Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 09:58 AM EDT

PDB ID	:	1QUN
Title	:	X-RAY STRUCTURE OF THE FIMC-FIMH CHAPERONE ADHESIN COMPLEX FROM UROPATHOGENIC E.COLI
Authors	:	Choudhury, D.; Thompson, A.; Stojanoff, V.; Langerman, S.; Pinkner, J.; Hultgren, S.J.; Knight, S.
Deposited on	:	1999-07-01
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

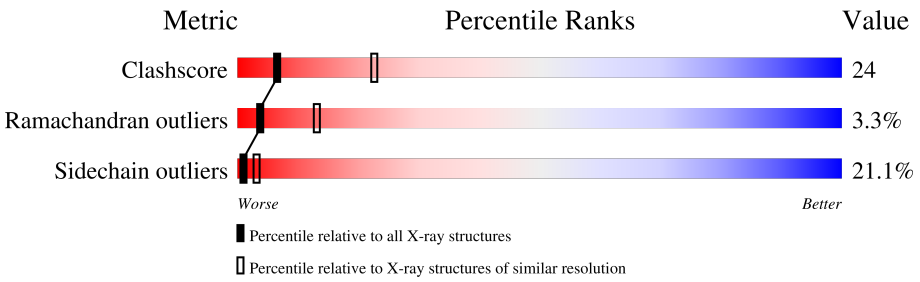
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	205	51% 35% 11% • •
1	C	205	53% 34% 9% • •
1	E	205	53% 34% 9% • •
1	G	205	52% 35% 9% • •
1	I	205	29% 41% 21% 5% •
1	K	205	30% 41% 20% 6% •
1	M	205	30% 40% 21% 5% •
1	O	205	28% 43% 21% • •

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Mol	Chain	Length	Quality of chain
2	B	279	50% 35% 8% 8%
2	D	279	49% 35% 8% 7%
2	F	279	49% 36% 8% 8%
2	H	279	50% 35% 8% 7%
2	J	279	49% 32% 15% •
2	L	279	48% 33% 16% •
2	N	279	48% 33% 15% •
2	P	279	48% 33% 16% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28864 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 PAPD-LIKE CHAPERONE FIMC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1553	985	268	294	6	5	0	0
1	C	200	1553	985	268	294	6	5	0	0
1	E	200	1553	985	268	294	6	5	0	0
1	G	200	1553	985	268	294	6	5	0	0
1	I	198	1543	979	266	292	6	177	0	0
1	K	198	1543	979	266	292	6	176	0	0
1	M	198	1543	979	266	292	6	177	0	0
1	O	198	1543	979	266	292	6	177	0	0

- Molecule 2 is a protein called MANNOSE-SPECIFIC ADHESIN FIMH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	279	2052	1297	342	409	4	42	0	0
2	D	279	2052	1297	342	409	4	42	0	0
2	F	279	2052	1297	342	409	4	42	0	0
2	H	279	2052	1297	342	409	4	42	0	0
2	J	279	2052	1297	342	409	4	67	0	0
2	L	279	2052	1297	342	409	4	67	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	279	2052	1297	342	409	4	67	0	0
			Total	C	N	O	S			
2	P	279	2052	1297	342	409	4	67	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	5	5	5	0	0
			Total	O		
3	B	10	10	10	0	0
			Total	O		
3	C	6	6	6	0	0
			Total	O		
3	D	11	11	11	0	0
			Total	O		
3	E	5	5	5	0	0
			Total	O		
3	F	12	12	12	0	0
			Total	O		
3	G	5	5	5	0	0
			Total	O		
3	H	10	10	10	0	0

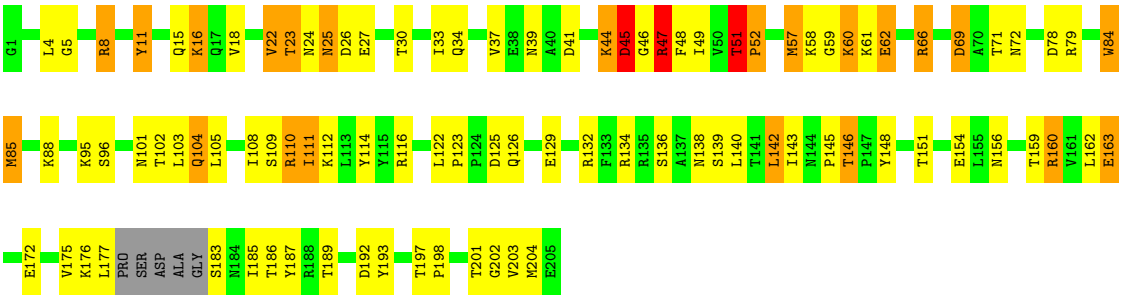
3 Residue-property plots (i)

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

Note EDS was not executed.

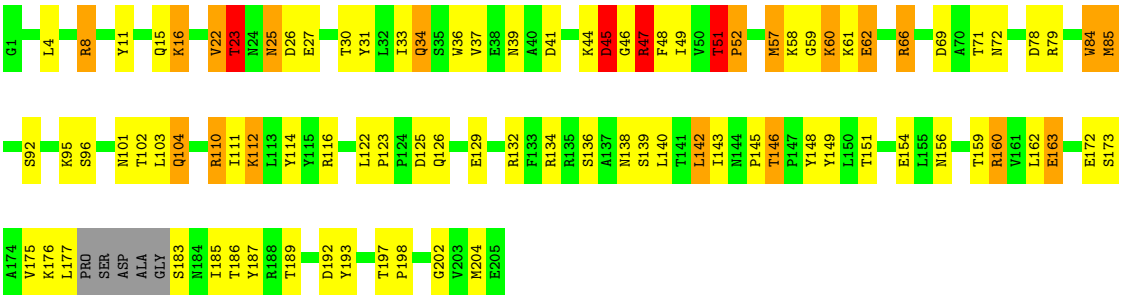
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain A:



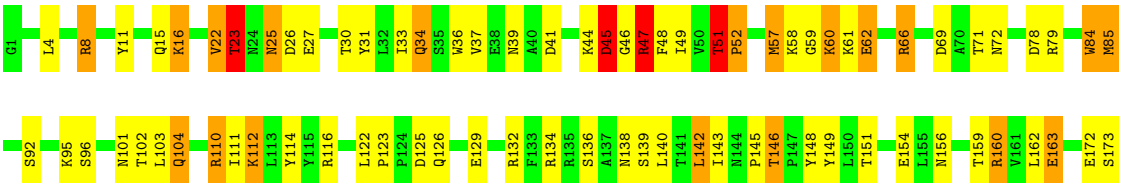
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

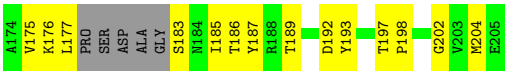
Chain C:



• Molecule 1: PAPD-LIKE CHAPERONE FIMC

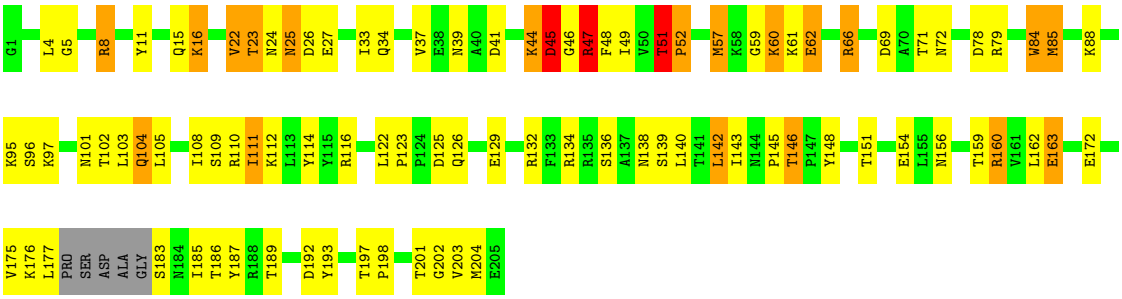
Chain E:





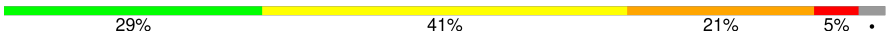
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

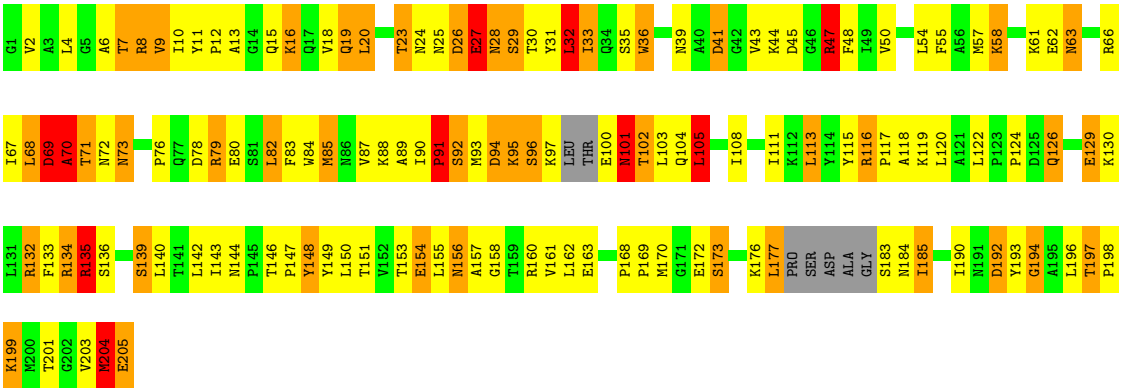
Chain G:



• Molecule 1: PAPD-LIKE CHAPERONE FIMC

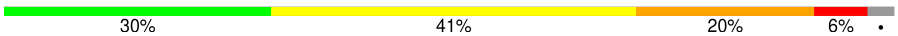
Chain I:

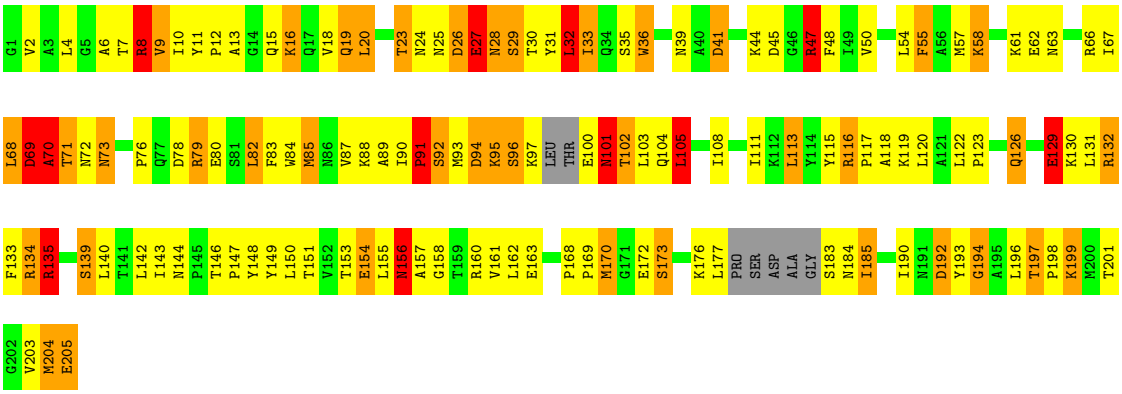




• Molecule 1: PAPD-LIKE CHAPERONE FIMC

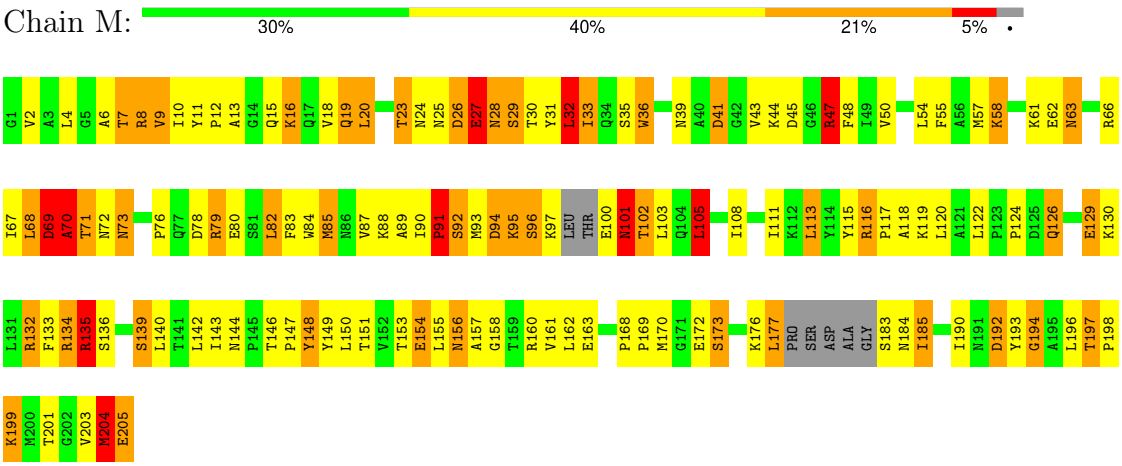
Chain K:





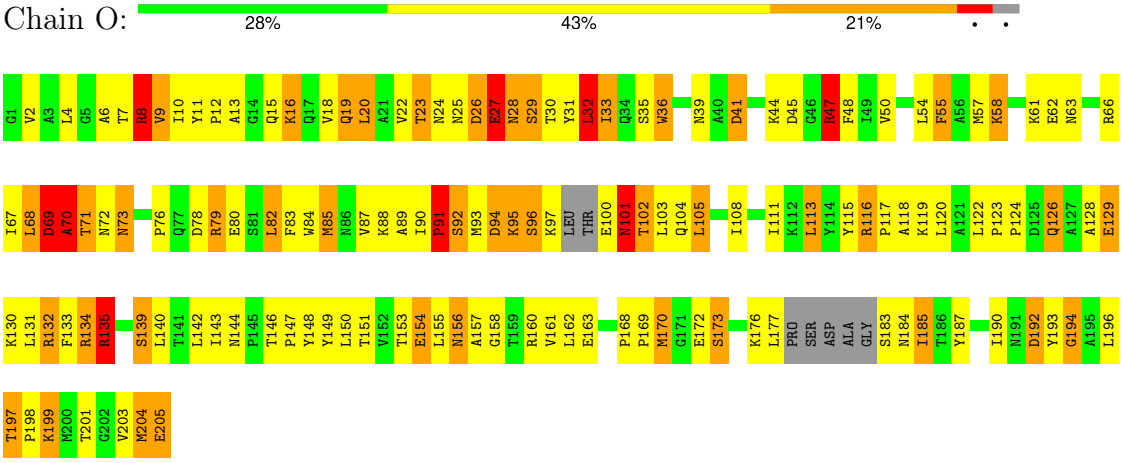
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain M:



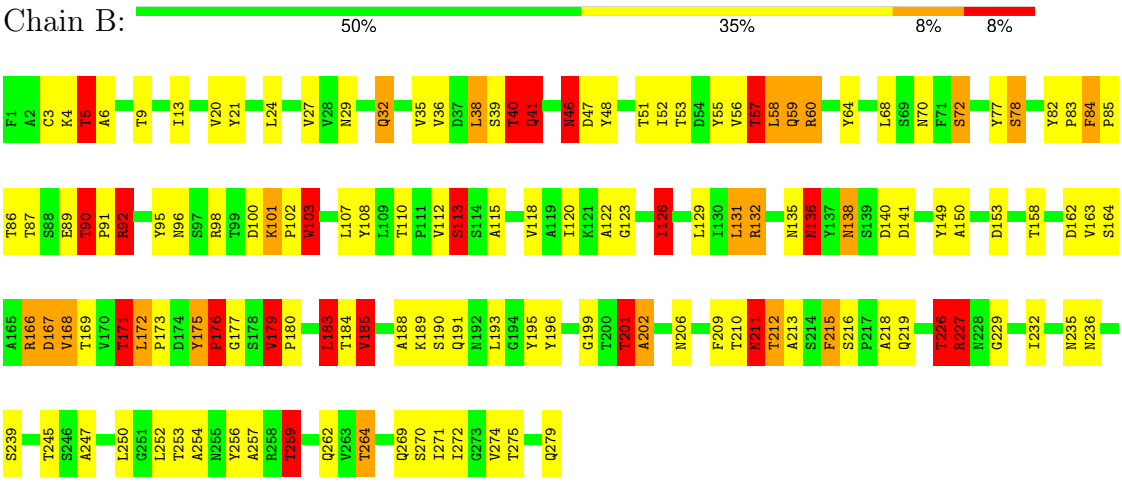
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain O:



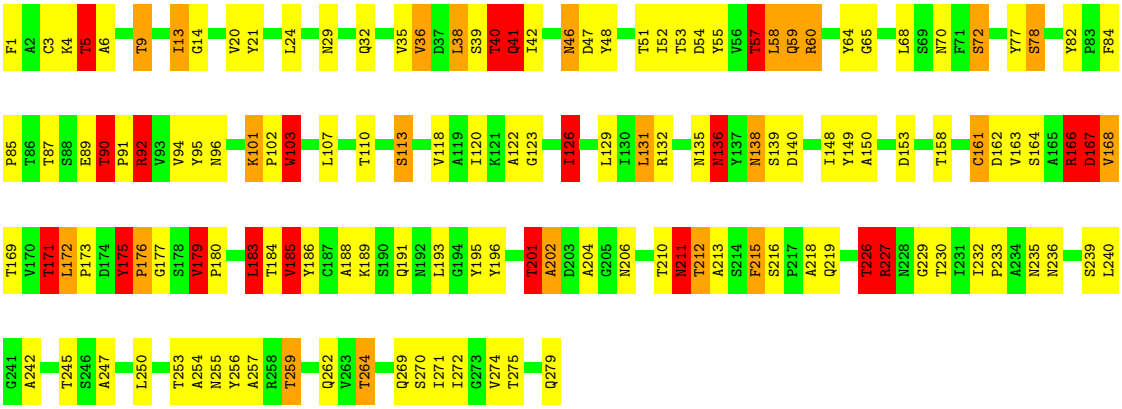
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain B:



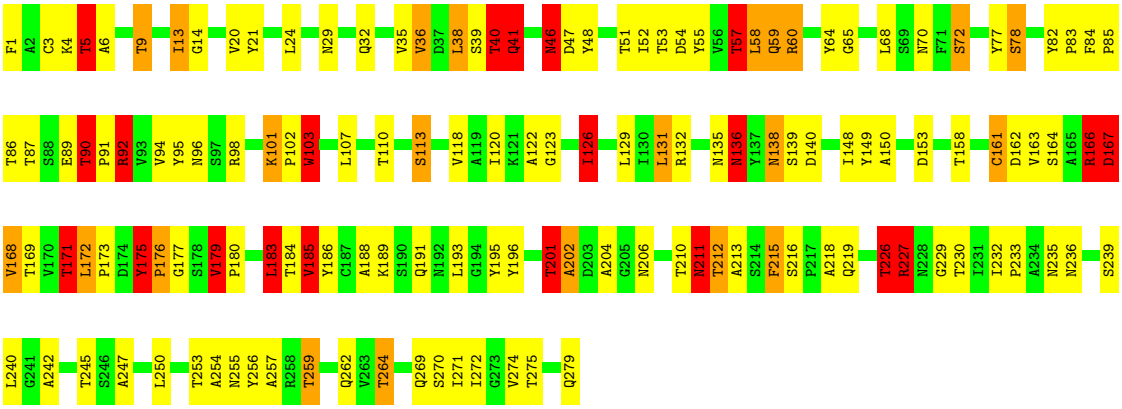
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain D:



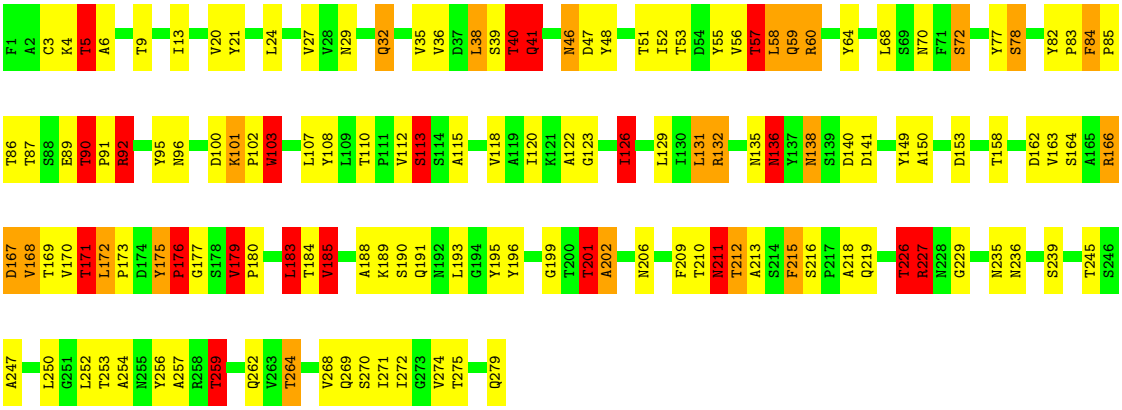
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain F:



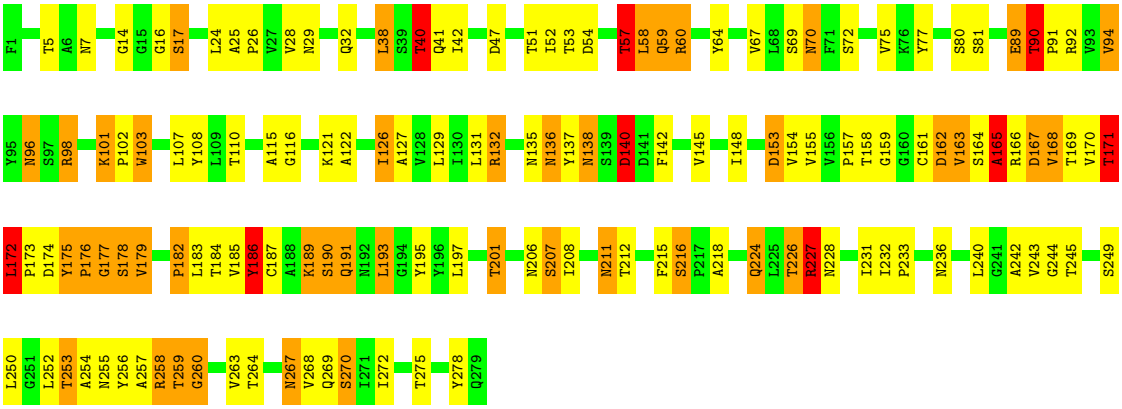
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain H:



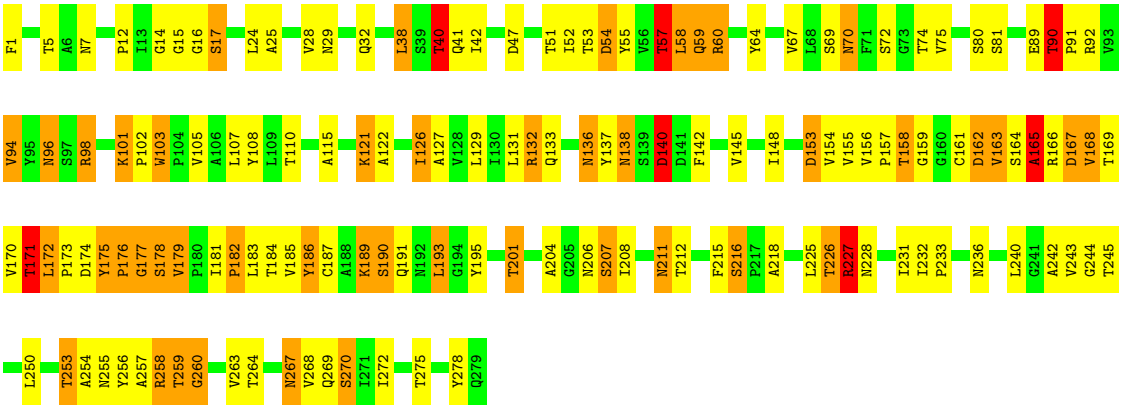
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain J:



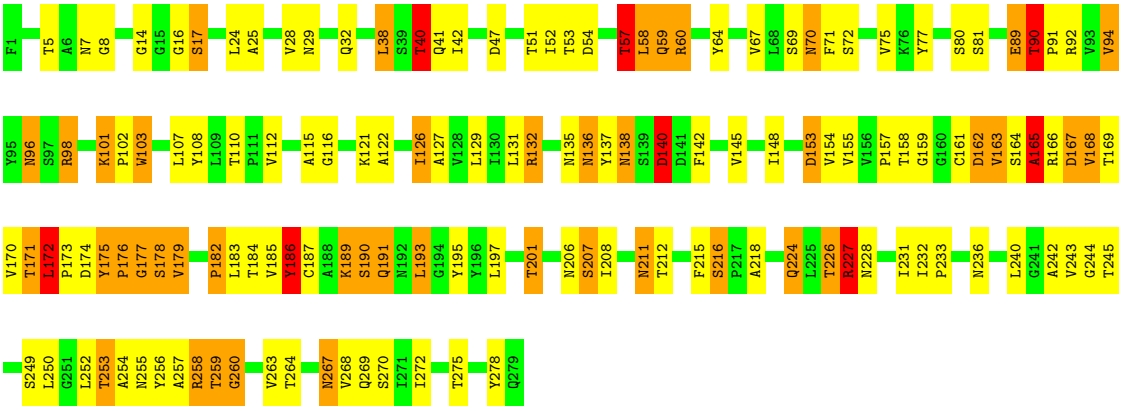
- Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain L:



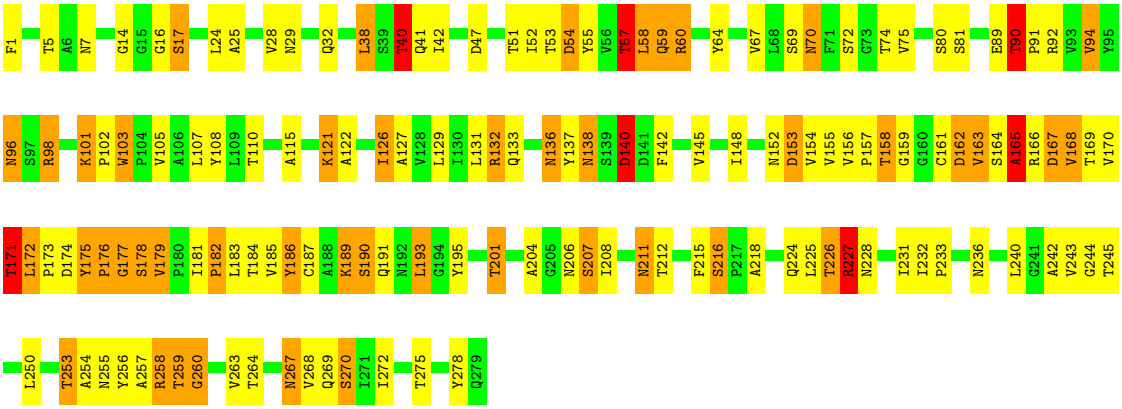
- Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain N:



- Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain P:


F1 T5 A6 N7 G14 G15 G16 S17 L24 A25 V28 N29 Q32 L38 S39 T40 Q41 I42 D47 T51 I52 T53 D54 Y55 V56 T57 L58 Q59 R60 Y64 V67 L68 S69 N70 F71 S72 G73 T74 V75 S80 S81 E89 T90 P91 R92 V93 V94 Y95
N96 S97 R98 K101 P102 W103 P104 V105 A106 L107 Y108 L109 T110 A115 K121 A122 I126 A127 V128 L129 I130 L131 R132 Q133 N136 Y137 N138 S139 D140 D141 F142 V145 I148 N152 D153 V154 V155 V156 P157 T158 G159 G160 C161 D162 V163 S164 A165 R166 D167 V168 T169 V170
T171 L172 P173 D174 Y175 P176 G177 S178 V179 P180 I181 P182 L183 T184 V185 Y186 C187 A188 K189 S190 Q191 N192 L193 G194 Y195 T201 A204 G205 N206 S207 I208 N211 T212 F215 S216 P217 A218 Q224 L225 T226 R227 N228 I231 I232 P233 N236 L240 G241 A242 V243 G244 T245
L250 T253 A254 N255 Y256 A257 R258 T259 G260 V263 T264 N267 V268 Q269 S270 I271 I272 T275 Y278 Q279

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.41Å 139.57Å 215.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.240 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28864	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.92	3/1580 (0.2%)	2.40	60/2146 (2.8%)
1	C	0.94	3/1580 (0.2%)	2.43	65/2146 (3.0%)
1	E	0.94	3/1580 (0.2%)	2.43	65/2146 (3.0%)
1	G	0.92	3/1580 (0.2%)	2.40	60/2146 (2.8%)
1	I	2.03	14/1568 (0.9%)	2.88	63/2126 (3.0%)
1	K	2.17	13/1568 (0.8%)	2.87	63/2126 (3.0%)
1	M	2.03	14/1568 (0.9%)	2.88	64/2126 (3.0%)
1	O	2.17	13/1568 (0.8%)	2.87	63/2126 (3.0%)
2	B	1.44	6/2097 (0.3%)	2.57	116/2881 (4.0%)
2	D	1.39	7/2097 (0.3%)	2.57	117/2881 (4.1%)
2	F	1.39	7/2097 (0.3%)	2.57	117/2881 (4.1%)
2	H	1.44	6/2097 (0.3%)	2.57	116/2881 (4.0%)
2	J	1.14	6/2096 (0.3%)	2.54	63/2878 (2.2%)
2	L	1.20	4/2097 (0.2%)	2.45	56/2881 (1.9%)
2	N	1.14	6/2096 (0.3%)	2.54	64/2878 (2.2%)
2	P	1.20	4/2097 (0.2%)	2.45	56/2881 (1.9%)
All	All	1.45	112/29366 (0.4%)	2.58	1208/40130 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	4
1	E	0	4
1	G	0	4
1	I	1	9
1	K	0	10
1	M	1	9
1	O	0	10
2	B	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	1	7
2	F	1	7
2	H	0	7
2	J	1	4
2	L	1	3
2	N	1	4
2	P	1	3
All	All	8	96

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	26	ASP	CG-OD1	43.75	2.25	1.25
1	M	26	ASP	CG-OD1	43.74	2.25	1.25
1	K	26	ASP	CG-OD1	40.57	2.18	1.25
1	O	26	ASP	CG-OD1	40.57	2.18	1.25
2	L	167	ASP	C-O	-35.59	0.55	1.23
2	P	167	ASP	C-O	-35.59	0.55	1.23
1	K	156	ASN	CG-OD1	-33.30	0.50	1.24
1	O	156	ASN	CG-OD1	-33.30	0.50	1.24
2	B	176	PRO	N-CA	-33.05	0.91	1.47
2	H	176	PRO	N-CA	-33.05	0.91	1.47
1	K	135	ARG	C-N	-32.83	0.58	1.34
1	O	135	ARG	C-N	-32.83	0.58	1.34
1	I	135	ARG	C-N	-30.75	0.63	1.34
1	M	135	ARG	C-N	-30.75	0.63	1.34
1	I	129	GLU	CG-CD	-30.15	1.06	1.51
1	M	129	GLU	CG-CD	-30.15	1.06	1.51
2	J	167	ASP	C-O	-29.58	0.67	1.23
2	N	167	ASP	C-O	-29.58	0.67	1.23
1	K	129	GLU	CG-CD	-29.35	1.07	1.51
1	O	129	GLU	CG-CD	-29.35	1.07	1.51
2	D	176	PRO	N-CA	-29.02	0.97	1.47
2	F	176	PRO	N-CA	-29.02	0.97	1.47
1	K	161	VAL	C-N	-27.25	0.71	1.34
1	O	161	VAL	C-N	-27.25	0.71	1.34
2	B	172	LEU	N-CA	-22.18	1.01	1.46
2	H	172	LEU	N-CA	-22.15	1.02	1.46
1	K	156	ASN	CG-ND2	21.50	1.86	1.32
1	O	156	ASN	CG-ND2	21.50	1.86	1.32
1	I	161	VAL	C-N	-20.15	0.87	1.34
1	M	161	VAL	C-N	-20.15	0.87	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	156	ASN	CA-C	-19.96	1.01	1.52
1	M	156	ASN	CA-C	-19.95	1.01	1.52
2	D	173	PRO	C-N	-19.02	0.90	1.34
2	F	173	PRO	C-N	-19.02	0.90	1.34
2	L	167	ASP	C-N	18.73	1.77	1.34
2	P	167	ASP	C-N	18.73	1.77	1.34
2	B	173	PRO	C-N	-18.59	0.91	1.34
2	H	173	PRO	C-N	-18.59	0.91	1.34
2	D	172	LEU	N-CA	-18.48	1.09	1.46
2	F	172	LEU	N-CA	-18.48	1.09	1.46
1	K	71	THR	N-CA	-18.41	1.09	1.46
1	O	71	THR	N-CA	-18.41	1.09	1.46
1	M	71	THR	N-CA	-18.19	1.09	1.46
1	I	71	THR	N-CA	-18.18	1.09	1.46
1	M	156	ASN	CG-ND2	17.66	1.76	1.32
1	I	156	ASN	CG-ND2	17.65	1.76	1.32
2	J	167	ASP	C-N	16.21	1.71	1.34
2	N	167	ASP	C-N	16.21	1.71	1.34
2	D	166	ARG	CD-NE	-14.06	1.22	1.46
2	F	166	ARG	CD-NE	-14.06	1.22	1.46
2	J	173	PRO	N-CA	-13.97	1.23	1.47
2	N	173	PRO	N-CA	-13.97	1.23	1.47
1	I	27	GLU	CA-C	-13.35	1.18	1.52
1	M	27	GLU	CA-C	-13.35	1.18	1.52
2	D	175	TYR	C-N	-13.04	1.09	1.34
2	F	175	TYR	C-N	-13.03	1.09	1.34
2	B	175	TYR	C-N	-12.56	1.10	1.34
2	H	175	TYR	C-N	-12.56	1.10	1.34
1	I	92	SER	N-CA	11.79	1.70	1.46
1	M	92	SER	N-CA	11.79	1.70	1.46
1	I	185	ILE	C-N	-11.34	1.07	1.34
1	M	185	ILE	C-N	-11.34	1.07	1.34
1	K	27	GLU	CA-C	-10.78	1.25	1.52
1	O	27	GLU	CA-C	-10.78	1.25	1.52
1	K	185	ILE	C-N	-10.68	1.09	1.34
1	O	185	ILE	C-N	-10.68	1.09	1.34
2	L	165	ALA	C-N	-8.91	1.13	1.34
2	P	165	ALA	C-N	-8.91	1.13	1.34
1	K	160	ARG	CG-CD	8.83	1.74	1.51
1	O	160	ARG	CG-CD	8.81	1.74	1.51
1	K	139	SER	C-N	-8.52	1.14	1.34
1	O	139	SER	C-N	-8.52	1.14	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	177	GLY	N-CA	-8.39	1.33	1.46
2	P	177	GLY	N-CA	-8.39	1.33	1.46
2	J	173	PRO	N-CD	8.22	1.59	1.47
2	N	173	PRO	N-CD	8.21	1.59	1.47
1	M	139	SER	C-N	-7.90	1.15	1.34
1	O	92	SER	N-CA	7.90	1.62	1.46
1	K	92	SER	N-CA	7.89	1.62	1.46
1	I	139	SER	C-N	-7.88	1.16	1.34
1	C	46	GLY	N-CA	7.54	1.57	1.46
1	E	46	GLY	N-CA	7.54	1.57	1.46
2	H	166	ARG	CD-NE	-7.15	1.34	1.46
2	B	166	ARG	CD-NE	-7.10	1.34	1.46
2	B	190	SER	CB-OG	6.35	1.50	1.42
2	H	190	SER	CB-OG	6.35	1.50	1.42
1	I	156	ASN	CA-CB	6.26	1.69	1.53
1	M	156	ASN	CA-CB	6.26	1.69	1.53
1	A	51	THR	C-O	6.25	1.35	1.23
1	G	51	THR	C-O	6.25	1.35	1.23
1	C	45	ASP	CA-CB	6.23	1.67	1.53
1	E	45	ASP	CA-CB	6.20	1.67	1.53
1	K	47	ARG	CZ-NH2	6.16	1.41	1.33
1	O	47	ARG	CZ-NH2	6.16	1.41	1.33
1	I	160	ARG	CG-CD	6.12	1.67	1.51
1	M	160	ARG	CG-CD	6.11	1.67	1.51
2	D	3	CYS	CB-SG	-6.08	1.72	1.82
2	F	3	CYS	CB-SG	-6.08	1.72	1.82
1	M	27	GLU	C-O	5.93	1.34	1.23
1	I	27	GLU	C-O	5.92	1.34	1.23
1	A	45	ASP	CA-CB	5.86	1.66	1.53
1	G	45	ASP	CA-CB	5.86	1.66	1.53
1	C	51	THR	C-O	5.85	1.34	1.23
1	E	51	THR	C-O	5.85	1.34	1.23
2	D	176	PRO	CA-CB	-5.79	1.42	1.53
2	F	176	PRO	CA-CB	-5.79	1.42	1.53
1	A	46	GLY	N-CA	5.79	1.54	1.46
1	G	46	GLY	N-CA	5.79	1.54	1.46
2	J	177	GLY	N-CA	-5.13	1.38	1.46
2	N	177	GLY	N-CA	-5.13	1.38	1.46
2	N	165	ALA	C-N	-5.11	1.22	1.34
2	J	165	ALA	C-N	-5.10	1.22	1.34

All (1208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	165	ALA	O-C-N	-61.51	24.29	122.70
2	N	165	ALA	O-C-N	-61.50	24.30	122.70
1	K	26	ASP	CB-CG-OD1	-61.39	63.05	118.30
1	O	26	ASP	CB-CG-OD1	-61.38	63.06	118.30
2	L	165	ALA	O-C-N	-60.60	25.74	122.70
2	P	165	ALA	O-C-N	-60.60	25.74	122.70
1	I	26	ASP	CB-CG-OD1	-60.10	64.21	118.30
1	M	26	ASP	CB-CG-OD1	-60.08	64.23	118.30
2	F	176	PRO	N-CA-CB	47.75	160.60	103.30
2	D	176	PRO	N-CA-CB	47.70	160.54	103.30
2	H	176	PRO	N-CA-CB	44.67	156.90	103.30
2	B	176	PRO	N-CA-CB	44.64	156.87	103.30
1	I	135	ARG	O-C-N	-36.54	64.23	122.70
1	M	135	ARG	O-C-N	-36.54	64.23	122.70
1	O	135	ARG	O-C-N	-35.58	65.78	122.70
1	K	135	ARG	O-C-N	-35.57	65.79	122.70
1	M	26	ASP	O-C-N	-33.16	69.65	122.70
1	K	71	THR	N-CA-CB	-33.14	47.33	110.30
1	O	71	THR	N-CA-CB	-33.14	47.33	110.30
1	I	26	ASP	O-C-N	-33.13	69.69	122.70
1	I	71	THR	N-CA-CB	-32.11	49.29	110.30
1	M	71	THR	N-CA-CB	-32.09	49.32	110.30
1	K	26	ASP	O-C-N	-32.05	71.42	122.70
1	O	26	ASP	O-C-N	-32.05	71.42	122.70
1	C	160	ARG	CG-CD-NE	-30.42	47.92	111.80
1	E	160	ARG	CG-CD-NE	-30.42	47.92	111.80
1	C	51	THR	CA-C-O	-28.57	60.10	120.10
1	E	51	THR	CA-C-O	-28.57	60.10	120.10
1	A	51	THR	CA-C-O	-28.19	60.90	120.10
1	G	51	THR	CA-C-O	-28.18	60.93	120.10
1	G	160	ARG	CG-CD-NE	-28.15	52.69	111.80
1	A	160	ARG	CG-CD-NE	-28.14	52.70	111.80
2	N	172	LEU	C-N-CD	-27.94	59.13	120.60
2	J	172	LEU	C-N-CD	-27.93	59.15	120.60
1	O	70	ALA	C-N-CA	-27.26	53.56	121.70
1	K	70	ALA	C-N-CA	-27.24	53.59	121.70
1	I	70	ALA	C-N-CA	-27.18	53.75	121.70
1	M	70	ALA	C-N-CA	-27.18	53.76	121.70
2	J	167	ASP	CA-C-O	-25.63	66.27	120.10
2	N	167	ASP	CA-C-O	-25.63	66.27	120.10
2	L	167	ASP	CA-C-O	-25.28	67.02	120.10
2	P	167	ASP	CA-C-O	-25.28	67.02	120.10
1	I	156	ASN	N-CA-CB	-23.43	68.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	156	ASN	N-CA-CB	-23.43	68.43	110.60
2	D	172	LEU	N-CA-C	-22.76	49.54	111.00
2	F	172	LEU	N-CA-C	-22.76	49.54	111.00
2	H	172	LEU	N-CA-C	-20.98	54.34	111.00
2	B	172	LEU	N-CA-C	-20.98	54.35	111.00
2	N	60	ARG	NE-CZ-NH1	20.75	130.68	120.30
2	J	60	ARG	NE-CZ-NH1	20.72	130.66	120.30
2	L	60	ARG	NE-CZ-NH1	20.71	130.65	120.30
2	P	60	ARG	NE-CZ-NH1	20.71	130.65	120.30
1	I	156	ASN	N-CA-C	20.70	166.89	111.00
1	M	156	ASN	N-CA-C	20.68	166.84	111.00
2	B	176	PRO	CA-N-CD	-20.62	82.63	111.50
2	H	176	PRO	CA-N-CD	-20.62	82.63	111.50
2	L	215	PHE	N-CA-CB	20.50	147.49	110.60
2	P	215	PHE	N-CA-CB	20.50	147.49	110.60
2	P	92	ARG	CD-NE-CZ	19.86	151.40	123.60
2	L	92	ARG	CD-NE-CZ	19.84	151.38	123.60
2	N	165	ALA	C-N-CA	19.47	170.39	121.70
2	J	165	ALA	C-N-CA	19.45	170.34	121.70
2	F	176	PRO	CA-N-CD	-19.20	84.62	111.50
2	D	176	PRO	CA-N-CD	-19.17	84.67	111.50
2	H	256	TYR	CB-CG-CD1	-17.98	110.21	121.00
2	B	256	TYR	CB-CG-CD1	-17.91	110.25	121.00
2	L	165	ALA	C-N-CA	17.90	166.46	121.70
2	P	165	ALA	C-N-CA	17.90	166.46	121.70
2	N	172	LEU	N-CA-CB	-17.90	74.60	110.40
2	J	172	LEU	N-CA-CB	-17.89	74.62	110.40
1	K	47	ARG	NE-CZ-NH2	-17.45	111.57	120.30
1	O	47	ARG	NE-CZ-NH2	-17.45	111.57	120.30
2	N	215	PHE	N-CA-CB	17.13	141.43	110.60
2	J	215	PHE	N-CA-CB	17.11	141.41	110.60
2	N	92	ARG	CD-NE-CZ	17.10	147.55	123.60
2	J	92	ARG	CD-NE-CZ	17.09	147.53	123.60
1	C	51	THR	O-C-N	-17.00	88.79	121.10
1	E	51	THR	O-C-N	-17.00	88.79	121.10
1	G	51	THR	O-C-N	-16.84	89.11	121.10
1	A	51	THR	O-C-N	-16.83	89.12	121.10
1	I	129	GLU	CB-CG-CD	16.55	158.89	114.20
1	M	129	GLU	CB-CG-CD	16.54	158.85	114.20
2	D	256	TYR	CB-CG-CD1	-16.31	111.22	121.00
2	F	256	TYR	CB-CG-CD1	-16.31	111.22	121.00
1	K	129	GLU	CB-CG-CD	16.10	157.67	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	129	GLU	CB-CG-CD	16.10	157.67	114.20
1	K	156	ASN	N-CA-CB	-16.07	81.67	110.60
1	O	156	ASN	N-CA-CB	-16.07	81.67	110.60
2	L	176	PRO	C-N-CA	15.72	155.31	122.30
2	P	176	PRO	C-N-CA	15.72	155.31	122.30
1	M	47	ARG	NE-CZ-NH1	15.69	128.14	120.30
1	C	110	ARG	NE-CZ-NH2	15.68	128.14	120.30
1	E	110	ARG	NE-CZ-NH2	15.68	128.14	120.30
1	I	47	ARG	NE-CZ-NH1	15.60	128.10	120.30
2	J	167	ASP	CA-C-N	15.22	150.69	117.20
2	N	167	ASP	CA-C-N	15.22	150.69	117.20
1	K	156	ASN	CA-C-N	-15.20	83.77	117.20
1	O	156	ASN	CA-C-N	-15.20	83.77	117.20
1	K	47	ARG	NE-CZ-NH1	14.92	127.76	120.30
1	O	47	ARG	NE-CZ-NH1	14.92	127.76	120.30
2	L	167	ASP	CA-C-N	14.79	149.74	117.20
2	P	167	ASP	CA-C-N	14.79	149.74	117.20
2	L	172	LEU	N-CA-CB	-14.78	80.83	110.40
2	P	172	LEU	N-CA-CB	-14.78	80.83	110.40
1	K	135	ARG	CA-C-N	14.74	149.63	117.20
1	O	135	ARG	CA-C-N	14.73	149.60	117.20
2	J	171	THR	C-N-CA	-14.47	85.52	121.70
2	N	171	THR	C-N-CA	-14.46	85.54	121.70
2	H	176	PRO	CA-CB-CG	-14.46	76.53	104.00
2	B	176	PRO	CA-CB-CG	-14.45	76.54	104.00
1	A	163	GLU	CA-CB-CG	14.25	144.74	113.40
1	G	163	GLU	CA-CB-CG	14.25	144.74	113.40
2	H	256	TYR	CB-CG-CD2	14.10	129.46	121.00
2	B	256	TYR	CB-CG-CD2	14.05	129.43	121.00
2	L	171	THR	C-N-CA	-13.72	87.40	121.70
2	P	171	THR	C-N-CA	-13.72	87.40	121.70
2	L	165	ALA	CA-C-N	13.57	147.06	117.20
2	P	165	ALA	CA-C-N	13.57	147.06	117.20
2	J	176	PRO	C-N-CA	13.52	150.69	122.30
1	K	161	VAL	O-C-N	13.51	144.32	122.70
1	O	161	VAL	O-C-N	13.51	144.32	122.70
2	N	176	PRO	C-N-CA	13.50	150.66	122.30
1	M	47	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	I	47	ARG	NE-CZ-NH2	-13.39	113.60	120.30
2	L	60	ARG	NE-CZ-NH2	-13.32	113.64	120.30
2	P	60	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	E	163	GLU	CA-CB-CG	13.20	142.44	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	163	GLU	CA-CB-CG	13.20	142.43	113.40
1	M	27	GLU	CA-C-O	13.11	147.63	120.10
1	I	27	GLU	CA-C-O	13.11	147.62	120.10
2	F	176	PRO	CA-CB-CG	-12.93	79.44	104.00
2	D	176	PRO	CA-CB-CG	-12.92	79.45	104.00
1	K	139	SER	O-C-N	-12.90	102.06	122.70
1	O	139	SER	O-C-N	-12.90	102.06	122.70
2	D	256	TYR	CB-CG-CD2	12.81	128.69	121.00
2	F	256	TYR	CB-CG-CD2	12.81	128.69	121.00
2	N	165	ALA	CA-C-N	12.78	145.32	117.20
2	J	165	ALA	CA-C-N	12.78	145.31	117.20
2	H	149	TYR	CB-CG-CD2	12.77	128.66	121.00
2	J	60	ARG	NE-CZ-NH2	-12.72	113.94	120.30
2	N	60	ARG	NE-CZ-NH2	-12.72	113.94	120.30
2	B	149	TYR	CB-CG-CD2	12.71	128.63	121.00
1	A	134	ARG	NE-CZ-NH1	12.50	126.55	120.30
1	G	134	ARG	NE-CZ-NH1	12.50	126.55	120.30
2	N	172	LEU	N-CA-C	12.36	144.38	111.00
2	J	172	LEU	N-CA-C	12.36	144.36	111.00
1	O	132	ARG	N-CA-CB	-12.21	88.62	110.60
1	K	132	ARG	N-CA-CB	-12.20	88.64	110.60
1	A	8	ARG	NE-CZ-NH2	12.19	126.39	120.30
1	I	135	ARG	CA-C-N	12.18	143.99	117.20
1	M	135	ARG	CA-C-N	12.16	143.96	117.20
1	G	8	ARG	NE-CZ-NH2	12.13	126.36	120.30
2	B	48	TYR	CB-CG-CD1	-12.02	113.79	121.00
2	H	48	TYR	CB-CG-CD1	-11.98	113.81	121.00
1	I	132	ARG	N-CA-CB	-11.97	89.05	110.60
1	M	132	ARG	N-CA-CB	-11.97	89.06	110.60
2	H	48	TYR	CB-CG-CD2	11.87	128.12	121.00
1	I	27	GLU	CA-C-N	-11.84	91.16	117.20
1	M	27	GLU	CA-C-N	-11.84	91.16	117.20
2	B	48	TYR	CB-CG-CD2	11.84	128.10	121.00
1	M	156	ASN	CB-CG-ND2	-11.51	89.08	116.70
1	I	156	ASN	CB-CG-ND2	-11.51	89.08	116.70
2	L	258	ARG	NE-CZ-NH1	11.48	126.04	120.30
2	P	258	ARG	NE-CZ-NH1	11.48	126.04	120.30
2	J	60	ARG	CD-NE-CZ	11.38	139.53	123.60
2	N	60	ARG	CD-NE-CZ	11.38	139.53	123.60
1	K	139	SER	C-N-CA	11.35	150.06	121.70
1	O	139	SER	C-N-CA	11.35	150.06	121.70
2	B	185	VAL	CB-CA-C	-11.22	90.08	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	185	VAL	CB-CA-C	-11.22	90.08	111.40
1	M	139	SER	C-N-CA	11.12	149.50	121.70
1	I	139	SER	C-N-CA	11.11	149.47	121.70
2	J	258	ARG	NE-CZ-NH1	11.05	125.82	120.30
2	N	258	ARG	NE-CZ-NH1	10.99	125.80	120.30
2	D	185	VAL	CB-CA-C	-10.93	90.63	111.40
2	F	185	VAL	CB-CA-C	-10.91	90.66	111.40
2	B	126	ILE	CA-CB-CG2	10.83	132.55	110.90
2	H	126	ILE	CA-CB-CG2	10.83	132.55	110.90
2	D	48	TYR	CB-CG-CD1	-10.76	114.55	121.00
2	F	48	TYR	CB-CG-CD1	-10.71	114.58	121.00
1	A	66	ARG	NE-CZ-NH2	10.65	125.62	120.30
1	G	66	ARG	NE-CZ-NH2	10.65	125.62	120.30
1	I	161	VAL	O-C-N	10.63	139.71	122.70
1	M	161	VAL	O-C-N	10.63	139.71	122.70
2	D	126	ILE	CA-CB-CG2	10.61	132.12	110.90
2	F	126	ILE	CA-CB-CG2	10.58	132.07	110.90
1	C	110	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	E	110	ARG	NE-CZ-NH1	-10.54	115.03	120.30
2	N	172	LEU	O-C-N	10.52	141.09	121.10
2	J	172	LEU	O-C-N	10.51	141.08	121.10
1	K	161	VAL	CA-C-N	-10.49	94.13	117.20
1	O	161	VAL	CA-C-N	-10.49	94.13	117.20
1	C	69	ASP	CB-CG-OD2	10.48	127.73	118.30
1	E	69	ASP	CB-CG-OD2	10.48	127.73	118.30
2	J	227	ARG	CD-NE-CZ	10.46	138.24	123.60
2	N	227	ARG	CD-NE-CZ	10.43	138.21	123.60
2	L	60	ARG	CD-NE-CZ	10.40	138.16	123.60
2	P	60	ARG	CD-NE-CZ	10.40	138.16	123.60
2	J	173	PRO	N-CA-CB	10.36	115.73	103.30
2	N	173	PRO	N-CA-CB	10.34	115.71	103.30
2	B	175	TYR	C-N-CA	10.25	165.04	122.00
2	H	175	TYR	C-N-CA	10.25	165.04	122.00
1	K	27	GLU	CA-C-N	-10.25	94.65	117.20
1	O	27	GLU	CA-C-N	-10.25	94.65	117.20
2	H	149	TYR	CB-CG-CD1	-10.23	114.86	121.00
2	B	149	TYR	CB-CG-CD1	-10.17	114.90	121.00
2	F	196	TYR	CB-CG-CD1	10.17	127.10	121.00
1	C	116	ARG	NE-CZ-NH1	-10.16	115.22	120.30
1	E	116	ARG	NE-CZ-NH1	-10.16	115.22	120.30
2	D	196	TYR	CB-CG-CD1	10.11	127.06	121.00
1	E	22	VAL	CB-CA-C	-10.09	92.23	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	45	ASP	CB-CG-OD2	10.08	127.38	118.30
1	C	22	VAL	CB-CA-C	-10.08	92.25	111.40
1	C	45	ASP	CB-CG-OD2	10.06	127.35	118.30
1	C	134	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	E	134	ARG	NE-CZ-NH1	10.04	125.32	120.30
2	F	149	TYR	CB-CG-CD2	10.02	127.01	121.00
2	D	149	TYR	CB-CG-CD2	10.01	127.01	121.00
1	A	78	ASP	CB-CG-OD2	9.98	127.28	118.30
1	G	78	ASP	CB-CG-OD2	9.96	127.27	118.30
1	K	27	GLU	CA-C-O	9.91	140.91	120.10
1	O	27	GLU	CA-C-O	9.91	140.91	120.10
1	E	45	ASP	CB-CG-OD1	-9.90	109.39	118.30
2	B	175	TYR	CA-C-N	-9.89	89.40	117.10
2	D	48	TYR	CB-CG-CD2	9.89	126.94	121.00
2	H	175	TYR	CA-C-N	-9.89	89.40	117.10
1	C	45	ASP	CB-CG-OD1	-9.87	109.41	118.30
2	F	48	TYR	CB-CG-CD2	9.85	126.91	121.00
1	G	22	VAL	CB-CA-C	-9.82	92.73	111.40
1	G	51	THR	CA-C-N	9.82	144.61	117.10
1	A	22	VAL	CB-CA-C	-9.82	92.74	111.40
1	I	161	VAL	CA-C-N	-9.82	95.60	117.20
1	M	161	VAL	CA-C-N	-9.82	95.60	117.20
1	A	51	THR	CA-C-N	9.81	144.56	117.10
1	C	8	ARG	NE-CZ-NH2	9.72	125.16	120.30
1	E	8	ARG	NE-CZ-NH2	9.72	125.16	120.30
1	C	160	ARG	CB-CG-CD	-9.71	86.37	111.60
1	E	160	ARG	CB-CG-CD	-9.71	86.37	111.60
1	G	116	ARG	NE-CZ-NH1	-9.66	115.47	120.30
2	P	64	TYR	CB-CG-CD2	-9.65	115.21	121.00
2	N	227	ARG	NE-CZ-NH2	9.64	125.12	120.30
2	F	175	TYR	CA-C-N	-9.63	90.14	117.10
2	D	175	TYR	CA-C-N	-9.62	90.17	117.10
2	L	64	TYR	CB-CG-CD2	-9.62	115.23	121.00
2	H	179	VAL	CB-CA-C	-9.61	93.14	111.40
2	B	179	VAL	CB-CA-C	-9.60	93.16	111.40
1	A	116	ARG	NE-CZ-NH1	-9.58	115.51	120.30
2	J	227	ARG	NE-CZ-NH2	9.57	125.08	120.30
1	K	129	GLU	CG-CD-OE2	-9.53	99.24	118.30
1	O	129	GLU	CG-CD-OE2	-9.53	99.24	118.30
1	A	45	ASP	CB-CG-OD1	-9.51	109.74	118.30
1	G	45	ASP	CB-CG-OD1	-9.51	109.74	118.30
1	C	85	MET	CA-CB-CG	9.48	129.42	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	85	MET	CA-CB-CG	9.48	129.42	113.30
2	D	179	VAL	CB-CA-C	-9.39	93.55	111.40
1	A	134	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	G	134	ARG	NE-CZ-NH2	-9.39	115.60	120.30
2	F	179	VAL	CB-CA-C	-9.38	93.57	111.40
1	K	156	ASN	OD1-CG-ND2	9.34	143.37	121.90
1	O	156	ASN	OD1-CG-ND2	9.34	143.37	121.90
1	A	110	ARG	NE-CZ-NH2	9.31	124.96	120.30
1	G	110	ARG	NE-CZ-NH2	9.26	124.93	120.30
1	C	51	THR	CA-C-N	9.25	143.01	117.10
1	E	51	THR	CA-C-N	9.25	143.01	117.10
2	D	175	TYR	C-N-CA	9.24	160.80	122.00
2	F	175	TYR	C-N-CA	9.23	160.77	122.00
1	G	85	MET	CA-CB-CG	9.19	128.93	113.30
1	A	85	MET	CA-CB-CG	9.19	128.93	113.30
2	L	92	ARG	NE-CZ-NH2	-9.18	115.71	120.30
2	P	227	ARG	NE-CZ-NH2	9.18	124.89	120.30
2	L	227	ARG	NE-CZ-NH2	9.17	124.89	120.30
2	P	92	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	I	139	SER	O-C-N	-9.11	108.12	122.70
1	M	139	SER	O-C-N	-9.11	108.12	122.70
1	A	45	ASP	CB-CG-OD2	9.11	126.50	118.30
1	G	45	ASP	CB-CG-OD2	9.11	126.50	118.30
1	A	148	TYR	CB-CG-CD2	-9.06	115.56	121.00
1	G	148	TYR	CB-CG-CD2	-9.03	115.58	121.00
2	J	64	TYR	CB-CG-CD2	-9.01	115.59	121.00
2	N	64	TYR	CB-CG-CD2	-9.01	115.59	121.00
1	I	28	ASN	CA-CB-CG	8.96	133.12	113.40
1	E	47	ARG	NE-CZ-NH1	-8.96	115.82	120.30
2	D	149	TYR	CB-CG-CD1	-8.95	115.63	121.00
2	F	149	TYR	CB-CG-CD1	-8.95	115.63	121.00
1	M	28	ASN	CA-CB-CG	8.95	133.09	113.40
1	C	47	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	G	160	ARG	CB-CG-CD	-8.94	88.37	111.60
1	A	160	ARG	CB-CG-CD	-8.93	88.37	111.60
1	A	148	TYR	CB-CG-CD1	8.93	126.36	121.00
1	G	148	TYR	CB-CG-CD1	8.93	126.36	121.00
1	C	192	ASP	CB-CG-OD1	8.84	126.25	118.30
1	E	192	ASP	CB-CG-OD1	8.84	126.25	118.30
1	G	47	ARG	NE-CZ-NH1	-8.82	115.89	120.30
2	D	202	ALA	CB-CA-C	-8.81	96.89	110.10
2	F	202	ALA	CB-CA-C	-8.81	96.89	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	129	GLU	CG-CD-OE2	-8.80	100.70	118.30
1	M	129	GLU	CG-CD-OE2	-8.80	100.70	118.30
1	G	23	THR	CA-CB-CG2	8.80	124.71	112.40
1	O	28	ASN	CA-CB-CG	8.77	132.70	113.40
1	C	114	TYR	CB-CG-CD2	-8.77	115.74	121.00
1	E	114	TYR	CB-CG-CD2	-8.77	115.74	121.00
1	A	23	THR	CA-CB-CG2	8.77	124.68	112.40
2	H	185	VAL	CG1-CB-CG2	8.77	124.93	110.90
1	K	28	ASN	CA-CB-CG	8.77	132.69	113.40
2	B	185	VAL	CG1-CB-CG2	8.75	124.90	110.90
1	G	116	ARG	NE-CZ-NH2	8.75	124.68	120.30
2	J	132	ARG	CD-NE-CZ	8.75	135.85	123.60
1	A	47	ARG	NE-CZ-NH1	-8.74	115.93	120.30
1	M	173	SER	N-CA-CB	8.74	123.61	110.50
1	C	23	THR	CA-CB-CG2	8.74	124.63	112.40
2	N	132	ARG	CD-NE-CZ	8.72	135.81	123.60
1	I	173	SER	N-CA-CB	8.72	123.58	110.50
2	L	227	ARG	CD-NE-CZ	8.71	135.80	123.60
2	P	227	ARG	CD-NE-CZ	8.71	135.79	123.60
1	E	23	THR	CA-CB-CG2	8.70	124.58	112.40
2	F	201	THR	N-CA-CB	-8.70	93.77	110.30
2	D	5	THR	N-CA-CB	-8.70	93.78	110.30
2	F	5	THR	N-CA-CB	-8.70	93.78	110.30
2	D	201	THR	N-CA-CB	-8.69	93.80	110.30
2	L	132	ARG	CD-NE-CZ	8.68	135.75	123.60
1	E	116	ARG	NE-CZ-NH2	8.67	124.64	120.30
2	P	132	ARG	CD-NE-CZ	8.66	135.72	123.60
1	A	192	ASP	CB-CG-OD1	8.65	126.09	118.30
1	G	192	ASP	CB-CG-OD1	8.65	126.09	118.30
1	C	116	ARG	NE-CZ-NH2	8.65	124.63	120.30
1	A	116	ARG	NE-CZ-NH2	8.63	124.62	120.30
2	B	202	ALA	CB-CA-C	-8.62	97.16	110.10
2	H	202	ALA	CB-CA-C	-8.62	97.18	110.10
2	F	185	VAL	CG1-CB-CG2	8.59	124.65	110.90
1	K	161	VAL	C-N-CA	-8.59	100.24	121.70
2	D	185	VAL	CG1-CB-CG2	8.58	124.63	110.90
2	D	13	ILE	CA-C-N	8.57	133.35	116.20
2	F	13	ILE	CA-C-N	8.57	133.35	116.20
1	O	161	VAL	C-N-CA	-8.57	100.26	121.70
2	N	132	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	J	132	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	K	173	SER	N-CA-CB	8.51	123.27	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	173	SER	N-CA-CB	8.49	123.23	110.50
2	J	140	ASP	CB-CG-OD1	-8.43	110.72	118.30
2	N	140	ASP	CB-CG-OD1	-8.43	110.72	118.30
1	A	69	ASP	CB-CG-OD2	8.40	125.86	118.30
2	N	98	ARG	NE-CZ-NH1	8.40	124.50	120.30
2	H	5	THR	N-CA-CB	-8.39	94.36	110.30
2	H	13	ILE	CA-C-N	8.39	132.98	116.20
2	B	5	THR	N-CA-CB	-8.39	94.36	110.30
1	I	156	ASN	OD1-CG-ND2	8.39	141.19	121.90
1	M	156	ASN	OD1-CG-ND2	8.38	141.18	121.90
2	J	98	ARG	NE-CZ-NH1	8.38	124.49	120.30
2	B	13	ILE	CA-C-N	8.37	132.95	116.20
1	G	69	ASP	CB-CG-OD2	8.37	125.84	118.30
1	C	78	ASP	CB-CG-OD2	8.36	125.83	118.30
1	E	78	ASP	CB-CG-OD2	8.36	125.83	118.30
1	A	25	ASN	CB-CA-C	-8.30	93.81	110.40
2	P	153	ASP	CB-CA-C	-8.30	93.80	110.40
2	L	153	ASP	CB-CA-C	-8.29	93.82	110.40
2	B	60	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	G	25	ASN	CB-CA-C	-8.28	93.84	110.40
2	H	60	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	B	103	TRP	CA-CB-CG	8.26	129.40	113.70
2	D	227	ARG	NE-CZ-NH2	8.26	124.43	120.30
2	F	227	ARG	NE-CZ-NH2	8.26	124.43	120.30
2	H	103	TRP	CA-CB-CG	8.26	129.40	113.70
2	H	215	PHE	CB-CG-CD2	8.21	126.55	120.80
1	K	204	MET	C-N-CA	8.21	142.22	121.70
1	O	204	MET	C-N-CA	8.21	142.22	121.70
1	K	26	ASP	OD1-CG-OD2	8.21	138.89	123.30
2	B	153	ASP	CB-CG-OD2	8.20	125.68	118.30
2	H	153	ASP	CB-CG-OD2	8.20	125.68	118.30
1	O	26	ASP	OD1-CG-OD2	8.18	138.84	123.30
1	C	148	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	E	148	TYR	CB-CG-CD2	-8.15	116.11	121.00
2	B	215	PHE	CB-CG-CD2	8.15	126.51	120.80
1	I	8	ARG	CD-NE-CZ	8.14	135.00	123.60
1	M	8	ARG	CD-NE-CZ	8.14	135.00	123.60
1	A	160	ARG	CD-NE-CZ	8.13	134.99	123.60
2	J	153	ASP	CB-CA-C	-8.13	94.15	110.40
2	N	153	ASP	CB-CA-C	-8.12	94.17	110.40
1	G	160	ARG	CD-NE-CZ	8.09	134.93	123.60
2	D	64	TYR	CB-CG-CD2	-8.02	116.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	167	ASP	CB-CG-OD2	8.02	125.52	118.30
2	F	64	TYR	CB-CG-CD2	-8.02	116.19	121.00
2	F	167	ASP	CB-CG-OD2	8.02	125.52	118.30
1	C	134	ARG	CD-NE-CZ	8.01	134.81	123.60
1	E	134	ARG	CD-NE-CZ	8.01	134.81	123.60
1	K	129	GLU	CG-CD-OE1	8.00	134.30	118.30
1	O	129	GLU	CG-CD-OE1	8.00	134.30	118.30
1	K	139	SER	CA-C-N	7.98	134.76	117.20
1	O	139	SER	CA-C-N	7.98	134.76	117.20
2	B	60	ARG	NE-CZ-NH2	-7.97	116.32	120.30
2	H	60	ARG	NE-CZ-NH2	-7.96	116.32	120.30
2	F	196	TYR	CB-CG-CD2	-7.96	116.22	121.00
2	N	47	ASP	CB-CG-OD2	-7.96	111.13	118.30
1	C	110	ARG	CD-NE-CZ	-7.95	112.47	123.60
1	E	110	ARG	CD-NE-CZ	-7.95	112.47	123.60
2	J	47	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	C	45	ASP	C-N-CA	-7.91	105.69	122.30
1	E	45	ASP	C-N-CA	-7.91	105.69	122.30
2	F	90	THR	N-CA-CB	-7.90	95.30	110.30
1	C	25	ASN	CB-CA-C	-7.88	94.63	110.40
1	E	25	ASN	CB-CA-C	-7.88	94.63	110.40
2	D	90	THR	N-CA-CB	-7.88	95.33	110.30
2	D	196	TYR	CB-CG-CD2	-7.87	116.28	121.00
2	D	60	ARG	NE-CZ-NH1	7.85	124.22	120.30
2	F	60	ARG	NE-CZ-NH1	7.85	124.22	120.30
2	J	259	THR	CA-CB-CG2	7.83	123.36	112.40
1	I	129	GLU	CG-CD-OE1	7.82	133.94	118.30
1	M	129	GLU	CG-CD-OE1	7.82	133.94	118.30
2	D	175	TYR	CB-CG-CD1	-7.82	116.31	121.00
2	D	215	PHE	CB-CG-CD2	7.82	126.27	120.80
2	F	175	TYR	CB-CG-CD1	-7.82	116.31	121.00
2	F	215	PHE	CB-CG-CD2	7.82	126.27	120.80
2	N	259	THR	CA-CB-CG2	7.81	123.34	112.40
2	D	103	TRP	CA-CB-CG	7.81	128.54	113.70
2	F	103	TRP	CA-CB-CG	7.81	128.54	113.70
2	B	175	TYR	CB-CG-CD1	-7.80	116.32	121.00
2	H	175	TYR	CB-CG-CD1	-7.80	116.32	121.00
1	I	79	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	C	45	ASP	CA-CB-CG	-7.79	96.27	113.40
1	E	45	ASP	CA-CB-CG	-7.78	96.28	113.40
1	O	204	MET	CA-C-O	7.76	136.40	120.10
1	K	26	ASP	CA-C-N	7.76	134.28	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	204	MET	CA-C-O	7.76	136.40	120.10
1	O	26	ASP	CA-C-N	7.76	134.27	117.20
2	L	259	THR	CA-CB-CG2	7.74	123.24	112.40
2	H	176	PRO	CB-CA-C	-7.74	92.66	112.00
2	B	176	PRO	CB-CA-C	-7.73	92.67	112.00
2	P	259	THR	CA-CB-CG2	7.73	123.22	112.40
1	M	79	ARG	NE-CZ-NH2	7.73	124.16	120.30
2	D	167	ASP	C-N-CA	7.71	140.98	121.70
2	F	167	ASP	C-N-CA	7.71	140.98	121.70
2	D	168	VAL	C-N-CA	7.71	140.97	121.70
2	F	168	VAL	C-N-CA	7.71	140.97	121.70
1	G	110	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	110	ARG	NE-CZ-NH1	-7.70	116.45	120.30
2	B	167	ASP	CB-CG-OD2	7.69	125.22	118.30
2	H	167	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	45	ASP	CA-CB-CG	-7.68	96.50	113.40
1	G	45	ASP	CA-CB-CG	-7.68	96.50	113.40
1	I	204	MET	C-N-CA	7.68	140.90	121.70
1	M	204	MET	C-N-CA	7.67	140.88	121.70
1	C	66	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	E	66	ARG	NE-CZ-NH2	7.64	124.12	120.30
2	D	82	TYR	CB-CG-CD2	-7.62	116.43	121.00
2	F	82	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	M	91	PRO	C-N-CA	-7.62	102.64	121.70
2	J	186	TYR	CA-CB-CG	7.62	127.87	113.40
2	N	186	TYR	CA-CB-CG	7.62	127.87	113.40
2	L	58	LEU	N-CA-CB	7.62	125.63	110.40
2	P	58	LEU	N-CA-CB	7.62	125.63	110.40
1	I	91	PRO	C-N-CA	-7.61	102.66	121.70
2	B	64	TYR	CB-CG-CD2	-7.60	116.44	121.00
2	H	64	TYR	CB-CG-CD2	-7.60	116.44	121.00
2	N	207	SER	N-CA-CB	7.58	121.87	110.50
2	J	207	SER	N-CA-CB	7.58	121.86	110.50
1	C	134	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	E	134	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	K	132	ARG	CA-CB-CG	7.57	130.05	113.40
1	O	132	ARG	CA-CB-CG	7.57	130.05	113.40
2	F	36	VAL	CA-CB-CG2	7.55	122.23	110.90
2	D	36	VAL	CA-CB-CG2	7.54	122.22	110.90
2	D	177	GLY	N-CA-C	7.54	131.95	113.10
2	F	177	GLY	N-CA-C	7.54	131.95	113.10
1	C	11	TYR	CB-CG-CD2	7.54	125.52	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	11	TYR	CB-CG-CD2	7.54	125.52	121.00
2	H	103	TRP	N-CA-CB	7.53	124.16	110.60
2	B	90	THR	N-CA-CB	-7.52	96.01	110.30
2	H	90	THR	N-CA-CB	-7.52	96.01	110.30
2	B	103	TRP	N-CA-CB	7.51	124.12	110.60
2	D	54	ASP	CB-CG-OD2	7.48	125.03	118.30
2	B	36	VAL	CA-CB-CG2	7.46	122.10	110.90
2	P	132	ARG	NE-CZ-NH1	7.46	124.03	120.30
2	F	54	ASP	CB-CG-OD2	7.46	125.01	118.30
2	H	36	VAL	CA-CB-CG2	7.46	122.08	110.90
1	I	204	MET	CA-C-O	7.46	135.76	120.10
1	M	204	MET	CA-C-O	7.46	135.76	120.10
1	A	66	ARG	NE-CZ-NH1	-7.45	116.57	120.30
2	B	175	TYR	O-C-N	7.45	135.26	121.10
1	G	66	ARG	NE-CZ-NH1	-7.45	116.57	120.30
2	H	175	TYR	O-C-N	7.45	135.26	121.10
2	F	40	THR	N-CA-CB	-7.45	96.14	110.30
1	A	134	ARG	CD-NE-CZ	7.45	134.03	123.60
1	G	134	ARG	CD-NE-CZ	7.45	134.03	123.60
1	M	26	ASP	OD1-CG-OD2	7.45	137.45	123.30
1	A	110	ARG	CD-NE-CZ	-7.45	113.18	123.60
2	B	168	VAL	C-N-CA	7.45	140.31	121.70
2	H	168	VAL	C-N-CA	7.45	140.31	121.70
1	G	110	ARG	CD-NE-CZ	-7.44	113.18	123.60
2	D	40	THR	N-CA-CB	-7.44	96.16	110.30
2	D	226	THR	N-CA-CB	-7.43	96.19	110.30
1	I	26	ASP	OD1-CG-OD2	7.43	137.41	123.30
2	P	186	TYR	CA-CB-CG	7.42	127.50	113.40
2	P	207	SER	N-CA-CB	7.42	121.62	110.50
2	B	21	TYR	CB-CG-CD1	7.41	125.45	121.00
2	H	21	TYR	CB-CG-CD1	7.41	125.45	121.00
2	F	226	THR	N-CA-CB	-7.41	96.22	110.30
2	L	186	TYR	CA-CB-CG	7.41	127.48	113.40
2	L	132	ARG	NE-CZ-NH1	7.41	124.00	120.30
2	L	207	SER	N-CA-CB	7.40	121.60	110.50
1	I	71	THR	CA-CB-CG2	-7.39	102.05	112.40
1	K	71	THR	CA-CB-CG2	-7.39	102.05	112.40
1	O	71	THR	CA-CB-CG2	-7.39	102.05	112.40
1	M	71	THR	CA-CB-CG2	-7.39	102.05	112.40
2	D	103	TRP	N-CA-CB	7.38	123.88	110.60
2	F	103	TRP	N-CA-CB	7.38	123.88	110.60
1	I	26	ASP	CB-CG-OD2	7.37	124.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	26	ASP	CB-CG-OD2	7.37	124.93	118.30
1	M	47	ARG	NH1-CZ-NH2	-7.34	111.32	119.40
1	K	91	PRO	C-N-CA	-7.34	103.35	121.70
1	O	91	PRO	C-N-CA	-7.33	103.37	121.70
2	B	57	THR	N-CA-CB	-7.32	96.39	110.30
1	C	132	ARG	NE-CZ-NH1	-7.32	116.64	120.30
2	D	92	ARG	CD-NE-CZ	7.31	133.84	123.60
2	F	92	ARG	CD-NE-CZ	7.31	133.84	123.60
2	H	57	THR	N-CA-CB	-7.31	96.42	110.30
1	I	47	ARG	NH1-CZ-NH2	-7.30	111.37	119.40
2	D	227	ARG	NE-CZ-NH1	-7.29	116.66	120.30
2	F	227	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	A	45	ASP	C-N-CA	-7.29	107.00	122.30
1	G	45	ASP	C-N-CA	-7.29	107.00	122.30
1	K	132	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	O	132	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	E	132	ARG	NE-CZ-NH1	-7.26	116.67	120.30
2	J	38	LEU	CA-CB-CG	-7.26	98.61	115.30
2	N	38	LEU	CA-CB-CG	-7.26	98.60	115.30
1	K	8	ARG	CD-NE-CZ	7.26	133.76	123.60
1	O	8	ARG	CD-NE-CZ	7.26	133.76	123.60
1	G	34	GLN	N-CA-CB	7.26	123.66	110.60
1	K	26	ASP	CB-CG-OD2	7.26	124.83	118.30
2	B	13	ILE	C-N-CA	-7.25	107.08	122.30
1	A	34	GLN	N-CA-CB	7.24	123.64	110.60
2	H	13	ILE	C-N-CA	-7.24	107.09	122.30
1	K	79	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	K	8	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	O	8	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	O	79	ARG	NE-CZ-NH2	7.22	123.91	120.30
2	F	13	ILE	C-N-CA	-7.21	107.16	122.30
2	D	13	ILE	C-N-CA	-7.20	107.17	122.30
1	O	26	ASP	CB-CG-OD2	7.20	124.78	118.30
1	E	47	ARG	NH1-CZ-NH2	7.20	127.32	119.40
1	C	47	ARG	NH1-CZ-NH2	7.17	127.29	119.40
2	B	82	TYR	CB-CG-CD2	-7.17	116.70	121.00
2	N	40	THR	N-CA-CB	-7.15	96.72	110.30
2	J	40	THR	N-CA-CB	-7.15	96.72	110.30
2	H	171	THR	N-CA-CB	7.14	123.86	110.30
2	B	171	THR	N-CA-CB	7.13	123.86	110.30
2	F	175	TYR	O-C-N	7.13	134.64	121.10
2	J	58	LEU	N-CA-CB	7.13	124.65	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	167	ASP	C-N-CA	-7.13	103.88	121.70
2	N	58	LEU	N-CA-CB	7.13	124.65	110.40
2	H	82	TYR	CB-CG-CD2	-7.12	116.73	121.00
2	N	167	ASP	C-N-CA	-7.12	103.89	121.70
2	B	177	GLY	N-CA-C	7.12	130.90	113.10
2	D	21	TYR	CB-CG-CD1	7.12	125.27	121.00
2	F	21	TYR	CB-CG-CD1	7.12	125.27	121.00
2	D	175	TYR	O-C-N	7.12	134.62	121.10
2	H	177	GLY	N-CA-C	7.11	130.87	113.10
1	M	92	SER	N-CA-CB	-7.10	99.84	110.50
1	K	156	ASN	CA-C-O	7.09	134.99	120.10
1	O	156	ASN	CA-C-O	7.09	134.99	120.10
1	I	92	SER	N-CA-CB	-7.08	99.87	110.50
2	P	38	LEU	CA-CB-CG	-7.08	99.02	115.30
2	L	38	LEU	CA-CB-CG	-7.07	99.05	115.30
1	A	8	ARG	NH1-CZ-NH2	-7.06	111.63	119.40
1	G	8	ARG	NH1-CZ-NH2	-7.06	111.63	119.40
1	A	163	GLU	OE1-CD-OE2	-7.06	114.83	123.30
1	G	163	GLU	OE1-CD-OE2	-7.06	114.83	123.30
1	C	11	TYR	CB-CG-CD1	-7.04	116.77	121.00
1	E	11	TYR	CB-CG-CD1	-7.04	116.77	121.00
2	B	167	ASP	C-N-CA	7.04	139.31	121.70
2	H	167	ASP	C-N-CA	7.04	139.31	121.70
1	I	26	ASP	CA-C-N	7.03	132.66	117.20
1	M	26	ASP	CA-C-N	7.03	132.66	117.20
2	F	171	THR	N-CA-CB	7.02	123.63	110.30
1	A	114	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	G	114	TYR	CB-CG-CD2	-7.00	116.80	121.00
2	B	226	THR	N-CA-CB	-7.00	97.00	110.30
2	F	175	TYR	CA-C-O	6.99	134.79	120.10
2	B	175	TYR	CA-C-O	6.99	134.78	120.10
2	D	171	THR	N-CA-CB	6.99	123.58	110.30
2	H	175	TYR	CA-C-O	6.99	134.78	120.10
2	D	175	TYR	CA-C-O	6.99	134.78	120.10
2	H	87	THR	CA-CB-CG2	-6.99	102.62	112.40
1	G	11	TYR	CB-CG-CD2	6.98	125.19	121.00
2	J	92	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	N	92	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	H	226	THR	N-CA-CB	-6.97	97.05	110.30
2	B	87	THR	CA-CB-CG2	-6.96	102.66	112.40
2	D	123	GLY	O-C-N	-6.96	111.57	122.70
2	F	123	GLY	O-C-N	-6.95	111.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	TYR	CB-CG-CD2	6.94	125.17	121.00
1	K	194	GLY	N-CA-C	6.94	130.45	113.10
1	O	194	GLY	N-CA-C	6.94	130.45	113.10
2	H	92	ARG	CD-NE-CZ	6.94	133.31	123.60
2	D	262	GLN	CB-CG-CD	6.92	129.60	111.60
2	F	262	GLN	CB-CG-CD	6.92	129.60	111.60
2	N	172	LEU	CA-C-O	-6.92	105.57	120.10
2	D	57	THR	N-CA-CB	-6.91	97.17	110.30
2	F	57	THR	N-CA-CB	-6.91	97.17	110.30
2	B	92	ARG	CD-NE-CZ	6.91	133.27	123.60
2	B	40	THR	N-CA-CB	-6.90	97.19	110.30
2	J	172	LEU	CA-C-O	-6.90	105.60	120.10
1	E	47	ARG	NE-CZ-NH2	-6.89	116.85	120.30
2	H	40	THR	N-CA-CB	-6.89	97.21	110.30
2	D	87	THR	CA-CB-CG2	-6.89	102.76	112.40
2	F	87	THR	CA-CB-CG2	-6.89	102.76	112.40
1	I	132	ARG	CA-CB-CG	6.88	128.54	113.40
1	M	132	ARG	CA-CB-CG	6.88	128.54	113.40
2	H	262	GLN	CB-CG-CD	6.87	129.47	111.60
2	B	262	GLN	CB-CG-CD	6.87	129.45	111.60
1	C	47	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	D	227	ARG	CD-NE-CZ	-6.85	114.01	123.60
2	F	227	ARG	CD-NE-CZ	-6.85	114.01	123.60
2	D	167	ASP	O-C-N	-6.84	111.75	122.70
1	C	34	GLN	N-CA-CB	6.83	122.90	110.60
1	E	34	GLN	N-CA-CB	6.83	122.90	110.60
1	A	8	ARG	CD-NE-CZ	-6.82	114.05	123.60
2	L	140	ASP	CB-CG-OD1	-6.82	112.16	118.30
2	P	140	ASP	CB-CG-OD1	-6.82	112.16	118.30
2	F	167	ASP	O-C-N	-6.81	111.80	122.70
1	G	8	ARG	CD-NE-CZ	-6.80	114.08	123.60
2	H	227	ARG	CB-CG-CD	6.80	129.28	111.60
2	B	227	ARG	CB-CG-CD	6.80	129.27	111.60
2	D	175	TYR	CB-CG-CD2	6.79	125.07	121.00
2	F	175	TYR	CB-CG-CD2	6.79	125.07	121.00
2	B	227	ARG	NE-CZ-NH1	-6.76	116.92	120.30
2	H	227	ARG	NE-CZ-NH1	-6.76	116.92	120.30
2	B	103	TRP	CH2-CZ2-CE2	-6.75	110.65	117.40
1	K	47	ARG	CD-NE-CZ	6.74	133.03	123.60
1	O	47	ARG	CD-NE-CZ	6.74	133.03	123.60
2	B	175	TYR	CB-CG-CD2	6.73	125.04	121.00
2	H	175	TYR	CB-CG-CD2	6.73	125.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	194	GLY	N-CA-C	6.71	129.87	113.10
1	M	194	GLY	N-CA-C	6.71	129.87	113.10
2	H	103	TRP	CH2-CZ2-CE2	-6.70	110.70	117.40
2	L	47	ASP	CB-CG-OD2	-6.70	112.27	118.30
2	P	47	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	K	69	ASP	CB-CG-OD1	6.68	124.31	118.30
1	O	69	ASP	CB-CG-OD1	6.68	124.31	118.30
2	B	6	ALA	O-C-N	-6.67	112.03	122.70
2	H	6	ALA	O-C-N	-6.65	112.06	122.70
1	M	161	VAL	C-N-CA	-6.63	105.11	121.70
2	L	108	TYR	CB-CG-CD2	6.62	124.97	121.00
2	P	108	TYR	CB-CG-CD2	6.62	124.97	121.00
1	I	161	VAL	C-N-CA	-6.62	105.16	121.70
2	B	21	TYR	CB-CG-CD2	-6.61	117.03	121.00
2	H	21	TYR	CB-CG-CD2	-6.61	117.03	121.00
2	D	215	PHE	CA-CB-CG	6.61	129.76	113.90
2	F	215	PHE	CA-CB-CG	6.61	129.76	113.90
1	I	132	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	L	258	ARG	NE-CZ-NH2	-6.60	117.00	120.30
2	P	258	ARG	NE-CZ-NH2	-6.60	117.00	120.30
2	H	196	TYR	CB-CG-CD1	6.60	124.96	121.00
1	E	163	GLU	OE1-CD-OE2	-6.59	115.39	123.30
1	C	163	GLU	OE1-CD-OE2	-6.58	115.41	123.30
1	M	132	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	41	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	G	41	ASP	CB-CG-OD1	-6.57	112.39	118.30
2	D	204	ALA	CB-CA-C	6.56	119.94	110.10
2	F	204	ALA	CB-CA-C	6.56	119.94	110.10
2	B	196	TYR	CB-CG-CD1	6.55	124.93	121.00
2	D	188	ALA	O-C-N	-6.55	112.22	122.70
2	F	188	ALA	O-C-N	-6.55	112.22	122.70
2	J	69	SER	CB-CA-C	-6.53	97.70	110.10
2	N	69	SER	CB-CA-C	-6.52	97.72	110.10
2	L	103	TRP	CA-CB-CG	6.51	126.07	113.70
2	P	103	TRP	CA-CB-CG	6.51	126.07	113.70
2	B	123	GLY	O-C-N	-6.50	112.30	122.70
1	G	11	TYR	CB-CG-CD1	-6.50	117.10	121.00
2	B	193	LEU	N-CA-CB	6.48	123.36	110.40
2	H	193	LEU	N-CA-CB	6.48	123.36	110.40
2	H	123	GLY	O-C-N	-6.47	112.34	122.70
2	D	47	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	A	78	ASP	CB-CG-OD1	-6.46	112.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	101	LYS	CA-CB-CG	6.45	127.59	113.40
2	L	167	ASP	C-N-CA	-6.45	105.58	121.70
2	P	101	LYS	CA-CB-CG	6.45	127.58	113.40
1	A	85	MET	N-CA-CB	-6.44	99.00	110.60
1	C	8	ARG	CD-NE-CZ	-6.44	114.58	123.60
1	E	8	ARG	CD-NE-CZ	-6.44	114.58	123.60
1	G	78	ASP	CB-CG-OD1	-6.44	112.51	118.30
1	G	85	MET	N-CA-CB	-6.44	99.02	110.60
2	P	167	ASP	C-N-CA	-6.44	105.61	121.70
2	F	9	THR	CA-CB-OG1	-6.43	95.49	109.00
2	D	9	THR	CA-CB-OG1	-6.42	95.51	109.00
1	A	11	TYR	CB-CG-CD1	-6.42	117.15	121.00
2	D	193	LEU	N-CA-CB	6.42	123.24	110.40
2	F	193	LEU	N-CA-CB	6.42	123.24	110.40
2	F	47	ASP	CB-CG-OD2	-6.42	112.52	118.30
2	B	201	THR	N-CA-CB	-6.41	98.12	110.30
2	D	153	ASP	CB-CG-OD2	6.40	124.06	118.30
2	F	153	ASP	CB-CG-OD2	6.40	124.06	118.30
2	H	201	THR	N-CA-CB	-6.39	98.15	110.30
2	D	166	ARG	CD-NE-CZ	-6.39	114.66	123.60
2	D	173	PRO	C-N-CA	-6.39	105.73	121.70
2	F	166	ARG	CD-NE-CZ	-6.39	114.66	123.60
2	F	173	PRO	C-N-CA	-6.39	105.73	121.70
2	L	172	LEU	CA-C-O	-6.39	106.69	120.10
2	P	172	LEU	CA-C-O	-6.39	106.69	120.10
2	D	103	TRP	CH2-CZ2-CE2	-6.38	111.02	117.40
1	A	84	TRP	CB-CG-CD2	6.37	134.88	126.60
2	H	196	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	K	29	SER	N-CA-CB	-6.36	100.96	110.50
2	B	113	SER	CA-CB-OG	-6.36	94.03	111.20
1	G	84	TRP	CB-CG-CD2	6.36	134.87	126.60
2	H	113	SER	CA-CB-OG	-6.36	94.03	111.20
1	O	29	SER	N-CA-CB	-6.35	100.97	110.50
1	K	92	SER	N-CA-CB	-6.35	100.98	110.50
2	F	103	TRP	CH2-CZ2-CE2	-6.34	111.06	117.40
2	B	46	ASN	CA-CB-CG	6.34	127.34	113.40
2	B	196	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	I	139	SER	CA-C-N	6.33	131.13	117.20
1	O	92	SER	N-CA-CB	-6.33	101.01	110.50
1	M	139	SER	CA-C-N	6.33	131.12	117.20
2	H	46	ASN	CA-CB-CG	6.33	127.31	113.40
1	I	197	THR	N-CA-CB	6.33	122.32	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	215	PHE	CA-CB-CG	6.32	129.08	113.90
1	I	172	GLU	CA-CB-CG	6.32	127.31	113.40
2	L	126	ILE	CB-CA-C	-6.32	98.96	111.60
2	P	126	ILE	CB-CA-C	-6.32	98.96	111.60
2	H	20	VAL	C-N-CA	6.32	137.50	121.70
2	H	215	PHE	CA-CB-CG	6.31	129.05	113.90
2	B	173	PRO	C-N-CA	-6.31	105.92	121.70
2	H	173	PRO	C-N-CA	-6.31	105.92	121.70
1	M	197	THR	N-CA-CB	6.31	122.29	110.30
2	B	20	VAL	C-N-CA	6.31	137.48	121.70
1	C	84	TRP	CB-CG-CD2	6.31	134.80	126.60
1	E	84	TRP	CB-CG-CD2	6.31	134.80	126.60
1	M	172	GLU	CA-CB-CG	6.31	127.28	113.40
2	N	126	ILE	CB-CA-C	-6.30	99.00	111.60
2	J	126	ILE	CB-CA-C	-6.29	99.02	111.60
1	A	51	THR	CA-CB-OG1	-6.29	95.79	109.00
1	G	51	THR	CA-CB-OG1	-6.29	95.79	109.00
2	B	141	ASP	CB-CG-OD1	6.28	123.95	118.30
2	H	141	ASP	CB-CG-OD1	6.28	123.95	118.30
2	B	176	PRO	N-CA-C	-6.28	95.78	112.10
2	D	126	ILE	N-CA-CB	-6.28	96.36	110.80
2	H	176	PRO	N-CA-C	-6.28	95.78	112.10
2	F	126	ILE	N-CA-CB	-6.28	96.37	110.80
2	F	78	SER	N-CA-CB	-6.27	101.10	110.50
1	C	78	ASP	CB-CG-OD1	-6.26	112.66	118.30
2	D	78	SER	N-CA-CB	-6.26	101.10	110.50
1	E	78	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	C	84	TRP	CH2-CZ2-CE2	-6.26	111.14	117.40
2	H	60	ARG	CA-CB-CG	6.26	127.17	113.40
1	O	172	GLU	CA-CB-CG	6.26	127.17	113.40
2	B	60	ARG	CA-CB-CG	6.25	127.16	113.40
1	K	172	GLU	CA-CB-CG	6.25	127.16	113.40
2	D	60	ARG	CA-CB-CG	6.25	127.15	113.40
2	B	100	ASP	O-C-N	6.25	132.69	122.70
2	H	100	ASP	O-C-N	6.25	132.69	122.70
2	H	126	ILE	N-CA-CB	-6.25	96.44	110.80
1	E	84	TRP	CH2-CZ2-CE2	-6.24	111.16	117.40
2	B	126	ILE	N-CA-CB	-6.23	96.46	110.80
2	F	60	ARG	CA-CB-CG	6.23	127.11	113.40
1	A	5	GLY	O-C-N	-6.23	112.73	122.70
1	G	5	GLY	O-C-N	-6.23	112.73	122.70
2	N	60	ARG	CA-CB-CG	6.23	127.10	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	60	ARG	CA-CB-CG	6.23	127.10	113.40
2	J	101	LYS	CA-CB-CG	6.19	127.01	113.40
2	N	101	LYS	CA-CB-CG	6.19	127.01	113.40
2	F	6	ALA	O-C-N	-6.18	112.81	122.70
2	D	122	ALA	N-CA-CB	-6.18	101.44	110.10
2	F	122	ALA	N-CA-CB	-6.18	101.44	110.10
1	I	47	ARG	CD-NE-CZ	6.18	132.25	123.60
1	K	71	THR	N-CA-C	6.17	127.67	111.00
2	D	6	ALA	O-C-N	-6.17	112.83	122.70
1	O	71	THR	N-CA-C	6.16	127.63	111.00
2	D	20	VAL	C-N-CA	6.15	137.08	121.70
1	M	47	ARG	CD-NE-CZ	6.15	132.21	123.60
2	F	20	VAL	C-N-CA	6.14	137.06	121.70
1	I	29	SER	N-CA-CB	-6.13	101.31	110.50
1	M	29	SER	N-CA-CB	-6.12	101.33	110.50
2	N	103	TRP	CA-CB-CG	6.10	125.29	113.70
2	B	257	ALA	CB-CA-C	6.09	119.24	110.10
2	J	103	TRP	CA-CB-CG	6.08	125.26	113.70
1	M	27	GLU	CB-CA-C	6.08	122.57	110.40
1	I	27	GLU	CB-CA-C	6.07	122.54	110.40
2	H	185	VAL	CA-CB-CG1	-6.07	101.79	110.90
1	G	57	MET	CA-CB-CG	6.07	123.61	113.30
2	H	257	ALA	CB-CA-C	6.06	119.19	110.10
2	B	185	VAL	CA-CB-CG1	-6.06	101.82	110.90
1	K	47	ARG	NH1-CZ-NH2	-6.05	112.74	119.40
1	O	47	ARG	NH1-CZ-NH2	-6.05	112.74	119.40
2	H	183	LEU	CA-C-O	6.05	132.81	120.10
2	B	183	LEU	CA-C-O	6.05	132.80	120.10
2	B	171	THR	CA-C-O	-6.05	107.40	120.10
1	A	57	MET	CA-CB-CG	6.03	123.56	113.30
1	K	197	THR	N-CA-CB	6.03	121.76	110.30
1	O	197	THR	N-CA-CB	6.03	121.76	110.30
2	H	171	THR	CA-C-O	-6.03	107.44	120.10
1	M	69	ASP	CB-CG-OD1	6.03	123.72	118.30
2	D	68	LEU	CA-CB-CG	6.00	129.11	115.30
2	D	113	SER	CA-CB-OG	-6.00	95.00	111.20
2	F	113	SER	CA-CB-OG	-6.00	95.00	111.20
2	L	60	ARG	CA-CB-CG	6.00	126.59	113.40
2	P	60	ARG	CA-CB-CG	6.00	126.59	113.40
2	F	68	LEU	CA-CB-CG	5.99	129.09	115.30
2	B	68	LEU	CA-CB-CG	5.99	129.08	115.30
2	H	68	LEU	CA-CB-CG	5.99	129.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	69	ASP	CB-CG-OD1	5.99	123.69	118.30
1	K	27	GLU	CB-CA-C	5.99	122.38	110.40
1	O	27	GLU	CB-CA-C	5.99	122.38	110.40
2	D	171	THR	C-N-CA	-5.96	106.79	121.70
2	F	171	THR	C-N-CA	-5.96	106.79	121.70
1	A	132	ARG	NE-CZ-NH1	-5.94	117.33	120.30
2	D	171	THR	CA-C-O	-5.94	107.62	120.10
2	F	171	THR	CA-C-O	-5.94	107.62	120.10
2	B	210	THR	OG1-CB-CG2	-5.94	96.33	110.00
2	H	210	THR	OG1-CB-CG2	-5.94	96.35	110.00
2	D	183	LEU	CA-C-O	5.93	132.56	120.10
2	F	183	LEU	CA-C-O	5.93	132.56	120.10
1	G	132	ARG	NE-CZ-NH1	-5.93	117.34	120.30
2	P	92	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	148	TYR	CB-CG-CD1	5.92	124.55	121.00
1	E	148	TYR	CB-CG-CD1	5.92	124.55	121.00
2	D	92	ARG	CB-CA-C	-5.92	98.57	110.40
2	F	92	ARG	CB-CA-C	-5.92	98.57	110.40
1	G	47	ARG	NH1-CZ-NH2	5.90	125.89	119.40
2	L	92	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	L	40	THR	N-CA-CB	-5.90	99.10	110.30
2	P	40	THR	N-CA-CB	-5.90	99.10	110.30
1	A	47	ARG	NH1-CZ-NH2	5.89	125.88	119.40
1	C	41	ASP	CA-CB-CG	-5.89	100.45	113.40
1	E	41	ASP	CA-CB-CG	-5.89	100.45	113.40
1	I	9	VAL	N-CA-CB	5.88	124.43	111.50
2	B	209	PHE	CB-CG-CD1	-5.87	116.69	120.80
1	M	9	VAL	CA-CB-CG2	5.87	119.70	110.90
2	B	199	GLY	O-C-N	-5.86	113.32	122.70
2	H	199	GLY	O-C-N	-5.86	113.32	122.70
2	B	227	ARG	CD-NE-CZ	-5.86	115.39	123.60
2	H	227	ARG	CD-NE-CZ	-5.86	115.39	123.60
2	N	175	TYR	N-CA-C	5.86	126.82	111.00
2	J	175	TYR	N-CA-C	5.85	126.80	111.00
1	M	9	VAL	N-CA-CB	5.85	124.37	111.50
2	D	72	SER	C-N-CA	-5.84	110.03	122.30
2	F	72	SER	C-N-CA	-5.84	110.03	122.30
1	I	9	VAL	CA-CB-CG2	5.84	119.66	110.90
2	H	9	THR	CA-CB-OG1	-5.82	96.77	109.00
2	N	162	ASP	CB-CG-OD2	5.82	123.54	118.30
2	H	209	PHE	CB-CG-CD1	-5.81	116.73	120.80
2	B	9	THR	CA-CB-OG1	-5.81	96.80	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	84	TRP	CB-CG-CD1	-5.81	119.45	127.00
1	E	84	TRP	CB-CG-CD1	-5.81	119.45	127.00
2	J	94	VAL	N-CA-CB	5.81	124.27	111.50
2	N	94	VAL	N-CA-CB	5.80	124.27	111.50
2	B	136	ASN	O-C-N	-5.80	113.42	122.70
2	J	162	ASP	CB-CG-OD2	5.80	123.52	118.30
2	L	175	TYR	N-CA-C	5.80	126.66	111.00
1	M	27	GLU	O-C-N	-5.80	113.42	122.70
2	P	175	TYR	N-CA-C	5.80	126.66	111.00
2	L	69	SER	CB-CA-C	-5.80	99.08	110.10
1	M	91	PRO	N-CA-CB	-5.80	96.22	102.60
1	I	91	PRO	N-CA-CB	-5.80	96.22	102.60
2	H	136	ASN	O-C-N	-5.78	113.45	122.70
2	P	69	SER	CB-CA-C	-5.78	99.11	110.10
1	I	27	GLU	O-C-N	-5.78	113.45	122.70
2	B	126	ILE	CA-CB-CG1	-5.78	100.02	111.00
2	H	126	ILE	CA-CB-CG1	-5.78	100.02	111.00
1	A	186	THR	N-CA-CB	5.78	121.27	110.30
1	G	186	THR	N-CA-CB	5.78	121.27	110.30
2	H	162	ASP	CB-CG-OD2	-5.77	113.10	118.30
2	D	136	ASN	O-C-N	-5.77	113.47	122.70
2	B	38	LEU	CA-CB-CG	-5.76	102.04	115.30
2	F	196	TYR	CD1-CE1-CZ	-5.76	114.61	119.80
2	H	38	LEU	CA-CB-CG	-5.76	102.04	115.30
2	H	103	TRP	NE1-CE2-CZ2	-5.76	124.06	130.40
2	F	136	ASN	O-C-N	-5.76	113.48	122.70
1	A	52	PRO	CA-N-CD	-5.76	103.44	111.50
1	G	52	PRO	CA-N-CD	-5.76	103.44	111.50
1	I	41	ASP	N-CA-CB	5.76	120.97	110.60
1	M	41	ASP	N-CA-CB	5.76	120.97	110.60
1	K	95	LYS	C-N-CA	5.76	136.09	121.70
1	O	95	LYS	C-N-CA	5.76	136.09	121.70
2	B	167	ASP	O-C-N	-5.75	113.50	122.70
2	H	167	ASP	O-C-N	-5.75	113.50	122.70
2	B	72	SER	C-N-CA	-5.75	110.23	122.30
2	H	72	SER	C-N-CA	-5.75	110.23	122.30
2	B	103	TRP	NE1-CE2-CZ2	-5.74	124.08	130.40
2	N	108	TYR	CB-CG-CD2	5.74	124.44	121.00
1	C	39	ASN	O-C-N	-5.74	113.52	122.70
1	E	39	ASN	O-C-N	-5.74	113.52	122.70
2	B	162	ASP	CB-CG-OD2	-5.73	113.14	118.30
2	B	201	THR	OG1-CB-CG2	5.73	123.18	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	176	PRO	CB-CA-C	-5.73	97.67	112.00
2	F	176	PRO	CB-CA-C	-5.73	97.67	112.00
2	H	201	THR	OG1-CB-CG2	5.73	123.18	110.00
2	B	78	SER	N-CA-CB	-5.73	101.91	110.50
2	H	78	SER	N-CA-CB	-5.73	101.91	110.50
1	M	95	LYS	C-N-CA	5.72	136.01	121.70
2	D	46	ASN	CA-CB-CG	5.72	125.98	113.40
2	F	46	ASN	CA-CB-CG	5.72	125.98	113.40
1	A	22	VAL	O-C-N	-5.72	113.55	122.70
2	D	21	TYR	CB-CG-CD2	-5.72	117.57	121.00
2	F	21	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	I	95	LYS	C-N-CA	5.71	135.99	121.70
2	J	108	TYR	CB-CG-CD2	5.71	124.43	121.00
2	L	98	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	P	98	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	B	101	LYS	N-CA-CB	-5.71	100.32	110.60
1	G	22	VAL	O-C-N	-5.71	113.57	122.70
2	H	101	LYS	N-CA-CB	-5.71	100.33	110.60
2	D	196	TYR	CD1-CE1-CZ	-5.70	114.67	119.80
1	C	193	TYR	C-N-CA	-5.70	110.33	122.30
1	E	193	TYR	C-N-CA	-5.70	110.33	122.30
2	B	47	ASP	CB-CG-OD2	-5.69	113.17	118.30
2	H	47	ASP	CB-CG-OD2	-5.69	113.17	118.30
1	A	105	LEU	CB-CG-CD1	-5.69	101.33	111.00
2	J	16	GLY	N-CA-C	5.67	127.28	113.10
2	N	16	GLY	N-CA-C	5.67	127.28	113.10
1	O	156	ASN	CB-CG-OD1	-5.67	110.26	121.60
1	K	156	ASN	CB-CG-OD1	-5.67	110.27	121.60
1	G	105	LEU	CB-CG-CD1	-5.66	101.38	111.00
2	B	210	THR	CA-CB-OG1	-5.66	97.12	109.00
2	H	210	THR	CA-CB-OG1	-5.66	97.11	109.00
2	N	153	ASP	CB-CG-OD2	-5.66	113.21	118.30
2	H	3	CYS	CA-CB-SG	5.65	124.18	114.00
2	B	13	ILE	O-C-N	-5.65	113.59	123.20
2	B	118	VAL	CG1-CB-CG2	-5.65	101.86	110.90
2	H	13	ILE	O-C-N	-5.65	113.59	123.20
2	D	103	TRP	NE1-CE2-CZ2	-5.64	124.19	130.40
2	N	70	ASN	CB-CG-OD1	5.64	132.89	121.60
2	D	82	TYR	CB-CG-CD1	5.64	124.39	121.00
2	F	82	TYR	CB-CG-CD1	5.64	124.39	121.00
2	J	153	ASP	CB-CG-OD2	-5.64	113.23	118.30
2	B	3	CYS	CA-CB-SG	5.63	124.14	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	118	VAL	CG1-CB-CG2	-5.63	101.89	110.90
1	O	91	PRO	N-CA-CB	-5.63	96.40	102.60
2	B	227	ARG	N-CA-CB	5.63	120.74	110.60
2	H	227	ARG	N-CA-CB	5.63	120.74	110.60
2	J	70	ASN	CB-CG-OD1	5.63	132.86	121.60
1	I	102	THR	C-N-CA	5.62	135.76	121.70
2	L	64	TYR	CB-CG-CD1	5.62	124.37	121.00
1	O	102	THR	C-N-CA	5.62	135.75	121.70
2	P	64	TYR	CB-CG-CD1	5.62	124.37	121.00
1	K	91	PRO	N-CA-CB	-5.62	96.42	102.60
1	K	102	THR	C-N-CA	5.62	135.75	121.70
1	K	9	VAL	N-CA-CB	5.62	123.86	111.50
1	O	9	VAL	N-CA-CB	5.62	123.86	111.50
2	F	103	TRP	NE1-CE2-CZ2	-5.61	124.23	130.40
1	M	102	THR	C-N-CA	5.61	135.73	121.70
2	D	38	LEU	CA-CB-CG	-5.61	102.40	115.30
2	F	38	LEU	CA-CB-CG	-5.61	102.40	115.30
2	L	167	ASP	O-C-N	5.60	131.66	122.70
2	P	167	ASP	O-C-N	5.60	131.66	122.70
2	N	90	THR	N-CA-CB	-5.59	99.68	110.30
2	J	69	SER	N-CA-CB	5.58	118.88	110.50
2	N	69	SER	N-CA-CB	5.58	118.88	110.50
2	B	32	GLN	O-C-N	-5.58	113.77	122.70
2	H	227	ARG	NE-CZ-NH2	5.58	123.09	120.30
2	L	162	ASP	CB-CG-OD2	5.58	123.32	118.30
2	P	162	ASP	CB-CG-OD2	5.58	123.32	118.30
2	D	211	ASN	N-CA-CB	5.58	120.64	110.60
2	F	211	ASN	N-CA-CB	5.58	120.64	110.60
2	H	56	VAL	CA-C-O	5.58	131.81	120.10
2	J	54	ASP	CB-CG-OD2	5.58	123.32	118.30
2	J	90	THR	N-CA-CB	-5.57	99.71	110.30
2	N	70	ASN	CB-CA-C	5.57	121.54	110.40
2	J	70	ASN	CB-CA-C	5.56	121.52	110.40
2	B	56	VAL	CA-C-O	5.56	131.77	120.10
1	A	41	ASP	CA-CB-CG	-5.56	101.18	113.40
1	G	41	ASP	CA-CB-CG	-5.56	101.18	113.40
2	H	32	GLN	O-C-N	-5.55	113.81	122.70
1	K	9	VAL	CA-CB-CG2	5.55	119.23	110.90
1	O	9	VAL	CA-CB-CG2	5.55	119.23	110.90
2	D	254	ALA	CB-CA-C	-5.54	101.79	110.10
2	F	254	ALA	CB-CA-C	-5.54	101.79	110.10
2	L	173	PRO	CA-N-CD	-5.54	103.75	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	173	PRO	CA-N-CD	-5.54	103.75	111.50
1	K	32	LEU	CA-CB-CG	5.53	128.03	115.30
1	O	32	LEU	CA-CB-CG	5.53	128.03	115.30
2	B	227	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	E	173	SER	O-C-N	5.53	131.54	122.70
1	I	7	THR	CA-CB-CG2	-5.53	104.66	112.40
2	N	54	ASP	CB-CG-OD2	5.53	123.27	118.30
2	B	188	ALA	O-C-N	-5.52	113.87	122.70
2	D	13	ILE	O-C-N	-5.52	113.82	123.20
1	C	173	SER	O-C-N	5.51	131.51	122.70
2	F	13	ILE	O-C-N	-5.51	113.84	123.20
1	M	7	THR	CA-CB-CG2	-5.50	104.69	112.40
2	N	172	LEU	CB-CA-C	5.50	120.66	110.20
2	D	257	ALA	CB-CA-C	5.50	118.35	110.10
1	C	51	THR	CA-CB-OG1	-5.50	97.45	109.00
2	H	188	ALA	O-C-N	-5.50	113.91	122.70
1	C	31	TYR	CB-CG-CD2	-5.49	117.70	121.00
2	D	139	SER	CB-CA-C	5.49	120.54	110.10
1	E	31	TYR	CB-CG-CD2	-5.49	117.70	121.00
2	F	139	SER	CB-CA-C	5.49	120.54	110.10
2	J	172	LEU	CB-CA-C	5.49	120.63	110.20
1	E	51	THR	CA-CB-OG1	-5.49	97.48	109.00
2	L	94	VAL	N-CA-CB	5.49	123.57	111.50
2	P	94	VAL	N-CA-CB	5.49	123.57	111.50
2	D	14	GLY	CA-C-N	5.48	127.17	116.20
2	F	14	GLY	CA-C-N	5.48	127.17	116.20
2	D	168	VAL	O-C-N	-5.48	113.93	122.70
2	F	168	VAL	O-C-N	-5.48	113.93	122.70
2	F	257	ALA	CB-CA-C	5.48	118.31	110.10
2	J	64	TYR	CB-CG-CD1	5.47	124.28	121.00
2	N	64	TYR	CB-CG-CD1	5.47	124.28	121.00
1	E	57	MET	CA-CB-CG	5.47	122.59	113.30
1	C	186	THR	N-CA-CB	5.46	120.67	110.30
1	E	186	THR	N-CA-CB	5.46	120.67	110.30
2	D	3	CYS	CA-CB-SG	5.46	123.82	114.00
2	F	3	CYS	CA-CB-SG	5.46	123.82	114.00
2	D	41	GLN	N-CA-CB	5.45	120.41	110.60
1	K	116	ARG	CD-NE-CZ	5.45	131.23	123.60
1	O	116	ARG	CD-NE-CZ	5.45	131.23	123.60
1	C	57	MET	CA-CB-CG	5.45	122.56	113.30
1	K	41	ASP	N-CA-CB	5.44	120.40	110.60
1	O	41	ASP	N-CA-CB	5.44	120.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	227	ARG	CB-CG-CD	5.44	125.74	111.60
2	F	227	ARG	CB-CG-CD	5.44	125.74	111.60
1	C	41	ASP	CB-CG-OD1	-5.44	113.41	118.30
1	E	41	ASP	CB-CG-OD1	-5.44	113.41	118.30
1	C	8	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
1	E	8	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
2	F	41	GLN	N-CA-CB	5.43	120.38	110.60
2	L	204	ALA	CB-CA-C	5.43	118.25	110.10
1	M	172	GLU	CA-C-O	5.43	131.51	120.10
2	P	204	ALA	CB-CA-C	5.43	118.25	110.10
2	J	94	VAL	CA-CB-CG1	5.43	119.04	110.90
2	N	94	VAL	CA-CB-CG1	5.43	119.04	110.90
1	I	172	GLU	CA-C-O	5.42	131.49	120.10
1	G	44	LYS	N-CA-CB	5.42	120.35	110.60
1	A	44	LYS	N-CA-CB	5.41	120.34	110.60
1	C	173	SER	N-CA-CB	5.41	118.61	110.50
1	E	173	SER	N-CA-CB	5.41	118.61	110.50
2	F	101	LYS	N-CA-CB	-5.40	100.88	110.60
2	D	101	LYS	N-CA-CB	-5.39	100.90	110.60
2	P	94	VAL	CA-CB-CG1	5.38	118.97	110.90
1	K	105	LEU	CA-CB-CG	5.38	127.67	115.30
1	O	105	LEU	CA-CB-CG	5.38	127.67	115.30
2	L	227	ARG	NH1-CZ-NH2	-5.38	113.49	119.40
2	P	227	ARG	NH1-CZ-NH2	-5.38	113.49	119.40
2	B	235	ASN	CB-CG-OD1	5.37	132.34	121.60
2	H	235	ASN	CB-CG-OD1	5.36	132.33	121.60
2	H	172	LEU	CB-CA-C	5.36	120.38	110.20
1	A	84	TRP	CB-CG-CD1	-5.36	120.03	127.00
2	L	94	VAL	CA-CB-CG1	5.36	118.94	110.90
2	D	169	THR	N-CA-C	5.36	125.47	111.00
2	F	169	THR	N-CA-C	5.36	125.47	111.00
2	H	132	ARG	CB-CG-CD	5.35	125.52	111.60
2	L	70	ASN	CB-CA-C	5.35	121.10	110.40
2	P	70	ASN	CB-CA-C	5.35	121.10	110.40
1	C	8	ARG	CG-CD-NE	-5.35	100.56	111.80
1	E	8	ARG	CG-CD-NE	-5.35	100.56	111.80
2	B	132	ARG	CB-CG-CD	5.35	125.50	111.60
2	B	172	LEU	CB-CA-C	5.34	120.36	110.20
1	G	84	TRP	CB-CG-CD1	-5.34	120.05	127.00
2	L	57	THR	N-CA-CB	-5.34	100.15	110.30
2	P	57	THR	N-CA-CB	-5.34	100.15	110.30
2	L	54	ASP	CB-CG-OD2	5.33	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	54	ASP	CB-CG-OD2	5.33	123.10	118.30
1	M	105	LEU	CA-CB-CG	5.33	127.56	115.30
2	L	90	THR	N-CA-CB	-5.33	100.18	110.30
2	P	90	THR	N-CA-CB	-5.33	100.18	110.30
1	I	105	LEU	CA-CB-CG	5.33	127.55	115.30
1	C	78	ASP	N-CA-CB	-5.32	101.03	110.60
1	E	78	ASP	N-CA-CB	-5.32	101.03	110.60
1	K	185	ILE	C-N-CA	5.31	134.98	121.70
1	O	185	ILE	C-N-CA	5.31	134.98	121.70
2	H	169	THR	N-CA-C	5.31	125.34	111.00
2	F	196	TYR	CG-CD1-CE1	5.31	125.55	121.30
2	B	169	THR	N-CA-C	5.30	125.31	111.00
2	D	60	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	F	60	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	78	ASP	N-CA-CB	-5.29	101.08	110.60
1	G	78	ASP	N-CA-CB	-5.29	101.08	110.60
2	H	236	ASN	CA-CB-CG	5.28	125.02	113.40
2	D	65	GLY	C-N-CA	5.28	133.38	122.30
1	C	132	ARG	NH1-CZ-NH2	5.27	125.19	119.40
2	D	126	ILE	CA-CB-CG1	-5.27	100.99	111.00
2	D	196	TYR	CG-CD1-CE1	5.26	125.51	121.30
1	I	32	LEU	CA-CB-CG	5.26	127.41	115.30
2	B	236	ASN	CA-CB-CG	5.26	124.98	113.40
2	F	242	ALA	CB-CA-C	5.26	117.99	110.10
1	M	32	LEU	CA-CB-CG	5.26	127.40	115.30
2	L	16	GLY	N-CA-C	5.26	126.25	113.10
2	P	16	GLY	N-CA-C	5.26	126.25	113.10
1	K	132	ARG	CD-NE-CZ	5.26	130.96	123.60
1	O	132	ARG	CD-NE-CZ	5.26	130.96	123.60
1	E	52	PRO	CA-N-CD	-5.25	104.14	111.50
2	F	65	GLY	C-N-CA	5.25	133.33	122.30
2	F	126	ILE	CA-CB-CG1	-5.24	101.04	111.00
1	C	52	PRO	CA-N-CD	-5.24	104.17	111.50
2	D	242	ALA	CB-CA-C	5.24	117.95	110.10
2	J	57	THR	N-CA-CB	-5.23	100.36	110.30
2	N	57	THR	N-CA-CB	-5.23	100.36	110.30
2	D	233	PRO	CA-C-N	5.23	128.71	117.20
2	F	233	PRO	CA-C-N	5.23	128.71	117.20
2	B	92	ARG	CB-CA-C	-5.23	99.94	110.40
2	H	92	ARG	CB-CA-C	-5.23	99.94	110.40
2	D	70	ASN	CB-CA-C	-5.23	99.94	110.40
1	E	22	VAL	O-C-N	-5.23	114.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	70	ASN	CB-CA-C	-5.23	99.94	110.40
1	E	132	ARG	NH1-CZ-NH2	5.22	125.15	119.40
2	J	197	LEU	C-N-CA	5.22	134.76	121.70
2	B	32	GLN	CA-C-O	5.22	131.06	120.10
1	M	148	TYR	CB-CG-CD1	5.21	124.13	121.00
2	D	185	VAL	CA-CB-CG1	-5.21	103.08	110.90
2	F	185	VAL	CA-CB-CG1	-5.21	103.08	110.90
2	H	32	GLN	CA-C-O	5.21	131.05	120.10
2	N	197	LEU	C-N-CA	5.21	134.73	121.70
1	C	22	VAL	O-C-N	-5.21	114.37	122.70
2	H	41	GLN	N-CA-CB	5.21	119.97	110.60
1	K	172	GLU	CA-C-O	5.20	131.01	120.10
2	B	41	GLN	N-CA-CB	5.19	119.94	110.60
2	D	229	GLY	CA-C-O	-5.19	111.26	120.60
2	L	103	TRP	CH2-CZ2-CE2	-5.19	112.21	117.40
2	P	103	TRP	CH2-CZ2-CE2	-5.19	112.21	117.40
2	F	236	ASN	CA-CB-CG	5.19	124.81	113.40
1	O	172	GLU	CA-C-O	5.18	130.99	120.10
2	D	118	VAL	CG1-CB-CG2	-5.18	102.61	110.90
2	F	118	VAL	CG1-CB-CG2	-5.18	102.61	110.90
2	B	254	ALA	CB-CA-C	-5.17	102.34	110.10
1	C	149	TYR	CB-CG-CD2	-5.17	117.90	121.00
2	D	236	ASN	CA-CB-CG	5.17	124.78	113.40
1	E	149	TYR	CB-CG-CD2	-5.17	117.90	121.00
2	F	229	GLY	CA-C-O	-5.17	111.29	120.60
2	H	254	ALA	CB-CA-C	-5.17	102.34	110.10
1	E	85	MET	CB-CA-C	5.17	120.75	110.40
1	C	85	MET	CB-CA-C	5.17	120.75	110.40
1	E	31	TYR	CB-CA-C	-5.17	100.06	110.40
1	A	193	TYR	CB-CG-CD1	-5.16	117.90	121.00
2	D	57	THR	OG1-CB-CG2	5.16	121.87	110.00
2	F	57	THR	OG1-CB-CG2	5.16	121.87	110.00
2	F	123	GLY	CA-C-N	5.16	128.56	117.20
1	G	193	TYR	CB-CG-CD1	-5.16	117.90	121.00
2	B	168	VAL	O-C-N	-5.16	114.45	122.70
2	H	168	VAL	O-C-N	-5.16	114.45	122.70
1	C	31	TYR	CB-CA-C	-5.16	100.09	110.40
2	D	123	GLY	CA-C-N	5.16	128.54	117.20
2	D	94	VAL	CG1-CB-CG2	-5.15	102.65	110.90
2	F	94	VAL	CG1-CB-CG2	-5.15	102.65	110.90
2	H	103	TRP	CD2-CE3-CZ3	-5.15	112.10	118.80
1	I	148	TYR	CB-CG-CD1	5.15	124.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	24	LEU	CA-C-O	-5.15	109.29	120.10
2	B	211	ASN	N-CA-CB	5.14	119.86	110.60
2	B	103	TRP	CD2-CE3-CZ3	-5.14	112.12	118.80
2	D	24	LEU	CA-C-O	-5.14	109.31	120.10
2	H	211	ASN	N-CA-CB	5.14	119.85	110.60
1	C	112	LYS	CB-CA-C	-5.14	100.12	110.40
2	J	172	LEU	C-N-CA	5.14	143.57	122.00
2	N	172	LEU	C-N-CA	5.14	143.57	122.00
2	B	108	TYR	CA-C-O	-5.12	109.34	120.10
2	H	108	TYR	CA-C-O	-5.12	109.34	120.10
2	D	172	LEU	CB-CA-C	5.12	119.93	110.20
2	F	172	LEU	CB-CA-C	5.12	119.93	110.20
1	M	204	MET	CA-CB-CG	5.12	122.01	113.30
1	M	8	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	E	112	LYS	CB-CA-C	-5.11	100.17	110.40
2	B	259	THR	CA-CB-CG2	-5.11	105.25	112.40
2	H	259	THR	CA-CB-CG2	-5.11	105.25	112.40
2	D	161	CYS	CA-CB-SG	-5.10	104.81	114.00
2	F	161	CYS	CA-CB-SG	-5.10	104.81	114.00
1	I	204	MET	CA-CB-CG	5.10	121.97	113.30
1	I	8	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	M	132	ARG	CD-NE-CZ	5.09	130.73	123.60
2	B	27	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	G	39	ASN	O-C-N	-5.09	114.55	122.70
1	M	73	ASN	CA-C-O	5.09	130.79	120.10
1	I	73	ASN	CA-C-O	5.09	130.78	120.10
2	J	89	GLU	OE1-CD-OE2	-5.08	117.20	123.30
2	H	27	VAL	CG1-CB-CG2	-5.08	102.78	110.90
1	I	132	ARG	CD-NE-CZ	5.08	130.71	123.60
1	K	73	ASN	CA-C-O	5.08	130.76	120.10
2	N	77	TYR	CB-CG-CD2	5.08	124.05	121.00
2	B	229	GLY	CA-C-O	-5.08	111.46	120.60
1	C	41	ASP	CA-C-O	-5.07	109.45	120.10
1	E	41	ASP	CA-C-O	-5.07	109.45	120.10
2	N	191	GLN	N-CA-CB	-5.07	101.47	110.60
1	O	73	ASN	CA-C-O	5.07	130.75	120.10
1	A	39	ASN	O-C-N	-5.07	114.58	122.70
2	H	185	VAL	N-CA-CB	5.07	122.66	111.50
2	B	185	VAL	N-CA-CB	5.07	122.65	111.50
1	C	36	TRP	CB-CG-CD2	5.07	133.19	126.60
2	J	191	GLN	N-CA-CB	-5.07	101.48	110.60
2	H	229	GLY	CA-C-O	-5.07	111.48	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	235	ASN	CB-CG-OD1	5.07	131.73	121.60
2	F	235	ASN	CB-CG-OD1	5.07	131.73	121.60
2	J	249	SER	CB-CA-C	-5.06	100.48	110.10
2	B	84	PHE	CZ-CE2-CD2	5.06	126.17	120.10
2	N	249	SER	CB-CA-C	-5.06	100.49	110.10
2	B	113	SER	CB-CA-C	-5.05	100.50	110.10
2	H	113	SER	CB-CA-C	-5.05	100.50	110.10
2	H	84	PHE	CZ-CE2-CD2	5.05	126.16	120.10
1	A	109	SER	N-CA-CB	5.05	118.08	110.50
2	N	89	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	E	36	TRP	CB-CG-CD2	5.04	133.15	126.60
2	N	258	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	G	109	SER	N-CA-CB	5.04	118.05	110.50
1	G	84	TRP	CH2-CZ2-CE2	-5.03	112.37	117.40
2	J	77	TYR	CB-CG-CD2	5.03	124.02	121.00
2	P	69	SER	N-CA-CB	5.03	118.05	110.50
1	I	116	ARG	CD-NE-CZ	5.02	130.63	123.60
2	D	162	ASP	CB-CG-OD2	-5.02	113.78	118.30
2	F	162	ASP	CB-CG-OD2	-5.02	113.78	118.30
2	J	258	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	N	227	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
2	L	69	SER	N-CA-CB	5.02	118.03	110.50
2	D	227	ARG	N-CA-CB	5.01	119.63	110.60
2	F	227	ARG	N-CA-CB	5.01	119.63	110.60
1	A	84	TRP	CH2-CZ2-CE2	-5.01	112.39	117.40
2	D	210	THR	CA-CB-OG1	-5.01	98.49	109.00
2	F	210	THR	CA-CB-OG1	-5.00	98.49	109.00
1	K	204	MET	CA-CB-CG	5.00	121.81	113.30
1	M	116	ARG	CD-NE-CZ	5.00	130.61	123.60
1	O	204	MET	CA-CB-CG	5.00	121.81	113.30
1	M	27	GLU	N-CA-C	5.00	124.51	111.00

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	176	PRO	CA
2	F	176	PRO	CA
1	I	156	ASN	CA
2	J	215	PHE	CA
2	L	215	PHE	CA
1	M	156	ASN	CA
2	N	215	PHE	CA

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Mol	Chain	Res	Type	Atom
2	P	215	PHE	CA

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ASN	Mainchain
1	A	45	ASP	Mainchain
1	A	51	THR	Peptide,Mainchain
2	B	103	TRP	Mainchain
2	B	122	ALA	Mainchain
2	B	171	THR	Mainchain
2	B	24	LEU	Mainchain
2	B	274	VAL	Mainchain
2	B	35	VAL	Mainchain
2	B	58	LEU	Mainchain
1	C	25	ASN	Mainchain
1	C	45	ASP	Mainchain
1	C	51	THR	Peptide,Mainchain
2	D	103	TRP	Mainchain
2	D	171	THR	Mainchain
2	D	175	TYR	Peptide
2	D	274	VAL	Mainchain
2	D	35	VAL	Mainchain
2	D	36	VAL	Mainchain
2	D	58	LEU	Mainchain
1	E	25	ASN	Mainchain
1	E	45	ASP	Mainchain
1	E	51	THR	Peptide,Mainchain
2	F	103	TRP	Mainchain
2	F	171	THR	Mainchain
2	F	175	TYR	Peptide
2	F	274	VAL	Mainchain
2	F	35	VAL	Mainchain
2	F	36	VAL	Mainchain
2	F	58	LEU	Mainchain
1	G	25	ASN	Mainchain
1	G	45	ASP	Mainchain
1	G	51	THR	Peptide,Mainchain
2	H	103	TRP	Mainchain
2	H	122	ALA	Mainchain
2	H	171	THR	Mainchain
2	H	24	LEU	Mainchain

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Mol	Chain	Res	Type	Group
2	H	274	VAL	Mainchain
2	H	35	VAL	Mainchain
2	H	58	LEU	Mainchain
1	I	135	ARG	Mainchain
1	I	139	SER	Peptide
1	I	156	ASN	Sidechain
1	I	26	ASP	Sidechain,Mainchain
1	I	27	GLU	Mainchain
1	I	47	ARG	Sidechain
1	I	70	ALA	Peptide,Mainchain
2	J	165	ALA	Peptide,Mainchain
2	J	171	THR	Mainchain
2	J	172	LEU	Peptide
1	K	135	ARG	Mainchain
1	K	139	SER	Peptide,Mainchain
1	K	156	ASN	Mainchain
1	K	26	ASP	Sidechain,Mainchain
1	K	27	GLU	Mainchain
1	K	47	ARG	Sidechain
1	K	70	ALA	Peptide,Mainchain
2	L	165	ALA	Peptide,Mainchain
2	L	171	THR	Mainchain
1	M	135	ARG	Mainchain
1	M	139	SER	Peptide
1	M	156	ASN	Sidechain
1	M	26	ASP	Sidechain,Mainchain
1	M	27	GLU	Mainchain
1	M	47	ARG	Sidechain
1	M	70	ALA	Peptide,Mainchain
2	N	165	ALA	Peptide,Mainchain
2	N	171	THR	Mainchain
2	N	172	LEU	Peptide
1	O	135	ARG	Mainchain
1	O	139	SER	Peptide,Mainchain
1	O	156	ASN	Mainchain
1	O	26	ASP	Sidechain,Mainchain
1	O	27	GLU	Mainchain
1	O	47	ARG	Sidechain
1	O	70	ALA	Peptide,Mainchain
2	P	165	ALA	Peptide,Mainchain
2	P	171	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1553	0	1587	48	0
1	C	1553	0	1587	42	0
1	E	1553	0	1587	41	0
1	G	1553	0	1587	44	0
1	I	1543	0	1576	110	0
1	K	1543	0	1576	107	0
1	M	1543	0	1576	109	0
1	O	1543	0	1576	105	0
2	B	2052	0	2006	83	0
2	D	2052	0	2006	80	0
2	F	2052	0	2006	82	0
2	H	2052	0	2006	81	0
2	J	2052	0	2003	114	0
2	L	2052	0	2004	118	0
2	N	2052	0	2003	114	0
2	P	2052	0	2004	114	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
3	C	6	0	0	0	0
3	D	11	0	0	1	0
3	E	5	0	0	0	0
3	F	12	0	0	1	0
3	G	5	0	0	0	0
3	H	10	0	0	1	0
All	All	28864	0	28690	1311	0

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

All (1311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:197:THR:HB	1:O:198:PRO:HD2	1.45	0.98
2:N:53:THR:H	2:N:136:ASN:HD21	1.08	0.98
2:J:53:THR:H	2:J:136:ASN:HD21	1.08	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:THR:HG22	2:B:253:THR:HB	1.45	0.98
1:I:197:THR:HB	1:I:198:PRO:HD2	1.46	0.98
1:K:197:THR:HB	1:K:198:PRO:HD2	1.45	0.98
2:L:53:THR:H	2:L:136:ASN:HD21	1.08	0.97
1:M:197:THR:HB	1:M:198:PRO:HD2	1.46	0.96
2:H:226:THR:HG22	2:H:253:THR:HB	1.45	0.95
1:K:6:ALA:HA	2:L:159:GLY:HA2	1.49	0.95
2:P:53:THR:H	2:P:136:ASN:HD21	1.08	0.94
2:L:53:THR:H	2:L:136:ASN:ND2	1.66	0.94
1:I:6:ALA:HA	2:J:159:GLY:HA2	1.50	0.94
2:D:226:THR:HG22	2:D:253:THR:HB	1.49	0.93
1:O:6:ALA:HA	2:P:159:GLY:HA2	1.49	0.93
1:O:4:LEU:HD21	1:O:87:VAL:HG21	1.49	0.93
2:N:53:THR:H	2:N:136:ASN:ND2	1.67	0.93
1:K:4:LEU:HD21	1:K:87:VAL:HG21	1.49	0.93
2:P:53:THR:H	2:P:136:ASN:ND2	1.66	0.93
2:J:53:THR:H	2:J:136:ASN:ND2	1.67	0.92
1:M:6:ALA:HA	2:N:159:GLY:HA2	1.50	0.92
2:F:226:THR:HG22	2:F:253:THR:HB	1.49	0.91
1:O:32:LEU:HD13	1:O:54:LEU:HD11	1.52	0.91
1:M:4:LEU:HD21	1:M:87:VAL:HG21	1.51	0.91
1:I:4:LEU:HD21	1:I:87:VAL:HG21	1.52	0.91
1:M:32:LEU:HD13	1:M:54:LEU:HD11	1.51	0.90
1:I:32:LEU:HD13	1:I:54:LEU:HD11	1.51	0.90
1:M:9:VAL:HB	1:M:113:LEU:HD13	1.54	0.89
1:K:32:LEU:HD13	1:K:54:LEU:HD11	1.52	0.89
1:O:9:VAL:HB	1:O:113:LEU:HD13	1.55	0.89
1:I:9:VAL:HB	1:I:113:LEU:HD13	1.54	0.88
2:H:5:THR:HG21	3:H:282:HOH:O	1.73	0.88
2:B:5:THR:HG21	3:B:282:HOH:O	1.73	0.87
1:K:9:VAL:HB	1:K:113:LEU:HD13	1.55	0.87
2:P:70:ASN:HB2	2:P:115:ALA:HB2	1.57	0.87
2:F:5:THR:HG21	3:F:284:HOH:O	1.75	0.85
2:N:70:ASN:HB2	2:N:115:ALA:HB2	1.57	0.85
2:J:70:ASN:HB2	2:J:115:ALA:HB2	1.57	0.85
1:A:197:THR:HB	1:A:198:PRO:HD2	1.59	0.85
1:G:197:THR:HB	1:G:198:PRO:HD2	1.59	0.84
1:M:151:THR:HG22	1:M:190:ILE:HD12	1.59	0.84
1:I:151:THR:HG22	1:I:190:ILE:HD12	1.59	0.84
2:H:219:GLN:HB2	2:H:264:THR:HB	1.60	0.84
2:L:70:ASN:HB2	2:L:115:ALA:HB2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:THR:HG21	3:D:284:HOH:O	1.76	0.83
2:D:92:ARG:HG2	2:D:92:ARG:HH11	1.43	0.83
2:H:163:VAL:HG22	2:H:185:VAL:HG13	1.60	0.83
2:D:163:VAL:HG22	2:D:185:VAL:HG13	1.59	0.82
2:F:163:VAL:HG22	2:F:185:VAL:HG13	1.59	0.82
1:K:151:THR:HG22	1:K:190:ILE:HD12	1.61	0.82
2:B:219:GLN:HB2	2:B:264:THR:HB	1.60	0.82
2:J:57:THR:HG21	2:J:89:GLU:OE2	1.80	0.82
1:O:18:VAL:HG12	1:O:19:GLN:H	1.45	0.82
2:B:163:VAL:HG22	2:B:185:VAL:HG13	1.60	0.82
1:E:112:LYS:NZ	2:F:279:GLN:O	2.13	0.81
2:F:92:ARG:HG2	2:F:92:ARG:HH11	1.43	0.81
1:I:18:VAL:HG12	1:I:19:GLN:H	1.45	0.81
1:M:133:PHE:O	1:M:134:ARG:HB2	1.80	0.81
1:O:151:THR:HG22	1:O:190:ILE:HD12	1.61	0.81
2:B:92:ARG:HH11	2:B:92:ARG:HG2	1.45	0.81
2:N:17:SER:HB3	2:N:145:VAL:HB	1.63	0.81
2:N:57:THR:HG21	2:N:89:GLU:OE2	1.80	0.81
2:H:92:ARG:HG2	2:H:92:ARG:HH11	1.45	0.81
1:C:112:LYS:NZ	2:D:279:GLN:O	2.13	0.80
2:J:17:SER:HB3	2:J:145:VAL:HB	1.63	0.80
1:K:18:VAL:HG12	1:K:19:GLN:H	1.45	0.80
1:A:51:THR:HG22	1:A:66:ARG:HG3	1.64	0.80
1:M:18:VAL:HG12	1:M:19:GLN:H	1.45	0.80
1:O:133:PHE:O	1:O:134:ARG:HB2	1.81	0.80
2:P:226:THR:HG22	2:P:253:THR:HB	1.64	0.80
2:B:184:THR:HG23	2:B:247:ALA:HB1	1.62	0.79
1:I:133:PHE:O	1:I:134:ARG:HB2	1.80	0.79
2:N:258:ARG:NH2	2:N:263:VAL:HG23	1.97	0.79
2:H:184:THR:HG23	2:H:247:ALA:HB1	1.62	0.79
2:L:57:THR:HG21	2:L:89:GLU:OE2	1.83	0.79
2:N:40:THR:CG2	2:N:41:GLN:HE21	1.96	0.79
2:P:17:SER:HB3	2:P:145:VAL:HB	1.65	0.79
2:J:258:ARG:NH2	2:J:263:VAL:HG23	1.97	0.79
2:L:40:THR:CG2	2:L:41:GLN:HE21	1.95	0.79
2:P:40:THR:CG2	2:P:41:GLN:HE21	1.95	0.79
2:N:14:GLY:HA2	2:N:142:PHE:CD1	2.18	0.79
1:G:51:THR:HG22	1:G:66:ARG:HG3	1.64	0.78
1:K:133:PHE:O	1:K:134:ARG:HB2	1.81	0.78
2:J:40:THR:CG2	2:J:41:GLN:HE21	1.96	0.78
2:P:57:THR:HG21	2:P:89:GLU:OE2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:14:GLY:HA2	2:J:142:PHE:CD1	2.18	0.78
2:D:184:THR:HG23	2:D:247:ALA:HB1	1.64	0.78
2:J:67:VAL:HG21	2:J:126:ILE:HG23	1.66	0.78
2:L:226:THR:HG22	2:L:253:THR:HB	1.64	0.78
2:P:29:ASN:HB2	2:P:32:GLN:NE2	1.99	0.78
2:J:29:ASN:HB2	2:J:32:GLN:NE2	1.99	0.77
2:L:17:SER:HB3	2:L:145:VAL:HB	1.65	0.77
2:J:167:ASP:O	2:J:168:VAL:N	2.18	0.77
1:A:112:LYS:NZ	2:B:279:GLN:O	2.17	0.77
1:G:112:LYS:NZ	2:H:279:GLN:O	2.17	0.77
2:L:29:ASN:HB2	2:L:32:GLN:NE2	1.99	0.77
2:L:167:ASP:O	2:L:168:VAL:N	2.17	0.77
2:D:40:THR:CG2	2:D:41:GLN:HE21	1.97	0.77
2:F:184:THR:HG23	2:F:247:ALA:HB1	1.64	0.77
1:C:197:THR:HB	1:C:198:PRO:HD2	1.67	0.77
2:F:40:THR:CG2	2:F:41:GLN:HE21	1.97	0.77
2:N:29:ASN:HB2	2:N:32:GLN:NE2	1.99	0.77
2:J:138:ASN:HD22	2:J:138:ASN:H	1.33	0.77
2:N:67:VAL:HG21	2:N:126:ILE:HG23	1.66	0.77
1:C:51:THR:HG22	1:C:66:ARG:HG3	1.67	0.76
1:E:51:THR:HG22	1:E:66:ARG:HG3	1.67	0.76
1:E:197:THR:HB	1:E:198:PRO:HD2	1.67	0.76
2:P:167:ASP:O	2:P:168:VAL:N	2.17	0.76
1:I:197:THR:HB	1:I:198:PRO:CD	2.15	0.76
2:P:14:GLY:HA2	2:P:142:PHE:CD1	2.21	0.76
1:E:162:LEU:HD21	1:E:177:LEU:HD12	1.68	0.76
2:L:14:GLY:HA2	2:L:142:PHE:CD1	2.21	0.76
2:F:219:GLN:HB2	2:F:264:THR:HB	1.68	0.76
2:D:219:GLN:HB2	2:D:264:THR:HB	1.68	0.75
1:A:162:LEU:HD21	1:A:177:LEU:HD12	1.68	0.75
1:K:197:THR:HB	1:K:198:PRO:CD	2.16	0.75
1:M:197:THR:HB	1:M:198:PRO:CD	2.15	0.75
2:N:167:ASP:O	2:N:168:VAL:N	2.18	0.75
2:N:138:ASN:HD22	2:N:138:ASN:H	1.32	0.75
2:B:201:THR:HG21	2:B:206:ASN:OD1	1.87	0.75
2:L:138:ASN:HD22	2:L:138:ASN:H	1.35	0.75
1:O:197:THR:HB	1:O:198:PRO:CD	2.16	0.75
2:B:40:THR:CG2	2:B:41:GLN:HE21	2.00	0.75
2:P:67:VAL:HG21	2:P:126:ILE:HG23	1.69	0.75
2:P:258:ARG:NH2	2:P:263:VAL:HG23	2.02	0.75
1:C:162:LEU:HD21	1:C:177:LEU:HD12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:226:THR:HG22	2:N:253:THR:HB	1.69	0.74
2:F:57:THR:HG21	2:F:89:GLU:OE1	1.87	0.74
2:L:67:VAL:HG21	2:L:126:ILE:HG23	1.69	0.74
2:H:55:TYR:HB3	2:H:92:ARG:HG3	1.70	0.74
2:L:258:ARG:NH2	2:L:263:VAL:HG23	2.02	0.74
2:D:57:THR:HG21	2:D:89:GLU:OE1	1.87	0.74
1:G:162:LEU:HD21	1:G:177:LEU:HD12	1.68	0.74
2:P:211:ASN:HD22	2:P:269:GLN:H	1.36	0.74
1:K:2:VAL:HG12	1:K:24:ASN:HA	1.69	0.74
2:H:40:THR:CG2	2:H:41:GLN:HE21	2.00	0.74
2:D:201:THR:HG21	2:D:206:ASN:OD1	1.89	0.73
2:F:184:THR:CG2	2:F:247:ALA:HB1	2.18	0.73
2:H:201:THR:HG21	2:H:206:ASN:OD1	1.87	0.73
1:O:2:VAL:HG12	1:O:24:ASN:HA	1.69	0.73
2:D:184:THR:CG2	2:D:247:ALA:HB1	2.18	0.73
2:N:40:THR:HG22	2:N:41:GLN:HE21	1.54	0.73
2:P:138:ASN:H	2:P:138:ASN:HD22	1.35	0.73
2:F:201:THR:HG21	2:F:206:ASN:OD1	1.89	0.73
2:B:55:TYR:HB3	2:B:92:ARG:HG3	1.70	0.73
2:J:226:THR:HG22	2:J:253:THR:HB	1.69	0.73
2:J:40:THR:HG22	2:J:41:GLN:HE21	1.54	0.73
1:O:50:VAL:HG21	1:O:85:MET:HE3	1.70	0.73
2:L:211:ASN:HD22	2:L:269:GLN:H	1.36	0.72
2:H:184:THR:CG2	2:H:247:ALA:HB1	2.19	0.72
2:N:211:ASN:HD22	2:N:269:GLN:H	1.38	0.72
2:N:122:ALA:HB2	2:N:153:ASP:H	1.54	0.72
2:B:184:THR:CG2	2:B:247:ALA:HB1	2.19	0.71
1:I:2:VAL:HG12	1:I:24:ASN:HA	1.72	0.71
2:L:29:ASN:HB2	2:L:32:GLN:HE22	1.54	0.71
2:B:57:THR:HG21	2:B:89:GLU:OE1	1.91	0.71
1:C:45:ASP:HB3	1:C:47:ARG:H	1.55	0.71
2:B:77:TYR:CD2	2:B:90:THR:HG21	2.26	0.71
2:P:58:LEU:H	2:P:90:THR:CG2	2.04	0.71
1:I:50:VAL:HG21	1:I:85:MET:HE3	1.71	0.71
2:J:29:ASN:HB2	2:J:32:GLN:HE22	1.54	0.71
2:J:122:ALA:HB2	2:J:153:ASP:H	1.54	0.71
2:P:40:THR:HG22	2:P:41:GLN:HE21	1.57	0.70
2:P:201:THR:HG21	2:P:206:ASN:ND2	2.06	0.70
2:L:201:THR:HG21	2:L:206:ASN:ND2	2.06	0.70
2:H:57:THR:HG21	2:H:89:GLU:OE1	1.91	0.70
2:N:29:ASN:HB2	2:N:32:GLN:HE22	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:THR:HG22	2:H:41:GLN:HE21	1.57	0.70
2:H:77:TYR:CD2	2:H:90:THR:HG21	2.26	0.70
1:I:169:PRO:O	1:I:170:MET:HB2	1.92	0.70
1:M:169:PRO:O	1:M:170:MET:HB2	1.92	0.70
2:N:101:LYS:HG2	2:N:102:PRO:HD2	1.73	0.70
2:B:211:ASN:ND2	2:B:269:GLN:H	1.90	0.70
2:L:58:LEU:H	2:L:90:THR:CG2	2.04	0.70
2:B:40:THR:HG22	2:B:41:GLN:HE21	1.57	0.69
2:D:138:ASN:HD21	2:D:140:ASP:HB2	1.57	0.69
2:H:211:ASN:ND2	2:H:269:GLN:H	1.90	0.69
2:J:211:ASN:HD22	2:J:269:GLN:H	1.38	0.69
2:J:101:LYS:HG2	2:J:102:PRO:HD2	1.73	0.69
2:F:55:TYR:HB3	2:F:92:ARG:HG3	1.75	0.69
2:F:138:ASN:HD21	2:F:140:ASP:HB2	1.57	0.69
1:K:50:VAL:HG21	1:K:85:MET:HE3	1.74	0.69
1:E:45:ASP:HB3	1:E:47:ARG:H	1.55	0.69
1:M:2:VAL:HG12	1:M:24:ASN:HA	1.72	0.69
2:L:40:THR:HG22	2:L:41:GLN:HE21	1.57	0.69
2:P:29:ASN:HB2	2:P:32:GLN:HE22	1.53	0.69
2:D:55:TYR:HB3	2:D:92:ARG:HG3	1.75	0.69
2:H:226:THR:CG2	2:H:253:THR:HB	2.22	0.69
1:M:50:VAL:HG21	1:M:85:MET:HE3	1.74	0.68
2:B:226:THR:CG2	2:B:253:THR:HB	2.21	0.68
2:J:58:LEU:H	2:J:90:THR:CG2	2.06	0.68
2:N:201:THR:HG21	2:N:206:ASN:ND2	2.09	0.68
1:O:7:THR:HG22	2:P:278:TYR:CD2	2.29	0.68
2:P:101:LYS:HG2	2:P:102:PRO:HD2	1.75	0.68
2:P:211:ASN:ND2	2:P:269:GLN:H	1.91	0.68
1:A:23:THR:HG22	1:A:62:GLU:HG3	1.76	0.67
2:J:58:LEU:H	2:J:90:THR:HG21	1.59	0.67
1:K:35:SER:HB3	1:K:50:VAL:HG11	1.77	0.67
1:K:7:THR:HG22	2:L:278:TYR:CD2	2.29	0.67
1:K:169:PRO:O	1:K:170:MET:HB2	1.93	0.67
2:B:38:LEU:HD13	2:B:129:LEU:HD11	1.77	0.67
1:G:23:THR:HG22	1:G:62:GLU:HG3	1.76	0.67
2:J:201:THR:HG21	2:J:206:ASN:ND2	2.09	0.67
2:L:211:ASN:ND2	2:L:269:GLN:H	1.91	0.67
2:N:58:LEU:H	2:N:90:THR:CG2	2.07	0.67
2:N:58:LEU:H	2:N:90:THR:HG21	1.59	0.67
2:P:211:ASN:HD21	2:P:268:VAL:HA	1.60	0.67
2:D:40:THR:HG23	2:D:41:GLN:HE21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:211:ASN:ND2	2:N:269:GLN:H	1.93	0.67
1:I:7:THR:HG22	2:J:278:TYR:CD2	2.31	0.66
1:O:169:PRO:O	1:O:170:MET:HB2	1.93	0.66
2:L:211:ASN:HD21	2:L:268:VAL:HA	1.60	0.66
1:M:7:THR:HG22	2:N:278:TYR:CD2	2.31	0.66
1:C:103:LEU:HD11	2:D:272:ILE:HD12	1.77	0.66
1:G:103:LEU:HD11	2:H:272:ILE:HD12	1.77	0.66
2:L:101:LYS:HG2	2:L:102:PRO:HD2	1.75	0.66
1:A:103:LEU:HD11	2:B:272:ILE:HD12	1.77	0.66
1:O:35:SER:HB3	1:O:50:VAL:HG11	1.77	0.66
2:D:226:THR:CG2	2:D:253:THR:HB	2.25	0.66
2:J:211:ASN:ND2	2:J:269:GLN:H	1.93	0.66
1:M:35:SER:HB3	1:M:50:VAL:HG11	1.78	0.66
1:K:156:ASN:ND2	1:K:156:ASN:OD1	2.28	0.66
1:E:103:LEU:HD11	2:F:272:ILE:HD12	1.77	0.65
2:H:38:LEU:HD13	2:H:129:LEU:HD11	1.77	0.65
1:I:147:PRO:O	1:I:169:PRO:HB3	1.96	0.65
1:I:35:SER:HB3	1:I:50:VAL:HG11	1.78	0.65
2:D:77:TYR:CD2	2:D:90:THR:HG21	2.32	0.65
2:J:259:THR:HG22	2:J:260:GLY:H	1.61	0.65
1:M:147:PRO:O	1:M:169:PRO:HB3	1.96	0.65
2:P:179:VAL:HG23	2:P:254:ALA:HB3	1.79	0.65
2:F:40:THR:HG23	2:F:41:GLN:HE21	1.60	0.65
2:J:211:ASN:HD21	2:J:268:VAL:HA	1.61	0.65
1:O:85:MET:HA	1:O:85:MET:HE2	1.77	0.65
2:P:122:ALA:HB2	2:P:153:ASP:H	1.61	0.65
1:C:23:THR:HG22	1:C:62:GLU:HG3	1.79	0.65
2:L:259:THR:HG22	2:L:260:GLY:H	1.61	0.65
2:F:77:TYR:CD2	2:F:90:THR:HG21	2.32	0.65
2:L:122:ALA:HB2	2:L:153:ASP:H	1.61	0.65
1:A:45:ASP:HB3	1:A:47:ARG:H	1.62	0.65
2:F:38:LEU:HD13	2:F:129:LEU:HD11	1.79	0.65
1:K:85:MET:HE2	1:K:85:MET:HA	1.78	0.65
1:I:23:THR:HB	1:I:62:GLU:HB2	1.79	0.64
2:J:195:TYR:CE1	2:J:240:LEU:HD21	2.32	0.64
2:D:38:LEU:HD13	2:D:129:LEU:HD11	1.79	0.64
2:N:195:TYR:CE1	2:N:240:LEU:HD21	2.32	0.64
2:N:259:THR:HG22	2:N:260:GLY:H	1.61	0.64
2:L:179:VAL:HG23	2:L:254:ALA:HB3	1.78	0.64
1:G:45:ASP:HB3	1:G:47:ARG:H	1.62	0.64
1:K:79:ARG:HB3	1:K:170:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:79:ARG:HB3	1:O:170:MET:CE	2.27	0.64
2:P:53:THR:N	2:P:136:ASN:HD21	1.90	0.64
1:M:79:ARG:HB3	1:M:170:MET:CE	2.28	0.64
2:N:211:ASN:HD21	2:N:268:VAL:HA	1.61	0.64
1:I:4:LEU:CD2	1:I:87:VAL:HG21	2.27	0.64
2:L:211:ASN:ND2	2:L:268:VAL:HA	2.13	0.64
2:P:259:THR:HG22	2:P:260:GLY:H	1.61	0.64
2:H:59:GLN:HE22	2:H:132:ARG:CZ	2.11	0.64
1:O:50:VAL:HG22	1:O:67:ILE:HG12	1.80	0.64
2:L:240:LEU:HD11	2:L:250:LEU:HD21	1.80	0.64
1:K:23:THR:HB	1:K:62:GLU:HB2	1.80	0.63
2:F:84:PHE:HA	2:F:85:PRO:C	2.19	0.63
2:F:138:ASN:C	2:F:138:ASN:HD22	2.01	0.63
1:K:50:VAL:HG22	1:K:67:ILE:HG12	1.80	0.63
1:O:23:THR:HB	1:O:62:GLU:HB2	1.80	0.63
2:D:84:PHE:HA	2:D:85:PRO:C	2.19	0.63
1:K:18:VAL:HG12	1:K:19:GLN:N	2.14	0.63
1:O:4:LEU:CD2	1:O:87:VAL:HG21	2.25	0.63
2:P:58:LEU:H	2:P:90:THR:HG21	1.63	0.63
1:E:23:THR:HG22	1:E:62:GLU:HG3	1.79	0.63
2:D:211:ASN:ND2	2:D:269:GLN:H	1.97	0.63
1:I:50:VAL:HG22	1:I:67:ILE:HG12	1.81	0.63
2:D:211:ASN:ND2	2:D:213:ALA:H	1.97	0.63
1:G:104:GLN:CG	2:H:168:VAL:HG23	2.29	0.63
1:A:104:GLN:CG	2:B:168:VAL:HG23	2.29	0.63
2:B:59:GLN:HE22	2:B:132:ARG:CZ	2.11	0.63
1:I:79:ARG:HB3	1:I:170:MET:CE	2.28	0.63
1:M:50:VAL:HG22	1:M:67:ILE:HG12	1.81	0.63
2:N:211:ASN:ND2	2:N:268:VAL:HA	2.14	0.63
1:E:104:GLN:CG	2:F:168:VAL:HG23	2.29	0.62
2:F:211:ASN:ND2	2:F:269:GLN:H	1.97	0.62
1:M:101:ASN:ND2	2:N:268:VAL:O	2.32	0.62
2:P:211:ASN:ND2	2:P:268:VAL:HA	2.13	0.62
2:F:226:THR:CG2	2:F:253:THR:HB	2.25	0.62
1:M:23:THR:HB	1:M:62:GLU:HB2	1.79	0.62
2:N:258:ARG:HH21	2:N:263:VAL:HG23	1.63	0.62
1:C:104:GLN:CG	2:D:168:VAL:HG23	2.29	0.62
2:D:138:ASN:C	2:D:138:ASN:HD22	2.01	0.62
2:P:240:LEU:HD11	2:P:250:LEU:HD21	1.80	0.62
2:J:211:ASN:ND2	2:J:268:VAL:HA	2.14	0.62
2:J:258:ARG:HH21	2:J:263:VAL:HG23	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:PRO:O	1:K:169:PRO:HB3	1.98	0.62
2:L:195:TYR:CE1	2:L:240:LEU:HD21	2.33	0.62
1:I:101:ASN:ND2	2:J:268:VAL:O	2.32	0.62
1:O:147:PRO:O	1:O:169:PRO:HB3	1.98	0.62
2:P:195:TYR:CE1	2:P:240:LEU:HD21	2.33	0.62
2:H:138:ASN:HD21	2:H:140:ASP:HB2	1.65	0.62
2:N:70:ASN:HB2	2:N:115:ALA:CB	2.29	0.62
2:B:138:ASN:HD21	2:B:140:ASP:HB2	1.65	0.62
2:F:211:ASN:ND2	2:F:213:ALA:H	1.97	0.62
1:K:4:LEU:CD2	1:K:87:VAL:HG21	2.25	0.62
1:M:4:LEU:CD2	1:M:87:VAL:HG21	2.27	0.62
2:N:14:GLY:HA2	2:N:142:PHE:CG	2.35	0.62
2:F:38:LEU:HD13	2:F:129:LEU:CD1	2.30	0.62
1:K:100:GLU:O	1:K:101:ASN:HB2	2.00	0.62
2:L:58:LEU:H	2:L:90:THR:HG21	1.63	0.62
1:O:100:GLU:O	1:O:101:ASN:HB2	2.00	0.62
1:O:144:ASN:HD22	1:O:170:MET:H	1.48	0.62
2:J:179:VAL:HG23	2:J:254:ALA:HB3	1.81	0.61
2:B:211:ASN:HD22	2:B:212:THR:H	1.48	0.61
1:I:85:MET:HE2	1:I:85:MET:HA	1.81	0.61
1:M:18:VAL:HG12	1:M:19:GLN:N	2.15	0.61
2:J:195:TYR:HE1	2:J:240:LEU:HD21	1.66	0.61
2:F:59:GLN:HE22	2:F:132:ARG:CZ	2.13	0.61
2:J:14:GLY:HA2	2:J:142:PHE:CG	2.35	0.61
2:D:38:LEU:HD13	2:D:129:LEU:CD1	2.30	0.61
2:N:179:VAL:HG23	2:N:254:ALA:HB3	1.81	0.61
1:O:24:ASN:HD21	1:O:31:TYR:HD1	1.48	0.61
1:M:100:GLU:O	1:M:101:ASN:HB2	2.01	0.61
1:I:100:GLU:O	1:I:101:ASN:HB2	2.01	0.61
2:J:70:ASN:HB2	2:J:115:ALA:CB	2.29	0.61
2:J:103:TRP:CE3	2:J:131:LEU:HD12	2.36	0.61
2:B:84:PHE:HA	2:B:85:PRO:C	2.21	0.61
2:H:84:PHE:HA	2:H:85:PRO:C	2.21	0.61
2:D:138:ASN:ND2	2:D:140:ASP:H	1.99	0.61
2:D:59:GLN:HE22	2:D:132:ARG:CZ	2.13	0.60
2:L:195:TYR:HE1	2:L:240:LEU:HD21	1.65	0.60
2:N:195:TYR:HE1	2:N:240:LEU:HD21	1.66	0.60
1:I:18:VAL:HG12	1:I:19:GLN:N	2.15	0.60
2:D:29:ASN:HB2	2:D:32:GLN:HG3	1.82	0.60
1:K:7:THR:HG22	2:L:278:TYR:HD2	1.65	0.60
1:K:24:ASN:HD21	1:K:31:TYR:HD1	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:103:TRP:CE3	2:N:131:LEU:HD12	2.36	0.60
2:B:38:LEU:HD13	2:B:129:LEU:CD1	2.31	0.60
1:I:32:LEU:HD11	1:I:54:LEU:HD21	1.83	0.60
2:L:40:THR:HG23	2:L:41:GLN:HE21	1.66	0.60
2:P:195:TYR:HE1	2:P:240:LEU:HD21	1.65	0.60
2:F:138:ASN:ND2	2:F:140:ASP:H	1.99	0.60
2:L:53:THR:N	2:L:136:ASN:HD21	1.90	0.60
1:M:85:MET:HE2	1:M:85:MET:HA	1.82	0.60
1:O:78:ASP:O	1:O:147:PRO:HB3	2.02	0.60
2:B:138:ASN:C	2:B:138:ASN:HD22	2.05	0.60
2:H:38:LEU:HD13	2:H:129:LEU:CD1	2.31	0.60
2:F:29:ASN:HB2	2:F:32:GLN:HG3	1.83	0.60
2:H:126:ILE:HD13	2:H:150:ALA:HB2	1.84	0.60
2:H:211:ASN:HD22	2:H:212:THR:H	1.48	0.60
2:L:70:ASN:HB2	2:L:115:ALA:CB	2.30	0.60
1:O:18:VAL:HG12	1:O:19:GLN:N	2.14	0.60
1:M:32:LEU:HD11	1:M:54:LEU:HD21	1.83	0.59
2:D:90:THR:HG23	2:D:91:PRO:O	2.02	0.59
1:K:16:LYS:O	1:K:68:LEU:HD23	2.03	0.59
1:O:7:THR:HG22	2:P:278:TYR:HD2	1.65	0.59
2:N:29:ASN:OD1	2:N:157:PRO:HG2	2.03	0.59
2:P:40:THR:HG23	2:P:41:GLN:HE21	1.67	0.59
1:K:24:ASN:HD22	1:K:57:MET:HB2	1.68	0.59
1:K:78:ASP:O	1:K:147:PRO:HB3	2.02	0.59
1:K:111:ILE:HG22	2:L:278:TYR:HB2	1.84	0.59
1:O:111:ILE:HG22	2:P:278:TYR:HB2	1.84	0.59
1:A:37:VAL:HG11	1:A:48:PHE:HB2	1.84	0.59
2:N:57:THR:HG22	2:N:132:ARG:HB3	1.85	0.59
1:G:104:GLN:HG3	2:H:168:VAL:HG23	1.84	0.59
2:H:29:ASN:HB2	2:H:32:GLN:HG3	1.85	0.59
1:A:197:THR:HB	1:A:198:PRO:CD	2.33	0.59
1:I:126:GLN:HG2	1:I:130:LYS:HZ2	1.67	0.59
1:C:104:GLN:HG3	2:D:168:VAL:HG23	1.84	0.59
1:E:104:GLN:HG3	2:F:168:VAL:HG23	1.84	0.59
2:H:189:LYS:O	2:H:191:GLN:HG2	2.03	0.59
2:J:29:ASN:OD1	2:J:157:PRO:HG2	2.03	0.59
1:K:144:ASN:HD22	1:K:170:MET:H	1.48	0.59
2:H:53:THR:H	2:H:136:ASN:ND2	2.01	0.59
1:K:48:PHE:HE1	1:K:113:LEU:HG	1.67	0.59
2:B:189:LYS:O	2:B:191:GLN:HG2	2.03	0.58
2:F:59:GLN:NE2	2:F:132:ARG:NH2	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:THR:HG23	2:F:91:PRO:O	2.02	0.58
2:P:70:ASN:HB2	2:P:115:ALA:CB	2.30	0.58
2:J:189:LYS:O	2:J:191:GLN:NE2	2.36	0.58
2:L:14:GLY:HA2	2:L:142:PHE:CG	2.39	0.58
1:M:48:PHE:HE1	1:M:113:LEU:HG	1.68	0.58
1:O:16:LYS:O	1:O:68:LEU:HD23	2.03	0.58
1:O:48:PHE:HE1	1:O:113:LEU:HG	1.67	0.58
2:B:29:ASN:HB2	2:B:32:GLN:HG3	1.85	0.58
1:G:37:VAL:HG11	1:G:48:PHE:HB2	1.84	0.58
1:I:144:ASN:HD22	1:I:170:MET:H	1.51	0.58
2:J:57:THR:HG22	2:J:132:ARG:HB3	1.85	0.58
1:O:32:LEU:HD11	1:O:54:LEU:HD21	1.85	0.58
2:B:53:THR:H	2:B:136:ASN:ND2	2.01	0.58
2:J:240:LEU:HD11	2:J:250:LEU:HD21	1.86	0.58
2:N:240:LEU:HD11	2:N:250:LEU:HD21	1.86	0.58
1:E:47:ARG:HG3	1:E:71:THR:HG22	1.85	0.58
2:F:183:LEU:HD13	2:F:250:LEU:HD12	1.86	0.58
2:F:211:ASN:HD22	2:F:212:THR:H	1.50	0.58
1:M:78:ASP:O	1:M:147:PRO:HB3	2.04	0.58
1:M:144:ASN:HD22	1:M:170:MET:H	1.51	0.58
1:M:162:LEU:HD22	1:M:176:LYS:O	2.04	0.58
1:O:24:ASN:HD22	1:O:57:MET:HB2	1.68	0.58
2:H:138:ASN:C	2:H:138:ASN:HD22	2.05	0.58
1:M:24:ASN:HD21	1:M:31:TYR:HD1	1.52	0.58
2:P:189:LYS:O	2:P:191:GLN:NE2	2.37	0.58
2:J:138:ASN:ND2	2:J:140:ASP:OD1	2.37	0.58
2:P:57:THR:HG22	2:P:132:ARG:HB3	1.86	0.58
2:D:211:ASN:HD22	2:D:212:THR:H	1.50	0.58
1:M:126:GLN:HG2	1:M:130:LYS:HZ2	1.68	0.58
1:C:47:ARG:HG3	1:C:71:THR:HG22	1.85	0.57
1:I:111:ILE:HG22	2:J:278:TYR:HB2	1.86	0.57
2:L:57:THR:HG22	2:L:132:ARG:HB3	1.86	0.57
2:B:113:SER:HB2	2:P:81:SER:HB2	1.86	0.57
2:B:211:ASN:ND2	2:B:213:ALA:H	2.02	0.57
2:D:59:GLN:NE2	2:D:132:ARG:NH2	2.51	0.57
2:F:40:THR:HG22	2:F:41:GLN:HE21	1.68	0.57
1:A:104:GLN:HG3	2:B:168:VAL:HG23	1.84	0.57
1:C:16:LYS:H	1:C:16:LYS:HD2	1.70	0.57
1:K:32:LEU:HD11	1:K:54:LEU:HD21	1.85	0.57
2:L:201:THR:HG21	2:L:206:ASN:HD22	1.68	0.57
2:N:138:ASN:ND2	2:N:140:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:162:LEU:HD22	1:O:176:LYS:O	2.05	0.57
2:P:201:THR:HG21	2:P:206:ASN:HD22	1.68	0.57
2:P:208:ILE:HD13	2:P:257:ALA:HB3	1.87	0.57
2:H:211:ASN:ND2	2:H:213:ALA:H	2.02	0.57
1:O:126:GLN:HG2	1:O:130:LYS:HZ2	1.68	0.57
2:B:126:ILE:HD13	2:B:150:ALA:HB2	1.84	0.57
1:C:37:VAL:HG11	1:C:48:PHE:HB2	1.87	0.57
1:I:24:ASN:HD21	1:I:31:TYR:HD1	1.51	0.57
1:K:162:LEU:HD22	1:K:176:LYS:O	2.05	0.57
2:L:189:LYS:O	2:L:191:GLN:NE2	2.37	0.57
1:M:35:SER:O	1:M:36:TRP:HB3	2.04	0.57
1:E:16:LYS:H	1:E:16:LYS:HD2	1.70	0.57
1:I:48:PHE:HE1	1:I:113:LEU:HG	1.69	0.57
1:I:78:ASP:O	1:I:147:PRO:HB3	2.04	0.57
1:C:151:THR:O	1:C:189:THR:HA	2.05	0.57
2:D:53:THR:H	2:D:136:ASN:ND2	2.02	0.57
2:D:183:LEU:HD13	2:D:250:LEU:HD12	1.86	0.57
2:F:53:THR:H	2:F:136:ASN:ND2	2.02	0.57
2:J:201:THR:HG21	2:J:206:ASN:HD22	1.70	0.57
1:I:35:SER:O	1:I:36:TRP:HB3	2.04	0.57
1:M:111:ILE:HG22	2:N:278:TYR:HB2	1.86	0.57
2:P:38:LEU:HD13	2:P:129:LEU:HD11	1.87	0.57
2:J:40:THR:HG23	2:J:41:GLN:HE21	1.70	0.57
1:K:126:GLN:HG2	1:K:130:LYS:HZ2	1.70	0.57
2:P:5:THR:HG22	2:P:7:ASN:H	1.69	0.57
2:D:126:ILE:HD13	2:D:150:ALA:HB2	1.87	0.56
1:I:162:LEU:HD22	1:I:176:LYS:O	2.04	0.56
2:L:5:THR:HG22	2:L:7:ASN:H	1.69	0.56
2:L:38:LEU:HD13	2:L:129:LEU:HD11	1.87	0.56
2:N:208:ILE:HD13	2:N:257:ALA:HB3	1.87	0.56
2:P:138:ASN:ND2	2:P:140:ASP:OD1	2.38	0.56
1:G:104:GLN:HB2	2:H:271:ILE:HG13	1.88	0.56
2:H:90:THR:HG23	2:H:91:PRO:O	2.05	0.56
2:L:208:ILE:HD13	2:L:257:ALA:HB3	1.87	0.56
2:F:77:TYR:CE2	2:F:90:THR:HG21	2.41	0.56
2:J:208:ILE:HD13	2:J:257:ALA:HB3	1.87	0.56
2:N:189:LYS:O	2:N:191:GLN:NE2	2.36	0.56
2:P:14:GLY:HA2	2:P:142:PHE:CG	2.39	0.56
2:F:126:ILE:HD13	2:F:150:ALA:HB2	1.87	0.56
2:H:113:SER:HB2	2:L:81:SER:HB2	1.88	0.56
2:N:122:ALA:HB2	2:N:153:ASP:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:THR:HG22	2:D:41:GLN:HE21	1.68	0.56
2:F:189:LYS:O	2:F:191:GLN:HG2	2.05	0.56
1:K:35:SER:O	1:K:36:TRP:HB3	2.06	0.56
2:L:138:ASN:ND2	2:L:140:ASP:OD1	2.38	0.56
1:M:68:LEU:O	1:M:69:ASP:HB2	2.06	0.56
2:N:201:THR:HG21	2:N:206:ASN:HD22	1.70	0.56
1:E:37:VAL:HG11	1:E:48:PHE:HB2	1.87	0.56
1:E:140:LEU:HB2	1:E:177:LEU:HD13	1.88	0.56
2:F:59:GLN:HE22	2:F:132:ARG:NH2	2.04	0.56
1:K:68:LEU:O	1:K:69:ASP:HB2	2.06	0.56
1:K:101:ASN:ND2	2:L:268:VAL:O	2.39	0.56
2:D:189:LYS:O	2:D:191:GLN:HG2	2.05	0.56
1:G:197:THR:HB	1:G:198:PRO:CD	2.33	0.56
1:E:151:THR:O	1:E:189:THR:HA	2.05	0.55
1:A:104:GLN:HB2	2:B:271:ILE:HG13	1.88	0.55
2:B:77:TYR:CE2	2:B:90:THR:HG21	2.41	0.55
2:B:90:THR:HG23	2:B:91:PRO:O	2.05	0.55
2:D:59:GLN:HE22	2:D:132:ARG:NH2	2.04	0.55
1:K:13:ALA:HB2	1:K:117:PRO:HA	1.89	0.55
1:O:35:SER:O	1:O:36:TRP:HB3	2.06	0.55
2:H:77:TYR:CE2	2:H:90:THR:HG21	2.41	0.55
2:L:170:VAL:O	2:L:179:VAL:HG11	2.07	0.55
1:M:12:PRO:HA	1:M:116:ARG:O	2.06	0.55
1:K:69:ASP:O	1:K:70:ALA:HB2	2.06	0.55
1:O:101:ASN:ND2	2:P:268:VAL:O	2.39	0.55
1:C:33:ILE:HG12	1:C:57:MET:CE	2.37	0.55
1:I:68:LEU:O	1:I:69:ASP:HB2	2.06	0.55
1:O:69:ASP:O	1:O:70:ALA:HB2	2.06	0.55
2:P:170:VAL:O	2:P:179:VAL:HG11	2.07	0.55
2:B:59:GLN:NE2	2:B:132:ARG:CZ	2.70	0.55
1:O:13:ALA:HB2	1:O:117:PRO:HA	1.89	0.55
2:B:57:THR:HG22	2:B:132:ARG:HB3	1.89	0.55
1:C:104:GLN:HB2	2:D:271:ILE:HG13	1.89	0.55
2:D:77:TYR:CE2	2:D:90:THR:HG21	2.41	0.55
1:O:12:PRO:HA	1:O:116:ARG:O	2.07	0.55
1:O:68:LEU:O	1:O:69:ASP:HB2	2.06	0.55
1:K:12:PRO:HA	1:K:116:ARG:O	2.07	0.55
1:M:7:THR:HG22	2:N:278:TYR:HD2	1.71	0.54
1:M:30:THR:HG23	1:M:58:LYS:CE	2.37	0.54
1:C:140:LEU:HB2	1:C:177:LEU:HD13	1.88	0.54
1:I:30:THR:HG23	1:I:58:LYS:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:VAL:CG2	2:B:185:VAL:HG13	2.35	0.54
1:O:30:THR:HG23	1:O:58:LYS:CE	2.38	0.54
1:E:33:ILE:HG12	1:E:57:MET:CE	2.37	0.54
2:N:53:THR:N	2:N:136:ASN:HD21	1.91	0.54
2:D:57:THR:HG22	2:D:132:ARG:HB3	1.90	0.54
2:J:5:THR:HA	2:J:41:GLN:O	2.08	0.54
2:J:170:VAL:O	2:J:179:VAL:HG11	2.07	0.54
2:L:258:ARG:HH21	2:L:263:VAL:HG23	1.70	0.54
2:N:5:THR:HA	2:N:41:GLN:O	2.08	0.54
1:K:30:THR:HG23	1:K:58:LYS:CE	2.38	0.54
1:I:9:VAL:HG12	1:I:10:ILE:N	2.23	0.54
2:P:258:ARG:HH21	2:P:263:VAL:HG23	1.70	0.54
1:I:24:ASN:HD22	1:I:57:MET:HB2	1.73	0.54
1:E:104:GLN:HB2	2:F:271:ILE:HG13	1.89	0.54
2:H:163:VAL:CG2	2:H:185:VAL:HG13	2.35	0.54
2:N:170:VAL:O	2:N:179:VAL:HG11	2.07	0.54
2:F:218:ALA:HB1	2:F:264:THR:O	2.08	0.53
1:K:9:VAL:HG12	1:K:10:ILE:N	2.23	0.53
1:M:9:VAL:HG12	1:M:10:ILE:N	2.23	0.53
1:M:69:ASP:O	1:M:70:ALA:HB2	2.08	0.53
1:G:123:PRO:HG2	1:G:126:GLN:HB2	1.90	0.53
2:H:57:THR:HG22	2:H:132:ARG:HB3	1.89	0.53
1:I:12:PRO:HA	1:I:116:ARG:O	2.06	0.53
1:E:162:LEU:HB3	1:E:175:VAL:HG11	1.90	0.53
1:G:151:THR:O	1:G:189:THR:HA	2.08	0.53
2:H:59:GLN:NE2	2:H:132:ARG:CZ	2.70	0.53
2:J:59:GLN:HG3	2:J:132:ARG:HD3	1.90	0.53
1:I:4:LEU:HD21	1:I:87:VAL:HG11	1.91	0.53
1:I:142:LEU:N	1:I:173:SER:O	2.41	0.53
2:J:201:THR:HG21	2:J:206:ASN:HA	1.90	0.53
2:P:201:THR:HG21	2:P:206:ASN:HA	1.90	0.53
1:C:162:LEU:HB3	1:C:175:VAL:HG11	1.90	0.53
2:L:201:THR:HG21	2:L:206:ASN:HA	1.90	0.53
2:P:122:ALA:HB2	2:P:153:ASP:N	2.23	0.53
1:A:185:ILE:O	1:A:202:GLY:N	2.37	0.53
2:F:163:VAL:CG2	2:F:185:VAL:HG13	2.35	0.53
1:A:123:PRO:HG2	1:A:126:GLN:HB2	1.90	0.53
1:C:185:ILE:O	1:C:202:GLY:N	2.37	0.53
1:I:7:THR:HG22	2:J:278:TYR:HD2	1.71	0.53
2:J:122:ALA:HB2	2:J:153:ASP:N	2.20	0.53
2:N:40:THR:HG23	2:N:41:GLN:HE21	1.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:THR:HG22	2:F:132:ARG:HB3	1.90	0.53
1:M:48:PHE:CE1	1:M:113:LEU:HG	2.44	0.53
1:A:151:THR:O	1:A:189:THR:HA	2.08	0.53
1:A:162:LEU:HD21	1:A:177:LEU:CD1	2.39	0.53
1:M:4:LEU:HD21	1:M:87:VAL:HG11	1.91	0.53
2:B:120:ILE:HG23	2:B:126:ILE:HD11	1.90	0.52
2:D:163:VAL:CG2	2:D:185:VAL:HG13	2.35	0.52
2:H:201:THR:CG2	2:H:206:ASN:HA	2.39	0.52
1:I:16:LYS:O	1:I:68:LEU:HD23	2.09	0.52
2:N:201:THR:HG21	2:N:206:ASN:HA	1.90	0.52
2:N:212:THR:N	2:N:269:GLN:O	2.43	0.52
1:I:48:PHE:CE1	1:I:113:LEU:HG	2.44	0.52
1:M:24:ASN:HD22	1:M:57:MET:HB2	1.73	0.52
1:O:9:VAL:HG12	1:O:10:ILE:N	2.24	0.52
1:A:16:LYS:H	1:A:16:LYS:HD2	1.75	0.52
2:D:218:ALA:HB1	2:D:264:THR:O	2.08	0.52
1:G:16:LYS:H	1:G:16:LYS:HD2	1.75	0.52
1:G:47:ARG:HG3	1:G:71:THR:HG22	1.90	0.52
1:A:101:ASN:HB2	2:B:171:THR:O	2.10	0.52
1:K:151:THR:CG2	1:K:190:ILE:HD12	2.37	0.52
2:N:59:GLN:HG3	2:N:132:ARG:HD3	1.90	0.52
1:A:47:ARG:HG3	1:A:71:THR:HG22	1.90	0.52
2:D:5:THR:HA	2:D:41:GLN:O	2.10	0.52
1:I:151:THR:CG2	1:I:190:ILE:HD12	2.37	0.52
1:O:126:GLN:HG2	1:O:130:LYS:NZ	2.25	0.52
2:B:201:THR:CG2	2:B:206:ASN:HA	2.39	0.52
1:I:10:ILE:HD11	1:I:192:ASP:HB3	1.91	0.52
1:K:126:GLN:HG2	1:K:130:LYS:NZ	2.25	0.52
2:P:59:GLN:HG3	2:P:132:ARG:HD3	1.91	0.52
1:C:197:THR:HB	1:C:198:PRO:CD	2.38	0.52
2:F:5:THR:HA	2:F:41:GLN:O	2.10	0.52
2:F:59:GLN:NE2	2:F:132:ARG:CZ	2.73	0.52
2:H:120:ILE:HG23	2:H:126:ILE:HD11	1.90	0.52
1:M:142:LEU:N	1:M:173:SER:O	2.41	0.52
2:J:212:THR:N	2:J:269:GLN:O	2.43	0.52
1:K:103:LEU:CD1	2:L:272:ILE:HD12	2.40	0.52
1:O:48:PHE:CE1	1:O:113:LEU:HG	2.45	0.52
1:C:51:THR:O	1:C:52:PRO:C	2.48	0.52
2:D:59:GLN:NE2	2:D:132:ARG:CZ	2.73	0.52
1:G:51:THR:O	1:G:52:PRO:C	2.46	0.52
2:H:218:ALA:HB1	2:H:264:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:16:LYS:O	1:M:68:LEU:HD23	2.09	0.52
2:P:59:GLN:HG3	2:P:132:ARG:CD	2.40	0.52
2:B:179:VAL:HG12	2:B:180:PRO:HD2	1.91	0.52
2:D:179:VAL:HG12	2:D:180:PRO:HD2	1.92	0.51
1:I:32:LEU:HD13	1:I:32:LEU:O	2.10	0.51
2:L:121:LYS:O	2:L:122:ALA:C	2.48	0.51
2:L:212:THR:N	2:L:269:GLN:O	2.43	0.51
1:M:102:THR:HA	2:N:169:THR:O	2.10	0.51
2:P:259:THR:CG2	2:P:260:GLY:H	2.23	0.51
1:I:69:ASP:O	1:I:70:ALA:HB2	2.08	0.51
2:L:59:GLN:HG3	2:L:132:ARG:HD3	1.91	0.51
2:L:259:THR:CG2	2:L:260:GLY:H	2.23	0.51
1:M:103:LEU:HD11	2:N:272:ILE:HD12	1.92	0.51
2:J:259:THR:CG2	2:J:260:GLY:H	2.24	0.51
1:K:102:THR:HA	2:L:169:THR:O	2.10	0.51
1:M:11:TYR:CE1	1:M:18:VAL:HG23	2.46	0.51
2:P:58:LEU:H	2:P:90:THR:HG22	1.76	0.51
2:B:218:ALA:HB1	2:B:264:THR:O	2.10	0.51
1:E:162:LEU:HD21	1:E:177:LEU:CD1	2.40	0.51
2:L:5:THR:HA	2:L:41:GLN:O	2.10	0.51
1:O:102:THR:HA	2:P:169:THR:O	2.10	0.51
1:O:103:LEU:CD1	2:P:272:ILE:HD12	2.40	0.51
2:D:120:ILE:HG23	2:D:126:ILE:HD11	1.93	0.51
1:G:162:LEU:HD21	1:G:177:LEU:CD1	2.39	0.51
1:I:13:ALA:HB2	1:I:117:PRO:HA	1.93	0.51
1:I:102:THR:HA	2:J:169:THR:O	2.10	0.51
1:I:120:LEU:HD22	1:I:147:PRO:HG3	1.93	0.51
2:L:122:ALA:HB2	2:L:153:ASP:N	2.23	0.51
1:O:134:ARG:HA	1:O:205:GLU:HB3	1.92	0.51
2:P:5:THR:HA	2:P:41:GLN:O	2.10	0.51
2:P:90:THR:HG23	2:P:91:PRO:O	2.10	0.51
2:B:59:GLN:NE2	2:B:132:ARG:NH2	2.59	0.51
2:J:121:LYS:O	2:J:122:ALA:C	2.48	0.51
2:L:59:GLN:HG3	2:L:132:ARG:CD	2.40	0.51
2:L:90:THR:HG23	2:L:91:PRO:O	2.10	0.51
2:N:195:TYR:HA	2:N:275:THR:O	2.11	0.51
1:I:103:LEU:HD11	2:J:272:ILE:HD12	1.92	0.51
2:J:195:TYR:HA	2:J:275:THR:O	2.11	0.51
1:M:13:ALA:HB2	1:M:117:PRO:HA	1.93	0.51
1:G:101:ASN:HB2	2:H:171:THR:O	2.10	0.51
2:H:179:VAL:HG12	2:H:180:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:ARG:HA	1:K:205:GLU:HB3	1.92	0.51
1:M:32:LEU:HD13	1:M:32:LEU:O	2.11	0.51
1:M:120:LEU:HD22	1:M:147:PRO:HG3	1.93	0.51
2:N:121:LYS:O	2:N:122:ALA:C	2.48	0.51
2:N:187:CYS:O	2:N:245:THR:HA	2.11	0.51
2:P:96:ASN:ND2	2:P:96:ASN:H	2.09	0.51
2:B:135:ASN:HD21	2:B:138:ASN:ND2	2.09	0.50
1:C:162:LEU:HD21	1:C:177:LEU:CD1	2.40	0.50
2:J:190:SER:HA	2:J:244:GLY:HA2	1.92	0.50
1:M:10:ILE:HD11	1:M:192:ASP:HB3	1.91	0.50
1:C:101:ASN:HB2	2:D:171:THR:O	2.12	0.50
1:E:101:ASN:HB2	2:F:171:THR:O	2.12	0.50
1:E:185:ILE:HB	1:E:202:GLY:HA3	1.93	0.50
2:H:59:GLN:NE2	2:H:132:ARG:NH2	2.59	0.50
2:H:135:ASN:HD21	2:H:138:ASN:ND2	2.09	0.50
2:J:52:ILE:HG23	2:J:137:TYR:HB2	1.93	0.50
2:J:187:CYS:O	2:J:245:THR:HA	2.11	0.50
2:L:231:ILE:HG22	2:L:232:ILE:N	2.26	0.50
2:B:201:THR:HG23	2:B:206:ASN:HA	1.93	0.50
1:C:185:ILE:HB	1:C:202:GLY:HA3	1.93	0.50
1:K:10:ILE:HD11	1:K:192:ASP:HB3	1.93	0.50
1:K:118:ALA:O	1:K:119:LYS:HB2	2.12	0.50
1:K:120:LEU:HD22	1:K:147:PRO:HG3	1.93	0.50
1:O:120:LEU:HD22	1:O:147:PRO:HG3	1.93	0.50
2:P:29:ASN:OD1	2:P:157:PRO:HD2	2.11	0.50
1:O:142:LEU:N	1:O:173:SER:O	2.44	0.50
2:H:201:THR:HG23	2:H:206:ASN:HA	1.93	0.50
2:L:29:ASN:OD1	2:L:157:PRO:HD2	2.11	0.50
2:N:90:THR:HG23	2:N:91:PRO:O	2.11	0.50
2:N:190:SER:HA	2:N:244:GLY:HA2	1.92	0.50
2:B:138:ASN:ND2	2:B:140:ASP:H	2.10	0.50
2:F:179:VAL:HG12	2:F:180:PRO:HD2	1.92	0.50
2:H:40:THR:HG23	2:H:41:GLN:HE21	1.75	0.50
2:J:90:THR:HG23	2:J:91:PRO:O	2.11	0.50
1:K:48:PHE:CE1	1:K:113:LEU:HG	2.45	0.50
1:E:27:GLU:OE2	1:E:60:LYS:HG3	2.12	0.50
1:M:151:THR:CG2	1:M:190:ILE:HD12	2.37	0.50
2:N:259:THR:CG2	2:N:260:GLY:H	2.24	0.50
1:O:103:LEU:HD11	2:P:272:ILE:HD12	1.93	0.50
2:L:96:ASN:H	2:L:96:ASN:ND2	2.09	0.50
1:O:10:ILE:HD11	1:O:192:ASP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:118:ALA:O	1:O:119:LYS:HB2	2.12	0.50
1:A:162:LEU:HB3	1:A:175:VAL:HG11	1.93	0.49
1:C:27:GLU:OE2	1:C:60:LYS:HG3	2.12	0.49
2:J:131:LEU:C	2:J:131:LEU:HD23	2.32	0.49
2:N:126:ILE:HG22	2:N:127:ALA:HB2	1.94	0.49
2:J:5:THR:HG22	2:J:7:ASN:H	1.77	0.49
1:K:103:LEU:HD11	2:L:272:ILE:HD12	1.93	0.49
2:P:231:ILE:HG22	2:P:232:ILE:N	2.26	0.49
2:D:103:TRP:CH2	2:D:131:LEU:HB2	2.48	0.49
1:E:185:ILE:O	1:E:202:GLY:N	2.37	0.49
2:F:103:TRP:CH2	2:F:131:LEU:HB2	2.47	0.49
2:H:138:ASN:ND2	2:H:140:ASP:H	2.10	0.49
1:I:11:TYR:CE1	1:I:18:VAL:HG23	2.46	0.49
1:M:18:VAL:CG1	1:M:19:GLN:H	2.22	0.49
2:N:131:LEU:HD23	2:N:131:LEU:C	2.32	0.49
1:O:79:ARG:HB3	1:O:170:MET:HE2	1.95	0.49
2:H:53:THR:H	2:H:136:ASN:HD21	1.59	0.49
1:I:30:THR:HG23	1:I:58:LYS:HE3	1.94	0.49
1:I:32:LEU:CD1	1:I:54:LEU:HD11	2.34	0.49
2:J:24:LEU:O	2:J:25:ALA:C	2.51	0.49
1:K:2:VAL:HG12	1:K:24:ASN:CA	2.41	0.49
2:B:211:ASN:HD21	2:B:269:GLN:H	1.61	0.49
2:D:138:ASN:HD21	2:D:140:ASP:CB	2.25	0.49
2:N:28:VAL:HG23	2:N:154:VAL:CG1	2.42	0.49
1:C:123:PRO:HG2	1:C:126:GLN:HB2	1.94	0.49
1:C:156:ASN:O	1:C:185:ILE:HA	2.12	0.49
1:E:51:THR:O	1:E:52:PRO:C	2.48	0.49
1:I:118:ALA:O	1:I:119:LYS:HB2	2.13	0.49
2:N:38:LEU:CD2	2:N:148:ILE:HD12	2.43	0.49
2:F:120:ILE:HG23	2:F:126:ILE:HD11	1.93	0.49
1:G:162:LEU:HB3	1:G:175:VAL:HG11	1.93	0.49
2:J:218:ALA:HA	2:J:264:THR:O	2.13	0.49
2:L:52:ILE:HG23	2:L:137:TYR:HB2	1.95	0.49
2:L:131:LEU:HD23	2:L:131:LEU:C	2.33	0.49
1:M:45:ASP:OD1	1:M:47:ARG:HD2	2.13	0.49
2:N:5:THR:HG22	2:N:7:ASN:H	1.77	0.49
2:P:212:THR:N	2:P:269:GLN:O	2.43	0.49
2:F:120:ILE:CG2	2:F:126:ILE:HD11	2.43	0.49
1:I:103:LEU:CD1	2:J:272:ILE:HD12	2.43	0.49
1:K:24:ASN:ND2	1:K:31:TYR:HD1	2.11	0.49
1:M:134:ARG:HA	1:M:205:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:THR:H	2:B:136:ASN:HD21	1.60	0.49
1:G:185:ILE:O	1:G:202:GLY:N	2.37	0.49
2:J:28:VAL:HG23	2:J:154:VAL:CG1	2.42	0.49
1:K:4:LEU:HD22	1:K:20:LEU:HD21	1.95	0.49
2:P:24:LEU:O	2:P:25:ALA:C	2.51	0.49
1:E:123:PRO:HG2	1:E:126:GLN:HB2	1.94	0.48
1:I:4:LEU:HD21	1:I:87:VAL:CG2	2.35	0.48
1:I:82:LEU:HD11	1:I:84:TRP:NE1	2.27	0.48
1:K:79:ARG:HB3	1:K:170:MET:HE2	1.94	0.48
1:M:32:LEU:CD1	1:M:54:LEU:HD11	2.34	0.48
1:O:30:THR:HG23	1:O:58:LYS:HE3	1.95	0.48
2:H:120:ILE:CG2	2:H:126:ILE:HD11	2.43	0.48
1:M:103:LEU:CD1	2:N:272:ILE:HD12	2.42	0.48
1:M:118:ALA:O	1:M:119:LYS:HB2	2.12	0.48
1:O:4:LEU:HD22	1:O:20:LEU:HD21	1.95	0.48
1:O:144:ASN:ND2	1:O:170:MET:H	2.11	0.48
2:P:218:ALA:HA	2:P:264:THR:O	2.13	0.48
1:A:140:LEU:HB2	1:A:177:LEU:HD13	1.95	0.48
2:H:211:ASN:HD21	2:H:269:GLN:H	1.61	0.48
1:I:82:LEU:HB3	1:I:149:TYR:CE1	2.48	0.48
2:L:187:CYS:O	2:L:245:THR:HA	2.14	0.48
1:M:126:GLN:HG2	1:M:130:LYS:NZ	2.29	0.48
2:N:96:ASN:H	2:N:96:ASN:ND2	2.11	0.48
1:O:24:ASN:ND2	1:O:31:TYR:HD1	2.11	0.48
1:O:151:THR:CG2	1:O:190:ILE:HD12	2.37	0.48
2:J:53:THR:N	2:J:136:ASN:HD21	1.91	0.48
1:K:30:THR:HG23	1:K:58:LYS:HE3	1.95	0.48
1:K:198:PRO:O	1:K:199:LYS:C	2.52	0.48
2:L:38:LEU:CD2	2:L:148:ILE:HD12	2.43	0.48
1:M:82:LEU:HB3	1:M:149:TYR:CE1	2.48	0.48
2:N:38:LEU:HD13	2:N:129:LEU:HD11	1.95	0.48
2:P:131:LEU:C	2:P:131:LEU:HD23	2.33	0.48
2:B:183:LEU:HD13	2:B:250:LEU:HD12	1.94	0.48
2:H:183:LEU:HD13	2:H:250:LEU:HD12	1.94	0.48
2:H:227:ARG:HH11	2:H:227:ARG:HD3	1.44	0.48
1:I:45:ASP:OD1	1:I:47:ARG:HD2	2.13	0.48
1:K:32:LEU:HD13	1:K:32:LEU:O	2.14	0.48
2:L:58:LEU:H	2:L:90:THR:HG22	1.76	0.48
2:L:191:GLN:O	2:L:242:ALA:HA	2.14	0.48
1:M:79:ARG:HB3	1:M:170:MET:HE2	1.96	0.48
1:M:82:LEU:HD11	1:M:84:TRP:NE1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:198:PRO:O	1:O:199:LYS:C	2.52	0.48
1:A:69:ASP:OD2	1:A:71:THR:OG1	2.28	0.48
2:B:120:ILE:CG2	2:B:126:ILE:HD11	2.43	0.48
1:E:156:ASN:O	1:E:185:ILE:HA	2.12	0.48
1:I:134:ARG:HA	1:I:205:GLU:HB3	1.94	0.48
2:J:96:ASN:H	2:J:96:ASN:ND2	2.11	0.48
1:M:30:THR:HG23	1:M:58:LYS:HE3	1.94	0.48
2:N:52:ILE:HG23	2:N:137:TYR:HB2	1.93	0.48
1:I:126:GLN:HG2	1:I:130:LYS:NZ	2.29	0.48
2:J:38:LEU:CD2	2:J:148:ILE:HD12	2.43	0.48
2:P:121:LYS:O	2:P:122:ALA:C	2.48	0.48
2:B:40:THR:HG23	2:B:41:GLN:HE21	1.75	0.48
1:E:197:THR:HB	1:E:198:PRO:CD	2.38	0.48
2:J:126:ILE:HG22	2:J:127:ALA:HB2	1.94	0.48
1:K:85:MET:HB2	1:K:111:ILE:HG13	1.96	0.48
2:L:195:TYR:HA	2:L:275:THR:O	2.14	0.48
2:L:216:SER:O	2:L:267:ASN:HB2	2.14	0.48
2:L:218:ALA:HA	2:L:264:THR:O	2.13	0.48
1:O:85:MET:HB2	1:O:111:ILE:HG13	1.96	0.48
1:G:140:LEU:HB2	1:G:177:LEU:HD13	1.95	0.48
1:I:9:VAL:HG12	1:I:10:ILE:H	1.78	0.48
1:I:150:LEU:HD23	1:I:150:LEU:HA	1.67	0.48
1:K:45:ASP:OD1	1:K:47:ARG:HD2	2.14	0.48
1:K:82:LEU:HB3	1:K:149:TYR:CE1	2.49	0.48
1:M:11:TYR:CD1	1:M:18:VAL:HG23	2.49	0.48
2:N:42:ILE:HB	2:N:103:TRP:CD1	2.49	0.48
2:D:120:ILE:CG2	2:D:126:ILE:HD11	2.43	0.48
2:L:28:VAL:HG23	2:L:154:VAL:CG1	2.43	0.48
1:M:24:ASN:H	1:M:57:MET:HE2	1.79	0.48
2:N:24:LEU:O	2:N:25:ALA:C	2.51	0.48
2:N:42:ILE:HB	2:N:103:TRP:HD1	1.78	0.48
1:O:82:LEU:HD11	1:O:84:TRP:NE1	2.29	0.48
2:P:28:VAL:HG23	2:P:154:VAL:CG1	2.43	0.48
2:J:42:ILE:HB	2:J:103:TRP:CD1	2.49	0.47
2:J:42:ILE:HB	2:J:103:TRP:HD1	1.78	0.47
2:J:208:ILE:HD13	2:J:257:ALA:CB	2.44	0.47
2:P:52:ILE:HG23	2:P:137:TYR:HB2	1.95	0.47
2:P:191:GLN:O	2:P:242:ALA:HA	2.14	0.47
2:H:195:TYR:HA	2:H:275:THR:O	2.14	0.47
2:J:38:LEU:HD13	2:J:129:LEU:HD11	1.95	0.47
2:N:218:ALA:HA	2:N:264:THR:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:216:SER:O	2:P:267:ASN:HB2	2.14	0.47
1:I:11:TYR:CD1	1:I:18:VAL:HG23	2.49	0.47
1:K:142:LEU:N	1:K:173:SER:O	2.44	0.47
2:N:231:ILE:HG22	2:N:232:ILE:N	2.29	0.47
1:O:4:LEU:HD21	1:O:87:VAL:HG11	1.97	0.47
2:P:38:LEU:CD2	2:P:148:ILE:HD12	2.43	0.47
2:P:126:ILE:HG22	2:P:127:ALA:HB2	1.96	0.47
1:A:51:THR:O	1:A:52:PRO:C	2.46	0.47
1:C:30:THR:OG1	1:C:58:LYS:HG2	2.15	0.47
1:G:27:GLU:OE2	1:G:60:LYS:HG3	2.14	0.47
1:O:45:ASP:OD1	1:O:47:ARG:HD2	2.14	0.47
2:P:103:TRP:CE3	2:P:131:LEU:HD12	2.50	0.47
2:B:195:TYR:HA	2:B:275:THR:O	2.14	0.47
1:I:2:VAL:HG12	1:I:24:ASN:CA	2.44	0.47
1:I:11:TYR:HB3	1:I:115:TYR:HA	1.96	0.47
1:M:198:PRO:O	1:M:199:LYS:C	2.53	0.47
1:O:13:ALA:CB	1:O:118:ALA:H	2.28	0.47
1:O:18:VAL:CG1	1:O:19:GLN:H	2.22	0.47
1:O:32:LEU:HD13	1:O:32:LEU:O	2.14	0.47
2:B:103:TRP:CH2	2:B:131:LEU:HB2	2.49	0.47
2:D:161:CYS:HB3	2:D:186:TYR:O	2.14	0.47
2:J:218:ALA:HB3	2:J:268:VAL:HG23	1.96	0.47
1:A:27:GLU:OE2	1:A:60:LYS:HG3	2.14	0.47
2:F:161:CYS:HB3	2:F:186:TYR:O	2.14	0.47
1:K:2:VAL:HG22	1:K:89:ALA:HB2	1.95	0.47
1:K:13:ALA:CB	1:K:118:ALA:H	2.28	0.47
2:N:208:ILE:HD13	2:N:257:ALA:CB	2.44	0.47
1:O:82:LEU:HB3	1:O:149:TYR:CE1	2.49	0.47
2:P:187:CYS:O	2:P:245:THR:HA	2.14	0.47
1:C:33:ILE:HG12	1:C:57:MET:HE2	1.97	0.47
2:L:103:TRP:CE3	2:L:131:LEU:HD12	2.50	0.47
1:O:2:VAL:HG22	1:O:89:ALA:HB2	1.95	0.47
1:A:33:ILE:HG12	1:A:57:MET:CE	2.45	0.47
2:B:5:THR:HA	2:B:41:GLN:O	2.15	0.47
2:D:202:ALA:CB	2:D:259:THR:CG2	2.93	0.47
2:F:138:ASN:ND2	2:F:140:ASP:HB2	2.28	0.47
1:I:24:ASN:ND2	1:I:31:TYR:HD1	2.13	0.47
1:K:11:TYR:CE1	1:K:18:VAL:HG23	2.50	0.47
1:K:144:ASN:ND2	1:K:170:MET:H	2.11	0.47
1:O:11:TYR:CE1	1:O:18:VAL:HG23	2.50	0.47
1:O:13:ALA:HB3	1:O:118:ALA:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:ASN:ND2	2:D:140:ASP:HB2	2.28	0.47
1:E:27:GLU:CD	1:E:60:LYS:HG3	2.36	0.47
2:F:131:LEU:C	2:F:131:LEU:HD23	2.36	0.47
2:F:202:ALA:CB	2:F:259:THR:CG2	2.93	0.47
2:H:103:TRP:CH2	2:H:131:LEU:HB2	2.49	0.47
1:K:82:LEU:HD11	1:K:84:TRP:NE1	2.29	0.47
2:L:42:ILE:HB	2:L:103:TRP:HD1	1.80	0.47
2:L:126:ILE:HG22	2:L:127:ALA:HB2	1.96	0.47
1:M:24:ASN:ND2	1:M:31:TYR:HD1	2.12	0.47
2:P:29:ASN:OD1	2:P:157:PRO:HG2	2.15	0.47
2:P:195:TYR:HA	2:P:275:THR:O	2.14	0.47
1:G:33:ILE:HG12	1:G:57:MET:CE	2.45	0.46
2:L:42:ILE:HB	2:L:103:TRP:CD1	2.50	0.46
2:P:190:SER:HA	2:P:244:GLY:HA2	1.97	0.46
1:I:18:VAL:CG1	1:I:19:GLN:H	2.22	0.46
2:J:216:SER:O	2:J:267:ASN:HB2	2.15	0.46
1:K:149:TYR:CE2	1:K:169:PRO:HD3	2.50	0.46
1:K:149:TYR:CZ	1:K:169:PRO:HD3	2.50	0.46
1:M:9:VAL:HG12	1:M:10:ILE:H	1.78	0.46
2:J:231:ILE:HG22	2:J:232:ILE:N	2.29	0.46
1:O:116:ARG:HA	1:O:117:PRO:HD2	1.77	0.46
2:D:29:ASN:HB2	2:D:32:GLN:CG	2.45	0.46
2:D:240:LEU:HD21	2:D:250:LEU:CD2	2.46	0.46
1:E:33:ILE:HG12	1:E:57:MET:HE2	1.96	0.46
1:G:156:ASN:O	1:G:185:ILE:HA	2.15	0.46
2:H:77:TYR:O	2:H:78:SER:C	2.54	0.46
1:I:90:ILE:HG23	1:I:91:PRO:HD2	1.98	0.46
2:N:189:LYS:HA	2:N:189:LYS:HD3	1.58	0.46
2:N:218:ALA:HB3	2:N:268:VAL:HG23	1.96	0.46
2:F:138:ASN:HD21	2:F:140:ASP:CB	2.25	0.46
2:P:42:ILE:HB	2:P:103:TRP:CD1	2.50	0.46
2:B:202:ALA:HB1	2:B:259:THR:HG22	1.98	0.46
1:I:198:PRO:O	1:I:199:LYS:C	2.53	0.46
2:J:29:ASN:OD1	2:J:157:PRO:HD2	2.16	0.46
2:L:190:SER:HA	2:L:244:GLY:HA2	1.97	0.46
1:O:149:TYR:CZ	1:O:169:PRO:HD3	2.50	0.46
1:A:24:ASN:O	1:A:60:LYS:HA	2.16	0.46
2:D:131:LEU:C	2:D:131:LEU:HD23	2.36	0.46
1:E:110:ARG:HH11	1:E:110:ARG:HD3	1.26	0.46
2:F:227:ARG:HH11	2:F:227:ARG:HD3	1.36	0.46
1:G:97:LYS:HZ2	2:H:170:VAL:HG23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:57:MET:HE1	1:M:63:ASN:H	1.81	0.46
2:P:42:ILE:HB	2:P:103:TRP:HD1	1.80	0.46
1:A:27:GLU:CD	1:A:60:LYS:HG3	2.36	0.46
2:B:202:ALA:CB	2:B:259:THR:CG2	2.94	0.46
2:F:240:LEU:HD21	2:F:250:LEU:CD2	2.46	0.46
1:G:27:GLU:CD	1:G:60:LYS:HG3	2.36	0.46
1:K:4:LEU:HD21	1:K:87:VAL:HG11	1.96	0.46
1:K:13:ALA:HB3	1:K:118:ALA:H	1.80	0.46
2:L:208:ILE:HD13	2:L:257:ALA:CB	2.46	0.46
2:N:140:ASP:HB3	2:N:142:PHE:CE1	2.51	0.46
2:H:202:ALA:HB1	2:H:259:THR:HG22	1.98	0.46
2:J:59:GLN:HG3	2:J:132:ARG:CD	2.46	0.46
2:N:216:SER:O	2:N:267:ASN:HB2	2.15	0.46
1:O:149:TYR:CE2	1:O:169:PRO:HD3	2.50	0.46
2:B:77:TYR:O	2:B:78:SER:C	2.54	0.46
2:D:53:THR:H	2:D:136:ASN:HD21	1.64	0.46
1:E:30:THR:OG1	1:E:58:LYS:HG2	2.15	0.46
2:H:5:THR:HA	2:H:41:GLN:O	2.15	0.46
1:A:156:ASN:O	1:A:185:ILE:HA	2.15	0.45
2:B:59:GLN:HE22	2:B:132:ARG:NH2	2.14	0.45
1:C:27:GLU:CD	1:C:60:LYS:HG3	2.36	0.45
1:E:59:GLY:O	1:E:61:LYS:HB2	2.15	0.45
2:H:70:ASN:HB3	2:H:115:ALA:HB2	1.98	0.45
1:I:120:LEU:HD23	1:I:120:LEU:HA	1.88	0.45
2:L:24:LEU:O	2:L:25:ALA:C	2.51	0.45
1:M:144:ASN:ND2	1:M:170:MET:H	2.14	0.45
1:M:150:LEU:HD23	1:M:150:LEU:HA	1.67	0.45
2:B:40:THR:CG2	2:B:41:GLN:NE2	2.76	0.45
2:F:92:ARG:HG2	2:F:92:ARG:NH1	2.18	0.45
2:J:140:ASP:HB3	2:J:142:PHE:CE1	2.51	0.45
1:K:11:TYR:HB3	1:K:115:TYR:HA	1.98	0.45
2:L:75:VAL:O	2:L:81:SER:HA	2.17	0.45
1:O:9:VAL:HG12	1:O:10:ILE:H	1.81	0.45
2:B:39:SER:O	2:B:102:PRO:HB3	2.17	0.45
2:F:39:SER:O	2:F:102:PRO:HB3	2.16	0.45
2:H:39:SER:O	2:H:102:PRO:HB3	2.17	0.45
2:H:77:TYR:CD2	2:H:90:THR:CG2	2.99	0.45
2:J:140:ASP:HB3	2:J:142:PHE:CZ	2.51	0.45
1:K:33:ILE:HG13	1:K:57:MET:HG2	1.98	0.45
1:K:133:PHE:CD2	1:K:140:LEU:HD11	2.51	0.45
2:D:211:ASN:HD22	2:D:212:THR:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:9:VAL:HG12	1:K:10:ILE:H	1.81	0.45
1:K:32:LEU:HD12	1:K:90:ILE:HD12	1.99	0.45
2:N:29:ASN:OD1	2:N:157:PRO:HD2	2.16	0.45
2:N:182:PRO:O	2:N:183:LEU:HG	2.16	0.45
2:B:70:ASN:HB3	2:B:115:ALA:HB2	1.98	0.45
1:C:59:GLY:O	1:C:61:LYS:HB2	2.16	0.45
2:F:166:ARG:HG3	2:F:167:ASP:OD1	2.17	0.45
1:I:88:LYS:HE3	1:I:108:ILE:HD11	1.99	0.45
1:K:126:GLN:HE21	1:K:126:GLN:HB2	1.47	0.45
1:M:11:TYR:HB3	1:M:115:TYR:HA	1.97	0.45
2:N:140:ASP:OD1	2:N:140:ASP:N	2.47	0.45
2:N:227:ARG:HG2	2:N:227:ARG:O	2.17	0.45
1:O:32:LEU:HD12	1:O:90:ILE:HD12	1.99	0.45
1:K:88:LYS:HE3	1:K:108:ILE:HD11	1.99	0.45
1:K:129:GLU:H	1:K:129:GLU:HG3	1.75	0.45
1:K:150:LEU:HD23	1:K:150:LEU:HA	1.70	0.45
2:N:140:ASP:HB3	2:N:142:PHE:CZ	2.51	0.45
1:O:4:LEU:HD21	1:O:87:VAL:CG2	2.33	0.45
1:A:27:GLU:OE1	1:A:60:LYS:HG3	2.17	0.45
2:B:77:TYR:CD2	2:B:90:THR:CG2	2.99	0.45
1:G:185:ILE:HB	1:G:202:GLY:HA3	1.99	0.45
2:H:202:ALA:CB	2:H:259:THR:CG2	2.94	0.45
1:I:2:VAL:HG22	1:I:89:ALA:HB2	1.98	0.45
1:I:144:ASN:ND2	1:I:170:MET:H	2.14	0.45
1:I:149:TYR:CZ	1:I:169:PRO:HD3	2.52	0.45
2:L:101:LYS:HA	2:L:102:PRO:HD3	1.90	0.45
1:M:2:VAL:HG22	1:M:89:ALA:HB2	1.98	0.45
2:P:75:VAL:O	2:P:81:SER:HA	2.16	0.45
2:P:208:ILE:HD13	2:P:257:ALA:CB	2.46	0.45
2:D:95:TYR:OH	2:D:103:TRP:HA	2.17	0.45
2:F:211:ASN:HD22	2:F:212:THR:N	2.13	0.45
2:J:250:LEU:HB2	2:J:252:LEU:HG	1.98	0.45
1:K:18:VAL:CG1	1:K:19:GLN:H	2.22	0.45
1:K:153:THR:O	1:K:154:GLU:C	2.54	0.45
1:M:149:TYR:CZ	1:M:169:PRO:HD3	2.52	0.45
2:F:95:TYR:OH	2:F:103:TRP:HA	2.17	0.45
1:I:33:ILE:HG13	1:I:57:MET:HG2	1.99	0.45
1:I:50:VAL:HG21	1:I:85:MET:CE	2.43	0.45
2:J:227:ARG:O	2:J:227:ARG:HG2	2.17	0.45
2:L:29:ASN:OD1	2:L:157:PRO:HG2	2.15	0.45
2:L:189:LYS:HA	2:L:189:LYS:HD3	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:ALA:CB	1:M:118:ALA:H	2.30	0.45
1:M:153:THR:O	1:M:154:GLU:C	2.55	0.45
1:O:33:ILE:HG13	1:O:57:MET:HG2	1.98	0.45
2:P:161:CYS:HB3	2:P:186:TYR:O	2.17	0.45
1:A:185:ILE:HB	1:A:202:GLY:HA3	1.99	0.45
2:D:166:ARG:HG3	2:D:167:ASP:OD1	2.17	0.45
1:G:24:ASN:O	1:G:60:LYS:HA	2.16	0.45
2:J:191:GLN:O	2:J:242:ALA:HA	2.17	0.45
2:J:258:ARG:HH21	2:J:263:VAL:CG2	2.30	0.45
1:M:13:ALA:HB3	1:M:118:ALA:H	1.82	0.45
1:O:153:THR:O	1:O:154:GLU:C	2.54	0.45
1:A:59:GLY:O	1:A:61:LYS:HB2	2.17	0.44
1:I:153:THR:O	1:I:154:GLU:C	2.55	0.44
2:J:182:PRO:O	2:J:183:LEU:HG	2.16	0.44
2:L:218:ALA:HB3	2:L:268:VAL:HG23	1.99	0.44
1:O:133:PHE:CD2	1:O:140:LEU:HD11	2.51	0.44
2:D:39:SER:O	2:D:102:PRO:HB3	2.16	0.44
2:F:168:VAL:O	2:F:168:VAL:HG13	2.18	0.44
1:M:90:ILE:HG23	1:M:91:PRO:HD2	1.98	0.44
1:M:153:THR:HB	1:M:190:ILE:HD11	1.99	0.44
2:N:250:LEU:HB2	2:N:252:LEU:HG	1.98	0.44
1:O:2:VAL:HG12	1:O:24:ASN:CA	2.41	0.44
1:C:4:LEU:HD13	1:C:111:ILE:HD13	1.98	0.44
1:E:4:LEU:HD13	1:E:111:ILE:HD13	1.98	0.44
1:E:145:PRO:HD2	1:E:146:THR:HG23	1.99	0.44
2:F:202:ALA:HB1	2:F:259:THR:HG22	1.99	0.44
2:J:129:LEU:HD12	2:J:148:ILE:HD11	1.99	0.44
2:J:138:ASN:H	2:J:138:ASN:ND2	2.10	0.44
1:M:80:GLU:OE2	1:M:148:TYR:HA	2.17	0.44
1:M:88:LYS:HE3	1:M:108:ILE:HD11	1.99	0.44
1:O:11:TYR:HB3	1:O:115:TYR:HA	1.98	0.44
1:O:80:GLU:OE2	1:O:148:TYR:HA	2.18	0.44
2:P:218:ALA:HB3	2:P:268:VAL:HG23	1.99	0.44
1:M:4:LEU:HD22	1:M:20:LEU:HD21	2.00	0.44
2:N:38:LEU:HD22	2:N:148:ILE:HD12	1.99	0.44
2:N:59:GLN:HG3	2:N:132:ARG:CD	2.46	0.44
2:N:75:VAL:O	2:N:81:SER:HA	2.18	0.44
2:P:227:ARG:O	2:P:227:ARG:HG2	2.18	0.44
2:F:29:ASN:HB2	2:F:32:GLN:CG	2.45	0.44
2:F:135:ASN:HD21	2:F:138:ASN:ND2	2.16	0.44
1:I:4:LEU:HD22	1:I:20:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:LEU:HD13	2:L:129:LEU:CD1	2.48	0.44
2:L:161:CYS:HB3	2:L:186:TYR:O	2.17	0.44
2:L:201:THR:CG2	2:L:206:ASN:HA	2.47	0.44
1:M:50:VAL:HG21	1:M:85:MET:CE	2.43	0.44
2:N:191:GLN:O	2:N:242:ALA:HA	2.17	0.44
2:B:227:ARG:HH11	2:B:227:ARG:HD3	1.44	0.44
1:C:51:THR:HB	1:C:66:ARG:HB2	2.00	0.44
2:D:202:ALA:HB1	2:D:259:THR:HG22	1.99	0.44
1:G:4:LEU:HD13	1:G:111:ILE:HD13	1.99	0.44
2:H:40:THR:CG2	2:H:41:GLN:NE2	2.76	0.44
1:I:149:TYR:CE2	1:I:169:PRO:HD3	2.52	0.44
2:J:136:ASN:H	2:J:136:ASN:HD22	1.66	0.44
2:J:224:GLN:CD	2:J:231:ILE:HD13	2.38	0.44
2:L:140:ASP:OD1	2:L:140:ASP:N	2.49	0.44
2:N:224:GLN:CD	2:N:231:ILE:HD13	2.38	0.44
2:P:193:LEU:HD21	2:P:278:TYR:CE2	2.53	0.44
1:C:145:PRO:HD2	1:C:146:THR:HG23	1.99	0.44
1:I:116:ARG:HA	1:I:117:PRO:HD2	1.80	0.44
1:K:7:THR:O	1:K:8:ARG:NH2	2.49	0.44
1:K:19:GLN:HB2	1:K:66:ARG:HD3	2.00	0.44
1:K:32:LEU:CD1	1:K:54:LEU:HD11	2.37	0.44
2:L:227:ARG:O	2:L:227:ARG:HG2	2.18	0.44
1:O:19:GLN:HB2	1:O:66:ARG:HD3	2.00	0.44
1:O:88:LYS:HE3	1:O:108:ILE:HD11	1.99	0.44
1:O:120:LEU:HD23	1:O:120:LEU:HA	1.86	0.44
2:D:135:ASN:HD21	2:D:138:ASN:ND2	2.16	0.44
2:D:195:TYR:HA	2:D:275:THR:O	2.18	0.44
2:D:226:THR:HA	2:D:230:THR:O	2.17	0.44
1:E:142:LEU:N	1:E:142:LEU:HD23	2.33	0.44
1:E:154:GLU:O	1:E:187:TYR:HA	2.18	0.44
2:F:226:THR:HA	2:F:230:THR:O	2.17	0.44
1:G:27:GLU:H	1:G:27:GLU:HG2	1.39	0.44
1:M:19:GLN:HB2	1:M:66:ARG:HD3	2.00	0.44
2:B:92:ARG:HG2	2:B:92:ARG:NH1	2.21	0.44
1:G:37:VAL:HA	1:G:84:TRP:O	2.18	0.44
1:G:59:GLY:O	1:G:61:LYS:HB2	2.17	0.44
1:I:13:ALA:CB	1:I:118:ALA:H	2.30	0.44
1:K:11:TYR:CD1	1:K:18:VAL:HG23	2.53	0.44
2:L:193:LEU:HD21	2:L:278:TYR:CE2	2.53	0.44
1:M:149:TYR:CE2	1:M:169:PRO:HD3	2.52	0.44
2:N:201:THR:CG2	2:N:206:ASN:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD23	1:A:142:LEU:N	2.33	0.43
2:B:112:VAL:HG12	2:P:74:THR:CG2	2.48	0.43
2:B:112:VAL:HG12	2:P:74:THR:HG22	2.00	0.43
1:C:110:ARG:HH11	1:C:110:ARG:HD3	1.26	0.43
1:I:101:ASN:HD21	2:J:268:VAL:H	1.66	0.43
1:I:116:ARG:HH12	1:I:124:PRO:HB3	1.83	0.43
2:J:75:VAL:O	2:J:81:SER:HA	2.18	0.43
2:J:201:THR:CG2	2:J:206:ASN:HA	2.47	0.43
1:M:32:LEU:HD12	1:M:90:ILE:HD12	2.00	0.43
2:N:162:ASP:HB3	2:N:186:TYR:CD2	2.53	0.43
2:P:38:LEU:HD13	2:P:129:LEU:CD1	2.48	0.43
2:P:163:VAL:HG12	2:P:185:VAL:HG12	2.00	0.43
2:P:201:THR:CG2	2:P:206:ASN:HA	2.47	0.43
1:C:154:GLU:O	1:C:187:TYR:HA	2.18	0.43
2:F:53:THR:H	2:F:136:ASN:HD21	1.63	0.43
1:G:27:GLU:OE1	1:G:60:LYS:HG3	2.17	0.43
1:K:29:SER:O	1:K:58:LYS:HA	2.17	0.43
2:N:161:CYS:HB3	2:N:186:TYR:O	2.18	0.43
1:O:11:TYR:CD1	1:O:18:VAL:HG23	2.53	0.43
2:P:136:ASN:H	2:P:136:ASN:HD22	1.66	0.43
2:P:189:LYS:HD3	2:P:189:LYS:HA	1.55	0.43
1:E:163:GLU:HB2	1:E:175:VAL:HG13	2.00	0.43
1:G:201:THR:O	1:G:203:VAL:HG23	2.18	0.43
1:I:79:ARG:HB3	1:I:170:MET:HE2	1.98	0.43
1:I:133:PHE:CD2	1:I:140:LEU:HD11	2.53	0.43
2:J:161:CYS:HB3	2:J:186:TYR:O	2.18	0.43
1:K:153:THR:HB	1:K:190:ILE:HD11	2.00	0.43
2:L:140:ASP:HB3	2:L:142:PHE:CZ	2.54	0.43
1:M:154:GLU:HG3	1:M:196:LEU:HD21	2.01	0.43
1:A:37:VAL:HA	1:A:84:TRP:O	2.18	0.43
1:A:201:THR:O	1:A:203:VAL:HG23	2.18	0.43
1:E:47:ARG:HH11	1:E:47:ARG:HD2	1.57	0.43
1:M:33:ILE:HG13	1:M:57:MET:HG2	1.99	0.43
1:O:29:SER:O	1:O:58:LYS:HA	2.17	0.43
1:A:4:LEU:HD13	1:A:111:ILE:HD13	1.99	0.43
1:A:145:PRO:HD2	1:A:146:THR:HG23	1.99	0.43
1:A:163:GLU:HB2	1:A:175:VAL:HG13	2.01	0.43
2:B:226:THR:O	2:B:252:LEU:HA	2.19	0.43
2:D:40:THR:CG2	2:D:41:GLN:NE2	2.76	0.43
1:E:51:THR:N	1:E:66:ARG:O	2.39	0.43
2:F:195:TYR:HA	2:F:275:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:GLN:HE22	2:H:132:ARG:NH2	2.14	0.43
2:J:25:ALA:HA	2:J:26:PRO:HD3	1.84	0.43
2:N:136:ASN:HD22	2:N:136:ASN:H	1.66	0.43
2:N:164:SER:HB3	2:N:184:THR:OG1	2.19	0.43
2:P:164:SER:HB3	2:P:184:THR:OG1	2.19	0.43
1:C:163:GLU:HB2	1:C:175:VAL:HG13	2.00	0.43
2:H:226:THR:O	2:H:252:LEU:HA	2.19	0.43
1:I:80:GLU:OE2	1:I:148:TYR:HA	2.17	0.43
2:L:163:VAL:HG12	2:L:185:VAL:HG12	2.00	0.43
1:M:133:PHE:CD2	1:M:140:LEU:HD11	2.53	0.43
2:N:129:LEU:HD12	2:N:148:ILE:HD11	1.99	0.43
1:O:153:THR:HB	1:O:190:ILE:HD11	2.00	0.43
2:H:126:ILE:CD1	2:H:150:ALA:HB2	2.49	0.43
1:K:50:VAL:HG21	1:K:85:MET:CE	2.46	0.43
1:O:128:ALA:O	1:O:187:TYR:OH	2.25	0.43
2:P:182:PRO:O	2:P:183:LEU:HG	2.18	0.43
1:I:13:ALA:HB3	1:I:118:ALA:H	1.82	0.43
1:I:144:ASN:ND2	1:I:168:PRO:O	2.52	0.43
2:J:38:LEU:HD22	2:J:148:ILE:HD12	1.99	0.43
1:M:39:ASN:HA	1:M:83:PHE:CD2	2.54	0.43
2:B:168:VAL:HG13	2:B:168:VAL:O	2.19	0.43
1:C:142:LEU:N	1:C:142:LEU:HD23	2.33	0.43
2:D:168:VAL:HG13	2:D:168:VAL:O	2.18	0.43
2:H:95:TYR:OH	2:H:103:TRP:HA	2.19	0.43
2:H:168:VAL:O	2:H:168:VAL:HG13	2.19	0.43
2:J:58:LEU:O	2:J:90:THR:HB	2.19	0.43
1:K:4:LEU:HD21	1:K:87:VAL:CG2	2.33	0.43
2:L:126:ILE:HD13	2:L:126:ILE:HG21	1.72	0.43
2:L:164:SER:HB3	2:L:184:THR:OG1	2.19	0.43
1:M:116:ARG:HH12	1:M:124:PRO:HB3	1.83	0.43
2:N:258:ARG:HH21	2:N:263:VAL:CG2	2.30	0.43
1:O:122:LEU:HD11	1:O:130:LYS:HE2	2.01	0.43
2:P:90:THR:HA	2:P:91:PRO:HD3	1.89	0.43
1:C:37:VAL:HA	1:C:84:TRP:O	2.19	0.43
1:G:145:PRO:HD2	1:G:146:THR:HG23	1.99	0.43
1:I:29:SER:O	1:I:58:LYS:HA	2.18	0.43
1:I:39:ASN:HA	1:I:83:PHE:CD2	2.54	0.43
2:J:162:ASP:HB3	2:J:186:TYR:CD2	2.53	0.43
2:J:193:LEU:HD21	2:J:278:TYR:CE2	2.54	0.43
1:K:80:GLU:OE2	1:K:148:TYR:HA	2.18	0.43
1:A:88:LYS:HB2	1:A:108:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:TYR:OH	2:B:103:TRP:HA	2.19	0.42
2:H:112:VAL:HG12	2:L:74:THR:CG2	2.49	0.42
1:I:32:LEU:HD12	1:I:90:ILE:HD12	2.01	0.42
1:I:153:THR:HB	1:I:190:ILE:HD11	1.99	0.42
2:L:136:ASN:HD22	2:L:136:ASN:H	1.66	0.42
2:L:182:PRO:O	2:L:183:LEU:HG	2.18	0.42
1:M:122:LEU:HD11	1:M:130:LYS:HE2	2.01	0.42
1:G:88:LYS:HB2	1:G:108:ILE:HG12	2.01	0.42
1:G:142:LEU:N	1:G:142:LEU:HD23	2.33	0.42
1:I:82:LEU:C	1:I:82:LEU:HD12	2.39	0.42
1:K:122:LEU:HD11	1:K:130:LYS:HE2	2.01	0.42
1:M:101:ASN:HD21	2:N:268:VAL:H	1.66	0.42
2:P:103:TRP:CE2	2:P:105:VAL:HG21	2.54	0.42
2:P:140:ASP:HB3	2:P:142:PHE:CZ	2.54	0.42
2:F:5:THR:HB	2:F:9:THR:O	2.20	0.42
1:I:19:GLN:HB2	1:I:66:ARG:HD3	2.00	0.42
1:I:57:MET:HE3	1:I:57:MET:HB3	1.94	0.42
2:L:103:TRP:CE2	2:L:105:VAL:HG21	2.54	0.42
1:M:2:VAL:HG12	1:M:24:ASN:CA	2.44	0.42
1:M:82:LEU:C	1:M:82:LEU:HD12	2.39	0.42
1:O:33:ILE:HG13	1:O:57:MET:CG	2.49	0.42
2:P:225:LEU:HD21	2:P:272:ILE:CD1	2.49	0.42
1:A:47:ARG:HH11	1:A:47:ARG:HD2	1.54	0.42
2:D:84:PHE:CA	2:D:85:PRO:C	2.87	0.42
2:D:211:ASN:HD21	2:D:269:GLN:H	1.67	0.42
1:E:27:GLU:OE1	1:E:60:LYS:HG3	2.20	0.42
1:I:126:GLN:HE21	1:I:126:GLN:HB2	1.46	0.42
1:I:154:GLU:HG3	1:I:196:LEU:HD21	2.01	0.42
2:J:164:SER:HB3	2:J:184:THR:OG1	2.19	0.42
1:M:33:ILE:HG13	1:M:57:MET:CG	2.49	0.42
1:M:144:ASN:ND2	1:M:168:PRO:O	2.52	0.42
2:B:126:ILE:CD1	2:B:150:ALA:HB2	2.49	0.42
2:J:103:TRP:CD2	2:J:131:LEU:HD12	2.54	0.42
1:K:103:LEU:CD2	2:L:181:ILE:HG12	2.50	0.42
2:N:193:LEU:HD21	2:N:278:TYR:CE2	2.54	0.42
1:O:150:LEU:HD23	1:O:150:LEU:HA	1.70	0.42
1:O:154:GLU:HG3	1:O:196:LEU:HD21	2.01	0.42
2:B:83:PRO:O	2:B:86:THR:HA	2.20	0.42
2:B:126:ILE:HD13	2:B:150:ALA:CB	2.49	0.42
1:E:51:THR:HB	1:E:66:ARG:HB2	2.00	0.42
2:F:40:THR:HG23	2:F:41:GLN:NE2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:PRO:O	2:H:86:THR:HA	2.20	0.42
1:K:168:PRO:HA	1:K:169:PRO:HD3	1.80	0.42
2:N:58:LEU:O	2:N:90:THR:HB	2.19	0.42
2:N:135:ASN:OD1	2:N:137:TYR:N	2.43	0.42
1:O:193:TYR:CB	2:P:155:VAL:HG11	2.50	0.42
2:P:126:ILE:HG21	2:P:126:ILE:HD13	1.72	0.42
2:J:163:VAL:HG12	2:J:185:VAL:HG12	2.01	0.42
1:K:104:GLN:N	2:L:270:SER:O	2.48	0.42
1:K:144:ASN:ND2	1:K:168:PRO:O	2.53	0.42
2:L:207:SER:HA	2:L:233:PRO:HA	2.01	0.42
2:N:103:TRP:CD2	2:N:131:LEU:HD12	2.54	0.42
2:N:126:ILE:HG21	2:N:126:ILE:HD13	1.66	0.42
2:P:55:TYR:O	2:P:133:GLN:HA	2.19	0.42
2:F:58:LEU:H	2:F:90:THR:CG2	2.33	0.42
1:G:163:GLU:HB2	1:G:175:VAL:HG13	2.01	0.42
2:H:138:ASN:ND2	2:H:140:ASP:HB2	2.33	0.42
1:I:33:ILE:HG13	1:I:57:MET:CG	2.49	0.42
1:K:116:ARG:HA	1:K:117:PRO:HD2	1.76	0.42
1:K:154:GLU:HG3	1:K:196:LEU:HD21	2.01	0.42
2:N:163:VAL:HG12	2:N:185:VAL:HG12	2.01	0.42
1:O:144:ASN:ND2	1:O:168:PRO:O	2.53	0.42
1:G:154:GLU:O	1:G:187:TYR:HA	2.20	0.42
1:K:39:ASN:HA	1:K:83:PHE:CD2	2.54	0.42
1:K:193:TYR:CB	2:L:155:VAL:HG11	2.50	0.42
2:L:55:TYR:O	2:L:133:GLN:HA	2.19	0.42
1:M:29:SER:O	1:M:58:LYS:HA	2.18	0.42
1:O:55:PHE:N	1:O:55:PHE:CD2	2.88	0.42
2:F:84:PHE:CA	2:F:85:PRO:C	2.87	0.42
2:H:112:VAL:HG12	2:L:74:THR:HG22	2.01	0.42
1:I:122:LEU:HD11	1:I:130:LYS:HE2	2.01	0.42
2:L:225:LEU:HD21	2:L:272:ILE:CD1	2.49	0.42
2:N:256:TYR:HE2	2:N:268:VAL:HG11	1.85	0.42
1:O:39:ASN:HA	1:O:83:PHE:CD2	2.54	0.42
1:O:103:LEU:CD2	2:P:181:ILE:HG12	2.50	0.42
2:P:1:PHE:HB2	2:P:54:ASP:OD2	2.20	0.42
1:A:197:THR:CB	1:A:198:PRO:CD	2.98	0.41
1:C:27:GLU:OE1	1:C:60:LYS:HG3	2.20	0.41
2:D:5:THR:HB	2:D:9:THR:O	2.20	0.41
2:F:211:ASN:HD21	2:F:269:GLN:H	1.67	0.41
1:G:33:ILE:HG12	1:G:57:MET:HE2	2.01	0.41
1:I:105:LEU:HA	2:J:272:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:THR:O	1:O:8:ARG:NH2	2.49	0.41
2:B:227:ARG:HD3	2:B:232:ILE:HG12	2.02	0.41
2:J:207:SER:HA	2:J:233:PRO:HA	2.01	0.41
1:K:33:ILE:HG13	1:K:57:MET:CG	2.49	0.41
1:K:55:PHE:CD2	1:K:55:PHE:N	2.88	0.41
2:L:158:THR:HB	2:L:189:LYS:HG2	2.02	0.41
1:O:90:ILE:HG23	1:O:91:PRO:HD2	2.01	0.41
2:P:207:SER:HA	2:P:233:PRO:HA	2.01	0.41
2:B:57:THR:HG23	2:B:89:GLU:HG3	2.03	0.41
1:I:153:THR:OG1	1:I:154:GLU:N	2.53	0.41
1:K:90:ILE:HG23	1:K:91:PRO:HD2	2.01	0.41
1:M:57:MET:SD	1:M:63:ASN:HB2	2.61	0.41
2:P:96:ASN:ND2	2:P:96:ASN:N	2.67	0.41
1:A:27:GLU:H	1:A:27:GLU:HG2	1.39	0.41
1:C:51:THR:N	1:C:66:ARG:O	2.39	0.41
2:D:227:ARG:HD3	2:D:232:ILE:HG12	2.01	0.41
1:E:37:VAL:HA	1:E:84:TRP:O	2.19	0.41
2:J:135:ASN:OD1	2:J:137:TYR:N	2.43	0.41
2:L:1:PHE:HB2	2:L:54:ASP:OD2	2.20	0.41
2:P:171:THR:HG22	2:P:256:TYR:CZ	2.55	0.41
1:A:101:ASN:O	2:B:171:THR:N	2.45	0.41
1:A:197:THR:CB	1:A:198:PRO:HD2	2.42	0.41
2:J:256:TYR:HE2	2:J:268:VAL:HG11	1.85	0.41
1:O:90:ILE:HA	1:O:91:PRO:HD3	1.92	0.41
1:I:43:VAL:O	1:I:45:ASP:N	2.54	0.41
2:J:40:THR:HG23	2:J:41:GLN:NE2	2.35	0.41
1:K:79:ARG:HA	1:K:147:PRO:CB	2.51	0.41
1:M:43:VAL:O	1:M:45:ASP:N	2.54	0.41
1:M:122:LEU:HD11	1:M:130:LYS:HZ1	1.85	0.41
2:N:207:SER:HA	2:N:233:PRO:HA	2.01	0.41
2:P:28:VAL:O	2:P:156:VAL:HA	2.20	0.41
1:A:110:ARG:HH11	1:A:110:ARG:HD3	1.34	0.41
1:A:154:GLU:O	1:A:187:TYR:HA	2.20	0.41
2:F:103:TRP:CZ3	2:F:131:LEU:HB2	2.55	0.41
1:I:140:LEU:HB2	1:I:177:LEU:CD1	2.51	0.41
1:K:122:LEU:HA	1:K:123:PRO:HD3	1.94	0.41
2:L:28:VAL:O	2:L:156:VAL:HA	2.20	0.41
1:M:105:LEU:HA	2:N:272:ILE:O	2.21	0.41
1:M:193:TYR:CB	2:N:155:VAL:HG11	2.51	0.41
2:N:38:LEU:HD13	2:N:129:LEU:CD1	2.51	0.41
2:P:158:THR:HB	2:P:189:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ASN:O	2:B:98:ARG:HA	2.21	0.41
2:F:77:TYR:O	2:F:78:SER:C	2.59	0.41
2:H:57:THR:HG23	2:H:89:GLU:HG3	2.03	0.41
2:H:131:LEU:C	2:H:131:LEU:HD23	2.40	0.41
2:J:38:LEU:HD13	2:J:129:LEU:CD1	2.51	0.41
2:L:12:PRO:O	2:L:15:GLY:HA3	2.21	0.41
2:L:256:TYR:HE2	2:L:268:VAL:HG11	1.86	0.41
1:M:4:LEU:HD21	1:M:87:VAL:CG2	2.35	0.41
2:N:96:ASN:ND2	2:N:96:ASN:N	2.68	0.41
2:B:131:LEU:HD23	2:B:131:LEU:C	2.40	0.41
2:B:138:ASN:ND2	2:B:140:ASP:HB2	2.33	0.41
2:D:38:LEU:HD22	2:D:148:ILE:HD12	2.03	0.41
2:D:58:LEU:H	2:D:90:THR:CG2	2.33	0.41
1:I:197:THR:CB	1:I:198:PRO:CD	2.89	0.41
2:J:58:LEU:H	2:J:90:THR:HG22	1.85	0.41
2:J:126:ILE:HD13	2:J:126:ILE:HG21	1.66	0.41
2:J:171:THR:HG22	2:J:256:TYR:CZ	2.56	0.41
2:J:267:ASN:HD22	2:J:267:ASN:HA	1.73	0.41
2:L:38:LEU:HD22	2:L:148:ILE:HD12	2.02	0.41
2:L:171:THR:HG22	2:L:256:TYR:CZ	2.55	0.41
2:L:240:LEU:HD21	2:L:250:LEU:HD22	2.03	0.41
2:L:267:ASN:HD22	2:L:267:ASN:HA	1.73	0.41
1:M:120:LEU:HD23	1:M:120:LEU:HA	1.88	0.41
1:M:153:THR:OG1	1:M:154:GLU:N	2.54	0.41
2:N:67:VAL:O	2:N:71:PHE:HB2	2.21	0.41
1:O:116:ARG:HH12	1:O:124:PRO:HB3	1.86	0.41
2:B:84:PHE:CA	2:B:85:PRO:C	2.89	0.41
2:D:40:THR:HG23	2:D:41:GLN:NE2	2.32	0.41
2:F:40:THR:CG2	2:F:41:GLN:NE2	2.76	0.41
2:F:83:PRO:O	2:F:86:THR:HA	2.21	0.41
2:H:211:ASN:HD22	2:H:212:THR:N	2.16	0.41
1:I:57:MET:SD	1:I:63:ASN:HB2	2.61	0.41
2:L:162:ASP:N	2:L:186:TYR:O	2.46	0.41
1:M:85:MET:HB2	1:M:111:ILE:HG13	2.03	0.41
1:O:79:ARG:HA	1:O:147:PRO:CB	2.51	0.41
1:O:104:GLN:N	2:P:270:SER:O	2.48	0.41
1:O:123:PRO:HA	1:O:124:PRO:HD2	1.95	0.41
2:P:152:ASN:OD1	2:P:152:ASN:N	2.54	0.41
1:A:101:ASN:CB	2:B:171:THR:O	2.69	0.40
2:D:42:ILE:HD12	2:D:103:TRP:HE1	1.87	0.40
2:D:103:TRP:CZ3	2:D:131:LEU:HB2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:189:LYS:HB3	2:F:189:LYS:HE3	1.93	0.40
1:G:101:ASN:OD1	2:H:268:VAL:N	2.45	0.40
2:H:58:LEU:H	2:H:90:THR:CG2	2.34	0.40
2:H:126:ILE:HD13	2:H:150:ALA:CB	2.49	0.40
1:I:104:GLN:N	2:J:270:SER:O	2.50	0.40
1:K:103:LEU:HD21	1:K:105:LEU:HD21	2.02	0.40
2:N:112:VAL:O	2:N:112:VAL:HG23	2.21	0.40
1:O:4:LEU:CD2	1:O:22:VAL:HG22	2.51	0.40
2:P:224:GLN:CD	2:P:231:ILE:HD13	2.41	0.40
1:C:47:ARG:HH11	1:C:47:ARG:HD2	1.58	0.40
2:D:1:PHE:O	2:D:13:ILE:HA	2.21	0.40
2:F:227:ARG:HD3	2:F:232:ILE:HG12	2.01	0.40
2:H:92:ARG:HG2	2:H:92:ARG:NH1	2.21	0.40
2:L:40:THR:HG23	2:L:41:GLN:NE2	2.34	0.40
1:M:140:LEU:HB2	1:M:177:LEU:CD1	2.51	0.40
1:A:30:THR:OG1	1:A:58:LYS:HG2	2.22	0.40
2:F:1:PHE:O	2:F:13:ILE:HA	2.21	0.40
1:G:101:ASN:CB	2:H:171:THR:O	2.69	0.40
2:L:58:LEU:O	2:L:90:THR:HB	2.21	0.40
2:N:136:ASN:HD22	2:N:136:ASN:N	2.19	0.40
2:P:256:TYR:HE2	2:P:268:VAL:HG11	1.86	0.40
2:D:77:TYR:O	2:D:78:SER:C	2.59	0.40
2:F:38:LEU:HD22	2:F:148:ILE:HD12	2.03	0.40
1:I:193:TYR:CB	2:J:155:VAL:HG11	2.51	0.40
1:M:204:MET:O	1:M:205:GLU:HB2	2.21	0.40
2:P:162:ASP:HB3	2:P:186:TYR:CD2	2.57	0.40
1:A:11:TYR:HA	1:A:18:VAL:HG21	2.03	0.40
2:B:29:ASN:HB2	2:B:32:GLN:CG	2.51	0.40
2:B:58:LEU:H	2:B:90:THR:CG2	2.34	0.40
1:C:101:ASN:O	2:D:171:THR:N	2.46	0.40
2:D:126:ILE:CD1	2:D:150:ALA:HB2	2.51	0.40
2:F:46:ASN:O	2:F:98:ARG:HA	2.21	0.40
1:G:197:THR:CB	1:G:198:PRO:CD	2.98	0.40
1:I:39:ASN:HB3	1:I:45:ASP:OD2	2.22	0.40
1:I:204:MET:O	1:I:205:GLU:HB2	2.21	0.40
1:M:39:ASN:HB3	1:M:45:ASP:OD2	2.22	0.40
2:N:5:THR:O	2:N:8:GLY:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	196/205 (96%)	185 (94%)	11 (6%)	0	100	100
1	C	196/205 (96%)	184 (94%)	12 (6%)	0	100	100
1	E	196/205 (96%)	184 (94%)	12 (6%)	0	100	100
1	G	196/205 (96%)	185 (94%)	11 (6%)	0	100	100
1	I	190/205 (93%)	135 (71%)	37 (20%)	18 (10%)	0	1
1	K	190/205 (93%)	134 (70%)	37 (20%)	19 (10%)	0	1
1	M	190/205 (93%)	135 (71%)	37 (20%)	18 (10%)	0	1
1	O	190/205 (93%)	134 (70%)	37 (20%)	19 (10%)	0	1
2	B	277/279 (99%)	253 (91%)	23 (8%)	1 (0%)	34	66
2	D	277/279 (99%)	254 (92%)	22 (8%)	1 (0%)	34	66
2	F	277/279 (99%)	254 (92%)	22 (8%)	1 (0%)	34	66
2	H	277/279 (99%)	253 (91%)	23 (8%)	1 (0%)	34	66
2	J	275/279 (99%)	238 (86%)	25 (9%)	12 (4%)	2	8
2	L	277/279 (99%)	242 (87%)	24 (9%)	11 (4%)	3	9
2	N	275/279 (99%)	238 (86%)	25 (9%)	12 (4%)	2	8
2	P	277/279 (99%)	242 (87%)	24 (9%)	11 (4%)	3	9
All	All	3756/3872 (97%)	3250 (86%)	382 (10%)	124 (3%)	4	13

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	176	PRO
2	D	176	PRO
2	F	176	PRO
2	H	176	PRO
1	I	68	LEU
1	I	70	ALA

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Mol	Chain	Res	Type
1	I	101	ASN
1	I	134	ARG
1	I	135	ARG
1	I	194	GLY
1	I	204	MET
2	J	166	ARG
2	J	168	VAL
2	J	175	TYR
2	J	177	GLY
1	K	68	LEU
1	K	70	ALA
1	K	101	ASN
1	K	134	ARG
1	K	135	ARG
1	K	194	GLY
1	K	204	MET
2	L	166	ARG
2	L	168	VAL
2	L	175	TYR
2	L	177	GLY
1	M	68	LEU
1	M	70	ALA
1	M	101	ASN
1	M	134	ARG
1	M	135	ARG
1	M	194	GLY
1	M	204	MET
2	N	166	ARG
2	N	168	VAL
2	N	175	TYR
2	N	177	GLY
1	O	68	LEU
1	O	70	ALA
1	O	101	ASN
1	O	134	ARG
1	O	135	ARG
1	O	194	GLY
1	O	204	MET
2	P	166	ARG
2	P	168	VAL
2	P	175	TYR
2	P	177	GLY

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Mol	Chain	Res	Type
1	I	33	ILE
1	I	44	LYS
1	I	69	ASP
1	I	157	ALA
1	I	158	GLY
2	J	165	ALA
2	J	260	GLY
1	K	33	ILE
1	K	44	LYS
1	K	157	ALA
2	L	260	GLY
1	M	33	ILE
1	M	44	LYS
1	M	69	ASP
1	M	157	ALA
1	M	158	GLY
2	N	165	ALA
2	N	260	GLY
1	O	33	ILE
1	O	44	LYS
1	O	157	ALA
2	P	260	GLY
1	I	96	SER
1	K	69	ASP
1	K	96	SER
1	K	154	GLU
2	L	243	VAL
1	M	96	SER
1	O	69	ASP
1	O	96	SER
1	O	154	GLU
2	P	243	VAL
1	I	94	ASP
1	I	154	GLU
1	K	94	ASP
2	L	165	ALA
1	M	94	ASP
1	M	154	GLU
1	O	94	ASP
2	P	165	ALA
1	I	36	TRP
1	K	36	TRP

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Mol	Chain	Res	Type
1	K	170	MET
2	L	216	SER
1	M	36	TRP
1	O	36	TRP
1	O	170	MET
2	P	216	SER
2	J	176	PRO
2	J	178	SER
2	J	182	PRO
2	J	216	SER
2	J	243	VAL
1	K	158	GLY
2	L	176	PRO
2	L	178	SER
2	N	176	PRO
2	N	178	SER
2	N	182	PRO
2	N	216	SER
2	N	243	VAL
1	O	158	GLY
2	P	176	PRO
2	P	178	SER
1	I	76	PRO
1	K	76	PRO
2	L	182	PRO
1	M	76	PRO
1	O	76	PRO
2	P	182	PRO
1	I	91	PRO
1	K	91	PRO
1	M	91	PRO
1	O	91	PRO
2	J	116	GLY
2	N	116	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/175 (97%)	134 (79%)	35 (21%)	1	3
1	C	169/175 (97%)	132 (78%)	37 (22%)	1	3
1	E	169/175 (97%)	132 (78%)	37 (22%)	1	3
1	G	169/175 (97%)	134 (79%)	35 (21%)	1	3
1	I	169/175 (97%)	121 (72%)	48 (28%)	0	1
1	K	169/175 (97%)	121 (72%)	48 (28%)	0	1
1	M	169/175 (97%)	121 (72%)	48 (28%)	0	1
1	O	169/175 (97%)	121 (72%)	48 (28%)	0	1
2	B	226/226 (100%)	181 (80%)	45 (20%)	1	4
2	D	226/226 (100%)	181 (80%)	45 (20%)	1	4
2	F	226/226 (100%)	181 (80%)	45 (20%)	1	4
2	H	226/226 (100%)	181 (80%)	45 (20%)	1	4
2	J	226/226 (100%)	188 (83%)	38 (17%)	2	6
2	L	226/226 (100%)	189 (84%)	37 (16%)	2	7
2	N	226/226 (100%)	188 (83%)	38 (17%)	2	6
2	P	226/226 (100%)	189 (84%)	37 (16%)	2	7
All	All	3160/3208 (98%)	2494 (79%)	666 (21%)	1	3

All (666) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	15	GLN
1	A	16	LYS
1	A	22	VAL
1	A	26	ASP
1	A	44	LYS
1	A	45	ASP
1	A	47	ARG
1	A	49	ILE
1	A	51	THR
1	A	60	LYS
1	A	62	GLU
1	A	72	ASN
1	A	79	ARG
1	A	85	MET
1	A	95	LYS

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Mol	Chain	Res	Type
1	A	96	SER
1	A	102	THR
1	A	104	GLN
1	A	111	ILE
1	A	122	LEU
1	A	125	ASP
1	A	129	GLU
1	A	136	SER
1	A	138	ASN
1	A	139	SER
1	A	142	LEU
1	A	143	ILE
1	A	146	THR
1	A	159	THR
1	A	160	ARG
1	A	172	GLU
1	A	176	LYS
1	A	183	SER
1	A	204	MET
2	B	4	LYS
2	B	5	THR
2	B	40	THR
2	B	41	GLN
2	B	46	ASN
2	B	51	THR
2	B	52	ILE
2	B	57	THR
2	B	59	GLN
2	B	60	ARG
2	B	72	SER
2	B	90	THR
2	B	92	ARG
2	B	96	ASN
2	B	101	LYS
2	B	103	TRP
2	B	107	LEU
2	B	110	THR
2	B	113	SER
2	B	126	ILE
2	B	131	LEU
2	B	136	ASN
2	B	138	ASN

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Mol	Chain	Res	Type
2	B	158	THR
2	B	164	SER
2	B	166	ARG
2	B	167	ASP
2	B	172	LEU
2	B	175	TYR
2	B	176	PRO
2	B	179	VAL
2	B	183	LEU
2	B	185	VAL
2	B	201	THR
2	B	211	ASN
2	B	212	THR
2	B	215	PHE
2	B	216	SER
2	B	226	THR
2	B	227	ARG
2	B	239	SER
2	B	245	THR
2	B	259	THR
2	B	264	THR
2	B	270	SER
1	C	8	ARG
1	C	15	GLN
1	C	16	LYS
1	C	22	VAL
1	C	23	THR
1	C	26	ASP
1	C	34	GLN
1	C	44	LYS
1	C	45	ASP
1	C	47	ARG
1	C	49	ILE
1	C	51	THR
1	C	60	LYS
1	C	62	GLU
1	C	72	ASN
1	C	79	ARG
1	C	85	MET
1	C	92	SER
1	C	95	LYS
1	C	96	SER

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Mol	Chain	Res	Type
1	C	102	THR
1	C	104	GLN
1	C	122	LEU
1	C	125	ASP
1	C	129	GLU
1	C	136	SER
1	C	138	ASN
1	C	139	SER
1	C	142	LEU
1	C	143	ILE
1	C	146	THR
1	C	159	THR
1	C	160	ARG
1	C	172	GLU
1	C	176	LYS
1	C	183	SER
1	C	204	MET
2	D	4	LYS
2	D	5	THR
2	D	40	THR
2	D	41	GLN
2	D	46	ASN
2	D	51	THR
2	D	52	ILE
2	D	57	THR
2	D	59	GLN
2	D	60	ARG
2	D	72	SER
2	D	90	THR
2	D	92	ARG
2	D	96	ASN
2	D	101	LYS
2	D	103	TRP
2	D	107	LEU
2	D	110	THR
2	D	113	SER
2	D	126	ILE
2	D	131	LEU
2	D	136	ASN
2	D	138	ASN
2	D	158	THR
2	D	164	SER

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Mol	Chain	Res	Type
2	D	166	ARG
2	D	167	ASP
2	D	172	LEU
2	D	175	TYR
2	D	179	VAL
2	D	183	LEU
2	D	185	VAL
2	D	201	THR
2	D	211	ASN
2	D	212	THR
2	D	215	PHE
2	D	216	SER
2	D	226	THR
2	D	227	ARG
2	D	239	SER
2	D	245	THR
2	D	255	ASN
2	D	259	THR
2	D	264	THR
2	D	270	SER
1	E	8	ARG
1	E	15	GLN
1	E	16	LYS
1	E	22	VAL
1	E	23	THR
1	E	26	ASP
1	E	34	GLN
1	E	44	LYS
1	E	45	ASP
1	E	47	ARG
1	E	49	ILE
1	E	51	THR
1	E	60	LYS
1	E	62	GLU
1	E	72	ASN
1	E	79	ARG
1	E	85	MET
1	E	92	SER
1	E	95	LYS
1	E	96	SER
1	E	102	THR
1	E	104	GLN

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Mol	Chain	Res	Type
1	E	122	LEU
1	E	125	ASP
1	E	129	GLU
1	E	136	SER
1	E	138	ASN
1	E	139	SER
1	E	142	LEU
1	E	143	ILE
1	E	146	THR
1	E	159	THR
1	E	160	ARG
1	E	172	GLU
1	E	176	LYS
1	E	183	SER
1	E	204	MET
2	F	4	LYS
2	F	5	THR
2	F	40	THR
2	F	41	GLN
2	F	46	ASN
2	F	51	THR
2	F	52	ILE
2	F	57	THR
2	F	59	GLN
2	F	60	ARG
2	F	72	SER
2	F	90	THR
2	F	92	ARG
2	F	96	ASN
2	F	101	LYS
2	F	103	TRP
2	F	107	LEU
2	F	110	THR
2	F	113	SER
2	F	126	ILE
2	F	131	LEU
2	F	136	ASN
2	F	138	ASN
2	F	158	THR
2	F	164	SER
2	F	166	ARG
2	F	167	ASP

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Mol	Chain	Res	Type
2	F	172	LEU
2	F	175	TYR
2	F	179	VAL
2	F	183	LEU
2	F	185	VAL
2	F	201	THR
2	F	211	ASN
2	F	212	THR
2	F	215	PHE
2	F	216	SER
2	F	226	THR
2	F	227	ARG
2	F	239	SER
2	F	245	THR
2	F	255	ASN
2	F	259	THR
2	F	264	THR
2	F	270	SER
1	G	8	ARG
1	G	15	GLN
1	G	16	LYS
1	G	22	VAL
1	G	26	ASP
1	G	44	LYS
1	G	45	ASP
1	G	47	ARG
1	G	49	ILE
1	G	51	THR
1	G	60	LYS
1	G	62	GLU
1	G	72	ASN
1	G	79	ARG
1	G	85	MET
1	G	95	LYS
1	G	96	SER
1	G	102	THR
1	G	104	GLN
1	G	111	ILE
1	G	122	LEU
1	G	125	ASP
1	G	129	GLU
1	G	136	SER

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Mol	Chain	Res	Type
1	G	138	ASN
1	G	139	SER
1	G	142	LEU
1	G	143	ILE
1	G	146	THR
1	G	159	THR
1	G	160	ARG
1	G	172	GLU
1	G	176	LYS
1	G	183	SER
1	G	204	MET
2	H	4	LYS
2	H	5	THR
2	H	40	THR
2	H	41	GLN
2	H	46	ASN
2	H	51	THR
2	H	52	ILE
2	H	57	THR
2	H	59	GLN
2	H	60	ARG
2	H	72	SER
2	H	90	THR
2	H	92	ARG
2	H	96	ASN
2	H	101	LYS
2	H	103	TRP
2	H	107	LEU
2	H	110	THR
2	H	113	SER
2	H	126	ILE
2	H	131	LEU
2	H	136	ASN
2	H	138	ASN
2	H	158	THR
2	H	164	SER
2	H	166	ARG
2	H	167	ASP
2	H	172	LEU
2	H	175	TYR
2	H	176	PRO
2	H	179	VAL

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Mol	Chain	Res	Type
2	H	183	LEU
2	H	185	VAL
2	H	201	THR
2	H	211	ASN
2	H	212	THR
2	H	215	PHE
2	H	216	SER
2	H	226	THR
2	H	227	ARG
2	H	239	SER
2	H	245	THR
2	H	259	THR
2	H	264	THR
2	H	270	SER
1	I	8	ARG
1	I	15	GLN
1	I	16	LYS
1	I	19	GLN
1	I	20	LEU
1	I	23	THR
1	I	25	ASN
1	I	27	GLU
1	I	28	ASN
1	I	32	LEU
1	I	41	ASP
1	I	47	ARG
1	I	55	PHE
1	I	58	LYS
1	I	61	LYS
1	I	63	ASN
1	I	71	THR
1	I	72	ASN
1	I	73	ASN
1	I	82	LEU
1	I	85	MET
1	I	91	PRO
1	I	92	SER
1	I	93	MET
1	I	94	ASP
1	I	95	LYS
1	I	96	SER
1	I	97	LYS

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Mol	Chain	Res	Type
1	I	101	ASN
1	I	105	LEU
1	I	113	LEU
1	I	126	GLN
1	I	129	GLU
1	I	132	ARG
1	I	136	SER
1	I	143	ILE
1	I	146	THR
1	I	155	LEU
1	I	163	GLU
1	I	177	LEU
1	I	183	SER
1	I	184	ASN
1	I	185	ILE
1	I	192	ASP
1	I	199	LYS
1	I	201	THR
1	I	203	VAL
1	I	205	GLU
2	J	17	SER
2	J	40	THR
2	J	51	THR
2	J	57	THR
2	J	59	GLN
2	J	60	ARG
2	J	72	SER
2	J	80	SER
2	J	90	THR
2	J	94	VAL
2	J	96	ASN
2	J	98	ARG
2	J	107	LEU
2	J	110	THR
2	J	136	ASN
2	J	138	ASN
2	J	140	ASP
2	J	158	THR
2	J	163	VAL
2	J	172	LEU
2	J	174	ASP
2	J	178	SER

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Mol	Chain	Res	Type
2	J	179	VAL
2	J	186	TYR
2	J	189	LYS
2	J	190	SER
2	J	193	LEU
2	J	201	THR
2	J	211	ASN
2	J	224	GLN
2	J	226	THR
2	J	227	ARG
2	J	228	ASN
2	J	236	ASN
2	J	253	THR
2	J	255	ASN
2	J	267	ASN
2	J	270	SER
1	K	8	ARG
1	K	15	GLN
1	K	16	LYS
1	K	19	GLN
1	K	20	LEU
1	K	23	THR
1	K	25	ASN
1	K	27	GLU
1	K	28	ASN
1	K	32	LEU
1	K	41	ASP
1	K	47	ARG
1	K	55	PHE
1	K	58	LYS
1	K	61	LYS
1	K	63	ASN
1	K	71	THR
1	K	72	ASN
1	K	73	ASN
1	K	82	LEU
1	K	85	MET
1	K	91	PRO
1	K	92	SER
1	K	93	MET
1	K	94	ASP
1	K	95	LYS

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Mol	Chain	Res	Type
1	K	96	SER
1	K	97	LYS
1	K	101	ASN
1	K	105	LEU
1	K	113	LEU
1	K	126	GLN
1	K	129	GLU
1	K	131	LEU
1	K	132	ARG
1	K	143	ILE
1	K	146	THR
1	K	155	LEU
1	K	163	GLU
1	K	177	LEU
1	K	183	SER
1	K	184	ASN
1	K	185	ILE
1	K	192	ASP
1	K	199	LYS
1	K	201	THR
1	K	203	VAL
1	K	205	GLU
2	L	17	SER
2	L	40	THR
2	L	51	THR
2	L	57	THR
2	L	59	GLN
2	L	60	ARG
2	L	72	SER
2	L	80	SER
2	L	90	THR
2	L	94	VAL
2	L	96	ASN
2	L	98	ARG
2	L	107	LEU
2	L	110	THR
2	L	121	LYS
2	L	136	ASN
2	L	138	ASN
2	L	140	ASP
2	L	158	THR
2	L	163	VAL

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Mol	Chain	Res	Type
2	L	172	LEU
2	L	174	ASP
2	L	178	SER
2	L	179	VAL
2	L	189	LYS
2	L	190	SER
2	L	193	LEU
2	L	201	THR
2	L	211	ASN
2	L	226	THR
2	L	227	ARG
2	L	228	ASN
2	L	236	ASN
2	L	253	THR
2	L	255	ASN
2	L	267	ASN
2	L	270	SER
1	M	8	ARG
1	M	15	GLN
1	M	16	LYS
1	M	19	GLN
1	M	20	LEU
1	M	23	THR
1	M	25	ASN
1	M	27	GLU
1	M	28	ASN
1	M	32	LEU
1	M	41	ASP
1	M	47	ARG
1	M	55	PHE
1	M	58	LYS
1	M	61	LYS
1	M	63	ASN
1	M	71	THR
1	M	72	ASN
1	M	73	ASN
1	M	82	LEU
1	M	85	MET
1	M	91	PRO
1	M	92	SER
1	M	93	MET
1	M	94	ASP

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Mol	Chain	Res	Type
1	M	95	LYS
1	M	96	SER
1	M	97	LYS
1	M	101	ASN
1	M	105	LEU
1	M	113	LEU
1	M	126	GLN
1	M	129	GLU
1	M	132	ARG
1	M	136	SER
1	M	143	ILE
1	M	146	THR
1	M	155	LEU
1	M	163	GLU
1	M	177	LEU
1	M	183	SER
1	M	184	ASN
1	M	185	ILE
1	M	192	ASP
1	M	199	LYS
1	M	201	THR
1	M	203	VAL
1	M	205	GLU
2	N	17	SER
2	N	40	THR
2	N	51	THR
2	N	57	THR
2	N	59	GLN
2	N	60	ARG
2	N	72	SER
2	N	80	SER
2	N	90	THR
2	N	94	VAL
2	N	96	ASN
2	N	98	ARG
2	N	107	LEU
2	N	110	THR
2	N	136	ASN
2	N	138	ASN
2	N	140	ASP
2	N	158	THR
2	N	163	VAL

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Mol	Chain	Res	Type
2	N	172	LEU
2	N	174	ASP
2	N	178	SER
2	N	179	VAL
2	N	186	TYR
2	N	189	LYS
2	N	190	SER
2	N	193	LEU
2	N	201	THR
2	N	211	ASN
2	N	224	GLN
2	N	226	THR
2	N	227	ARG
2	N	228	ASN
2	N	236	ASN
2	N	253	THR
2	N	255	ASN
2	N	267	ASN
2	N	270	SER
1	O	8	ARG
1	O	15	GLN
1	O	16	LYS
1	O	19	GLN
1	O	20	LEU
1	O	23	THR
1	O	25	ASN
1	O	27	GLU
1	O	28	ASN
1	O	32	LEU
1	O	41	ASP
1	O	47	ARG
1	O	55	PHE
1	O	58	LYS
1	O	61	LYS
1	O	63	ASN
1	O	71	THR
1	O	72	ASN
1	O	73	ASN
1	O	82	LEU
1	O	85	MET
1	O	91	PRO
1	O	92	SER

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Mol	Chain	Res	Type
1	O	93	MET
1	O	94	ASP
1	O	95	LYS
1	O	96	SER
1	O	97	LYS
1	O	101	ASN
1	O	105	LEU
1	O	113	LEU
1	O	126	GLN
1	O	129	GLU
1	O	131	LEU
1	O	132	ARG
1	O	143	ILE
1	O	146	THR
1	O	155	LEU
1	O	163	GLU
1	O	177	LEU
1	O	183	SER
1	O	184	ASN
1	O	185	ILE
1	O	192	ASP
1	O	199	LYS
1	O	201	THR
1	O	203	VAL
1	O	205	GLU
2	P	17	SER
2	P	40	THR
2	P	51	THR
2	P	57	THR
2	P	59	GLN
2	P	60	ARG
2	P	72	SER
2	P	80	SER
2	P	90	THR
2	P	94	VAL
2	P	96	ASN
2	P	98	ARG
2	P	107	LEU
2	P	110	THR
2	P	121	LYS
2	P	136	ASN
2	P	138	ASN

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Mol	Chain	Res	Type
2	P	140	ASP
2	P	158	THR
2	P	163	VAL
2	P	172	LEU
2	P	174	ASP
2	P	178	SER
2	P	179	VAL
2	P	189	LYS
2	P	190	SER
2	P	193	LEU
2	P	201	THR
2	P	211	ASN
2	P	226	THR
2	P	227	ARG
2	P	228	ASN
2	P	236	ASN
2	P	253	THR
2	P	255	ASN
2	P	267	ASN
2	P	270	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
2	B	33	ASN
2	B	41	GLN
2	B	59	GLN
2	B	96	ASN
2	B	136	ASN
2	B	138	ASN
2	B	211	ASN
2	B	236	ASN
2	B	255	ASN
2	B	267	ASN
2	B	279	GLN
1	C	74	GLN
2	D	33	ASN
2	D	41	GLN
2	D	59	GLN
2	D	96	ASN
2	D	136	ASN

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Mol	Chain	Res	Type
2	D	138	ASN
2	D	211	ASN
2	D	255	ASN
2	D	267	ASN
2	D	279	GLN
1	E	74	GLN
2	F	33	ASN
2	F	41	GLN
2	F	59	GLN
2	F	96	ASN
2	F	136	ASN
2	F	138	ASN
2	F	211	ASN
2	F	255	ASN
2	F	267	ASN
2	F	279	GLN
1	G	74	GLN
2	H	33	ASN
2	H	41	GLN
2	H	59	GLN
2	H	96	ASN
2	H	136	ASN
2	H	138	ASN
2	H	211	ASN
2	H	236	ASN
2	H	255	ASN
2	H	267	ASN
2	H	279	GLN
1	I	24	ASN
1	I	63	ASN
1	I	101	ASN
1	I	104	GLN
1	I	126	GLN
1	I	144	ASN
2	J	41	GLN
2	J	70	ASN
2	J	96	ASN
2	J	136	ASN
2	J	138	ASN
2	J	206	ASN
2	J	211	ASN
2	J	219	GLN

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Mol	Chain	Res	Type
2	J	228	ASN
2	J	267	ASN
2	J	279	GLN
1	K	24	ASN
1	K	63	ASN
1	K	101	ASN
1	K	104	GLN
1	K	126	GLN
1	K	144	ASN
2	L	41	GLN
2	L	70	ASN
2	L	96	ASN
2	L	136	ASN
2	L	138	ASN
2	L	211	ASN
2	L	219	GLN
2	L	228	ASN
2	L	267	ASN
2	L	279	GLN
1	M	24	ASN
1	M	63	ASN
1	M	101	ASN
1	M	104	GLN
1	M	126	GLN
1	M	144	ASN
2	N	41	GLN
2	N	70	ASN
2	N	96	ASN
2	N	136	ASN
2	N	138	ASN
2	N	206	ASN
2	N	211	ASN
2	N	219	GLN
2	N	228	ASN
2	N	267	ASN
2	N	279	GLN
1	O	24	ASN
1	O	63	ASN
1	O	101	ASN
1	O	104	GLN
1	O	126	GLN
1	O	144	ASN

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Mol	Chain	Res	Type
2	P	41	GLN
2	P	70	ASN
2	P	96	ASN
2	P	136	ASN
2	P	138	ASN
2	P	206	ASN
2	P	211	ASN
2	P	219	GLN
2	P	228	ASN
2	P	267	ASN
2	P	279	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	5

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Mol	Chain	Number of breaks
1	M	5
1	K	5
1	O	5
2	J	2
2	N	2
2	L	2
2	P	2
2	B	2
2	H	2
2	D	2
2	F	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	173:PRO	C	174:ASP	N	2.75
1	N	173:PRO	C	174:ASP	N	2.75
1	I	74:GLN	C	75:LEU	N	2.13
1	M	74:GLN	C	75:LEU	N	2.13
1	K	74:GLN	C	75:LEU	N	2.05
1	O	74:GLN	C	75:LEU	N	2.05
1	L	167:ASP	C	168:VAL	N	1.77
1	P	167:ASP	C	168:VAL	N	1.77
1	J	167:ASP	C	168:VAL	N	1.71
1	N	167:ASP	C	168:VAL	N	1.71
1	I	139:SER	C	140:LEU	N	1.15
1	M	139:SER	C	140:LEU	N	1.15
1	K	139:SER	C	140:LEU	N	1.14
1	O	139:SER	C	140:LEU	N	1.14
1	L	165:ALA	C	166:ARG	N	1.13
1	P	165:ALA	C	166:ARG	N	1.13
1	B	175:TYR	C	176:PRO	N	1.10
1	H	175:TYR	C	176:PRO	N	1.10
1	D	175:TYR	C	176:PRO	N	1.09
1	F	175:TYR	C	176:PRO	N	1.09
1	K	185:ILE	C	186:THR	N	1.09
1	O	185:ILE	C	186:THR	N	1.09
1	I	185:ILE	C	186:THR	N	1.08
1	M	185:ILE	C	186:THR	N	1.08
1	B	173:PRO	C	174:ASP	N	0.91
1	H	173:PRO	C	174:ASP	N	0.91
1	D	173:PRO	C	174:ASP	N	0.90
1	F	173:PRO	C	174:ASP	N	0.90

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	161:VAL	C	162:LEU	N	0.87
1	M	161:VAL	C	162:LEU	N	0.87
1	K	161:VAL	C	162:LEU	N	0.71
1	O	161:VAL	C	162:LEU	N	0.71
1	I	135:ARG	C	136:SER	N	0.63
1	M	135:ARG	C	136:SER	N	0.63
1	K	135:ARG	C	136:SER	N	0.58
1	O	135:ARG	C	136:SER	N	0.58

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.