06	97.72	103.80
1	A	181	LEU	O-C-N	5.05	129.31	122.59
1	A	1	ASP	CB-CA-C	-5.05	100.50	110.10
2	D	94	ARG	CB-CG-CD	5.05	122.92	111.30
1	A	110	ASP	CA-CB-CG	5.05	117.65	112.60
3	F	869	GLU	CB-CG-CD	5.05	121.18	112.60
2	B	134	SER	CA-CB-OG	5.04	121.19	111.10
2	D	88	ALA	CA-C-N	-5.04	115.76	122.72
2	D	88	ALA	C-N-CA	-5.04	115.76	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	LEU	CA-C-N	5.04	128.63	121.42
1	A	179	LEU	C-N-CA	5.04	128.63	121.42
2	D	9	PRO	N-CD-CG	-5.04	95.64	103.20
1	C	146	VAL	O-C-N	5.03	128.86	122.57
2	B	208	LYS	N-CA-C	5.03	116.50	107.80
1	C	27	GLN	CG-CD-NE2	-5.03	108.86	116.40
1	C	111	ALA	CA-C-N	5.03	128.29	120.60
1	C	111	ALA	C-N-CA	5.03	128.29	120.60
1	C	213	GLU	CA-C-N	-5.02	112.66	121.70
1	C	213	GLU	C-N-CA	-5.02	112.66	121.70
1	A	205	ILE	CA-C-N	5.02	129.72	123.14
1	A	205	ILE	C-N-CA	5.02	129.72	123.14
1	A	27(C)	LEU	CA-C-O	5.02	126.58	120.81
1	C	55	GLU	N-CA-CB	-5.02	102.59	109.97
1	A	159	VAL	CA-CB-CG1	5.02	118.93	110.40
2	B	164	HIS	N-CA-C	-5.02	100.12	110.80
1	C	196	ALA	N-CA-C	5.01	116.77	108.20
2	D	162	GLY	CA-C-N	-5.01	115.17	122.68
2	D	162	GLY	C-N-CA	-5.01	115.17	122.68
3	F	824	LYS	N-CA-CB	-5.01	101.76	110.17
1	C	54	ARG	CD-NE-CZ	-5.00	117.39	124.40
2	D	198	ALA	N-CA-CB	-5.00	103.09	110.90
1	A	103	LYS	CA-C-O	-5.00	114.78	120.58
3	F	821	VAL	CB-CA-C	5.00	119.49	111.29

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	83	GLN	CA
2	B	177	LEU	CA
3	E	820	GLU	CA
3	E	828	ILE	CB
2	D	132	THR	CA
2	D	134	SER	CA
2	D	188	TRP	CA
3	F	818	LYS	CA

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	PRO	Mainchain
1	A	125	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	152	GLY	Peptide
1	A	156	GLN	Mainchain,Sidechain
1	A	157	ASN	Mainchain,Sidechain
1	A	158	GLY	Peptide
1	A	159	VAL	Mainchain
1	A	160	LEU	Mainchain
1	A	173	TYR	Mainchain,Sidechain
1	A	190	ASN	Peptide
1	A	198	HIS	Mainchain
1	A	2	ILE	Mainchain
1	A	200	THR	Mainchain
1	A	204	PRO	Peptide
1	A	208	SER	Peptide
1	A	76	SER	Mainchain
2	B	101	ASP	Mainchain
2	B	125	ALA	Mainchain
2	B	130	ALA	Mainchain
2	B	135	MET	Mainchain
2	B	148	GLU	Peptide,Mainchain
2	B	149	PRO	Mainchain
2	B	156	SER	Mainchain
2	B	189	PRO	Peptide
2	B	191	GLU	Mainchain
2	B	2	ILE	Mainchain
2	B	45	LEU	Mainchain
2	B	70	SER	Mainchain
2	B	9	PRO	Mainchain
1	C	21	MET	Mainchain
1	C	27(D)	ASN	Peptide
1	C	59	PRO	Mainchain
1	C	84	ALA	Mainchain
2	D	125	ALA	Mainchain
2	D	133	ASN	Sidechain
2	D	134	SER	Peptide
2	D	149	PRO	Peptide
2	D	188	TRP	Peptide,Mainchain
2	D	213	ARG	Sidechain
2	D	23	LYS	Mainchain
2	D	30	THR	Mainchain
2	D	38	ASN	Mainchain
2	D	60	ALA	Mainchain
2	D	9	PRO	Mainchain

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Mol	Chain	Res	Type	Group
2	D	91	PHE	Peptide
3	E	818	LYS	Peptide
3	E	820	GLU	Peptide
3	E	839	PHE	Mainchain
3	E	850	ALA	Mainchain
3	F	818	LYS	Peptide
3	F	820	GLU	Mainchain
3	F	831	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1657	203	1
1	C	1708	0	1658	182	0
2	B	1660	0	1615	141	0
2	D	1660	0	1615	142	1
3	E	516	0	496	38	0
3	F	516	0	496	54	0
4	A	30	0	0	4	0
4	B	31	0	0	5	0
4	C	20	0	0	2	0
4	D	26	0	0	4	0
4	E	6	0	0	1	0
4	F	3	0	0	1	0
All	All	7884	0	7537	727	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (727) 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:147:LYS:CG	1:C:147:LYS:CD	1.75	1.65
1:A:45:LYS:CD	1:A:45:LYS:CG	1.75	1.65
1:C:79:GLN:CG	1:C:79:GLN:CB	1.75	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:LYS:CD	2:B:43:LYS:CG	1.76	1.64
2:D:97:LEU:CD2	2:D:97:LEU:CG	1.75	1.62
1:C:24:LYS:CE	1:C:24:LYS:CD	1.78	1.61
1:C:160:LEU:CD2	1:C:160:LEU:CG	1.74	1.61
2:D:205:LYS:CG	2:D:205:LYS:CD	1.77	1.60
1:C:100:ALA:CB	1:C:100:ALA:CA	1.75	1.59
2:B:5:VAL:CB	2:B:5:VAL:CG1	1.75	1.59
3:E:840:LYS:CD	3:E:840:LYS:CG	1.74	1.58
1:C:106:LEU:CG	1:C:106:LEU:CD1	1.75	1.58
1:C:4:MET:CG	1:C:4:MET:CB	1.78	1.57
1:C:142:LYS:CD	1:C:142:LYS:CG	1.76	1.57
2:B:97:LEU:CD2	2:B:97:LEU:CG	1.82	1.56
3:E:824:LYS:CG	3:E:824:LYS:CB	1.78	1.56
3:E:834:ILE:CD1	3:E:834:ILE:CG1	1.82	1.56
1:A:180:THR:CG2	1:A:180:THR:CB	1.78	1.55
1:C:205:ILE:CD1	1:C:205:ILE:CG1	1.84	1.55
1:C:45:LYS:CD	1:C:45:LYS:CG	1.82	1.52
1:A:1:ASP:N	1:A:1:ASP:CA	1.69	1.51
3:E:840:LYS:CD	3:E:840:LYS:CE	1.84	1.49
1:C:103:LYS:CE	1:C:103:LYS:CD	1.89	1.48
1:A:119:PRO:CB	1:A:119:PRO:CG	1.77	1.47
2:D:212:PRO:CG	2:D:212:PRO:CB	1.77	1.47
1:C:30:LYS:CE	1:C:30:LYS:NZ	1.78	1.46
1:A:210:ASN:HB3	2:B:129:ALA:CB	1.55	1.35
2:B:97:LEU:HD22	2:B:97:LEU:H	1.03	1.19
1:C:198:HIS:HD2	1:C:200:THR:OG1	1.32	1.12
2:B:125:ALA:HB1	2:B:126:PRO:HD2	1.31	1.11
2:B:188:TRP:O	2:B:189:PRO:C	1.90	1.09
2:D:189:PRO:CB	2:D:212:PRO:HG3	1.83	1.08
1:A:210:ASN:HB3	2:B:129:ALA:HB2	1.27	1.08
2:D:189:PRO:HB2	2:D:212:PRO:HG3	1.19	1.07
2:D:138:LEU:HD23	2:D:210:ILE:HG21	1.31	1.04
1:A:156:GLN:HE21	1:A:159:VAL:HG22	1.18	1.03
2:D:138:LEU:HD23	2:D:210:ILE:CG2	1.88	1.03
3:F:830:ALA:HB2	3:F:880:ALA:HA	1.40	1.02
1:A:148:TRP:CD1	1:A:179:LEU:HG	1.96	1.00
1:A:210:ASN:CB	2:B:129:ALA:HB2	1.92	0.99
2:B:97:LEU:CD2	2:B:97:LEU:H	1.76	0.98
3:F:866:TRP:HE3	3:F:868:LEU:HD21	1.26	0.98
2:B:160:SER:O	2:B:163:VAL:HG23	1.65	0.97
2:B:46:ASN:HB3	4:B:237:HOH:O	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TRP:HD1	1:A:159:VAL:HG12	1.31	0.96
2:B:83:LYS:HG3	2:B:85:GLU:HG2	1.50	0.94
1:A:210:ASN:CB	2:B:129:ALA:CB	2.45	0.94
1:A:148:TRP:NE1	1:A:179:LEU:HB2	1.83	0.93
1:C:183:LYS:HD3	1:C:187:GLU:OE2	1.70	0.92
1:C:180:THR:O	1:C:181:LEU:HD23	1.70	0.91
3:F:866:TRP:CE3	3:F:868:LEU:HD21	2.05	0.91
1:C:135:PHE:C	1:C:136:LEU:HD12	1.95	0.91
3:E:840:LYS:CE	3:E:840:LYS:HB3	2.01	0.90
1:C:2:ILE:HD12	1:C:2:ILE:H	1.34	0.90
1:A:148:TRP:CD1	1:A:179:LEU:HB2	2.06	0.90
1:A:160:LEU:CD2	2:B:171:GLN:OE1	2.20	0.89
1:A:115:VAL:HA	1:A:135:PHE:O	1.73	0.89
2:B:97:LEU:HD22	2:B:97:LEU:N	1.88	0.89
1:C:136:LEU:HD12	1:C:136:LEU:N	1.88	0.89
3:E:831:ASP:OD2	3:E:833:LYS:HG3	1.72	0.88
2:D:89:THR:HG22	2:D:108:THR:OG1	1.72	0.88
2:B:188:TRP:HB3	2:B:189:PRO:HD2	1.55	0.88
3:F:864:TYR:CD2	3:F:877:ILE:HG23	2.10	0.87
3:F:869:GLU:HG3	3:F:870:ASP:O	1.75	0.87
3:E:840:LYS:CD	3:E:840:LYS:CB	2.51	0.87
1:C:147:LYS:NZ	1:C:156:GLN:NE2	2.23	0.87
2:B:188:TRP:O	2:B:189:PRO:O	1.91	0.86
1:A:193:THR:CG2	1:A:206:VAL:HG13	2.06	0.86
2:B:118:PRO:O	2:B:119:PRO:O	1.93	0.86
2:D:55:GLY:O	2:D:57:PRO:HD3	1.73	0.86
1:C:198:HIS:CD2	1:C:200:THR:OG1	2.24	0.85
1:A:139:PHE:CD2	1:A:139:PHE:O	2.29	0.85
2:B:125:ALA:HB1	2:B:126:PRO:CD	2.06	0.85
1:A:108:ARG:HH11	1:A:172:THR:CG2	1.90	0.85
1:A:148:TRP:CD1	1:A:179:LEU:CG	2.58	0.85
1:A:77:SER:O	1:A:78:VAL:C	2.11	0.85
1:A:118:PHE:HZ	2:B:137:THR:O	1.60	0.84
2:D:138:LEU:CD2	2:D:210:ILE:HG21	2.07	0.84
1:A:160:LEU:HD21	2:B:171:GLN:NE2	1.91	0.83
1:C:168:SER:HB3	4:C:223:HOH:O	1.78	0.83
2:D:59:TYR:HB3	2:D:63:PHE:O	1.79	0.83
2:B:150:VAL:CG2	2:B:177:LEU:HD11	2.09	0.82
1:A:148:TRP:HD1	1:A:179:LEU:HG	1.42	0.82
1:A:115:VAL:HG12	1:A:116:SER:H	1.43	0.82
1:C:106:LEU:CD1	1:C:106:LEU:CD2	2.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD21	2:B:171:GLN:CD	2.05	0.81
1:A:160:LEU:HD21	2:B:171:GLN:OE1	1.80	0.81
1:C:155:ARG:HG2	1:C:155:ARG:HH11	1.44	0.80
2:B:97:LEU:CD2	2:B:97:LEU:CB	2.60	0.80
1:C:123:GLU:HA	1:C:126:THR:OG1	1.81	0.80
1:C:27(C):LEU:HD23	1:C:27(D):ASN:N	1.97	0.79
1:A:210:ASN:HB3	2:B:129:ALA:HB3	1.61	0.79
2:D:117:THR:HG21	2:D:174:LEU:HD21	1.63	0.79
1:A:193:THR:CG2	1:A:206:VAL:CG1	2.62	0.77
3:E:824:LYS:CG	3:E:824:LYS:CA	2.62	0.77
2:B:66:ARG:HG3	4:B:244:HOH:O	1.84	0.77
1:C:148:TRP:CE3	1:C:193:THR:O	2.38	0.77
2:D:38:ASN:ND2	2:D:46:ASN:HB2	1.98	0.76
1:A:7:SER:HB2	1:A:22:SER:OG	1.85	0.76
1:A:19:VAL:HG12	1:A:75:ILE:HB	1.68	0.76
1:A:156:GLN:NE2	1:A:159:VAL:HG22	1.98	0.76
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.21	0.76
3:F:826:ASN:HB2	3:F:876:ASN:HD22	1.51	0.76
1:A:108:ARG:HH11	1:A:172:THR:HG22	1.51	0.75
1:A:115:VAL:HG12	1:A:116:SER:N	2.00	0.75
1:C:27:GLN:C	1:C:69:THR:HG22	2.12	0.75
1:A:160:LEU:HD21	2:B:171:GLN:HE22	1.48	0.75
1:C:79:GLN:HE21	1:C:79:GLN:HB2	1.51	0.75
2:D:150:VAL:HG23	2:D:150:VAL:O	1.87	0.75
2:B:82(A):ASN:O	2:B:82(B):SER:C	2.30	0.75
1:A:45:LYS:CG	1:A:45:LYS:CE	2.64	0.75
2:B:125:ALA:CB	2:B:126:PRO:HD2	2.14	0.75
1:C:27(C):LEU:O	1:C:92:TYR:CE1	2.40	0.75
1:C:79:GLN:CB	1:C:79:GLN:CD	2.60	0.74
1:C:24:LYS:CE	1:C:24:LYS:CG	2.65	0.74
1:A:148:TRP:CE3	1:A:193:THR:O	2.41	0.74
1:C:202:THR:O	1:C:204:PRO:HD3	1.88	0.74
1:A:148:TRP:HD1	1:A:159:VAL:CG1	2.01	0.74
2:B:163:VAL:HG12	2:B:164:HIS:N	2.02	0.74
2:B:124:LEU:HD12	2:B:139:GLY:HA3	1.69	0.74
1:A:148:TRP:CD1	1:A:159:VAL:HG12	2.21	0.74
1:C:145:ASN:HB2	1:C:197:THR:HB	1.68	0.74
2:D:82:ILE:HG22	2:D:82(C):LEU:HD23	1.68	0.74
1:C:45:LYS:CD	1:C:45:LYS:CB	2.62	0.74
1:A:148:TRP:CD1	1:A:179:LEU:CB	2.71	0.74
1:C:117:ILE:HG12	1:C:118:PHE:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ALA:CB	1:C:100:ALA:C	2.60	0.73
2:B:5:VAL:CG1	2:B:5:VAL:CA	2.64	0.73
1:A:160:LEU:HD22	2:B:171:GLN:OE1	1.86	0.73
3:F:823:ILE:O	3:F:823:ILE:HG13	1.88	0.73
2:D:97:LEU:CD2	2:D:97:LEU:CB	2.67	0.73
1:A:115:VAL:HG12	1:A:134:CYS:SG	2.29	0.72
1:A:150:ILE:HD12	1:A:150:ILE:H	1.52	0.72
1:A:124:GLN:HG3	2:B:122:TYR:CE2	2.24	0.72
1:A:210:ASN:OD1	1:A:210:ASN:O	2.08	0.72
2:D:154:TRP:CZ3	2:D:195:CYS:HB3	2.25	0.72
1:A:24:LYS:HE2	1:A:70:ASP:OD1	1.89	0.72
1:A:210:ASN:O	1:A:214:CYS:HB3	1.89	0.72
1:C:119:PRO:HG2	2:D:213:ARG:HH12	1.55	0.72
1:A:187:GLU:HA	1:A:211:ARG:HH22	1.55	0.72
2:B:125:ALA:CB	2:B:126:PRO:CD	2.66	0.71
1:A:118:PHE:CZ	2:B:137:THR:O	2.43	0.71
3:F:826:ASN:HB2	3:F:876:ASN:ND2	2.05	0.71
1:A:115:VAL:CG1	1:A:134:CYS:SG	2.79	0.71
1:A:160:LEU:O	1:A:161:ASN:OD1	2.07	0.71
1:A:146:VAL:HG11	1:A:161:ASN:ND2	2.05	0.71
2:B:188:TRP:HB3	2:B:189:PRO:CD	2.21	0.71
1:A:141:PRO:HD2	1:A:198:HIS:CE1	2.25	0.71
2:B:199:HIS:O	2:B:200:PRO:C	2.32	0.71
1:A:28:THR:O	1:A:29:ARG:HB2	1.90	0.71
1:C:147:LYS:HE3	1:C:156:GLN:HE22	1.55	0.70
2:B:64:LYS:HA	2:B:64:LYS:HZ3	1.53	0.70
2:B:150:VAL:HG22	2:B:177:LEU:HD11	1.74	0.70
1:A:178:THR:HG22	1:A:178:THR:O	1.90	0.70
1:C:146:VAL:HG13	1:C:146:VAL:O	1.91	0.70
3:F:866:TRP:HE3	3:F:868:LEU:CD2	2.04	0.70
1:A:140:TYR:HB3	1:A:141:PRO:HD3	1.74	0.70
2:D:199:HIS:CD2	2:D:202:SER:HB3	2.27	0.70
1:C:188:ARG:O	1:C:189:HIS:HB2	1.91	0.69
1:A:150:ILE:HG13	1:A:192:TYR:CE1	2.26	0.69
1:C:178:THR:O	1:C:178:THR:HG22	1.91	0.69
2:D:70:SER:O	2:D:71:LEU:HD23	1.93	0.69
2:D:153:THR:O	2:D:195:CYS:HA	1.92	0.69
1:A:148:TRP:HE3	1:A:193:THR:O	1.75	0.69
2:B:199:HIS:ND1	2:B:202:SER:HB2	2.07	0.69
1:C:2:ILE:H	1:C:2:ILE:CD1	2.04	0.69
1:C:100:ALA:CB	1:C:100:ALA:N	2.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:HZ1	1:C:156:GLN:NE2	1.90	0.69
2:D:126:PRO:HG3	2:D:136:VAL:CG2	2.23	0.69
2:B:64:LYS:HA	2:B:64:LYS:NZ	2.06	0.69
1:C:125:LEU:O	1:C:127:SER:N	2.25	0.69
1:A:19:VAL:CG1	1:A:75:ILE:HB	2.23	0.68
2:B:18:VAL:HG22	2:B:19:LYS:N	2.07	0.68
2:B:46:ASN:CB	4:B:237:HOH:O	2.34	0.68
3:F:860:VAL:O	3:F:861:ASN:OD1	2.12	0.68
2:B:196:ASN:ND2	2:B:207:ASP:OD2	2.27	0.68
1:A:107:LYS:HA	1:A:140:TYR:OH	1.93	0.68
1:A:27:GLN:HG3	4:A:220:HOH:O	1.93	0.68
2:D:199:HIS:HB3	2:D:204:THR:HB	1.75	0.68
1:A:9:SER:HB3	3:E:840:LYS:HE3	1.76	0.68
2:D:11:LEU:HG	2:D:147:PRO:HG3	1.75	0.68
3:F:849:GLU:OE2	3:F:852:ARG:NH1	2.27	0.67
1:C:29:ARG:HG3	1:C:29:ARG:O	1.93	0.67
2:D:67:PHE:CD2	2:D:82:ILE:HG12	2.30	0.67
1:A:117:ILE:HD13	1:A:118:PHE:H	1.60	0.67
2:B:64:LYS:HZ2	2:B:65:GLY:H	1.39	0.67
1:A:108:ARG:NH1	1:A:172:THR:CG2	2.58	0.67
3:E:821:VAL:N	3:E:841:GLY:O	2.27	0.67
1:C:2:ILE:HD12	1:C:2:ILE:N	2.06	0.67
1:C:133:VAL:HG21	2:D:124:LEU:HD21	1.76	0.67
2:D:82:ILE:HG22	2:D:82(C):LEU:CD2	2.24	0.67
2:D:126:PRO:HD2	2:D:188:TRP:CH2	2.30	0.67
2:D:66:ARG:HD2	2:D:82(A):ASN:O	1.95	0.67
2:D:147:PRO:C	2:D:149:PRO:HD2	2.19	0.66
2:B:177:LEU:O	2:B:178:SER:HB3	1.96	0.66
3:E:845:GLU:HG2	4:E:108:HOH:O	1.94	0.66
1:A:127:SER:HB3	4:A:226:HOH:O	1.95	0.66
1:C:106:LEU:CD1	1:C:106:LEU:CB	2.69	0.66
3:F:864:TYR:HA	3:F:878:LYS:O	1.96	0.66
1:C:4:MET:HB3	1:C:4:MET:HE3	1.78	0.66
1:C:22:SER:HB2	1:C:24:LYS:HZ2	1.61	0.66
1:A:162:SER:O	1:A:175:MET:HB2	1.96	0.66
2:D:189:PRO:CB	2:D:212:PRO:CG	2.70	0.66
1:C:79:GLN:HB2	1:C:79:GLN:NE2	2.11	0.65
1:C:142:LYS:CD	1:C:142:LYS:CB	2.74	0.65
1:A:159:VAL:HG12	1:A:179:LEU:HG	1.78	0.65
2:D:82:ILE:CG2	2:D:82(C):LEU:CD2	2.74	0.65
3:F:864:TYR:CD2	3:F:877:ILE:CG2	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27(D):ASN:O	1:C:29:ARG:N	2.27	0.65
1:A:150:ILE:HG21	1:A:189:HIS:HB3	1.77	0.65
1:A:162:SER:O	1:A:175:MET:CB	2.44	0.65
1:C:39:LYS:O	1:C:40:PRO:C	2.37	0.65
2:D:148:GLU:N	2:D:149:PRO:HD2	2.12	0.65
1:A:150:ILE:O	1:A:190:ASN:ND2	2.29	0.65
2:B:1:GLN:OE1	2:B:1:GLN:N	2.24	0.65
2:B:64:LYS:NZ	2:B:65:GLY:H	1.95	0.65
1:A:119:PRO:O	1:A:120:PRO:O	2.15	0.65
1:A:55:GLU:HG3	1:A:56:SER:N	2.12	0.64
2:D:52:ASN:OD1	2:D:54:THR:HG23	1.97	0.64
1:A:122:SER:O	1:A:124:GLN:N	2.30	0.64
1:C:66:GLY:HA3	1:C:71:PHE:CD1	2.32	0.64
1:A:92:TYR:CD2	1:A:93:ILE:HG22	2.33	0.64
1:C:160:LEU:HD21	2:D:171:GLN:NE2	2.12	0.64
2:D:194:THR:HB	2:D:209:LYS:HA	1.79	0.63
1:A:150:ILE:O	1:A:190:ASN:CG	2.41	0.63
1:C:13:VAL:HG21	1:C:19:VAL:CG2	2.28	0.63
1:A:193:THR:HG21	1:A:206:VAL:CG1	2.28	0.63
1:C:136:LEU:N	1:C:136:LEU:CD1	2.59	0.63
3:E:840:LYS:CD	3:E:840:LYS:HB3	2.29	0.63
1:C:22:SER:HB2	1:C:24:LYS:NZ	2.14	0.63
1:C:155:ARG:HG2	1:C:155:ARG:NH1	2.08	0.63
2:D:136:VAL:HG22	2:D:137:THR:H	1.64	0.63
2:B:64:LYS:HZ2	2:B:65:GLY:N	1.97	0.63
2:B:83:LYS:O	2:B:84:ASN:C	2.40	0.63
1:A:148:TRP:CZ3	1:A:194:CYS:HA	2.34	0.63
1:C:148:TRP:HE3	1:C:193:THR:O	1.81	0.63
1:C:179:LEU:HD13	1:C:180:THR:N	2.14	0.62
2:D:38:ASN:HD22	2:D:46:ASN:HB2	1.64	0.62
3:F:829:PHE:C	3:F:831:ASP:H	2.07	0.62
1:A:134:CYS:HB2	1:A:148:TRP:CH2	2.35	0.62
1:C:27(C):LEU:O	1:C:92:TYR:CZ	2.52	0.62
1:C:179:LEU:HD13	1:C:179:LEU:C	2.24	0.62
1:C:107:LYS:HA	1:C:140:TYR:OH	2.00	0.62
1:C:137:ASN:N	1:C:137:ASN:ND2	2.44	0.62
1:A:134:CYS:HB2	1:A:148:TRP:HH2	1.65	0.62
1:C:119:PRO:HG2	2:D:213:ARG:NH1	2.14	0.62
3:F:849:GLU:O	3:F:850:ALA:C	2.37	0.62
2:B:126:PRO:O	2:B:213:ARG:HG3	2.00	0.62
1:C:150:ILE:HD13	1:C:155:ARG:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:LEU:HD22	2:D:97:LEU:H	1.64	0.61
2:D:12:LYS:O	2:D:111:VAL:HA	2.01	0.61
1:C:31:ASN:O	1:C:50:TRP:HA	2.01	0.61
1:A:7:SER:HB2	1:A:22:SER:HG	1.64	0.61
1:A:63:THR:HG22	1:A:64:GLY:N	2.16	0.61
1:C:147:LYS:CE	1:C:156:GLN:NE2	2.64	0.61
1:A:193:THR:HG22	1:A:206:VAL:HG13	1.81	0.61
1:A:115:VAL:HG11	1:A:194:CYS:SG	2.39	0.61
1:A:158:GLY:O	1:A:180:THR:HB	2.01	0.61
2:D:139:GLY:HA2	2:D:154:TRP:CH2	2.36	0.61
3:E:830:ALA:C	3:E:832:GLY:H	2.09	0.61
1:A:194:CYS:O	1:A:206:VAL:HA	2.00	0.60
2:B:5:VAL:CG1	2:B:5:VAL:CG2	2.73	0.60
1:C:45:LYS:CG	1:C:45:LYS:CE	2.77	0.60
1:C:148:TRP:CZ3	1:C:194:CYS:HB3	2.37	0.60
1:A:194:CYS:HB3	1:A:207:LYS:O	2.00	0.60
1:C:137:ASN:N	1:C:137:ASN:HD22	1.99	0.60
3:E:840:LYS:HB3	3:E:840:LYS:HE2	1.84	0.60
2:B:2:ILE:C	2:B:2:ILE:HD13	2.26	0.60
1:C:142:LYS:CG	1:C:142:LYS:CE	2.74	0.60
2:D:70:SER:C	2:D:71:LEU:HD23	2.27	0.60
3:F:837:ALA:O	3:F:838:GLU:HB2	2.01	0.60
1:A:210:ASN:HB3	2:B:129:ALA:HB1	1.72	0.60
3:E:828:ILE:HG22	3:E:828:ILE:O	2.01	0.60
2:D:115:LYS:O	2:D:117:THR:HG22	2.01	0.60
2:D:148:GLU:N	2:D:149:PRO:CD	2.65	0.60
1:A:31:ASN:HD21	1:A:68:GLY:H	1.50	0.60
2:B:82(B):SER:O	2:B:82(C):LEU:O	2.19	0.60
3:E:834:ILE:CD1	3:E:834:ILE:HG21	2.31	0.60
2:D:137:THR:HA	2:D:181:VAL:O	2.01	0.60
1:A:14:SER:O	1:A:17:GLU:HB2	2.02	0.60
2:D:138:LEU:N	2:D:138:LEU:HD12	2.17	0.60
1:C:79:GLN:CB	1:C:79:GLN:NE2	2.65	0.60
1:C:125:LEU:O	1:C:126:THR:C	2.43	0.60
3:F:869:GLU:CG	3:F:870:ASP:O	2.49	0.60
1:A:138:ASN:OD1	2:B:164:HIS:NE2	2.35	0.59
2:B:204:THR:HG22	2:B:206:VAL:HG23	1.84	0.59
1:A:195:GLU:HB2	4:A:236:HOH:O	2.02	0.59
3:F:823:ILE:HD11	3:F:850:ALA:HB2	1.84	0.59
3:E:834:ILE:HG21	3:E:834:ILE:HD13	1.85	0.59
2:B:59:TYR:OH	2:B:68:ALA:HA	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:THR:HG21	1:A:32:TYR:OH	2.02	0.58
3:F:821:VAL:O	3:F:840:LYS:HA	2.03	0.58
1:C:13:VAL:HG21	1:C:19:VAL:HG22	1.84	0.58
2:D:138:LEU:CD2	2:D:210:ILE:CG2	2.71	0.58
1:A:1:ASP:HA	4:A:231:HOH:O	2.03	0.58
2:B:20:ILE:HB	4:B:235:HOH:O	2.03	0.58
2:B:82:ILE:HG22	2:B:82(C):LEU:HD23	1.85	0.58
2:B:138:LEU:HD23	2:B:210:ILE:CG2	2.33	0.58
2:D:82(B):SER:O	2:D:82(C):LEU:C	2.43	0.58
1:C:119:PRO:HB2	1:C:120:PRO:CD	2.34	0.58
2:D:39:GLN:HE21	2:D:44:GLY:HA2	1.68	0.58
2:D:126:PRO:CG	2:D:136:VAL:CG2	2.82	0.58
1:C:83:GLN:OE1	1:C:106:LEU:HB2	2.04	0.58
1:C:207:LYS:NZ	2:D:133:ASN:OD1	2.37	0.58
1:A:150:ILE:HG21	1:A:189:HIS:CB	2.34	0.58
1:A:198:HIS:CD2	1:A:200:THR:H	2.22	0.58
2:B:82:ILE:CG2	2:B:82(C):LEU:HD23	2.34	0.58
2:B:202:SER:O	2:B:203:SER:C	2.44	0.58
2:B:2:ILE:C	2:B:2:ILE:CD1	2.76	0.57
1:C:206:VAL:CG1	1:C:207:LYS:N	2.67	0.57
1:C:160:LEU:CD2	1:C:160:LEU:CB	2.77	0.57
1:A:11:LEU:HD13	1:A:19:VAL:HG23	1.86	0.57
3:E:860:VAL:HG12	3:E:861:ASN:ND2	2.19	0.57
1:C:119:PRO:HB2	1:C:120:PRO:HD2	1.87	0.57
1:A:183:LYS:C	1:A:185:GLU:H	2.13	0.57
1:C:160:LEU:CD2	1:C:160:LEU:HG	2.18	0.57
2:B:163:VAL:HG12	2:B:164:HIS:H	1.67	0.57
2:D:13:LYS:HB2	2:D:16:GLU:OE1	2.05	0.57
2:B:83:LYS:CG	2:B:85:GLU:HG2	2.32	0.56
1:A:150:ILE:O	1:A:190:ASN:HB2	2.06	0.56
1:C:4:MET:CG	1:C:4:MET:CA	2.74	0.56
1:C:13:VAL:O	1:C:106:LEU:HD22	2.05	0.56
1:C:119:PRO:CB	1:C:120:PRO:CD	2.83	0.56
1:A:161:ASN:HB3	1:A:175:MET:HE2	1.86	0.56
3:E:834:ILE:CD1	3:E:834:ILE:CB	2.78	0.56
2:D:13:LYS:NZ	2:D:113:SER:O	2.38	0.56
3:F:875:MET:HE2	3:F:877:ILE:HD11	1.87	0.56
1:A:186:TYR:OH	1:A:214:CYS:SG	2.64	0.56
2:B:118:PRO:C	2:B:119:PRO:O	2.47	0.56
2:B:154:TRP:HB3	2:B:159:LEU:HB2	1.88	0.56
1:C:161:ASN:ND2	1:C:175:MET:HE1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:VAL:HG12	1:C:207:LYS:N	2.20	0.56
2:D:126:PRO:HG2	2:D:188:TRP:CZ3	2.41	0.56
3:E:834:ILE:CD1	3:E:834:ILE:CG2	2.85	0.56
2:B:163:VAL:HA	2:B:180:SER:O	2.06	0.55
3:F:827:LEU:HD12	3:F:879:PHE:HE1	1.71	0.55
1:A:207:LYS:HB2	1:A:207:LYS:NZ	2.20	0.55
3:F:827:LEU:N	3:F:835:GLN:O	2.39	0.55
1:A:110:ASP:OD1	1:A:141:PRO:HG2	2.06	0.55
3:F:834:ILE:HD13	3:F:834:ILE:N	2.21	0.55
1:C:161:ASN:CG	1:C:175:MET:CE	2.80	0.55
3:F:860:VAL:C	3:F:861:ASN:OD1	2.49	0.55
1:A:178:THR:O	1:A:178:THR:CG2	2.55	0.55
1:C:144:ILE:CD1	1:C:175:MET:SD	2.95	0.55
1:C:147:LYS:HZ1	1:C:156:GLN:HE21	1.53	0.55
2:D:83:LYS:C	2:D:111:VAL:HG11	2.32	0.55
3:F:866:TRP:O	3:F:867:ASP:C	2.46	0.55
1:A:117:ILE:HB	1:A:207:LYS:HG3	1.89	0.55
1:C:33:LEU:CD2	1:C:71:PHE:CG	2.90	0.55
1:A:122:SER:C	1:A:124:GLN:H	2.14	0.55
2:B:82(A):ASN:O	2:B:82(B):SER:O	2.25	0.55
1:C:147:LYS:HE3	1:C:156:GLN:NE2	2.20	0.55
3:E:865:THR:OG1	3:E:878:LYS:HD3	2.08	0.54
1:C:107:LYS:NZ	3:F:836:THR:HG23	2.22	0.54
2:D:136:VAL:CG2	2:D:137:THR:H	2.20	0.54
2:D:202:SER:OG	2:D:202:SER:O	2.24	0.54
1:A:21:MET:HE3	1:A:73:LEU:HD23	1.89	0.54
1:A:201:SER:HB2	1:A:203:SER:O	2.07	0.54
2:D:124:LEU:O	2:D:138:LEU:HB3	2.07	0.54
1:C:170:ASP:OD1	1:C:170:ASP:C	2.48	0.54
2:D:59:TYR:OH	2:D:68:ALA:HA	2.06	0.54
2:D:126:PRO:HG3	2:D:136:VAL:HG23	1.88	0.54
2:B:163:VAL:CG1	2:B:164:HIS:N	2.71	0.54
1:C:179:LEU:C	1:C:179:LEU:CD1	2.80	0.54
1:A:110:ASP:OD2	1:A:199:LYS:HE2	2.06	0.54
1:A:185:GLU:HA	1:A:188:ARG:HG2	1.89	0.54
1:A:117:ILE:CD1	1:A:118:PHE:H	2.21	0.54
2:B:199:HIS:ND1	2:B:202:SER:CB	2.70	0.54
1:C:204:PRO:O	1:C:206:VAL:HG23	2.08	0.53
1:A:150:ILE:HD12	1:A:150:ILE:N	2.22	0.53
2:D:73:THR:O	2:D:74:SER:C	2.50	0.53
1:A:108:ARG:O	1:A:140:TYR:CE2	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PRO:HD2	1:A:198:HIS:HE1	1.71	0.53
1:C:27:GLN:C	1:C:69:THR:CG2	2.80	0.53
1:C:150:ILE:CD1	1:C:155:ARG:HG3	2.39	0.53
1:C:117:ILE:HG12	1:C:118:PHE:H	1.70	0.53
1:A:109:ALA:O	1:A:110:ASP:C	2.44	0.53
1:C:49:TYR:O	1:C:50:TRP:HB2	2.07	0.53
1:C:110:ASP:OD2	1:C:199:LYS:NZ	2.42	0.53
2:B:123:PRO:HG3	2:B:208:LYS:HG2	1.91	0.53
1:C:144:ILE:HD11	1:C:175:MET:SD	2.49	0.53
1:A:1:ASP:N	1:A:1:ASP:CB	2.66	0.53
1:A:139:PHE:O	1:A:139:PHE:CG	2.62	0.53
2:B:97:LEU:CD2	2:B:97:LEU:N	2.58	0.53
2:B:150:VAL:HG12	2:B:199:HIS:HB2	1.91	0.52
2:B:36:TRP:O	2:B:48:MET:HB2	2.08	0.52
2:D:126:PRO:HG2	2:D:136:VAL:HG21	1.91	0.52
2:D:154:TRP:CE3	2:D:195:CYS:HB3	2.43	0.52
2:B:154:TRP:CB	2:B:159:LEU:HB2	2.40	0.52
1:C:180:THR:C	1:C:181:LEU:HD23	2.34	0.52
2:D:199:HIS:CD2	2:D:202:SER:CB	2.92	0.52
3:F:875:MET:CE	3:F:877:ILE:HD11	2.39	0.52
1:A:108:ARG:O	1:A:140:TYR:CD2	2.63	0.52
1:A:148:TRP:CZ3	1:A:193:THR:O	2.63	0.52
1:C:77:SER:O	1:C:78:VAL:C	2.53	0.52
1:A:12:ALA:HA	1:A:105:GLU:O	2.09	0.52
2:B:70:SER:O	2:B:71:LEU:HD23	2.10	0.52
1:C:27(C):LEU:HD23	1:C:27(D):ASN:H	1.73	0.52
2:D:38:ASN:ND2	2:D:38:ASN:C	2.67	0.52
1:A:149:LYS:C	1:A:151:ASP:H	2.18	0.52
2:B:153:THR:OG1	2:B:196:ASN:HB2	2.09	0.52
2:D:191:GLU:HG3	2:D:192:THR:H	1.75	0.52
1:A:147:LYS:HG2	1:A:154:GLU:OE2	2.10	0.52
1:A:193:THR:HG21	1:A:206:VAL:HG13	1.87	0.52
1:C:150:ILE:HD13	1:C:155:ARG:CG	2.40	0.52
1:C:210:ASN:HB3	1:C:213:GLU:HG3	1.90	0.52
1:A:121:SER:O	1:A:122:SER:C	2.53	0.51
2:B:121:VAL:O	2:B:122:TYR:CD1	2.63	0.51
2:B:170:LEU:HD12	2:B:174:LEU:O	2.10	0.51
1:C:79:GLN:CB	1:C:79:GLN:HE21	2.23	0.51
3:F:864:TYR:HD2	3:F:877:ILE:HG23	1.73	0.51
1:C:33:LEU:HD22	1:C:71:PHE:CG	2.45	0.51
1:C:147:LYS:CE	1:C:156:GLN:HE22	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:LYS:O	2:D:84:ASN:C	2.47	0.51
2:D:116:THR:HA	2:D:146:PHE:O	2.11	0.51
1:A:148:TRP:CG	1:A:179:LEU:HD12	2.45	0.51
2:B:124:LEU:HD12	2:B:139:GLY:CA	2.40	0.51
1:C:210:ASN:CB	1:C:213:GLU:OE2	2.58	0.51
2:D:57:PRO:HB3	2:D:59:TYR:CE2	2.45	0.51
1:A:135:PHE:HE1	1:A:176:SER:HB2	1.75	0.51
1:C:33:LEU:HD22	1:C:71:PHE:CD2	2.46	0.51
2:B:38:ASN:HD22	2:B:48:MET:HG3	1.75	0.51
1:A:146:VAL:CG1	1:A:161:ASN:ND2	2.72	0.51
2:B:18:VAL:CG2	2:B:19:LYS:N	2.72	0.51
2:D:66:ARG:O	2:D:82(A):ASN:N	2.43	0.51
2:D:117:THR:CG2	2:D:174:LEU:HD21	2.38	0.51
3:F:847:THR:HG22	3:F:851:TYR:CE2	2.45	0.51
1:C:149:LYS:O	1:C:193:THR:HB	2.11	0.51
3:F:866:TRP:O	3:F:868:LEU:HD23	2.10	0.51
2:D:150:VAL:O	2:D:150:VAL:CG2	2.57	0.51
1:A:13:VAL:HG12	1:A:14:SER:H	1.76	0.50
2:D:155:ASN:HB2	2:D:158:SER:OG	2.11	0.50
1:A:159:VAL:CG1	1:A:179:LEU:HG	2.39	0.50
1:A:214:CYS:SG	1:A:214:CYS:OXT	2.69	0.50
1:C:64:GLY:HA2	1:C:72:THR:O	2.11	0.50
1:C:139:PHE:CZ	1:C:144:ILE:HG12	2.46	0.50
1:A:140:TYR:O	1:A:140:TYR:CD1	2.65	0.50
1:A:148:TRP:HZ3	1:A:194:CYS:CA	2.25	0.50
2:B:82(B):SER:C	2:B:82(C):LEU:O	2.53	0.50
1:C:50:TRP:O	1:C:51:ALA:HB3	2.11	0.50
1:C:79:GLN:CG	1:C:79:GLN:CA	2.82	0.50
1:C:150:ILE:O	1:C:150:ILE:HG22	2.11	0.50
2:D:192:THR:HA	4:D:222:HOH:O	2.11	0.50
3:F:849:GLU:O	3:F:851:TYR:N	2.45	0.50
1:A:11:LEU:HD13	1:A:19:VAL:CG2	2.41	0.50
1:C:4:MET:HB3	1:C:4:MET:CE	2.41	0.50
1:C:24:LYS:HG3	1:C:70:ASP:OD1	2.11	0.50
1:A:9:SER:CB	3:E:840:LYS:HE3	2.42	0.50
1:A:135:PHE:CE1	1:A:176:SER:HB2	2.47	0.50
1:A:192:TYR:CB	1:A:209:PHE:CE2	2.95	0.50
2:B:145:TYR:N	2:B:174:LEU:HD12	2.27	0.50
1:C:115:VAL:CG1	1:C:134:CYS:SG	3.00	0.50
2:D:123:PRO:HB3	2:D:210:ILE:HD13	1.94	0.50
1:A:122:SER:C	1:A:124:GLN:N	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HH21	1:C:82:ASP:CG	2.19	0.50
1:C:147:LYS:HZ2	1:C:156:GLN:NE2	2.08	0.50
1:C:161:ASN:ND2	1:C:175:MET:CE	2.75	0.50
1:C:190:ASN:HD21	1:C:212:ASN:ND2	2.10	0.50
1:A:133:VAL:HA	1:A:177:SER:O	2.12	0.49
1:A:140:TYR:CB	1:A:141:PRO:HD3	2.38	0.49
2:B:82:ILE:CG2	2:B:82(C):LEU:CD2	2.90	0.49
1:C:4:MET:CB	1:C:4:MET:SD	2.93	0.49
1:C:13:VAL:HG12	1:C:14:SER:N	2.26	0.49
3:F:858:ALA:O	3:F:860:VAL:N	2.44	0.49
1:A:210:ASN:O	1:A:210:ASN:CG	2.56	0.49
2:B:15:GLY:O	2:B:82(B):SER:HA	2.12	0.49
3:E:840:LYS:HB3	3:E:840:LYS:HE3	1.90	0.49
1:C:4:MET:CB	1:C:4:MET:CE	2.91	0.49
2:B:138:LEU:HD23	2:B:210:ILE:HG21	1.94	0.49
2:B:183:VAL:HG23	2:B:183:VAL:O	2.12	0.49
2:B:123:PRO:HB3	2:B:210:ILE:HG13	1.94	0.49
1:C:168:SER:CB	4:C:223:HOH:O	2.50	0.49
1:A:24:LYS:NZ	1:A:24:LYS:HB3	2.28	0.49
1:A:148:TRP:HE1	1:A:179:LEU:HB2	1.73	0.49
1:A:56:SER:HB3	2:D:27:TYR:O	2.12	0.49
2:D:97:LEU:C	2:D:99:GLN:H	2.21	0.49
2:B:199:HIS:CE1	2:B:202:SER:HB2	2.47	0.49
1:C:147:LYS:CD	1:C:147:LYS:CB	2.81	0.49
1:A:187:GLU:HA	1:A:211:ARG:NH2	2.24	0.48
3:E:858:ALA:O	3:E:859:LYS:C	2.54	0.48
3:E:879:PHE:N	3:E:879:PHE:CD1	2.79	0.48
1:C:66:GLY:HA3	1:C:71:PHE:HD1	1.78	0.48
2:D:136:VAL:HG22	2:D:137:THR:N	2.28	0.48
3:F:842:THR:O	3:F:844:GLU:N	2.46	0.48
1:A:78:VAL:HG22	1:A:106:LEU:HD11	1.95	0.48
1:A:186:TYR:HE1	1:A:209:PHE:HZ	1.62	0.48
2:D:83:LYS:O	2:D:86:ASP:HB2	2.14	0.48
2:D:97:LEU:CD2	2:D:97:LEU:CD1	2.79	0.48
2:D:4:LEU:O	2:D:104:GLY:HA2	2.13	0.48
2:D:191:GLU:HG3	2:D:192:THR:OG1	2.13	0.48
1:A:194:CYS:N	1:A:207:LYS:O	2.47	0.48
2:D:20:ILE:HD11	2:D:80:LEU:HD23	1.95	0.48
3:F:854:ALA:HB2	3:F:877:ILE:HD13	1.93	0.48
3:F:873:ASN:O	3:F:874:HIS:HB2	2.13	0.48
1:A:146:VAL:HG13	1:A:146:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TRP:HZ3	1:A:194:CYS:HA	1.78	0.48
1:C:147:LYS:O	1:C:195:GLU:N	2.38	0.48
3:F:842:THR:O	3:F:843:PHE:C	2.56	0.48
1:A:86:TYR:N	1:A:86:TYR:CD1	2.82	0.48
3:F:858:ALA:O	3:F:861:ASN:O	2.31	0.48
1:C:4:MET:CB	1:C:4:MET:HE3	2.43	0.48
1:C:106:LEU:HA	1:C:106:LEU:HD23	1.57	0.48
1:C:133:VAL:HG12	1:C:134:CYS:N	2.29	0.48
1:A:107:LYS:HE3	3:E:836:THR:HG23	1.95	0.48
2:B:138:LEU:HD21	2:B:188:TRP:CE2	2.49	0.48
2:B:211:VAL:O	2:B:211:VAL:HG23	2.13	0.48
1:C:89:LYS:HG3	1:C:98:PHE:CE2	2.49	0.48
1:C:11:LEU:HD13	1:C:19:VAL:HG11	1.94	0.47
2:D:66:ARG:NH1	2:D:86:ASP:OD2	2.45	0.47
1:A:34:ALA:O	1:A:88:CYS:HA	2.14	0.47
1:A:108:ARG:HE	1:A:108:ARG:HB2	1.40	0.47
1:A:211:ARG:HE	1:A:211:ARG:HA	1.79	0.47
3:E:840:LYS:CE	3:E:840:LYS:CB	2.83	0.47
3:F:858:ALA:HA	3:F:861:ASN:O	2.14	0.47
1:A:150:ILE:O	1:A:190:ASN:CB	2.61	0.47
2:B:154:TRP:CZ3	2:B:195:CYS:HB3	2.49	0.47
1:C:119:PRO:CG	2:D:213:ARG:NH1	2.77	0.47
2:D:177:LEU:HD23	2:D:178:SER:N	2.28	0.47
1:A:13:VAL:HG12	1:A:14:SER:N	2.29	0.47
1:A:148:TRP:CD1	1:A:159:VAL:CG1	2.90	0.47
1:C:11:LEU:HD13	1:C:19:VAL:CG1	2.44	0.47
1:C:89:LYS:HB3	1:C:89:LYS:HE2	1.55	0.47
2:B:185:SER:C	2:B:187:THR:N	2.72	0.47
1:A:136:LEU:O	1:A:174:SER:HA	2.14	0.47
2:B:40:ALA:HB1	2:B:41:PRO:HD2	1.96	0.47
1:C:188:ARG:O	1:C:189:HIS:CB	2.58	0.47
2:D:138:LEU:HD22	2:D:193:VAL:HG11	1.96	0.47
2:D:163:VAL:HG12	2:D:164:HIS:N	2.30	0.47
1:A:132:VAL:HG12	1:A:133:VAL:N	2.29	0.47
2:B:160:SER:O	2:B:163:VAL:CG2	2.50	0.47
1:C:24:LYS:N	1:C:24:LYS:HE2	2.30	0.47
1:C:133:VAL:CG1	1:C:134:CYS:N	2.77	0.47
2:B:125:ALA:HB2	2:B:210:ILE:CG2	2.45	0.46
1:C:48:ILE:HG22	1:C:49:TYR:N	2.29	0.46
1:C:190:ASN:HD22	1:C:211:ARG:HB3	1.80	0.46
1:C:4:MET:CE	1:C:23:CYS:SG	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82(C):LEU:HD13	2:D:111:VAL:HG22	1.98	0.46
2:D:148:GLU:O	2:D:150:VAL:N	2.49	0.46
2:D:209:LYS:HD2	2:D:210:ILE:H	1.81	0.46
1:A:110:ASP:OD1	1:A:141:PRO:CG	2.63	0.46
2:D:20:ILE:HD13	2:D:20:ILE:HG21	1.75	0.46
2:D:177:LEU:HD23	2:D:177:LEU:C	2.40	0.46
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.97	0.46
2:B:211:VAL:O	2:B:211:VAL:CG2	2.63	0.46
3:F:834:ILE:HD13	3:F:834:ILE:H	1.79	0.46
3:E:829:PHE:CD1	3:E:829:PHE:N	2.84	0.46
1:A:77:SER:O	1:A:78:VAL:O	2.32	0.46
1:A:115:VAL:CG1	1:A:194:CYS:SG	3.04	0.46
2:B:124:LEU:HD21	2:B:141:LEU:HB3	1.97	0.46
2:B:146:PHE:CD1	2:B:147:PRO:HA	2.51	0.46
1:C:148:TRP:CH2	1:C:194:CYS:HB3	2.50	0.46
2:D:170:LEU:HD12	2:D:171:GLN:N	2.30	0.46
2:B:170:LEU:HD12	2:B:171:GLN:H	1.79	0.46
2:D:47:TRP:CE2	2:D:49:GLY:HA2	2.49	0.46
2:D:99:GLN:HE21	2:D:99:GLN:HB3	1.46	0.46
1:A:139:PHE:CD2	1:A:139:PHE:C	2.92	0.46
1:C:27(C):LEU:HG	1:C:31:ASN:ND2	2.30	0.46
3:F:829:PHE:C	3:F:831:ASP:N	2.74	0.46
2:D:155:ASN:HD21	2:D:192:THR:C	2.24	0.46
3:F:848:ALA:HB1	3:F:852:ARG:NH2	2.31	0.46
1:C:161:ASN:O	1:C:162:SER:HB2	2.16	0.45
2:D:117:THR:CG2	2:D:174:LEU:CD2	2.94	0.45
2:B:48:MET:HE1	2:B:80:LEU:HD22	1.98	0.45
2:D:189:PRO:HB3	2:D:212:PRO:HG3	1.87	0.45
1:C:123:GLU:OE1	1:C:123:GLU:N	2.49	0.45
1:A:210:ASN:OD1	1:A:213:GLU:HB3	2.16	0.45
1:C:27:GLN:O	1:C:69:THR:HG22	2.16	0.45
2:D:97:LEU:CD2	2:D:97:LEU:H	2.29	0.45
3:F:842:THR:OG1	3:F:845:GLU:HB2	2.17	0.45
3:F:854:ALA:CB	3:F:877:ILE:HD13	2.46	0.45
1:A:9:SER:HB3	3:E:840:LYS:CE	2.46	0.45
1:A:33:LEU:HG	1:A:34:ALA:N	2.31	0.45
1:A:119:PRO:O	1:A:120:PRO:C	2.50	0.45
2:B:167:PRO:O	2:B:168:ALA:C	2.56	0.45
2:D:188:TRP:CH2	2:D:212:PRO:HA	2.51	0.45
1:A:140:TYR:CD1	1:A:140:TYR:C	2.94	0.45
1:A:151:ASP:OD1	1:A:191:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASP:O	1:C:172:THR:HG23	2.17	0.45
2:D:192:THR:C	2:D:193:VAL:HG23	2.42	0.45
1:C:94:PRO:HA	1:C:95:PRO:C	2.42	0.45
3:E:822:THR:HA	3:E:839:PHE:O	2.17	0.45
1:A:79:GLN:C	1:A:81:GLU:N	2.73	0.45
1:A:125:LEU:O	1:A:127:SER:N	2.49	0.45
1:A:150:ILE:H	1:A:150:ILE:CD1	2.26	0.45
1:A:160:LEU:C	1:A:161:ASN:OD1	2.60	0.45
2:B:153:THR:O	2:B:196:ASN:N	2.39	0.45
1:C:189:HIS:ND1	1:C:190:ASN:N	2.64	0.45
2:D:66:ARG:HB3	2:D:82(A):ASN:O	2.17	0.45
2:B:5:VAL:CG1	2:B:5:VAL:C	2.90	0.45
2:D:30:THR:CG2	4:D:227:HOH:O	2.65	0.45
2:D:102:VAL:HG12	2:D:103:TRP:N	2.32	0.45
1:A:61:ARG:O	1:A:75:ILE:HA	2.16	0.44
1:C:107:LYS:NZ	3:F:836:THR:OG1	2.50	0.44
1:A:13:VAL:O	1:A:107:LYS:N	2.41	0.44
2:D:19:LYS:HD3	2:D:81:GLN:OE1	2.17	0.44
2:D:139:GLY:HA2	2:D:154:TRP:CZ2	2.52	0.44
2:B:13:LYS:HA	2:B:14:PRO:HD3	1.80	0.44
2:D:18:VAL:O	2:D:18:VAL:HG13	2.15	0.44
1:A:210:ASN:CG	1:A:213:GLU:HB3	2.43	0.44
1:C:39:LYS:HB3	1:C:40:PRO:HD2	1.99	0.44
2:D:126:PRO:CG	2:D:136:VAL:HG21	2.47	0.44
1:A:150:ILE:CG2	1:A:189:HIS:HB3	2.45	0.44
2:B:88:ALA:HB3	2:B:90:TYR:CE2	2.52	0.44
2:D:163:VAL:CG1	2:D:164:HIS:N	2.79	0.44
2:B:7:SER:OG	4:B:218:HOH:O	2.21	0.44
2:B:117:THR:O	2:B:145:TYR:HB2	2.18	0.44
2:B:127:GLY:HA2	2:B:213:ARG:CG	2.47	0.44
2:D:48:MET:HA	2:D:63:PHE:CD2	2.52	0.44
2:B:43:LYS:CG	2:B:43:LYS:CE	2.84	0.43
3:E:823:ILE:HD13	3:E:823:ILE:HG21	1.68	0.43
1:C:13:VAL:HG21	1:C:19:VAL:HG21	1.97	0.43
1:C:71:PHE:C	1:C:72:THR:HG23	2.43	0.43
2:D:59:TYR:CB	2:D:63:PHE:O	2.60	0.43
1:A:148:TRP:CZ3	1:A:194:CYS:CA	3.01	0.43
3:E:853:TYR:O	3:E:854:ALA:C	2.60	0.43
2:D:38:ASN:HD21	2:D:46:ASN:HB2	1.81	0.43
2:D:138:LEU:HD23	2:D:210:ILE:HG22	1.87	0.43
1:A:24:LYS:HA	1:A:69:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:842:THR:O	3:E:843:PHE:C	2.61	0.43
2:D:97:LEU:HD22	2:D:97:LEU:N	2.33	0.43
3:F:824:LYS:HB3	4:F:102:HOH:O	2.17	0.43
1:C:19:VAL:HG12	1:C:20:THR:N	2.33	0.43
1:C:141:PRO:O	1:C:198:HIS:HE1	2.01	0.43
2:B:55:GLY:O	2:B:57:PRO:HD3	2.18	0.43
1:A:12:ALA:C	1:A:13:VAL:HG23	2.43	0.43
3:E:853:TYR:O	3:E:856:LEU:N	2.51	0.43
1:C:23:CYS:C	1:C:24:LYS:HE2	2.44	0.43
2:D:135:MET:HB3	2:D:136:VAL:H	1.70	0.43
3:F:828:ILE:HG12	3:F:834:ILE:CG2	2.49	0.43
1:A:100:ALA:HB1	3:E:818:LYS:HG2	2.00	0.43
1:C:107:LYS:HZ1	3:F:836:THR:HG23	1.84	0.43
2:D:47:TRP:CH2	2:D:49:GLY:HA2	2.53	0.43
2:D:191:GLU:HG3	2:D:192:THR:N	2.34	0.43
1:A:108:ARG:NH1	1:A:172:THR:HG22	2.24	0.43
2:B:40:ALA:HB1	2:B:41:PRO:CD	2.48	0.43
2:D:37:VAL:HG12	2:D:38:ASN:N	2.32	0.43
1:A:78:VAL:CG2	1:A:106:LEU:HD21	2.49	0.43
1:A:122:SER:O	1:A:125:LEU:N	2.52	0.43
1:A:186:TYR:CE1	1:A:209:PHE:HZ	2.36	0.43
1:C:73:LEU:HD12	1:C:73:LEU:HA	1.85	0.43
2:B:94:ARG:HD3	2:B:101:ASP:OD2	2.19	0.42
1:C:22:SER:CB	1:C:24:LYS:HZ2	2.29	0.42
1:C:125:LEU:C	1:C:127:SER:N	2.77	0.42
2:B:51:VAL:HG22	2:B:52:ASN:N	2.33	0.42
2:B:124:LEU:HB2	2:B:139:GLY:C	2.44	0.42
2:B:150:VAL:HG12	2:B:199:HIS:CB	2.49	0.42
2:B:194:THR:HB	2:B:209:LYS:HA	2.01	0.42
2:D:89:THR:CG2	2:D:108:THR:OG1	2.56	0.42
2:D:168:ALA:HB2	2:D:177:LEU:HD12	2.01	0.42
1:A:150:ILE:CG1	1:A:192:TYR:CE1	2.99	0.42
1:C:161:ASN:HB3	1:C:175:MET:HE3	2.01	0.42
2:D:196:ASN:ND2	2:D:207:ASP:OD2	2.45	0.42
1:A:122:SER:O	1:A:123:GLU:C	2.63	0.42
3:E:830:ALA:O	3:E:832:GLY:N	2.49	0.42
2:D:67:PHE:CE2	2:D:82:ILE:HG12	2.54	0.42
2:D:162:GLY:O	2:D:181:VAL:HA	2.20	0.42
3:F:828:ILE:HA	3:F:834:ILE:HG22	2.01	0.42
3:F:845:GLU:O	3:F:846:ALA:C	2.61	0.42
2:B:138:LEU:HD23	2:B:210:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:PHE:HA	2:D:167:PRO:HD3	1.83	0.42
3:F:864:TYR:CA	3:F:878:LYS:O	2.65	0.42
2:B:11:LEU:HG	2:B:147:PRO:HG3	2.02	0.42
2:D:97:LEU:C	2:D:99:GLN:N	2.77	0.42
2:D:137:THR:O	4:D:224:HOH:O	2.22	0.42
2:D:146:PHE:HA	2:D:147:PRO:HA	1.79	0.42
2:B:188:TRP:CB	2:B:189:PRO:CD	2.89	0.42
1:C:5:SER:O	1:C:24:LYS:HE2	2.20	0.42
1:C:29:ARG:O	1:C:29:ARG:CG	2.64	0.42
1:C:49:TYR:CZ	1:C:53:THR:HG21	2.55	0.42
2:D:138:LEU:N	2:D:138:LEU:CD1	2.83	0.42
2:D:188:TRP:CH2	2:D:212:PRO:HB3	2.54	0.42
2:D:82:ILE:HG21	2:D:82(C):LEU:CD2	2.48	0.42
1:A:124:GLN:HE22	1:A:131:SER:H	1.68	0.41
1:C:86:TYR:CD1	1:C:86:TYR:N	2.87	0.41
2:B:150:VAL:HA	2:B:198:ALA:O	2.20	0.41
1:C:34:ALA:HB1	1:C:48:ILE:O	2.19	0.41
1:C:133:VAL:HG21	2:D:124:LEU:CD2	2.47	0.41
1:A:27(A):SER:O	1:A:27(B):LEU:HD23	2.20	0.41
3:F:853:TYR:CZ	3:F:857:LEU:HD21	2.56	0.41
2:B:52:ASN:OD1	2:B:53:GLU:N	2.53	0.41
2:B:127:GLY:HA2	2:B:213:ARG:HG3	2.03	0.41
2:B:185:SER:C	2:B:187:THR:H	2.29	0.41
2:B:205:LYS:O	2:B:206:VAL:CG2	2.68	0.41
3:F:882:LYS:C	3:F:882:LYS:HD3	2.46	0.41
1:A:131:SER:HA	1:A:179:LEU:O	2.20	0.41
1:A:146:VAL:HG11	1:A:161:ASN:HD22	1.84	0.41
2:B:2:ILE:O	2:B:3:GLN:HB3	2.20	0.41
1:C:7:SER:HA	1:C:8:PRO:HA	1.83	0.41
1:C:209:PHE:CD1	1:C:209:PHE:C	2.99	0.41
2:D:30:THR:HG21	4:D:227:HOH:O	2.19	0.41
2:D:52:ASN:OD1	2:D:54:THR:N	2.53	0.41
2:D:117:THR:O	2:D:145:TYR:HA	2.20	0.41
1:A:31:ASN:ND2	1:A:68:GLY:H	2.15	0.41
1:A:154:GLU:O	1:A:154:GLU:HG3	2.21	0.41
2:B:139:GLY:HA2	2:B:179:SER:O	2.20	0.41
1:C:37:GLN:HB2	1:C:47:LEU:HD11	2.03	0.41
2:B:125:ALA:HA	2:B:126:PRO:HD3	1.84	0.41
1:A:104:LEU:C	1:A:104:LEU:CD2	2.94	0.41
2:B:32:PHE:O	2:B:52(A):THR:OG1	2.36	0.41
1:C:124:GLN:HE22	1:C:131:SER:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:CG1	1:A:133:VAL:N	2.82	0.41
1:A:186:TYR:HA	1:A:192:TYR:OH	2.21	0.41
2:B:24:ALA:HB2	2:B:29:PHE:HD1	1.85	0.41
2:B:38:ASN:ND2	2:B:48:MET:HG3	2.36	0.41
3:E:830:ALA:C	3:E:832:GLY:N	2.74	0.41
1:C:24:LYS:HA	1:C:69:THR:O	2.20	0.41
1:C:44:PRO:HG2	2:D:45:LEU:HD21	2.02	0.41
2:D:117:THR:HG21	2:D:174:LEU:CD2	2.41	0.41
3:F:823:ILE:CD1	3:F:850:ALA:HB2	2.51	0.41
1:A:148:TRP:O	1:A:154:GLU:HA	2.20	0.41
2:B:120:SER:HB3	2:B:122:TYR:CZ	2.56	0.41
1:A:120:PRO:HG2	1:A:186:TYR:CE2	2.56	0.40
1:A:192:TYR:HB3	1:A:209:PHE:CD2	2.56	0.40
1:A:196:ALA:HB3	1:A:205:ILE:O	2.21	0.40
2:B:2:ILE:O	2:B:3:GLN:CB	2.67	0.40
1:A:35:TRP:HA	1:A:87:TYR:O	2.21	0.40
1:A:50:TRP:C	1:A:52:SER:H	2.29	0.40
2:B:163:VAL:CG1	2:B:164:HIS:H	2.31	0.40
2:D:38:ASN:HD21	2:D:46:ASN:HD22	1.69	0.40
2:D:177:LEU:HD23	2:D:178:SER:CA	2.52	0.40
1:C:63:THR:HG22	1:C:64:GLY:N	2.30	0.40
2:D:59:TYR:CE1	2:D:67:PHE:O	2.75	0.40
1:A:125:LEU:O	1:A:126:THR:C	2.65	0.40
1:A:156:GLN:HE21	1:A:159:VAL:CG2	2.07	0.40
2:B:70:SER:HB2	2:B:71:LEU:H	1.63	0.40
3:E:824:LYS:CB	3:E:824:LYS:CD	2.83	0.40
3:F:822:THR:HA	3:F:839:PHE:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27(F):ARG:NH1	2:D:127:GLY:O[2_555]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/220 (99%)	182 (84%)	24 (11%)	12 (6%)	1	1
1	C	218/220 (99%)	184 (84%)	23 (11%)	11 (5%)	1	2
2	B	216/218 (99%)	185 (86%)	20 (9%)	11 (5%)	1	2
2	D	216/218 (99%)	180 (83%)	30 (14%)	6 (3%)	4	6
3	E	63/65 (97%)	56 (89%)	6 (10%)	1 (2%)	7	16
3	F	63/65 (97%)	39 (62%)	16 (25%)	8 (13%)	0	0
All	All	994/1006 (99%)	826 (83%)	119 (12%)	49 (5%)	1	2

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	THR
1	A	154	GLU
1	A	190	ASN
2	B	189	PRO
1	C	126	THR
1	C	151	ASP
2	D	131	GLN
2	D	156	SER
3	F	830	ALA
1	A	51	ALA
1	A	122	SER
2	B	82(B)	SER
1	C	122	SER
1	C	152	GLY
1	C	158	GLY
1	C	205	ILE
3	F	846	ALA
3	F	859	LYS
3	F	860	VAL
1	A	120	PRO
1	A	125	LEU
1	A	151	ASP
1	A	167	ASP
1	A	191	SER
2	B	144	GLY
2	B	171	GLN

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Mol	Chain	Res	Type
2	B	186	SER
2	D	189	PRO
3	F	843	PHE
1	A	83	GLN
2	B	148	GLU
1	C	204	PRO
2	D	45	LEU
2	D	212	PRO
3	F	858	ALA
3	F	874	HIS
2	B	66	ARG
2	B	188	TRP
3	E	830	ALA
1	C	68	GLY
3	F	847	THR
2	B	119	PRO
1	C	84	ALA
1	C	150	ILE
2	D	98	ARG
1	A	150	ILE
2	B	57	PRO
2	B	212	PRO
1	C	2	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/195 (100%)	153 (78%)	42 (22%)	1	2
1	C	195/195 (100%)	163 (84%)	32 (16%)	2	4
2	B	187/187 (100%)	158 (84%)	29 (16%)	2	5
2	D	187/187 (100%)	157 (84%)	30 (16%)	2	4
3	E	51/51 (100%)	38 (74%)	13 (26%)	0	1
3	F	51/51 (100%)	43 (84%)	8 (16%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	866/866 (100%)	712 (82%)	154 (18%)	2 3

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	21	MET
1	A	45	LYS
1	A	55	GLU
1	A	56	SER
1	A	78	VAL
1	A	83	GLN
1	A	93	ILE
1	A	96	LEU
1	A	97	THR
1	A	104	LEU
1	A	105	GLU
1	A	110	ASP
1	A	115	VAL
1	A	117	ILE
1	A	127	SER
1	A	136	LEU
1	A	142	LYS
1	A	143	ASP
1	A	144	ILE
1	A	147	LYS
1	A	149	LYS
1	A	150	ILE
1	A	151	ASP
1	A	153	SER
1	A	154	GLU
1	A	155	ARG
1	A	156	GLN
1	A	160	LEU
1	A	169	LYS
1	A	176	SER
1	A	178	THR
1	A	179	LEU
1	A	183	LYS
1	A	184	ASP
1	A	187	GLU
1	A	190	ASN

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Mol	Chain	Res	Type
1	A	202	THR
1	A	203	SER
1	A	205	ILE
1	A	207	LYS
1	A	209	PHE
2	B	1	GLN
2	B	2	ILE
2	B	11	LEU
2	B	17	THR
2	B	20	ILE
2	B	30	THR
2	B	45	LEU
2	B	46	ASN
2	B	64	LYS
2	B	70	SER
2	B	76	SER
2	B	96	LEU
2	B	97	LEU
2	B	109	VAL
2	B	111	VAL
2	B	115	LYS
2	B	128	SER
2	B	131	GLN
2	B	149	PRO
2	B	158	SER
2	B	161	SER
2	B	174	LEU
2	B	177	LEU
2	B	186	SER
2	B	194	THR
2	B	205	LYS
2	B	208	LYS
2	B	209	LYS
2	B	210	ILE
3	E	818	LYS
3	E	820	GLU
3	E	821	VAL
3	E	822	THR
3	E	827	LEU
3	E	829	PHE
3	E	840	LYS
3	E	844	GLU

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Mol	Chain	Res	Type
3	E	860	VAL
3	E	873	ASN
3	E	875	MET
3	E	877	ILE
3	E	879	PHE
1	C	11	LEU
1	C	22	SER
1	C	28	THR
1	C	29	ARG
1	C	43	SER
1	C	67	SER
1	C	78	VAL
1	C	79	GLN
1	C	104	LEU
1	C	106	LEU
1	C	117	ILE
1	C	125	LEU
1	C	127	SER
1	C	136	LEU
1	C	137	ASN
1	C	142	LYS
1	C	144	ILE
1	C	150	ILE
1	C	155	ARG
1	C	156	GLN
1	C	163	TRP
1	C	169	LYS
1	C	176	SER
1	C	177	SER
1	C	179	LEU
1	C	180	THR
1	C	191	SER
1	C	199	LYS
1	C	200	THR
1	C	207	LYS
1	C	208	SER
1	C	212	ASN
2	D	11	LEU
2	D	14	PRO
2	D	21	SER
2	D	25	SER
2	D	38	ASN

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Mol	Chain	Res	Type
2	D	61	ASP
2	D	74	SER
2	D	76	SER
2	D	81	GLN
2	D	85	GLU
2	D	87	THR
2	D	113	SER
2	D	117	THR
2	D	119	PRO
2	D	120	SER
2	D	128	SER
2	D	131	GLN
2	D	132	THR
2	D	133	ASN
2	D	134	SER
2	D	138	LEU
2	D	143	LYS
2	D	169	VAL
2	D	172	SER
2	D	179	SER
2	D	190	SER
2	D	192	THR
2	D	194	THR
2	D	205	LYS
2	D	208	LYS
3	F	818	LYS
3	F	821	VAL
3	F	834	ILE
3	F	845	GLU
3	F	859	LYS
3	F	860	VAL
3	F	869	GLU
3	F	882	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	37	GLN
1	A	38	GLN
1	A	42	GLN
1	A	156	GLN

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Mol	Chain	Res	Type
1	A	157	ASN
1	A	198	HIS
2	B	39	GLN
2	B	131	GLN
1	C	31	ASN
1	C	37	GLN
1	C	38	GLN
1	C	42	GLN
1	C	79	GLN
1	C	124	GLN
1	C	137	ASN
1	C	145	ASN
1	C	156	GLN
1	C	190	ASN
1	C	198	HIS
1	C	210	ASN
1	C	212	ASN
2	D	3	GLN
2	D	38	ASN
2	D	39	GLN
2	D	99	GLN
2	D	171	GLN
2	D	199	HIS
3	F	874	HIS
3	F	876	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 oligosaccharides 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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	220/220 (100%)	0.16	15 (6%) 23 19	15, 58, 108, 123	3 (1%)
1	C	220/220 (100%)	-0.06	4 (1%) 67 63	16, 66, 103, 122	3 (1%)
2	B	218/218 (100%)	0.08	9 (4%) 41 36	17, 60, 100, 136	2 (0%)
2	D	218/218 (100%)	0.10	10 (4%) 37 32	24, 68, 110, 137	2 (0%)
3	E	65/65 (100%)	-0.06	1 (1%) 72 68	22, 67, 94, 124	1 (1%)
3	F	65/65 (100%)	0.44	6 (9%) 14 11	30, 84, 115, 123	1 (1%)
All	All	1006/1006 (100%)	0.08	45 (4%) 38 32	15, 66, 107, 137	12 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	SER	6.5
2	B	127	GLY	5.6
2	D	140	CYS	5.3
1	A	183	LYS	4.6
2	B	140	CYS	4.3
2	B	128	SER	4.1
2	D	128	SER	4.0
1	C	176	SER	3.9
2	D	210	ILE	3.9
1	A	186	TYR	3.7
1	C	78	VAL	3.6
2	B	129	ALA	3.6
2	B	46	ASN	3.5
3	F	871	GLY	3.5
3	F	845	GLU	3.5
1	A	182	THR	3.4
2	D	46	ASN	3.2
2	D	213	ARG	3.1
3	F	881	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	130	ALA	3.1
1	A	78	VAL	3.0
2	D	132	THR	2.9
1	C	65	ARG	2.7
2	B	132	THR	2.7
2	D	129	ALA	2.7
1	A	194	CYS	2.6
1	A	65	ARG	2.6
3	F	870	ASP	2.6
1	A	181	LEU	2.6
3	E	845	GLU	2.5
1	A	210	ASN	2.5
2	D	127	GLY	2.5
1	A	158	GLY	2.5
1	A	205	ILE	2.4
3	F	882	LYS	2.4
1	A	177	SER	2.3
1	A	152	GLY	2.3
1	A	129	GLY	2.2
2	B	134	SER	2.2
1	A	148	TRP	2.2
3	F	872	GLY	2.1
2	D	182	THR	2.1
2	B	131	GLN	2.1
1	C	214	CYS	2.1
2	D	185	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.