



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZS2  
Title : TYRB25,NMEPHEB26,LYSB28,PROB29-INSULIN ANALOGUE CRYSTAL STRUCTURE  
Authors : Antolikova, E.; Zakova, L.; Turkenburg, J.P.; Watson, C.J.; Hanclova, I.; Sanda, M.; Cooper, A.; Kraus, T.; Brzozowski, A.M.; Jiracek, J.A.  
Deposited on : 2011-06-21  
Resolution : 1.97 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

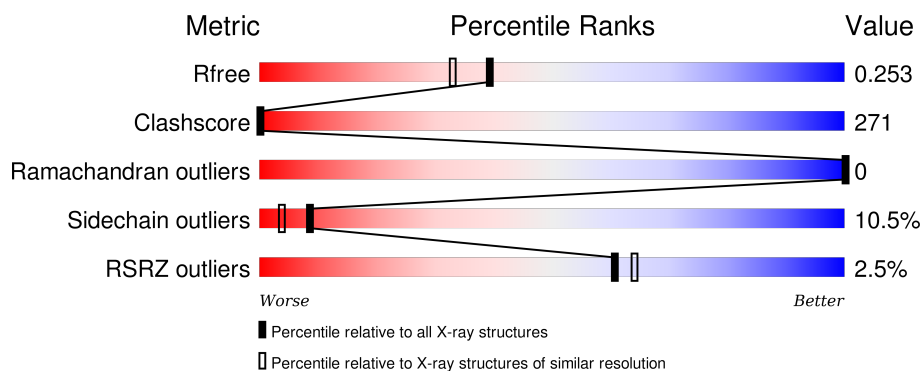
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	21	<div> <div>19%</div> <div>86%</div> <div>10%</div> <div>5%</div> </div>
1	C	21	<div> <div>5%</div> <div>90%</div> <div>5%</div> </div>
1	E	21	<div> <div>81%</div> <div>19%</div> </div>
1	G	21	<div> <div>14%</div> <div>67%</div> <div>14%</div> <div>5%</div> </div>
1	I	21	<div> <div>5%</div> <div>90%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	21	
2	B	30	
2	D	30	
2	F	30	
2	H	30	
2	J	30	
2	L	30	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MEA	D	26	-	X	-	-
2	MEA	F	26	-	X	X	-
2	MEA	H	26	-	X	-	-
2	MEA	J	26	-	X	-	-
2	MEA	L	26	-	X	-	-
3	IPH	A	1022	-	X	-	-
3	IPH	C	1022	-	X	-	-
3	IPH	E	1022	-	X	-	-
3	IPH	G	1022	-	X	-	-
3	IPH	I	1022	-	X	-	-
3	IPH	K	1022	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2440 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 INSULIN A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	20	Total	C	N	O	S	0	0	0
			159	97	24	34	4			
1	C	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	E	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	G	20	Total	C	N	O	S	0	0	0
			159	97	24	34	4			
1	I	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	K	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			219	144	36	37	2			
2	D	25	Total	C	N	O	S	0	0	0
			194	125	34	33	2			
2	F	25	Total	C	N	O	S	0	0	0
			194	125	34	33	2			
2	H	28	Total	C	N	O	S	0	0	1
			220	144	37	37	2			
2	J	29	Total	C	N	O	S	0	0	0
			235	155	39	39	2			
2	L	26	Total	C	N	O	S	0	0	0
			212	140	35	35	2			

There are 24 discrepancies between the modelled and reference sequences:

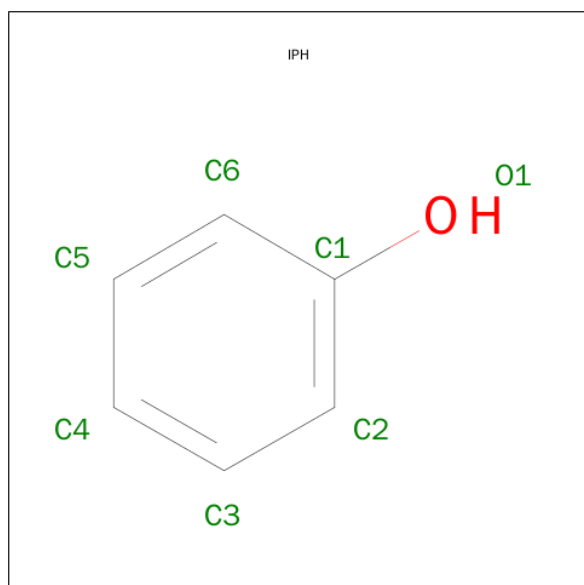
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
B	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
B	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
D	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
D	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
D	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
D	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
F	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
F	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
F	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
F	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
H	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
H	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
H	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
H	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
J	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
J	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
J	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
J	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
L	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
L	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
L	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
L	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308

- Molecule 3 is PHENOL (three-letter code: IPH) (formula: C<sub>6</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 6 1	0	0
3	C	1	Total C O 7 6 1	0	0
3	E	1	Total C O 7 6 1	0	0
3	G	1	Total C O 7 6 1	0	0
3	I	1	Total C O 7 6 1	0	0
3	K	1	Total C O 7 6 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	17	Total O 17 17	0	0
6	C	17	Total O 17 17	0	0
6	D	10	Total O 10 10	0	0
6	E	7	Total O 7 7	0	0

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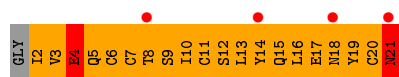
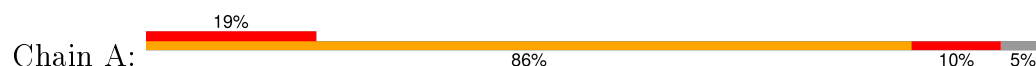
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	15	Total 15	O 15	0	0
6	G	17	Total 17	O 17	0	0
6	H	17	Total 17	O 17	0	0
6	I	19	Total 19	O 19	0	0
6	J	16	Total 16	O 16	0	0
6	K	9	Total 9	O 9	0	0
6	L	4	Total 4	O 4	0	0

### 3 Residue-property plots [i](#)

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

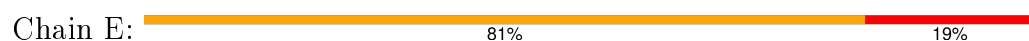
- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN



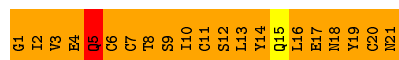
- Molecule 1: INSULIN A CHAIN



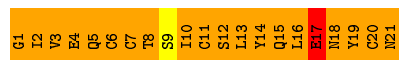
- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN

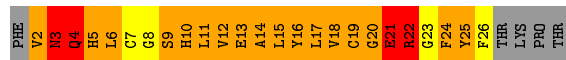
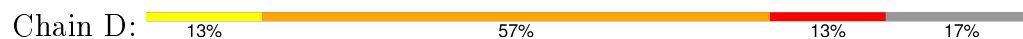




## • Molecule 2: INSULIN B CHAIN



## • Molecule 2: INSULIN B CHAIN



## • Molecule 2: INSULIN B CHAIN



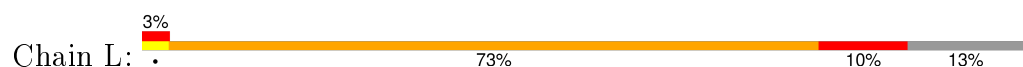
## • Molecule 2: INSULIN B CHAIN



## • Molecule 2: INSULIN B CHAIN



## • Molecule 2: INSULIN B CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.68 Å 62.17 Å 57.66 Å 90.00° 111.32° 90.00°	Depositor
Resolution (Å)	53.68 – 1.97 29.03 – 1.97	Depositor EDS
% Data completeness (in resolution range)	89.9 (53.68-1.97) 56.7 (29.03-1.97)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.97 (at 1.96 Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, $R_{free}$	0.193 , 0.252 0.196 , 0.253	Depositor DCC
$R_{free}$ test set	617 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.1	EDS
Estimated twinning fraction	0.051 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 12370 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.26% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MEA, IPH, CL

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	8.64	89/160 (55.6%)	6.45	74/215 (34.4%)
1	C	9.23	114/164 (69.5%)	5.50	68/220 (30.9%)
1	E	8.84	92/164 (56.1%)	5.86	98/220 (44.5%)
1	G	8.32	76/160 (47.5%)	5.40	68/215 (31.6%)
1	I	9.44	104/164 (63.4%)	5.56	77/220 (35.0%)
1	K	9.06	106/164 (64.6%)	5.30	78/220 (35.5%)
2	B	9.26	128/211 (60.7%)	6.53	115/283 (40.6%)
2	D	8.05	104/185 (56.2%)	5.47	87/249 (34.9%)
2	F	7.48	89/185 (48.1%)	5.67	111/249 (44.6%)
2	H	8.79	116/212 (54.7%)	5.73	103/285 (36.1%)
2	J	8.32	130/228 (57.0%)	5.93	102/306 (33.3%)
2	L	8.93	133/205 (64.9%)	6.40	100/276 (36.2%)
All	All	8.70	1281/2202 (58.2%)	5.85	1081/2958 (36.5%)

All (1281) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	CYS	CB-SG	29.76	2.32	1.82
1	I	12	SER	CB-OG	28.65	1.79	1.42
1	K	20	CYS	CB-SG	28.63	2.31	1.82
2	H	25	TYR	CG-CD2	25.70	1.72	1.39
1	G	6	CYS	CB-SG	25.51	2.25	1.82
1	K	17	GLU	CG-CD	25.44	1.90	1.51
1	K	12	SER	CB-OG	24.93	1.74	1.42
2	H	25	TYR	CE1-CZ	24.57	1.70	1.38
2	L	22	ARG	CZ-NH2	24.10	1.64	1.33
1	I	14	TYR	CD1-CE1	23.84	1.75	1.39
1	I	14	TYR	CD2-CE2	23.82	1.75	1.39
1	A	14	TYR	CE1-CZ	23.49	1.69	1.38
1	G	9	SER	CA-CB	23.31	1.88	1.52
2	H	7	CYS	CB-SG	23.12	2.21	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	14	TYR	CB-CG	23.02	1.86	1.51
2	D	13	GLU	CD-OE1	22.96	1.50	1.25
1	G	11	CYS	CB-SG	-22.64	1.43	1.82
1	A	14	TYR	CG-CD2	22.47	1.68	1.39
1	E	19	TYR	CG-CD1	22.43	1.68	1.39
1	I	20	CYS	CB-SG	22.36	2.20	1.82
1	A	17	GLU	CD-OE1	-22.35	1.01	1.25
2	H	9	SER	CA-CB	22.17	1.86	1.52
1	A	12	SER	CA-CB	22.12	1.86	1.52
1	C	19	TYR	CG-CD2	22.09	1.67	1.39
1	G	19	TYR	CE1-CZ	-21.84	1.10	1.38
1	A	11	CYS	CB-SG	-21.73	1.45	1.82
2	B	13	GLU	CB-CG	21.48	1.93	1.52
1	E	19	TYR	CE2-CZ	21.33	1.66	1.38
2	H	24	PHE	CB-CG	21.31	1.87	1.51
1	G	19	TYR	CG-CD2	-21.28	1.11	1.39
1	E	9	SER	CB-OG	-21.27	1.14	1.42
1	C	14	TYR	CE2-CZ	-21.20	1.10	1.38
1	E	1	GLY	CA-C	21.15	1.85	1.51
1	C	17	GLU	CD-OE2	21.13	1.48	1.25
1	K	1	GLY	CA-C	21.05	1.85	1.51
1	K	4	GLU	CD-OE2	20.81	1.48	1.25
1	G	14	TYR	CB-CG	-20.77	1.20	1.51
2	B	21	GLU	CD-OE2	-20.31	1.03	1.25
1	C	9	SER	N-CA	20.24	1.86	1.46
2	J	16	TYR	CE1-CZ	20.09	1.64	1.38
2	J	25	TYR	CE1-CZ	-20.05	1.12	1.38
1	E	4	GLU	CD-OE1	-20.01	1.03	1.25
2	F	20	GLY	CA-C	19.83	1.83	1.51
2	J	25	TYR	CG-CD2	-19.81	1.13	1.39
2	H	13	GLU	CB-CG	19.81	1.89	1.52
2	J	16	TYR	CG-CD2	19.80	1.64	1.39
1	A	6	CYS	CB-SG	19.80	2.15	1.82
1	A	19	TYR	CE2-CZ	-19.73	1.12	1.38
1	C	4	GLU	CD-OE2	-19.64	1.04	1.25
1	C	19	TYR	CE1-CZ	19.62	1.64	1.38
1	G	12	SER	CA-CB	19.61	1.82	1.52
1	A	19	TYR	CG-CD1	-19.55	1.13	1.39
2	B	16	TYR	CE1-CZ	-19.52	1.13	1.38
2	B	25	TYR	CG-CD2	19.45	1.64	1.39
1	I	19	TYR	CG-CD1	19.31	1.64	1.39
1	I	14	TYR	CZ-OH	19.25	1.70	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	21	GLU	CG-CD	18.91	1.80	1.51
2	L	24	PHE	CA-CB	18.88	1.95	1.53
2	J	10	HIS	CB-CG	18.84	1.83	1.50
1	K	21	ASN	N-CA	18.74	1.83	1.46
1	C	14	TYR	CG-CD1	-18.66	1.14	1.39
2	F	12	VAL	CA-CB	18.54	1.93	1.54
1	G	14	TYR	CD1-CE1	-18.41	1.11	1.39
2	H	23	GLY	C-O	18.39	1.53	1.23
2	F	7	CYS	C-N	18.27	1.66	1.33
2	B	25	TYR	CE1-CZ	18.18	1.62	1.38
2	L	16	TYR	CE1-CZ	18.14	1.62	1.38
1	I	9	SER	CB-OG	18.11	1.65	1.42
2	L	13	GLU	CG-CD	-18.05	1.24	1.51
1	G	14	TYR	CD2-CE2	-17.95	1.12	1.39
2	J	9	SER	CA-CB	17.94	1.79	1.52
2	H	24	PHE	CD1-CE1	17.91	1.75	1.39
1	C	19	TYR	N-CA	17.89	1.82	1.46
2	B	23	GLY	N-CA	17.88	1.72	1.46
2	H	18	VAL	N-CA	17.86	1.82	1.46
1	E	6	CYS	CB-SG	-17.85	1.51	1.82
1	C	17	GLU	CG-CD	17.81	1.78	1.51
2	F	21	GLU	CG-CD	17.78	1.78	1.51
1	E	14	TYR	CG-CD1	-17.73	1.16	1.39
2	L	19	CYS	N-CA	17.66	1.81	1.46
2	D	12	VAL	CA-CB	17.62	1.91	1.54
2	L	16	TYR	CG-CD1	17.49	1.61	1.39
1	I	4	GLU	CA-CB	17.49	1.92	1.53
2	B	16	TYR	CG-CD2	-17.41	1.16	1.39
1	G	7	CYS	N-CA	17.32	1.80	1.46
2	J	22	ARG	C-N	17.30	1.64	1.33
2	J	13	GLU	CD-OE1	-17.27	1.06	1.25
2	J	22	ARG	CZ-NH1	17.27	1.55	1.33
2	B	14	ALA	N-CA	17.23	1.80	1.46
2	L	1	PHE	CB-CG	17.20	1.80	1.51
2	H	16	TYR	CA-CB	17.17	1.91	1.53
2	J	25	TYR	CA-CB	17.12	1.91	1.53
2	L	22	ARG	CD-NE	17.11	1.75	1.46
2	B	7	CYS	N-CA	17.09	1.80	1.46
2	L	20	GLY	CA-C	17.01	1.79	1.51
2	D	17	LEU	N-CA	16.99	1.80	1.46
1	A	12	SER	CB-OG	-16.94	1.20	1.42
2	J	13	GLU	CA-CB	16.82	1.91	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	GLU	CD-OE2	-16.82	1.07	1.25
1	I	1	GLY	CA-C	16.81	1.78	1.51
2	H	18	VAL	CB-CG1	16.79	1.88	1.52
1	K	20	CYS	CA-C	16.75	1.96	1.52
1	I	19	TYR	CE2-CZ	16.71	1.60	1.38
2	F	13	GLU	CD-OE2	-16.71	1.07	1.25
1	E	14	TYR	CE2-CZ	-16.68	1.16	1.38
1	I	4	GLU	CG-CD	-16.67	1.26	1.51
2	L	1	PHE	CG-CD2	16.67	1.63	1.38
2	H	16	TYR	CG-CD2	-16.61	1.17	1.39
2	B	24	PHE	CG-CD1	-16.60	1.13	1.38
2	D	2	VAL	CA-C	16.59	1.96	1.52
2	B	5	HIS	CA-CB	16.56	1.90	1.53
2	D	10	HIS	N-CA	16.55	1.79	1.46
2	B	24	PHE	CG-CD2	16.54	1.63	1.38
2	D	21	GLU	C-O	16.53	1.54	1.23
2	D	25	TYR	N-CA	16.49	1.79	1.46
2	D	7	CYS	C-N	16.44	1.62	1.33
2	H	21	GLU	CB-CG	-16.17	1.21	1.52
1	I	14	TYR	N-CA	16.10	1.78	1.46
1	I	18	ASN	N-CA	16.09	1.78	1.46
2	F	21	GLU	N-CA	16.05	1.78	1.46
2	B	10	HIS	CG-CD2	16.01	1.62	1.35
2	H	24	PHE	CD2-CE2	15.96	1.71	1.39
2	L	3	ASN	CB-CG	15.94	1.87	1.51
2	L	13	GLU	CA-CB	15.91	1.89	1.53
2	H	11	LEU	N-CA	15.85	1.78	1.46
1	E	16	LEU	C-O	15.84	1.53	1.23
2	H	14	ALA	N-CA	15.83	1.78	1.46
2	J	2	VAL	CA-CB	15.79	1.88	1.54
2	L	16	TYR	CG-CD2	15.78	1.59	1.39
2	B	22	ARG	CZ-NH2	-15.73	1.12	1.33
1	A	9	SER	CA-CB	15.71	1.76	1.52
1	C	12	SER	C-O	15.69	1.53	1.23
1	C	5	GLN	N-CA	15.68	1.77	1.46
2	H	6	LEU	N-CA	-15.67	1.15	1.46
2	F	8	GLY	C-O	-15.66	0.98	1.23
2	H	16	TYR	CE1-CZ	-15.66	1.18	1.38
2	D	3	ASN	N-CA	15.64	1.77	1.46
1	E	12	SER	C-O	15.64	1.53	1.23
1	E	19	TYR	CE1-CZ	15.62	1.58	1.38
2	B	9	SER	CA-CB	15.61	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	29	PRO	CA-CB	-15.61	1.22	1.53
2	B	12	VAL	CA-CB	15.60	1.87	1.54
1	E	5	GLN	C-O	15.58	1.52	1.23
1	G	14	TYR	CZ-OH	-15.57	1.11	1.37
2	D	20	GLY	C-O	15.55	1.48	1.23
1	G	14	TYR	N-CA	15.50	1.77	1.46
2	D	9	SER	CA-C	15.44	1.93	1.52
1	C	1	GLY	CA-C	15.43	1.76	1.51
1	C	9	SER	CB-OG	-15.41	1.22	1.42
2	B	6	LEU	CA-C	15.40	1.93	1.52
2	F	21	GLU	C-O	15.37	1.52	1.23
1	C	15	GLN	N-CA	15.36	1.77	1.46
1	E	15	GLN	C-O	15.35	1.52	1.23
2	J	24	PHE	CB-CG	15.33	1.77	1.51
1	I	6	CYS	N-CA	15.32	1.76	1.46
2	B	1	PHE	CB-CG	-15.28	1.25	1.51
2	H	7	CYS	N-CA	15.26	1.76	1.46
1	K	12	SER	CA-CB	-15.23	1.30	1.52
2	D	19	CYS	CA-CB	15.21	1.87	1.53
1	I	2	ILE	N-CA	15.19	1.76	1.46
1	K	18	ASN	C-O	15.18	1.52	1.23
2	F	22	ARG	CG-CD	15.18	1.89	1.51
2	J	5	HIS	CG-CD2	15.16	1.61	1.35
1	I	6	CYS	C-O	15.15	1.52	1.23
2	L	15	LEU	N-CA	15.11	1.76	1.46
1	E	19	TYR	N-CA	15.10	1.76	1.46
2	B	24	PHE	CB-CG	15.06	1.76	1.51
2	D	24	PHE	CA-C	15.05	1.92	1.52
2	D	22	ARG	CB-CG	14.98	1.93	1.52
1	E	2	ILE	C-O	14.98	1.51	1.23
2	H	22	ARG	CZ-NH1	-14.90	1.13	1.33
1	I	6	CYS	CB-SG	14.88	2.07	1.82
1	A	14	TYR	CE2-CZ	-14.87	1.19	1.38
2	J	15	LEU	N-CA	14.83	1.76	1.46
2	L	6	LEU	CA-CB	14.80	1.87	1.53
1	E	11	CYS	CA-CB	14.71	1.86	1.53
1	A	7	CYS	N-CA	14.67	1.75	1.46
2	J	10	HIS	CD2-NE2	14.66	1.72	1.42
2	B	18	VAL	C-O	14.60	1.51	1.23
2	H	5	HIS	CA-CB	14.60	1.86	1.53
1	G	10	ILE	C-O	14.59	1.51	1.23
2	H	2	VAL	CA-CB	14.59	1.85	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	14	TYR	C-O	14.53	1.50	1.23
2	L	10	HIS	CB-CG	14.51	1.76	1.50
1	E	9	SER	N-CA	14.46	1.75	1.46
2	D	4	GLN	N-CA	-14.39	1.17	1.46
2	J	12	VAL	C-N	14.36	1.67	1.34
2	J	19	CYS	N-CA	14.36	1.75	1.46
2	D	13	GLU	CB-CG	14.32	1.79	1.52
1	G	4	GLU	CG-CD	14.31	1.73	1.51
2	B	11	LEU	CA-CB	-14.30	1.20	1.53
1	E	11	CYS	N-CA	-14.30	1.17	1.46
2	B	13	GLU	CA-C	14.25	1.90	1.52
1	E	18	ASN	CA-C	14.23	1.90	1.52
2	L	8	GLY	N-CA	14.21	1.67	1.46
2	F	16	TYR	CG-CD1	14.21	1.57	1.39
1	K	14	TYR	CD2-CE2	14.17	1.60	1.39
1	I	16	LEU	N-CA	-14.15	1.18	1.46
1	E	2	ILE	N-CA	14.14	1.74	1.46
1	A	11	CYS	C-N	14.13	1.66	1.34
2	B	15	LEU	C-O	14.13	1.50	1.23
2	L	12	VAL	C-N	14.12	1.66	1.34
1	A	19	TYR	CA-CB	14.06	1.84	1.53
2	H	17	LEU	CA-C	14.01	1.89	1.52
1	A	14	TYR	CG-CD1	-13.98	1.21	1.39
2	L	2	VAL	CA-CB	13.96	1.84	1.54
2	J	19	CYS	C-N	13.95	1.58	1.33
2	H	10	HIS	CB-CG	13.93	1.75	1.50
1	I	17	GLU	CA-C	13.92	1.89	1.52
2	B	22	ARG	N-CA	-13.90	1.18	1.46
1	A	21	ASN	CB-CG	13.89	1.83	1.51
1	C	17	GLU	N-CA	-13.89	1.18	1.46
2	L	1	PHE	CE1-CZ	13.88	1.63	1.37
1	I	16	LEU	CA-CB	13.87	1.85	1.53
2	F	16	TYR	CE2-CZ	13.86	1.56	1.38
2	H	2	VAL	CB-CG1	-13.85	1.23	1.52
1	K	17	GLU	CA-C	13.85	1.89	1.52
2	D	22	ARG	NE-CZ	-13.77	1.15	1.33
1	C	4	GLU	CA-C	13.74	1.88	1.52
2	J	1	PHE	C-N	13.73	1.65	1.34
2	J	28	LYS	CA-CB	13.70	1.84	1.53
2	B	4	GLN	CA-CB	-13.69	1.23	1.53
2	B	6	LEU	CB-CG	13.69	1.92	1.52
2	B	25	TYR	CG-CD1	-13.67	1.21	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	11	CYS	CB-SG	13.67	2.05	1.82
2	D	21	GLU	CD-OE2	-13.65	1.10	1.25
2	J	22	ARG	CA-CB	-13.64	1.24	1.53
1	C	8	THR	CA-C	13.64	1.88	1.52
2	L	25	TYR	CE2-CZ	-13.63	1.20	1.38
2	B	18	VAL	N-CA	13.62	1.73	1.46
1	I	15	GLN	CD-OE1	13.62	1.53	1.24
2	L	25	TYR	CG-CD1	-13.62	1.21	1.39
2	L	25	TYR	CB-CG	13.61	1.72	1.51
2	F	21	GLU	CA-CB	-13.59	1.24	1.53
2	J	22	ARG	NE-CZ	13.59	1.50	1.33
2	L	16	TYR	CE2-CZ	13.59	1.56	1.38
1	G	15	GLN	N-CA	-13.58	1.19	1.46
2	L	19	CYS	C-O	13.56	1.49	1.23
2	L	5	HIS	CE1-NE2	13.49	1.63	1.32
2	J	25	TYR	C-O	-13.49	0.97	1.23
1	A	18	ASN	N-CA	-13.47	1.19	1.46
2	F	2	VAL	CB-CG2	13.46	1.81	1.52
1	A	11	CYS	N-CA	13.46	1.73	1.46
1	C	19	TYR	CE2-CZ	13.46	1.56	1.38
2	L	1	PHE	CD2-CE2	13.45	1.66	1.39
2	L	22	ARG	C-O	13.42	1.48	1.23
2	F	4	GLN	CD-OE1	13.41	1.53	1.24
1	C	5	GLN	CA-CB	-13.40	1.24	1.53
2	B	12	VAL	CB-CG2	-13.40	1.24	1.52
1	C	19	TYR	C-O	13.39	1.48	1.23
1	K	8	THR	C-O	13.38	1.48	1.23
2	B	9	SER	CB-OG	-13.36	1.24	1.42
1	G	8	THR	CB-OG1	13.36	1.70	1.43
2	H	24	PHE	C-O	13.36	1.48	1.23
2	L	18	VAL	CA-C	13.34	1.87	1.52
2	L	12	VAL	CB-CG1	-13.34	1.24	1.52
2	D	8	GLY	N-CA	-13.33	1.26	1.46
2	L	12	VAL	CB-CG2	13.33	1.80	1.52
1	C	3	VAL	CB-CG1	-13.32	1.24	1.52
1	E	4	GLU	CG-CD	13.32	1.72	1.51
1	I	5	GLN	CA-C	13.32	1.87	1.52
2	H	13	GLU	CD-OE2	-13.31	1.11	1.25
2	H	12	VAL	CB-CG2	-13.30	1.25	1.52
2	H	13	GLU	N-CA	-13.29	1.19	1.46
2	J	22	ARG	CZ-NH2	-13.29	1.15	1.33
1	E	8	THR	CA-C	13.28	1.87	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	21	GLU	CG-CD	-13.29	1.32	1.51
1	E	19	TYR	C-O	13.27	1.48	1.23
2	B	2	VAL	CB-CG1	-13.26	1.25	1.52
2	F	18	VAL	C-N	13.24	1.64	1.34
1	E	1	GLY	C-O	13.23	1.44	1.23
2	L	22	ARG	CA-CB	-13.21	1.24	1.53
1	C	17	GLU	CA-CB	13.20	1.82	1.53
1	C	20	CYS	CA-CB	13.20	1.82	1.53
1	G	14	TYR	CA-C	-13.17	1.18	1.52
1	K	5	GLN	CA-C	13.17	1.87	1.52
1	I	13	LEU	CA-C	13.15	1.87	1.52
1	G	18	ASN	C-N	13.15	1.64	1.34
2	H	12	VAL	CA-CB	13.14	1.82	1.54
1	K	2	ILE	N-CA	13.14	1.72	1.46
2	J	29	PRO	C-O	13.13	1.49	1.23
2	L	25	TYR	CD2-CE2	13.13	1.59	1.39
1	E	17	GLU	CG-CD	-13.13	1.32	1.51
1	A	6	CYS	N-CA	-13.12	1.20	1.46
1	C	3	VAL	CA-CB	13.09	1.82	1.54
2	H	15	LEU	C-N	13.06	1.64	1.34
1	E	5	GLN	CA-CB	-13.06	1.25	1.53
2	H	21	GLU	CD-OE2	13.06	1.40	1.25
1	C	15	GLN	CA-CB	-13.06	1.25	1.53
2	J	1	PHE	CA-CB	13.06	1.82	1.53
2	L	16	TYR	CB-CG	-13.05	1.32	1.51
2	H	4	GLN	C-N	13.03	1.64	1.34
1	I	14	TYR	CA-CB	-13.03	1.25	1.53
1	C	14	TYR	CA-C	13.01	1.86	1.52
1	C	19	TYR	CG-CD1	13.00	1.56	1.39
1	A	4	GLU	CG-CD	12.99	1.71	1.51
1	E	7	CYS	N-CA	-12.98	1.20	1.46
1	E	19	TYR	CG-CD2	12.98	1.56	1.39
2	B	24	PHE	CE1-CZ	12.96	1.61	1.37
1	I	21	ASN	CA-CB	-12.96	1.19	1.53
2	D	15	LEU	CA-CB	12.93	1.83	1.53
2	J	4	GLN	CA-CB	12.91	1.82	1.53
1	I	7	CYS	N-CA	12.90	1.72	1.46
1	C	16	LEU	C-O	12.88	1.47	1.23
2	F	10	HIS	N-CA	12.82	1.72	1.46
2	J	5	HIS	CE1-NE2	12.82	1.62	1.32
1	G	6	CYS	CA-C	12.79	1.86	1.52
1	K	4	GLU	N-CA	-12.78	1.20	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	14	TYR	CD1-CE1	12.78	1.58	1.39
1	I	18	ASN	C-O	12.76	1.47	1.23
2	J	11	LEU	N-CA	12.74	1.71	1.46
1	I	8	THR	C-O	12.74	1.47	1.23
2	L	22	ARG	CG-CD	-12.70	1.20	1.51
2	H	25	TYR	CE2-CZ	12.68	1.55	1.38
2	L	1	PHE	CD1-CE1	12.65	1.64	1.39
2	J	12	VAL	CB-CG2	12.64	1.79	1.52
1	K	15	GLN	CD-OE1	12.62	1.51	1.24
2	L	14	ALA	CA-C	12.62	1.85	1.52
2	J	2	VAL	CB-CG1	12.60	1.79	1.52
2	F	22	ARG	C-O	12.60	1.47	1.23
1	I	3	VAL	C-N	12.59	1.63	1.34
2	B	1	PHE	CD1-CE1	-12.59	1.14	1.39
2	D	16	TYR	CA-C	12.59	1.85	1.52
2	D	18	VAL	C-N	12.59	1.62	1.34
2	B	10	HIS	CG-ND1	-12.58	1.11	1.38
1	K	6	CYS	N-CA	12.58	1.71	1.46
2	L	1	PHE	C-N	12.58	1.62	1.34
2	B	15	LEU	CG-CD2	12.55	1.98	1.51
2	B	3	ASN	N-CA	12.54	1.71	1.46
1	K	14	TYR	CE1-CZ	12.50	1.54	1.38
2	J	19	CYS	C-O	12.50	1.47	1.23
2	L	5	HIS	N-CA	-12.48	1.21	1.46
2	B	25	TYR	CE2-CZ	-12.47	1.22	1.38
2	B	17	LEU	CA-C	12.45	1.85	1.52
1	I	7	CYS	C-O	12.45	1.47	1.23
2	B	24	PHE	CE2-CZ	-12.43	1.13	1.37
2	B	16	TYR	CA-CB	12.41	1.81	1.53
1	C	11	CYS	N-CA	-12.41	1.21	1.46
2	L	5	HIS	C-N	12.41	1.62	1.34
1	K	21	ASN	C-O	-12.32	0.99	1.23
2	H	15	LEU	CA-CB	-12.32	1.25	1.53
1	K	14	TYR	CZ-OH	12.31	1.58	1.37
2	H	1	PHE	CA-CB	12.30	1.81	1.53
1	E	2	ILE	CB-CG1	12.29	1.88	1.54
2	H	25	TYR	CG-CD1	12.27	1.55	1.39
2	F	16	TYR	CE1-CZ	12.27	1.54	1.38
2	J	9	SER	CB-OG	12.26	1.58	1.42
1	C	7	CYS	CA-CB	12.25	1.80	1.53
2	H	18	VAL	C-O	12.22	1.46	1.23
1	E	9	SER	C-O	12.21	1.46	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	24	PHE	C-O	12.21	1.46	1.23
1	A	3	VAL	N-CA	12.20	1.70	1.46
1	K	14	TYR	CA-CB	-12.17	1.27	1.53
1	C	7	CYS	C-O	-12.17	1.00	1.23
2	B	10	HIS	CA-C	12.16	1.84	1.52
2	J	22	ARG	N-CA	12.16	1.70	1.46
1	E	14	TYR	C-N	-12.13	1.06	1.34
2	H	27	THR	N-CA	-12.11	1.22	1.46
1	C	3	VAL	N-CA	-12.11	1.22	1.46
1	E	19	TYR	CA-CB	-12.10	1.27	1.53
1	C	21	ASN	C-O	12.09	1.46	1.23
2	B	2	VAL	N-CA	-12.09	1.22	1.46
2	F	15	LEU	C-O	-12.09	1.00	1.23
2	D	8	GLY	C-O	-12.08	1.04	1.23
1	K	16	LEU	N-CA	-12.07	1.22	1.46
2	L	23	GLY	C-O	-12.06	1.04	1.23
1	C	2	ILE	N-CA	12.06	1.70	1.46
1	E	17	GLU	N-CA	-12.05	1.22	1.46
1	A	17	GLU	CA-CB	12.04	1.80	1.53
1	C	12	SER	N-CA	12.01	1.70	1.46
2	B	4	GLN	C-N	12.01	1.61	1.34
1	G	11	CYS	CA-C	-12.00	1.21	1.52
1	E	21	ASN	C-OXT	11.97	1.46	1.23
1	G	2	ILE	CB-CG2	11.97	1.90	1.52
2	F	16	TYR	C-O	-11.96	1.00	1.23
1	K	8	THR	CB-OG1	11.96	1.67	1.43
2	D	15	LEU	N-CA	-11.95	1.22	1.46
1	C	16	LEU	CA-C	-11.93	1.22	1.52
2	L	9	SER	CA-CB	11.92	1.70	1.52
2	H	10	HIS	CA-C	11.91	1.83	1.52
1	I	21	ASN	N-CA	11.91	1.70	1.46
2	L	21	GLU	CB-CG	11.90	1.74	1.52
1	K	15	GLN	C-O	11.89	1.46	1.23
2	D	6	LEU	N-CA	11.89	1.70	1.46
1	I	15	GLN	CA-C	-11.88	1.22	1.52
2	B	22	ARG	CD-NE	-11.87	1.26	1.46
2	L	4	GLN	N-CA	11.87	1.70	1.46
1	I	14	TYR	CG-CD1	11.87	1.54	1.39
2	L	10	HIS	CD2-NE2	11.87	1.66	1.42
1	E	4	GLU	C-N	-11.86	1.06	1.34
1	G	15	GLN	CD-OE1	11.86	1.50	1.24
2	H	5	HIS	CA-C	-11.86	1.22	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	12	VAL	CA-C	-11.84	1.22	1.52
1	C	9	SER	C-N	11.84	1.61	1.34
1	C	4	GLU	CG-CD	11.84	1.69	1.51
2	H	8	GLY	C-N	11.81	1.61	1.34
1	G	12	SER	CB-OG	11.80	1.57	1.42
2	J	21	GLU	CA-C	11.79	1.83	1.52
2	B	24	PHE	CD1-CE1	11.78	1.62	1.39
2	D	23	GLY	N-CA	11.77	1.63	1.46
2	L	1	PHE	CG-CD1	-11.74	1.21	1.38
2	J	4	GLN	CG-CD	11.74	1.78	1.51
2	B	10	HIS	C-N	-11.73	1.07	1.34
1	E	13	LEU	C-O	11.72	1.45	1.23
2	L	5	HIS	CB-CG	-11.72	1.28	1.50
1	E	16	LEU	N-CA	11.72	1.69	1.46
1	K	18	ASN	N-CA	11.71	1.69	1.46
2	J	18	VAL	CB-CG1	11.67	1.77	1.52
1	K	13	LEU	C-N	-11.67	1.07	1.34
1	K	15	GLN	CB-CG	-11.63	1.21	1.52
1	I	3	VAL	N-CA	11.63	1.69	1.46
2	D	3	ASN	CA-C	-11.62	1.22	1.52
2	B	2	VAL	CA-CB	11.61	1.79	1.54
1	E	17	GLU	CD-OE1	11.61	1.38	1.25
1	K	4	GLU	CA-CB	11.61	1.79	1.53
1	C	2	ILE	CB-CG1	11.60	1.86	1.54
2	B	23	GLY	C-O	11.60	1.42	1.23
2	L	17	LEU	CA-CB	11.60	1.80	1.53
2	B	2	VAL	CB-CG2	11.59	1.77	1.52
2	B	11	LEU	N-CA	11.55	1.69	1.46
2	F	15	LEU	CA-CB	11.54	1.80	1.53
1	G	12	SER	N-CA	-11.53	1.23	1.46
2	J	3	ASN	C-N	11.52	1.60	1.34
2	F	22	ARG	NE-CZ	11.52	1.48	1.33
2	J	8	GLY	C-N	11.49	1.60	1.34
2	J	24	PHE	CD2-CE2	11.49	1.62	1.39
2	F	19	CYS	C-O	-11.48	1.01	1.23
2	J	28	LYS	CB-CG	-11.48	1.21	1.52
1	K	17	GLU	CD-OE2	11.47	1.38	1.25
2	L	4	GLN	CG-CD	11.47	1.77	1.51
2	H	6	LEU	CB-CG	11.47	1.85	1.52
1	K	10	ILE	CA-C	11.46	1.82	1.52
1	A	16	LEU	C-N	11.45	1.60	1.34
1	K	3	VAL	N-CA	11.39	1.69	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	23	GLY	CA-C	-11.39	1.33	1.51
2	B	21	GLU	CD-OE1	11.38	1.38	1.25
1	E	7	CYS	C-O	-11.37	1.01	1.23
1	C	18	ASN	CA-C	11.37	1.82	1.52
2	D	14	ALA	N-CA	11.37	1.69	1.46
2	L	16	TYR	CD1-CE1	-11.37	1.22	1.39
2	B	11	LEU	C-O	11.36	1.45	1.23
1	C	14	TYR	CA-CB	11.35	1.78	1.53
1	E	6	CYS	N-CA	11.35	1.69	1.46
2	F	16	TYR	CG-CD2	11.34	1.53	1.39
2	L	2	VAL	C-N	-11.33	1.07	1.34
2	J	10	HIS	C-N	11.33	1.60	1.34
1	C	6	CYS	CB-SG	-11.33	1.62	1.82
2	D	25	TYR	CA-C	-11.32	1.23	1.52
1	E	10	ILE	CA-CB	11.31	1.80	1.54
1	K	11	CYS	N-CA	11.31	1.69	1.46
2	B	8	GLY	CA-C	-11.30	1.33	1.51
2	L	22	ARG	NE-CZ	-11.29	1.18	1.33
2	B	25	TYR	N-CA	11.29	1.69	1.46
2	J	12	VAL	CB-CG1	-11.28	1.29	1.52
2	F	4	GLN	N-CA	-11.25	1.23	1.46
2	F	11	LEU	C-N	11.25	1.59	1.34
1	A	2	ILE	N-CA	-11.22	1.24	1.46
1	A	5	GLN	CA-CB	11.22	1.78	1.53
2	H	13	GLU	CA-C	11.21	1.82	1.52
1	I	13	LEU	CB-CG	11.20	1.85	1.52
1	K	7	CYS	C-N	-11.19	1.08	1.34
2	B	4	GLN	N-CA	11.19	1.68	1.46
2	D	14	ALA	C-N	11.18	1.59	1.34
2	J	2	VAL	C-N	-11.16	1.08	1.34
2	L	16	TYR	CD2-CE2	-11.16	1.22	1.39
2	J	3	ASN	CA-CB	-11.15	1.24	1.53
2	H	22	ARG	C-O	-11.14	1.02	1.23
2	D	12	VAL	C-O	-11.14	1.02	1.23
2	H	22	ARG	C-N	11.14	1.53	1.33
1	A	18	ASN	CB-CG	-11.14	1.25	1.51
2	H	1	PHE	CB-CG	-11.14	1.32	1.51
2	F	14	ALA	C-N	11.13	1.59	1.34
2	J	22	ARG	CD-NE	-11.12	1.27	1.46
2	F	25	TYR	CA-C	-11.12	1.24	1.52
2	L	21	GLU	CD-OE1	-11.11	1.13	1.25
2	B	21	GLU	CA-C	-11.09	1.24	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	2	ILE	CB-CG1	-11.07	1.23	1.54
1	A	5	GLN	N-CA	11.07	1.68	1.46
1	E	6	CYS	C-O	11.04	1.44	1.23
2	H	21	GLU	CA-C	-11.02	1.24	1.52
2	D	11	LEU	C-N	11.02	1.59	1.34
1	K	3	VAL	C-O	11.01	1.44	1.23
1	K	14	TYR	CG-CD2	11.01	1.53	1.39
1	A	18	ASN	C-N	10.99	1.59	1.34
2	D	22	ARG	C-N	-10.97	1.13	1.33
1	K	6	CYS	C-O	10.97	1.44	1.23
1	G	18	ASN	CB-CG	10.97	1.76	1.51
1	K	14	TYR	CB-CG	10.96	1.68	1.51
2	B	1	PHE	CD2-CE2	-10.95	1.17	1.39
1	E	7	CYS	CA-CB	10.95	1.78	1.53
1	K	2	ILE	CA-C	10.93	1.81	1.52
2	D	16	TYR	C-O	-10.92	1.02	1.23
1	I	17	GLU	CD-OE1	-10.92	1.13	1.25
2	L	25	TYR	CG-CD2	10.92	1.53	1.39
1	A	10	ILE	CA-C	10.91	1.81	1.52
1	G	13	LEU	CA-CB	-10.90	1.28	1.53
2	F	3	ASN	N-CA	10.90	1.68	1.46
1	E	18	ASN	N-CA	10.88	1.68	1.46
1	A	6	CYS	C-O	-10.87	1.02	1.23
1	I	20	CYS	CA-C	10.86	1.81	1.52
1	I	6	CYS	CA-C	10.83	1.81	1.52
1	I	20	CYS	C-N	-10.82	1.09	1.34
1	C	21	ASN	N-CA	-10.81	1.24	1.46
1	A	3	VAL	C-N	-10.80	1.09	1.34
2	B	23	GLY	CA-C	-10.79	1.34	1.51
2	D	16	TYR	CG-CD1	10.79	1.53	1.39
2	L	11	LEU	C-N	-10.78	1.09	1.34
2	H	6	LEU	CA-C	10.76	1.80	1.52
1	I	2	ILE	CB-CG1	10.76	1.84	1.54
1	C	8	THR	CB-CG2	10.75	1.87	1.52
1	K	10	ILE	CA-CB	10.74	1.79	1.54
2	J	28	LYS	C-N	-10.74	1.13	1.34
1	C	13	LEU	CA-CB	10.72	1.78	1.53
2	J	10	HIS	CA-C	10.71	1.80	1.52
2	B	4	GLN	CB-CG	10.69	1.81	1.52
2	J	14	ALA	CA-C	10.68	1.80	1.52
1	K	3	VAL	CB-CG2	-10.68	1.30	1.52
1	G	10	ILE	CA-CB	-10.68	1.30	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	11	LEU	C-N	-10.65	1.09	1.34
2	B	3	ASN	CB-CG	-10.64	1.26	1.51
2	H	4	GLN	CA-CB	-10.64	1.30	1.53
1	I	21	ASN	C-OXT	10.64	1.43	1.23
2	F	12	VAL	C-O	-10.62	1.03	1.23
1	I	4	GLU	N-CA	-10.62	1.25	1.46
2	H	22	ARG	CA-CB	10.62	1.77	1.53
1	K	7	CYS	N-CA	10.60	1.67	1.46
2	D	5	HIS	CA-C	10.60	1.80	1.52
2	H	24	PHE	CG-CD1	-10.58	1.22	1.38
2	B	11	LEU	CG-CD2	10.58	1.91	1.51
2	D	3	ASN	CG-ND2	10.58	1.59	1.32
1	A	3	VAL	CB-CG1	10.57	1.75	1.52
1	A	19	TYR	C-O	10.57	1.43	1.23
2	B	24	PHE	CD2-CE2	10.57	1.60	1.39
2	B	19	CYS	CB-SG	-10.57	1.64	1.82
1	A	13	LEU	CA-CB	-10.57	1.29	1.53
1	C	7	CYS	N-CA	-10.55	1.25	1.46
1	I	7	CYS	CB-SG	-10.55	1.64	1.82
1	A	8	THR	CA-CB	-10.53	1.25	1.53
1	E	4	GLU	CA-C	10.52	1.80	1.52
2	H	17	LEU	CG-CD1	10.52	1.90	1.51
2	J	6	LEU	N-CA	10.51	1.67	1.46
2	L	16	TYR	C-N	10.51	1.58	1.34
2	B	22	ARG	CZ-NH1	-10.50	1.19	1.33
2	F	20	GLY	C-N	-10.50	1.09	1.34
1	I	11	CYS	CB-SG	10.49	2.00	1.82
2	F	10	HIS	CG-CD2	-10.49	1.18	1.35
2	H	11	LEU	CA-CB	-10.49	1.29	1.53
2	H	15	LEU	CG-CD2	10.49	1.90	1.51
1	C	16	LEU	CB-CG	-10.48	1.22	1.52
1	C	6	CYS	N-CA	10.48	1.67	1.46
2	J	10	HIS	CG-ND1	10.46	1.61	1.38
2	F	4	GLN	C-O	-10.46	1.03	1.23
1	I	19	TYR	CB-CG	-10.45	1.35	1.51
2	J	13	GLU	CB-CG	10.45	1.72	1.52
2	L	3	ASN	C-N	10.43	1.58	1.34
1	G	11	CYS	C-N	10.42	1.58	1.34
2	H	2	VAL	CB-CG2	10.40	1.74	1.52
1	A	7	CYS	CB-SG	-10.40	1.64	1.82
1	E	5	GLN	CA-C	10.40	1.79	1.52
2	B	13	GLU	N-CA	-10.38	1.25	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	TYR	N-CA	10.38	1.67	1.46
1	A	4	GLU	CA-CB	-10.37	1.31	1.53
2	J	29	PRO	N-CA	10.37	1.64	1.47
1	G	21	ASN	CG-ND2	10.36	1.58	1.32
2	L	21	GLU	C-O	10.34	1.43	1.23
2	L	4	GLN	CB-CG	-10.32	1.24	1.52
2	F	22	ARG	CZ-NH1	10.32	1.46	1.33
2	J	22	ARG	CG-CD	-10.31	1.26	1.51
1	K	12	SER	C-O	10.31	1.43	1.23
1	G	20	CYS	CA-CB	-10.31	1.31	1.53
1	E	10	ILE	CA-C	-10.30	1.26	1.52
1	K	18	ASN	CB-CG	-10.30	1.27	1.51
2	J	5	HIS	CB-CG	-10.29	1.31	1.50
1	E	5	GLN	N-CA	10.29	1.67	1.46
1	G	13	LEU	CG-CD2	10.28	1.89	1.51
1	G	11	CYS	C-O	10.28	1.42	1.23
1	K	19	TYR	CG-CD2	10.27	1.52	1.39
2	B	10	HIS	N-CA	10.27	1.66	1.46
2	H	2	VAL	N-CA	-10.26	1.25	1.46
1	K	14	TYR	N-CA	10.25	1.66	1.46
1	I	10	ILE	CA-C	10.24	1.79	1.52
1	A	21	ASN	CA-CB	10.23	1.79	1.53
1	A	17	GLU	CB-CG	10.23	1.71	1.52
1	G	5	GLN	CD-OE1	10.22	1.46	1.24
1	A	6	CYS	CA-C	10.21	1.79	1.52
2	J	9	SER	C-N	-10.21	1.10	1.34
2	F	3	ASN	CA-C	-10.19	1.26	1.52
2	J	28	LYS	CE-NZ	10.19	1.74	1.49
1	A	2	ILE	C-N	10.19	1.57	1.34
1	K	19	TYR	CE2-CZ	10.17	1.51	1.38
2	D	14	ALA	CA-C	-10.13	1.26	1.52
1	I	4	GLU	CD-OE2	-10.13	1.14	1.25
2	L	5	HIS	CG-ND1	10.13	1.61	1.38
2	J	3	ASN	CB-CG	10.13	1.74	1.51
2	B	6	LEU	N-CA	-10.12	1.26	1.46
2	H	4	GLN	N-CA	10.10	1.66	1.46
1	E	8	THR	C-N	-10.10	1.10	1.34
2	B	17	LEU	CB-CG	-10.09	1.23	1.52
2	L	25	TYR	CD1-CE1	10.09	1.54	1.39
1	G	19	TYR	CA-CB	10.08	1.76	1.53
2	H	19	CYS	CB-SG	-10.08	1.65	1.82
2	J	27	THR	C-O	-10.07	1.04	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	10	HIS	ND1-CE1	10.07	1.59	1.34
1	G	13	LEU	C-N	10.02	1.57	1.34
2	J	2	VAL	N-CA	10.02	1.66	1.46
2	D	7	CYS	CA-C	-10.02	1.26	1.52
1	C	18	ASN	N-CA	10.01	1.66	1.46
2	L	13	GLU	C-N	-10.00	1.11	1.34
1	K	17	GLU	CD-OE1	-10.00	1.14	1.25
1	G	12	SER	C-O	-9.99	1.04	1.23
1	I	5	GLN	CD-OE1	-9.98	1.01	1.24
1	I	19	TYR	C-O	-9.98	1.04	1.23
1	G	14	TYR	CA-CB	9.98	1.75	1.53
2	J	5	HIS	N-CA	-9.97	1.26	1.46
1	K	16	LEU	CA-C	9.97	1.78	1.52
1	K	16	LEU	CB-CG	9.96	1.81	1.52
2	B	22	ARG	C-O	-9.95	1.04	1.23
1	G	5	GLN	C-N	9.94	1.56	1.34
1	C	2	ILE	C-N	9.94	1.56	1.34
2	L	6	LEU	CG-CD1	9.93	1.88	1.51
1	A	21	ASN	C-O	-9.92	1.04	1.23
2	H	3	ASN	CA-C	9.91	1.78	1.52
2	D	20	GLY	CA-C	9.88	1.67	1.51
1	C	17	GLU	CD-OE1	-9.85	1.14	1.25
1	A	5	GLN	CA-C	-9.84	1.27	1.52
2	L	11	LEU	N-CA	9.82	1.66	1.46
1	C	15	GLN	CG-CD	-9.79	1.28	1.51
2	B	21	GLU	CA-CB	9.78	1.75	1.53
1	C	2	ILE	CA-C	-9.76	1.27	1.52
1	I	11	CYS	N-CA	9.75	1.65	1.46
2	H	22	ARG	N-CA	-9.74	1.26	1.46
2	L	13	GLU	CD-OE2	9.73	1.36	1.25
2	D	10	HIS	CB-CG	-9.73	1.32	1.50
2	B	16	TYR	CD2-CE2	-9.73	1.24	1.39
1	K	9	SER	C-O	9.72	1.41	1.23
2	J	24	PHE	CD1-CE1	9.70	1.58	1.39
2	L	21	GLU	N-CA	9.68	1.65	1.46
2	D	22	ARG	C-O	9.65	1.41	1.23
2	F	11	LEU	C-O	-9.64	1.05	1.23
2	B	3	ASN	CA-C	9.64	1.78	1.52
1	E	21	ASN	CA-CB	9.63	1.78	1.53
2	H	24	PHE	C-N	-9.63	1.11	1.34
1	I	15	GLN	C-O	9.63	1.41	1.23
2	F	9	SER	CA-CB	-9.61	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PHE	CA-C	-9.61	1.27	1.52
2	H	19	CYS	CA-CB	-9.61	1.32	1.53
2	B	1	PHE	CA-C	-9.60	1.27	1.52
2	J	22	ARG	C-O	9.60	1.41	1.23
2	B	5	HIS	CA-C	-9.59	1.28	1.52
1	K	7	CYS	C-O	9.59	1.41	1.23
1	K	5	GLN	C-N	-9.58	1.12	1.34
1	K	13	LEU	CA-C	9.58	1.77	1.52
2	F	2	VAL	C-O	-9.57	1.05	1.23
1	K	17	GLU	N-CA	9.56	1.65	1.46
1	I	10	ILE	CB-CG1	9.54	1.80	1.54
2	L	25	TYR	CE1-CZ	9.54	1.50	1.38
2	D	11	LEU	N-CA	-9.53	1.27	1.46
2	H	10	HIS	CG-ND1	-9.53	1.17	1.38
2	B	1	PHE	C-O	9.52	1.41	1.23
2	B	22	ARG	CA-C	9.52	1.77	1.52
2	B	15	LEU	CA-CB	-9.51	1.31	1.53
1	E	20	CYS	CA-CB	9.50	1.74	1.53
2	B	16	TYR	CB-CG	-9.50	1.37	1.51
1	A	17	GLU	CA-C	-9.48	1.28	1.52
1	I	14	TYR	CE2-CZ	9.48	1.50	1.38
2	B	14	ALA	C-O	9.48	1.41	1.23
2	H	4	GLN	CG-CD	-9.46	1.29	1.51
1	A	10	ILE	CB-CG1	9.45	1.80	1.54
1	K	17	GLU	C-O	9.43	1.41	1.23
1	E	15	GLN	CA-C	9.41	1.77	1.52
2	F	23	GLY	N-CA	-9.40	1.31	1.46
1	K	19	TYR	CE1-CZ	9.40	1.50	1.38
1	E	3	VAL	CB-CG2	9.40	1.72	1.52
1	G	3	VAL	N-CA	9.40	1.65	1.46
2	B	3	ASN	C-N	-9.39	1.12	1.34
2	L	25	TYR	CZ-OH	9.38	1.53	1.37
1	K	10	ILE	CB-CG1	9.38	1.80	1.54
2	J	18	VAL	CA-C	9.38	1.77	1.52
2	F	10	HIS	CB-CG	-9.37	1.33	1.50
2	J	2	VAL	CB-CG2	-9.34	1.33	1.52
2	D	12	VAL	CB-CG1	9.32	1.72	1.52
2	H	13	GLU	CG-CD	9.31	1.66	1.51
2	B	4	GLN	CD-OE1	9.31	1.44	1.24
2	D	16	TYR	CE2-CZ	9.29	1.50	1.38
1	E	9	SER	C-N	9.28	1.55	1.34
2	J	5	HIS	CD2-NE2	-9.28	1.17	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	18	ASN	CB-CG	9.27	1.72	1.51
2	D	6	LEU	CA-CB	-9.27	1.32	1.53
1	G	19	TYR	C-O	9.26	1.41	1.23
1	K	10	ILE	C-O	-9.25	1.05	1.23
2	F	9	SER	C-N	9.24	1.55	1.34
1	C	19	TYR	CA-CB	-9.23	1.33	1.53
1	I	19	TYR	N-CA	-9.21	1.27	1.46
2	L	20	GLY	N-CA	-9.21	1.32	1.46
2	L	4	GLN	CA-C	-9.20	1.29	1.52
1	E	4	GLU	CB-CG	9.20	1.69	1.52
2	D	19	CYS	C-O	-9.19	1.05	1.23
1	G	16	LEU	N-CA	9.18	1.64	1.46
2	D	20	GLY	C-N	-9.18	1.12	1.34
2	J	11	LEU	CB-CG	-9.18	1.25	1.52
2	F	22	ARG	CA-CB	9.16	1.74	1.53
1	G	10	ILE	N-CA	-9.16	1.28	1.46
2	J	13	GLU	C-N	-9.16	1.12	1.34
2	B	12	VAL	C-O	9.16	1.40	1.23
2	B	24	PHE	C-N	-9.16	1.12	1.34
2	D	13	GLU	CA-C	9.16	1.76	1.52
2	F	20	GLY	C-O	9.16	1.38	1.23
2	L	25	TYR	CA-CB	9.16	1.74	1.53
1	K	5	GLN	CG-CD	9.15	1.72	1.51
2	J	13	GLU	CD-OE2	9.14	1.35	1.25
1	A	9	SER	C-N	-9.13	1.13	1.34
1	E	15	GLN	CA-CB	-9.13	1.33	1.53
1	I	19	TYR	CD2-CE2	-9.13	1.25	1.39
2	B	18	VAL	CA-CB	-9.12	1.35	1.54
2	F	9	SER	C-O	-9.12	1.06	1.23
1	A	2	ILE	CB-CG1	-9.09	1.28	1.54
1	C	6	CYS	C-O	9.09	1.40	1.23
1	A	3	VAL	CA-CB	9.08	1.73	1.54
1	C	8	THR	C-O	-9.06	1.06	1.23
1	K	3	VAL	CB-CG1	9.04	1.71	1.52
2	B	10	HIS	ND1-CE1	9.02	1.57	1.34
2	H	14	ALA	C-N	-9.01	1.13	1.34
2	J	11	LEU	CA-CB	9.00	1.74	1.53
1	A	9	SER	CB-OG	-8.98	1.30	1.42
2	B	16	TYR	CD1-CE1	-8.98	1.25	1.39
2	H	1	PHE	CD1-CE1	-8.98	1.21	1.39
1	A	8	THR	CB-OG1	8.97	1.61	1.43
2	D	12	VAL	N-CA	-8.96	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	19	CYS	CA-CB	8.96	1.73	1.53
1	I	12	SER	CA-CB	-8.96	1.39	1.52
2	F	10	HIS	ND1-CE1	-8.96	1.12	1.34
2	J	12	VAL	CA-CB	-8.96	1.35	1.54
1	A	2	ILE	CB-CG2	8.95	1.80	1.52
1	A	7	CYS	CA-CB	8.94	1.73	1.53
1	E	6	CYS	CA-C	-8.94	1.29	1.52
2	F	17	LEU	CB-CG	8.93	1.78	1.52
1	I	19	TYR	CD1-CE1	-8.93	1.25	1.39
1	K	6	CYS	CB-SG	8.91	1.97	1.82
1	K	19	TYR	CD1-CE1	-8.91	1.25	1.39
2	F	15	LEU	CG-CD1	8.89	1.84	1.51
2	B	17	LEU	C-N	-8.89	1.13	1.34
1	I	3	VAL	CA-C	-8.86	1.29	1.52
1	I	10	ILE	CA-CB	8.86	1.75	1.54
2	D	21	GLU	CB-CG	8.85	1.69	1.52
1	C	8	THR	CB-OG1	-8.84	1.25	1.43
1	E	3	VAL	N-CA	-8.83	1.28	1.46
1	E	16	LEU	CB-CG	-8.83	1.26	1.52
1	G	11	CYS	N-CA	8.82	1.64	1.46
2	D	5	HIS	CA-CB	8.81	1.73	1.53
1	C	21	ASN	C-OXT	-8.81	1.06	1.23
1	I	16	LEU	CG-CD1	8.79	1.84	1.51
2	L	21	GLU	C-N	-8.78	1.13	1.34
1	K	15	GLN	CA-C	-8.78	1.30	1.52
2	D	9	SER	CA-CB	-8.77	1.39	1.52
1	K	3	VAL	CA-C	-8.77	1.30	1.52
1	A	2	ILE	CA-C	8.76	1.75	1.52
1	I	17	GLU	CG-CD	-8.75	1.38	1.51
2	J	24	PHE	CG-CD1	8.75	1.51	1.38
2	L	3	ASN	CA-C	8.73	1.75	1.52
1	A	10	ILE	C-O	8.71	1.40	1.23
2	F	24	PHE	CA-C	8.71	1.75	1.52
2	F	10	HIS	CA-CB	8.70	1.73	1.53
2	L	14	ALA	C-N	8.70	1.54	1.34
2	B	2	VAL	CA-C	8.69	1.75	1.52
1	C	17	GLU	CB-CG	8.69	1.68	1.52
1	I	18	ASN	CB-CG	-8.69	1.31	1.51
1	A	17	GLU	N-CA	8.67	1.63	1.46
1	K	9	SER	CB-OG	-8.66	1.30	1.42
1	C	12	SER	CA-CB	8.66	1.66	1.52
2	J	1	PHE	CG-CD1	-8.65	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	23	GLY	C-O	-8.65	1.09	1.23
1	A	14	TYR	CA-CB	8.65	1.73	1.53
1	I	19	TYR	CZ-OH	-8.65	1.23	1.37
2	D	11	LEU	CA-C	-8.63	1.30	1.52
2	L	4	GLN	CA-CB	8.61	1.72	1.53
2	H	10	HIS	CE1-NE2	-8.61	1.12	1.32
2	D	11	LEU	CG-CD2	8.61	1.83	1.51
2	F	3	ASN	CG-ND2	8.60	1.54	1.32
2	L	22	ARG	C-N	8.60	1.48	1.33
1	K	15	GLN	CG-CD	8.59	1.70	1.51
1	E	14	TYR	C-O	8.59	1.39	1.23
2	H	11	LEU	C-N	8.59	1.53	1.34
1	G	15	GLN	C-N	8.59	1.53	1.34
1	E	3	VAL	CA-CB	8.59	1.72	1.54
2	L	1	PHE	CE2-CZ	-8.58	1.21	1.37
1	G	12	SER	C-N	-8.57	1.14	1.34
1	I	14	TYR	C-O	8.56	1.39	1.23
2	D	23	GLY	C-O	8.56	1.37	1.23
1	A	4	GLU	C-N	8.55	1.53	1.34
2	L	14	ALA	N-CA	-8.55	1.29	1.46
2	J	16	TYR	CD2-CE2	-8.54	1.26	1.39
2	L	19	CYS	CB-SG	-8.52	1.67	1.82
1	A	5	GLN	CG-CD	8.51	1.70	1.51
2	F	14	ALA	N-CA	8.51	1.63	1.46
2	L	25	TYR	C-O	8.50	1.39	1.23
2	F	6	LEU	N-CA	8.49	1.63	1.46
2	F	16	TYR	C-N	8.49	1.53	1.34
2	F	13	GLU	C-O	-8.46	1.07	1.23
1	C	15	GLN	CA-C	8.46	1.75	1.52
1	A	8	THR	C-N	8.45	1.53	1.34
2	D	4	GLN	CD-OE1	8.44	1.42	1.24
2	J	27	THR	CA-CB	8.44	1.75	1.53
1	C	6	CYS	CA-C	-8.43	1.31	1.52
1	C	11	CYS	CA-C	8.42	1.74	1.52
2	L	18	VAL	CA-CB	-8.39	1.37	1.54
1	K	5	GLN	CD-NE2	-8.34	1.11	1.32
2	B	7	CYS	C-O	8.32	1.39	1.23
1	E	14	TYR	CA-C	8.31	1.74	1.52
1	C	16	LEU	CG-CD2	8.31	1.82	1.51
1	I	13	LEU	C-N	-8.30	1.15	1.34
2	D	18	VAL	CA-C	-8.30	1.31	1.52
2	J	24	PHE	CE2-CZ	8.27	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	ASN	CB-CG	8.25	1.70	1.51
2	J	4	GLN	CA-C	-8.24	1.31	1.52
1	C	15	GLN	C-O	8.23	1.39	1.23
1	A	15	GLN	CD-NE2	-8.23	1.12	1.32
2	B	18	VAL	CB-CG1	8.22	1.70	1.52
2	F	25	TYR	N-CA	8.22	1.62	1.46
1	G	10	ILE	CA-C	8.22	1.74	1.52
2	L	6	LEU	CG-CD2	-8.22	1.21	1.51
2	F	12	VAL	CB-CG2	-8.22	1.35	1.52
1	E	14	TYR	CA-CB	8.22	1.72	1.53
2	B	1	PHE	CA-CB	8.20	1.72	1.53
2	F	9	SER	CA-C	8.19	1.74	1.52
2	B	22	ARG	C-N	8.19	1.47	1.33
1	G	15	GLN	C-O	-8.16	1.07	1.23
1	I	3	VAL	CA-CB	-8.16	1.37	1.54
1	C	4	GLU	CA-CB	8.15	1.71	1.53
1	K	19	TYR	CG-CD1	8.15	1.49	1.39
2	B	17	LEU	CG-CD1	8.14	1.81	1.51
2	F	21	GLU	CD-OE1	8.13	1.34	1.25
1	C	14	TYR	C-N	-8.13	1.15	1.34
2	D	10	HIS	CE1-NE2	8.12	1.51	1.32
1	G	10	ILE	CB-CG1	8.10	1.76	1.54
2	F	5	HIS	C-O	-8.10	1.07	1.23
2	B	8	GLY	C-O	8.09	1.36	1.23
1	C	19	TYR	CB-CG	-8.09	1.39	1.51
2	D	22	ARG	CA-C	8.09	1.74	1.52
1	I	7	CYS	CA-CB	-8.08	1.36	1.53
1	G	6	CYS	C-N	-8.07	1.15	1.34
2	J	10	HIS	ND1-CE1	8.07	1.54	1.34
2	D	15	LEU	CG-CD1	8.07	1.81	1.51
2	J	19	CYS	CB-SG	-8.05	1.68	1.82
2	L	15	LEU	CA-CB	8.03	1.72	1.53
2	L	10	HIS	C-N	8.02	1.52	1.34
1	A	21	ASN	CA-C	8.02	1.73	1.52
1	I	3	VAL	CB-CG2	-8.02	1.36	1.52
1	K	19	TYR	CD2-CE2	-8.01	1.27	1.39
2	F	2	VAL	CA-CB	-8.01	1.38	1.54
2	B	11	LEU	C-N	8.00	1.52	1.34
1	E	2	ILE	CA-C	-7.99	1.32	1.52
2	B	10	HIS	CB-CG	7.97	1.64	1.50
2	L	24	PHE	C-N	-7.97	1.15	1.34
2	J	27	THR	CB-OG1	7.97	1.59	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	17	LEU	N-CA	7.96	1.62	1.46
1	G	4	GLU	CD-OE1	-7.95	1.17	1.25
2	B	15	LEU	C-N	7.94	1.52	1.34
1	C	6	CYS	C-N	7.94	1.52	1.34
1	A	17	GLU	CG-CD	-7.91	1.40	1.51
1	A	10	ILE	CA-CB	-7.91	1.36	1.54
1	K	2	ILE	CB-CG1	7.90	1.76	1.54
2	D	12	VAL	CB-CG2	-7.90	1.36	1.52
2	B	9	SER	N-CA	-7.90	1.30	1.46
1	E	19	TYR	CB-CG	-7.89	1.39	1.51
1	E	2	ILE	CB-CG2	7.89	1.77	1.52
2	J	4	GLN	N-CA	7.89	1.62	1.46
2	L	10	HIS	CG-ND1	7.89	1.56	1.38
1	K	5	GLN	CA-CB	7.88	1.71	1.53
1	C	14	TYR	CB-CG	-7.87	1.39	1.51
2	F	2	VAL	C-N	7.86	1.52	1.34
2	L	17	LEU	CB-CG	7.83	1.75	1.52
2	J	12	VAL	N-CA	-7.82	1.30	1.46
2	F	2	VAL	CA-C	7.82	1.73	1.52
2	H	21	GLU	CD-OE1	7.81	1.34	1.25
1	G	5	GLN	CA-CB	7.80	1.71	1.53
1	C	16	LEU	C-N	7.80	1.51	1.34
2	B	14	ALA	C-N	-7.80	1.16	1.34
1	I	3	VAL	C-O	7.79	1.38	1.23
2	L	1	PHE	N-CA	7.79	1.61	1.46
2	F	17	LEU	C-O	-7.79	1.08	1.23
2	J	16	TYR	N-CA	-7.77	1.30	1.46
1	C	13	LEU	N-CA	-7.76	1.30	1.46
2	L	7	CYS	CA-C	7.75	1.73	1.52
2	D	10	HIS	CA-C	-7.73	1.32	1.52
1	A	16	LEU	CB-CG	7.71	1.75	1.52
2	H	4	GLN	CB-CG	7.71	1.73	1.52
1	K	13	LEU	CB-CG	-7.70	1.30	1.52
2	B	4	GLN	C-O	7.68	1.38	1.23
1	I	19	TYR	CA-CB	7.67	1.70	1.53
1	K	6	CYS	CA-C	7.66	1.72	1.52
1	A	4	GLU	CD-OE1	-7.66	1.17	1.25
2	F	23	GLY	C-O	7.66	1.35	1.23
1	G	21	ASN	CA-CB	7.66	1.73	1.53
1	K	21	ASN	CA-CB	-7.65	1.33	1.53
2	H	14	ALA	CA-C	7.64	1.72	1.52
2	L	24	PHE	N-CA	-7.63	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	13	GLU	N-CA	7.63	1.61	1.46
2	L	7	CYS	C-N	7.62	1.46	1.33
2	H	15	LEU	N-CA	7.62	1.61	1.46
1	K	7	CYS	CB-SG	-7.62	1.69	1.82
1	I	18	ASN	CA-C	-7.59	1.33	1.52
1	G	2	ILE	N-CA	-7.59	1.31	1.46
2	L	24	PHE	C-O	-7.55	1.09	1.23
1	A	5	GLN	CB-CG	7.54	1.72	1.52
1	K	19	TYR	CA-CB	7.53	1.70	1.53
1	A	18	ASN	CG-ND2	7.53	1.51	1.32
1	K	8	THR	N-CA	7.53	1.61	1.46
2	L	15	LEU	C-N	-7.53	1.16	1.34
2	J	3	ASN	CG-ND2	7.52	1.51	1.32
1	E	5	GLN	CD-OE1	-7.52	1.07	1.24
1	I	2	ILE	CA-C	7.52	1.72	1.52
2	D	13	GLU	CA-CB	-7.50	1.37	1.53
1	C	5	GLN	CB-CG	7.50	1.72	1.52
1	C	10	ILE	CA-C	-7.50	1.33	1.52
2	F	2	VAL	CB-CG1	7.49	1.68	1.52
1	K	19	TYR	CB-CG	-7.47	1.40	1.51
1	C	11	CYS	CA-CB	7.46	1.70	1.53
1	K	16	LEU	CA-CB	7.45	1.70	1.53
1	C	16	LEU	N-CA	7.45	1.61	1.46
1	G	15	GLN	CB-CG	7.45	1.72	1.52
1	I	14	TYR	CG-CD2	7.43	1.48	1.39
1	E	10	ILE	CB-CG1	-7.42	1.33	1.54
2	L	5	HIS	ND1-CE1	-7.40	1.16	1.34
2	D	10	HIS	CG-ND1	7.38	1.54	1.38
2	J	16	TYR	CD1-CE1	-7.38	1.28	1.39
1	K	19	TYR	CZ-OH	-7.37	1.25	1.37
2	F	22	ARG	C-N	-7.36	1.19	1.33
2	D	15	LEU	C-O	-7.36	1.09	1.23
2	D	24	PHE	CG-CD2	7.35	1.49	1.38
1	C	19	TYR	CD1-CE1	-7.33	1.28	1.39
2	D	2	VAL	CB-CG1	7.33	1.68	1.52
2	L	10	HIS	CA-C	7.33	1.72	1.52
2	L	16	TYR	CZ-OH	-7.32	1.25	1.37
1	E	17	GLU	CA-C	7.31	1.72	1.52
2	J	28	LYS	CG-CD	7.31	1.77	1.52
2	J	6	LEU	CA-CB	7.30	1.70	1.53
2	D	11	LEU	CG-CD1	7.29	1.78	1.51
1	C	4	GLU	CB-CG	-7.29	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	12	VAL	CA-C	-7.29	1.34	1.52
1	A	16	LEU	N-CA	7.29	1.60	1.46
1	A	18	ASN	CG-OD1	7.28	1.40	1.24
2	D	2	VAL	CB-CG2	-7.28	1.37	1.52
1	I	14	TYR	CE1-CZ	7.27	1.48	1.38
1	G	18	ASN	CG-ND2	7.26	1.51	1.32
2	J	1	PHE	CB-CG	7.26	1.63	1.51
2	D	11	LEU	CA-CB	7.25	1.70	1.53
2	L	10	HIS	CA-CB	7.25	1.69	1.53
1	I	5	GLN	CA-CB	7.25	1.69	1.53
2	L	7	CYS	CA-CB	-7.24	1.38	1.53
1	K	4	GLU	CG-CD	7.24	1.62	1.51
1	E	4	GLU	CA-CB	7.23	1.69	1.53
2	H	11	LEU	C-O	7.22	1.37	1.23
1	C	4	GLU	C-N	-7.21	1.17	1.34
2	H	19	CYS	C-O	7.21	1.37	1.23
2	H	7	CYS	C-N	-7.21	1.20	1.33
1	G	13	LEU	CA-C	7.21	1.71	1.52
2	H	24	PHE	CE2-CZ	-7.21	1.23	1.37
2	L	4	GLN	C-N	-7.20	1.17	1.34
2	J	12	VAL	CA-C	7.19	1.71	1.52
2	D	23	GLY	C-N	7.19	1.50	1.34
1	K	2	ILE	CB-CG2	-7.18	1.30	1.52
2	D	5	HIS	C-O	-7.17	1.09	1.23
2	H	12	VAL	CB-CG1	-7.17	1.37	1.52
2	D	21	GLU	CA-C	7.16	1.71	1.52
1	I	18	ASN	C-N	7.16	1.50	1.34
1	G	8	THR	CA-CB	-7.16	1.34	1.53
1	E	6	CYS	CA-CB	-7.15	1.38	1.53
1	I	15	GLN	C-N	7.15	1.50	1.34
2	F	10	HIS	CG-ND1	7.14	1.54	1.38
2	J	3	ASN	CA-C	7.14	1.71	1.52
1	K	13	LEU	C-O	7.13	1.36	1.23
1	K	9	SER	C-N	7.13	1.50	1.34
1	C	19	TYR	CD2-CE2	-7.12	1.28	1.39
2	D	10	HIS	ND1-CE1	-7.10	1.17	1.34
1	E	17	GLU	CA-CB	7.10	1.69	1.53
2	H	15	LEU	CG-CD1	-7.09	1.25	1.51
1	C	5	GLN	CD-NE2	7.09	1.50	1.32
2	L	6	LEU	N-CA	7.08	1.60	1.46
2	H	3	ASN	C-O	-7.08	1.09	1.23
1	I	8	THR	CB-CG2	7.08	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	ILE	CB-CG2	7.06	1.74	1.52
1	E	11	CYS	CB-SG	7.06	1.94	1.82
1	I	2	ILE	CB-CG2	-7.05	1.30	1.52
2	B	23	GLY	C-N	7.04	1.50	1.34
2	D	7	CYS	CB-SG	7.04	1.94	1.82
1	I	21	ASN	CG-OD1	-7.03	1.08	1.24
2	B	16	TYR	C-O	7.03	1.36	1.23
1	E	15	GLN	N-CA	7.03	1.60	1.46
2	J	16	TYR	CB-CG	-7.02	1.41	1.51
1	G	18	ASN	N-CA	-7.01	1.32	1.46
1	C	2	ILE	C-O	7.00	1.36	1.23
2	J	24	PHE	C-O	-6.98	1.10	1.23
1	G	13	LEU	CB-CG	-6.96	1.32	1.52
2	B	4	GLN	CG-CD	-6.95	1.35	1.51
2	H	3	ASN	C-N	-6.95	1.18	1.34
1	C	14	TYR	CD2-CE2	-6.93	1.28	1.39
2	D	16	TYR	CG-CD2	-6.93	1.30	1.39
2	H	1	PHE	CD2-CE2	-6.93	1.25	1.39
2	D	21	GLU	CD-OE1	6.92	1.33	1.25
2	H	20	GLY	C-O	-6.91	1.12	1.23
1	C	6	CYS	CA-CB	-6.90	1.38	1.53
2	D	24	PHE	CE1-CZ	6.89	1.50	1.37
1	I	5	GLN	CB-CG	-6.89	1.33	1.52
1	I	10	ILE	C-N	-6.88	1.18	1.34
2	B	24	PHE	N-CA	-6.87	1.32	1.46
2	B	17	LEU	C-O	6.86	1.36	1.23
1	A	15	GLN	C-O	-6.85	1.10	1.23
2	B	11	LEU	CG-CD1	-6.84	1.26	1.51
2	H	10	HIS	C-N	-6.80	1.18	1.34
1	I	1	GLY	C-O	-6.80	1.12	1.23
1	I	16	LEU	CB-CG	6.79	1.72	1.52
2	J	4	GLN	CD-NE2	-6.78	1.15	1.32
1	I	12	SER	C-O	6.78	1.36	1.23
2	H	11	LEU	CG-CD2	6.76	1.76	1.51
1	C	21	ASN	CA-C	6.76	1.70	1.52
1	I	15	GLN	CB-CG	-6.76	1.34	1.52
2	J	27	THR	CA-C	6.74	1.70	1.52
1	E	4	GLU	C-O	6.73	1.36	1.23
2	D	16	TYR	N-CA	-6.73	1.32	1.46
2	L	6	LEU	C-N	-6.72	1.18	1.34
1	C	18	ASN	CG-OD1	-6.72	1.09	1.24
2	B	16	TYR	N-CA	-6.72	1.32	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	22	ARG	N-CA	6.72	1.59	1.46
2	H	25	TYR	C-O	6.72	1.36	1.23
2	F	19	CYS	CB-SG	-6.71	1.70	1.82
1	G	5	GLN	CG-CD	6.71	1.66	1.51
1	I	20	CYS	N-CA	-6.71	1.32	1.46
2	L	4	GLN	CD-OE1	-6.71	1.09	1.24
1	K	21	ASN	CG-ND2	-6.71	1.16	1.32
2	F	3	ASN	C-N	6.70	1.49	1.34
2	H	21	GLU	C-N	6.70	1.49	1.34
1	I	5	GLN	N-CA	-6.69	1.32	1.46
1	C	18	ASN	CB-CG	6.69	1.66	1.51
2	D	24	PHE	C-O	6.68	1.36	1.23
2	F	3	ASN	CG-OD1	6.68	1.38	1.24
2	L	21	GLU	CA-C	6.68	1.70	1.52
1	K	16	LEU	CG-CD1	6.67	1.76	1.51
2	D	3	ASN	CG-OD1	6.67	1.38	1.24
2	B	21	GLU	CG-CD	6.67	1.61	1.51
2	F	11	LEU	N-CA	-6.66	1.33	1.46
1	G	4	GLU	N-CA	6.65	1.59	1.46
1	C	13	LEU	CG-CD2	6.65	1.76	1.51
2	D	13	GLU	N-CA	6.64	1.59	1.46
1	A	13	LEU	C-N	6.64	1.49	1.34
2	F	16	TYR	CA-C	6.63	1.70	1.52
1	G	7	CYS	C-O	6.63	1.35	1.23
1	A	8	THR	CB-CG2	6.63	1.74	1.52
2	H	11	LEU	CG-CD1	-6.62	1.27	1.51
2	J	29	PRO	CB-CG	6.61	1.82	1.50
2	J	21	GLU	CG-CD	6.61	1.61	1.51
1	G	15	GLN	CD-NE2	6.59	1.49	1.32
2	J	5	HIS	CA-C	6.59	1.70	1.52
1	A	7	CYS	C-O	6.58	1.35	1.23
2	H	9	SER	N-CA	-6.57	1.33	1.46
1	G	2	ILE	C-O	-6.57	1.10	1.23
2	F	10	HIS	CA-C	-6.56	1.35	1.52
1	C	19	TYR	C-N	6.54	1.49	1.34
1	C	19	TYR	CZ-OH	-6.53	1.26	1.37
2	F	12	VAL	CB-CG1	6.53	1.66	1.52
2	B	16	TYR	CZ-OH	-6.51	1.26	1.37
1	I	20	CYS	C-O	6.50	1.35	1.23
1	C	17	GLU	C-O	-6.49	1.11	1.23
2	B	22	ARG	CA-CB	6.49	1.68	1.53
2	B	13	GLU	CG-CD	6.49	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	16	LEU	CA-C	-6.48	1.36	1.52
2	D	3	ASN	C-N	6.47	1.49	1.34
2	L	16	TYR	N-CA	-6.47	1.33	1.46
1	I	19	TYR	CA-C	-6.46	1.36	1.52
1	G	6	CYS	N-CA	-6.44	1.33	1.46
1	K	11	CYS	CA-CB	6.44	1.68	1.53
2	H	27	THR	CA-CB	6.43	1.70	1.53
1	K	2	ILE	CA-CB	-6.42	1.40	1.54
2	B	24	PHE	CA-C	6.42	1.69	1.52
2	L	3	ASN	CA-CB	-6.40	1.36	1.53
2	J	15	LEU	CA-CB	6.40	1.68	1.53
2	D	7	CYS	N-CA	6.40	1.59	1.46
1	A	15	GLN	CA-C	6.40	1.69	1.52
1	E	17	GLU	CD-OE2	-6.39	1.18	1.25
2	F	5	HIS	CA-C	6.39	1.69	1.52
2	H	1	PHE	C-N	6.38	1.48	1.34
1	A	16	LEU	CG-CD1	-6.38	1.28	1.51
1	A	18	ASN	CA-C	6.38	1.69	1.52
2	L	15	LEU	C-O	6.36	1.35	1.23
2	D	5	HIS	CG-CD2	-6.36	1.25	1.35
1	A	10	ILE	N-CA	-6.36	1.33	1.46
2	B	19	CYS	C-O	6.35	1.35	1.23
1	I	13	LEU	CA-CB	6.33	1.68	1.53
2	H	16	TYR	CA-C	-6.32	1.36	1.52
2	H	13	GLU	CA-CB	6.32	1.67	1.53
1	I	18	ASN	CA-CB	-6.32	1.36	1.53
1	C	10	ILE	CA-CB	6.30	1.69	1.54
1	E	12	SER	CB-OG	6.29	1.50	1.42
1	I	7	CYS	C-N	-6.29	1.19	1.34
1	A	4	GLU	CA-C	6.28	1.69	1.52
1	K	17	GLU	C-N	-6.27	1.19	1.34
1	K	5	GLN	N-CA	-6.27	1.33	1.46
2	J	15	LEU	CA-C	-6.27	1.36	1.52
2	L	10	HIS	ND1-CE1	6.27	1.50	1.34
2	D	12	VAL	CA-C	6.25	1.69	1.52
2	H	6	LEU	C-O	-6.23	1.11	1.23
2	D	19	CYS	N-CA	-6.22	1.33	1.46
1	E	18	ASN	C-O	6.22	1.35	1.23
2	H	10	HIS	CG-CD2	6.21	1.46	1.35
2	H	15	LEU	C-O	6.21	1.35	1.23
1	C	14	TYR	N-CA	-6.20	1.33	1.46
2	L	22	ARG	N-CA	6.20	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	27	THR	CB-CG2	6.19	1.72	1.52
1	A	17	GLU	C-N	-6.18	1.19	1.34
1	G	2	ILE	CA-C	6.18	1.69	1.52
1	K	3	VAL	CA-CB	-6.16	1.41	1.54
1	C	13	LEU	C-O	6.15	1.35	1.23
1	C	20	CYS	N-CA	-6.14	1.34	1.46
1	E	20	CYS	CB-SG	6.14	1.92	1.82
2	J	28	LYS	CD-CE	6.14	1.66	1.51
1	I	8	THR	C-N	6.14	1.48	1.34
1	K	19	TYR	N-CA	-6.13	1.34	1.46
1	I	4	GLU	CA-C	-6.11	1.37	1.52
2	H	8	GLY	CA-C	-6.10	1.42	1.51
2	H	17	LEU	N-CA	-6.10	1.34	1.46
2	F	6	LEU	C-O	-6.09	1.11	1.23
1	G	9	SER	N-CA	-6.09	1.34	1.46
2	J	1	PHE	CE2-CZ	-6.08	1.25	1.37
1	G	17	GLU	CG-CD	6.08	1.61	1.51
2	H	3	ASN	CG-OD1	-6.08	1.10	1.24
2	B	12	VAL	CB-CG1	-6.07	1.40	1.52
2	F	3	ASN	CA-CB	6.06	1.68	1.53
2	H	16	TYR	CB-CG	-6.05	1.42	1.51
1	K	3	VAL	C-N	6.04	1.48	1.34
1	G	16	LEU	CB-CG	6.02	1.70	1.52
1	I	5	GLN	C-O	-6.01	1.11	1.23
1	C	11	CYS	C-N	6.01	1.47	1.34
2	J	11	LEU	CG-CD1	6.00	1.74	1.51
2	J	21	GLU	C-O	-6.00	1.11	1.23
1	K	4	GLU	CD-OE1	-5.99	1.19	1.25
1	A	15	GLN	C-N	-5.99	1.20	1.34
2	F	4	GLN	CD-NE2	5.97	1.47	1.32
1	E	19	TYR	CD1-CE1	-5.97	1.30	1.39
2	J	3	ASN	CG-OD1	-5.97	1.10	1.24
1	G	3	VAL	CA-CB	5.96	1.67	1.54
2	L	1	PHE	CA-CB	5.95	1.67	1.53
2	L	13	GLU	CB-CG	5.95	1.63	1.52
1	C	14	TYR	CZ-OH	-5.93	1.27	1.37
2	H	17	LEU	CB-CG	-5.92	1.35	1.52
1	A	13	LEU	CB-CG	5.92	1.69	1.52
1	E	15	GLN	CG-CD	-5.92	1.37	1.51
2	D	24	PHE	CG-CD1	5.90	1.47	1.38
2	H	18	VAL	CA-CB	-5.89	1.42	1.54
1	A	19	TYR	CB-CG	-5.89	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	LEU	N-CA	5.89	1.58	1.46
2	J	14	ALA	C-N	5.89	1.47	1.34
2	D	24	PHE	CE2-CZ	5.88	1.48	1.37
1	I	4	GLU	C-O	-5.87	1.12	1.23
2	B	25	TYR	C-O	5.86	1.34	1.23
2	F	18	VAL	C-O	-5.86	1.12	1.23
2	L	13	GLU	CD-OE1	5.85	1.32	1.25
1	A	4	GLU	CD-OE2	-5.80	1.19	1.25
1	C	5	GLN	CA-C	5.80	1.68	1.52
1	C	8	THR	N-CA	-5.80	1.34	1.46
2	L	25	TYR	CA-C	5.80	1.68	1.52
2	D	4	GLN	CD-NE2	5.80	1.47	1.32
2	L	2	VAL	CB-CG2	-5.78	1.40	1.52
1	C	12	SER	CA-C	-5.78	1.38	1.52
2	D	4	GLN	C-N	5.76	1.47	1.34
2	L	5	HIS	CG-CD2	5.74	1.45	1.35
1	E	18	ASN	CA-CB	-5.73	1.38	1.53
1	A	2	ILE	CA-CB	-5.72	1.41	1.54
2	B	14	ALA	CA-C	5.72	1.67	1.52
1	E	20	CYS	C-N	5.72	1.47	1.34
2	L	17	LEU	C-N	-5.72	1.20	1.34
2	J	1	PHE	CD1-CE1	5.72	1.50	1.39
1	C	7	CYS	CA-C	-5.71	1.38	1.52
2	L	13	GLU	N-CA	5.68	1.57	1.46
2	L	2	VAL	CB-CG1	5.68	1.64	1.52
2	L	5	HIS	CA-C	5.67	1.67	1.52
2	L	8	GLY	C-O	5.67	1.32	1.23
1	G	15	GLN	CA-C	5.66	1.67	1.52
1	I	12	SER	CA-C	-5.66	1.38	1.52
1	I	18	ASN	CG-ND2	-5.64	1.18	1.32
1	A	13	LEU	CG-CD2	5.64	1.72	1.51
2	H	16	TYR	CD1-CE1	-5.61	1.30	1.39
2	J	16	TYR	CZ-OH	-5.61	1.28	1.37
2	D	13	GLU	CG-CD	-5.60	1.43	1.51
2	J	17	LEU	CA-CB	5.59	1.66	1.53
2	L	13	GLU	CA-C	-5.59	1.38	1.52
2	B	24	PHE	C-O	5.58	1.33	1.23
2	J	1	PHE	CD2-CE2	5.58	1.50	1.39
1	K	8	THR	C-N	5.57	1.46	1.34
1	A	15	GLN	CG-CD	5.54	1.63	1.51
1	K	15	GLN	N-CA	5.53	1.57	1.46
2	D	22	ARG	CA-CB	5.53	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	10	ILE	CB-CG2	-5.51	1.35	1.52
2	L	11	LEU	CA-CB	5.50	1.66	1.53
1	K	18	ASN	CA-CB	-5.50	1.38	1.53
2	H	1	PHE	C-O	5.49	1.33	1.23
2	J	1	PHE	CE1-CZ	5.49	1.47	1.37
2	J	1	PHE	CG-CD2	5.49	1.47	1.38
2	B	9	SER	CA-C	5.48	1.67	1.52
2	F	5	HIS	C-N	5.48	1.46	1.34
2	H	25	TYR	CA-CB	-5.48	1.42	1.53
2	F	5	HIS	CG-CD2	5.46	1.45	1.35
2	J	21	GLU	N-CA	-5.46	1.35	1.46
1	C	15	GLN	CB-CG	5.45	1.67	1.52
2	D	19	CYS	CB-SG	-5.45	1.73	1.81
2	J	21	GLU	C-N	-5.44	1.21	1.34
1	C	18	ASN	CG-ND2	5.43	1.46	1.32
2	L	19	CYS	CA-C	-5.43	1.38	1.52
2	F	7	CYS	CB-SG	-5.41	1.73	1.81
2	D	15	LEU	CG-CD2	5.40	1.71	1.51
1	K	19	TYR	C-O	-5.39	1.13	1.23
2	B	8	GLY	C-N	5.39	1.46	1.34
1	K	18	ASN	CA-C	-5.39	1.39	1.52
2	F	21	GLU	CA-C	5.37	1.67	1.52
1	E	3	VAL	C-O	5.37	1.33	1.23
2	J	6	LEU	CG-CD1	5.37	1.71	1.51
2	L	11	LEU	CB-CG	-5.36	1.37	1.52
1	I	17	GLU	CD-OE2	5.36	1.31	1.25
2	J	28	LYS	CA-C	5.36	1.66	1.52
1	K	2	ILE	C-O	5.35	1.33	1.23
2	L	8	GLY	CA-C	-5.34	1.43	1.51
2	H	1	PHE	N-CA	-5.34	1.35	1.46
2	B	8	GLY	N-CA	5.33	1.54	1.46
2	J	3	ASN	N-CA	-5.33	1.35	1.46
1	A	14	TYR	C-N	5.32	1.46	1.34
2	J	19	CYS	CA-C	-5.32	1.39	1.52
1	C	15	GLN	CD-NE2	-5.32	1.19	1.32
2	F	13	GLU	N-CA	5.32	1.56	1.46
2	D	4	GLN	CG-CD	-5.32	1.38	1.51
1	C	10	ILE	C-N	-5.31	1.21	1.34
1	E	7	CYS	CB-SG	-5.31	1.73	1.81
1	C	12	SER	C-N	5.30	1.46	1.34
1	C	18	ASN	CA-CB	-5.30	1.39	1.53
1	G	21	ASN	CA-C	5.29	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	21	ASN	C-OXT	-5.29	1.13	1.23
1	K	9	SER	N-CA	-5.29	1.35	1.46
2	J	5	HIS	C-N	5.29	1.46	1.34
2	L	16	TYR	C-O	5.28	1.33	1.23
2	L	16	TYR	CA-CB	-5.28	1.42	1.53
1	E	10	ILE	N-CA	-5.28	1.35	1.46
2	L	9	SER	CB-OG	-5.28	1.35	1.42
1	C	7	CYS	CB-SG	-5.27	1.73	1.81
1	G	21	ASN	C-OXT	-5.27	1.13	1.23
2	J	18	VAL	CB-CG2	5.27	1.64	1.52
2	D	2	VAL	C-N	5.26	1.46	1.34
1	C	1	GLY	C-O	-5.25	1.15	1.23
2	D	10	HIS	C-N	5.25	1.46	1.34
2	F	4	GLN	CB-CG	5.25	1.66	1.52
2	D	4	GLN	C-O	-5.25	1.13	1.23
2	J	25	TYR	CE2-CZ	-5.24	1.31	1.38
2	D	17	LEU	CG-CD1	-5.21	1.32	1.51
2	L	12	VAL	C-O	5.20	1.33	1.23
2	H	23	GLY	CA-C	-5.20	1.43	1.51
2	D	19	CYS	CA-C	-5.20	1.39	1.52
2	B	19	CYS	C-N	-5.20	1.23	1.33
2	H	10	HIS	C-O	-5.15	1.13	1.23
2	B	1	PHE	CG-CD2	-5.15	1.31	1.38
1	K	7	CYS	CA-CB	-5.15	1.42	1.53
2	H	23	GLY	N-CA	5.14	1.53	1.46
1	E	1	GLY	N-CA	-5.13	1.38	1.46
1	I	13	LEU	N-CA	-5.13	1.36	1.46
1	E	18	ASN	CG-OD1	-5.13	1.12	1.24
2	H	8	GLY	C-O	5.12	1.31	1.23
1	I	10	ILE	C-O	-5.12	1.13	1.23
2	H	12	VAL	C-O	5.12	1.33	1.23
2	J	22	ARG	CB-CG	5.11	1.66	1.52
2	L	17	LEU	CG-CD1	-5.11	1.32	1.51
1	K	7	CYS	CA-C	5.10	1.66	1.52
1	E	2	ILE	CA-CB	-5.10	1.43	1.54
1	A	19	TYR	CZ-OH	-5.09	1.29	1.37
1	C	9	SER	CA-CB	5.08	1.60	1.52
1	I	9	SER	C-N	5.08	1.45	1.34
2	B	3	ASN	CG-OD1	-5.08	1.12	1.24
2	L	14	ALA	CA-CB	-5.06	1.41	1.52
2	J	14	ALA	CA-CB	-5.05	1.41	1.52
2	J	11	LEU	CA-C	-5.04	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	PHE	CA-C	5.03	1.66	1.52
1	C	14	TYR	CD1-CE1	-5.03	1.31	1.39
2	F	13	GLU	CA-C	5.02	1.66	1.52
1	G	18	ASN	C-O	-5.01	1.13	1.23
1	G	16	LEU	CA-C	5.01	1.66	1.52
2	B	25	TYR	CB-CG	5.01	1.59	1.51
2	J	18	VAL	C-N	-5.00	1.22	1.34

All (1081) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	22	ARG	NE-CZ-NH1	-39.15	100.72	120.30
1	A	14	TYR	CB-CG-CD1	-33.41	100.95	121.00
2	J	16	TYR	CB-CG-CD1	-29.25	103.45	121.00
2	J	22	ARG	NE-CZ-NH1	29.24	134.92	120.30
2	B	24	PHE	CB-CG-CD2	26.18	139.13	120.80
1	I	19	TYR	CB-CG-CD2	-25.92	105.45	121.00
1	A	14	TYR	CG-CD1-CE1	-25.73	100.71	121.30
2	B	25	TYR	CB-CG-CD1	-25.40	105.76	121.00
1	A	14	TYR	CB-CG-CD2	24.00	135.40	121.00
2	L	1	PHE	CB-CG-CD2	23.97	137.58	120.80
2	L	25	TYR	CB-CG-CD2	23.88	135.32	121.00
1	A	14	TYR	CZ-CE2-CD2	-22.86	99.22	119.80
2	H	24	PHE	CB-CG-CD2	22.62	136.63	120.80
2	B	25	TYR	CB-CG-CD2	22.29	134.38	121.00
2	J	16	TYR	CG-CD1-CE1	-21.48	104.11	121.30
2	B	1	PHE	CB-CG-CD2	-19.82	106.92	120.80
2	B	25	TYR	CG-CD1-CE1	-18.85	106.22	121.30
2	D	16	TYR	CB-CG-CD2	-18.81	109.71	121.00
2	J	16	TYR	CZ-CE2-CD2	-18.77	102.90	119.80
2	J	22	ARG	NE-CZ-NH2	-18.70	110.95	120.30
1	A	14	TYR	CG-CD2-CE2	18.65	136.22	121.30
1	G	19	TYR	CB-CG-CD1	18.62	132.18	121.00
1	I	19	TYR	CG-CD2-CE2	-18.59	106.43	121.30
1	I	19	TYR	CD1-CE1-CZ	-18.02	103.58	119.80
2	B	25	TYR	CZ-CE2-CD2	-17.40	104.14	119.80
2	J	25	TYR	CB-CG-CD1	17.32	131.39	121.00
2	H	25	TYR	CB-CG-CD1	-17.22	110.67	121.00
2	B	24	PHE	CG-CD2-CE2	17.01	139.51	120.80
1	C	19	TYR	CB-CG-CD1	-16.97	110.82	121.00
2	B	22	ARG	NE-CZ-NH1	16.79	128.70	120.30
1	A	19	TYR	CB-CG-CD2	16.71	131.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	22	ARG	NE-CZ-NH2	16.53	128.56	120.30
1	G	14	TYR	CB-CG-CD2	-16.40	111.16	121.00
2	B	25	TYR	CG-CD2-CE2	16.40	134.42	121.30
1	A	14	TYR	CD1-CE1-CZ	16.36	134.52	119.80
2	L	25	TYR	CG-CD2-CE2	16.21	134.27	121.30
2	F	22	ARG	NE-CZ-NH1	16.17	128.38	120.30
1	G	8	THR	CA-CB-CG2	-16.13	89.82	112.40
2	B	16	TYR	CB-CG-CD2	-16.08	111.35	121.00
1	K	20	CYS	O-C-N	-15.86	97.33	122.70
2	L	25	TYR	CD1-CE1-CZ	15.59	133.83	119.80
2	B	25	TYR	CD1-CE1-CZ	15.42	133.68	119.80
2	L	16	TYR	CB-CG-CD1	-15.41	111.75	121.00
2	L	1	PHE	CG-CD2-CE2	15.38	137.72	120.80
2	L	16	TYR	CD1-CG-CD2	15.27	134.70	117.90
2	D	6	LEU	CB-CG-CD1	-15.17	85.21	111.00
1	E	19	TYR	CB-CG-CD2	-15.12	111.93	121.00
1	C	8	THR	O-C-N	-14.86	98.92	122.70
2	B	24	PHE	CD1-CE1-CZ	14.76	137.81	120.10
2	H	24	PHE	CD1-CG-CD2	-14.70	99.19	118.30
2	H	24	PHE	CG-CD2-CE2	14.69	136.96	120.80
2	L	22	ARG	NH1-CZ-NH2	14.44	135.28	119.40
2	F	6	LEU	CB-CG-CD1	-14.43	86.48	111.00
2	D	21	GLU	N-CA-CB	-14.30	84.87	110.60
1	G	6	CYS	O-C-N	-14.21	99.97	122.70
1	E	19	TYR	CG-CD2-CE2	-14.13	110.00	121.30
2	L	1	PHE	CD1-CE1-CZ	14.04	136.95	120.10
1	I	5	GLN	O-C-N	-13.99	100.31	122.70
1	G	14	TYR	CG-CD2-CE2	-13.95	110.14	121.30
2	H	17	LEU	CB-CG-CD2	-13.95	87.29	111.00
1	G	19	TYR	CG-CD1-CE1	13.89	132.41	121.30
1	K	5	GLN	O-C-N	-13.81	100.61	122.70
1	C	4	GLU	O-C-N	-13.68	100.81	122.70
2	B	27	THR	CA-CB-CG2	-13.55	93.43	112.40
1	A	9	SER	N-CA-CB	13.54	130.81	110.50
1	C	14	TYR	O-C-N	-13.54	101.04	122.70
1	C	19	TYR	CG-CD1-CE1	-13.49	110.50	121.30
1	C	14	TYR	CB-CG-CD1	-13.44	112.94	121.00
2	H	10	HIS	O-C-N	-13.31	101.41	122.70
2	J	5	HIS	CG-ND1-CE1	-13.29	88.42	105.70
1	K	19	TYR	CB-CG-CD1	-13.26	113.05	121.00
2	F	6	LEU	CB-CA-C	-13.23	85.06	110.20
2	H	24	PHE	CD1-CE1-CZ	13.19	135.92	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	13	LEU	O-C-N	-13.18	101.61	122.70
2	B	24	PHE	CB-CG-CD1	-13.06	111.66	120.80
2	L	13	GLU	OE1-CD-OE2	13.06	138.97	123.30
2	B	17	LEU	CB-CG-CD1	-13.04	88.84	111.00
1	E	16	LEU	CB-CG-CD2	-13.01	88.88	111.00
1	K	17	GLU	OE1-CD-OE2	-12.96	107.75	123.30
2	H	3	ASN	O-C-N	-12.95	101.98	122.70
2	J	1	PHE	CB-CG-CD2	12.93	129.85	120.80
1	C	14	TYR	CB-CG-CD2	12.91	128.75	121.00
2	H	25	TYR	CG-CD1-CE1	-12.83	111.04	121.30
2	J	25	TYR	CG-CD1-CE1	12.64	131.41	121.30
1	A	8	THR	CA-CB-CG2	-12.62	94.74	112.40
2	B	16	TYR	CB-CG-CD1	12.58	128.55	121.00
2	L	16	TYR	CB-CG-CD2	-12.55	113.47	121.00
2	D	16	TYR	O-C-N	-12.52	102.66	122.70
1	G	19	TYR	CZ-CE2-CD2	12.51	131.06	119.80
2	J	21	GLU	O-C-N	-12.51	102.69	122.70
2	J	29	PRO	N-CD-CG	-12.47	84.49	103.20
2	J	18	VAL	CG1-CB-CG2	12.47	130.86	110.90
2	F	17	LEU	CB-CG-CD2	12.47	132.20	111.00
1	C	14	TYR	CG-CD1-CE1	-12.46	111.33	121.30
2	H	16	TYR	CB-CG-CD1	12.45	128.47	121.00
1	E	4	GLU	OE1-CD-OE2	-12.43	108.39	123.30
1	A	19	TYR	CG-CD2-CE2	12.36	131.19	121.30
1	G	4	GLU	CB-CA-C	-12.35	85.71	110.40
2	H	10	HIS	ND1-CG-CD2	-12.34	88.72	106.00
1	E	19	TYR	CD1-CG-CD2	12.28	131.41	117.90
2	L	10	HIS	CA-CB-CG	12.28	134.47	113.60
1	C	16	LEU	O-C-N	12.26	142.31	122.70
1	C	19	TYR	CZ-CE2-CD2	-12.25	108.78	119.80
2	B	1	PHE	CG-CD2-CE2	-12.24	107.33	120.80
1	I	10	ILE	O-C-N	-12.22	103.14	122.70
1	G	14	TYR	CD1-CG-CD2	12.17	131.29	117.90
2	H	25	TYR	CZ-CE2-CD2	-12.16	108.85	119.80
2	D	5	HIS	O-C-N	-12.11	103.32	122.70
2	B	16	TYR	CG-CD2-CE2	-12.08	111.64	121.30
2	B	6	LEU	O-C-N	-12.00	103.50	122.70
1	I	12	SER	CB-CA-C	-11.87	87.55	110.10
1	E	19	TYR	CD1-CE1-CZ	-11.81	109.17	119.80
1	K	10	ILE	O-C-N	-11.80	103.82	122.70
1	E	8	THR	O-C-N	-11.79	103.84	122.70
2	L	16	TYR	CG-CD1-CE1	-11.76	111.89	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	TYR	CB-CG-CD2	11.71	128.03	121.00
1	A	13	LEU	CB-CG-CD1	-11.70	91.11	111.00
1	K	9	SER	N-CA-CB	-11.69	92.96	110.50
2	L	11	LEU	CB-CG-CD1	-11.65	91.19	111.00
2	D	21	GLU	OE1-CD-OE2	-11.62	109.35	123.30
2	H	25	TYR	N-CA-CB	-11.62	89.69	110.60
2	H	16	TYR	CB-CG-CD2	-11.56	114.06	121.00
1	C	14	TYR	CG-CD2-CE2	11.53	130.52	121.30
1	E	16	LEU	CA-C-N	-11.49	91.92	117.20
2	D	9	SER	O-C-N	-11.49	104.31	122.70
2	H	2	VAL	CG1-CB-CG2	-11.48	92.53	110.90
1	K	14	TYR	CB-CG-CD2	11.46	127.88	121.00
1	E	20	CYS	CA-CB-SG	11.42	134.56	114.00
1	G	11	CYS	O-C-N	11.39	140.93	122.70
1	E	17	GLU	N-CA-CB	-11.38	90.12	110.60
1	A	4	GLU	OE1-CD-OE2	-11.37	109.66	123.30
1	C	19	TYR	CD1-CG-CD2	11.37	130.40	117.90
1	E	8	THR	OG1-CB-CG2	-11.36	83.88	110.00
1	G	14	TYR	CD1-CE1-CZ	-11.33	109.60	119.80
1	I	15	GLN	O-C-N	11.28	140.75	122.70
2	H	24	PHE	CE1-CZ-CE2	-11.26	99.73	120.00
1	A	19	TYR	CB-CG-CD1	-11.24	114.26	121.00
2	B	2	VAL	CA-CB-CG2	11.21	127.72	110.90
2	F	13	GLU	CB-CA-C	-11.17	88.06	110.40
2	J	5	HIS	ND1-CG-CD2	11.16	124.42	108.80
1	I	14	TYR	CB-CG-CD1	11.15	127.69	121.00
1	C	4	GLU	OE1-CD-OE2	-11.14	109.93	123.30
2	J	16	TYR	CD1-CG-CD2	11.13	130.15	117.90
2	L	5	HIS	CG-CD2-NE2	-11.13	88.05	109.20
2	F	11	LEU	CB-CG-CD1	-11.08	92.16	111.00
2	F	7	CYS	CA-C-O	-11.05	96.90	120.10
1	A	19	TYR	CD1-CE1-CZ	11.02	129.72	119.80
2	B	1	PHE	CD1-CE1-CZ	-10.99	106.91	120.10
2	J	25	TYR	CZ-CE2-CD2	10.98	129.68	119.80
2	L	5	HIS	ND1-CG-CD2	10.98	124.17	108.80
1	A	11	CYS	CA-C-O	-10.96	97.08	120.10
1	K	1	GLY	O-C-N	-10.90	105.26	122.70
1	K	19	TYR	CD1-CG-CD2	10.85	129.84	117.90
1	A	13	LEU	CA-CB-CG	-10.84	90.36	115.30
2	B	16	TYR	CD1-CE1-CZ	-10.83	110.06	119.80
2	L	1	PHE	CB-CG-CD1	-10.83	113.22	120.80
2	L	16	TYR	CG-CD2-CE2	-10.81	112.65	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	21	ASN	CA-C-O	-10.80	97.41	120.10
2	D	16	TYR	CG-CD2-CE2	-10.78	112.68	121.30
1	I	7	CYS	C-N-CA	-10.78	94.76	121.70
2	F	6	LEU	CA-CB-CG	-10.73	90.62	115.30
1	E	5	GLN	N-CA-CB	-10.69	91.36	110.60
2	H	17	LEU	O-C-N	-10.64	105.67	122.70
1	E	14	TYR	CG-CD2-CE2	10.61	129.79	121.30
1	G	17	GLU	CB-CA-C	-10.61	89.19	110.40
2	L	10	HIS	CB-CA-C	10.60	131.59	110.40
2	F	10	HIS	N-CA-CB	10.59	129.66	110.60
1	I	3	VAL	O-C-N	10.56	139.59	122.70
2	J	29	PRO	CA-N-CD	10.55	126.46	111.70
2	B	22	ARG	NH1-CZ-NH2	-10.53	107.81	119.40
1	E	15	GLN	N-CA-CB	-10.53	91.64	110.60
2	F	3	ASN	N-CA-CB	10.53	129.55	110.60
1	C	11	CYS	N-CA-CB	-10.51	91.69	110.60
1	C	10	ILE	CA-CB-CG1	10.50	130.96	111.00
1	C	2	ILE	O-C-N	10.46	139.44	122.70
1	G	11	CYS	CA-CB-SG	-10.41	95.27	114.00
2	J	6	LEU	CB-CG-CD1	10.39	128.66	111.00
2	D	16	TYR	CD1-CE1-CZ	-10.38	110.46	119.80
1	I	7	CYS	CA-CB-SG	-10.38	95.32	114.00
2	F	19	CYS	N-CA-CB	10.37	129.26	110.60
2	J	7	CYS	CB-CA-C	-10.35	89.70	110.40
1	E	2	ILE	O-C-N	10.33	139.23	122.70
2	B	3	ASN	O-C-N	-10.31	106.21	122.70
2	L	12	VAL	CG1-CB-CG2	10.29	127.36	110.90
2	B	2	VAL	CB-CA-C	10.28	130.94	111.40
2	D	12	VAL	O-C-N	-10.27	106.27	122.70
1	I	14	TYR	CD1-CG-CD2	-10.24	106.63	117.90
2	D	3	ASN	O-C-N	10.24	139.08	122.70
1	I	17	GLU	O-C-N	-10.21	106.37	122.70
2	B	9	SER	CB-CA-C	10.20	129.47	110.10
2	F	24	PHE	CB-CA-C	10.19	130.77	110.40
2	D	6	LEU	CA-CB-CG	-10.17	91.91	115.30
2	B	15	LEU	CB-CG-CD1	-10.16	93.72	111.00
2	D	18	VAL	CG1-CB-CG2	-10.15	94.66	110.90
2	D	10	HIS	CG-CD2-NE2	-10.14	89.93	109.20
2	L	16	TYR	CE1-CZ-CE2	10.14	136.03	119.80
2	H	16	TYR	CG-CD1-CE1	10.14	129.41	121.30
2	J	18	VAL	CA-CB-CG2	-10.14	95.69	110.90
2	D	18	VAL	CA-C-O	-10.12	98.84	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	15	GLN	O-C-N	10.12	138.89	122.70
2	F	16	TYR	CB-CG-CD2	-10.12	114.93	121.00
1	I	19	TYR	CD1-CG-CD2	10.10	129.01	117.90
2	B	16	TYR	CB-CA-C	10.07	130.55	110.40
2	F	20	GLY	CA-C-O	10.05	138.69	120.60
2	F	22	ARG	CA-C-N	-10.05	96.10	116.20
1	G	9	SER	N-CA-CB	10.04	125.56	110.50
2	H	12	VAL	CA-CB-CG2	-10.04	95.84	110.90
2	L	18	VAL	CG1-CB-CG2	-10.02	94.88	110.90
2	L	18	VAL	CA-CB-CG2	-10.01	95.88	110.90
2	D	7	CYS	O-C-N	10.01	140.21	123.20
1	I	18	ASN	O-C-N	10.00	138.71	122.70
2	D	14	ALA	O-C-N	9.98	138.68	122.70
2	J	12	VAL	CA-CB-CG1	-9.98	95.92	110.90
2	L	25	TYR	CA-CB-CG	9.93	132.27	113.40
2	D	3	ASN	N-CA-CB	9.92	128.46	110.60
2	F	18	VAL	CA-C-O	-9.92	99.27	120.10
2	D	10	HIS	N-CA-CB	9.92	128.45	110.60
2	H	23	GLY	CA-C-N	-9.90	95.42	117.20
2	D	20	GLY	CA-C-O	9.89	138.40	120.60
2	F	11	LEU	CA-C-O	-9.85	99.42	120.10
2	J	28	LYS	N-CA-CB	9.83	128.30	110.60
1	K	15	GLN	CA-C-N	-9.78	95.69	117.20
2	H	1	PHE	O-C-N	9.75	138.30	122.70
2	F	22	ARG	C-N-CA	-9.73	101.86	122.30
2	F	18	VAL	CG1-CB-CG2	-9.72	95.34	110.90
1	A	12	SER	N-CA-CB	9.68	125.03	110.50
2	J	17	LEU	CB-CA-C	9.68	128.59	110.20
1	E	16	LEU	O-C-N	9.67	138.18	122.70
1	E	6	CYS	O-C-N	9.67	138.17	122.70
2	L	12	VAL	CB-CA-C	9.65	129.73	111.40
2	L	11	LEU	CB-CA-C	-9.64	91.88	110.20
2	B	1	PHE	CD1-CG-CD2	9.62	130.81	118.30
2	B	13	GLU	N-CA-CB	-9.58	93.35	110.60
2	B	16	TYR	CG-CD1-CE1	9.57	128.95	121.30
2	J	27	THR	O-C-N	-9.55	107.42	122.70
1	E	14	TYR	CA-C-O	9.53	140.12	120.10
2	J	10	HIS	CG-ND1-CE1	9.50	121.50	108.20
2	D	6	LEU	CB-CA-C	-9.49	92.16	110.20
1	C	14	TYR	CZ-CE2-CD2	-9.46	111.29	119.80
1	K	3	VAL	O-C-N	9.45	137.82	122.70
1	I	1	GLY	O-C-N	-9.44	107.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	18	VAL	O-C-N	9.42	137.78	122.70
1	C	9	SER	CA-C-O	-9.42	100.32	120.10
2	B	1	PHE	O-C-N	9.40	137.74	122.70
1	G	13	LEU	CB-CA-C	-9.40	92.35	110.20
2	F	16	TYR	CD1-CG-CD2	9.39	128.23	117.90
1	C	20	CYS	CA-CB-SG	9.37	130.87	114.00
2	D	12	VAL	CA-CB-CG1	9.36	124.94	110.90
1	E	12	SER	N-CA-C	-9.35	85.74	111.00
2	J	24	PHE	N-CA-CB	-9.35	93.78	110.60
2	H	21	GLU	O-C-N	9.32	137.61	122.70
2	B	27	THR	N-CA-CB	-9.31	92.61	110.30
1	I	9	SER	N-CA-CB	-9.30	96.55	110.50
2	F	16	TYR	CG-CD2-CE2	-9.30	113.86	121.30
1	C	6	CYS	O-C-N	9.29	137.57	122.70
2	H	10	HIS	CG-CD2-NE2	9.28	126.83	109.20
1	E	4	GLU	CA-C-O	9.26	139.54	120.10
1	K	7	CYS	N-CA-C	9.26	135.99	111.00
2	H	1	PHE	CB-CG-CD2	-9.25	114.32	120.80
1	E	13	LEU	N-CA-CB	-9.25	91.90	110.40
1	K	16	LEU	N-CA-CB	-9.22	91.95	110.40
1	A	20	CYS	CB-CA-C	-9.21	91.97	110.40
2	F	17	LEU	N-CA-CB	9.20	128.80	110.40
2	L	11	LEU	CA-CB-CG	-9.20	94.14	115.30
1	K	3	VAL	CA-CB-CG2	-9.15	97.18	110.90
1	C	14	TYR	CD1-CE1-CZ	9.14	128.03	119.80
2	B	13	GLU	O-C-N	-9.12	108.11	122.70
1	E	3	VAL	CG1-CB-CG2	-9.11	96.33	110.90
1	C	12	SER	O-C-N	9.10	137.27	122.70
2	H	22	ARG	CA-C-N	9.10	134.40	116.20
2	H	16	TYR	CG-CD2-CE2	-9.10	114.02	121.30
2	H	23	GLY	N-CA-C	-9.09	90.36	113.10
2	J	24	PHE	CB-CG-CD1	9.09	127.16	120.80
1	E	2	ILE	CA-C-N	-9.08	97.22	117.20
1	K	13	LEU	CA-C-O	9.08	139.17	120.10
2	B	22	ARG	CA-C-N	9.08	134.35	116.20
1	E	13	LEU	CB-CG-CD1	9.08	126.43	111.00
2	F	6	LEU	CB-CG-CD2	9.05	126.39	111.00
1	K	12	SER	CB-CA-C	-9.04	92.93	110.10
2	L	5	HIS	CA-CB-CG	-9.03	98.25	113.60
2	F	7	CYS	N-CA-C	-9.01	86.66	111.00
2	H	2	VAL	CB-CA-C	8.99	128.49	111.40
2	F	20	GLY	O-C-N	-8.99	108.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	27	THR	N-CA-CB	-8.99	93.22	110.30
2	B	10	HIS	O-C-N	-8.95	108.38	122.70
2	D	22	ARG	CG-CD-NE	8.94	130.58	111.80
2	L	18	VAL	O-C-N	-8.92	108.43	122.70
1	A	4	GLU	CB-CA-C	-8.90	92.59	110.40
1	G	5	GLN	N-CA-C	-8.90	86.96	111.00
2	J	16	TYR	CB-CG-CD2	8.90	126.34	121.00
1	G	20	CYS	CA-CB-SG	-8.90	97.98	114.00
1	A	14	TYR	N-CA-C	-8.88	87.02	111.00
1	C	18	ASN	O-C-N	-8.87	108.52	122.70
1	I	3	VAL	CA-CB-CG2	-8.86	97.61	110.90
1	E	20	CYS	CB-CA-C	8.85	128.11	110.40
2	F	14	ALA	CA-C-O	-8.85	101.52	120.10
2	F	14	ALA	N-CA-CB	8.85	122.49	110.10
2	H	24	PHE	C-N-CA	-8.85	99.58	121.70
1	K	16	LEU	CB-CA-C	8.85	127.01	110.20
1	G	14	TYR	N-CA-CB	8.85	126.53	110.60
2	B	4	GLN	CG-CD-NE2	-8.83	95.51	116.70
2	J	4	GLN	OE1-CD-NE2	-8.83	101.60	121.90
1	A	6	CYS	O-C-N	-8.82	108.58	122.70
1	C	10	ILE	CG1-CB-CG2	-8.82	91.99	111.40
2	B	10	HIS	CA-C-O	8.82	138.62	120.10
2	D	7	CYS	CA-C-O	-8.82	101.58	120.10
1	A	15	GLN	O-C-N	-8.82	108.59	122.70
2	J	1	PHE	CG-CD2-CE2	8.81	130.49	120.80
1	G	14	TYR	CE1-CZ-CE2	8.80	133.88	119.80
1	I	7	CYS	CA-C-N	-8.78	97.89	117.20
2	D	16	TYR	CB-CG-CD1	8.77	126.26	121.00
2	H	7	CYS	N-CA-CB	8.76	126.37	110.60
2	H	9	SER	CB-CA-C	8.76	126.74	110.10
2	D	2	VAL	O-C-N	-8.75	108.69	122.70
1	E	17	GLU	OE1-CD-OE2	8.75	133.80	123.30
2	L	15	LEU	CB-CG-CD2	-8.74	96.13	111.00
1	G	4	GLU	OE1-CD-OE2	-8.74	112.82	123.30
1	G	20	CYS	CB-CA-C	-8.73	92.93	110.40
1	G	21	ASN	CB-CG-OD1	-8.72	104.17	121.60
1	G	14	TYR	O-C-N	8.71	136.63	122.70
2	D	11	LEU	CA-C-O	-8.68	101.87	120.10
1	G	3	VAL	CG1-CB-CG2	8.66	124.75	110.90
2	F	17	LEU	CB-CA-C	-8.66	93.75	110.20
1	K	14	TYR	CA-CB-CG	-8.64	96.97	113.40
2	D	17	LEU	CB-CA-C	-8.64	93.78	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	HIS	CE1-NE2-CD2	-8.63	85.01	106.60
2	D	17	LEU	N-CA-CB	8.63	127.65	110.40
1	C	1	GLY	O-C-N	-8.63	108.90	122.70
2	J	17	LEU	CB-CG-CD1	8.62	125.66	111.00
1	A	19	TYR	CG-CD1-CE1	-8.62	114.41	121.30
2	D	20	GLY	CA-C-N	-8.61	98.26	117.20
1	E	3	VAL	CB-CA-C	8.61	127.75	111.40
2	F	3	ASN	O-C-N	8.60	136.46	122.70
1	K	18	ASN	CA-C-N	-8.60	98.28	117.20
2	B	23	GLY	O-C-N	8.58	136.43	122.70
2	B	19	CYS	N-CA-CB	-8.57	95.17	110.60
1	E	3	VAL	CA-CB-CG1	8.57	123.75	110.90
1	E	9	SER	O-C-N	8.57	136.41	122.70
2	D	13	GLU	OE1-CD-OE2	8.56	133.58	123.30
2	J	18	VAL	O-C-N	-8.56	109.00	122.70
1	A	19	TYR	CZ-CE2-CD2	-8.55	112.10	119.80
2	F	10	HIS	CG-CD2-NE2	-8.54	92.98	109.20
1	G	13	LEU	CB-CG-CD1	-8.53	96.49	111.00
2	L	7	CYS	CB-CA-C	-8.52	93.35	110.40
1	K	8	THR	O-C-N	8.51	136.32	122.70
1	E	14	TYR	CD1-CE1-CZ	8.51	127.46	119.80
2	J	18	VAL	CB-CA-C	-8.51	95.24	111.40
2	D	11	LEU	O-C-N	8.47	136.26	122.70
2	F	6	LEU	N-CA-CB	8.47	127.34	110.40
2	B	21	GLU	CG-CD-OE1	8.47	135.24	118.30
1	K	6	CYS	N-CA-CB	-8.46	95.36	110.60
2	L	1	PHE	CA-CB-CG	8.46	134.21	113.90
2	L	16	TYR	CD1-CE1-CZ	-8.46	112.18	119.80
1	K	14	TYR	CG-CD2-CE2	8.45	128.06	121.30
2	D	18	VAL	CA-CB-CG2	-8.45	98.22	110.90
1	C	19	TYR	CE1-CZ-CE2	8.44	133.31	119.80
2	L	25	TYR	CB-CG-CD1	-8.44	115.94	121.00
2	J	1	PHE	CB-CA-C	8.42	127.25	110.40
2	B	17	LEU	CA-C-O	8.42	137.78	120.10
2	B	21	GLU	O-C-N	8.41	136.15	122.70
1	E	2	ILE	C-N-CA	-8.40	100.69	121.70
2	L	17	LEU	CA-CB-CG	8.37	134.55	115.30
2	D	22	ARG	NE-CZ-NH2	-8.36	116.12	120.30
2	H	13	GLU	OE1-CD-OE2	-8.36	113.27	123.30
2	J	13	GLU	CG-CD-OE1	-8.36	101.58	118.30
1	E	12	SER	C-N-CA	-8.36	100.81	121.70
2	F	12	VAL	N-CA-CB	8.35	129.88	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	24	PHE	CA-C-N	-8.34	98.86	117.20
1	C	19	TYR	O-C-N	8.33	136.03	122.70
1	K	7	CYS	CA-C-O	8.33	137.59	120.10
2	L	25	TYR	CD1-CG-CD2	-8.33	108.74	117.90
1	I	20	CYS	O-C-N	-8.30	109.41	122.70
2	F	11	LEU	CB-CA-C	-8.29	94.44	110.20
1	C	11	CYS	CB-CA-C	8.29	126.97	110.40
1	G	3	VAL	CA-CB-CG1	-8.28	98.48	110.90
2	J	10	HIS	CA-CB-CG	8.28	127.67	113.60
1	A	14	TYR	OH-CZ-CE2	-8.27	97.77	120.10
1	E	8	THR	CA-C-O	8.26	137.45	120.10
2	D	16	TYR	CA-C-N	8.25	135.34	117.20
1	K	5	GLN	CA-C-O	8.24	137.41	120.10
2	F	13	GLU	N-CA-CB	8.23	125.42	110.60
2	L	14	ALA	N-CA-CB	-8.22	98.59	110.10
2	F	13	GLU	CB-CG-CD	-8.19	92.09	114.20
1	E	18	ASN	O-C-N	-8.19	109.60	122.70
1	G	19	TYR	CB-CG-CD2	-8.19	116.09	121.00
2	L	17	LEU	CB-CA-C	8.18	125.75	110.20
2	J	28	LYS	CD-CE-NZ	8.17	130.49	111.70
1	E	13	LEU	CB-CG-CD2	-8.16	97.12	111.00
1	I	14	TYR	CG-CD1-CE1	8.16	127.83	121.30
2	B	8	GLY	O-C-N	8.16	135.75	122.70
2	L	22	ARG	N-CA-CB	-8.15	95.93	110.60
2	B	24	PHE	CG-CD1-CE1	-8.14	111.84	120.80
1	I	20	CYS	CA-C-O	8.13	137.18	120.10
2	H	2	VAL	CA-CB-CG2	8.12	123.08	110.90
2	L	16	TYR	CZ-CE2-CD2	-8.12	112.49	119.80
1	K	18	ASN	C-N-CA	-8.11	101.42	121.70
2	F	11	LEU	CB-CG-CD2	8.11	124.79	111.00
2	J	24	PHE	CA-CB-CG	8.11	133.37	113.90
2	H	6	LEU	O-C-N	-8.11	109.73	122.70
1	A	13	LEU	CB-CG-CD2	8.10	124.77	111.00
2	H	25	TYR	CD1-CG-CD2	8.10	126.81	117.90
1	G	18	ASN	CB-CA-C	8.10	126.59	110.40
2	L	21	GLU	CA-C-O	8.09	137.10	120.10
1	E	14	TYR	CB-CG-CD1	-8.07	116.16	121.00
2	H	12	VAL	O-C-N	8.07	135.61	122.70
1	K	11	CYS	N-CA-CB	8.06	125.11	110.60
2	D	22	ARG	CA-C-O	8.05	137.00	120.10
1	E	19	TYR	CE1-CZ-CE2	8.05	132.68	119.80
2	D	17	LEU	CA-CB-CG	-8.04	96.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	LEU	CA-CB-CG	8.03	133.78	115.30
2	F	16	TYR	CD1-CE1-CZ	-8.03	112.57	119.80
1	E	12	SER	CA-C-N	-8.02	99.57	117.20
2	H	27	THR	CA-CB-OG1	-8.01	92.17	109.00
1	A	20	CYS	CA-CB-SG	-8.00	99.60	114.00
1	K	18	ASN	O-C-N	7.97	135.46	122.70
2	J	18	VAL	N-CA-C	7.97	132.52	111.00
2	B	10	HIS	ND1-CE1-NE2	7.97	127.43	109.90
2	F	9	SER	CA-C-N	7.96	134.71	117.20
1	K	14	TYR	CD1-CE1-CZ	7.96	126.96	119.80
1	K	19	TYR	CZ-CE2-CD2	-7.94	112.66	119.80
1	E	4	GLU	O-C-N	-7.93	110.00	122.70
2	H	16	TYR	CZ-CE2-CD2	7.93	126.94	119.80
1	E	11	CYS	CB-CA-C	7.93	126.26	110.40
2	F	16	TYR	CA-C-N	7.92	134.63	117.20
2	F	5	HIS	N-CA-CB	7.92	124.85	110.60
1	E	17	GLU	CG-CD-OE2	-7.91	102.48	118.30
2	H	13	GLU	CA-CB-CG	7.91	130.79	113.40
1	K	15	GLN	C-N-CA	-7.90	101.95	121.70
1	E	4	GLU	CG-CD-OE2	7.90	134.10	118.30
2	D	2	VAL	CA-CB-CG2	7.90	122.75	110.90
1	K	14	TYR	N-CA-CB	-7.90	96.39	110.60
1	C	17	GLU	CG-CD-OE2	7.88	134.06	118.30
2	H	1	PHE	CD1-CG-CD2	7.87	128.53	118.30
1	C	12	SER	N-CA-C	-7.87	89.75	111.00
2	D	10	HIS	ND1-CG-CD2	7.87	119.81	108.80
1	E	6	CYS	CA-C-N	-7.85	99.92	117.20
2	L	19	CYS	CA-C-N	-7.85	100.49	116.20
1	A	7	CYS	N-CA-CB	7.85	124.73	110.60
2	B	12	VAL	CA-C-N	-7.84	99.95	117.20
2	J	1	PHE	CD1-CE1-CZ	7.84	129.51	120.10
1	K	17	GLU	CA-C-O	7.82	136.53	120.10
1	E	21	ASN	N-CA-C	-7.81	89.91	111.00
2	B	10	HIS	CG-CD2-NE2	7.80	124.03	109.20
2	H	17	LEU	CA-CB-CG	-7.79	97.38	115.30
2	B	17	LEU	O-C-N	-7.79	110.24	122.70
1	A	13	LEU	CB-CA-C	-7.78	95.41	110.20
2	L	10	HIS	CG-ND1-CE1	7.78	119.09	108.20
1	A	18	ASN	OD1-CG-ND2	7.77	139.77	121.90
2	D	2	VAL	CG1-CB-CG2	-7.77	98.47	110.90
2	J	16	TYR	CE1-CZ-CE2	7.77	132.23	119.80
1	K	19	TYR	N-CA-CB	-7.76	96.63	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	19	CYS	O-C-N	7.74	136.36	123.20
2	B	24	PHE	CZ-CE2-CD2	-7.74	110.81	120.10
2	H	24	PHE	CA-C-O	7.73	136.33	120.10
1	I	19	TYR	CE1-CZ-CE2	7.72	132.16	119.80
2	H	15	LEU	CB-CG-CD1	-7.72	97.88	111.00
2	L	19	CYS	O-C-N	7.71	136.31	123.20
2	F	5	HIS	CA-CB-CG	7.70	126.69	113.60
1	E	20	CYS	N-CA-CB	-7.69	96.75	110.60
1	I	14	TYR	CB-CG-CD2	7.67	125.60	121.00
2	D	14	ALA	CA-C-O	-7.66	104.02	120.10
1	E	5	GLN	CA-CB-CG	-7.64	96.59	113.40
1	C	21	ASN	CA-C-O	7.64	136.14	120.10
1	I	18	ASN	CB-CA-C	-7.63	95.14	110.40
2	J	8	GLY	N-CA-C	-7.63	94.03	113.10
2	H	16	TYR	CD1-CE1-CZ	-7.62	112.94	119.80
2	H	2	VAL	N-CA-C	-7.62	90.43	111.00
1	K	19	TYR	CE1-CZ-CE2	7.62	131.98	119.80
2	H	8	GLY	CA-C-O	-7.59	106.93	120.60
2	F	22	ARG	CB-CG-CD	7.58	131.31	111.60
2	H	13	GLU	O-C-N	-7.57	110.59	122.70
2	H	22	ARG	NH1-CZ-NH2	-7.57	111.08	119.40
2	H	22	ARG	CA-C-O	-7.56	104.22	120.10
2	J	27	THR	CA-C-N	7.56	133.83	117.20
2	F	22	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	I	19	TYR	CB-CG-CD1	7.55	125.53	121.00
2	B	10	HIS	N-CA-C	7.54	131.37	111.00
2	F	15	LEU	CB-CG-CD2	7.53	123.80	111.00
1	G	18	ASN	N-CA-C	-7.53	90.68	111.00
2	J	5	HIS	CB-CG-ND1	-7.52	104.41	123.20
1	E	16	LEU	C-N-CA	-7.51	102.91	121.70
2	B	16	TYR	CZ-CE2-CD2	7.51	126.56	119.80
1	C	12	SER	CA-C-N	-7.51	100.68	117.20
1	G	18	ASN	CA-C-O	-7.50	104.35	120.10
1	A	3	VAL	CA-CB-CG1	7.49	122.13	110.90
1	K	7	CYS	C-N-CA	-7.48	102.99	121.70
2	L	4	GLN	OE1-CD-NE2	-7.48	104.69	121.90
1	A	10	ILE	CG1-CB-CG2	7.48	127.85	111.40
1	E	19	TYR	CA-CB-CG	-7.47	99.21	113.40
2	B	2	VAL	CA-CB-CG1	-7.46	99.71	110.90
1	G	16	LEU	CD1-CG-CD2	-7.46	88.12	110.50
1	C	10	ILE	CA-C-N	-7.46	100.80	117.20
2	F	15	LEU	N-CA-CB	7.45	125.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	18	VAL	C-N-CA	-7.44	103.09	121.70
2	J	27	THR	CA-CB-OG1	7.44	124.62	109.00
1	C	12	SER	CA-CB-OG	-7.43	91.13	111.20
2	F	16	TYR	C-N-CA	7.43	140.28	121.70
1	K	17	GLU	CG-CD-OE2	7.42	133.15	118.30
1	I	8	THR	N-CA-CB	-7.41	96.22	110.30
2	F	22	ARG	N-CA-CB	-7.41	97.27	110.60
2	L	25	TYR	CB-CA-C	7.40	125.20	110.40
2	B	18	VAL	CA-CB-CG1	-7.39	99.81	110.90
1	E	2	ILE	CG1-CB-CG2	7.39	127.67	111.40
2	B	15	LEU	O-C-N	7.39	134.52	122.70
2	L	22	ARG	NE-CZ-NH2	7.39	124.00	120.30
2	J	10	HIS	ND1-CG-CD2	-7.38	95.67	106.00
1	C	21	ASN	CB-CA-C	7.36	125.12	110.40
1	C	8	THR	CA-C-N	7.35	133.37	117.20
2	H	7	CYS	CA-CB-SG	7.34	127.21	114.00
2	F	3	ASN	CA-C-O	-7.34	104.69	120.10
2	J	14	ALA	CB-CA-C	-7.33	99.10	110.10
1	A	6	CYS	CA-C-N	7.32	133.31	117.20
2	F	7	CYS	CA-C-N	7.32	130.85	116.20
2	D	24	PHE	CB-CA-C	7.32	125.04	110.40
2	J	13	GLU	CG-CD-OE2	7.31	132.92	118.30
2	H	14	ALA	O-C-N	-7.31	111.01	122.70
2	F	19	CYS	CA-CB-SG	-7.30	100.85	114.00
2	B	25	TYR	CB-CA-C	7.30	125.00	110.40
1	C	13	LEU	CB-CG-CD2	-7.29	98.60	111.00
1	C	21	ASN	CA-CB-CG	7.28	129.42	113.40
2	H	9	SER	N-CA-C	-7.27	91.36	111.00
2	J	2	VAL	CA-CB-CG1	7.27	121.80	110.90
1	E	19	TYR	CB-CG-CD1	-7.27	116.64	121.00
1	I	16	LEU	CB-CA-C	7.26	124.00	110.20
2	J	1	PHE	CA-CB-CG	7.26	131.33	113.90
2	H	24	PHE	N-CA-C	-7.26	91.40	111.00
1	G	5	GLN	CB-CA-C	7.25	124.91	110.40
1	C	21	ASN	N-CA-C	-7.25	91.43	111.00
1	K	19	TYR	CG-CD1-CE1	-7.25	115.50	121.30
1	C	4	GLU	CG-CD-OE1	7.22	132.74	118.30
2	D	24	PHE	N-CA-CB	-7.22	97.60	110.60
2	J	5	HIS	CG-CD2-NE2	-7.21	95.49	109.20
1	E	19	TYR	C-N-CA	-7.21	103.68	121.70
2	F	13	GLU	CA-CB-CG	-7.21	97.54	113.40
1	E	12	SER	CA-CB-OG	-7.20	91.76	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	24	PHE	O-C-N	-7.20	111.18	122.70
1	C	2	ILE	CG1-CB-CG2	7.20	127.23	111.40
2	H	22	ARG	CD-NE-CZ	7.20	133.67	123.60
2	H	15	LEU	O-C-N	7.18	134.18	122.70
2	L	21	GLU	N-CA-C	7.18	130.37	111.00
1	E	6	CYS	CA-CB-SG	-7.17	101.09	114.00
2	F	13	GLU	O-C-N	-7.17	111.24	122.70
2	B	17	LEU	N-CA-C	7.16	130.34	111.00
2	B	12	VAL	O-C-N	7.16	134.15	122.70
2	J	13	GLU	N-CA-CB	7.15	123.48	110.60
2	H	23	GLY	O-C-N	7.14	134.12	122.70
1	G	12	SER	O-C-N	-7.12	111.31	122.70
1	G	21	ASN	N-CA-CB	-7.12	97.79	110.60
1	C	14	TYR	CB-CA-C	7.11	124.62	110.40
2	B	1	PHE	CA-C-N	-7.11	101.56	117.20
2	F	2	VAL	CA-C-N	7.11	132.83	117.20
1	A	11	CYS	O-C-N	7.10	134.06	122.70
1	K	10	ILE	CA-C-N	7.10	132.82	117.20
1	E	14	TYR	CG-CD1-CE1	-7.10	115.62	121.30
2	D	10	HIS	O-C-N	7.09	134.04	122.70
2	D	10	HIS	CB-CA-C	-7.08	96.25	110.40
2	F	21	GLU	CA-C-N	-7.07	101.65	117.20
2	F	18	VAL	CA-CB-CG1	7.06	121.49	110.90
2	B	12	VAL	CA-CB-CG1	7.04	121.46	110.90
2	L	3	ASN	OD1-CG-ND2	-7.04	105.70	121.90
1	E	13	LEU	CB-CA-C	7.04	123.57	110.20
1	E	21	ASN	CB-CA-C	7.04	124.47	110.40
2	J	25	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	I	16	LEU	CA-CB-CG	7.03	131.46	115.30
2	L	11	LEU	CB-CG-CD2	-7.02	99.06	111.00
2	B	22	ARG	O-C-N	-7.02	111.27	123.20
2	L	1	PHE	CD1-CG-CD2	-7.00	109.20	118.30
2	L	1	PHE	CB-CA-C	7.00	124.40	110.40
2	B	24	PHE	CD1-CG-CD2	-7.00	109.20	118.30
2	B	5	HIS	O-C-N	6.99	133.89	122.70
2	B	22	ARG	C-N-CA	6.98	136.96	122.30
2	L	12	VAL	N-CA-CB	-6.95	96.21	111.50
2	F	16	TYR	CB-CG-CD1	-6.95	116.83	121.00
2	J	8	GLY	CA-C-O	-6.95	108.10	120.60
2	B	24	PHE	CA-C-O	6.94	134.67	120.10
1	C	14	TYR	CA-C-O	6.92	134.63	120.10
1	I	7	CYS	N-CA-C	6.92	129.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	3	VAL	C-N-CA	-6.92	104.41	121.70
1	C	13	LEU	CB-CG-CD1	6.91	122.75	111.00
2	B	14	ALA	CA-C-O	6.89	134.57	120.10
2	J	16	TYR	OH-CZ-CE2	-6.88	101.52	120.10
1	E	12	SER	CB-CA-C	6.88	123.17	110.10
1	G	15	GLN	CA-C-N	6.87	132.31	117.20
1	E	13	LEU	CA-CB-CG	6.87	131.10	115.30
2	H	5	HIS	O-C-N	6.87	133.69	122.70
1	I	14	TYR	CZ-CE2-CD2	6.87	125.98	119.80
1	I	15	GLN	CA-CB-CG	-6.87	98.29	113.40
1	K	19	TYR	CG-CD2-CE2	-6.86	115.81	121.30
2	D	18	VAL	CB-CA-C	-6.86	98.37	111.40
1	A	5	GLN	O-C-N	6.86	133.67	122.70
1	A	21	ASN	OD1-CG-ND2	-6.86	106.13	121.90
1	E	10	ILE	O-C-N	6.84	133.65	122.70
1	E	3	VAL	CA-CB-CG2	6.84	121.16	110.90
2	B	12	VAL	CA-CB-CG2	-6.84	100.64	110.90
2	D	10	HIS	CA-CB-CG	-6.82	102.00	113.60
2	D	19	CYS	N-CA-CB	6.82	122.88	110.60
2	J	22	ARG	CD-NE-CZ	-6.82	114.05	123.60
2	B	11	LEU	CB-CG-CD1	-6.81	99.42	111.00
1	A	17	GLU	CA-CB-CG	6.79	128.34	113.40
2	D	2	VAL	N-CA-C	6.79	129.32	111.00
2	F	5	HIS	CA-C-N	6.78	132.12	117.20
1	A	16	LEU	CD1-CG-CD2	-6.77	90.19	110.50
2	L	1	PHE	CZ-CE2-CD2	-6.77	111.97	120.10
1	A	5	GLN	N-CA-CB	6.77	122.79	110.60
2	H	13	GLU	CB-CA-C	6.77	123.94	110.40
2	D	21	GLU	CG-CD-OE1	6.76	131.83	118.30
2	F	10	HIS	CE1-NE2-CD2	6.76	123.50	106.60
2	L	23	GLY	CA-C-O	-6.76	108.43	120.60
1	C	16	LEU	CA-C-N	-6.76	102.33	117.20
2	D	22	ARG	C-N-CA	-6.76	108.11	122.30
1	C	4	GLU	CA-C-O	6.75	134.28	120.10
2	H	27	THR	OG1-CB-CG2	6.74	125.51	110.00
2	H	21	GLU	CB-CA-C	-6.74	96.93	110.40
1	K	8	THR	CA-C-N	-6.74	102.38	117.20
2	L	25	TYR	CZ-CE2-CD2	-6.73	113.74	119.80
1	A	6	CYS	C-N-CA	6.72	138.51	121.70
1	G	16	LEU	N-CA-CB	6.72	123.84	110.40
1	E	19	TYR	CA-C-N	-6.71	102.43	117.20
1	I	13	LEU	CA-C-O	6.71	134.19	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	ILE	CG1-CB-CG2	-6.71	96.65	111.40
2	F	11	LEU	CA-C-N	6.71	131.95	117.20
1	I	8	THR	CA-CB-OG1	-6.71	94.92	109.00
1	I	5	GLN	CA-C-N	6.70	131.95	117.20
1	K	21	ASN	CA-CB-CG	-6.70	98.65	113.40
1	E	14	TYR	N-CA-CB	-6.70	98.54	110.60
2	F	2	VAL	CB-CA-C	-6.70	98.68	111.40
1	K	19	TYR	CB-CG-CD2	-6.69	116.98	121.00
2	L	18	VAL	N-CA-C	6.69	129.07	111.00
1	G	18	ASN	CA-C-N	6.68	131.91	117.20
1	A	9	SER	CB-CA-C	-6.68	97.40	110.10
2	B	12	VAL	C-N-CA	-6.68	105.01	121.70
2	D	19	CYS	C-N-CA	6.67	136.31	122.30
2	B	19	CYS	C-N-CA	-6.67	108.30	122.30
2	D	6	LEU	CB-CG-CD2	6.67	122.34	111.00
2	L	5	HIS	CG-ND1-CE1	-6.67	97.03	105.70
2	L	15	LEU	CA-C-N	-6.66	102.55	117.20
2	F	2	VAL	CA-CB-CG2	-6.63	100.95	110.90
1	I	10	ILE	CA-CB-CG1	6.63	123.60	111.00
2	F	9	SER	C-N-CA	6.63	138.28	121.70
2	H	17	LEU	CD1-CG-CD2	6.63	130.38	110.50
1	A	20	CYS	C-N-CA	6.62	138.26	121.70
2	B	1	PHE	CE1-CZ-CE2	6.62	131.91	120.00
1	K	13	LEU	O-C-N	-6.61	112.12	122.70
2	D	13	GLU	O-C-N	-6.61	112.13	122.70
1	I	18	ASN	CA-C-N	-6.61	102.67	117.20
1	A	19	TYR	N-CA-CB	6.61	122.49	110.60
1	I	8	THR	OG1-CB-CG2	6.60	125.17	110.00
2	D	13	GLU	CB-CA-C	-6.59	97.21	110.40
1	A	21	ASN	N-CA-CB	-6.59	98.73	110.60
2	B	17	LEU	N-CA-CB	-6.59	97.22	110.40
2	H	22	ARG	C-N-CA	6.59	136.14	122.30
2	L	1	PHE	CG-CD1-CE1	-6.58	113.56	120.80
1	K	10	ILE	CA-CB-CG1	6.58	123.50	111.00
1	A	16	LEU	CB-CG-CD2	6.58	122.18	111.00
2	D	16	TYR	C-N-CA	6.58	138.15	121.70
2	H	16	TYR	CB-CA-C	6.58	123.56	110.40
2	H	19	CYS	N-CA-CB	-6.58	98.76	110.60
1	A	5	GLN	CA-CB-CG	6.58	127.86	113.40
2	L	16	TYR	N-CA-CB	-6.57	98.77	110.60
1	G	10	ILE	CA-CB-CG2	-6.56	97.78	110.90
2	J	21	GLU	CB-CG-CD	-6.55	96.50	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	SER	CA-C-N	6.55	131.61	117.20
1	E	1	GLY	CA-C-O	6.55	132.39	120.60
1	K	5	GLN	CG-CD-OE1	6.55	134.70	121.60
1	E	5	GLN	N-CA-C	6.54	128.67	111.00
2	H	5	HIS	CA-CB-CG	6.54	124.73	113.60
2	J	6	LEU	CB-CA-C	6.54	122.63	110.20
2	F	17	LEU	CA-CB-CG	6.54	130.35	115.30
2	F	22	ARG	CA-CB-CG	6.54	127.79	113.40
1	G	7	CYS	N-CA-CB	6.51	122.32	110.60
1	K	4	GLU	CB-CA-C	6.51	123.41	110.40
2	B	3	ASN	CA-C-O	6.50	133.76	120.10
2	F	22	ARG	CA-C-O	6.50	133.76	120.10
2	D	13	GLU	CG-CD-OE2	-6.50	105.30	118.30
2	J	2	VAL	N-CA-CB	6.49	125.77	111.50
2	B	25	TYR	CA-C-O	-6.48	106.49	120.10
2	H	6	LEU	CA-C-N	6.48	131.46	117.20
2	D	17	LEU	CB-CG-CD2	6.48	122.01	111.00
2	J	3	ASN	CB-CG-ND2	6.48	132.25	116.70
2	H	15	LEU	CA-CB-CG	-6.47	100.42	115.30
2	H	10	HIS	CG-ND1-CE1	6.47	117.25	108.20
2	D	4	GLN	CA-C-O	-6.46	106.53	120.10
1	I	3	VAL	CB-CA-C	-6.46	99.12	111.40
2	J	24	PHE	CA-C-O	-6.46	106.53	120.10
1	K	9	SER	CB-CA-C	-6.46	97.84	110.10
1	I	4	GLU	OE1-CD-OE2	6.45	131.04	123.30
1	K	7	CYS	N-CA-CB	-6.45	98.99	110.60
2	B	22	ARG	CB-CA-C	6.44	123.29	110.40
1	G	8	THR	CB-CA-C	-6.43	94.23	111.60
2	J	12	VAL	N-CA-CB	-6.43	97.35	111.50
1	G	19	TYR	CG-CD2-CE2	-6.43	116.16	121.30
2	F	21	GLU	OE1-CD-OE2	-6.43	115.59	123.30
1	K	19	TYR	CB-CA-C	6.43	123.26	110.40
2	L	16	TYR	CB-CA-C	-6.42	97.55	110.40
1	I	4	GLU	N-CA-C	-6.42	93.66	111.00
2	F	4	GLN	CA-CB-CG	-6.39	99.34	113.40
1	K	21	ASN	N-CA-CB	6.39	122.10	110.60
1	I	8	THR	O-C-N	6.39	132.92	122.70
2	B	22	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	B	22	ARG	CA-CB-CG	6.38	127.44	113.40
2	J	4	GLN	CB-CG-CD	6.38	128.18	111.60
2	H	22	ARG	N-CA-C	-6.38	93.79	111.00
1	E	4	GLU	CB-CG-CD	6.37	131.39	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	GLN	CA-C-N	6.34	131.14	117.20
1	C	17	GLU	CA-CB-CG	6.33	127.33	113.40
2	F	18	VAL	N-CA-C	-6.33	93.90	111.00
2	B	18	VAL	CA-C-N	-6.33	103.28	117.20
1	G	5	GLN	CA-C-O	-6.33	106.81	120.10
1	A	2	ILE	CA-CB-CG1	-6.32	98.99	111.00
2	F	4	GLN	CG-CD-NE2	-6.32	101.52	116.70
2	B	18	VAL	C-N-CA	-6.32	105.90	121.70
2	F	7	CYS	C-N-CA	6.32	135.57	122.30
2	L	24	PHE	CA-CB-CG	6.32	129.06	113.90
2	F	18	VAL	CA-CB-CG2	-6.32	101.43	110.90
2	D	20	GLY	C-N-CA	-6.31	105.92	121.70
1	K	5	GLN	OE1-CD-NE2	-6.31	107.39	121.90
1	G	6	CYS	CA-C-O	6.31	133.35	120.10
2	L	20	GLY	O-C-N	-6.30	112.61	122.70
1	A	10	ILE	CA-CB-CG1	-6.30	99.03	111.00
1	E	19	TYR	O-C-N	6.30	132.78	122.70
2	B	27	THR	CA-CB-OG1	6.30	122.23	109.00
2	L	11	LEU	CA-C-O	6.29	133.32	120.10
2	B	19	CYS	N-CA-C	6.29	127.98	111.00
2	J	10	HIS	CB-CA-C	6.29	122.97	110.40
1	C	10	ILE	O-C-N	6.28	132.75	122.70
1	E	18	ASN	CA-C-O	6.27	133.26	120.10
1	E	21	ASN	N-CA-CB	6.27	121.88	110.60
2	J	28	LYS	CB-CA-C	6.27	122.93	110.40
2	B	2	VAL	O-C-N	-6.26	112.68	122.70
2	H	22	ARG	CB-CA-C	6.26	122.93	110.40
2	L	15	LEU	N-CA-CB	6.26	122.93	110.40
1	E	2	ILE	CB-CA-C	-6.26	99.08	111.60
1	E	21	ASN	CA-CB-CG	6.26	127.18	113.40
1	I	16	LEU	CB-CG-CD1	6.26	121.64	111.00
2	J	16	TYR	CG-CD2-CE2	6.26	126.31	121.30
1	A	14	TYR	CB-CA-C	6.25	122.91	110.40
1	K	17	GLU	O-C-N	-6.25	112.69	122.70
1	C	5	GLN	CB-CA-C	-6.25	97.89	110.40
2	B	6	LEU	N-CA-CB	-6.25	97.90	110.40
2	J	28	LYS	O-C-N	-6.25	109.23	121.10
1	K	19	TYR	CD1-CE1-CZ	-6.25	114.18	119.80
2	J	24	PHE	CG-CD1-CE1	6.24	127.67	120.80
2	H	1	PHE	CG-CD2-CE2	-6.23	113.94	120.80
2	F	16	TYR	N-CA-CB	6.22	121.81	110.60
2	B	1	PHE	C-N-CA	-6.22	106.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	11	CYS	CA-CB-SG	6.21	125.19	114.00
2	J	6	LEU	CA-CB-CG	6.21	129.59	115.30
2	F	9	SER	N-CA-CB	6.21	119.81	110.50
2	D	14	ALA	CB-CA-C	-6.21	100.79	110.10
2	J	14	ALA	N-CA-C	6.21	127.77	111.00
2	D	11	LEU	CB-CG-CD1	-6.21	100.45	111.00
2	D	19	CYS	CA-C-O	-6.20	107.09	120.10
2	D	24	PHE	CB-CG-CD1	-6.20	116.46	120.80
1	K	16	LEU	CB-CG-CD1	6.20	121.53	111.00
2	F	15	LEU	CB-CA-C	-6.19	98.43	110.20
2	D	17	LEU	CB-CG-CD1	-6.19	100.48	111.00
2	F	4	GLN	OE1-CD-NE2	6.18	136.12	121.90
1	G	3	VAL	N-CA-CB	6.18	125.09	111.50
1	K	14	TYR	C-N-CA	-6.17	106.27	121.70
2	H	14	ALA	CA-C-O	6.17	133.06	120.10
2	B	24	PHE	N-CA-CB	6.17	121.70	110.60
1	E	11	CYS	N-CA-C	-6.16	94.37	111.00
2	J	4	GLN	O-C-N	6.15	132.54	122.70
2	L	9	SER	CB-CA-C	-6.15	98.41	110.10
1	E	19	TYR	CB-CA-C	-6.14	98.12	110.40
2	F	18	VAL	CA-C-N	6.14	130.71	117.20
2	L	6	LEU	CB-CG-CD1	6.14	121.43	111.00
1	K	20	CYS	CA-C-N	6.13	130.70	117.20
2	L	10	HIS	ND1-CG-CD2	-6.13	97.41	106.00
2	F	25	TYR	CA-C-O	-6.13	107.23	120.10
2	F	16	TYR	CE1-CZ-CE2	6.12	129.59	119.80
2	F	24	PHE	CA-CB-CG	-6.12	99.22	113.90
1	K	16	LEU	O-C-N	-6.11	112.92	122.70
2	H	8	GLY	O-C-N	6.10	132.46	122.70
1	A	14	TYR	CE1-CZ-OH	6.10	136.56	120.10
2	D	22	ARG	N-CA-CB	-6.10	99.62	110.60
2	L	8	GLY	O-C-N	6.10	132.46	122.70
2	J	28	LYS	CG-CD-CE	6.09	130.17	111.90
1	I	6	CYS	N-CA-C	6.09	127.44	111.00
2	D	5	HIS	CA-CB-CG	6.08	123.93	113.60
2	F	7	CYS	CA-CB-SG	6.08	124.94	114.00
1	A	15	GLN	OE1-CD-NE2	-6.07	107.93	121.90
2	B	18	VAL	CA-CB-CG2	6.07	120.01	110.90
2	D	24	PHE	CA-CB-CG	-6.07	99.33	113.90
2	L	2	VAL	CA-CB-CG2	-6.07	101.80	110.90
1	I	14	TYR	CE1-CZ-CE2	-6.06	110.10	119.80
2	J	11	LEU	CA-C-N	-6.06	103.88	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	CYS	CB-CA-C	6.05	122.51	110.40
1	K	1	GLY	CA-C-O	6.05	131.50	120.60
2	J	14	ALA	N-CA-CB	-6.05	101.63	110.10
2	B	16	TYR	N-CA-CB	-6.04	99.72	110.60
1	I	15	GLN	CA-C-N	-6.04	103.90	117.20
1	C	9	SER	O-C-N	6.04	132.37	122.70
2	B	5	HIS	C-N-CA	-6.04	106.61	121.70
2	F	12	VAL	N-CA-C	-6.03	94.72	111.00
1	I	4	GLU	CG-CD-OE2	-6.03	106.24	118.30
2	J	28	LYS	N-CA-C	-6.03	94.73	111.00
2	B	3	ASN	N-CA-C	6.00	127.20	111.00
2	D	10	HIS	CE1-NE2-CD2	6.00	121.61	106.60
1	E	9	SER	CB-CA-C	5.99	121.48	110.10
2	H	25	TYR	CE1-CZ-CE2	5.99	129.39	119.80
1	C	10	ILE	N-CA-CB	5.99	124.57	110.80
1	C	6	CYS	CA-CB-SG	-5.97	103.25	114.00
2	F	13	GLU	C-N-CA	5.97	136.63	121.70
1	K	2	ILE	O-C-N	-5.97	113.14	122.70
2	L	4	GLN	CG-CD-NE2	5.97	131.03	116.70
2	B	19	CYS	CA-CB-SG	-5.97	103.26	114.00
2	H	6	LEU	CB-CA-C	5.97	121.54	110.20
2	L	3	ASN	CB-CA-C	5.97	122.33	110.40
1	G	9	SER	C-N-CA	-5.96	106.79	121.70
2	B	15	LEU	CD1-CG-CD2	5.96	128.38	110.50
1	I	14	TYR	CG-CD2-CE2	5.96	126.07	121.30
2	J	15	LEU	CB-CG-CD1	5.96	121.13	111.00
2	H	17	LEU	N-CA-C	5.96	127.08	111.00
2	L	4	GLN	N-CA-CB	5.95	121.31	110.60
2	F	3	ASN	N-CA-C	-5.95	94.95	111.00
2	D	20	GLY	N-CA-C	-5.94	98.24	113.10
2	F	13	GLU	CG-CD-OE1	5.94	130.19	118.30
1	C	19	TYR	CB-CA-C	-5.93	98.54	110.40
1	I	3	VAL	CA-C-O	-5.93	107.65	120.10
2	H	17	LEU	CA-C-O	5.92	132.53	120.10
1	A	8	THR	OG1-CB-CG2	5.91	123.60	110.00
2	D	24	PHE	CD1-CG-CD2	5.91	125.99	118.30
1	E	9	SER	N-CA-C	-5.91	95.03	111.00
2	F	12	VAL	CA-C-N	5.91	130.20	117.20
1	I	13	LEU	N-CA-CB	-5.91	98.58	110.40
1	G	19	TYR	CD1-CE1-CZ	-5.91	114.48	119.80
2	D	12	VAL	CA-C-N	5.90	130.19	117.20
1	C	18	ASN	CB-CG-ND2	5.90	130.85	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	14	ALA	N-CA-C	-5.90	95.08	111.00
2	J	7	CYS	N-CA-C	5.89	126.91	111.00
1	E	17	GLU	CB-CA-C	5.89	122.19	110.40
2	L	4	GLN	CA-C-N	-5.89	104.24	117.20
2	J	17	LEU	CD1-CG-CD2	-5.88	92.85	110.50
2	B	15	LEU	CA-CB-CG	-5.88	101.78	115.30
1	K	9	SER	CA-CB-OG	-5.87	95.34	111.20
2	D	22	ARG	NH1-CZ-NH2	5.86	125.85	119.40
1	K	4	GLU	N-CA-CB	-5.86	100.05	110.60
2	L	22	ARG	O-C-N	5.86	133.16	123.20
2	F	21	GLU	N-CA-CB	-5.86	100.06	110.60
2	H	10	HIS	CE1-NE2-CD2	-5.86	91.96	106.60
2	D	7	CYS	N-CA-C	-5.85	95.20	111.00
2	B	4	GLN	OE1-CD-NE2	5.84	135.33	121.90
1	C	4	GLU	CB-CA-C	5.83	122.06	110.40
1	K	18	ASN	CA-CB-CG	-5.82	100.59	113.40
2	B	4	GLN	O-C-N	5.82	132.01	122.70
1	K	2	ILE	CA-C-O	5.82	132.32	120.10
1	G	14	TYR	CB-CG-CD1	-5.82	117.51	121.00
2	J	16	TYR	CB-CA-C	-5.82	98.77	110.40
1	K	3	VAL	CA-C-N	-5.81	104.41	117.20
2	L	8	GLY	N-CA-C	-5.81	98.57	113.10
2	B	24	PHE	O-C-N	-5.81	113.41	122.70
2	H	21	GLU	CA-C-O	-5.81	107.90	120.10
1	E	17	GLU	O-C-N	-5.81	113.41	122.70
2	L	15	LEU	C-N-CA	-5.80	107.19	121.70
2	F	19	CYS	CB-CA-C	-5.80	98.81	110.40
1	E	14	TYR	CZ-CE2-CD2	-5.79	114.59	119.80
2	J	11	LEU	C-N-CA	-5.79	107.22	121.70
1	C	19	TYR	CA-CB-CG	-5.78	102.42	113.40
2	J	22	ARG	O-C-N	5.77	133.01	123.20
2	J	11	LEU	CB-CA-C	-5.77	99.24	110.20
2	L	11	LEU	N-CA-C	5.77	126.57	111.00
1	I	13	LEU	CB-CA-C	5.76	121.15	110.20
1	G	19	TYR	CD1-CG-CD2	-5.76	111.56	117.90
2	L	12	VAL	CA-CB-CG1	-5.76	102.26	110.90
2	B	13	GLU	CG-CD-OE1	5.76	129.82	118.30
1	E	7	CYS	CB-CA-C	5.76	121.92	110.40
1	G	6	CYS	N-CA-C	5.75	126.53	111.00
1	I	2	ILE	O-C-N	-5.75	113.50	122.70
2	J	25	TYR	CD1-CE1-CZ	-5.75	114.62	119.80
2	J	4	GLN	N-CA-CB	5.75	120.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	10	HIS	N-CA-C	-5.75	95.49	111.00
2	J	1	PHE	CB-CG-CD1	-5.75	116.78	120.80
2	H	4	GLN	CA-C-O	-5.75	108.03	120.10
2	F	23	GLY	C-N-CA	-5.74	107.34	121.70
2	F	2	VAL	CA-CB-CG1	5.74	119.51	110.90
2	B	24	PHE	CB-CA-C	-5.74	98.93	110.40
1	A	18	ASN	C-N-CA	5.73	136.03	121.70
2	L	21	GLU	CA-C-N	-5.73	104.58	117.20
2	L	1	PHE	CA-C-O	-5.73	108.07	120.10
2	J	20	GLY	N-CA-C	-5.72	98.79	113.10
2	F	12	VAL	O-C-N	-5.72	113.55	122.70
2	B	15	LEU	C-N-CA	-5.72	107.40	121.70
1	K	18	ASN	CB-CG-OD1	-5.71	110.17	121.60
2	B	13	GLU	CB-CA-C	5.70	121.81	110.40
1	A	21	ASN	N-CA-C	5.70	126.39	111.00
2	J	11	LEU	N-CA-CB	5.70	121.80	110.40
1	K	18	ASN	N-CA-C	5.70	126.38	111.00
1	E	8	THR	N-CA-C	5.69	126.36	111.00
1	G	13	LEU	CD1-CG-CD2	5.69	127.57	110.50
2	H	14	ALA	N-CA-CB	5.69	118.07	110.10
1	I	19	TYR	CE1-CZ-OH	-5.68	104.76	120.10
2	L	19	CYS	C-N-CA	-5.68	110.36	122.30
1	C	8	THR	C-N-CA	5.68	135.90	121.70
1	E	13	LEU	CA-C-N	-5.68	104.70	117.20
1	C	13	LEU	N-CA-CB	-5.68	99.04	110.40
2	J	5	HIS	ND1-CE1-NE2	5.68	122.39	109.90
1	I	8	THR	CB-CA-C	5.67	126.92	111.60
1	G	2	ILE	O-C-N	-5.67	113.63	122.70
1	I	18	ASN	CA-CB-CG	-5.66	100.94	113.40
1	C	19	TYR	N-CA-CB	5.66	120.78	110.60
2	H	10	HIS	CA-C-O	5.66	131.98	120.10
2	H	12	VAL	CA-CB-CG1	5.66	119.39	110.90
2	B	21	GLU	CG-CD-OE2	-5.65	107.01	118.30
1	K	20	CYS	CA-C-O	5.64	131.94	120.10
2	F	10	HIS	ND1-CE1-NE2	-5.63	97.52	109.90
1	G	19	TYR	CB-CA-C	-5.63	99.15	110.40
1	K	7	CYS	CA-C-N	-5.62	104.83	117.20
2	D	21	GLU	CA-C-N	-5.62	104.84	117.20
2	L	6	LEU	CB-CG-CD2	-5.60	101.47	111.00
2	J	11	LEU	CB-CG-CD2	-5.59	101.49	111.00
2	D	24	PHE	O-C-N	-5.59	113.76	122.70
2	H	19	CYS	CA-CB-SG	-5.58	103.95	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	13	GLU	CA-C-N	5.58	129.47	117.20
1	E	13	LEU	O-C-N	5.57	131.61	122.70
2	D	5	HIS	CA-C-N	5.57	129.45	117.20
1	G	16	LEU	CB-CG-CD1	5.57	120.47	111.00
1	C	12	SER	N-CA-CB	5.56	118.84	110.50
1	E	14	TYR	CA-C-N	-5.56	104.96	117.20
1	I	15	GLN	CG-CD-NE2	-5.56	103.35	116.70
2	D	16	TYR	CD1-CG-CD2	5.56	124.01	117.90
1	A	18	ASN	CA-C-O	-5.55	108.44	120.10
1	I	21	ASN	CA-C-O	-5.55	108.45	120.10
2	L	2	VAL	CG1-CB-CG2	5.55	119.78	110.90
1	C	2	ILE	CA-C-O	-5.54	108.46	120.10
1	E	7	CYS	CA-C-N	5.54	129.40	117.20
2	H	11	LEU	O-C-N	5.54	131.57	122.70
1	A	17	GLU	CG-CD-OE2	5.54	129.38	118.30
1	G	4	GLU	N-CA-CB	5.54	120.57	110.60
1	K	6	CYS	CB-CA-C	5.54	121.47	110.40
2	D	8	GLY	O-C-N	-5.54	113.84	122.70
2	H	25	TYR	CA-C-O	-5.53	108.48	120.10
1	E	4	GLU	CB-CA-C	5.53	121.46	110.40
1	E	6	CYS	C-N-CA	-5.53	107.88	121.70
2	J	25	TYR	CD1-CG-CD2	-5.53	111.82	117.90
1	C	19	TYR	CA-C-N	-5.52	105.05	117.20
2	J	1	PHE	CA-C-O	-5.52	108.51	120.10
2	F	16	TYR	N-CA-C	-5.52	96.10	111.00
2	F	14	ALA	O-C-N	5.51	131.51	122.70
2	L	5	HIS	N-CA-CB	-5.51	100.69	110.60
2	D	22	ARG	CB-CA-C	5.50	121.40	110.40
2	J	17	LEU	N-CA-C	-5.48	96.20	111.00
2	L	5	HIS	CE1-NE2-CD2	5.48	120.30	106.60
2	L	21	GLU	C-N-CA	-5.48	108.01	121.70
2	D	18	VAL	CA-CB-CG1	5.47	119.11	110.90
1	E	3	VAL	N-CA-CB	-5.47	99.47	111.50
2	H	3	ASN	N-CA-CB	5.47	120.44	110.60
1	I	19	TYR	CA-C-O	-5.47	108.62	120.10
2	H	23	GLY	CA-C-O	5.46	130.44	120.60
2	J	12	VAL	CA-C-O	-5.46	108.62	120.10
1	A	17	GLU	O-C-N	5.46	131.44	122.70
1	I	18	ASN	CB-CG-ND2	-5.46	103.59	116.70
2	B	14	ALA	CA-C-N	-5.46	105.19	117.20
1	G	2	ILE	CB-CA-C	-5.45	100.70	111.60
1	K	9	SER	O-C-N	5.45	131.42	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	HIS	N-CA-CB	5.45	120.40	110.60
1	K	21	ASN	CB-CA-C	-5.44	99.51	110.40
1	E	15	GLN	CB-CA-C	5.44	121.29	110.40
2	L	6	LEU	N-CA-CB	5.44	121.28	110.40
2	L	21	GLU	CA-CB-CG	-5.44	101.43	113.40
2	D	21	GLU	CB-CA-C	5.42	121.25	110.40
1	K	17	GLU	CB-CG-CD	5.42	128.84	114.20
1	A	18	ASN	N-CA-CB	-5.42	100.85	110.60
1	E	18	ASN	OD1-CG-ND2	-5.42	109.44	121.90
1	A	17	GLU	CA-C-N	-5.41	105.30	117.20
2	H	22	ARG	CA-CB-CG	5.41	125.30	113.40
1	C	12	SER	CB-CA-C	5.41	120.37	110.10
1	A	11	CYS	C-N-CA	5.41	135.21	121.70
2	H	3	ASN	CA-C-O	5.41	131.45	120.10
2	J	4	GLN	CG-CD-OE1	5.40	132.41	121.60
2	F	10	HIS	CB-CA-C	-5.40	99.60	110.40
1	G	12	SER	CA-CB-OG	5.40	125.78	111.20
1	I	12	SER	O-C-N	5.39	131.33	122.70
2	H	12	VAL	CB-CA-C	-5.39	101.16	111.40
2	D	4	GLN	OE1-CD-NE2	5.39	134.29	121.90
1	G	21	ASN	CB-CG-ND2	5.38	129.62	116.70
1	I	15	GLN	CB-CG-CD	-5.38	97.61	111.60
2	B	3	ASN	CB-CG-OD1	-5.38	110.85	121.60
1	I	13	LEU	N-CA-C	5.36	125.47	111.00
1	A	21	ASN	CA-CB-CG	5.35	125.18	113.40
1	G	10	ILE	N-CA-CB	-5.35	98.49	110.80
1	G	15	GLN	C-N-CA	5.35	135.08	121.70
1	K	18	ASN	N-CA-CB	-5.35	100.97	110.60
2	J	6	LEU	CD1-CG-CD2	-5.34	94.47	110.50
1	I	13	LEU	CA-CB-CG	5.34	127.58	115.30
2	B	13	GLU	OE1-CD-OE2	-5.34	116.90	123.30
1	A	18	ASN	CA-C-N	5.33	128.94	117.20
1	A	15	GLN	CB-CA-C	-5.33	99.73	110.40
2	F	23	GLY	CA-C-N	-5.33	105.47	117.20
1	E	5	GLN	CA-C-O	5.33	131.28	120.10
2	F	16	TYR	CA-CB-CG	5.33	123.52	113.40
1	I	5	GLN	CG-CD-NE2	5.33	129.48	116.70
2	L	22	ARG	CA-CB-CG	-5.33	101.69	113.40
2	F	7	CYS	O-C-N	5.32	132.25	123.20
1	I	17	GLU	CG-CD-OE1	-5.32	107.66	118.30
1	A	16	LEU	CA-CB-CG	5.32	127.54	115.30
2	F	24	PHE	N-CA-C	-5.32	96.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	LEU	CB-CG-CD2	5.32	120.04	111.00
2	D	13	GLU	N-CA-CB	5.32	120.17	110.60
1	E	19	TYR	CE1-CZ-OH	-5.31	105.76	120.10
2	L	3	ASN	CB-CG-OD1	5.31	132.22	121.60
1	I	2	ILE	CA-CB-CG1	5.30	121.06	111.00
1	A	11	CYS	CA-C-N	5.29	128.85	117.20
2	F	5	HIS	C-N-CA	5.29	134.93	121.70
2	B	11	LEU	O-C-N	5.29	131.17	122.70
1	I	17	GLU	CA-C-O	5.29	131.21	120.10
2	F	11	LEU	CA-CB-CG	-5.29	103.14	115.30
2	J	25	TYR	CG-CD2-CE2	-5.28	117.07	121.30
1	G	16	LEU	CA-CB-CG	5.28	127.44	115.30
2	F	2	VAL	C-N-CA	5.26	134.86	121.70
1	A	11	CYS	N-CA-C	5.26	125.21	111.00
1	K	2	ILE	CA-CB-CG2	-5.26	100.38	110.90
1	G	13	LEU	CA-C-N	5.26	128.76	117.20
1	A	17	GLU	N-CA-CB	5.25	120.06	110.60
1	G	19	TYR	N-CA-C	5.25	125.17	111.00
2	H	1	PHE	CB-CG-CD1	-5.25	117.13	120.80
1	I	7	CYS	CA-C-O	5.25	131.12	120.10
2	F	18	VAL	CB-CA-C	-5.23	101.45	111.40
1	C	16	LEU	CB-CG-CD2	-5.23	102.10	111.00
2	L	1	PHE	CE1-CZ-CE2	-5.23	110.58	120.00
1	G	19	TYR	CA-CB-CG	-5.22	103.47	113.40
1	A	14	TYR	CD1-CG-CD2	5.22	123.65	117.90
2	B	2	VAL	N-CA-CB	-5.22	100.03	111.50
2	B	11	LEU	N-CA-CB	-5.20	100.01	110.40
2	B	25	TYR	OH-CZ-CE2	-5.19	106.08	120.10
1	I	9	SER	CA-CB-OG	5.19	125.21	111.20
2	H	24	PHE	CB-CA-C	-5.18	100.03	110.40
2	H	1	PHE	CD1-CE1-CZ	-5.18	113.88	120.10
1	G	19	TYR	CA-C-N	-5.18	105.81	117.20
1	G	2	ILE	CA-CB-CG2	5.17	121.25	110.90
2	J	10	HIS	ND1-CE1-NE2	-5.17	98.52	109.90
1	E	6	CYS	CB-CA-C	-5.17	100.06	110.40
1	G	11	CYS	CB-CA-C	-5.17	100.06	110.40
1	A	19	TYR	O-C-N	5.17	130.96	122.70
2	L	12	VAL	N-CA-C	-5.16	97.06	111.00
2	H	14	ALA	CB-CA-C	-5.15	102.37	110.10
2	B	18	VAL	N-CA-CB	-5.15	100.16	111.50
2	F	9	SER	O-C-N	-5.15	114.46	122.70
2	B	15	LEU	N-CA-CB	-5.15	100.11	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2	ILE	CA-CB-CG2	-5.14	100.61	110.90
2	L	4	GLN	O-C-N	5.14	130.93	122.70
2	J	10	HIS	CA-C-N	5.14	128.50	117.20
2	J	14	ALA	O-C-N	-5.14	114.48	122.70
1	E	8	THR	CA-CB-OG1	5.13	119.77	109.00
2	F	24	PHE	CA-C-O	5.13	130.87	120.10
1	I	5	GLN	CB-CA-C	5.13	120.66	110.40
1	E	13	LEU	C-N-CA	-5.13	108.89	121.70
1	I	18	ASN	C-N-CA	-5.12	108.89	121.70
2	J	18	VAL	CA-C-O	5.12	130.86	120.10
1	A	21	ASN	CB-CG-OD1	5.12	131.83	121.60
2	B	24	PHE	CE1-CZ-CE2	-5.11	110.81	120.00
2	F	15	LEU	CA-C-N	5.11	128.44	117.20
1	K	8	THR	CA-CB-CG2	5.10	119.55	112.40
1	A	16	LEU	CB-CA-C	5.10	119.89	110.20
2	L	6	LEU	CA-CB-CG	5.10	127.02	115.30
1	E	1	GLY	O-C-N	-5.09	114.56	122.70
2	B	9	SER	N-CA-C	-5.08	97.28	111.00
1	I	1	GLY	CA-C-N	5.08	128.37	117.20
1	I	11	CYS	N-CA-CB	5.08	119.74	110.60
2	F	15	LEU	CB-CG-CD1	-5.07	102.39	111.00
2	H	17	LEU	CB-CG-CD1	5.07	119.62	111.00
1	A	14	TYR	CA-C-O	-5.06	109.47	120.10
1	I	11	CYS	N-CA-C	-5.06	97.34	111.00
2	F	16	TYR	CA-C-O	-5.05	109.49	120.10
1	G	2	ILE	CA-C-N	5.05	128.32	117.20
2	D	4	GLN	CA-CB-CG	-5.04	102.31	113.40
2	B	16	TYR	CE1-CZ-OH	-5.04	106.50	120.10
2	L	4	GLN	C-N-CA	-5.04	109.11	121.70
2	H	16	TYR	N-CA-C	-5.03	97.41	111.00
1	A	14	TYR	N-CA-CB	5.03	119.65	110.60
1	I	3	VAL	CG1-CB-CG2	-5.03	102.85	110.90
2	J	5	HIS	CB-CA-C	-5.03	100.34	110.40
2	L	17	LEU	CB-CG-CD1	5.02	119.54	111.00
1	A	17	GLU	CG-CD-OE1	-5.02	108.26	118.30
1	C	14	TYR	N-CA-CB	-5.02	101.57	110.60
2	J	28	LYS	CA-C-O	5.02	130.63	120.10
1	E	15	GLN	C-N-CA	-5.01	109.17	121.70
1	C	18	ASN	CB-CA-C	-5.01	100.39	110.40
1	G	4	GLU	CG-CD-OE2	5.01	128.31	118.30
2	H	18	VAL	CA-C-N	-5.00	106.19	117.20
2	B	13	GLU	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

There are no planarity outliers.

## 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	159	0	142	88	0
1	C	163	0	149	108	0
1	E	163	0	148	131	0
1	G	159	0	143	73	0
1	I	163	0	149	112	0
1	K	163	0	146	122	0
2	B	219	0	205	146	0
2	D	194	0	178	94	0
2	F	194	0	180	63	0
2	H	220	0	206	96	0
2	J	235	0	219	132	0
2	L	212	0	195	117	0
3	A	7	0	5	2	0
3	C	7	0	6	0	0
3	E	7	0	5	0	0
3	G	7	0	6	2	0
3	I	7	0	5	1	0
3	K	7	0	5	2	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	2	0	0	0	0
6	B	17	0	0	5	0
6	C	17	0	0	3	0
6	D	10	0	0	6	0
6	E	7	0	0	1	0
6	F	15	0	0	5	0
6	G	17	0	0	6	0
6	H	17	0	0	3	0
6	I	19	0	0	6	0
6	J	16	0	0	1	0
6	K	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	4	0	0	0	0
All	All	2440	0	2092	1179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 271.

All (1179) 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)
2:H:10:HIS:CB	2:H:10:HIS:CG	1.75	1.70
1:I:14:TYR:CE1	1:I:14:TYR:CD1	1.75	1.70
1:I:14:TYR:CD2	1:I:14:TYR:CE2	1.75	1.68
2:B:24:PHE:CB	2:B:24:PHE:CG	1.77	1.68
2:H:24:PHE:CD1	2:H:24:PHE:CE1	1.75	1.65
1:I:8:THR:CB	1:I:8:THR:CG2	1.75	1.65
2:L:10:HIS:CB	2:L:10:HIS:CG	1.76	1.63
2:H:22:ARG:CB	2:H:22:ARG:CA	1.77	1.62
1:A:9:SER:CB	1:A:9:SER:CA	1.76	1.62
1:K:2:ILE:CG1	1:K:2:ILE:CB	1.76	1.62
1:G:14:TYR:CA	1:G:14:TYR:CB	1.75	1.62
1:C:2:ILE:CG2	1:C:2:ILE:CB	1.74	1.62
2:J:24:PHE:CB	2:J:24:PHE:CG	1.77	1.61
1:C:13:LEU:CA	1:C:13:LEU:CB	1.78	1.61
2:B:2:VAL:CB	2:B:2:VAL:CG2	1.77	1.61
2:L:17:LEU:CB	2:L:17:LEU:CG	1.75	1.61
2:J:11:LEU:CB	2:J:11:LEU:CA	1.74	1.61
1:K:10:ILE:CD1	1:K:10:ILE:CG1	1.78	1.61
2:J:28:LYS:CG	2:J:28:LYS:CD	1.77	1.61
2:D:11:LEU:CD1	2:D:11:LEU:CG	1.78	1.61
1:E:10:ILE:CD1	1:E:10:ILE:CG1	1.75	1.61
2:D:13:GLU:CG	2:D:13:GLU:CB	1.79	1.61
1:E:21:ASN:CB	1:E:21:ASN:CA	1.78	1.61
1:G:10:ILE:CG1	1:G:10:ILE:CB	1.76	1.60
2:L:1:PHE:CG	2:L:1:PHE:CB	1.80	1.60
2:J:10:HIS:CG	2:J:10:HIS:CB	1.84	1.60
2:B:2:VAL:CB	2:B:2:VAL:CA	1.79	1.60
2:J:2:VAL:CB	2:J:2:VAL:CG1	1.79	1.60
2:J:9:SER:CA	2:J:9:SER:CB	1.79	1.59
1:K:10:ILE:CB	1:K:10:ILE:CA	1.79	1.59
2:J:18:VAL:CB	2:J:18:VAL:CG1	1.77	1.59
1:A:5:GLN:CA	1:A:5:GLN:CB	1.78	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:TYR:CA	1:C:14:TYR:CB	1.78	1.59
1:K:10:ILE:CB	1:K:10:ILE:CG1	1.80	1.59
1:A:3:VAL:CB	1:A:3:VAL:CG1	1.75	1.59
1:E:7:CYS:CB	1:E:7:CYS:CA	1.78	1.59
2:F:2:VAL:CG2	2:F:2:VAL:CB	1.81	1.59
1:I:10:ILE:CG1	1:I:10:ILE:CB	1.80	1.59
1:I:10:ILE:CA	1:I:10:ILE:CB	1.75	1.59
2:H:2:VAL:CB	2:H:2:VAL:CG2	1.74	1.59
1:C:13:LEU:CD2	1:C:13:LEU:CG	1.76	1.59
1:G:19:TYR:CA	1:G:19:TYR:CB	1.76	1.59
1:A:17:GLU:CA	1:A:17:GLU:CB	1.80	1.58
1:A:10:ILE:CG1	1:A:10:ILE:CB	1.80	1.58
2:F:17:LEU:CG	2:F:17:LEU:CB	1.78	1.58
2:L:17:LEU:CA	2:L:17:LEU:CB	1.80	1.58
2:L:12:VAL:CB	2:L:12:VAL:CG2	1.80	1.58
1:K:16:LEU:CG	1:K:16:LEU:CB	1.81	1.57
1:K:16:LEU:CD1	1:K:16:LEU:CG	1.76	1.57
2:H:11:LEU:CG	2:H:11:LEU:CD2	1.76	1.57
2:F:15:LEU:CA	2:F:15:LEU:CB	1.80	1.57
1:G:12:SER:CA	1:G:12:SER:CB	1.82	1.57
1:E:10:ILE:CB	1:E:10:ILE:CA	1.80	1.57
2:J:27:THR:CB	2:J:27:THR:CA	1.75	1.56
1:C:16:LEU:CG	1:C:16:LEU:CD2	1.82	1.56
1:A:2:ILE:CB	1:A:2:ILE:CG2	1.80	1.56
2:H:12:VAL:CB	2:H:12:VAL:CA	1.82	1.56
2:J:1:PHE:CA	2:J:1:PHE:CB	1.82	1.56
2:B:25:TYR:CA	2:B:25:TYR:N	1.68	1.56
2:H:24:PHE:CB	2:H:24:PHE:CG	1.87	1.56
2:J:4:GLN:CA	2:J:4:GLN:CB	1.82	1.56
2:B:21:GLU:CB	2:B:21:GLU:CA	1.75	1.56
2:L:2:VAL:CA	2:L:2:VAL:CB	1.84	1.56
1:E:20:CYS:CB	1:E:20:CYS:CA	1.74	1.56
1:K:18:ASN:CA	1:K:18:ASN:N	1.69	1.55
2:F:26:MEA:CA	2:F:26:MEA:C	1.84	1.55
1:I:10:ILE:CG1	1:I:10:ILE:CD1	1.82	1.55
1:A:16:LEU:CB	1:A:16:LEU:CG	1.74	1.55
1:I:14:TYR:CG	1:I:14:TYR:CB	1.86	1.55
1:C:11:CYS:C	1:C:11:CYS:CA	1.74	1.55
2:J:12:VAL:CG2	2:J:12:VAL:CB	1.79	1.55
1:K:4:GLU:CA	1:K:4:GLU:CB	1.79	1.55
2:B:16:TYR:CB	2:B:16:TYR:CA	1.81	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:LEU:CG	2:F:15:LEU:CD1	1.84	1.55
2:B:4:GLN:CB	2:B:4:GLN:CG	1.81	1.55
2:B:9:SER:CA	2:B:9:SER:CB	1.76	1.55
1:I:16:LEU:CB	1:I:16:LEU:CA	1.85	1.55
1:I:13:LEU:CB	1:I:13:LEU:CG	1.85	1.55
2:B:17:LEU:CD1	2:B:17:LEU:CG	1.82	1.55
1:C:17:GLU:CB	1:C:17:GLU:CA	1.83	1.55
2:H:6:LEU:CG	2:H:6:LEU:CB	1.85	1.54
1:C:15:GLN:CA	1:C:15:GLN:C	1.74	1.54
2:J:28:LYS:CA	2:J:28:LYS:CB	1.84	1.54
1:E:16:LEU:N	1:E:16:LEU:CA	1.69	1.54
1:K:11:CYS:CA	1:K:11:CYS:N	1.69	1.54
1:G:18:ASN:CG	1:G:18:ASN:CB	1.76	1.54
1:A:21:ASN:CB	1:A:21:ASN:CA	1.79	1.54
1:C:3:VAL:CB	1:C:3:VAL:CA	1.82	1.54
1:A:12:SER:CB	1:A:12:SER:CA	1.86	1.54
2:L:21:GLU:CB	2:L:21:GLU:CG	1.74	1.54
1:E:2:ILE:CG2	1:E:2:ILE:CB	1.77	1.54
1:I:21:ASN:CA	1:I:21:ASN:N	1.70	1.54
1:K:6:CYS:N	1:K:6:CYS:CA	1.71	1.54
2:H:9:SER:CB	2:H:9:SER:CA	1.86	1.54
1:I:2:ILE:CG1	1:I:2:ILE:CB	1.84	1.54
1:A:2:ILE:CA	1:A:2:ILE:C	1.75	1.53
2:D:14:ALA:CA	2:D:14:ALA:N	1.69	1.53
1:C:20:CYS:CB	1:C:20:CYS:CA	1.83	1.53
2:B:2:VAL:C	2:B:2:VAL:CA	1.75	1.53
1:E:11:CYS:CB	1:E:11:CYS:CA	1.86	1.53
2:H:2:VAL:CA	2:H:2:VAL:CB	1.85	1.53
2:H:5:HIS:CB	2:H:5:HIS:CA	1.86	1.53
1:C:12:SER:CA	1:C:12:SER:N	1.70	1.53
2:B:11:LEU:N	2:B:11:LEU:CA	1.69	1.53
2:D:19:CYS:CB	2:D:19:CYS:CA	1.87	1.53
2:L:4:GLN:CA	2:L:4:GLN:N	1.70	1.53
2:H:1:PHE:CA	2:H:1:PHE:CB	1.81	1.52
1:I:7:CYS:N	1:I:7:CYS:CA	1.72	1.52
1:G:9:SER:CA	1:G:9:SER:CB	1.87	1.52
1:I:16:LEU:CG	1:I:16:LEU:CD1	1.84	1.52
1:A:11:CYS:CA	1:A:11:CYS:N	1.73	1.52
2:J:22:ARG:CA	2:J:22:ARG:N	1.70	1.52
1:I:3:VAL:CA	1:I:3:VAL:N	1.69	1.52
1:K:2:ILE:N	1:K:2:ILE:CA	1.72	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ASN:CA	1:E:18:ASN:N	1.68	1.52
2:L:4:GLN:CG	2:L:4:GLN:CD	1.77	1.52
2:B:18:VAL:CA	2:B:18:VAL:N	1.73	1.52
1:C:17:GLU:CG	1:C:17:GLU:CD	1.78	1.52
2:D:11:LEU:CG	2:D:11:LEU:CD2	1.83	1.52
2:F:10:HIS:CA	2:F:10:HIS:N	1.72	1.52
2:J:2:VAL:CA	2:J:2:VAL:CB	1.87	1.52
2:F:3:ASN:N	2:F:3:ASN:CA	1.68	1.52
2:D:6:LEU:N	2:D:6:LEU:CA	1.70	1.51
1:C:7:CYS:CB	1:C:7:CYS:CA	1.80	1.51
1:E:15:GLN:C	1:E:15:GLN:CA	1.77	1.51
2:B:12:VAL:CB	2:B:12:VAL:CA	1.87	1.51
1:I:1:GLY:CA	1:I:1:GLY:C	1.78	1.51
2:L:13:GLU:CA	2:L:13:GLU:CB	1.89	1.51
2:L:6:LEU:CA	2:L:6:LEU:CB	1.87	1.51
2:D:15:LEU:CG	2:D:15:LEU:CD1	1.81	1.51
1:C:2:ILE:CA	1:C:2:ILE:N	1.70	1.51
1:K:13:LEU:CA	1:K:13:LEU:C	1.77	1.51
1:E:6:CYS:CA	1:E:6:CYS:N	1.69	1.51
1:E:2:ILE:CG1	1:E:2:ILE:CB	1.88	1.51
2:J:18:VAL:CA	2:J:18:VAL:C	1.77	1.51
1:K:16:LEU:C	1:K:16:LEU:CA	1.78	1.51
2:D:15:LEU:CB	2:D:15:LEU:CA	1.83	1.51
2:D:13:GLU:C	2:D:13:GLU:CA	1.76	1.51
2:J:11:LEU:N	2:J:11:LEU:CA	1.71	1.50
2:L:6:LEU:CD1	2:L:6:LEU:CG	1.88	1.50
1:A:3:VAL:CA	1:A:3:VAL:N	1.70	1.50
1:K:7:CYS:N	1:K:7:CYS:CA	1.67	1.50
2:F:21:GLU:CD	2:F:21:GLU:CG	1.78	1.50
1:C:1:GLY:CA	1:C:1:GLY:C	1.76	1.50
2:F:22:ARG:CD	2:F:22:ARG:CG	1.89	1.50
1:E:9:SER:CA	1:E:9:SER:N	1.75	1.50
2:D:5:HIS:CA	2:D:5:HIS:C	1.80	1.50
1:A:5:GLN:CA	1:A:5:GLN:N	1.68	1.50
2:B:4:GLN:N	2:B:4:GLN:CA	1.68	1.50
1:E:14:TYR:CA	1:E:14:TYR:C	1.74	1.50
1:A:19:TYR:CB	1:A:19:TYR:CA	1.84	1.49
1:E:5:GLN:CA	1:E:5:GLN:C	1.80	1.49
2:B:5:HIS:CA	2:B:5:HIS:CB	1.90	1.49
2:L:3:ASN:C	2:L:3:ASN:CA	1.75	1.49
1:C:8:THR:CG2	1:C:8:THR:CB	1.87	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LEU:CG	2:B:11:LEU:CD2	1.91	1.49
1:A:10:ILE:C	1:A:10:ILE:CA	1.81	1.49
2:H:18:VAL:CG1	2:H:18:VAL:CB	1.88	1.49
2:F:24:PHE:CA	2:F:24:PHE:C	1.75	1.49
2:L:22:ARG:NE	2:L:22:ARG:CD	1.75	1.49
2:J:4:GLN:CD	2:J:4:GLN:CG	1.78	1.49
1:A:7:CYS:CA	1:A:7:CYS:N	1.75	1.49
2:B:22:ARG:C	2:B:22:ARG:CA	1.77	1.49
2:L:20:GLY:C	2:L:20:GLY:CA	1.79	1.49
2:J:13:GLU:CA	2:J:13:GLU:CB	1.91	1.49
1:C:2:ILE:CB	1:C:2:ILE:CG1	1.86	1.49
2:H:13:GLU:CB	2:H:13:GLU:CG	1.89	1.49
2:H:17:LEU:CD1	2:H:17:LEU:CG	1.90	1.49
2:J:25:TYR:CB	2:J:25:TYR:CA	1.91	1.48
2:B:3:ASN:C	2:B:3:ASN:CA	1.78	1.48
1:E:19:TYR:N	1:E:19:TYR:CA	1.76	1.48
2:H:15:LEU:CG	2:H:15:LEU:CD2	1.90	1.48
2:J:14:ALA:CA	2:J:14:ALA:C	1.80	1.48
2:J:19:CYS:N	2:J:19:CYS:CA	1.75	1.48
2:J:28:LYS:CE	2:J:28:LYS:NZ	1.74	1.48
2:D:26:MEA:C1	2:D:26:MEA:N	1.74	1.48
2:H:16:TYR:CB	2:H:16:TYR:CA	1.91	1.48
2:J:10:HIS:C	2:J:10:HIS:CA	1.80	1.48
2:H:3:ASN:C	2:H:3:ASN:CA	1.78	1.48
2:H:7:CYS:CA	2:H:7:CYS:N	1.76	1.48
2:H:6:LEU:C	2:H:6:LEU:CA	1.80	1.48
1:K:3:VAL:CA	1:K:3:VAL:N	1.69	1.48
1:A:6:CYS:CA	1:A:6:CYS:C	1.79	1.48
1:G:2:ILE:CB	1:G:2:ILE:CG2	1.90	1.48
1:I:6:CYS:CA	1:I:6:CYS:C	1.81	1.47
1:G:13:LEU:CD2	1:G:13:LEU:CG	1.89	1.47
2:B:6:LEU:CG	2:B:6:LEU:CB	1.92	1.47
1:I:10:ILE:C	1:I:10:ILE:CA	1.79	1.47
2:H:14:ALA:CA	2:H:14:ALA:N	1.78	1.47
1:A:21:ASN:CG	1:A:21:ASN:CB	1.83	1.47
2:B:23:GLY:CA	2:B:23:GLY:N	1.72	1.47
1:E:2:ILE:N	1:E:2:ILE:CA	1.74	1.47
1:K:10:ILE:C	1:K:10:ILE:CA	1.82	1.47
1:E:4:GLU:CA	1:E:4:GLU:C	1.80	1.47
1:I:20:CYS:C	1:I:20:CYS:CA	1.81	1.47
2:J:15:LEU:CA	2:J:15:LEU:N	1.76	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ASN:CA	2:B:3:ASN:N	1.71	1.47
1:I:2:ILE:N	1:I:2:ILE:CA	1.76	1.46
2:D:22:ARG:CB	2:D:22:ARG:CG	1.93	1.46
1:C:15:GLN:CA	1:C:15:GLN:N	1.77	1.46
2:D:21:GLU:CG	2:D:21:GLU:CD	1.80	1.46
2:D:3:ASN:CA	2:D:3:ASN:N	1.77	1.46
2:H:13:GLU:C	2:H:13:GLU:CA	1.82	1.46
2:J:26:MEA:CA	2:J:26:MEA:CB	1.93	1.46
2:H:11:LEU:N	2:H:11:LEU:CA	1.78	1.46
1:I:4:GLU:CB	1:I:4:GLU:CA	1.92	1.46
1:K:2:ILE:CA	1:K:2:ILE:C	1.81	1.45
2:F:21:GLU:CA	2:F:21:GLU:N	1.78	1.45
1:I:6:CYS:CA	1:I:6:CYS:N	1.77	1.45
2:L:14:ALA:CA	2:L:14:ALA:C	1.85	1.45
1:C:18:ASN:CA	1:C:18:ASN:C	1.82	1.45
2:L:15:LEU:N	2:L:15:LEU:CA	1.76	1.45
2:B:13:GLU:CB	2:B:13:GLU:CG	1.93	1.45
2:J:21:GLU:CA	2:J:21:GLU:C	1.83	1.45
2:F:20:GLY:C	2:F:20:GLY:CA	1.83	1.45
1:C:5:GLN:N	1:C:5:GLN:CA	1.77	1.45
2:D:12:VAL:CA	2:D:12:VAL:CB	1.91	1.45
2:H:10:HIS:C	2:H:10:HIS:CA	1.83	1.44
2:D:16:TYR:CA	2:D:16:TYR:C	1.85	1.44
2:L:24:PHE:CB	2:L:24:PHE:CA	1.95	1.44
2:B:10:HIS:CA	2:B:10:HIS:C	1.84	1.44
1:E:1:GLY:CA	1:E:1:GLY:C	1.85	1.44
1:I:14:TYR:N	1:I:14:TYR:CA	1.78	1.43
1:I:14:TYR:CZ	1:I:14:TYR:OH	1.70	1.43
2:F:12:VAL:CA	2:F:12:VAL:CB	1.93	1.43
1:K:5:GLN:CA	1:K:5:GLN:C	1.87	1.43
2:B:14:ALA:CA	2:B:14:ALA:N	1.80	1.43
2:L:19:CYS:N	2:L:19:CYS:CA	1.81	1.43
2:H:18:VAL:CA	2:H:18:VAL:N	1.82	1.43
2:D:25:TYR:CA	2:D:25:TYR:N	1.79	1.43
1:I:18:ASN:N	1:I:18:ASN:CA	1.78	1.43
1:G:6:CYS:C	1:G:6:CYS:CA	1.86	1.43
1:G:14:TYR:CA	1:G:14:TYR:N	1.77	1.43
2:B:17:LEU:CA	2:B:17:LEU:C	1.85	1.42
1:C:11:CYS:CB	1:C:11:CYS:SG	2.05	1.42
2:L:3:ASN:CB	2:L:3:ASN:CG	1.87	1.42
1:K:1:GLY:CA	1:K:1:GLY:C	1.85	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:SER:CB	1:I:9:SER:OG	1.65	1.42
1:G:7:CYS:N	1:G:7:CYS:CA	1.81	1.42
2:B:7:CYS:N	2:B:7:CYS:CA	1.80	1.42
1:K:8:THR:CB	1:K:8:THR:OG1	1.67	1.42
2:L:18:VAL:C	2:L:18:VAL:CA	1.87	1.42
1:I:5:GLN:CA	1:I:5:GLN:C	1.87	1.41
1:I:13:LEU:CA	1:I:13:LEU:C	1.87	1.41
1:C:4:GLU:C	1:C:4:GLU:CA	1.88	1.41
2:D:17:LEU:N	2:D:17:LEU:CA	1.80	1.41
1:K:17:GLU:CA	1:K:17:GLU:C	1.88	1.41
2:B:15:LEU:CG	2:B:15:LEU:CD2	1.98	1.41
1:I:6:CYS:SG	1:I:6:CYS:CB	2.07	1.40
1:C:14:TYR:CA	1:C:14:TYR:C	1.86	1.40
2:D:10:HIS:CA	2:D:10:HIS:N	1.79	1.40
1:K:17:GLU:CG	1:K:17:GLU:CD	1.90	1.40
1:E:8:THR:CA	1:E:8:THR:C	1.87	1.40
1:C:8:THR:CA	1:C:8:THR:C	1.88	1.40
1:C:19:TYR:N	1:C:19:TYR:CA	1.82	1.40
2:H:17:LEU:CA	2:H:17:LEU:C	1.89	1.39
1:E:18:ASN:CA	1:E:18:ASN:C	1.89	1.39
1:I:17:GLU:C	1:I:17:GLU:CA	1.89	1.39
2:B:13:GLU:CA	2:B:13:GLU:C	1.90	1.39
1:K:21:ASN:N	1:K:21:ASN:CA	1.83	1.38
1:C:9:SER:N	1:C:9:SER:CA	1.86	1.37
2:B:6:LEU:CA	2:B:6:LEU:C	1.93	1.37
2:D:24:PHE:CA	2:D:24:PHE:C	1.92	1.36
2:D:9:SER:C	2:D:9:SER:CA	1.93	1.36
1:G:8:THR:OG1	1:G:8:THR:CB	1.70	1.36
2:D:2:VAL:CA	2:D:2:VAL:C	1.96	1.34
1:K:20:CYS:C	1:K:20:CYS:CA	1.96	1.34
2:J:29:PRO:CG	2:J:29:PRO:CB	1.83	1.33
1:K:12:SER:CB	1:K:12:SER:OG	1.74	1.33
1:A:6:CYS:CB	1:A:6:CYS:SG	2.15	1.32
1:I:12:SER:CB	1:I:12:SER:OG	1.79	1.31
1:I:20:CYS:SG	1:I:20:CYS:CB	2.20	1.29
2:H:7:CYS:SG	2:H:7:CYS:CB	2.21	1.28
2:J:10:HIS:NE2	2:J:10:HIS:CD2	1.72	1.27
1:G:6:CYS:SG	1:G:6:CYS:CB	2.25	1.23
2:H:2:VAL:CG1	2:H:2:VAL:CG2	2.18	1.22
2:B:17:LEU:CD1	2:B:17:LEU:CB	2.17	1.21
1:K:20:CYS:CB	1:K:20:CYS:SG	2.30	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:CYS:SG	2:B:7:CYS:CB	2.32	1.16
1:E:3:VAL:HG22	6:E:2001:HOH:O	1.46	1.12
2:B:17:LEU:CD1	2:B:17:LEU:HB2	1.80	1.09
2:H:12:VAL:CG2	2:H:12:VAL:CA	2.31	1.09
1:I:8:THR:HG23	6:I:2011:HOH:O	1.53	1.08
2:B:18:VAL:HA	1:G:13:LEU:HD21	1.29	1.07
1:G:18:ASN:HB3	6:G:2010:HOH:O	1.53	1.07
2:B:2:VAL:CG1	2:B:2:VAL:CA	2.34	1.04
2:F:26:MEA:HC3	2:F:26:MEA:C	1.88	1.03
2:F:2:VAL:N	6:F:2001:HOH:O	1.93	1.01
2:J:28:LYS:CB	2:J:28:LYS:HA	1.87	1.01
1:G:14:TYR:CG	1:G:14:TYR:CA	2.45	1.00
2:B:24:PHE:CB	2:B:24:PHE:CD1	2.42	1.00
1:C:16:LEU:CD2	1:C:16:LEU:CB	2.39	1.00
2:J:28:LYS:HD2	2:L:20:GLY:HA2	1.44	0.99
2:F:26:MEA:C1	2:F:26:MEA:C	2.38	0.99
2:B:11:LEU:N	2:B:11:LEU:CB	2.24	0.99
2:D:26:MEA:C1	2:D:26:MEA:C	2.40	0.99
1:E:14:TYR:CA	1:E:15:GLN:N	2.26	0.99
2:L:18:VAL:C	2:L:18:VAL:HG22	1.83	0.98
2:H:11:LEU:CD1	2:H:11:LEU:CD2	2.40	0.98
2:D:26:MEA:CA	2:D:26:MEA:C1	2.40	0.98
2:L:4:GLN:CB	2:L:4:GLN:CD	2.32	0.98
2:B:6:LEU:HD22	2:J:10:HIS:CG	1.98	0.98
2:J:12:VAL:HG12	2:L:12:VAL:HG13	1.44	0.97
2:B:21:GLU:CB	2:B:21:GLU:C	2.32	0.97
1:A:10:ILE:CG1	1:A:10:ILE:CA	2.42	0.97
1:C:12:SER:C	1:C:12:SER:N	2.18	0.97
2:B:12:VAL:CA	2:B:12:VAL:CG2	2.43	0.97
1:E:21:ASN:HA	1:E:21:ASN:CB	1.93	0.96
1:I:21:ASN:N	1:I:21:ASN:CB	2.28	0.96
2:F:3:ASN:C	2:F:3:ASN:N	2.18	0.96
2:J:28:LYS:CD	2:J:28:LYS:CB	2.44	0.95
2:J:27:THR:HB	2:J:27:THR:CA	1.94	0.95
1:A:10:ILE:HG22	1:A:10:ILE:C	1.86	0.94
1:G:14:TYR:C	1:G:14:TYR:CB	2.34	0.94
2:D:13:GLU:CB	2:D:13:GLU:C	2.36	0.94
2:J:18:VAL:C	2:J:18:VAL:CG1	2.35	0.93
2:B:10:HIS:C	2:B:11:LEU:CA	2.36	0.93
2:F:2:VAL:CA	2:F:2:VAL:CG2	2.47	0.93
1:G:21:ASN:HA	6:G:2016:HOH:O	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:C	2:H:12:VAL:CB	2.38	0.92
2:H:17:LEU:HG	2:H:17:LEU:CD1	2.00	0.92
1:K:4:GLU:CB	1:K:4:GLU:N	2.33	0.91
2:L:12:VAL:HB	2:L:12:VAL:CG2	2.00	0.91
1:I:10:ILE:HA	1:I:10:ILE:CB	2.00	0.91
2:B:24:PHE:C	2:B:25:TYR:CA	2.39	0.91
2:B:2:VAL:CB	2:B:2:VAL:N	2.33	0.91
1:I:20:CYS:C	1:I:21:ASN:CA	2.38	0.91
1:E:7:CYS:CB	1:E:7:CYS:N	2.34	0.91
1:A:16:LEU:CB	1:A:16:LEU:HG	1.98	0.91
1:G:19:TYR:CA	1:G:19:TYR:CG	2.54	0.90
1:K:13:LEU:CA	1:K:14:TYR:N	2.34	0.90
2:J:18:VAL:C	2:J:18:VAL:CB	2.39	0.90
1:A:10:ILE:C	1:A:10:ILE:CG2	2.39	0.90
1:I:10:ILE:CA	1:I:10:ILE:HB	2.01	0.90
2:J:1:PHE:CB	2:J:1:PHE:HA	1.97	0.90
2:L:1:PHE:CB	2:L:1:PHE:CD1	2.53	0.90
2:F:21:GLU:CB	2:F:21:GLU:N	2.34	0.90
1:A:9:SER:CB	1:A:9:SER:C	2.39	0.90
2:B:2:VAL:O	2:B:6:LEU:HG	1.71	0.90
1:I:2:ILE:CG2	1:I:2:ILE:CG1	2.49	0.90
2:F:12:VAL:HA	2:F:12:VAL:CB	2.00	0.90
1:A:21:ASN:ND2	2:B:22:ARG:HE	1.69	0.89
2:B:2:VAL:CG1	2:B:2:VAL:CG2	2.47	0.89
1:E:20:CYS:CB	1:E:20:CYS:N	2.34	0.89
2:J:25:TYR:OH	1:K:21:ASN:ND2	2.05	0.89
1:K:7:CYS:CB	1:K:7:CYS:N	2.36	0.89
1:I:8:THR:HB	1:I:8:THR:CG2	1.99	0.89
2:J:11:LEU:CB	2:J:11:LEU:C	2.40	0.89
1:C:3:VAL:O	1:C:7:CYS:HB2	1.73	0.89
2:H:22:ARG:HA	2:H:22:ARG:CB	2.02	0.89
2:F:19:CYS:O	2:F:22:ARG:HD3	1.73	0.89
2:L:6:LEU:CD1	2:L:6:LEU:CD2	2.50	0.89
1:K:10:ILE:HB	1:K:10:ILE:CG1	2.03	0.89
1:C:3:VAL:CA	1:C:3:VAL:CG1	2.50	0.89
2:H:5:HIS:C	2:H:5:HIS:CB	2.41	0.88
2:J:12:VAL:CG2	2:J:12:VAL:CG1	2.49	0.88
1:A:17:GLU:C	1:A:17:GLU:CB	2.40	0.88
2:D:19:CYS:O	2:D:22:ARG:HG3	1.73	0.88
2:L:22:ARG:NE	2:L:22:ARG:CG	2.36	0.88
2:D:11:LEU:HG	2:D:11:LEU:CD2	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:ILE:CG2	1:K:2:ILE:CG1	2.52	0.88
2:B:9:SER:OG	2:D:13:GLU:OE1	1.90	0.88
1:G:10:ILE:CG1	1:G:10:ILE:CA	2.52	0.88
1:E:10:ILE:CA	1:E:10:ILE:CG1	2.52	0.88
1:K:6:CYS:CB	1:K:6:CYS:N	2.35	0.88
1:C:13:LEU:N	1:C:13:LEU:CB	2.37	0.88
1:C:13:LEU:CD2	1:C:13:LEU:CB	2.51	0.87
2:J:25:TYR:CZ	1:K:21:ASN:ND2	2.43	0.87
2:L:21:GLU:CB	2:L:21:GLU:CD	2.43	0.87
1:K:14:TYR:CD1	1:K:14:TYR:C	2.45	0.87
2:H:6:LEU:HD22	2:L:10:HIS:CD2	2.10	0.87
2:B:3:ASN:HA	2:B:3:ASN:N	1.86	0.87
1:C:15:GLN:CB	1:C:15:GLN:C	2.43	0.87
2:F:10:HIS:C	2:F:10:HIS:N	2.29	0.87
2:F:17:LEU:HG	2:F:17:LEU:CB	2.05	0.86
2:D:26:MEA:HC3	2:D:26:MEA:C	2.04	0.86
1:E:2:ILE:HD12	1:E:19:TYR:CD1	2.10	0.86
2:B:4:GLN:CG	2:B:4:GLN:CA	2.53	0.86
2:D:11:LEU:CD1	2:D:11:LEU:CB	2.53	0.86
2:L:18:VAL:C	2:L:18:VAL:CG2	2.44	0.86
2:B:10:HIS:O	2:B:11:LEU:CA	2.24	0.86
2:D:14:ALA:N	2:D:14:ALA:C	2.29	0.86
2:L:2:VAL:CG2	2:L:2:VAL:CA	2.53	0.86
1:K:18:ASN:N	1:K:18:ASN:CB	2.38	0.86
2:B:18:VAL:N	2:B:18:VAL:CB	2.38	0.86
1:G:4:GLU:H	1:G:4:GLU:CD	1.79	0.85
1:E:4:GLU:CA	1:E:5:GLN:N	2.39	0.85
2:B:17:LEU:C	2:B:18:VAL:CA	2.45	0.85
2:H:9:SER:CB	2:H:9:SER:HA	2.05	0.85
2:J:11:LEU:CG	2:J:11:LEU:CA	2.53	0.85
2:L:21:GLU:CA	2:L:21:GLU:CG	2.54	0.85
1:I:14:TYR:CG	1:I:14:TYR:CA	2.57	0.85
1:I:2:ILE:HD13	2:J:15:LEU:HD11	1.58	0.84
1:K:6:CYS:C	1:K:7:CYS:CA	2.46	0.84
2:B:22:ARG:C	2:B:22:ARG:N	2.30	0.84
2:J:27:THR:CB	2:J:27:THR:HA	2.04	0.84
2:B:16:TYR:CG	2:B:16:TYR:CA	2.60	0.84
1:A:5:GLN:NE2	1:A:19:TYR:OH	2.11	0.84
1:C:2:ILE:HB	1:C:2:ILE:CG1	2.05	0.84
1:E:2:ILE:HD12	1:E:19:TYR:CG	2.12	0.84
1:E:2:ILE:CG2	1:E:2:ILE:HB	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:TYR:CA	1:C:14:TYR:CG	2.60	0.84
1:C:2:ILE:CG2	1:C:2:ILE:CA	2.56	0.84
2:J:14:ALA:C	2:J:14:ALA:CB	2.46	0.83
1:I:2:ILE:CD1	2:J:15:LEU:HD11	2.09	0.83
1:K:5:GLN:OE1	1:K:19:TYR:OH	1.96	0.83
2:B:16:TYR:CB	2:B:16:TYR:N	2.42	0.83
2:J:18:VAL:CG1	2:J:18:VAL:HB	2.02	0.83
2:H:6:LEU:N	2:H:6:LEU:C	2.32	0.83
1:C:17:GLU:CB	1:C:17:GLU:N	2.40	0.83
1:E:14:TYR:C	1:E:14:TYR:HA	1.96	0.83
2:F:20:GLY:C	2:F:21:GLU:CA	2.47	0.83
2:H:2:VAL:CG1	2:H:2:VAL:CA	2.56	0.83
2:F:15:LEU:CB	2:F:15:LEU:C	2.46	0.83
1:G:2:ILE:CG1	1:G:2:ILE:CG2	2.57	0.82
2:D:9:SER:HA	2:D:12:VAL:HG22	1.60	0.82
2:J:18:VAL:C	2:J:18:VAL:HG12	1.98	0.82
2:L:6:LEU:HA	2:L:6:LEU:CB	2.09	0.82
1:I:13:LEU:C	1:I:13:LEU:HA	1.98	0.82
1:K:16:LEU:HG	1:K:16:LEU:CD1	2.08	0.82
1:C:14:TYR:N	1:C:14:TYR:CB	2.43	0.81
1:A:10:ILE:CB	1:A:10:ILE:C	2.48	0.81
2:H:10:HIS:CA	2:H:10:HIS:CG	2.62	0.81
2:H:5:HIS:HB2	1:K:10:ILE:HD11	1.63	0.81
2:J:2:VAL:CG2	2:J:2:VAL:CG1	2.57	0.81
1:E:6:CYS:N	1:E:7:CYS:N	2.27	0.81
1:E:15:GLN:HA	1:E:15:GLN:C	1.99	0.81
1:E:19:TYR:N	1:E:19:TYR:CD1	2.48	0.81
2:B:4:GLN:N	2:B:4:GLN:CB	2.40	0.81
1:C:18:ASN:CB	1:C:18:ASN:C	2.48	0.81
1:E:1:GLY:C	1:E:4:GLU:HG2	2.00	0.81
1:K:16:LEU:CD2	1:K:16:LEU:CB	2.58	0.80
1:E:15:GLN:C	1:E:16:LEU:CA	2.49	0.80
1:E:9:SER:C	1:E:9:SER:N	2.34	0.80
1:C:2:ILE:C	1:C:2:ILE:N	2.34	0.80
2:B:9:SER:N	2:B:9:SER:CB	2.43	0.80
2:L:22:ARG:HH11	2:L:22:ARG:CD	1.94	0.80
1:A:21:ASN:HB3	2:B:22:ARG:HB3	1.64	0.80
1:A:10:ILE:CB	1:A:10:ILE:CD1	2.60	0.80
2:D:3:ASN:N	2:D:3:ASN:C	2.36	0.80
1:E:5:GLN:C	1:E:6:CYS:CA	2.49	0.80
1:K:12:SER:C	1:K:12:SER:OG	2.19	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:TYR:C	1:I:14:TYR:CG	2.55	0.79
1:E:6:CYS:N	1:E:6:CYS:CB	2.43	0.79
2:J:28:LYS:CG	2:J:28:LYS:CA	2.57	0.79
2:D:3:ASN:N	2:D:4:GLN:N	2.29	0.79
1:A:21:ASN:N	1:A:21:ASN:CB	2.45	0.79
1:I:7:CYS:N	1:I:7:CYS:CB	2.43	0.79
2:J:11:LEU:N	2:J:11:LEU:HA	1.94	0.79
1:K:10:ILE:CG2	1:K:10:ILE:CA	2.60	0.79
1:E:8:THR:C	1:E:8:THR:HA	2.00	0.79
1:K:16:LEU:C	1:K:16:LEU:HA	2.03	0.79
1:E:4:GLU:HA	1:E:4:GLU:C	2.02	0.79
2:H:13:GLU:N	2:H:13:GLU:C	2.35	0.79
2:D:6:LEU:HA	2:D:6:LEU:N	1.96	0.78
2:F:24:PHE:N	2:F:24:PHE:C	2.35	0.78
1:E:13:LEU:O	1:E:17:GLU:HG3	1.82	0.78
2:J:2:VAL:CA	2:J:2:VAL:CG2	2.61	0.78
2:J:12:VAL:CG2	2:J:12:VAL:CA	2.58	0.78
2:J:15:LEU:N	2:J:16:TYR:N	2.30	0.78
1:G:19:TYR:CB	1:G:19:TYR:C	2.51	0.78
1:E:11:CYS:CB	1:E:11:CYS:N	2.45	0.78
1:C:4:GLU:O	1:C:8:THR:HG23	1.82	0.78
2:L:17:LEU:HA	2:L:17:LEU:CB	2.08	0.78
2:J:22:ARG:CB	2:J:22:ARG:N	2.44	0.78
2:J:25:TYR:CE2	1:K:21:ASN:ND2	2.52	0.78
1:G:10:ILE:CG1	1:G:10:ILE:CG2	2.59	0.78
1:A:3:VAL:CG1	1:A:3:VAL:CG2	2.60	0.78
2:B:9:SER:HA	2:B:9:SER:CB	2.11	0.78
1:G:14:TYR:C	1:G:14:TYR:N	2.37	0.78
1:K:17:GLU:C	1:K:18:ASN:CA	2.49	0.77
2:J:13:GLU:OE1	2:L:9:SER:OG	2.02	0.77
1:C:15:GLN:CB	1:C:15:GLN:N	2.43	0.77
2:H:2:VAL:HG11	2:H:2:VAL:CG2	2.15	0.77
2:D:17:LEU:N	2:D:17:LEU:HA	1.97	0.77
2:F:24:PHE:CA	2:F:25:TYR:N	2.48	0.77
1:E:5:GLN:C	1:E:5:GLN:HA	2.02	0.77
1:I:10:ILE:CG1	1:I:10:ILE:CG2	2.62	0.77
1:K:8:THR:OG1	1:K:8:THR:CG2	2.32	0.77
1:I:6:CYS:C	1:I:7:CYS:CA	2.53	0.77
1:I:17:GLU:HA	1:I:20:CYS:SG	2.24	0.77
1:G:12:SER:N	1:G:12:SER:CB	2.46	0.77
1:I:20:CYS:O	1:I:21:ASN:CA	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:VAL:CB	1:K:3:VAL:N	2.45	0.76
1:E:6:CYS:N	1:E:7:CYS:H	1.82	0.76
2:J:28:LYS:HD2	2:L:20:GLY:CA	2.16	0.76
2:F:15:LEU:CB	2:F:15:LEU:CD1	2.62	0.76
1:A:2:ILE:CG2	1:A:2:ILE:CG1	2.61	0.76
2:B:2:VAL:C	2:B:2:VAL:N	2.36	0.76
2:B:2:VAL:CG2	2:B:2:VAL:HB	2.08	0.76
2:J:12:VAL:CG1	2:L:12:VAL:HG13	2.14	0.76
1:E:2:ILE:CG2	1:E:2:ILE:CA	2.64	0.76
2:F:9:SER:HA	2:F:12:VAL:HG22	1.67	0.76
1:E:2:ILE:HB	1:E:19:TYR:CD2	2.20	0.76
2:H:2:VAL:HA	2:H:2:VAL:CB	2.07	0.76
1:G:13:LEU:CD2	1:G:13:LEU:CB	2.60	0.76
2:F:17:LEU:HD23	2:L:17:LEU:HD12	1.67	0.76
1:C:16:LEU:HA	1:C:16:LEU:HD23	1.68	0.75
2:B:3:ASN:C	2:B:4:GLN:CA	2.48	0.75
1:E:10:ILE:CB	1:E:10:ILE:C	2.53	0.75
2:F:17:LEU:CD1	2:F:17:LEU:CB	2.62	0.75
1:I:20:CYS:CA	1:I:21:ASN:N	2.45	0.75
1:E:8:THR:C	1:E:9:SER:CA	2.52	0.75
1:I:6:CYS:CB	1:I:11:CYS:SG	2.75	0.75
1:K:2:ILE:C	1:K:3:VAL:CA	2.54	0.75
2:B:18:VAL:CA	1:G:13:LEU:HD21	2.11	0.75
1:A:2:ILE:C	1:A:2:ILE:N	2.40	0.75
1:A:5:GLN:CB	1:A:5:GLN:C	2.52	0.75
1:K:2:ILE:CG1	1:K:2:ILE:CA	2.62	0.74
2:B:25:TYR:CB	2:B:25:TYR:N	2.48	0.74
2:H:7:CYS:HA	2:H:7:CYS:N	1.99	0.74
2:D:25:TYR:C	2:D:25:TYR:N	2.39	0.74
2:F:20:GLY:O	2:F:21:GLU:CA	2.34	0.74
2:L:17:LEU:CB	2:L:17:LEU:CD2	2.64	0.74
2:D:13:GLU:CB	2:D:13:GLU:CD	2.54	0.74
2:H:5:HIS:HB2	1:K:10:ILE:CD1	2.18	0.74
1:K:5:GLN:O	1:K:6:CYS:CA	2.35	0.74
1:C:2:ILE:N	1:C:3:VAL:N	2.35	0.74
1:K:2:ILE:CD1	1:K:2:ILE:CB	2.64	0.74
1:A:10:ILE:N	1:A:10:ILE:CG1	2.50	0.74
1:E:18:ASN:CB	1:E:18:ASN:N	2.47	0.73
1:I:16:LEU:CB	1:I:16:LEU:N	2.46	0.73
2:J:9:SER:C	2:J:9:SER:CB	2.55	0.73
2:D:12:VAL:HB	2:D:12:VAL:CA	2.15	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:PHE:C	2:B:2:VAL:C	2.46	0.73
2:L:4:GLN:N	2:L:4:GLN:HA	1.99	0.73
2:H:12:VAL:C	2:H:13:GLU:C	2.46	0.73
1:C:5:GLN:N	1:C:5:GLN:CB	2.49	0.73
1:I:7:CYS:SG	1:I:7:CYS:N	2.62	0.73
1:E:10:ILE:CD1	2:J:2:VAL:HA	2.18	0.73
2:J:18:VAL:CA	2:J:18:VAL:CG1	2.65	0.73
1:A:2:ILE:CA	1:A:2:ILE:CG2	2.65	0.73
1:A:5:GLN:C	1:A:5:GLN:N	2.39	0.73
1:G:4:GLU:HG2	6:G:2001:HOH:O	1.88	0.73
2:H:24:PHE:HE2	2:H:26:MEA:HB2	1.54	0.72
2:F:20:GLY:CA	2:F:21:GLU:N	2.47	0.72
2:J:8:GLY:HA3	2:L:16:TYR:OH	1.89	0.72
2:B:10:HIS:CA	2:B:11:LEU:N	2.46	0.72
1:E:9:SER:O	1:E:9:SER:N	2.22	0.72
2:H:6:LEU:HD22	2:L:10:HIS:CG	2.24	0.72
2:J:8:GLY:HA3	2:L:16:TYR:CZ	2.25	0.72
1:C:12:SER:O	1:C:12:SER:N	2.23	0.72
1:K:17:GLU:HA	1:K:20:CYS:SG	2.30	0.72
2:B:17:LEU:O	2:B:18:VAL:CA	2.38	0.71
2:D:15:LEU:CB	2:D:15:LEU:CD1	2.67	0.71
2:B:7:CYS:HB2	2:F:6:LEU:HD11	1.72	0.71
2:J:13:GLU:CB	2:J:13:GLU:HA	2.12	0.71
2:L:22:ARG:CD	2:L:22:ARG:NH1	2.52	0.71
2:B:17:LEU:CA	2:B:18:VAL:N	2.50	0.71
1:I:10:ILE:N	1:I:10:ILE:C	2.44	0.71
1:I:3:VAL:N	1:I:3:VAL:C	2.41	0.71
1:C:20:CYS:CB	1:C:20:CYS:N	2.51	0.71
2:F:3:ASN:N	2:F:4:GLN:N	2.39	0.71
1:G:21:ASN:ND2	2:H:25:TYR:CE2	2.58	0.71
2:L:2:VAL:CB	2:L:2:VAL:C	2.57	0.71
2:B:9:SER:CA	2:B:9:SER:OG	2.36	0.71
2:F:20:GLY:O	6:F:2010:HOH:O	2.09	0.71
1:E:16:LEU:N	1:E:16:LEU:CB	2.52	0.70
1:E:5:GLN:CA	1:E:6:CYS:N	2.54	0.70
1:A:11:CYS:CB	1:A:11:CYS:N	2.51	0.70
1:I:13:LEU:CB	1:I:13:LEU:CD1	2.69	0.70
2:B:24:PHE:O	2:B:25:TYR:CA	2.39	0.70
2:J:4:GLN:HA	2:J:4:GLN:CB	2.11	0.70
2:B:3:ASN:O	2:B:4:GLN:CA	2.39	0.70
2:D:12:VAL:CB	2:D:12:VAL:HA	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:LEU:HD22	2:J:10:HIS:CD2	2.26	0.70
1:E:1:GLY:C	1:E:2:ILE:CA	2.59	0.70
1:E:8:THR:O	1:E:9:SER:CA	2.39	0.70
2:J:15:LEU:N	2:J:15:LEU:C	2.42	0.70
2:F:10:HIS:N	2:F:11:LEU:N	2.40	0.70
2:L:10:HIS:HB3	2:L:10:HIS:CG	2.19	0.69
1:I:14:TYR:CE2	6:I:2012:HOH:O	2.45	0.69
1:C:8:THR:HA	6:C:2007:HOH:O	1.93	0.69
2:B:17:LEU:HB2	2:B:17:LEU:HD13	1.74	0.69
1:C:14:TYR:HA	1:C:14:TYR:C	2.08	0.69
1:E:10:ILE:HD11	2:J:2:VAL:HA	1.75	0.69
2:L:19:CYS:C	2:L:20:GLY:C	2.52	0.69
1:A:12:SER:C	1:A:12:SER:CB	2.61	0.69
1:I:20:CYS:N	1:I:20:CYS:C	2.46	0.69
1:E:2:ILE:CG1	1:E:2:ILE:CA	2.68	0.69
1:A:10:ILE:C	1:A:11:CYS:CA	2.61	0.68
1:E:2:ILE:HB	1:E:19:TYR:CE2	2.28	0.68
2:H:1:PHE:CG	2:H:1:PHE:CA	2.72	0.68
1:I:2:ILE:C	1:I:3:VAL:CA	2.58	0.68
1:E:15:GLN:CA	1:E:16:LEU:N	2.55	0.68
1:K:5:GLN:C	1:K:6:CYS:CA	2.52	0.68
1:I:13:LEU:O	1:I:14:TYR:CA	2.42	0.68
2:B:11:LEU:N	2:B:11:LEU:HB2	2.09	0.68
2:F:26:MEA:N	2:F:26:MEA:C	2.50	0.68
1:E:2:ILE:C	1:E:2:ILE:CG1	2.61	0.68
1:C:11:CYS:C	1:C:11:CYS:HA	2.03	0.68
2:H:14:ALA:HA	2:H:14:ALA:N	2.00	0.68
1:E:5:GLN:CB	1:E:5:GLN:C	2.56	0.68
2:J:6:LEU:O	2:J:9:SER:HB3	1.94	0.68
1:K:7:CYS:SG	1:K:7:CYS:N	2.67	0.68
2:L:10:HIS:CG	2:L:10:HIS:HB2	2.19	0.68
1:G:6:CYS:O	1:G:7:CYS:CA	2.40	0.68
1:E:19:TYR:N	1:E:19:TYR:CG	2.62	0.67
1:E:5:GLN:HG3	1:E:5:GLN:C	2.15	0.67
1:K:6:CYS:O	1:K:7:CYS:HA	1.95	0.67
1:A:19:TYR:C	1:A:19:TYR:CB	2.63	0.67
1:A:13:LEU:HD11	2:H:18:VAL:HA	1.75	0.67
2:H:2:VAL:O	2:H:6:LEU:HG	1.94	0.67
1:C:15:GLN:CA	1:C:16:LEU:N	2.53	0.67
1:C:16:LEU:CA	1:C:16:LEU:CD2	2.72	0.67
2:B:6:LEU:CB	2:B:6:LEU:HG	2.18	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:TYR:CB	1:G:14:TYR:HA	2.15	0.67
1:K:3:VAL:HG23	1:K:3:VAL:N	2.08	0.67
1:A:5:GLN:N	1:A:6:CYS:N	2.41	0.67
1:I:18:ASN:N	1:I:19:TYR:N	2.43	0.67
1:G:21:ASN:ND2	2:H:25:TYR:CD2	2.63	0.67
2:L:22:ARG:CZ	2:L:22:ARG:CD	2.65	0.67
1:I:2:ILE:N	1:I:2:ILE:HA	1.99	0.66
1:A:16:LEU:CB	1:A:16:LEU:CD1	2.62	0.66
1:K:13:LEU:C	1:K:13:LEU:HA	2.06	0.66
1:K:2:ILE:HD13	2:L:15:LEU:HD11	1.76	0.66
2:H:3:ASN:C	2:H:3:ASN:CB	2.63	0.66
1:K:12:SER:O	1:K:16:LEU:HG	1.96	0.66
2:B:23:GLY:C	2:B:23:GLY:N	2.46	0.66
2:B:26:MEA:HC2	2:D:24:PHE:O	1.96	0.66
1:G:14:TYR:N	1:G:15:GLN:N	2.43	0.66
1:G:3:VAL:O	1:G:7:CYS:N	2.28	0.66
1:E:10:ILE:CD1	1:E:10:ILE:CB	2.65	0.66
2:D:6:LEU:N	2:D:6:LEU:HG	2.11	0.66
2:D:15:LEU:O	2:D:19:CYS:HB2	1.96	0.66
2:H:6:LEU:HG	2:H:6:LEU:CB	2.18	0.66
1:A:5:GLN:CB	1:A:5:GLN:HA	2.15	0.65
2:L:19:CYS:O	2:L:20:GLY:C	2.34	0.65
1:C:2:ILE:HG23	1:C:3:VAL:N	2.11	0.65
2:H:1:PHE:C	2:H:1:PHE:CB	2.57	0.65
2:H:15:LEU:CD2	2:H:15:LEU:HG	2.20	0.65
1:K:17:GLU:CA	1:K:18:ASN:N	2.56	0.65
6:B:2015:HOH:O	1:G:13:LEU:HG	1.96	0.65
1:C:13:LEU:O	1:C:17:GLU:HG3	1.97	0.65
1:K:7:CYS:CB	2:L:7:CYS:SG	2.83	0.65
1:G:9:SER:CB	1:G:10:ILE:N	2.59	0.65
1:G:17:GLU:HG2	1:G:17:GLU:O	1.95	0.65
1:K:16:LEU:CD2	1:K:16:LEU:CD1	2.67	0.65
2:J:9:SER:OG	2:L:13:GLU:OE2	2.15	0.65
2:J:16:TYR:CZ	2:L:8:GLY:HA3	2.32	0.65
2:J:19:CYS:N	2:J:20:GLY:N	2.45	0.65
2:B:11:LEU:CD1	2:B:11:LEU:CD2	2.69	0.65
2:J:2:VAL:HB	2:J:2:VAL:CG1	2.17	0.65
1:K:7:CYS:CA	2:L:7:CYS:SG	2.85	0.65
1:A:6:CYS:N	1:A:6:CYS:C	2.42	0.65
2:D:2:VAL:CA	6:D:2002:HOH:O	2.45	0.65
1:I:6:CYS:CA	1:I:7:CYS:N	2.59	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:PRO:O	2:L:21:GLU:OE1	2.14	0.64
2:B:24:PHE:CA	2:B:24:PHE:CG	2.75	0.64
2:L:5:HIS:CD2	2:L:5:HIS:C	2.71	0.64
1:I:12:SER:O	1:I:16:LEU:HG	1.97	0.64
1:K:17:GLU:HA	1:K:17:GLU:C	2.08	0.64
1:A:21:ASN:HB3	2:B:22:ARG:CB	2.26	0.64
2:F:15:LEU:CG	2:F:15:LEU:CA	2.74	0.64
1:K:2:ILE:CB	1:K:2:ILE:C	2.62	0.64
1:C:14:TYR:O	1:C:15:GLN:CA	2.45	0.64
1:K:11:CYS:N	1:K:11:CYS:C	2.51	0.64
1:E:1:GLY:O	1:E:4:GLU:HG2	1.98	0.64
1:E:7:CYS:SG	2:F:11:LEU:CD1	2.85	0.64
2:D:2:VAL:C	2:D:2:VAL:HA	2.13	0.64
1:K:12:SER:CA	1:K:12:SER:OG	2.41	0.64
2:H:10:HIS:C	2:H:10:HIS:CB	2.63	0.64
2:D:2:VAL:HA	6:D:2002:HOH:O	1.98	0.64
2:D:6:LEU:N	2:D:6:LEU:CG	2.61	0.64
1:A:21:ASN:ND2	2:B:22:ARG:NE	2.45	0.64
1:E:17:GLU:C	1:E:18:ASN:CA	2.57	0.64
2:H:4:GLN:NE2	6:H:2005:HOH:O	2.27	0.64
2:J:18:VAL:C	2:J:19:CYS:CA	2.60	0.63
2:B:15:LEU:HG	2:B:15:LEU:CD2	2.21	0.63
1:E:10:ILE:CD1	1:E:10:ILE:HG23	2.28	0.63
6:B:2015:HOH:O	1:G:13:LEU:N	2.30	0.63
1:C:2:ILE:HD12	1:C:19:TYR:CB	2.27	0.63
1:I:16:LEU:CD1	1:I:16:LEU:HG	2.14	0.63
2:B:24:PHE:C	2:B:24:PHE:CG	2.70	0.63
2:B:20:GLY:O	2:B:23:GLY:N	2.31	0.63
1:C:11:CYS:N	1:C:11:CYS:C	2.45	0.63
2:B:3:ASN:CA	2:B:4:GLN:N	2.53	0.63
1:C:4:GLU:O	1:C:8:THR:CG2	2.47	0.63
1:I:2:ILE:O	1:I:6:CYS:N	2.32	0.63
1:G:4:GLU:N	1:G:4:GLU:CD	2.52	0.63
1:E:16:LEU:N	1:E:17:GLU:N	2.46	0.63
2:D:3:ASN:N	2:D:4:GLN:H	1.96	0.63
1:G:3:VAL:HG23	1:G:7:CYS:HB2	1.81	0.63
2:L:3:ASN:C	2:L:3:ASN:N	2.49	0.63
2:H:16:TYR:CB	2:H:16:TYR:HA	2.21	0.63
1:E:10:ILE:HD13	2:J:2:VAL:HG22	1.81	0.63
2:J:21:GLU:C	2:J:21:GLU:CB	2.66	0.63
2:J:15:LEU:N	2:J:16:TYR:H	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:GLU:C	2:B:22:ARG:C	2.57	0.62
1:C:14:TYR:O	1:C:17:GLU:HB2	1.98	0.62
1:E:19:TYR:N	1:E:19:TYR:CB	2.54	0.62
2:D:6:LEU:HD11	2:H:7:CYS:HB2	1.80	0.62
2:B:3:ASN:C	2:B:3:ASN:CB	2.66	0.62
1:E:11:CYS:C	1:E:12:SER:O	2.36	0.62
2:F:14:ALA:O	2:F:18:VAL:N	2.26	0.62
4:C:1028:CL:CL	2:H:6:LEU:HB3	2.36	0.62
1:G:2:ILE:N	6:G:2001:HOH:O	2.32	0.62
1:G:10:ILE:CB	1:G:10:ILE:CD1	2.67	0.62
1:I:3:VAL:CB	1:I:3:VAL:N	2.55	0.62
1:K:15:GLN:C	1:K:16:LEU:C	2.57	0.62
2:D:16:TYR:C	2:D:16:TYR:N	2.49	0.62
1:G:13:LEU:CD2	1:G:13:LEU:HG	2.22	0.62
2:F:12:VAL:CA	2:F:12:VAL:CG2	2.72	0.62
2:L:20:GLY:N	2:L:20:GLY:C	2.50	0.62
1:C:7:CYS:SG	1:C:7:CYS:CA	2.86	0.61
2:H:1:PHE:N	2:H:1:PHE:CB	2.57	0.61
2:B:17:LEU:HD12	6:B:2007:HOH:O	1.99	0.61
1:I:16:LEU:HB3	2:J:15:LEU:HD23	1.81	0.61
2:B:13:GLU:HA	2:B:13:GLU:C	2.12	0.61
1:A:14:TYR:O	1:A:17:GLU:HB3	2.00	0.61
1:I:14:TYR:O	1:I:14:TYR:CD1	2.54	0.61
1:C:3:VAL:CB	1:C:3:VAL:N	2.52	0.61
1:K:3:VAL:N	1:K:3:VAL:CG2	2.63	0.61
1:C:10:ILE:HD11	6:C:2011:HOH:O	2.01	0.61
1:C:11:CYS:C	1:C:12:SER:O	2.39	0.61
1:C:7:CYS:CB	1:C:7:CYS:C	2.61	0.61
2:B:6:LEU:HA	2:B:6:LEU:C	2.11	0.61
2:L:21:GLU:CG	2:L:21:GLU:N	2.64	0.61
3:A:1022:IPH:C5	2:B:11:LEU:HG	2.31	0.61
1:A:10:ILE:N	1:A:10:ILE:HG13	2.16	0.61
1:A:17:GLU:O	1:A:18:ASN:C	2.39	0.61
2:H:15:LEU:CD2	2:H:15:LEU:CD1	2.69	0.61
1:I:6:CYS:N	1:I:6:CYS:CB	2.60	0.61
2:H:16:TYR:HA	2:H:24:PHE:CE1	2.36	0.61
1:I:8:THR:HG22	6:I:2005:HOH:O	2.00	0.61
1:C:19:TYR:N	1:C:19:TYR:CD1	2.69	0.60
2:L:19:CYS:N	2:L:20:GLY:N	2.49	0.60
1:G:12:SER:C	1:G:12:SER:CB	2.67	0.60
1:K:2:ILE:CD1	2:L:15:LEU:HD11	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ILE:N	1:E:3:VAL:N	2.49	0.60
1:C:17:GLU:OE1	1:C:17:GLU:CG	2.40	0.60
2:J:21:GLU:OE1	2:J:21:GLU:N	2.20	0.60
2:H:24:PHE:CG	2:H:24:PHE:C	2.74	0.60
2:L:17:LEU:CB	2:L:17:LEU:CD1	2.66	0.60
1:K:8:THR:HG1	1:K:8:THR:N	1.99	0.60
1:E:14:TYR:O	1:E:17:GLU:HB2	2.02	0.60
1:E:1:GLY:N	1:E:4:GLU:CG	2.65	0.60
1:E:5:GLN:CG	1:E:5:GLN:C	2.70	0.60
1:E:10:ILE:HD12	1:E:10:ILE:HG23	1.82	0.60
1:I:5:GLN:HG2	6:I:2015:HOH:O	2.00	0.60
2:H:18:VAL:CG1	2:H:18:VAL:CA	2.73	0.60
2:H:12:VAL:CB	2:H:13:GLU:N	2.65	0.60
2:B:17:LEU:HA	2:B:17:LEU:C	2.12	0.59
1:I:6:CYS:O	1:I:7:CYS:HA	2.02	0.59
1:C:10:ILE:HG13	1:C:11:CYS:O	2.03	0.59
2:B:2:VAL:HA	2:B:2:VAL:C	2.10	0.59
1:E:18:ASN:O	1:E:19:TYR:HA	2.02	0.59
1:K:10:ILE:HA	1:K:10:ILE:C	2.10	0.59
1:C:8:THR:CG2	1:C:8:THR:HB	2.19	0.59
1:A:9:SER:CB	1:A:10:ILE:N	2.64	0.59
1:A:21:ASN:HA	2:B:23:GLY:O	2.01	0.59
1:K:19:TYR:O	2:L:24:PHE:HA	2.03	0.59
2:H:10:HIS:O	2:H:11:LEU:CA	2.50	0.59
1:I:13:LEU:C	1:I:14:TYR:CA	2.60	0.59
2:D:15:LEU:CB	2:D:15:LEU:C	2.65	0.59
1:E:2:ILE:CG1	1:E:2:ILE:HB	2.22	0.59
1:I:4:GLU:OE2	2:J:29:PRO:HB3	2.03	0.59
1:A:5:GLN:HG2	1:A:11:CYS:SG	2.42	0.59
2:H:18:VAL:CG1	2:H:18:VAL:CG2	2.78	0.59
1:I:18:ASN:N	1:I:19:TYR:H	2.01	0.59
1:K:8:THR:CB	1:K:8:THR:HG1	2.10	0.59
1:K:2:ILE:N	1:K:2:ILE:CB	2.60	0.59
2:B:10:HIS:C	2:B:10:HIS:CB	2.69	0.59
1:K:10:ILE:N	1:K:10:ILE:CB	2.57	0.58
1:I:13:LEU:CB	1:I:13:LEU:CD2	2.73	0.58
1:K:16:LEU:HD13	2:L:14:ALA:HB1	1.83	0.58
1:A:20:CYS:SG	2:B:19:CYS:HA	2.43	0.58
2:L:22:ARG:CB	2:L:22:ARG:NE	2.65	0.58
2:J:16:TYR:OH	2:L:8:GLY:HA3	2.03	0.58
1:I:14:TYR:N	1:I:14:TYR:CB	2.53	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:ARG:HH11	2:D:22:ARG:HG3	1.68	0.58
1:E:1:GLY:H3	1:E:4:GLU:CD	2.07	0.58
1:C:3:VAL:CG2	1:C:3:VAL:CA	2.74	0.58
2:L:1:PHE:HB3	2:L:1:PHE:CG	2.24	0.58
2:L:21:GLU:OE1	2:L:21:GLU:CB	2.50	0.58
2:B:9:SER:CA	2:B:9:SER:HG	2.15	0.58
1:C:4:GLU:O	1:C:5:GLN:CA	2.51	0.58
1:C:2:ILE:HB	1:C:19:TYR:CD2	2.39	0.58
2:H:16:TYR:HA	2:H:24:PHE:HE1	1.69	0.58
2:J:26:MEA:O	2:L:23:GLY:HA2	2.04	0.58
2:D:14:ALA:N	2:D:15:LEU:N	2.51	0.58
1:A:19:TYR:CG	1:A:19:TYR:CA	2.78	0.57
2:J:28:LYS:CD	2:J:28:LYS:HB2	2.34	0.57
2:L:22:ARG:HH11	2:L:22:ARG:HD2	1.67	0.57
1:E:10:ILE:CA	1:E:10:ILE:CG2	2.72	0.57
1:E:10:ILE:CB	1:E:10:ILE:N	2.62	0.57
2:J:18:VAL:HG12	2:J:19:CYS:N	2.19	0.57
1:A:2:ILE:HD13	2:B:15:LEU:HD11	1.85	0.57
1:I:17:GLU:C	1:I:17:GLU:CB	2.68	0.57
1:E:6:CYS:N	1:E:6:CYS:SG	2.77	0.57
1:C:10:ILE:HG21	2:L:1:PHE:HB3	1.86	0.57
2:D:13:GLU:CG	2:D:13:GLU:C	2.72	0.57
1:I:9:SER:CB	1:I:9:SER:HG	2.09	0.57
2:H:24:PHE:CA	2:H:24:PHE:CG	2.84	0.57
1:E:10:ILE:HA	1:E:10:ILE:HD13	1.87	0.57
1:E:12:SER:O	1:E:13:LEU:C	2.39	0.57
1:E:7:CYS:SG	2:F:11:LEU:HD12	2.45	0.57
2:H:2:VAL:HB	2:H:2:VAL:CA	2.16	0.57
1:I:6:CYS:HA	1:I:6:CYS:C	2.09	0.57
1:G:6:CYS:O	1:G:7:CYS:HA	2.04	0.57
1:K:2:ILE:CA	1:K:3:VAL:N	2.58	0.57
1:C:19:TYR:N	1:C:20:CYS:N	2.53	0.57
1:G:9:SER:CB	1:G:9:SER:C	2.65	0.57
1:E:2:ILE:N	1:E:2:ILE:CB	2.61	0.57
2:L:21:GLU:N	2:L:21:GLU:HG2	2.19	0.56
2:B:15:LEU:C	2:B:17:LEU:N	2.59	0.56
1:G:6:CYS:C	1:G:7:CYS:CA	2.64	0.56
1:C:15:GLN:O	1:C:18:ASN:HB3	2.05	0.56
1:C:16:LEU:CA	1:C:16:LEU:HD23	2.36	0.56
2:L:17:LEU:HG	2:L:17:LEU:CB	2.17	0.56
2:J:2:VAL:C	2:J:2:VAL:CB	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:11:CYS:N	3:K:1022:IPH:O1	2.33	0.56
2:H:2:VAL:HG13	2:H:2:VAL:CG2	2.30	0.56
2:J:10:HIS:C	2:J:10:HIS:N	2.52	0.56
1:A:3:VAL:N	1:A:3:VAL:C	2.56	0.56
1:E:2:ILE:HG23	1:E:3:VAL:HG13	1.85	0.56
2:L:6:LEU:O	2:L:9:SER:HB3	2.06	0.56
1:G:2:ILE:HG21	1:G:2:ILE:HD13	1.88	0.56
1:C:14:TYR:C	1:C:15:GLN:CA	2.62	0.56
1:E:1:GLY:CA	1:E:2:ILE:N	2.65	0.56
1:A:2:ILE:CB	1:A:2:ILE:C	2.63	0.56
2:L:4:GLN:HB3	2:L:4:GLN:CD	2.24	0.56
2:J:19:CYS:C	2:J:19:CYS:N	2.51	0.56
2:L:18:VAL:C	2:L:18:VAL:CB	2.66	0.56
1:K:1:GLY:C	1:K:2:ILE:CA	2.64	0.56
2:J:22:ARG:CZ	2:J:22:ARG:HB2	2.36	0.56
1:C:20:CYS:SG	2:D:19:CYS:HA	2.46	0.55
2:D:9:SER:CA	2:D:12:VAL:HG22	2.34	0.55
1:I:20:CYS:O	1:I:21:ASN:HA	2.05	0.55
2:L:18:VAL:HA	2:L:18:VAL:C	2.15	0.55
2:D:2:VAL:HG12	1:G:8:THR:O	2.07	0.55
1:I:3:VAL:N	1:I:4:GLU:N	2.54	0.55
1:C:14:TYR:CA	1:C:14:TYR:CD1	2.88	0.55
1:I:14:TYR:C	1:I:14:TYR:CD1	2.79	0.55
1:C:2:ILE:HD12	1:C:19:TYR:HB2	1.87	0.55
2:L:19:CYS:N	2:L:20:GLY:H	2.03	0.55
1:E:19:TYR:HA	1:E:19:TYR:N	2.06	0.55
2:F:7:CYS:O	2:F:11:LEU:N	2.40	0.55
1:E:20:CYS:CA	1:E:20:CYS:HB3	2.18	0.55
1:E:2:ILE:O	1:E:2:ILE:CG1	2.54	0.55
2:D:3:ASN:ND2	2:D:4:GLN:N	2.55	0.55
2:L:11:LEU:O	2:L:12:VAL:C	2.42	0.55
2:B:22:ARG:O	2:B:22:ARG:CA	2.40	0.55
2:D:19:CYS:CB	2:D:19:CYS:C	2.67	0.55
2:B:1:PHE:O	2:B:2:VAL:C	2.45	0.55
2:J:28:LYS:CG	2:L:20:GLY:O	2.55	0.55
1:G:9:SER:CB	1:G:10:ILE:H	2.19	0.55
2:D:24:PHE:CD2	2:D:24:PHE:N	2.69	0.55
1:C:2:ILE:N	1:C:3:VAL:H	2.05	0.55
1:K:17:GLU:O	1:K:18:ASN:CA	2.54	0.54
1:A:21:ASN:HD22	2:B:22:ARG:HE	1.50	0.54
2:F:2:VAL:CG2	2:F:2:VAL:HA	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:4:GLN:N	2:L:5:HIS:N	2.54	0.54
1:E:3:VAL:O	1:E:7:CYS:HB2	2.08	0.54
2:J:26:MEA:HA	2:J:26:MEA:CB	2.24	0.54
1:K:6:CYS:HB2	2:L:11:LEU:HD11	1.88	0.54
1:K:7:CYS:HA	2:L:7:CYS:SG	2.47	0.54
2:B:25:TYR:CG	2:B:25:TYR:N	2.75	0.54
1:E:10:ILE:CD1	1:E:10:ILE:CG2	2.85	0.54
2:D:15:LEU:CB	2:D:15:LEU:N	2.59	0.54
1:I:18:ASN:N	1:I:18:ASN:CB	2.61	0.54
1:I:2:ILE:HA	1:I:5:GLN:HB3	1.89	0.54
1:A:10:ILE:CA	1:A:11:CYS:N	2.65	0.54
2:D:19:CYS:O	2:D:22:ARG:CG	2.51	0.54
6:H:2001:HOH:O	1:K:10:ILE:HG13	2.08	0.54
2:F:21:GLU:OE1	2:F:21:GLU:N	2.41	0.54
1:E:20:CYS:HB2	1:E:20:CYS:CA	2.18	0.54
2:B:12:VAL:CB	2:B:12:VAL:N	2.64	0.54
1:G:9:SER:HB2	1:G:10:ILE:H	1.71	0.53
2:H:12:VAL:HG23	2:H:12:VAL:CA	2.35	0.53
1:E:10:ILE:CG1	2:J:2:VAL:HA	2.39	0.53
2:B:8:GLY:O	2:B:9:SER:C	2.47	0.53
1:G:10:ILE:CG1	1:G:10:ILE:N	2.72	0.53
2:B:5:HIS:HB2	1:I:10:ILE:HD11	1.91	0.53
2:J:24:PHE:HB3	2:J:24:PHE:CG	2.21	0.53
1:C:7:CYS:SG	2:D:11:LEU:CD1	2.96	0.53
1:G:9:SER:CB	1:G:9:SER:HA	2.22	0.53
1:G:2:ILE:CG2	1:G:2:ILE:HD13	2.39	0.53
1:G:6:CYS:O	3:G:1022:IPH:O1	2.27	0.53
2:F:5:HIS:HD2	6:H:2007:HOH:O	1.90	0.53
1:A:12:SER:OG	1:A:15:GLN:HG3	2.08	0.53
2:B:19:CYS:HB3	2:B:23:GLY:O	2.09	0.53
2:B:2:VAL:C	2:B:3:ASN:CA	2.71	0.53
2:L:25:TYR:C	2:L:26:MEA:HD1	2.30	0.53
1:I:16:LEU:CD2	1:I:16:LEU:CD1	2.79	0.52
1:E:18:ASN:C	1:E:19:TYR:CA	2.64	0.52
1:C:2:ILE:CG2	1:C:3:VAL:N	2.72	0.52
2:D:12:VAL:CG2	2:D:12:VAL:CA	2.78	0.52
2:B:10:HIS:C	2:B:10:HIS:HA	2.15	0.52
2:H:24:PHE:CE2	2:H:26:MEA:HB2	2.40	0.52
1:I:10:ILE:CA	1:I:10:ILE:CG2	2.78	0.52
1:G:8:THR:CB	1:G:8:THR:HG1	2.13	0.52
1:C:2:ILE:HD12	1:C:19:TYR:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:SER:C	1:E:14:TYR:N	2.61	0.52
1:C:2:ILE:HD13	2:D:15:LEU:HD11	1.90	0.52
2:D:16:TYR:HA	6:D:2007:HOH:O	2.09	0.52
1:A:2:ILE:CA	1:A:2:ILE:O	2.48	0.52
1:C:21:ASN:HA	6:C:2017:HOH:O	2.09	0.52
1:C:2:ILE:C	1:C:2:ILE:CG2	2.77	0.52
1:A:21:ASN:HD22	2:B:22:ARG:NE	2.07	0.51
2:L:12:VAL:CA	2:L:12:VAL:CG2	2.76	0.51
1:I:21:ASN:CG	1:I:21:ASN:N	2.64	0.51
1:A:20:CYS:SG	2:B:19:CYS:CA	2.98	0.51
1:E:1:GLY:H2	1:E:4:GLU:CG	2.24	0.51
2:D:13:GLU:HG3	2:D:13:GLU:C	2.31	0.51
2:J:18:VAL:O	2:J:19:CYS:CA	2.57	0.51
2:D:3:ASN:HD22	2:D:4:GLN:N	2.08	0.51
2:H:17:LEU:HA	2:H:17:LEU:C	2.18	0.51
1:A:21:ASN:CB	2:B:22:ARG:HB3	2.38	0.51
1:E:10:ILE:HG12	2:J:2:VAL:HA	1.92	0.51
2:D:3:ASN:HD22	2:D:4:GLN:H	1.58	0.51
1:C:19:TYR:N	1:C:20:CYS:H	2.08	0.51
1:I:6:CYS:C	1:I:6:CYS:CB	2.70	0.51
2:B:15:LEU:CB	2:B:15:LEU:CD2	2.82	0.51
2:L:15:LEU:N	2:L:16:TYR:N	2.59	0.51
1:E:7:CYS:SG	2:F:11:LEU:HD11	2.51	0.51
1:K:1:GLY:O	1:K:2:ILE:CA	2.59	0.50
2:J:28:LYS:HG3	2:L:20:GLY:O	2.11	0.50
2:J:25:TYR:CG	2:J:25:TYR:CA	2.83	0.50
1:E:2:ILE:HG23	1:E:3:VAL:N	2.27	0.50
2:F:2:VAL:O	2:F:6:LEU:N	2.41	0.50
2:D:18:VAL:O	2:D:18:VAL:CG1	2.59	0.50
2:B:11:LEU:O	2:B:14:ALA:N	2.45	0.50
2:D:21:GLU:HB3	6:D:2010:HOH:O	2.11	0.50
2:J:21:GLU:O	2:J:22:ARG:CA	2.59	0.50
6:D:2009:HOH:O	1:I:13:LEU:HG	2.11	0.50
2:D:19:CYS:HA	2:D:19:CYS:CB	2.22	0.50
2:D:13:GLU:CG	2:D:13:GLU:CA	2.73	0.50
2:F:10:HIS:N	2:F:11:LEU:H	2.10	0.50
2:L:13:GLU:C	2:L:13:GLU:CB	2.71	0.50
2:B:21:GLU:CG	2:B:21:GLU:CA	2.81	0.50
1:G:2:ILE:CD1	1:G:2:ILE:CG2	2.89	0.50
1:G:6:CYS:C	1:G:6:CYS:CB	2.72	0.50
1:E:6:CYS:HA	1:E:11:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:ILE:HG23	1:K:2:ILE:C	2.33	0.49
2:D:19:CYS:SG	2:D:19:CYS:CA	2.97	0.49
1:I:10:ILE:HA	3:I:1022:IPH:O1	2.12	0.49
2:H:12:VAL:HG22	2:H:12:VAL:CA	2.35	0.49
1:C:7:CYS:SG	2:D:11:LEU:HD12	2.53	0.49
1:E:2:ILE:CB	1:E:19:TYR:CE2	2.95	0.49
2:J:12:VAL:HG12	2:L:12:VAL:CG1	2.31	0.49
2:J:7:CYS:C	2:J:9:SER:N	2.65	0.49
2:B:11:LEU:CB	2:B:11:LEU:CD2	2.84	0.49
1:E:11:CYS:CB	1:E:11:CYS:HA	2.21	0.49
2:B:4:GLN:N	2:B:4:GLN:C	2.55	0.49
2:L:25:TYR:O	2:L:26:MEA:HB2	2.13	0.49
2:J:15:LEU:HD13	2:J:24:PHE:CD2	2.48	0.49
1:C:1:GLY:C	1:C:1:GLY:N	2.58	0.49
2:J:26:MEA:HC3	2:L:24:PHE:H	1.77	0.49
1:C:15:GLN:HG3	1:C:15:GLN:N	2.27	0.49
2:F:15:LEU:O	2:F:19:CYS:HB2	2.12	0.49
2:H:19:CYS:HB3	2:H:23:GLY:O	2.13	0.49
1:K:20:CYS:HA	2:L:23:GLY:O	2.12	0.49
2:D:10:HIS:C	2:D:10:HIS:N	2.56	0.49
1:A:5:GLN:N	1:A:6:CYS:H	2.09	0.49
1:C:11:CYS:HA	1:C:15:GLN:HE21	1.78	0.49
1:E:16:LEU:N	1:E:17:GLU:H	2.10	0.49
1:E:2:ILE:CD1	1:E:19:TYR:CD1	2.91	0.49
1:A:7:CYS:N	1:A:8:THR:N	2.59	0.49
1:I:2:ILE:HG13	1:I:6:CYS:SG	2.53	0.48
2:J:7:CYS:O	2:J:8:GLY:C	2.50	0.48
2:B:15:LEU:CD2	2:B:15:LEU:CA	2.90	0.48
1:E:1:GLY:H2	1:E:4:GLU:HG3	1.78	0.48
1:A:9:SER:HB2	1:A:10:ILE:N	2.28	0.48
2:B:15:LEU:O	2:B:16:TYR:C	2.50	0.48
2:H:5:HIS:C	2:H:6:LEU:C	2.70	0.48
2:D:10:HIS:N	2:D:10:HIS:HA	2.07	0.48
2:F:20:GLY:HA2	6:F:2011:HOH:O	2.12	0.48
2:L:25:TYR:HA	2:L:26:MEA:HC1	1.66	0.48
1:K:6:CYS:C	1:K:7:CYS:HA	2.30	0.48
1:E:5:GLN:O	1:E:6:CYS:HA	2.13	0.48
1:K:2:ILE:O	1:K:3:VAL:CA	2.62	0.48
1:K:3:VAL:N	1:K:4:GLU:N	2.61	0.48
1:C:2:ILE:CD1	2:D:15:LEU:HD11	2.44	0.48
2:D:10:HIS:N	2:D:11:LEU:N	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2:ILE:N	1:K:2:ILE:HA	2.04	0.48
2:L:15:LEU:HA	2:L:15:LEU:N	2.10	0.48
2:B:6:LEU:HD22	2:J:10:HIS:CB	2.44	0.48
2:J:19:CYS:N	2:J:20:GLY:H	2.10	0.48
2:B:7:CYS:N	2:B:7:CYS:HA	2.12	0.48
2:B:15:LEU:HA	2:B:15:LEU:CD2	2.44	0.48
1:C:2:ILE:HB	1:C:2:ILE:CG2	2.19	0.48
1:C:4:GLU:C	1:C:4:GLU:HA	2.17	0.48
1:K:5:GLN:OE1	1:K:19:TYR:CZ	2.66	0.47
2:L:1:PHE:CG	2:L:1:PHE:HB2	2.24	0.47
1:I:4:GLU:OE2	2:J:29:PRO:CB	2.62	0.47
1:I:8:THR:CG2	1:I:8:THR:N	2.78	0.47
2:B:2:VAL:CB	2:B:2:VAL:HA	2.18	0.47
2:J:25:TYR:HE2	1:K:21:ASN:OD1	1.96	0.47
2:J:4:GLN:C	2:J:4:GLN:CB	2.67	0.47
2:D:15:LEU:O	2:D:19:CYS:CB	2.62	0.47
1:E:12:SER:OG	1:E:14:TYR:HB3	2.13	0.47
2:L:18:VAL:O	2:L:18:VAL:HG22	2.10	0.47
2:J:25:TYR:HE1	2:J:27:THR:HG1	1.60	0.47
2:J:20:GLY:HA3	6:J:2012:HOH:O	2.14	0.47
2:B:18:VAL:HG22	1:G:13:LEU:CD2	2.45	0.47
1:C:3:VAL:CB	1:C:3:VAL:HA	2.22	0.47
1:K:14:TYR:CD1	1:K:14:TYR:O	2.67	0.47
1:E:6:CYS:H	1:E:7:CYS:H	1.61	0.47
1:A:17:GLU:CB	1:A:18:ASN:N	2.75	0.47
1:K:20:CYS:O	1:K:21:ASN:CA	2.62	0.47
2:D:24:PHE:C	2:D:24:PHE:CD1	2.87	0.47
2:B:17:LEU:HD11	3:G:1022:IPH:H3	1.96	0.47
1:C:12:SER:H	1:C:15:GLN:NE2	2.13	0.47
1:E:10:ILE:HA	1:E:10:ILE:CD1	2.45	0.47
2:B:21:GLU:CB	2:B:22:ARG:N	2.78	0.47
2:L:17:LEU:HB3	2:L:17:LEU:CG	2.19	0.47
1:E:4:GLU:HA	2:F:4:GLN:HE22	1.79	0.47
2:D:13:GLU:CB	6:D:2006:HOH:O	2.63	0.47
1:K:5:GLN:O	1:K:6:CYS:HA	2.14	0.47
1:E:2:ILE:N	1:E:3:VAL:H	2.12	0.47
2:H:11:LEU:CB	2:H:11:LEU:CD2	2.80	0.47
1:K:15:GLN:O	1:K:16:LEU:C	2.54	0.47
3:K:1022:IPH:H4	2:L:10:HIS:HB3	1.97	0.47
1:A:7:CYS:N	1:A:7:CYS:HA	2.06	0.47
2:J:11:LEU:CD2	2:J:11:LEU:CA	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:CYS:O	3:A:1022:IPH:O1	2.33	0.46
1:G:17:GLU:O	1:G:18:ASN:C	2.53	0.46
1:C:10:ILE:CG2	2:L:1:PHE:CB	2.93	0.46
2:J:24:PHE:CD2	2:J:24:PHE:CB	2.76	0.46
1:K:6:CYS:HB2	2:L:11:LEU:CD1	2.45	0.46
1:A:20:CYS:SG	2:B:18:VAL:HG12	2.55	0.46
2:B:17:LEU:CB	2:B:17:LEU:C	2.73	0.46
2:B:18:VAL:HB	2:B:18:VAL:N	2.28	0.46
1:C:12:SER:C	1:C:14:TYR:N	2.63	0.46
2:B:9:SER:O	2:B:13:GLU:HG3	2.14	0.46
2:J:15:LEU:HB2	2:J:24:PHE:CZ	2.50	0.46
2:B:15:LEU:HA	2:B:15:LEU:HD23	1.96	0.46
2:B:21:GLU:HB2	2:B:21:GLU:C	2.31	0.46
1:G:2:ILE:O	1:G:6:CYS:HB2	2.16	0.46
2:H:6:LEU:O	2:H:10:HIS:CD2	2.69	0.46
1:K:4:GLU:CB	1:K:4:GLU:H	2.24	0.46
1:I:14:TYR:O	1:I:14:TYR:CG	2.69	0.46
1:G:21:ASN:HB2	2:H:22:ARG:O	2.16	0.46
1:E:16:LEU:O	1:E:17:GLU:C	2.54	0.46
1:E:2:ILE:CG2	1:E:3:VAL:N	2.79	0.46
2:H:12:VAL:O	2:H:13:GLU:C	2.54	0.46
1:G:13:LEU:O	1:G:17:GLU:N	2.48	0.46
2:J:24:PHE:CG	2:J:24:PHE:HB2	2.21	0.46
1:K:18:ASN:N	1:K:18:ASN:CG	2.69	0.46
2:B:16:TYR:OH	2:D:5:HIS:HA	2.16	0.46
2:H:18:VAL:C	2:H:18:VAL:CG1	2.83	0.46
2:J:26:MEA:HC2	2:J:26:MEA:CB	2.46	0.46
1:I:14:TYR:CZ	6:I:2012:HOH:O	2.66	0.46
1:A:2:ILE:HG12	2:B:11:LEU:HD22	1.98	0.46
2:B:9:SER:HB2	2:D:16:TYR:CE1	2.51	0.46
1:I:7:CYS:HA	2:J:7:CYS:SG	2.56	0.45
2:F:26:MEA:HZ	2:H:16:TYR:HE1	1.80	0.45
1:C:13:LEU:H	1:C:13:LEU:CB	2.26	0.45
1:C:15:GLN:O	1:C:18:ASN:CB	2.63	0.45
1:I:14:TYR:N	1:I:14:TYR:HA	2.12	0.45
2:D:13:GLU:HG3	2:D:13:GLU:O	2.16	0.45
2:L:3:ASN:O	2:L:3:ASN:CA	2.49	0.45
1:K:2:ILE:N	1:K:2:ILE:HG22	2.32	0.45
1:A:9:SER:CB	1:A:9:SER:HA	2.20	0.45
2:B:14:ALA:O	2:B:17:LEU:HB3	2.15	0.45
2:D:5:HIS:O	2:D:6:LEU:CA	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASN:O	1:C:19:TYR:HA	2.17	0.45
2:F:2:VAL:CA	6:F:2001:HOH:O	2.54	0.45
1:E:8:THR:CA	1:E:9:SER:N	2.59	0.45
1:I:8:THR:CA	1:I:8:THR:CG2	2.83	0.45
2:L:17:LEU:HB2	2:L:17:LEU:CG	2.19	0.45
2:J:2:VAL:HA	2:J:2:VAL:CB	2.23	0.45
1:E:2:ILE:O	1:E:3:VAL:C	2.54	0.45
1:E:2:ILE:C	1:E:4:GLU:N	2.62	0.45
2:H:12:VAL:CG1	2:H:12:VAL:CA	2.77	0.45
2:J:27:THR:CB	2:J:27:THR:N	2.71	0.45
2:J:18:VAL:O	2:J:18:VAL:CG1	2.64	0.45
1:I:2:ILE:O	1:I:3:VAL:CA	2.64	0.45
1:C:7:CYS:CB	1:C:7:CYS:N	2.60	0.45
2:D:22:ARG:HH11	2:D:22:ARG:CG	2.28	0.45
1:A:2:ILE:CG2	1:A:2:ILE:N	2.78	0.45
2:J:22:ARG:HB2	2:J:22:ARG:N	2.32	0.45
1:K:7:CYS:N	6:K:2004:HOH:O	2.49	0.44
2:H:16:TYR:CA	2:H:24:PHE:CE1	3.00	0.44
2:J:16:TYR:HB2	2:L:12:VAL:HG11	1.98	0.44
2:L:10:HIS:O	2:L:13:GLU:HB3	2.17	0.44
2:D:15:LEU:CG	2:D:15:LEU:CA	2.83	0.44
2:D:20:GLY:O	2:D:21:GLU:C	2.55	0.44
1:K:16:LEU:CA	1:K:17:GLU:N	2.67	0.44
1:A:2:ILE:C	1:A:2:ILE:CG1	2.86	0.44
1:A:19:TYR:HB2	2:B:15:LEU:HD22	1.99	0.44
2:J:25:TYR:HE2	1:K:21:ASN:CG	2.21	0.44
1:A:2:ILE:HB	1:A:2:ILE:CG2	2.22	0.44
2:L:22:ARG:HB2	2:L:22:ARG:NE	2.32	0.44
1:K:10:ILE:CG2	1:K:10:ILE:CG1	2.82	0.44
1:K:5:GLN:HG2	1:K:6:CYS:SG	2.57	0.44
2:B:16:TYR:CB	2:B:16:TYR:HA	2.22	0.44
2:J:18:VAL:CA	2:J:19:CYS:N	2.60	0.44
2:B:23:GLY:N	2:B:23:GLY:O	2.50	0.44
1:I:3:VAL:CG1	1:I:3:VAL:O	2.65	0.43
2:J:11:LEU:HD23	2:J:11:LEU:CA	2.48	0.43
1:A:10:ILE:O	1:A:10:ILE:HG22	2.18	0.43
1:C:15:GLN:HA	1:C:15:GLN:C	2.14	0.43
1:G:6:CYS:SG	1:G:6:CYS:N	2.91	0.43
1:K:2:ILE:CG2	1:K:2:ILE:C	2.86	0.43
1:A:12:SER:CB	1:A:13:LEU:N	2.80	0.43
2:L:21:GLU:OE1	2:L:21:GLU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:GLN:CG	1:C:15:GLN:N	2.81	0.43
1:K:6:CYS:HB3	2:L:11:LEU:HD21	2.00	0.43
1:E:17:GLU:O	1:E:18:ASN:CA	2.66	0.43
1:E:2:ILE:HG22	1:E:2:ILE:H	1.84	0.43
2:L:24:PHE:N	2:L:24:PHE:CB	2.68	0.43
1:A:2:ILE:O	1:A:6:CYS:HB2	2.19	0.43
1:A:3:VAL:HG22	2:B:26:MEA:HZ	2.01	0.43
2:B:26:MEA:C1	2:D:24:PHE:O	2.66	0.43
1:K:12:SER:CB	1:K:12:SER:HG	2.17	0.43
1:C:2:ILE:CA	1:C:2:ILE:CG1	2.86	0.43
1:E:2:ILE:O	1:E:2:ILE:HG12	2.19	0.43
2:L:2:VAL:O	2:L:3:ASN:C	2.56	0.43
2:J:11:LEU:CB	2:J:12:VAL:N	2.80	0.43
1:K:21:ASN:N	1:K:21:ASN:CG	2.72	0.43
1:E:1:GLY:O	1:E:2:ILE:CA	2.67	0.43
1:I:16:LEU:HD13	2:J:14:ALA:HB1	2.01	0.43
1:K:5:GLN:OE1	1:K:19:TYR:CE2	2.72	0.43
1:E:18:ASN:O	1:E:19:TYR:CA	2.63	0.43
1:I:5:GLN:O	1:I:6:CYS:CA	2.67	0.42
1:E:1:GLY:N	1:E:4:GLU:HG3	2.33	0.42
1:K:8:THR:CA	1:K:8:THR:OG1	2.56	0.42
1:K:18:ASN:N	1:K:19:TYR:N	2.67	0.42
1:C:11:CYS:HA	1:C:15:GLN:NE2	2.34	0.42
1:E:16:LEU:HD23	1:E:16:LEU:HA	1.55	0.42
1:K:2:ILE:HA	1:K:5:GLN:HB3	2.01	0.42
1:G:13:LEU:CD2	1:G:13:LEU:HB3	2.47	0.42
2:H:2:VAL:HG21	2:H:2:VAL:HG11	1.97	0.42
1:I:5:GLN:HE21	1:I:5:GLN:HB2	1.77	0.42
1:K:5:GLN:HA	1:K:5:GLN:C	2.17	0.42
2:L:9:SER:O	2:L:10:HIS:C	2.56	0.42
2:F:26:MEA:HE2	2:H:16:TYR:CD1	2.55	0.42
1:I:17:GLU:O	1:I:18:ASN:CA	2.67	0.42
1:K:13:LEU:O	1:K:14:TYR:C	2.56	0.42
2:J:5:HIS:C	2:J:5:HIS:CD2	2.91	0.42
1:A:2:ILE:N	1:A:4:GLU:OE1	2.53	0.42
1:G:2:ILE:N	6:G:2002:HOH:O	2.52	0.42
2:F:26:MEA:HE2	2:H:16:TYR:HD1	1.84	0.42
2:F:15:LEU:O	2:F:19:CYS:CB	2.67	0.42
2:F:9:SER:O	2:F:13:GLU:HG3	2.20	0.42
1:A:21:ASN:HD21	2:B:22:ARG:HE	1.63	0.42
2:B:4:GLN:C	2:B:4:GLN:CG	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:12:SER:C	1:I:12:SER:OG	2.57	0.41
1:K:17:GLU:O	1:K:20:CYS:CB	2.68	0.41
2:D:6:LEU:H	2:D:6:LEU:HG	1.83	0.41
6:B:2015:HOH:O	1:G:12:SER:HA	2.19	0.41
2:B:21:GLU:CB	2:B:21:GLU:N	2.68	0.41
2:B:4:GLN:CG	2:B:4:GLN:O	2.68	0.41
2:F:10:HIS:ND1	6:F:2006:HOH:O	2.35	0.41
2:H:6:LEU:O	2:H:10:HIS:HD2	2.02	0.41
2:J:8:GLY:CA	2:L:16:TYR:CZ	2.98	0.41
1:G:2:ILE:HB	1:G:2:ILE:CG2	2.27	0.41
1:E:10:ILE:HG22	1:E:11:CYS:O	2.20	0.41
2:D:13:GLU:HA	2:D:16:TYR:HB3	2.02	0.41
2:H:9:SER:O	2:H:13:GLU:HG3	2.20	0.41
1:I:1:GLY:O	1:I:5:GLN:HB2	2.20	0.41
6:B:2015:HOH:O	1:G:12:SER:CA	2.69	0.41
1:G:21:ASN:HB3	6:G:2017:HOH:O	2.20	0.41
2:J:15:LEU:CD1	2:J:24:PHE:CD2	3.03	0.41
1:E:1:GLY:O	1:E:2:ILE:HA	2.21	0.41
1:K:2:ILE:CG2	1:K:2:ILE:N	2.83	0.41
2:L:21:GLU:H	2:L:21:GLU:CG	2.33	0.41
1:K:18:ASN:HD22	1:K:18:ASN:HA	1.24	0.41
1:I:8:THR:CG2	6:I:2011:HOH:O	2.36	0.41
1:E:2:ILE:CG2	1:E:2:ILE:N	2.84	0.41
2:F:2:VAL:HA	2:F:5:HIS:HB3	2.01	0.41
1:G:5:GLN:NE2	1:G:19:TYR:OH	2.53	0.41
2:H:2:VAL:HG23	1:K:10:ILE:N	2.36	0.41
2:B:6:LEU:H	2:B:6:LEU:HG	1.85	0.41
2:J:22:ARG:C	2:J:22:ARG:N	2.63	0.41
2:F:21:GLU:HB2	2:F:21:GLU:N	2.32	0.41
1:I:2:ILE:HG23	1:I:3:VAL:N	2.33	0.40
1:A:2:ILE:HG23	1:A:3:VAL:N	2.36	0.40
2:H:1:PHE:HB3	2:H:3:ASN:OD1	2.21	0.40
2:L:11:LEU:HD23	2:L:11:LEU:HA	1.39	0.40
2:F:15:LEU:HD13	2:F:24:PHE:HB2	2.02	0.40
1:I:4:GLU:CB	1:I:4:GLU:C	2.76	0.40
1:C:15:GLN:O	1:C:18:ASN:N	2.54	0.40
2:D:2:VAL:CG1	1:G:8:THR:O	2.69	0.40
1:A:15:GLN:O	1:A:18:ASN:HB3	2.22	0.40
1:I:13:LEU:HD22	2:J:18:VAL:CG2	2.51	0.40
1:C:10:ILE:HG13	1:C:11:CYS:C	2.41	0.40

There are no symmetry-related clashes.

## 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	18/21 (86%)	17 (94%)	1 (6%)	0	100	100
1	C	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	E	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	G	18/21 (86%)	17 (94%)	1 (6%)	0	100	100
1	I	19/21 (90%)	19 (100%)	0	0	100	100
1	K	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
2	B	24/30 (80%)	24 (100%)	0	0	100	100
2	D	23/30 (77%)	22 (96%)	1 (4%)	0	100	100
2	F	23/30 (77%)	22 (96%)	1 (4%)	0	100	100
2	H	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
2	J	26/30 (87%)	24 (92%)	2 (8%)	0	100	100
2	L	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
All	All	257/306 (84%)	244 (95%)	13 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	20/20 (100%)	18 (90%)	2 (10%)	9	4
1	C	20/20 (100%)	19 (95%)	1 (5%)	30	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	20/20 (100%)	16 (80%)	4 (20%)	1	0
1	G	20/20 (100%)	17 (85%)	3 (15%)	3	1
1	I	20/20 (100%)	19 (95%)	1 (5%)	30	22
1	K	20/20 (100%)	19 (95%)	1 (5%)	30	22
2	B	22/25 (88%)	20 (91%)	2 (9%)	12	6
2	D	19/25 (76%)	15 (79%)	4 (21%)	1	0
2	F	19/25 (76%)	18 (95%)	1 (5%)	28	20
2	H	22/25 (88%)	20 (91%)	2 (9%)	12	6
2	J	24/25 (96%)	22 (92%)	2 (8%)	14	7
2	L	21/25 (84%)	18 (86%)	3 (14%)	4	1
All	All	247/270 (92%)	221 (90%)	26 (10%)	8	4

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	21	ASN
2	B	17	LEU
2	B	21	GLU
1	C	10	ILE
2	D	3	ASN
2	D	4	GLN
2	D	21	GLU
2	D	22	ARG
1	E	4	GLU
1	E	5	GLN
1	E	8	THR
1	E	9	SER
2	F	3	ASN
1	G	3	VAL
1	G	4	GLU
1	G	13	LEU
2	H	17	LEU
2	H	27	THR
1	I	5	GLN
2	J	4	GLN
2	J	22	ARG
1	K	17	GLU

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Mol	Chain	Res	Type
2	L	12	VAL
2	L	17	LEU
2	L	21	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	21	ASN
2	B	10	HIS
1	C	5	GLN
1	C	15	GLN
2	D	3	ASN
2	D	4	GLN
1	E	5	GLN
1	E	21	ASN
2	F	3	ASN
2	F	4	GLN
1	G	5	GLN
1	I	5	GLN
1	I	21	ASN
1	K	18	ASN
1	K	21	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MEA	B	26	2	10,12,13	6.33	6 (60%)	10,14,16	3.84	7 (70%)
2	MEA	D	26	2	10,12,13	9.90	7 (70%)	10,14,16	8.88	10 (100%)
2	MEA	F	26	2	10,12,13	9.23	7 (70%)	10,14,16	7.87	8 (80%)
2	MEA	H	26	2	10,12,13	6.13	6 (60%)	10,14,16	2.94	8 (80%)
2	MEA	J	26	2	10,12,13	25.75	6 (60%)	10,14,16	41.74	10 (100%)
2	MEA	L	26	2	10,12,13	4.99	9 (90%)	10,14,16	5.33	8 (80%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEA	B	26	2	-	0/4/8/10	0/1/1/1
2	MEA	D	26	2	-	0/4/8/10	0/1/1/1
2	MEA	F	26	2	-	0/4/8/10	0/1/1/1
2	MEA	H	26	2	-	0/4/8/10	0/1/1/1
2	MEA	J	26	2	-	0/4/8/10	1/1/1/1
2	MEA	L	26	2	-	0/4/8/10	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	26	MEA	CA-N	-16.73	1.16	1.47
2	D	26	MEA	CA-N	-15.90	1.18	1.47
2	F	26	MEA	CB-CG	-9.06	1.29	1.51
2	F	26	MEA	CE2-CD2	-8.61	1.21	1.38
2	D	26	MEA	CE1-CD1	-8.51	1.21	1.38
2	D	26	MEA	CB-CG	-8.18	1.31	1.51
2	D	26	MEA	CE2-CD2	-8.17	1.22	1.38
2	F	26	MEA	CE1-CD1	-8.10	1.22	1.38
2	L	26	MEA	C1-N	-8.08	1.24	1.46
2	J	26	MEA	C1-N	-8.07	1.24	1.46
2	L	26	MEA	CD2-CG	-5.08	1.28	1.38
2	L	26	MEA	CZ-CE1	-3.78	1.28	1.38
2	J	26	MEA	O-C	-2.27	1.09	1.19
2	L	26	MEA	O-C	-2.18	1.09	1.19
2	B	26	MEA	CZ-CE1	3.63	1.47	1.38
2	B	26	MEA	CD2-CG	4.65	1.48	1.38
2	L	26	MEA	CB-CG	4.87	1.63	1.51
2	L	26	MEA	CE2-CD2	4.93	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	26	MEA	CE1-CD1	4.94	1.49	1.38
2	L	26	MEA	CE2-CZ	5.38	1.51	1.38
2	F	26	MEA	C1-N	5.67	1.62	1.46
2	L	26	MEA	CD1-CG	6.06	1.51	1.38
2	H	26	MEA	C1-N	6.64	1.65	1.46
2	B	26	MEA	O-C	6.70	1.50	1.19
2	H	26	MEA	CZ-CE1	7.07	1.56	1.38
2	H	26	MEA	O-C	7.14	1.52	1.19
2	B	26	MEA	CA-N	7.39	1.60	1.47
2	H	26	MEA	CE2-CZ	7.67	1.57	1.38
2	H	26	MEA	CD2-CG	8.26	1.56	1.38
2	D	26	MEA	C1-N	9.85	1.74	1.46
2	H	26	MEA	CD1-CG	10.11	1.60	1.38
2	B	26	MEA	CE2-CZ	10.32	1.64	1.38
2	F	26	MEA	CE2-CZ	12.23	1.69	1.38
2	B	26	MEA	CD1-CG	12.23	1.64	1.38
2	F	26	MEA	CD1-CG	12.85	1.66	1.38
2	D	26	MEA	CE2-CZ	13.56	1.72	1.38
2	D	26	MEA	CD1-CG	15.48	1.71	1.38
2	J	26	MEA	CE2-CZ	28.90	2.12	1.38
2	J	26	MEA	CD1-CG	35.65	2.14	1.38
2	J	26	MEA	CZ-CE1	42.16	2.46	1.38
2	J	26	MEA	CD2-CG	51.64	2.48	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	26	MEA	CZ-CE1-CD1	-63.73	26.90	120.19
2	J	26	MEA	CZ-CE2-CD2	-60.21	32.04	120.19
2	J	26	MEA	CE2-CD2-CG	-59.28	26.44	120.65
2	J	26	MEA	CE1-CD1-CG	-56.06	31.55	120.65
2	J	26	MEA	CD2-CG-CD1	-37.48	58.13	118.13
2	J	26	MEA	CE2-CZ-CE1	-34.87	58.73	119.93
2	D	26	MEA	CZ-CE1-CD1	-15.20	97.94	120.19
2	F	26	MEA	CZ-CE1-CD1	-13.76	100.04	120.19
2	D	26	MEA	CE2-CD2-CG	-13.74	98.82	120.65
2	F	26	MEA	CE2-CD2-CG	-12.17	101.30	120.65
2	L	26	MEA	CG-CB-CA	-10.65	95.91	114.26
2	D	26	MEA	CB-CG-CD2	-10.45	99.04	120.90
2	F	26	MEA	CB-CG-CD2	-9.72	100.56	120.90
2	L	26	MEA	O-C-CA	-6.70	107.74	125.44
2	B	26	MEA	CZ-CE1-CD1	-6.06	111.31	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	MEA	CE2-CD2-CG	-5.37	112.12	120.65
2	D	26	MEA	CG-CB-CA	-5.02	105.61	114.26
2	B	26	MEA	CB-CG-CD2	-4.18	112.16	120.90
2	L	26	MEA	CZ-CE1-CD1	-4.12	114.15	120.19
2	J	26	MEA	O-C-CA	-3.51	116.16	125.44
2	L	26	MEA	CE2-CD2-CG	-3.50	115.08	120.65
2	D	26	MEA	O-C-CA	-3.44	116.36	125.44
2	H	26	MEA	CE2-CD2-CG	-3.04	115.82	120.65
2	L	26	MEA	CB-CG-CD2	-2.89	114.85	120.90
2	H	26	MEA	CZ-CE1-CD1	-2.69	116.25	120.19
2	H	26	MEA	CB-CG-CD2	-2.49	115.69	120.90
2	H	26	MEA	CZ-CE2-CD2	-2.30	116.82	120.19
2	H	26	MEA	CE1-CD1-CG	-2.27	117.04	120.65
2	H	26	MEA	O-C-CA	2.04	130.82	125.44
2	F	26	MEA	CB-CG-CD1	2.22	125.55	120.90
2	D	26	MEA	CB-CG-CD1	2.57	126.28	120.90
2	B	26	MEA	CG-CB-CA	2.97	119.37	114.26
2	F	26	MEA	CZ-CE2-CD2	2.99	124.56	120.19
2	F	26	MEA	CE1-CD1-CG	3.49	126.19	120.65
2	B	26	MEA	CE2-CZ-CE1	3.51	126.09	119.93
2	D	26	MEA	CZ-CE2-CD2	3.85	125.82	120.19
2	L	26	MEA	CB-CG-CD1	3.96	129.19	120.90
2	B	26	MEA	CD2-CG-CD1	4.14	124.76	118.13
2	D	26	MEA	CE1-CD1-CG	4.19	127.30	120.65
2	H	26	MEA	CE2-CZ-CE1	4.31	127.49	119.93
2	B	26	MEA	O-C-CA	4.51	137.34	125.44
2	H	26	MEA	CD2-CG-CD1	5.26	126.55	118.13
2	L	26	MEA	CE1-CD1-CG	5.68	129.67	120.65
2	J	26	MEA	CG-CB-CA	5.77	124.20	114.26
2	L	26	MEA	CZ-CE2-CD2	5.88	128.80	120.19
2	F	26	MEA	CE2-CZ-CE1	8.04	134.04	119.93
2	D	26	MEA	CE2-CZ-CE1	8.87	135.50	119.93
2	F	26	MEA	CD2-CG-CD1	9.83	133.86	118.13
2	D	26	MEA	CD2-CG-CD1	10.28	134.60	118.13
2	J	26	MEA	CB-CG-CD1	13.18	148.49	120.90
2	J	26	MEA	CB-CG-CD2	15.51	153.38	120.90

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	26	MEA	CD1-CD2-CE1-CE2-CG-CZ

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	26	MEA	3	0
2	D	26	MEA	4	0
2	F	26	MEA	7	0
2	H	26	MEA	2	0
2	J	26	MEA	5	0
2	L	26	MEA	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	IPH	A	1022	-	7,7,7	8.26	5 (71%)	8,8,8	7.51	8 (100%)
3	IPH	C	1022	-	7,7,7	4.58	4 (57%)	8,8,8	3.65	6 (75%)
3	IPH	E	1022	-	7,7,7	2.20	2 (28%)	8,8,8	2.53	6 (75%)
3	IPH	G	1022	-	7,7,7	7.72	7 (100%)	8,8,8	7.77	7 (87%)
3	IPH	I	1022	-	7,7,7	2.36	4 (57%)	8,8,8	3.00	5 (62%)
3	IPH	K	1022	-	7,7,7	6.59	5 (71%)	8,8,8	4.83	7 (87%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPH	A	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	C	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	E	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	G	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	I	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	K	1022	-	-	0/0/0/0	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1022	IPH	C3-C2	-9.77	1.18	1.38
3	K	1022	IPH	C5-C6	-9.49	1.19	1.38
3	K	1022	IPH	O1-C1	-7.66	1.18	1.37
3	G	1022	IPH	C2-C1	-6.44	1.25	1.38
3	K	1022	IPH	C6-C1	-5.64	1.27	1.38
3	K	1022	IPH	C4-C3	-5.20	1.24	1.38
3	G	1022	IPH	C5-C4	-5.15	1.24	1.38
3	E	1022	IPH	C2-C1	-4.96	1.28	1.38
3	I	1022	IPH	C6-C1	-3.48	1.31	1.38
3	E	1022	IPH	C5-C4	-2.70	1.31	1.38
3	I	1022	IPH	C4-C3	-2.54	1.31	1.38
3	A	1022	IPH	O1-C1	-2.47	1.31	1.37
3	A	1022	IPH	C5-C6	-2.12	1.34	1.38
3	A	1022	IPH	C3-C2	-2.05	1.34	1.38
3	I	1022	IPH	C2-C1	2.16	1.43	1.38
3	I	1022	IPH	C5-C4	2.73	1.45	1.38
3	G	1022	IPH	O1-C1	2.82	1.43	1.37
3	C	1022	IPH	C5-C4	2.93	1.45	1.38
3	C	1022	IPH	C2-C1	3.81	1.46	1.38
3	G	1022	IPH	C5-C6	5.38	1.50	1.38
3	G	1022	IPH	C3-C2	6.22	1.51	1.38
3	C	1022	IPH	C4-C3	7.10	1.56	1.38
3	C	1022	IPH	C6-C1	8.26	1.55	1.38
3	G	1022	IPH	C4-C3	10.62	1.65	1.38
3	G	1022	IPH	C6-C1	12.66	1.64	1.38
3	A	1022	IPH	C4-C3	13.30	1.72	1.38
3	A	1022	IPH	C6-C1	16.91	1.73	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1022	IPH	C4-C5-C6	-11.69	103.07	120.19
3	A	1022	IPH	C3-C2-C1	-11.27	102.45	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1022	IPH	C4-C5-C6	-11.14	103.88	120.19
3	G	1022	IPH	C3-C2-C1	-11.11	102.69	119.37
3	K	1022	IPH	C5-C6-C1	-7.99	107.37	119.37
3	K	1022	IPH	C4-C3-C2	-7.18	109.68	120.19
3	C	1022	IPH	C4-C5-C6	-6.80	110.23	120.19
3	A	1022	IPH	O1-C1-C2	-6.54	101.54	120.05
3	G	1022	IPH	O1-C1-C2	-5.48	104.53	120.05
3	I	1022	IPH	C5-C6-C1	-4.77	112.21	119.37
3	I	1022	IPH	C4-C3-C2	-4.24	113.98	120.19
3	C	1022	IPH	C3-C2-C1	-3.97	113.41	119.37
3	E	1022	IPH	C4-C5-C6	-3.62	114.88	120.19
3	K	1022	IPH	O1-C1-C6	-2.79	112.16	120.05
3	E	1022	IPH	O1-C1-C2	-2.50	112.96	120.05
3	C	1022	IPH	O1-C1-C2	-2.43	113.18	120.05
3	E	1022	IPH	C3-C2-C1	-2.08	116.24	119.37
3	G	1022	IPH	C6-C1-C2	2.41	123.23	119.79
3	I	1022	IPH	C6-C1-C2	2.44	123.28	119.79
3	E	1022	IPH	O1-C1-C6	2.52	127.18	120.05
3	A	1022	IPH	O1-C1-C6	2.69	127.66	120.05
3	E	1022	IPH	C4-C3-C2	2.86	124.38	120.19
3	K	1022	IPH	C3-C2-C1	2.87	123.69	119.37
3	C	1022	IPH	C5-C6-C1	2.89	123.72	119.37
3	I	1022	IPH	C3-C2-C1	3.00	123.89	119.37
3	C	1022	IPH	C6-C1-C2	3.16	124.29	119.79
3	K	1022	IPH	C4-C5-C6	3.24	124.93	120.19
3	I	1022	IPH	C4-C5-C6	3.53	125.35	120.19
3	E	1022	IPH	C5-C6-C1	3.57	124.73	119.37
3	K	1022	IPH	C5-C4-C3	3.74	126.49	119.93
3	G	1022	IPH	O1-C1-C6	4.28	132.16	120.05
3	C	1022	IPH	C5-C4-C3	4.42	127.69	119.93
3	A	1022	IPH	C5-C6-C1	4.50	126.14	119.37
3	A	1022	IPH	C4-C3-C2	4.60	126.91	120.19
3	K	1022	IPH	C6-C1-C2	5.59	127.75	119.79
3	A	1022	IPH	C5-C4-C3	6.07	130.58	119.93
3	A	1022	IPH	C6-C1-C2	7.72	130.80	119.79
3	G	1022	IPH	C4-C3-C2	9.31	133.82	120.19
3	G	1022	IPH	C5-C6-C1	9.64	133.85	119.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1022	IPH	2	0
3	G	1022	IPH	2	0
3	I	1022	IPH	1	0
3	K	1022	IPH	2	0

## 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, 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	20/21 (95%)	0.81	4 (20%) <span>1</span> <span>1</span>	39, 54, 68, 70	0
1	C	21/21 (100%)	-0.47	0 <span>100</span> <span>100</span>	27, 36, 48, 55	0
1	E	21/21 (100%)	-0.39	0 <span>100</span> <span>100</span>	28, 39, 57, 73	0
1	G	20/21 (95%)	-0.30	0 <span>100</span> <span>100</span>	31, 36, 57, 66	0
1	I	21/21 (100%)	-0.55	0 <span>100</span> <span>100</span>	27, 32, 44, 59	0
1	K	21/21 (100%)	-0.50	0 <span>100</span> <span>100</span>	27, 37, 53, 59	0
2	B	26/30 (86%)	0.17	1 (3%) <span>44</span> <span>48</span>	24, 30, 69, 94	0
2	D	24/30 (80%)	0.10	0 <span>100</span> <span>100</span>	21, 30, 59, 64	0
2	F	24/30 (80%)	0.08	0 <span>100</span> <span>100</span>	24, 30, 52, 66	0
2	H	27/30 (90%)	0.12	1 (3%) <span>45</span> <span>49</span>	23, 30, 62, 76	0
2	J	28/30 (93%)	0.09	0 <span>100</span> <span>100</span>	24, 29, 55, 73	0
2	L	25/30 (83%)	0.37	1 (4%) <span>42</span> <span>46</span>	23, 32, 55, 67	0
All	All	278/306 (90%)	-0.02	7 (2%) <span>61</span> <span>64</span>	21, 35, 65, 94	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	ASN	3.4
2	L	1	PHE	3.1
1	A	21	ASN	3.0
1	A	14	TYR	2.9
1	A	8	THR	2.7
2	B	25	TYR	2.3
2	H	22	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MEA	D	26	12/13	0.89	0.10	-	53,65,71,73	0
2	MEA	B	26	12/13	0.84	0.17	-	83,90,94,95	0
2	MEA	L	26	12/13	0.76	0.19	-	58,69,80,82	0
2	MEA	J	26	12/13	0.97	0.11	-	28,31,37,39	0
2	MEA	H	26	12/13	0.95	0.07	-	36,41,45,46	0
2	MEA	F	26	12/13	0.95	0.11	-	44,49,53,53	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	IPH	C	1022	7/7	0.97	0.14	1.45	27,32,33,34	0
3	IPH	G	1022	7/7	0.99	0.14	0.90	25,27,29,32	0
3	IPH	K	1022	7/7	0.96	0.13	0.88	28,28,31,32	0
4	CL	B	1028	1/1	1.00	0.12	0.43	27,27,27,27	0
3	IPH	A	1022	7/7	0.96	0.09	-0.06	29,31,36,36	0
3	IPH	I	1022	7/7	0.98	0.09	-0.22	25,26,28,30	0
5	ZN	B	1030	1/1	1.00	0.10	-0.33	25,25,25,25	0
3	IPH	E	1022	7/7	0.96	0.09	-0.39	32,33,35,35	0
4	CL	C	1028	1/1	0.99	0.12	-1.24	25,25,25,25	0
5	ZN	D	1030	1/1	1.00	0.07	-4.75	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.