



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:47 PM GMT

PDB ID : 1YMH  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

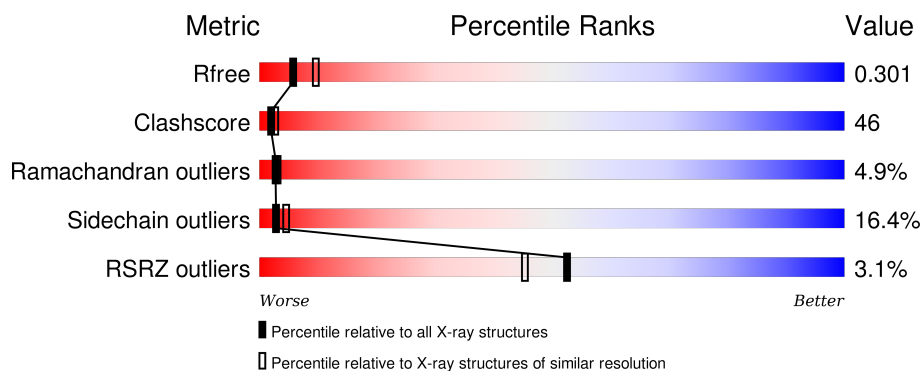
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	<div> <div>2%</div> <div>13% 36% 39% 13%</div> </div>
1	C	220	<div> <div>%</div> <div>13% 46% 34% 8%</div> </div>
2	B	218	<div> <div>3%</div> <div>18% 50% 23% 8%</div> </div>
2	D	218	<div> <div>5%</div> <div>17% 50% 27% 6%</div> </div>
3	E	65	<div> <div>3%</div> <div>8% 58% 25% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	65	<p>9% 11% 45% 31% 14%</p>

## 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	C	20	Total	O	0	0
			20	20		
4	D	26	Total	O	0	0
			26	26		

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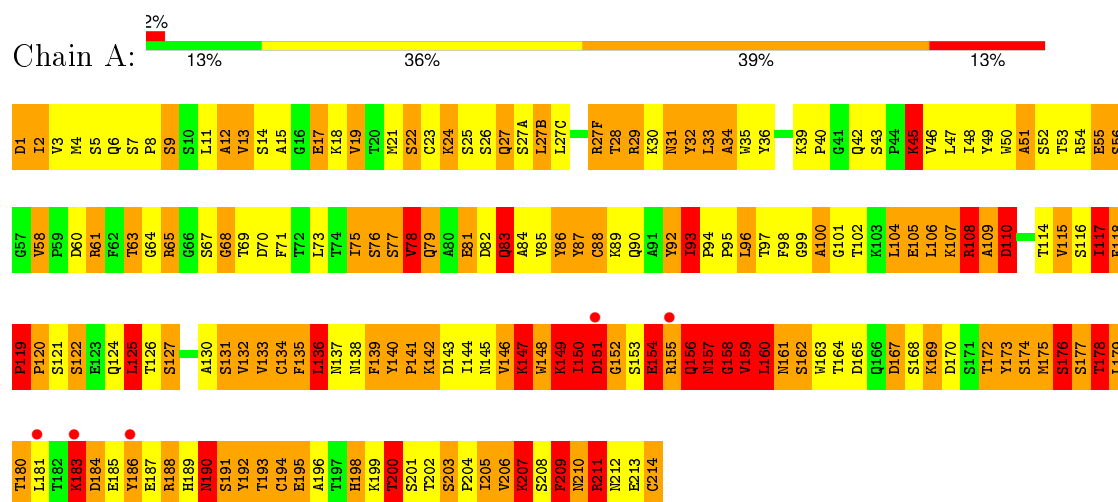
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	6	Total	O	0	0
			6	6		
4	F	3	Total	O	0	0
			3	3		

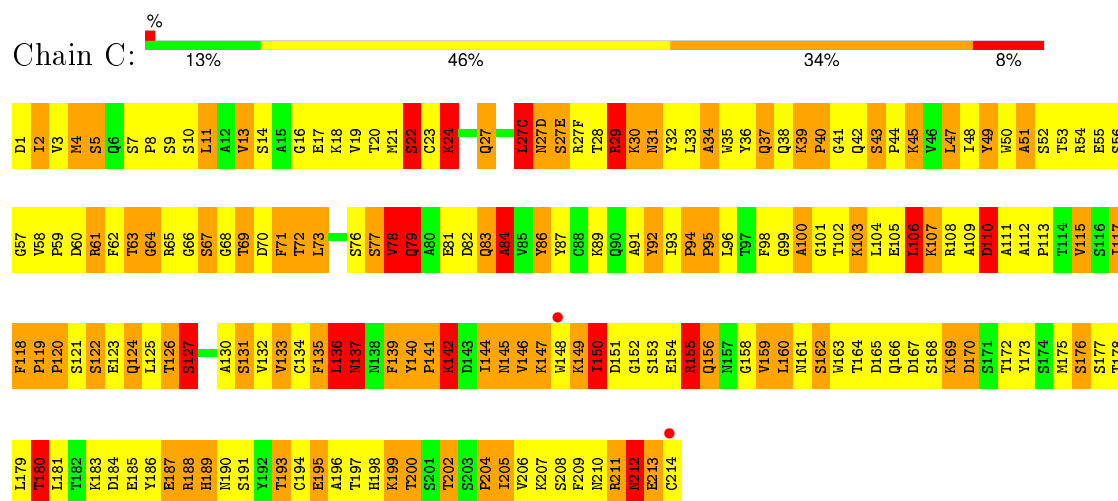
### 3 Residue-property plots

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

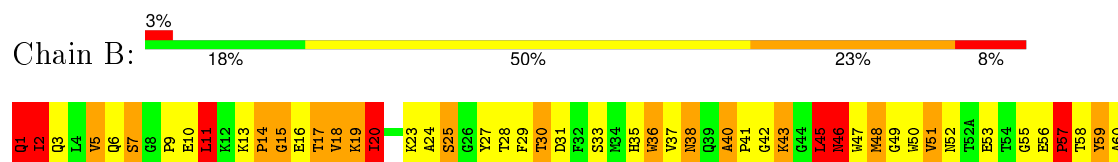
- Molecule 1: Fab 16D9D6, light chain

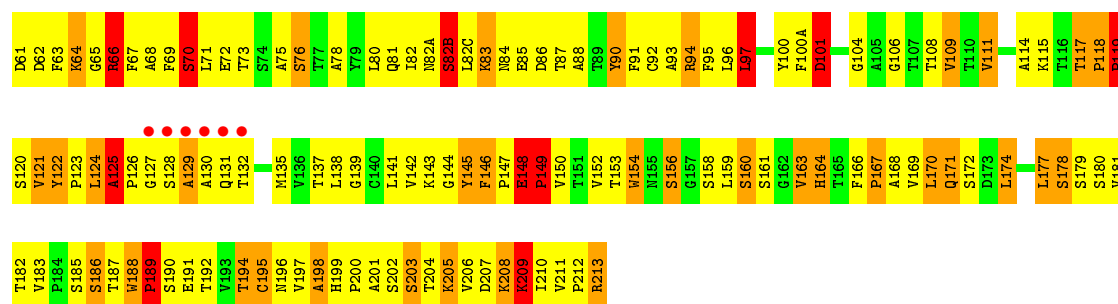


- Molecule 1: Fab 16D9D6, light chain

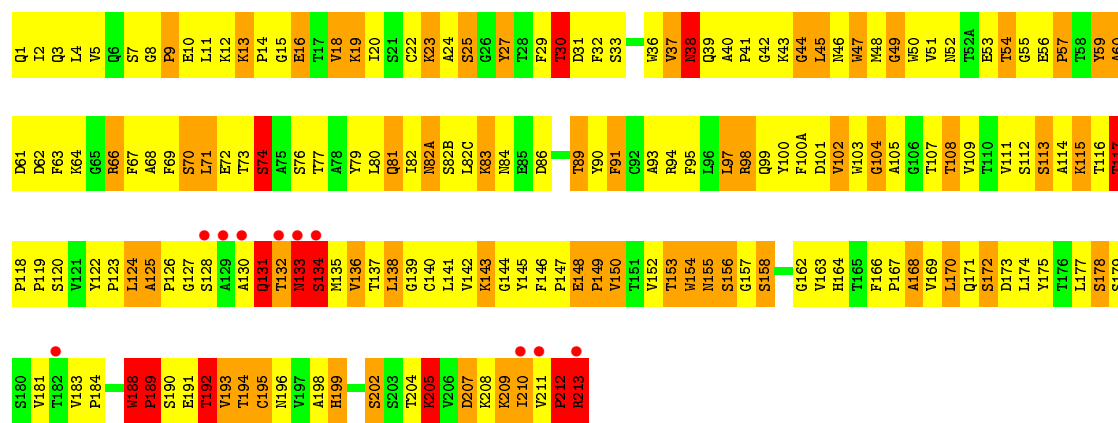


- Molecule 2: Fab 16D9D6, heavy chain

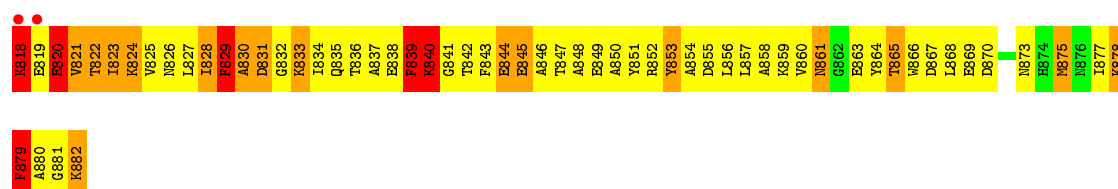
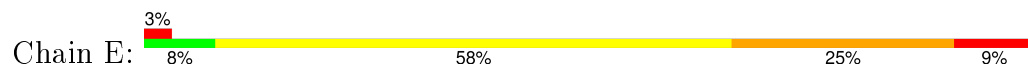




• Molecule 2: Fab 16D9D6, heavy chain



• 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, $\alpha$ , $\beta$ , $\gamma$	77.14Å 111.47Å 148.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.60 89.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (87.71-2.60) 97.5 (89.19-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 40049 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	3.19	192/1745 (11.0%)	2.31	98/2366 (4.1%)
1	C	3.03	173/1745 (9.9%)	2.02	48/2366 (2.0%)
2	B	2.90	134/1707 (7.9%)	2.23	68/2335 (2.9%)
2	D	2.88	151/1707 (8.8%)	2.15	67/2335 (2.9%)
3	E	3.37	73/525 (13.9%)	2.25	29/704 (4.1%)
3	F	2.81	34/525 (6.5%)	2.18	16/704 (2.3%)
All	All	3.02	757/7954 (9.5%)	2.18	326/10810 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	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 (757) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	TYR	CD2-CE2	19.94	1.69	1.39
1	A	50	TRP	CE3-CZ3	15.38	1.64	1.38
1	C	103	LYS	CD-CE	15.16	1.89	1.51
1	A	43	SER	CB-OG	-15.14	1.22	1.42
3	F	849	GLU	CD-OE2	14.76	1.41	1.25
1	A	78	VAL	CB-CG1	-14.47	1.22	1.52
1	A	105	GLU	CD-OE2	14.45	1.41	1.25
1	A	17	GLU	CD-OE1	14.06	1.41	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	GLU	CD-OE1	13.99	1.41	1.25
2	B	10	GLU	CD-OE2	13.65	1.40	1.25
3	E	840	LYS	CD-CE	13.34	1.84	1.51
1	C	49	TYR	CD1-CE1	13.06	1.58	1.39
2	D	25	SER	CB-OG	-12.93	1.25	1.42
2	B	149	PRO	N-CD	12.79	1.65	1.47
3	E	866	TRP	CB-CG	12.57	1.72	1.50
1	A	86	TYR	CG-CD1	-12.11	1.23	1.39
2	D	100	TYR	CD1-CE1	-11.96	1.21	1.39
1	A	52	SER	CB-OG	11.82	1.57	1.42
1	C	30	LYS	CE-NZ	11.82	1.78	1.49
3	F	849	GLU	CD-OE1	11.78	1.38	1.25
2	B	56	GLU	CD-OE1	11.71	1.38	1.25
2	B	7	SER	CA-CB	11.67	1.70	1.52
2	D	189	PRO	N-CD	11.63	1.64	1.47
1	C	166	GLN	C-O	-11.48	1.01	1.23
2	B	27	TYR	CD1-CE1	-11.48	1.22	1.39
2	D	69	PHE	CE2-CZ	-11.47	1.15	1.37
2	D	79	TYR	CD1-CE1	-11.42	1.22	1.39
1	A	1	ASP	N-CA	11.39	1.69	1.46
2	B	122	TYR	CD2-CE2	11.36	1.56	1.39
2	D	72	GLU	CD-OE2	11.20	1.38	1.25
1	A	46	VAL	CA-CB	-11.16	1.31	1.54
1	C	24	LYS	CD-CE	11.05	1.78	1.51
1	C	100	ALA	CA-CB	10.91	1.75	1.52
1	A	81	GLU	CG-CD	10.89	1.68	1.51
1	A	32	TYR	CD1-CE1	10.85	1.55	1.39
1	C	92	TYR	CD1-CE1	10.82	1.55	1.39
1	C	49	TYR	CD2-CE2	10.76	1.55	1.39
2	B	5	VAL	CB-CG1	10.58	1.75	1.52
1	C	51	ALA	CA-CB	-10.52	1.30	1.52
2	B	76	SER	CB-OG	-10.51	1.28	1.42
1	A	46	VAL	CB-CG2	-10.49	1.30	1.52
1	C	209	PHE	CD1-CE1	10.48	1.60	1.39
2	B	15	GLY	C-O	10.42	1.40	1.23
2	D	142	VAL	CB-CG1	-10.40	1.31	1.52
1	C	45	LYS	CB-CG	-10.33	1.24	1.52
2	B	40	ALA	CA-CB	10.30	1.74	1.52
2	D	195	CYS	CB-SG	10.28	1.99	1.82
2	B	36	TRP	CG-CD1	-10.24	1.22	1.36
2	D	51	VAL	CB-CG2	10.24	1.74	1.52
3	E	866	TRP	CG-CD1	10.21	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	TYR	CE2-CZ	10.19	1.51	1.38
2	D	33	SER	C-O	-10.17	1.04	1.23
1	C	78	VAL	CB-CG1	-10.10	1.31	1.52
3	E	864	TYR	C-O	-10.08	1.04	1.23
2	B	92	CYS	CB-SG	-10.05	1.65	1.82
1	A	25	SER	CB-OG	-9.97	1.29	1.42
2	B	27	TYR	CG-CD2	-9.89	1.26	1.39
3	E	824	LYS	CB-CG	9.75	1.78	1.52
1	A	133	VAL	CB-CG1	9.67	1.73	1.52
2	B	2	ILE	C-O	-9.62	1.05	1.23
1	A	23	CYS	CB-SG	-9.55	1.66	1.82
1	A	186	TYR	CZ-OH	9.52	1.54	1.37
2	B	50	TRP	C-O	-9.49	1.05	1.23
2	B	63	PHE	CD1-CE1	9.46	1.58	1.39
2	D	7	SER	CA-CB	-9.45	1.38	1.52
1	C	34	ALA	CA-CB	-9.44	1.32	1.52
3	F	843	PHE	CE2-CZ	9.32	1.55	1.37
2	B	69	PHE	CE1-CZ	9.28	1.54	1.37
2	B	67	PHE	CE2-CZ	9.26	1.54	1.37
3	E	863	GLU	CD-OE1	9.22	1.35	1.25
3	E	825	VAL	CB-CG2	9.19	1.72	1.52
2	D	152	VAL	CB-CG2	-9.19	1.33	1.52
1	C	147	LYS	CD-CE	9.18	1.74	1.51
2	B	111	VAL	CB-CG2	-9.18	1.33	1.52
2	B	197	VAL	CA-CB	9.18	1.74	1.54
2	D	72	GLU	CD-OE1	9.14	1.35	1.25
1	A	13	VAL	CA-CB	-9.12	1.35	1.54
1	A	98	PHE	CE1-CZ	9.12	1.54	1.37
1	C	185	GLU	CD-OE1	9.08	1.35	1.25
1	C	105	GLU	CD-OE2	9.06	1.35	1.25
1	A	206	VAL	CB-CG2	9.04	1.71	1.52
1	C	56	SER	CA-CB	-9.01	1.39	1.52
3	F	841	GLY	CA-C	9.00	1.66	1.51
1	C	87	TYR	CA-CB	-8.99	1.34	1.53
3	F	882	LYS	CD-CE	8.95	1.73	1.51
2	D	157	GLY	C-O	8.94	1.38	1.23
3	E	839	PHE	C-O	-8.94	1.06	1.23
2	D	193	VAL	CB-CG2	8.91	1.71	1.52
2	B	109	VAL	CB-CG1	-8.84	1.34	1.52
2	B	125	ALA	C-N	8.82	1.51	1.34
1	A	184	ASP	CB-CG	8.82	1.70	1.51
1	C	62	PHE	CD2-CE2	-8.81	1.21	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	846	ALA	CA-CB	8.81	1.71	1.52
1	A	60	ASP	CA-CB	8.79	1.73	1.53
1	C	95	PRO	C-O	8.74	1.40	1.23
3	F	851	TYR	CE1-CZ	8.72	1.49	1.38
1	C	45	LYS	CG-CD	8.71	1.82	1.52
1	A	9	SER	C-O	8.70	1.39	1.23
3	F	879	PHE	CE2-CZ	8.70	1.53	1.37
1	C	91	ALA	CA-CB	8.67	1.70	1.52
1	C	115	VAL	CB-CG2	8.65	1.71	1.52
1	C	145	ASN	CB-CG	8.65	1.71	1.51
2	B	1	GLN	CD-NE2	8.64	1.54	1.32
2	D	95	PHE	C-O	-8.63	1.06	1.23
3	F	860	VAL	CB-CG2	8.60	1.71	1.52
2	D	100	TYR	C-O	-8.59	1.07	1.23
3	E	848	ALA	CA-CB	8.58	1.70	1.52
3	E	853	TYR	C-O	8.58	1.39	1.23
1	C	10	SER	CA-CB	-8.56	1.40	1.52
1	A	89	LYS	CE-NZ	-8.55	1.27	1.49
2	D	64	LYS	CD-CE	8.55	1.72	1.51
3	E	851	TYR	CE1-CZ	-8.54	1.27	1.38
1	C	38	GLN	CG-CD	8.53	1.70	1.51
1	C	27	GLN	CD-OE1	8.51	1.42	1.24
2	D	90	TYR	CB-CG	8.50	1.64	1.51
1	C	71	PHE	CD1-CE1	8.48	1.56	1.39
2	B	190	SER	CA-CB	8.48	1.65	1.52
1	A	22	SER	CB-OG	8.46	1.53	1.42
1	A	105	GLU	CD-OE1	8.45	1.34	1.25
1	C	159	VAL	CB-CG2	-8.42	1.35	1.52
2	D	212	PRO	C-O	8.40	1.40	1.23
1	C	79	GLN	CB-CG	8.37	1.75	1.52
1	A	68	GLY	C-O	8.37	1.37	1.23
1	C	4	MET	CB-CG	8.37	1.78	1.51
3	F	839	PHE	CD2-CE2	8.36	1.55	1.39
1	A	169	LYS	CD-CE	8.35	1.72	1.51
2	D	205	LYS	CD-CE	8.32	1.72	1.51
3	E	851	TYR	CG-CD2	-8.31	1.28	1.39
3	E	829	PHE	CD1-CE1	-8.31	1.22	1.39
3	E	826	ASN	C-O	-8.30	1.07	1.23
2	D	152	VAL	CB-CG1	-8.30	1.35	1.52
2	D	79	TYR	C-O	8.29	1.39	1.23
2	B	145	TYR	CD2-CE2	-8.29	1.26	1.39
1	A	61	ARG	CZ-NH2	8.28	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	LEU	C-O	-8.28	1.07	1.23
1	A	4	MET	CG-SD	-8.26	1.59	1.81
2	B	27	TYR	CE2-CZ	-8.25	1.27	1.38
2	B	97	LEU	CG-CD2	8.23	1.82	1.51
1	A	177	SER	CB-OG	8.18	1.52	1.42
1	C	118	PHE	CD1-CE1	-8.18	1.22	1.39
1	A	163	TRP	CB-CG	8.17	1.65	1.50
3	E	839	PHE	CA-CB	-8.16	1.35	1.53
1	A	143	ASP	C-O	8.16	1.38	1.23
1	A	162	SER	CB-OG	8.15	1.52	1.42
1	C	107	LYS	CD-CE	8.13	1.71	1.51
2	B	72	GLU	CG-CD	8.12	1.64	1.51
1	A	209	PHE	CD2-CE2	8.09	1.55	1.39
3	E	837	ALA	CA-CB	-8.09	1.35	1.52
2	D	144	GLY	C-O	8.09	1.36	1.23
2	D	98	ARG	NE-CZ	-8.08	1.22	1.33
2	B	46	ASN	CG-ND2	8.07	1.53	1.32
2	B	48	MET	C-O	-8.06	1.08	1.23
1	C	176	SER	CA-CB	-8.04	1.40	1.52
2	D	90	TYR	CG-CD2	-8.03	1.28	1.39
1	C	55	GLU	CD-OE2	-8.02	1.16	1.25
1	A	98	PHE	CD1-CE1	8.01	1.55	1.39
1	A	135	PHE	CE2-CZ	-8.01	1.22	1.37
2	B	59	TYR	CE1-CZ	-8.01	1.28	1.38
3	E	855	ASP	CA-C	-7.98	1.32	1.52
1	A	87	TYR	CD2-CE2	7.97	1.51	1.39
2	D	40	ALA	CA-CB	7.97	1.69	1.52
3	F	863	GLU	CD-OE1	7.96	1.34	1.25
2	B	57	PRO	CA-C	7.95	1.68	1.52
1	A	27	GLN	CD-OE1	7.93	1.41	1.24
2	B	1	GLN	N-CA	7.92	1.62	1.46
1	A	15	ALA	CA-CB	-7.90	1.35	1.52
1	C	115	VAL	CB-CG1	7.90	1.69	1.52
1	A	180	THR	CB-CG2	7.88	1.78	1.52
2	B	1	GLN	CG-CD	7.87	1.69	1.51
2	D	100	TYR	CE1-CZ	-7.86	1.28	1.38
2	D	27	TYR	CD2-CE2	-7.86	1.27	1.39
1	A	24	LYS	CD-CE	7.85	1.70	1.51
1	A	190	ASN	CB-CG	7.85	1.69	1.51
3	E	847	THR	CA-CB	-7.84	1.32	1.53
2	D	74	SER	CA-CB	7.81	1.64	1.52
1	A	173	TYR	CD1-CE1	-7.79	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	VAL	CA-CB	-7.78	1.38	1.54
1	A	93	ILE	N-CA	-7.78	1.30	1.46
2	B	47	TRP	CG-CD1	-7.75	1.25	1.36
2	B	10	GLU	CD-OE1	7.72	1.34	1.25
3	E	840	LYS	CA-C	-7.69	1.32	1.52
1	C	83	GLN	CD-OE1	7.68	1.40	1.24
1	C	52	SER	C-O	7.66	1.37	1.23
1	C	146	VAL	C-O	7.64	1.37	1.23
3	E	845	GLU	CD-OE1	7.63	1.34	1.25
1	A	36	TYR	CE2-CZ	-7.62	1.28	1.38
1	A	76	SER	CA-CB	-7.62	1.41	1.52
1	A	82	ASP	CA-CB	-7.61	1.37	1.53
1	A	186	TYR	CA-CB	7.60	1.70	1.53
2	D	3	GLN	CA-CB	7.59	1.70	1.53
2	B	37	VAL	N-CA	-7.59	1.31	1.46
1	A	92	TYR	C-O	-7.59	1.08	1.23
2	B	67	PHE	CD1-CE1	7.59	1.54	1.39
1	C	186	TYR	CE2-CZ	-7.57	1.28	1.38
1	A	92	TYR	CD2-CE2	7.56	1.50	1.39
1	A	134	CYS	CB-SG	7.56	1.95	1.82
2	B	169	VAL	CA-CB	-7.56	1.38	1.54
3	F	860	VAL	CA-CB	7.55	1.70	1.54
1	C	149	LYS	CD-CE	7.54	1.70	1.51
2	D	91	PHE	CD1-CE1	-7.54	1.24	1.39
3	E	840	LYS	CB-CG	7.53	1.72	1.52
2	D	16	GLU	CG-CD	-7.53	1.40	1.51
2	B	47	TRP	CA-CB	-7.52	1.37	1.53
1	A	110	ASP	C-O	7.51	1.37	1.23
3	E	835	GLN	CG-CD	-7.49	1.33	1.51
1	C	132	VAL	CB-CG2	-7.46	1.37	1.52
1	C	135	PHE	CD2-CE2	7.45	1.54	1.39
1	A	45	LYS	N-CA	7.43	1.61	1.46
1	A	51	ALA	CA-CB	-7.41	1.36	1.52
3	E	869	GLU	CG-CD	7.41	1.63	1.51
1	A	79	GLN	CG-CD	7.40	1.68	1.51
2	B	69	PHE	N-CA	-7.40	1.31	1.46
1	A	192	TYR	CD2-CE2	7.39	1.50	1.39
1	C	173	TYR	CE2-CZ	7.38	1.48	1.38
2	B	27	TYR	CD2-CE2	-7.38	1.28	1.39
1	C	55	GLU	CG-CD	-7.38	1.40	1.51
1	C	93	ILE	CA-CB	7.38	1.71	1.54
2	B	152	VAL	CB-CG1	7.36	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	845	GLU	CD-OE2	7.36	1.33	1.25
1	C	78	VAL	CB-CG2	-7.35	1.37	1.52
1	A	135	PHE	CB-CG	7.34	1.63	1.51
2	D	81	GLN	CA-C	-7.34	1.33	1.52
3	E	867	ASP	C-O	-7.34	1.09	1.23
1	A	110	ASP	CB-CG	7.33	1.67	1.51
2	D	24	ALA	CA-CB	-7.32	1.37	1.52
2	D	205	LYS	CG-CD	7.29	1.77	1.52
2	B	19	LYS	N-CA	7.28	1.60	1.46
2	D	32	PHE	CE2-CZ	7.28	1.51	1.37
2	B	93	ALA	CA-CB	-7.27	1.37	1.52
2	B	11	LEU	C-O	-7.27	1.09	1.23
2	B	18	VAL	CA-CB	-7.27	1.39	1.54
1	C	36	TYR	CG-CD2	-7.27	1.29	1.39
1	C	169	LYS	CD-CE	7.26	1.69	1.51
1	C	164	THR	C-O	-7.25	1.09	1.23
1	A	188	ARG	NE-CZ	7.25	1.42	1.33
1	A	107	LYS	CE-NZ	7.24	1.67	1.49
1	A	87	TYR	CG-CD2	-7.24	1.29	1.39
2	D	33	SER	CA-C	-7.21	1.34	1.52
2	D	148	GLU	CD-OE1	7.21	1.33	1.25
1	C	180	THR	CA-CB	-7.21	1.34	1.53
2	D	148	GLU	C-O	7.20	1.37	1.23
3	F	876	ASN	CB-CG	7.20	1.67	1.51
1	C	213	GLU	CD-OE1	7.19	1.33	1.25
2	D	43	LYS	N-CA	7.19	1.60	1.46
3	F	844	GLU	CD-OE2	-7.18	1.17	1.25
2	B	142	VAL	CB-CG2	7.17	1.68	1.52
2	B	25	SER	CA-CB	-7.17	1.42	1.52
3	E	844	GLU	CG-CD	7.17	1.62	1.51
2	B	70	SER	CB-OG	7.16	1.51	1.42
2	B	72	GLU	CD-OE1	7.16	1.33	1.25
1	A	81	GLU	CD-OE1	7.15	1.33	1.25
2	D	56	GLU	CD-OE2	7.13	1.33	1.25
2	D	100(A)	PHE	CB-CG	-7.13	1.39	1.51
1	A	45	LYS	CE-NZ	7.11	1.66	1.49
2	D	90	TYR	CD2-CE2	-7.11	1.28	1.39
2	B	58	THR	CB-CG2	-7.10	1.28	1.52
2	B	197	VAL	CA-C	-7.08	1.34	1.52
3	E	881	GLY	C-O	-7.08	1.12	1.23
1	C	84	ALA	N-CA	7.07	1.60	1.46
1	C	162	SER	CB-OG	7.07	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	MET	N-CA	7.06	1.60	1.46
1	C	3	VAL	CB-CG1	7.06	1.67	1.52
2	B	209	LYS	CB-CG	7.06	1.71	1.52
1	A	58	VAL	CA-CB	7.06	1.69	1.54
1	A	36	TYR	CG-CD2	-7.03	1.30	1.39
1	C	142	LYS	CG-CD	7.02	1.76	1.52
2	D	205	LYS	CB-CG	7.00	1.71	1.52
2	D	81	GLN	CB-CG	6.99	1.71	1.52
1	A	140	TYR	CG-CD1	6.95	1.48	1.39
1	A	139	PHE	CD1-CE1	6.94	1.53	1.39
1	C	211	ARG	CB-CG	6.94	1.71	1.52
2	B	43	LYS	CG-CD	6.93	1.76	1.52
1	C	109	ALA	CA-CB	6.93	1.67	1.52
1	C	214	CYS	CA-CB	6.93	1.69	1.53
3	F	843	PHE	CG-CD2	6.91	1.49	1.38
2	D	27	TYR	CD1-CE1	-6.90	1.28	1.39
2	D	77	THR	C-O	-6.90	1.10	1.23
1	A	214	CYS	CB-SG	6.90	1.94	1.82
1	C	52	SER	CA-CB	6.90	1.63	1.52
3	E	864	TYR	CD2-CE2	-6.90	1.28	1.39
1	C	91	ALA	C-O	6.90	1.36	1.23
2	B	154	TRP	CD2-CE2	-6.88	1.33	1.41
3	E	833	LYS	CD-CE	6.87	1.68	1.51
3	F	825	VAL	CA-CB	-6.86	1.40	1.54
1	A	168	SER	C-O	6.85	1.36	1.23
2	B	5	VAL	N-CA	-6.84	1.32	1.46
3	E	861	ASN	C-O	6.83	1.36	1.23
1	A	86	TYR	CE1-CZ	-6.82	1.29	1.38
1	A	45	LYS	CA-CB	-6.80	1.39	1.53
3	E	880	ALA	CA-CB	6.80	1.66	1.52
3	E	831	ASP	CB-CG	6.79	1.66	1.51
1	C	99	GLY	C-O	-6.79	1.12	1.23
1	A	164	THR	N-CA	-6.78	1.32	1.46
2	B	7	SER	CB-OG	6.77	1.51	1.42
1	C	22	SER	CB-OG	6.77	1.51	1.42
1	C	43	SER	CA-CB	-6.77	1.42	1.52
1	A	101	GLY	CA-C	-6.76	1.41	1.51
2	B	75	ALA	C-O	-6.76	1.10	1.23
1	A	29	ARG	NE-CZ	6.75	1.41	1.33
1	C	87	TYR	CB-CG	-6.75	1.41	1.51
2	D	56	GLU	CG-CD	6.74	1.62	1.51
1	C	121	SER	CB-OG	6.73	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	ASP	CB-CG	-6.73	1.37	1.51
2	D	193	VAL	CB-CG1	-6.73	1.38	1.52
1	A	39	LYS	CA-CB	-6.72	1.39	1.53
1	A	90	GLN	CD-NE2	-6.72	1.16	1.32
2	B	36	TRP	CB-CG	6.71	1.62	1.50
3	E	851	TYR	CB-CG	6.71	1.61	1.51
1	A	176	SER	CA-CB	-6.71	1.42	1.52
2	D	1	GLN	CG-CD	6.71	1.66	1.51
2	D	41	PRO	C-O	6.70	1.36	1.23
2	B	100(A)	PHE	CE1-CZ	6.69	1.50	1.37
1	C	147	LYS	CG-CD	6.69	1.75	1.52
1	C	65	ARG	CB-CG	-6.68	1.34	1.52
1	C	150	ILE	C-O	6.67	1.36	1.23
2	D	2	ILE	CA-CB	-6.66	1.39	1.54
1	C	17	GLU	CB-CG	6.66	1.64	1.52
2	B	75	ALA	CA-CB	6.65	1.66	1.52
2	D	42	GLY	C-O	6.65	1.34	1.23
1	A	137	ASN	N-CA	-6.64	1.33	1.46
2	D	37	VAL	CB-CG1	-6.64	1.39	1.52
2	D	77	THR	CA-CB	-6.64	1.36	1.53
1	A	45	LYS	CG-CD	6.64	1.75	1.52
1	A	176	SER	N-CA	-6.64	1.33	1.46
2	B	81	GLN	CD-OE1	6.63	1.38	1.24
2	D	210	ILE	C-O	6.62	1.35	1.23
1	C	100	ALA	C-O	-6.62	1.10	1.23
1	A	186	TYR	CE2-CZ	6.60	1.47	1.38
1	A	192	TYR	CZ-OH	6.59	1.49	1.37
2	D	154	TRP	CD2-CE2	-6.59	1.33	1.41
3	E	843	PHE	CE2-CZ	6.58	1.49	1.37
3	F	879	PHE	CG-CD1	6.58	1.48	1.38
1	C	30	LYS	C-O	6.57	1.35	1.23
3	E	838	GLU	CD-OE2	6.57	1.32	1.25
1	C	18	LYS	C-O	-6.56	1.10	1.23
3	E	818	LYS	CB-CG	6.56	1.70	1.52
3	F	870	ASP	CA-C	6.56	1.70	1.52
3	E	840	LYS	CG-CD	6.54	1.74	1.52
1	A	168	SER	CB-OG	-6.54	1.33	1.42
1	A	86	TYR	CG-CD2	6.53	1.47	1.39
2	B	145	TYR	CZ-OH	6.53	1.49	1.37
1	A	152	GLY	C-O	6.52	1.34	1.23
2	D	83	LYS	CA-C	6.51	1.69	1.52
2	D	115	LYS	CB-CG	6.51	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	42	GLN	CD-OE1	6.49	1.38	1.24
1	A	108	ARG	C-O	6.47	1.35	1.23
1	C	196	ALA	CA-CB	-6.47	1.38	1.52
2	D	74	SER	CB-OG	6.46	1.50	1.42
1	C	35	TRP	CG-CD1	-6.46	1.27	1.36
2	D	79	TYR	CG-CD2	-6.46	1.30	1.39
1	A	61	ARG	NE-CZ	-6.46	1.24	1.33
1	C	43	SER	CB-OG	6.46	1.50	1.42
1	C	61	ARG	CZ-NH1	6.46	1.41	1.33
1	C	214	CYS	CB-SG	6.44	1.93	1.82
2	B	142	VAL	CA-C	-6.44	1.36	1.52
1	C	77	SER	N-CA	-6.43	1.33	1.46
1	A	42	GLN	CA-CB	6.43	1.68	1.53
1	C	27	GLN	CD-NE2	6.43	1.49	1.32
2	D	195	CYS	C-O	6.42	1.35	1.23
2	D	29	PHE	CB-CG	-6.41	1.40	1.51
1	A	68	GLY	CA-C	-6.41	1.41	1.51
1	A	26	SER	C-O	-6.41	1.11	1.23
2	D	93	ALA	N-CA	-6.40	1.33	1.46
2	D	50	TRP	CE3-CZ3	6.39	1.49	1.38
1	A	99	GLY	CA-C	-6.38	1.41	1.51
2	B	198	ALA	CA-CB	6.37	1.65	1.52
1	C	9	SER	CB-OG	6.36	1.50	1.42
2	B	51	VAL	N-CA	-6.35	1.33	1.46
1	C	173	TYR	CE1-CZ	6.35	1.46	1.38
3	E	844	GLU	CD-OE2	6.33	1.32	1.25
2	D	64	LYS	CE-NZ	6.33	1.64	1.49
1	A	86	TYR	CA-C	6.33	1.69	1.52
1	A	190	ASN	CA-C	6.32	1.69	1.52
1	A	61	ARG	CB-CG	-6.32	1.35	1.52
1	A	13	VAL	CB-CG1	6.31	1.66	1.52
2	D	29	PHE	CG-CD2	-6.31	1.29	1.38
2	B	78	ALA	C-O	6.30	1.35	1.23
1	C	213	GLU	CD-OE2	6.30	1.32	1.25
1	C	127	SER	CA-C	6.30	1.69	1.52
1	C	106	LEU	CG-CD1	6.30	1.75	1.51
3	E	870	ASP	CB-CG	6.29	1.65	1.51
2	D	97	LEU	CG-CD2	6.28	1.75	1.51
1	A	86	TYR	CE2-CZ	-6.27	1.30	1.38
2	B	166	PHE	CB-CG	6.27	1.62	1.51
3	E	851	TYR	CA-C	-6.27	1.36	1.52
1	C	111	ALA	CA-CB	6.27	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	197	VAL	CB-CG2	6.27	1.66	1.52
1	A	149	LYS	CE-NZ	6.26	1.64	1.49
2	D	56	GLU	CD-OE1	6.25	1.32	1.25
1	C	196	ALA	N-CA	-6.24	1.33	1.46
2	D	49	GLY	C-O	-6.24	1.13	1.23
3	F	869	GLU	CB-CG	6.22	1.64	1.52
2	D	178	SER	C-O	6.21	1.35	1.23
2	D	157	GLY	CA-C	6.21	1.61	1.51
2	B	49	GLY	C-O	-6.20	1.13	1.23
1	C	160	LEU	CG-CD2	6.20	1.74	1.51
2	D	150	VAL	CB-CG1	-6.19	1.39	1.52
2	D	59	TYR	C-O	-6.19	1.11	1.23
3	E	853	TYR	CG-CD2	-6.18	1.31	1.39
1	A	27	GLN	CG-CD	6.18	1.65	1.51
3	E	852	ARG	N-CA	6.18	1.58	1.46
2	B	10	GLU	CA-C	6.17	1.69	1.52
2	B	28	THR	CA-CB	-6.17	1.37	1.53
1	C	120	PRO	CG-CD	6.17	1.71	1.50
2	B	154	TRP	CB-CG	6.17	1.61	1.50
2	B	213	ARG	CB-CG	6.17	1.69	1.52
2	D	213	ARG	CB-CG	6.15	1.69	1.52
2	D	173	ASP	CB-CG	6.14	1.64	1.51
2	D	211	VAL	CA-CB	6.14	1.67	1.54
3	F	823	ILE	C-O	-6.14	1.11	1.23
1	A	90	GLN	CA-CB	-6.13	1.40	1.53
3	E	826	ASN	CB-CG	6.13	1.65	1.51
2	D	150	VAL	CA-CB	-6.12	1.42	1.54
2	B	87	THR	C-O	-6.12	1.11	1.23
2	B	2	ILE	CB-CG2	6.09	1.71	1.52
1	C	78	VAL	N-CA	-6.09	1.34	1.46
1	A	61	ARG	CZ-NH1	6.08	1.41	1.33
1	A	6	GLN	CA-C	-6.08	1.37	1.52
1	C	64	GLY	C-O	6.07	1.33	1.23
1	A	39	LYS	CD-CE	6.07	1.66	1.51
1	A	110	ASP	CG-OD1	6.07	1.39	1.25
2	D	54	THR	C-O	6.07	1.34	1.23
1	C	76	SER	CA-CB	-6.06	1.43	1.52
2	D	188	TRP	C-O	6.05	1.34	1.23
3	E	875	MET	CG-SD	6.05	1.96	1.81
1	C	17	GLU	C-O	6.05	1.34	1.23
2	D	32	PHE	CD1-CE1	6.04	1.51	1.39
1	A	78	VAL	N-CA	-6.04	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	79	TYR	CZ-OH	6.04	1.48	1.37
3	F	867	ASP	CB-CG	6.04	1.64	1.51
2	D	101	ASP	C-O	-6.03	1.11	1.23
1	C	149	LYS	C-O	6.03	1.34	1.23
1	A	65	ARG	N-CA	-6.02	1.34	1.46
1	C	67	SER	CB-OG	6.02	1.50	1.42
2	B	63	PHE	CB-CG	-6.00	1.41	1.51
1	C	73	LEU	CG-CD2	-6.00	1.29	1.51
1	A	119	PRO	CA-C	-6.00	1.40	1.52
2	B	169	VAL	CB-CG1	-5.99	1.40	1.52
1	C	141	PRO	CA-C	-5.98	1.40	1.52
1	A	71	PHE	CD1-CE1	5.97	1.51	1.39
2	D	205	LYS	CE-NZ	5.97	1.64	1.49
2	D	89	THR	CA-CB	5.97	1.68	1.53
2	D	168	ALA	C-O	-5.97	1.12	1.23
2	D	59	TYR	CE1-CZ	-5.96	1.30	1.38
1	A	65	ARG	NE-CZ	-5.96	1.25	1.33
2	B	17	THR	CA-CB	-5.96	1.37	1.53
3	E	819	GLU	CD-OE2	5.96	1.32	1.25
1	C	188	ARG	CG-CD	5.95	1.66	1.51
2	B	167	PRO	CG-CD	5.94	1.70	1.50
2	D	54	THR	CA-CB	5.94	1.68	1.53
2	D	8	GLY	C-O	5.94	1.33	1.23
2	D	192	THR	C-O	5.92	1.34	1.23
3	E	839	PHE	CG-CD1	5.91	1.47	1.38
1	C	54	ARG	CG-CD	5.91	1.66	1.51
1	A	161	ASN	C-O	5.91	1.34	1.23
2	D	43	LYS	CG-CD	5.90	1.72	1.52
1	C	112	ALA	CA-CB	5.90	1.64	1.52
1	C	11	LEU	C-O	5.90	1.34	1.23
1	C	31	ASN	CA-C	5.89	1.68	1.52
2	D	158	SER	CA-C	5.89	1.68	1.52
1	C	150	ILE	N-CA	5.89	1.58	1.46
2	B	104	GLY	CA-C	-5.88	1.42	1.51
2	B	209	LYS	CD-CE	5.88	1.66	1.51
2	B	33	SER	N-CA	-5.87	1.34	1.46
1	C	185	GLU	CD-OE2	5.86	1.32	1.25
2	D	122	TYR	CE1-CZ	5.86	1.46	1.38
2	B	60	ALA	C-O	5.85	1.34	1.23
2	B	203	SER	C-O	-5.85	1.12	1.23
2	D	57	PRO	CG-CD	5.85	1.70	1.50
1	A	82	ASP	CG-OD2	5.84	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	113	SER	N-CA	5.83	1.58	1.46
1	C	139	PHE	CE1-CZ	5.83	1.48	1.37
1	A	33	LEU	CG-CD2	-5.82	1.30	1.51
2	B	18	VAL	CB-CG2	-5.82	1.40	1.52
1	C	86	TYR	CE1-CZ	-5.82	1.30	1.38
3	F	846	ALA	CA-CB	5.81	1.64	1.52
2	D	115	LYS	CG-CD	5.79	1.72	1.52
2	B	30	THR	C-O	-5.79	1.12	1.23
1	A	173	TYR	CA-CB	5.79	1.66	1.53
2	D	91	PHE	CE2-CZ	-5.78	1.26	1.37
1	C	69	THR	C-O	5.78	1.34	1.23
1	C	153	SER	CB-OG	5.78	1.49	1.42
3	E	852	ARG	CG-CD	5.77	1.66	1.51
1	C	31	ASN	CA-CB	-5.77	1.38	1.53
2	D	1	GLN	N-CA	5.77	1.57	1.46
1	C	186	TYR	CZ-OH	-5.77	1.28	1.37
1	C	93	ILE	C-N	-5.77	1.23	1.34
2	B	70	SER	N-CA	5.76	1.57	1.46
1	C	119	PRO	CA-C	-5.76	1.41	1.52
1	C	57	GLY	C-O	5.75	1.32	1.23
2	B	178	SER	C-O	5.74	1.34	1.23
1	A	90	GLN	CA-C	-5.74	1.38	1.52
2	D	32	PHE	CG-CD1	-5.74	1.30	1.38
1	A	195	GLU	CD-OE1	5.74	1.31	1.25
1	C	41	GLY	N-CA	5.74	1.54	1.46
2	D	156	SER	CA-CB	-5.74	1.44	1.52
2	B	181	VAL	CB-CG1	-5.72	1.40	1.52
3	E	824	LYS	C-O	-5.72	1.12	1.23
2	D	172	SER	CA-CB	5.72	1.61	1.52
1	A	100	ALA	CA-C	5.72	1.67	1.52
1	A	27(C)	LEU	C-O	5.71	1.34	1.23
2	D	77	THR	CB-CG2	5.71	1.71	1.52
2	B	91	PHE	C-O	-5.71	1.12	1.23
2	D	209	LYS	CD-CE	5.70	1.65	1.51
1	C	60	ASP	CG-OD2	5.70	1.38	1.25
1	C	61	ARG	NE-CZ	-5.69	1.25	1.33
2	D	50	TRP	N-CA	-5.69	1.34	1.46
2	D	22	CYS	CB-SG	-5.69	1.72	1.81
1	C	36	TYR	CG-CD1	5.68	1.46	1.39
1	A	2	ILE	CA-CB	-5.68	1.41	1.54
1	A	146	VAL	CB-CG1	5.68	1.64	1.52
1	A	118	PHE	CA-CB	5.67	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	169	VAL	CA-CB	-5.67	1.42	1.54
2	B	95	PHE	CE1-CZ	5.67	1.48	1.37
2	B	100	TYR	CD2-CE2	-5.67	1.30	1.39
2	B	114	ALA	CA-CB	5.66	1.64	1.52
1	A	186	TYR	CE1-CZ	5.65	1.45	1.38
3	F	870	ASP	C-O	5.65	1.34	1.23
1	A	96	LEU	CG-CD2	5.64	1.72	1.51
2	D	82(A)	ASN	N-CA	5.64	1.57	1.46
1	A	177	SER	CA-CB	5.64	1.61	1.52
1	A	148	TRP	CA-C	5.63	1.67	1.52
3	E	878	LYS	CD-CE	5.63	1.65	1.51
3	E	882	LYS	CD-CE	5.63	1.65	1.51
1	A	43	SER	CA-CB	-5.63	1.44	1.52
1	C	32	TYR	CB-CG	5.63	1.60	1.51
1	A	19	VAL	CB-CG1	-5.62	1.41	1.52
2	D	3	GLN	CB-CG	-5.62	1.37	1.52
2	D	155	ASN	C-O	5.61	1.34	1.23
1	A	194	CYS	CB-SG	5.61	1.91	1.82
1	C	47	LEU	N-CA	5.61	1.57	1.46
2	B	37	VAL	CB-CG2	5.60	1.64	1.52
1	A	26	SER	CB-OG	5.60	1.49	1.42
1	C	202	THR	CB-CG2	5.60	1.70	1.52
2	B	31	ASP	C-O	-5.59	1.12	1.23
2	B	104	GLY	N-CA	5.58	1.54	1.46
1	C	1	ASP	C-O	5.58	1.33	1.23
2	D	47	TRP	CG-CD1	-5.58	1.28	1.36
1	A	30	LYS	CB-CG	5.58	1.67	1.52
1	C	94	PRO	CA-C	-5.56	1.41	1.52
1	A	32	TYR	C-O	5.55	1.33	1.23
2	B	38	ASN	CB-CG	5.55	1.63	1.51
2	B	45	LEU	C-O	5.55	1.33	1.23
1	C	36	TYR	CA-CB	-5.55	1.41	1.53
3	E	818	LYS	CD-CE	5.55	1.65	1.51
1	C	16	GLY	C-O	5.55	1.32	1.23
1	A	104	LEU	CA-CB	-5.55	1.41	1.53
1	A	98	PHE	CG-CD2	5.54	1.47	1.38
1	A	43	SER	C-N	-5.54	1.23	1.34
1	C	195	GLU	CD-OE2	5.53	1.31	1.25
2	D	154	TRP	CZ3-CH2	-5.53	1.31	1.40
2	D	212	PRO	CB-CG	5.53	1.77	1.50
2	B	143	LYS	CD-CE	5.53	1.65	1.51
1	A	87	TYR	CZ-OH	5.52	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	878	LYS	CB-CG	5.52	1.67	1.52
1	A	119	PRO	CB-CG	5.52	1.77	1.50
1	C	101	GLY	N-CA	-5.52	1.37	1.46
1	A	93	ILE	CA-CB	5.51	1.67	1.54
1	A	88	CYS	CB-SG	5.51	1.91	1.82
2	B	43	LYS	CE-NZ	5.50	1.62	1.49
2	D	53	GLU	CA-C	5.49	1.67	1.52
2	D	5	VAL	CA-CB	5.48	1.66	1.54
2	D	95	PHE	CE2-CZ	-5.48	1.26	1.37
2	B	57	PRO	CG-CD	5.48	1.68	1.50
1	C	72	THR	CB-CG2	5.47	1.70	1.52
1	C	195	GLU	CG-CD	5.46	1.60	1.51
2	D	79	TYR	CD2-CE2	5.45	1.47	1.39
3	F	866	TRP	CE2-CZ2	5.45	1.49	1.39
2	D	59	TYR	CG-CD1	5.45	1.46	1.39
3	E	853	TYR	CB-CG	-5.45	1.43	1.51
3	F	874	HIS	C-O	-5.45	1.13	1.23
2	B	23	LYS	C-O	-5.44	1.13	1.23
2	B	27	TYR	CB-CG	-5.44	1.43	1.51
1	A	8	PRO	C-O	-5.44	1.12	1.23
1	A	24	LYS	CE-NZ	5.44	1.62	1.49
3	E	861	ASN	C-N	5.44	1.42	1.33
3	E	828	ILE	CA-CB	-5.44	1.42	1.54
2	B	156	SER	N-CA	-5.43	1.35	1.46
2	B	198	ALA	N-CA	5.43	1.57	1.46
2	D	136	VAL	CB-CG1	-5.43	1.41	1.52
2	B	81	GLN	CG-CD	5.43	1.63	1.51
2	D	154	TRP	C-O	5.43	1.33	1.23
2	B	197	VAL	N-CA	-5.43	1.35	1.46
1	A	28	THR	CB-CG2	5.41	1.70	1.52
1	A	50	TRP	CZ2-CH2	5.41	1.47	1.37
1	C	17	GLU	CD-OE1	5.41	1.31	1.25
2	D	107	THR	CA-CB	-5.41	1.39	1.53
1	A	76	SER	N-CA	5.41	1.57	1.46
3	F	845	GLU	CD-OE1	5.41	1.31	1.25
1	C	17	GLU	CD-OE2	5.40	1.31	1.25
3	E	838	GLU	CB-CG	-5.40	1.41	1.52
3	F	859	LYS	CE-NZ	5.40	1.62	1.49
1	A	205	ILE	CA-CB	5.40	1.67	1.54
2	B	122	TYR	CE1-CZ	5.39	1.45	1.38
1	A	125	LEU	CG-CD1	5.39	1.71	1.51
1	C	212	ASN	CB-CG	5.39	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	173	TYR	CB-CG	5.39	1.59	1.51
3	E	857	LEU	C-O	5.38	1.33	1.23
1	A	27(F)	ARG	NE-CZ	5.38	1.40	1.33
1	A	27	GLN	C-O	-5.38	1.13	1.23
1	A	193	THR	CA-CB	5.38	1.67	1.53
3	E	863	GLU	CB-CG	5.38	1.62	1.52
2	D	25	SER	CA-CB	-5.38	1.44	1.52
2	B	160	SER	CB-OG	-5.37	1.35	1.42
2	B	119	PRO	C-O	-5.36	1.12	1.23
3	E	851	TYR	CG-CD1	-5.36	1.32	1.39
1	C	27(F)	ARG	C-O	5.36	1.33	1.23
1	C	39	LYS	CG-CD	5.36	1.70	1.52
1	A	40	PRO	C-O	5.36	1.33	1.23
1	C	150	ILE	CA-C	5.36	1.66	1.52
1	A	183	LYS	CB-CG	5.36	1.67	1.52
2	B	16	GLU	CG-CD	-5.35	1.44	1.51
2	D	117	THR	CA-CB	5.35	1.67	1.53
2	B	163	VAL	CA-CB	-5.35	1.43	1.54
3	E	835	GLN	CA-CB	-5.35	1.42	1.53
1	A	34	ALA	C-O	5.34	1.33	1.23
1	C	214	CYS	C-OXT	5.34	1.33	1.23
1	A	54	ARG	NE-CZ	5.34	1.40	1.33
1	C	140	TYR	CD2-CE2	5.34	1.47	1.39
1	C	124	GLN	CB-CG	5.33	1.67	1.52
2	D	122	TYR	CE2-CZ	5.33	1.45	1.38
1	A	117	ILE	CB-CG2	5.33	1.69	1.52
3	E	853	TYR	CA-CB	5.33	1.65	1.53
1	A	177	SER	CA-C	5.32	1.66	1.52
1	A	176	SER	CA-C	-5.32	1.39	1.52
1	C	212	ASN	N-CA	5.31	1.56	1.46
3	F	866	TRP	CE3-CZ3	5.31	1.47	1.38
1	C	3	VAL	C-O	5.31	1.33	1.23
1	A	174	SER	CA-CB	5.31	1.60	1.52
3	F	869	GLU	CA-CB	5.30	1.65	1.53
1	A	90	GLN	CB-CG	5.30	1.66	1.52
2	D	125	ALA	C-N	5.29	1.44	1.34
1	A	6	GLN	CB-CG	5.29	1.66	1.52
1	C	122	SER	CB-OG	5.29	1.49	1.42
1	A	173	TYR	C-O	5.28	1.33	1.23
2	D	69	PHE	CB-CG	5.28	1.60	1.51
2	B	59	TYR	C-O	5.28	1.33	1.23
2	D	70	SER	N-CA	-5.28	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	833	LYS	C-O	5.28	1.33	1.23
1	C	86	TYR	CB-CG	-5.28	1.43	1.51
2	D	82(A)	ASN	CA-C	-5.27	1.39	1.52
2	D	101	ASP	CB-CG	-5.27	1.40	1.51
1	A	67	SER	CA-CB	-5.26	1.45	1.52
1	A	141	PRO	CG-CD	5.26	1.68	1.50
2	B	95	PHE	CG-CD2	5.26	1.46	1.38
2	D	66	ARG	CG-CD	-5.26	1.38	1.51
2	B	45	LEU	CA-CB	5.25	1.65	1.53
2	B	203	SER	CB-OG	5.25	1.49	1.42
1	A	29	ARG	CB-CG	5.25	1.66	1.52
1	A	48	ILE	N-CA	-5.24	1.35	1.46
2	D	13	LYS	CD-CE	5.24	1.64	1.51
3	F	882	LYS	CG-CD	5.24	1.70	1.52
1	A	146	VAL	C-O	5.23	1.33	1.23
2	B	35	HIS	N-CA	-5.23	1.35	1.46
2	B	121	VAL	CB-CG2	5.23	1.63	1.52
2	D	101	ASP	CG-OD1	5.23	1.37	1.25
3	E	849	GLU	CB-CG	5.23	1.62	1.52
1	C	118	PHE	CB-CG	-5.22	1.42	1.51
1	A	94	PRO	C-O	-5.22	1.12	1.23
2	B	154	TRP	CZ3-CH2	-5.21	1.31	1.40
2	D	53	GLU	CD-OE1	5.21	1.31	1.25
1	A	163	TRP	CG-CD1	5.21	1.44	1.36
3	E	879	PHE	CG-CD2	-5.21	1.30	1.38
2	D	30	THR	CB-CG2	5.21	1.69	1.52
1	C	45	LYS	CD-CE	5.20	1.64	1.51
1	C	58	VAL	CA-CB	5.20	1.65	1.54
1	A	81	GLU	C-O	5.20	1.33	1.23
1	A	169	LYS	C-O	5.20	1.33	1.23
3	E	840	LYS	C-O	5.20	1.33	1.23
1	A	172	THR	CA-C	-5.20	1.39	1.52
1	A	3	VAL	CB-CG2	-5.20	1.42	1.52
1	A	18	LYS	CG-CD	5.20	1.70	1.52
1	A	87	TYR	CG-CD1	-5.19	1.32	1.39
3	E	820	GLU	CG-CD	5.19	1.59	1.51
1	C	40	PRO	N-CD	5.19	1.55	1.47
2	D	114	ALA	CA-CB	-5.19	1.41	1.52
2	D	213	ARG	CG-CD	5.19	1.65	1.51
1	C	130	ALA	C-O	5.18	1.33	1.23
1	C	103	LYS	CE-NZ	5.18	1.62	1.49
2	D	57	PRO	C-O	-5.18	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	823	ILE	N-CA	-5.18	1.35	1.46
2	B	213	ARG	CG-CD	5.17	1.64	1.51
1	C	106	LEU	N-CA	5.17	1.56	1.46
1	C	139	PHE	CG-CD2	-5.17	1.30	1.38
1	C	211	ARG	NE-CZ	5.17	1.39	1.33
1	A	174	SER	C-O	5.16	1.33	1.23
2	D	112	SER	CB-OG	-5.15	1.35	1.42
3	F	839	PHE	CA-CB	-5.15	1.42	1.53
2	D	210	ILE	CA-CB	5.15	1.66	1.54
1	C	35	TRP	N-CA	5.14	1.56	1.46
1	C	154	GLU	CD-OE2	5.14	1.31	1.25
1	A	205	ILE	CB-CG2	5.14	1.68	1.52
1	A	133	VAL	N-CA	-5.14	1.36	1.46
2	D	142	VAL	CB-CG2	-5.14	1.42	1.52
2	D	24	ALA	N-CA	-5.13	1.36	1.46
1	C	186	TYR	C-O	5.13	1.33	1.23
1	A	50	TRP	N-CA	5.13	1.56	1.46
1	A	145	ASN	CB-CG	5.13	1.62	1.51
1	C	35	TRP	CD2-CE2	-5.13	1.35	1.41
2	B	6	GLN	CD-OE1	5.13	1.35	1.24
1	C	140	TYR	CD1-CE1	5.13	1.47	1.39
1	A	50	TRP	CD2-CE2	-5.12	1.35	1.41
2	B	66	ARG	CB-CG	5.12	1.66	1.52
1	C	18	LYS	CE-NZ	5.12	1.61	1.49
2	D	178	SER	CA-CB	-5.12	1.45	1.52
1	C	10	SER	CB-OG	-5.11	1.35	1.42
3	E	844	GLU	CD-OE1	5.11	1.31	1.25
2	B	81	GLN	N-CA	5.11	1.56	1.46
1	A	75	ILE	C-O	5.10	1.33	1.23
1	C	37	GLN	CB-CG	-5.10	1.38	1.52
2	B	20	ILE	CA-C	-5.10	1.39	1.52
1	A	12	ALA	N-CA	5.10	1.56	1.46
3	E	852	ARG	CZ-NH1	5.09	1.39	1.33
1	A	73	LEU	C-O	5.08	1.33	1.23
2	B	109	VAL	CA-CB	-5.08	1.44	1.54
1	A	85	VAL	CB-CG1	-5.08	1.42	1.52
2	B	42	GLY	CA-C	5.08	1.59	1.51
1	C	13	VAL	CB-CG1	-5.08	1.42	1.52
1	C	101	GLY	C-O	-5.08	1.15	1.23
2	D	199	HIS	C-O	-5.08	1.13	1.23
1	A	210	ASN	C-O	5.07	1.32	1.23
3	E	877	ILE	CB-CG2	-5.07	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32	TYR	CE2-CZ	-5.07	1.31	1.38
1	A	173	TYR	CD2-CE2	-5.06	1.31	1.39
2	D	74	SER	C-O	-5.06	1.13	1.23
3	E	867	ASP	CG-OD2	5.06	1.36	1.25
3	E	837	ALA	CA-C	-5.06	1.39	1.52
2	D	198	ALA	C-O	5.06	1.32	1.23
1	A	27(B)	LEU	CA-C	-5.06	1.39	1.52
1	A	195	GLU	CG-CD	5.06	1.59	1.51
1	C	43	SER	C-N	-5.05	1.24	1.34
2	D	100(A)	PHE	C-N	-5.05	1.22	1.34
3	E	824	LYS	N-CA	5.05	1.56	1.46
2	D	140	CYS	CA-C	-5.05	1.39	1.52
1	A	31	ASN	C-O	5.05	1.32	1.23
2	D	143	LYS	CG-CD	5.05	1.69	1.52
2	D	175	TYR	CZ-OH	5.05	1.46	1.37
1	A	95	PRO	CA-CB	5.04	1.63	1.53
2	D	124	LEU	N-CA	-5.04	1.36	1.46
1	C	76	SER	C-O	5.04	1.32	1.23
3	E	864	TYR	CE1-CZ	-5.03	1.32	1.38
1	C	29	ARG	CG-CD	5.03	1.64	1.51
1	C	105	GLU	CG-CD	5.03	1.59	1.51
2	D	115	LYS	CD-CE	5.03	1.63	1.51
2	B	142	VAL	CA-CB	5.03	1.65	1.54
3	F	851	TYR	CZ-OH	5.02	1.46	1.37
2	B	195	CYS	C-O	-5.02	1.13	1.23
1	C	81	GLU	CD-OE1	5.02	1.31	1.25
2	B	172	SER	CA-CB	5.02	1.60	1.52
3	F	858	ALA	C-O	5.01	1.32	1.23
2	B	72	GLU	C-O	5.01	1.32	1.23
2	B	94	ARG	CD-NE	-5.01	1.38	1.46
1	A	42	GLN	C-O	-5.01	1.13	1.23
1	A	106	LEU	CG-CD1	-5.01	1.33	1.51
1	C	131	SER	CA-C	-5.00	1.40	1.52
1	A	26	SER	CA-CB	5.00	1.60	1.52
2	B	14	PRO	CA-CB	-5.00	1.43	1.53

All (326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	94	ARG	NE-CZ-NH2	-15.19	112.71	120.30
1	A	61	ARG	NE-CZ-NH1	-14.70	112.95	120.30
1	C	60	ASP	CB-CG-OD1	-13.37	106.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	149	PRO	CA-N-CD	-13.29	92.89	111.50
1	C	60	ASP	CB-CG-OD2	13.14	130.12	118.30
2	D	189	PRO	CA-N-CD	-13.13	93.12	111.50
3	F	819	GLU	OE1-CD-OE2	-12.26	108.59	123.30
2	D	207	ASP	CB-CG-OD2	11.93	129.04	118.30
2	B	124	LEU	CB-CG-CD1	-11.59	91.30	111.00
1	A	63	THR	CA-CB-CG2	-11.31	96.56	112.40
2	D	183	VAL	C-N-CD	11.13	151.78	128.40
2	B	62	ASP	CB-CG-OD1	-10.98	108.42	118.30
2	D	94	ARG	NE-CZ-NH1	10.80	125.70	120.30
2	D	79	TYR	CB-CG-CD2	10.53	127.32	121.00
1	A	155	ARG	NE-CZ-NH2	10.22	125.41	120.30
1	A	4	MET	CG-SD-CE	10.07	116.31	100.20
2	D	207	ASP	CB-CG-OD1	-10.07	109.24	118.30
2	B	92	CYS	CA-CB-SG	10.00	132.00	114.00
2	B	108	THR	OG1-CB-CG2	-9.98	87.04	110.00
2	B	124	LEU	CB-CG-CD2	9.58	127.29	111.00
3	E	840	LYS	CB-CA-C	-9.51	91.38	110.40
2	B	189	PRO	N-CD-CG	-9.34	89.19	103.20
2	B	62	ASP	CB-CG-OD2	9.33	126.69	118.30
1	A	158	GLY	C-N-CA	9.32	145.00	121.70
1	C	110	ASP	CB-CG-OD2	9.29	126.66	118.30
2	B	2	ILE	O-C-N	-9.17	108.03	122.70
2	D	62	ASP	CB-CG-OD2	9.17	126.55	118.30
1	A	27(B)	LEU	CB-CG-CD1	9.00	126.31	111.00
2	B	76	SER	CB-CA-C	9.00	127.20	110.10
2	D	79	TYR	CG-CD1-CE1	8.99	128.50	121.30
1	A	95	PRO	N-CD-CG	8.89	116.54	103.20
1	A	108	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	C	78	VAL	CG1-CB-CG2	-8.82	96.78	110.90
1	A	115	VAL	CB-CA-C	-8.80	94.67	111.40
1	A	108	ARG	NE-CZ-NH2	-8.78	115.91	120.30
2	B	94	ARG	NE-CZ-NH1	-8.77	115.92	120.30
3	F	867	ASP	CB-CG-OD1	8.72	126.15	118.30
2	D	188	TRP	O-C-N	-8.72	104.54	121.10
2	D	108	THR	OG1-CB-CG2	-8.63	90.16	110.00
2	B	129	ALA	O-C-N	-8.62	108.91	122.70
1	A	27(F)	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	165	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	A	93	ILE	CA-CB-CG2	8.39	127.68	110.90
2	B	2	ILE	CB-CA-C	8.39	128.38	111.60
2	B	91	PHE	CB-CG-CD2	8.32	126.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	853	TYR	CB-CG-CD2	-8.24	116.05	121.00
1	A	167	ASP	CB-CG-OD1	8.21	125.69	118.30
2	B	91	PHE	CB-CG-CD1	-8.19	115.07	120.80
1	C	184	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	114	THR	OG1-CB-CG2	-8.08	91.42	110.00
2	D	140	CYS	CA-CB-SG	-8.03	99.55	114.00
2	D	44	GLY	N-CA-C	7.98	133.04	113.10
3	E	828	ILE	CA-CB-CG1	7.87	125.95	111.00
2	D	118	PRO	N-CD-CG	-7.87	91.39	103.20
2	D	18	VAL	CG1-CB-CG2	7.82	123.42	110.90
2	D	184	PRO	CA-N-CD	-7.82	100.56	111.50
2	D	81	GLN	CB-CA-C	-7.78	94.83	110.40
1	A	114	THR	N-CA-C	-7.71	90.17	111.00
1	C	54	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	C	165	ASP	CB-CG-OD2	7.64	125.18	118.30
3	F	869	GLU	N-CA-CB	7.64	124.35	110.60
1	A	60	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	110	ASP	CB-CG-OD2	-7.53	111.53	118.30
2	B	61	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	81	GLU	OE1-CD-OE2	-7.49	114.32	123.30
1	A	83	GLN	N-CA-CB	7.49	124.08	110.60
1	C	84	ALA	CB-CA-C	-7.47	98.89	110.10
2	D	188	TRP	CA-C-N	7.46	138.00	117.10
3	F	818	LYS	C-N-CA	7.46	140.36	121.70
1	A	159	VAL	CA-CB-CG2	7.43	122.04	110.90
1	C	155	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	108	ARG	NE-CZ-NH1	7.32	123.96	120.30
3	E	868	LEU	CB-CG-CD2	-7.28	98.63	111.00
1	C	96	LEU	CA-CB-CG	7.24	131.95	115.30
1	A	184	ASP	CB-CG-OD2	7.24	124.81	118.30
3	F	821	VAL	CA-CB-CG1	7.20	121.70	110.90
2	B	125	ALA	CB-CA-C	7.19	120.88	110.10
3	E	840	LYS	CB-CG-CD	-7.18	92.94	111.60
2	D	10	GLU	OE1-CD-OE2	-7.11	114.77	123.30
1	A	21	MET	CG-SD-CE	7.08	111.52	100.20
2	D	105	ALA	C-N-CA	-7.07	107.46	122.30
2	D	104	GLY	N-CA-C	-7.06	95.44	113.10
1	A	130	ALA	O-C-N	-7.06	111.41	122.70
1	A	109	ALA	CB-CA-C	7.05	120.68	110.10
1	A	131	SER	CB-CA-C	7.05	123.49	110.10
2	D	188	TRP	CB-CA-C	7.04	124.48	110.40
1	A	200	THR	CA-CB-CG2	7.02	122.23	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	A	173	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	A	102	THR	CA-CB-CG2	-6.98	102.63	112.40
2	B	148	GLU	N-CA-CB	6.97	123.16	110.60
1	C	139	PHE	CB-CG-CD2	-6.97	115.92	120.80
1	A	136	LEU	CB-CG-CD2	-6.96	99.16	111.00
1	A	104	LEU	CB-CA-C	-6.96	96.97	110.20
2	B	146	PHE	O-C-N	-6.95	107.89	121.10
1	A	110	ASP	CB-CG-OD1	6.94	124.55	118.30
1	C	167	ASP	CB-CG-OD1	-6.93	112.06	118.30
2	B	129	ALA	CA-C-N	6.89	132.37	117.20
1	A	195	GLU	CA-C-N	-6.88	102.06	117.20
1	C	112	ALA	CB-CA-C	-6.83	99.86	110.10
1	A	194	CYS	CA-CB-SG	6.82	126.28	114.00
3	E	823	ILE	CG1-CB-CG2	-6.76	96.52	111.40
1	C	176	SER	CB-CA-C	-6.75	97.27	110.10
2	D	62	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	C	188	ARG	CA-CB-CG	6.71	128.17	113.40
3	F	868	LEU	CB-CG-CD2	6.71	122.40	111.00
2	D	130	ALA	C-N-CA	6.68	138.39	121.70
1	A	190	ASN	N-CA-C	6.65	128.96	111.00
1	A	211	ARG	C-N-CA	6.64	138.30	121.70
1	C	147	LYS	CD-CE-NZ	6.64	126.97	111.70
3	E	840	LYS	N-CA-CB	-6.63	98.66	110.60
3	F	869	GLU	N-CA-C	-6.63	93.11	111.00
2	B	47	TRP	CG-CD1-NE1	6.60	116.70	110.10
1	A	29	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	61	ARG	NE-CZ-NH1	-6.58	117.01	120.30
2	D	125	ALA	C-N-CD	6.57	142.19	128.40
1	A	49	TYR	CG-CD2-CE2	-6.57	116.05	121.30
3	E	869	GLU	O-C-N	-6.56	112.20	122.70
2	B	86	ASP	CB-CG-OD2	-6.56	112.40	118.30
2	D	148	GLU	OE1-CD-OE2	-6.54	115.45	123.30
2	B	63	PHE	CZ-CE2-CD2	6.53	127.94	120.10
1	A	87	TYR	CG-CD1-CE1	6.53	126.52	121.30
1	A	27(C)	LEU	CB-CG-CD1	6.49	122.03	111.00
1	A	33	LEU	CA-CB-CG	-6.49	100.39	115.30
2	D	141	LEU	CA-CB-CG	6.48	130.19	115.30
1	C	5	SER	CA-CB-OG	-6.44	93.80	111.20
1	A	150	ILE	C-N-CA	6.42	137.75	121.70
1	A	77	SER	N-CA-CB	-6.41	100.89	110.50
3	E	839	PHE	C-N-CA	6.39	137.68	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	VAL	CB-CA-C	-6.39	99.26	111.40
1	A	54	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	A	45	LYS	CD-CE-NZ	-6.36	97.07	111.70
1	A	178	THR	CA-C-N	-6.34	103.26	117.20
1	C	119	PRO	N-CD-CG	-6.31	93.74	103.20
1	A	181	LEU	CB-CG-CD1	6.30	121.71	111.00
2	D	173	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	170	ASP	CB-CG-OD2	6.29	123.97	118.30
3	E	820	GLU	N-CA-C	6.29	127.99	111.00
1	A	175	MET	CB-CA-C	-6.25	97.91	110.40
1	A	92	TYR	CZ-CE2-CD2	-6.23	114.19	119.80
3	E	870	ASP	CB-CG-OD2	6.23	123.90	118.30
1	A	78	VAL	CB-CA-C	6.22	123.22	111.40
2	B	33	SER	N-CA-CB	-6.21	101.19	110.50
1	C	47	LEU	CB-CG-CD2	-6.16	100.53	111.00
2	B	117	THR	CA-CB-CG2	6.15	121.01	112.40
1	C	173	TYR	CD1-CE1-CZ	-6.15	114.27	119.80
1	A	147	LYS	CA-C-N	-6.14	103.68	117.20
2	B	121	VAL	C-N-CA	-6.14	106.34	121.70
2	B	56	GLU	CB-CG-CD	-6.14	97.63	114.20
1	A	85	VAL	O-C-N	-6.13	112.88	122.70
2	B	66	ARG	CG-CD-NE	-6.13	98.92	111.80
1	A	142	LYS	CD-CE-NZ	6.13	125.80	111.70
1	A	212	ASN	N-CA-C	6.13	127.55	111.00
1	A	136	LEU	CB-CG-CD1	6.12	121.41	111.00
2	B	18	VAL	CA-CB-CG2	-6.10	101.75	110.90
2	D	56	GLU	N-CA-C	6.09	127.44	111.00
1	C	102	THR	CA-CB-CG2	-6.09	103.88	112.40
3	E	855	ASP	CB-CG-OD2	6.06	123.75	118.30
1	C	27(C)	LEU	CB-CG-CD1	6.06	121.30	111.00
2	D	170	LEU	CB-CG-CD2	6.05	121.29	111.00
2	D	29	PHE	CB-CG-CD1	6.02	125.01	120.80
2	D	156	SER	N-CA-CB	-6.02	101.47	110.50
1	A	157	ASN	N-CA-CB	6.01	121.43	110.60
2	B	10	GLU	OE1-CD-OE2	6.01	130.52	123.30
1	C	133	VAL	CG1-CB-CG2	6.01	120.51	110.90
1	A	188	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	61	ARG	NH1-CZ-NH2	6.00	126.00	119.40
1	C	104	LEU	CB-CG-CD1	5.99	121.19	111.00
3	F	821	VAL	C-N-CA	5.99	136.68	121.70
2	B	66	ARG	N-CA-C	5.99	127.16	111.00
2	B	121	VAL	CA-CB-CG1	5.98	119.87	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27(C)	LEU	CA-CB-CG	-5.98	101.55	115.30
2	B	56	GLU	N-CA-CB	-5.96	99.88	110.60
2	D	31	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	62	PHE	CB-CG-CD2	-5.95	116.63	120.80
3	F	822	THR	O-C-N	-5.95	113.18	122.70
3	E	857	LEU	CB-CG-CD2	-5.94	100.90	111.00
3	E	842	THR	OG1-CB-CG2	-5.94	96.34	110.00
1	A	186	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	A	27(B)	LEU	N-CA-C	-5.90	95.07	111.00
1	C	130	ALA	C-N-CA	-5.88	106.99	121.70
2	B	164	HIS	N-CA-CB	5.87	121.17	110.60
2	B	90	TYR	CB-CG-CD1	5.86	124.52	121.00
1	A	200	THR	O-C-N	-5.86	113.33	122.70
2	D	79	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	A	132	VAL	CB-CA-C	-5.82	100.33	111.40
1	C	78	VAL	CA-CB-CG1	-5.82	102.17	110.90
3	E	851	TYR	CB-CG-CD2	5.82	124.49	121.00
2	D	23	LYS	CA-CB-CG	5.81	126.19	113.40
2	B	121	VAL	O-C-N	-5.79	113.43	122.70
1	A	90	GLN	O-C-N	5.79	131.96	122.70
2	D	131	GLN	C-N-CA	5.78	136.15	121.70
1	A	155	ARG	CD-NE-CZ	5.76	131.67	123.60
1	A	143	ASP	CB-CG-OD1	-5.76	113.12	118.30
2	D	79	TYR	CA-C-N	-5.76	104.53	117.20
1	A	151	ASP	N-CA-C	5.75	126.53	111.00
2	B	163	VAL	CB-CA-C	-5.75	100.48	111.40
2	B	73	THR	OG1-CB-CG2	-5.73	96.81	110.00
1	A	130	ALA	N-CA-CB	5.73	118.12	110.10
2	B	197	VAL	CG1-CB-CG2	5.73	120.06	110.90
2	B	48	MET	O-C-N	-5.72	113.48	123.20
2	B	80	LEU	CB-CG-CD2	5.72	120.72	111.00
2	B	170	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	C	11	LEU	CB-CA-C	-5.71	99.36	110.20
3	F	851	TYR	N-CA-CB	5.70	120.87	110.60
3	E	820	GLU	N-CA-CB	5.70	120.85	110.60
2	D	36	TRP	N-CA-CB	5.69	120.84	110.60
1	C	63	THR	CA-CB-CG2	-5.69	104.44	112.40
1	A	188	ARG	NE-CZ-NH2	5.67	123.13	120.30
3	F	866	TRP	CA-CB-CG	5.66	124.45	113.70
1	C	155	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	D	19	LYS	CD-CE-NZ	-5.66	98.69	111.70
3	F	825	VAL	CG1-CB-CG2	5.66	119.95	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	136	LEU	CB-CG-CD2	5.65	120.60	111.00
2	B	192	THR	N-CA-C	-5.64	95.77	111.00
2	B	86	ASP	CB-CG-OD1	5.64	123.38	118.30
2	B	148	GLU	O-C-N	-5.63	110.40	121.10
2	D	107	THR	CA-CB-CG2	-5.63	104.52	112.40
2	D	213	ARG	NE-CZ-NH1	-5.62	117.49	120.30
2	B	213	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	82	ASP	CB-CG-OD1	-5.60	113.26	118.30
2	D	202	SER	N-CA-CB	-5.60	102.10	110.50
1	C	211	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	201	ALA	C-N-CA	5.58	135.65	121.70
3	E	851	TYR	CB-CG-CD1	-5.57	117.66	121.00
2	D	175	TYR	CA-CB-CG	5.57	123.98	113.40
2	B	106	GLY	CA-C-O	-5.56	110.59	120.60
1	A	156	GLN	CG-CD-OE1	-5.55	110.49	121.60
2	B	80	LEU	CB-CG-CD1	-5.55	101.57	111.00
1	C	43	SER	N-CA-CB	-5.55	102.18	110.50
2	B	66	ARG	N-CA-CB	-5.50	100.69	110.60
2	D	173	ASP	OD1-CG-OD2	-5.50	112.84	123.30
2	B	60	ALA	N-CA-CB	5.49	117.79	110.10
2	D	189	PRO	CB-CA-C	5.49	125.73	112.00
2	D	125	ALA	O-C-N	5.48	131.51	121.10
3	E	854	ALA	N-CA-CB	5.47	117.76	110.10
2	D	188	TRP	CA-C-O	-5.47	108.61	120.10
1	C	113	PRO	N-CD-CG	-5.46	95.00	103.20
1	A	109	ALA	O-C-N	-5.46	113.96	122.70
3	E	853	TYR	CB-CG-CD1	5.46	124.28	121.00
1	A	100	ALA	CB-CA-C	-5.45	101.93	110.10
3	E	838	GLU	OE1-CD-OE2	5.43	129.82	123.30
2	B	30	THR	CA-CB-CG2	5.43	120.00	112.40
1	A	82	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	148	TRP	CA-C-N	-5.42	105.28	117.20
1	C	61	ARG	CD-NE-CZ	-5.42	116.01	123.60
2	D	173	ASP	CB-CG-OD1	5.42	123.18	118.30
2	D	134	SER	C-N-CA	5.42	135.24	121.70
3	F	823	ILE	O-C-N	-5.41	114.04	122.70
2	D	188	TRP	N-CA-CB	5.40	120.31	110.60
1	A	146	VAL	CA-C-N	-5.39	105.34	117.20
1	A	207	LYS	CD-CE-NZ	5.39	124.09	111.70
2	D	150	VAL	CB-CA-C	-5.38	101.17	111.40
1	C	72	THR	CA-CB-CG2	-5.38	104.87	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	LEU	CB-CG-CD2	-5.37	101.86	111.00
2	B	190	SER	N-CA-CB	5.37	118.55	110.50
3	E	865	THR	CA-CB-CG2	-5.36	104.90	112.40
1	A	159	VAL	CA-CB-CG1	5.35	118.93	110.90
1	C	11	LEU	CA-CB-CG	5.35	127.61	115.30
3	E	827	LEU	CB-CG-CD1	-5.35	101.91	111.00
2	B	132	THR	CA-CB-CG2	5.34	119.87	112.40
3	E	828	ILE	O-C-N	-5.34	114.16	122.70
1	A	151	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	160	LEU	CA-C-N	-5.33	105.47	117.20
1	C	27(E)	SER	O-C-N	5.33	131.23	122.70
1	A	139	PHE	CD1-CE1-CZ	-5.33	113.71	120.10
1	A	84	ALA	CB-CA-C	-5.32	102.11	110.10
2	D	124	LEU	CA-CB-CG	5.32	127.54	115.30
3	E	825	VAL	CB-CA-C	-5.32	101.30	111.40
1	A	186	TYR	CB-CG-CD2	5.31	124.19	121.00
2	D	30	THR	CA-C-O	-5.31	108.95	120.10
1	A	188	ARG	NH1-CZ-NH2	-5.30	113.56	119.40
1	A	130	ALA	CB-CA-C	5.30	118.05	110.10
1	A	86	TYR	CD1-CE1-CZ	5.29	124.56	119.80
1	A	3	VAL	CB-CA-C	-5.29	101.36	111.40
1	A	84	ALA	N-CA-CB	-5.28	102.71	110.10
3	E	869	GLU	OE1-CD-OE2	-5.27	116.97	123.30
3	E	819	GLU	N-CA-C	5.27	125.23	111.00
2	B	46	ASN	CB-CG-OD1	-5.26	111.07	121.60
3	F	875	MET	CG-SD-CE	5.26	108.61	100.20
1	C	193	THR	N-CA-CB	-5.25	100.33	110.30
2	B	66	ARG	NE-CZ-NH1	-5.24	117.68	120.30
3	E	829	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	A	53	THR	OG1-CB-CG2	-5.21	98.00	110.00
2	B	83	LYS	CA-CB-CG	5.21	124.86	113.40
3	F	844	GLU	CG-CD-OE1	5.21	128.71	118.30
2	B	60	ALA	N-CA-C	-5.21	96.95	111.00
2	B	148	GLU	CA-C-N	5.18	131.60	117.10
2	D	71	LEU	CB-CG-CD1	-5.17	102.20	111.00
2	D	15	GLY	N-CA-C	5.17	126.03	113.10
1	C	189	HIS	C-N-CA	-5.16	108.80	121.70
1	C	87	TYR	CG-CD2-CE2	5.15	125.42	121.30
3	E	855	ASP	OD1-CG-OD2	-5.15	113.51	123.30
3	E	864	TYR	CE1-CZ-OH	-5.15	106.19	120.10
1	A	78	VAL	CA-CB-CG1	-5.14	103.18	110.90
2	D	60	ALA	CB-CA-C	-5.14	102.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	83	LYS	N-CA-C	5.14	124.88	111.00
2	D	153	THR	CA-C-O	5.14	130.90	120.10
1	C	187	GLU	CB-CA-C	5.12	120.65	110.40
1	A	18	LYS	CB-CG-CD	5.12	124.91	111.60
2	B	91	PHE	N-CA-C	5.12	124.82	111.00
2	B	109	VAL	CA-CB-CG1	-5.12	103.22	110.90
2	B	189	PRO	C-N-CA	5.12	134.49	121.70
1	C	137	ASN	N-CA-C	5.11	124.80	111.00
2	D	40	ALA	CB-CA-C	5.11	117.76	110.10
2	D	102	VAL	CA-CB-CG2	5.10	118.55	110.90
1	A	175	MET	CG-SD-CE	5.08	108.33	100.20
2	D	109	VAL	CG1-CB-CG2	-5.08	102.77	110.90
2	B	166	PHE	CB-CG-CD1	5.07	124.35	120.80
2	D	98	ARG	NE-CZ-NH2	-5.07	117.76	120.30
2	D	134	SER	CB-CA-C	5.07	119.73	110.10
2	B	182	THR	CA-CB-CG2	5.04	119.46	112.40
2	B	201	ALA	N-CA-C	5.04	124.61	111.00
2	D	9	PRO	N-CD-CG	-5.04	95.64	103.20
2	D	132	THR	N-CA-CB	5.04	119.87	110.30
2	B	118	PRO	CA-C-O	5.04	132.29	120.20
1	A	135	PHE	CB-CG-CD1	5.04	124.33	120.80
1	A	207	LYS	N-CA-C	-5.03	97.41	111.00
1	A	157	ASN	OD1-CG-ND2	-5.03	110.33	121.90
1	A	162	SER	CA-CB-OG	5.03	124.78	111.20
1	C	27(F)	ARG	O-C-N	5.02	130.74	122.70
2	D	148	GLU	CG-CD-OE1	5.01	128.33	118.30
1	A	152	GLY	O-C-N	5.00	130.70	122.70
2	D	198	ALA	N-CA-CB	-5.00	103.09	110.10
3	F	871	GLY	CA-C-O	-5.00	111.59	120.60

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
1	A	152	GLY	Peptide
1	A	156	GLN	Sidechain,Mainchain
1	A	157	ASN	Sidechain,Mainchain
1	A	158	GLY	Peptide
1	A	159	VAL	Mainchain
1	A	160	LEU	Mainchain
1	A	173	TYR	Sidechain,Mainchain
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	Mainchain,Peptide
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	Mainchain,Peptide
2	D	213	ARG	Sidechain
2	D	23	LYS	Mainchain
2	D	30	THR	Mainchain
2	D	38	ASN	Mainchain

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Mol	Chain	Res	Type	Group
2	D	60	ALA	Mainchain
2	D	9	PRO	Mainchain
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	196	1
1	C	1708	0	1658	177	0
2	B	1660	0	1615	137	0
2	D	1660	0	1614	140	1
3	E	516	0	495	36	0
3	F	516	0	496	55	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	7535	708	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 46.

All (708) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:CG	1:A:45:LYS:CD	1.75	1.65
1:C:79:GLN:CB	1:C:79:GLN:CG	1.75	1.65
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:CG	3:E:840:LYS:CD	1.74	1.58
1:C:106:LEU:CD1	1:C:106:LEU:CG	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:CG	2:B:97:LEU:CD2	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:CB	1:A:180:THR:CG2	1.78	1.55
1:C:205:ILE:CD1	1:C:205:ILE:CG1	1.84	1.55
1:C:45:LYS:CG	1:C:45:LYS:CD	1.82	1.52
1:A:1:ASP:N	1:A:1:ASP:CA	1.69	1.51
3:E:840:LYS:CE	3:E:840:LYS:CD	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:NZ	1:C:30:LYS:CE	1.78	1.46
1:A:210:ASN:HB3	2:B:129:ALA:CB	1.55	1.35
2:B:97:LEU:H	2:B:97:LEU:HD22	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: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:B:188:TRP:O	2:B:189:PRO:C	1.90	1.04
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:H	2:B:97:LEU:CD2	1.76	0.98
3:F:866:TRP:HE3	3:F:868:LEU:HD21	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:E:840:LYS:CE	3:E:840:LYS:HB3	2.01	0.90
1:C:2:ILE:H	1:C:2:ILE:HD12	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
2:B:97:LEU:N	2:B:97:LEU:HD22	1.88	0.89
1:A:115:VAL:HA	1:A:135:PHE:O	1.73	0.89
1:C:136:LEU:N	1:C:136:LEU:HD12	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
2:B:188:TRP:O	2:B:189:PRO:O	1.91	0.87
3:F:869:GLU:HG3	3:F:870:ASP:O	1.75	0.87
3:F:864:TYR:CD2	3:F:877:ILE:HG23	2.10	0.87
3:E:840:LYS:CB	3:E:840:LYS:CD	2.51	0.87
1:C:147:LYS:NZ	1:C:156:GLN:NE2	2.23	0.87
1:C:135:PHE:C	1:C:136:LEU:HD12	1.95	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:148:TRP:CD1	1:A:179:LEU:CG	2.58	0.85
1:A:108:ARG:HH11	1:A:172:THR:CG2	1.90	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
2:D:59:TYR:HB3	2:D:63:PHE:O	1.79	0.83
1:C:168:SER:HB3	4:C:223:HOH:O	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:CD1	1:C:106:LEU:CD2	2.58	0.81
1:A:160:LEU:HD21	2:B:171:GLN:OE1	1.80	0.81
1:C:155:ARG:HH11	1:C:155:ARG:HG2	1.44	0.80
2:B:97:LEU:CB	2:B:97:LEU:CD2	2.60	0.80
1:A:77:SER:O	1:A:78:VAL:C	2.11	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
1:A:160:LEU:HD21	2:B:171:GLN:CD	2.05	0.76
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:79:GLN:HB2	1:C:79:GLN:HE21	1.51	0.75
1:A:160:LEU:HD21	2:B:171:GLN:HE22	1.48	0.75
2:D:150:VAL:O	2:D:150:VAL:HG23	1.87	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: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:CB	1:C:45:LYS:CD	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
2:B:5:VAL:CA	2:B:5:VAL:CG1	2.64	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CB	2:D:97:LEU:CD2	2.67	0.73
1:A:150:ILE:HD12	1:A:150:ILE:H	1.52	0.72
1:A:115:VAL:HG12	1:A:134:CYS:SG	2.29	0.72
1:A:210:ASN:OD1	1:A:210:ASN:O	2.08	0.72
1:A:124:GLN:HG3	2:B:122:TYR:CE2	2.24	0.72
2:D:154:TRP:CZ3	2:D:195:CYS:HB3	2.25	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:24:LYS:HE2	1:A:70:ASP:OD1	1.89	0.72
1:A:187:GLU:HA	1:A:211:ARG:HH22	1.55	0.72
3:F:845:GLU:CA	3:F:845:GLU:OE2	2.36	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:178:THR:HG22	1:A:178:THR:O	1.90	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
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
1:C:27:GLN:C	1:C:69:THR:HG22	2.12	0.70
2:B:64:LYS:HA	2:B:64:LYS:HZ3	1.53	0.70
2:B:82(A):ASN:O	2:B:82(B):SER:C	2.30	0.70
2:B:150:VAL:HG22	2:B:177:LEU:HD11	1.74	0.70
3:F:866:TRP:HE3	3:F:868:LEU:CD2	2.04	0.70
1:C:146:VAL:O	1:C:146:VAL:HG13	1.91	0.70
1:C:79:GLN:CD	1:C:79:GLN:CB	2.60	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
2:B:1:GLN:OE1	2:B:1:GLN:N	2.24	0.69
1:A:148:TRP:HE3	1:A:193:THR:O	1.75	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:2:ILE:CD1	1:C:2:ILE:H	2.04	0.69
2:B:199:HIS:ND1	2:B:202:SER:HB2	2.07	0.69
1:C:100:ALA:CB	1:C:100:ALA:C	2.60	0.69
2:D:126:PRO:HG3	2:D:136:VAL:CG2	2.23	0.69
1:C:125:LEU:O	1:C:127:SER:N	2.25	0.69
2:B:64:LYS:HA	2:B:64:LYS:NZ	2.06	0.69
1:A:19:VAL:CG1	1:A:75:ILE:HB	2.23	0.68
2:B:46:ASN:CB	4:B:237:HOH:O	2.34	0.68
2:B:18:VAL:HG22	2:B:19:LYS:N	2.07	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
2:D:199:HIS:HB3	2:D:204:THR:HB	1.75	0.68
1:A:27:GLN:HG3	4:A:220:HOH:O	1.93	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
2:D:67:PHE:CD2	2:D:82:ILE:HG12	2.30	0.67
1:C:29:ARG:HG3	1:C:29:ARG:O	1.93	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
2:D:126:PRO:HD2	2:D:188:TRP:CH2	2.30	0.67
1:C:133:VAL:HG21	2:D:124:LEU:HD21	1.76	0.67
1:C:2:ILE:N	1:C:2:ILE:HD12	2.06	0.67
2:D:82:ILE:HG22	2:D:82(C):LEU:CD2	2.24	0.67
2:D:66:ARG:HD2	2:D:82(A):ASN:O	1.95	0.67
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:CB	1:C:106:LEU:CD1	2.69	0.66
3:F:864:TYR:HA	3:F:878:LYS:O	1.96	0.66
2:B:199:HIS:O	2:B:200:PRO:C	2.32	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:CB	1:C:142:LYS:CD	2.74	0.65
1:A:159:VAL:HG12	1:A:179:LEU:HG	1.78	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)
2:D:82:ILE:CG2	2:D:82(C):LEU:CD2	2.74	0.65
1:C:27(D):ASN:O	1:C:29:ARG:N	2.27	0.65
1:C:137:ASN:N	1:C:137:ASN:ND2	2.44	0.65
1:A:150:ILE:HG21	1:A:189:HIS:HB3	1.77	0.65
2:D:148:GLU:N	2:D:149:PRO:HD2	2.12	0.65
1:A:162:SER:O	1:A:175:MET:CB	2.44	0.65
1:A:150:ILE:O	1:A:190:ASN:ND2	2.29	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:C:147:LYS:HZ1	1:C:156:GLN:NE2	1.94	0.64
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: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:CD1	1:C:136:LEU:N	2.59	0.63
1:C:22:SER:HB2	1:C:24:LYS:NZ	2.14	0.63
3:E:840:LYS:CD	3:E:840:LYS:HB3	2.29	0.63
2:D:136:VAL:HG22	2:D:137:THR:H	1.64	0.63
1:C:155:ARG:HG2	1:C:155:ARG:NH1	2.08	0.63
2:B:64:LYS:HZ2	2:B:65:GLY:N	1.97	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
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:107:LYS:HA	1:C:140:TYR:OH	2.00	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
2:D:147:PRO:C	2:D:149:PRO:HD2	2.19	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
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:C:147:LYS:CE	1:C:156:GLN:NE2	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HG22	1:A:64:GLY:N	2.16	0.61
1:A:193:THR:HG22	1:A:206:VAL:HG13	1.81	0.61
1:A:158:GLY:O	1:A:180:THR:HB	2.01	0.61
1:A:115:VAL:HG11	1:A:194:CYS:SG	2.39	0.61
2:D:139:GLY:HA2	2:D:154:TRP:CH2	2.36	0.61
2:B:5:VAL:CG2	2:B:5:VAL:CG1	2.73	0.60
1:C:45:LYS:CE	1:C:45:LYS:CG	2.77	0.60
1:A:194:CYS:O	1:A:206:VAL:HA	2.00	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:HE2	3:E:840:LYS:HB3	1.84	0.60
1:C:39:LYS:O	1:C:40:PRO:C	2.37	0.60
1:C:142:LYS:CE	1:C:142:LYS:CG	2.74	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
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
3:E:828:ILE:HG22	3:E:828:ILE:O	2.01	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
3:F:845:GLU:C	3:F:845:GLU:OE2	2.40	0.60
2:B:82(B):SER:O	2:B:82(C):LEU:O	2.19	0.60
1:A:31:ASN:HD21	1:A:68:GLY:H	1.50	0.60
2:D:138:LEU:HD12	2:D:138:LEU:N	2.17	0.60
1:A:14:SER:O	1:A:17:GLU:HB2	2.02	0.60
1:C:79:GLN:CB	1:C:79:GLN:NE2	2.65	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:HD13	3:E:834:ILE:HG21	1.85	0.59
1:A:150:ILE:O	1:A:190:ASN:CG	2.41	0.59
2:B:59:TYR:OH	2:B:68:ALA:HA	2.01	0.59
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:138:LEU:HD23	2:B:210:ILE:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:LYS:O	2:B:84:ASN:C	2.40	0.58
2:B:82:ILE:HG22	2:B:82(C):LEU:HD23	1.85	0.58
2:B:20:ILE:HB	4:B:235:HOH:O	2.03	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
3:F:829:PHE:C	3:F:831:ASP:H	2.07	0.58
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
3:F:849:GLU:O	3:F:850:ALA:C	2.37	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: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
1:C:179:LEU:HD13	1:C:179:LEU:C	2.24	0.57
2:B:83:LYS:CG	2:B:85:GLU:HG2	2.32	0.56
1:C:13:VAL:O	1:C:106:LEU:HD22	2.05	0.56
1:C:4:MET:CA	1:C:4:MET:CG	2.74	0.56
1:A:150:ILE:O	1:A:190:ASN:HB2	2.06	0.56
1:C:119:PRO:CB	1:C:120:PRO:CD	2.83	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:E:830:ALA:C	3:E:832:GLY:H	2.09	0.56
2:D:126:PRO:HG2	2:D:188:TRP:CZ3	2.41	0.56
1:C:206:VAL:HG12	1:C:207:LYS:N	2.20	0.56
2:B:154:TRP:HB3	2:B:159:LEU:HB2	1.88	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
2:D:70:SER:C	2:D:71:LEU:HD23	2.27	0.55
2:B:2:ILE:C	2:B:2:ILE:HD13	2.26	0.55
3:F:827:LEU:HD12	3:F:879:PHE:HE1	1.71	0.55
1:A:207:LYS:NZ	1:A:207:LYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:834:ILE:N	3:F:834:ILE:HD13	2.21	0.55
1:C:125:LEU:O	1:C:126:THR:C	2.43	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:HZ2	1:C:156:GLN:NE2	2.03	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:C:147:LYS:HE3	1:C:156:GLN:NE2	2.20	0.55
2:B:82(A):ASN:O	2:B:82(B):SER:O	2.25	0.55
3:E:865:THR:OG1	3:E:878:LYS:HD3	2.08	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:C:107:LYS:NZ	3:F:836:THR:HG23	2.22	0.54
2:D:124:LEU:O	2:D:138:LEU:HB3	2.07	0.54
1:A:201:SER:HB2	1:A:203:SER:O	2.07	0.54
2:D:126:PRO:HG3	2:D:136:VAL:HG23	1.88	0.54
2:D:59:TYR:OH	2:D:68:ALA:HA	2.06	0.54
2:B:163:VAL:CG1	2:B:164:HIS:N	2.71	0.54
2:D:82(B):SER:O	2:D:82(C):LEU:C	2.43	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:83:LYS:O	2:D:84:ASN:C	2.47	0.53
1:A:108:ARG:O	1:A:140:TYR:CE2	2.61	0.53
1:A:141:PRO:HD2	1:A:198:HIS:HE1	1.71	0.53
1:C:150:ILE:CD1	1:C:155:ARG:HG3	2.39	0.53
2:B:202:SER:O	2:B:203:SER:C	2.44	0.53
1:C:117:ILE:HG12	1:C:118:PHE:H	1.70	0.53
2:B:2:ILE:CD1	2:B:2:ILE:C	2.76	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
2:B:97:LEU:N	2:B:97:LEU:CD2	2.58	0.53
1:A:1:ASP:CB	1:A:1:ASP:N	2.66	0.53
1:A:139:PHE:CG	1:A:139:PHE:O	2.62	0.53
2:B:150:VAL:HG12	2:B:199:HIS:HB2	1.91	0.52
2:D:126:PRO:HG2	2:D:136:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TRP:O	2:B:48:MET:HB2	2.08	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:170:ASP:OD1	1:C:170:ASP:C	2.48	0.52
3:F:875:MET:CE	3:F:877:ILE:HD11	2.39	0.52
2:D:199:HIS:CD2	2:D:202:SER:CB	2.92	0.52
1:A:148:TRP:CZ3	1:A:193:THR:O	2.63	0.52
1:A:108:ARG:O	1:A:140:TYR:CD2	2.63	0.52
1:C:27(C):LEU:HD23	1:C:27(D):ASN:H	1.73	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
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:A:183:LYS:C	1:A:185:GLU:H	2.13	0.52
1:C:210:ASN:HB3	1:C:213:GLU:HG3	1.90	0.52
1:C:79:GLN:CB	1:C:79:GLN:HE21	2.23	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
3:F:864:TYR:HD2	3:F:877:ILE:HG23	1.73	0.51
1:C:147:LYS:CE	1:C:156:GLN:HE22	2.21	0.51
2:D:116:THR:HA	2:D:146:PHE:O	2.11	0.51
1:C:33:LEU:HD22	1:C:71:PHE:CG	2.45	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
2:D:57:PRO:HB3	2:D:59:TYR:CE2	2.45	0.51
1:C:210:ASN:CB	1:C:213:GLU:OE2	2.58	0.51
1:A:135:PHE:HE1	1:A:176:SER:HB2	1.75	0.51
2:B:118:PRO:C	2:B:119:PRO:O	2.47	0.51
1:C:33:LEU:HD22	1:C:71:PHE:CD2	2.46	0.51
1:C:147:LYS:HZ1	1:C:156:GLN:HE21	1.57	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: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
2:B:18:VAL:CG2	2:B:19:LYS:N	2.72	0.51
3:F:866:TRP:O	3:F:868:LEU:HD23	2.10	0.51
1:C:149:LYS:O	1:C:193:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:4:MET:CE	1:C:4:MET:HB3	2.41	0.50
1:A:159:VAL:CG1	1:A:179:LEU:HG	2.39	0.50
1:A:109:ALA:O	1:A:110:ASP:C	2.44	0.50
1:C:161:ASN:CG	1:C:175:MET:CE	2.80	0.50
3:F:866:TRP:O	3:F:867:ASP:C	2.46	0.50
1:C:139:PHE:CZ	1:C:144:ILE:HG12	2.46	0.50
1:C:64:GLY:HA2	1:C:72:THR:O	2.11	0.50
1:C:79:GLN:CG	1:C:79:GLN:CA	2.82	0.50
1:A:122:SER:C	1:A:124:GLN:H	2.14	0.50
1:A:148:TRP:HZ3	1:A:194:CYS:CA	2.25	0.50
1:C:179:LEU:CD1	1:C:179:LEU:C	2.80	0.50
1:A:140:TYR:CD1	1:A:140:TYR:O	2.65	0.50
1:C:150:ILE:HG22	1:C:150:ILE:O	2.11	0.50
1:C:50:TRP:O	1:C:51:ALA:HB3	2.11	0.50
3:F:849:GLU:O	3:F:851:TYR:N	2.45	0.50
2:D:192:THR:HA	4:D:222:HOH:O	2.11	0.50
1:C:24:LYS:HG3	1:C:70:ASP:OD1	2.11	0.50
1:A:11:LEU:HD13	1:A:19:VAL:CG2	2.41	0.50
1:A:9:SER:CB	3:E:840:LYS:HE3	2.42	0.50
1:A:192:TYR:CB	1:A:209:PHE:CE2	2.95	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:135:PHE:CE1	1:A:176:SER:HB2	2.47	0.50
2:B:145:TYR:N	2:B:174:LEU:HD12	2.27	0.50
2:D:83:LYS:C	2:D:111:VAL:HG11	2.32	0.50
1:C:190:ASN:HD21	1:C:212:ASN:ND2	2.10	0.50
1:C:161:ASN:ND2	1:C:175:MET:CE	2.75	0.50
1:A:214:CYS:SG	1:A:214:CYS:OXT	2.69	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
3:F:860:VAL:C	3:F:861:ASN:OD1	2.49	0.49
1:A:133:VAL:HA	1:A:177:SER:O	2.12	0.49
1:C:13:VAL:HG12	1:C:14:SER:N	2.26	0.49
1:C:4:MET:SD	1:C:4:MET:CB	2.93	0.49
3:F:858:ALA:O	3:F:860:VAL:N	2.44	0.49
2:B:183:VAL:O	2:B:183:VAL:HG23	2.12	0.49
2:B:15:GLY:O	2:B:82(B):SER:HA	2.12	0.49
3:E:840:LYS:HE3	3:E:840:LYS:HB3	1.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:MET:CE	1:C:4:MET:CB	2.91	0.49
2:B:138:LEU:HD23	2:B:210:ILE:HG21	1.94	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:148:TRP:HE1	1:A:179:LEU:HB2	1.73	0.49
1:A:24:LYS:NZ	1:A:24:LYS:HB3	2.28	0.49
3:F:875:MET:HE2	3:F:877:ILE:HD11	1.94	0.49
1:A:56:SER:HB3	2:D:27:TYR:O	2.12	0.49
1:C:147:LYS:CD	1:C:147:LYS:CB	2.81	0.49
2:B:199:HIS:CE1	2:B:202:SER:HB2	2.47	0.49
1:C:27:GLN:C	1:C:69:THR:CG2	2.80	0.49
2:D:73:THR:O	2:D:74:SER:C	2.50	0.48
2:D:136:VAL:HG22	2:D:137:THR:N	2.28	0.48
1:A:187:GLU:HA	1:A:211:ARG:NH2	2.24	0.48
1:C:66:GLY:HA3	1:C:71:PHE:HD1	1.78	0.48
3:E:879:PHE:CD1	3:E:879:PHE:N	2.79	0.48
3:F:842:THR:O	3:F:844:GLU:N	2.46	0.48
2:D:97:LEU:CD2	2:D:97:LEU:CD1	2.79	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
1:A:78:VAL:HG22	1:A:106:LEU:HD11	1.95	0.48
1:A:186:TYR:OH	1:A:214:CYS:SG	2.64	0.48
3:F:845:GLU:HA	3:F:845:GLU:OE2	2.14	0.48
2:D:191:GLU:HG3	2:D:192:THR:OG1	2.13	0.48
2:D:4:LEU:O	2:D:104:GLY:HA2	2.13	0.48
1:A:194:CYS:N	1:A:207:LYS:O	2.47	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
2:D:20:ILE:HD11	2:D:80:LEU:HD23	1.95	0.48
1:C:147:LYS:O	1:C:195:GLU:N	2.38	0.48
1:A:148:TRP:HZ3	1:A:194:CYS:HA	1.78	0.48
1:A:146:VAL:O	1:A:146:VAL:HG13	2.13	0.48
3:F:858:ALA:O	3:F:861:ASN:O	2.31	0.48
1:A:86:TYR:N	1:A:86:TYR:CD1	2.82	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
2:B:138:LEU:HD21	2:B:188:TRP:CE2	2.49	0.48
1:A:107:LYS:HE3	3:E:836:THR:HG23	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:ARG:NH1	2:D:86:ASP:OD2	2.45	0.47
3:E:840:LYS:CE	3:E:840:LYS:CB	2.83	0.47
1:C:180:THR:C	1:C:181:LEU:HD23	2.34	0.47
1:A:108:ARG:HB2	1:A:108:ARG:HE	1.40	0.47
1:A:211:ARG:HA	1:A:211:ARG:HE	1.79	0.47
3:F:858:ALA:HA	3:F:861:ASN:O	2.14	0.47
3:E:845:GLU:HA	3:E:845:GLU:OE2	2.14	0.47
1:A:34:ALA:O	1:A:88:CYS:HA	2.14	0.47
1:A:150:ILE:O	1:A:190:ASN:CB	2.61	0.47
1:C:119:PRO:CG	2:D:213:ARG:NH1	2.77	0.47
2:B:154:TRP:CZ3	2:B:195:CYS:HB3	2.49	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:C:11:LEU:HD13	1:C:19:VAL:CG1	2.44	0.47
1:A:148:TRP:CD1	1:A:159:VAL:CG1	2.90	0.47
1:C:89:LYS:HB3	1:C:89:LYS:HE2	1.55	0.47
1:C:77:SER:O	1:C:78:VAL:C	2.53	0.47
2:D:38:ASN:ND2	2:D:38:ASN:C	2.67	0.47
1:A:149:LYS:C	1:A:151:ASP:H	2.18	0.47
2:D:138:LEU:HD22	2:D:193:VAL:HG11	1.96	0.47
1:C:188:ARG:O	1:C:189:HIS:CB	2.58	0.47
1:C:63:THR:HG22	1:C:64:GLY:N	2.30	0.47
2:B:40:ALA:HB1	2:B:41:PRO:HD2	1.96	0.47
1:A:136:LEU:O	1:A:174:SER:HA	2.14	0.47
2:D:163:VAL:HG12	2:D:164:HIS:N	2.30	0.47
1:A:121:SER:O	1:A:122:SER:C	2.53	0.47
2:B:160:SER:O	2:B:163:VAL:CG2	2.50	0.47
1:A:132:VAL:HG12	1:A:133:VAL:N	2.29	0.47
2:B:82(B):SER:C	2:B:82(C):LEU:O	2.53	0.47
1:C:24:LYS:HE2	1:C:24:LYS:N	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
2:D:209:LYS:HD2	2:D:210:ILE:H	1.81	0.46
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
1:A:110:ASP:OD1	1:A:141:PRO:CG	2.63	0.46
2:D:20:ILE:HG21	2:D:20:ILE:HD13	1.75	0.46
3:F:834:ILE:HD13	3:F:834:ILE:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:VAL:CG2	2:B:211:VAL:O	2.63	0.46
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.97	0.46
3:E:829:PHE:N	3:E:829:PHE:CD1	2.84	0.46
2:D:170:LEU:HD12	2:D:171:GLN:N	2.30	0.46
1:A:115:VAL:CG1	1:A:194:CYS:SG	3.04	0.46
1:A:77:SER:O	1:A:78:VAL:O	2.32	0.46
1:C:148:TRP:CH2	1:C:194:CYS:HB3	2.50	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
2:D:99:GLN:HE21	2:D:99:GLN:HB3	1.46	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
1:C:27(C):LEU:HG	1:C:31:ASN:ND2	2.30	0.46
3:F:848:ALA:HB1	3:F:852:ARG:NH2	2.31	0.46
2:D:163:VAL:CG1	2:D:164:HIS:N	2.79	0.46
2:D:117:THR:CG2	2:D:174:LEU:CD2	2.94	0.45
1:C:161:ASN:O	1:C:162:SER:HB2	2.16	0.45
2:D:189:PRO:HB3	2:D:212:PRO:HG3	1.87	0.45
1:C:123:GLU:N	1:C:123:GLU:OE1	2.49	0.45
1:C:161:ASN:ND2	1:C:175:MET:HE3	2.32	0.45
2:D:97:LEU:CD2	2:D:97:LEU:H	2.29	0.45
1:C:27:GLN:O	1:C:69:THR:HG22	2.16	0.45
1:A:210:ASN:OD1	1:A:213:GLU:HB3	2.16	0.45
3:F:854:ALA:CB	3:F:877:ILE:HD13	2.46	0.45
3:F:842:THR:OG1	3:F:845:GLU:HB2	2.17	0.45
1:C:159:VAL:HG12	1:C:160:LEU:N	2.32	0.45
1:A:9:SER:HB3	3:E:840:LYS:CE	2.46	0.45
2:D:188:TRP:CH2	2:D:212:PRO:HA	2.51	0.45
1:A:122:SER:C	1:A:124:GLN:N	2.70	0.45
1:A:33:LEU:HG	1:A:34:ALA:N	2.31	0.45
1:A:65:ARG:HG2	1:A:65:ARG:HH21	1.81	0.45
1:C:170:ASP:O	1:C:172:THR:HG23	2.17	0.45
1:A:151:ASP:OD1	1:A:191:SER:HB3	2.16	0.45
1:A:119:PRO:O	1:A:120:PRO:C	2.50	0.45
3:E:822:THR:HA	3:E:839:PHE:O	2.17	0.45
1:A:150:ILE:CD1	1:A:150:ILE:H	2.26	0.45
1:A:210:ASN:CG	1:A:210:ASN:O	2.56	0.45
1:A:125:LEU:O	1:A:127:SER:N	2.49	0.45
2:D:66:ARG:HB3	2:D:82(A):ASN:O	2.17	0.45
1:C:189:HIS:ND1	1:C:190:ASN:N	2.64	0.45
2:B:153:THR:O	2:B:196:ASN:N	2.39	0.45

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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	0.45
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:139:GLY:HA2	2:D:154:TRP:CZ2	2.52	0.44
2:D:19:LYS:HD3	2:D:81:GLN:OE1	2.17	0.44
2:D:18:VAL:O	2:D:18:VAL:HG13	2.15	0.44
2:B:13:LYS:HA	2:B:14:PRO:HD3	1.80	0.44
2:D:126:PRO:CG	2:D:136:VAL:HG21	2.47	0.44
1:C:39:LYS:HB3	1:C:40:PRO:HD2	1.99	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:B:127:GLY:HA2	2:B:213:ARG:CG	2.47	0.44
2:B:117:THR:O	2:B:145:TYR:HB2	2.18	0.44
2:D:37:VAL:HG12	2:D:38:ASN:N	2.32	0.44
2:D:48:MET:HA	2:D:63:PHE:CD2	2.52	0.44
3:E:858:ALA:O	3:E:859:LYS:C	2.54	0.44
2:B:43:LYS:CE	2:B:43:LYS:CG	2.84	0.43
1:C:13:VAL:HG21	1:C:19:VAL:HG21	1.97	0.43
2:D:59:TYR:CB	2:D:63:PHE:O	2.60	0.43
3:E:823:ILE:HD13	3:E:823:ILE:HG21	1.68	0.43
2:D:97:LEU:C	2:D:99:GLN:H	2.21	0.43
2:D:138:LEU:HD23	2:D:210:ILE:HG22	1.87	0.43
1:A:148:TRP:CZ3	1:A:194:CYS:CA	3.01	0.43
2:D:38:ASN:HD21	2:D:46:ASN:HB2	1.81	0.43
3:F:842:THR:O	3:F:843:PHE:C	2.56	0.43
2:D:97:LEU:HD22	2:D:97:LEU:N	2.33	0.43
1:C:19:VAL:HG12	1:C:20:THR:N	2.33	0.43
1:A:24:LYS:HA	1:A:69:THR:O	2.18	0.43
3:F:824:LYS:HB3	4:F:102:HOH:O	2.17	0.43
1:C:141:PRO:O	1:C:198:HIS:HE1	2.01	0.43
2:B:185:SER:C	2:B:187:THR:N	2.72	0.43
2:B:55:GLY:O	2:B:57:PRO:HD3	2.18	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
3:E:853:TYR:O	3:E:856:LEU:N	2.51	0.43
2:D:47:TRP:CH2	2:D:49:GLY:HA2	2.53	0.43
1:C:107:LYS:HZ1	3:F:836:THR:HG23	1.84	0.43
2:D:191:GLU:HG3	2:D:192:THR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:HB1	3:E:818:LYS:HG2	2.00	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:B:51:VAL:HG22	2:B:52:ASN:N	2.33	0.43
2:B:167:PRO:O	2:B:168:ALA:C	2.56	0.43
1:A:186:TYR:CE1	1:A:209:PHE:HZ	2.36	0.43
1:A:122:SER:O	1:A:125:LEU:N	2.52	0.43
1:A:78:VAL:CG2	1:A:106:LEU:HD21	2.49	0.43
1:C:73:LEU:HA	1:C:73:LEU:HD12	1.85	0.43
1:C:22:SER:CB	1:C:24:LYS:HZ2	2.29	0.42
2:B:94:ARG:HD3	2:B:101:ASP:OD2	2.19	0.42
2:B:150:VAL:HG12	2:B:199:HIS:CB	2.49	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
2:B:194:THR:HB	2:B:209:LYS:HA	2.01	0.42
1:A:150:ILE:CG1	1:A:192:TYR:CE1	2.99	0.42
2:D:196:ASN:ND2	2:D:207:ASP:OD2	2.45	0.42
2:D:162:GLY:O	2:D:181:VAL:HA	2.20	0.42
2:D:67:PHE:CE2	2:D:82:ILE:HG12	2.54	0.42
3:E:830:ALA:O	3:E:832:GLY:N	2.49	0.42
3:F:828:ILE:HA	3:F:834:ILE:HG22	2.01	0.42
1:A:65:ARG:HH21	1:A:65:ARG:CG	2.32	0.42
2:B:138:LEU:HD23	2:B:210:ILE:HB	2.01	0.42
2:D:166:PHE:HA	2:D:167:PRO:HD3	1.83	0.42
1:A:79:GLN:C	1:A:81:GLU:N	2.73	0.42
3:F:864:TYR:CA	3:F:878:LYS:O	2.65	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
1:A:132:VAL:CG1	1:A:133:VAL:N	2.82	0.42
2:B:11:LEU:HG	2:B:147:PRO:HG3	2.02	0.42
1:C:5:SER:O	1:C:24:LYS:HE2	2.20	0.42
2:D:188:TRP:CH2	2:D:212:PRO:HB3	2.54	0.42
2:B:188:TRP:CB	2:B:189:PRO:CD	2.89	0.42
2:D:138:LEU:CD1	2:D:138:LEU:N	2.83	0.42
1:C:29:ARG:CG	1:C:29:ARG:O	2.64	0.42
1:C:49:TYR:CZ	1:C:53:THR:HG21	2.55	0.42
2:D:82:ILE:HG21	2:D:82(C):LEU:CD2	2.48	0.42
2:B:7:SER:OG	4:B:218:HOH:O	2.21	0.42
1:A:124:GLN:HE22	1:A:131:SER:H	1.68	0.41
2:D:177:LEU:HD23	2:D:177:LEU:C	2.40	0.41
1:C:86:TYR:CD1	1:C:86:TYR:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:VAL:HG21	2:D:124:LEU:CD2	2.47	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
2:B:153:THR:HG1	2:B:196:ASN:HB2	1.85	0.41
3:F:853:TYR:CZ	3:F:857:LEU:HD21	2.56	0.41
1:A:27(A):SER:O	1:A:27(B):LEU:HD23	2.20	0.41
2:B:127:GLY:HA2	2:B:213:ARG:HG3	2.03	0.41
2:B:205:LYS:O	2:B:206:VAL:CG2	2.68	0.41
2:B:52:ASN:OD1	2:B:53:GLU:N	2.53	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:D:117:THR:O	2:D:145:TYR:HA	2.20	0.41
2:D:52:ASN:OD1	2:D:54:THR:N	2.53	0.41
2:B:2:ILE:O	2:B:3:GLN:HB3	2.20	0.41
2:D:30:THR:HG21	4:D:227:HOH:O	2.19	0.41
1:C:7:SER:HA	1:C:8:PRO:HA	1.83	0.41
1:A:154:GLU:HG3	1:A:154:GLU:O	2.21	0.41
2:B:139:GLY:HA2	2:B:179:SER:O	2.20	0.41
1:A:31:ASN:ND2	1:A:68:GLY:H	2.15	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
3:F:829:PHE:C	3:F:831:ASP:N	2.74	0.41
1:C:4:MET:HB3	1:C:4:MET:HE3	2.02	0.41
1:A:139:PHE:CD2	1:A:139:PHE:C	2.92	0.41
1:C:124:GLN:HE22	1:C:131:SER:CB	2.34	0.41
1:C:24:LYS:HA	1:C:69:THR:O	2.20	0.41
1:A:186:TYR:HA	1:A:192:TYR:OH	2.21	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
2:B:38:ASN:ND2	2:B:48:MET:HG3	2.36	0.41
2:D:155:ASN:HD21	2:D:192:THR:C	2.24	0.41
1:C:44:PRO:HG2	2:D:45:LEU:HD21	2.02	0.41
2:B:24:ALA:HB2	2:B:29:PHE:HD1	1.85	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
2:B:2:ILE:O	2:B:3:GLN:CB	2.67	0.40
1:A:196:ALA:HB3	1:A:205:ILE:O	2.21	0.40
1:A:35:TRP:HA	1:A:87:TYR:O	2.21	0.40
2:B:163:VAL:CG1	2:B:164:HIS:H	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TYR:CD1	1:A:140:TYR:C	2.94	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:94:PRO:HA	1:C:95:PRO:C	2.42	0.40
2:D:59:TYR:CE1	2:D:67:PHE:O	2.75	0.40
3:E:824:LYS:CD	3:E:824:LYS:CB	2.83	0.40
1:A:156:GLN:HE21	1:A:159:VAL:CG2	2.07	0.40
1:A:7:SER:HB2	1:A:22:SER:HG	1.82	0.40
2:B:70:SER:HB2	2:B:71:LEU:H	1.63	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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

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

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
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

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Mol	Chain	Res	Type
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%)	156 (80%)	39 (20%)	1	2
1	C	195/195 (100%)	165 (85%)	30 (15%)	3	5
2	B	187/187 (100%)	157 (84%)	30 (16%)	3	5
2	D	187/187 (100%)	163 (87%)	24 (13%)	5	10
3	E	51/51 (100%)	40 (78%)	11 (22%)	1	2
3	F	51/51 (100%)	43 (84%)	8 (16%)	3	5
All	All	866/866 (100%)	724 (84%)	142 (16%)	3	4

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
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	108	ARG
1	A	110	ASP

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Mol	Chain	Res	Type
1	A	117	ILE
1	A	127	SER
1	A	136	LEU
1	A	142	LYS
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	157	ASN
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	190	ASN
1	A	202	THR
1	A	203	SER
1	A	207	LYS
1	A	209	PHE
1	A	211	ARG
2	B	1	GLN
2	B	2	ILE
2	B	11	LEU
2	B	17	THR
2	B	20	ILE
2	B	25	SER
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	82(B)	SER
2	B	96	LEU
2	B	97	LEU

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Mol	Chain	Res	Type
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
3	E	818	LYS
3	E	820	GLU
3	E	821	VAL
3	E	822	THR
3	E	829	PHE
3	E	840	LYS
3	E	844	GLU
3	E	873	ASN
3	E	875	MET
3	E	879	PHE
3	E	882	LYS
1	C	22	SER
1	C	24	LYS
1	C	27(C)	LEU
1	C	27(E)	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	106	LEU
1	C	110	ASP
1	C	117	ILE
1	C	127	SER
1	C	136	LEU
1	C	137	ASN

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Mol	Chain	Res	Type
1	C	142	LYS
1	C	144	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	180	THR
1	C	191	SER
1	C	199	LYS
1	C	200	THR
1	C	208	SER
1	C	212	ASN
2	D	14	PRO
2	D	25	SER
2	D	38	ASN
2	D	61	ASP
2	D	74	SER
2	D	76	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	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
2	D	213	ARG
3	F	818	LYS
3	F	821	VAL
3	F	834	ILE
3	F	845	GLU

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Mol	Chain	Res	Type
3	F	859	LYS
3	F	860	VAL
3	F	869	GLU
3	F	882	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	42	GLN
1	A	156	GLN
1	A	157	ASN
1	A	198	HIS
2	B	3	GLN
2	B	131	GLN
1	C	31	ASN
1	C	38	GLN
1	C	42	GLN
1	C	79	GLN
1	C	124	GLN
1	C	137	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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	220/220 (100%)	-0.17	5 (2%) 64 57	28, 58, 108, 123	3 (1%)
1	C	220/220 (100%)	-0.33	2 (0%) 85 83	33, 66, 103, 122	3 (1%)
2	B	218/218 (100%)	-0.14	6 (2%) 56 49	29, 60, 100, 136	2 (0%)
2	D	218/218 (100%)	-0.12	10 (4%) 36 29	32, 68, 110, 137	2 (0%)
3	E	65/65 (100%)	-0.20	2 (3%) 52 45	43, 67, 94, 124	1 (1%)
3	F	65/65 (100%)	0.10	6 (9%) 11 7	56, 84, 115, 123	1 (1%)
All	All	1006/1006 (100%)	-0.17	31 (3%) 52 45	28, 66, 107, 137	12 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	132	THR	6.5
2	B	128	SER	6.3
2	D	129	ALA	6.0
2	D	128	SER	5.3
2	D	210	ILE	5.1
2	D	213	ARG	5.0
2	B	127	GLY	5.0
1	A	183	LYS	4.9
3	F	818	LYS	4.3
2	B	130	ALA	3.9
2	D	133	ASN	3.7
3	F	870	ASP	3.6
2	D	134	SER	3.5
1	A	186	TYR	3.2
3	F	881	GLY	3.1
3	E	818	LYS	3.0
3	F	882	LYS	3.0
1	C	214	CYS	2.9
2	B	132	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	182	THR	2.9
3	F	871	GLY	2.8
2	D	211	VAL	2.8
2	B	129	ALA	2.7
3	F	873	ASN	2.7
2	B	131	GLN	2.6
3	E	819	GLU	2.6
1	A	151	ASP	2.5
1	A	155	ARG	2.4
2	D	130	ALA	2.3
1	C	148	TRP	2.1
1	A	181	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.