Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 02:14 PM EDT

PDB ID	:	3QD8
Title	:	Crystal structure of Mycobacterium tuberculosis BfrB
Authors	:	Khare, G.; Gupta, V.; Nangpal, P.; Gupta, R.K.; Sauter, N.K.; Tyagi, A.K.
Deposited on	:	2011-01-18
Resolution	:	3.00 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 (1)) were used in the production of this report:

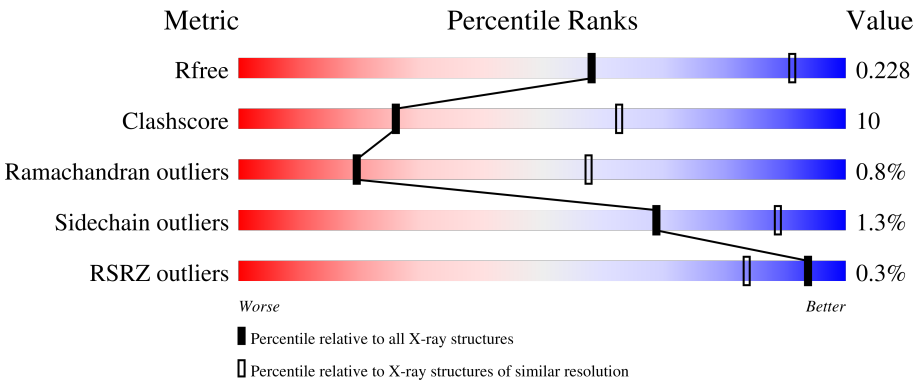
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	181	2%, 71%, 19%, 5%, 5%
1	B	181	%, 72%, 17%, •, 10%
1	C	181	75%, 14%, •, 10%
1	D	181	72%, 16%, •, 10%
1	E	181	71%, 18%, •, 10%

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Mol	Chain	Length	Quality of chain
1	F	181	75% 14% • 10%
1	G	181	74% 15% • 10%
1	H	181	73% 15% • 10%
1	I	181	% 74% 13% • 10%
1	J	181	76% 12% • 10%
1	K	181	69% 19% • 10%
1	L	181	73% 14% • 10%
1	M	181	71% 17% • 10%
1	N	181	71% 18% • 10%
1	O	181	% 72% 17% • 10%
1	P	181	% 75% 14% • 10%
1	Q	181	72% 16% • 10%
1	R	181	72% 15% • 10%
1	S	181	72% 16% •• 10%
1	T	181	% 71% 17% • 10%
1	U	181	67% 20% • 10%
1	V	181	75% 13% • 10%
1	W	181	% 70% 18% • 10%
1	X	181	72% 17% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 31864 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 Probable bacterioferritin BfrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	172	1357	852	244	256	5	0	0	0
1	B	162	1304	819	234	246	5	0	0	0
1	C	162	1298	816	231	246	5	0	0	0
1	D	162	1304	819	234	246	5	0	0	0
1	E	162	1304	819	234	246	5	0	0	0
1	F	162	1304	819	234	246	5	0	0	0
1	G	162	1304	819	234	246	5	0	0	0
1	H	162	1298	816	231	246	5	0	0	0
1	I	162	1314	827	236	246	5	0	1	0
1	J	162	1304	819	234	246	5	0	0	0
1	K	162	1304	819	234	246	5	0	0	0
1	L	162	1304	819	234	246	5	0	0	0
1	M	162	1304	819	234	246	5	0	0	0
1	N	162	1304	819	234	246	5	0	0	0
1	O	162	1304	819	234	246	5	0	0	0
1	P	162	1304	819	234	246	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	162	1304	819	234	246	5	0	0	0
1	R	162	1304	819	234	246	5	0	0	0
1	S	162	1304	819	234	246	5	0	0	0
1	T	162	1304	819	234	246	5	0	0	0
1	U	162	1304	819	234	246	5	0	0	0
1	V	162	1304	819	234	246	5	0	0	0
1	W	162	1304	819	234	246	5	0	0	0
1	X	162	1304	819	234	246	5	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	21	21	21	0	0
2	B	27	27	27	0	0
2	C	23	23	23	0	0
2	D	20	20	20	0	0
2	E	31	31	31	0	0
2	F	24	24	24	0	0
2	G	19	19	19	0	0
2	H	22	22	22	0	0
2	I	19	19	19	0	0
2	J	32	32	32	0	0
2	K	21	21	21	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	L	19	19	19	0	0
			Total	O		
2	M	22	22	22	0	0
			Total	O		
2	N	21	21	21	0	0
			Total	O		
2	O	18	18	18	0	0
			Total	O		
2	P	15	15	15	0	0
			Total	O		
2	Q	20	20	20	0	0
			Total	O		
2	R	23	23	23	0	0
			Total	O		
2	S	16	16	16	0	0
			Total	O		
2	T	19	19	19	0	0
			Total	O		
2	U	24	24	24	0	0
			Total	O		
2	V	16	16	16	0	0
			Total	O		
2	W	26	26	26	0	0
			Total	O		
2	X	19	19	19	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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Probable bacterioferritin BfrB

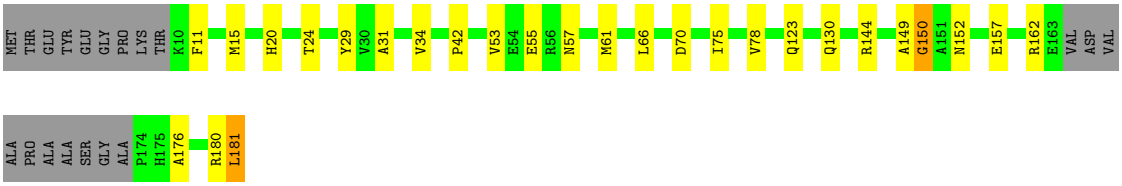
Chain A: 2% 71% 19% 5% 5%

• Molecule 1: Probable bacterioferritin BfrB

Chain B: % 72% 17% • 10%

• Molecule 1: Probable bacterioferritin BfrB

Chain C: 75% 14% • 10%

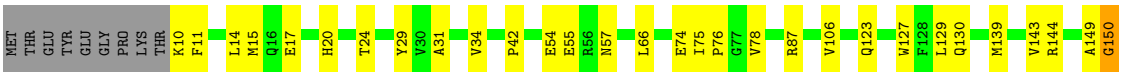


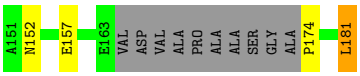
• Molecule 1: Probable bacterioferritin BfrB

Chain D: 72% 16% • 10%

• Molecule 1: Probable bacterioferritin BfrB

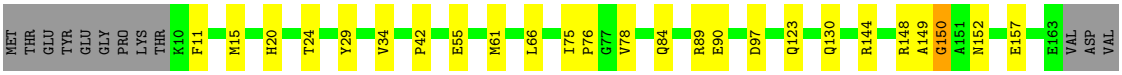
Chain E:

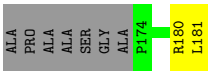




• Molecule 1: Probable bacterioferritin BfrB

Chain F:





• Molecule 1: Probable bacterioferritin BfrB

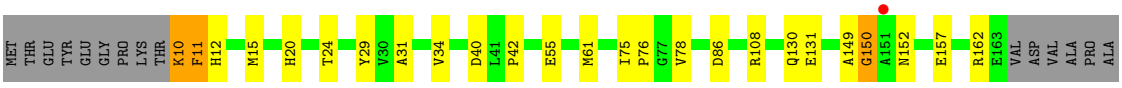
Chain G:

• Molecule 1: Probable bacterioferritin BfrB

Chain H:

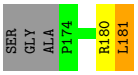
• Molecule 1: Probable bacterioferritin BfrB

Chain I:



• Molecule 1: Probable bacterioferritin BfrB

Chain J:

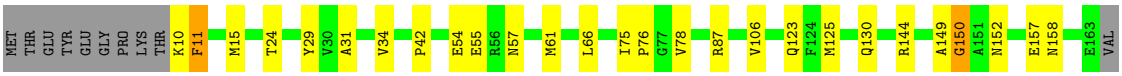


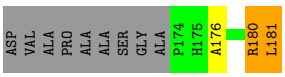
• Molecule 1: Probable bacterioferritin BfrB

Chain K:

• Molecule 1: Probable bacterioferritin BfrB

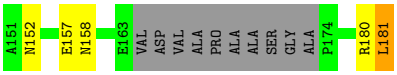
Chain L:





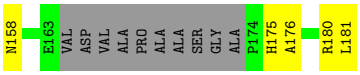
• Molecule 1: Probable bacterioferritin BfrB

Chain M:



• Molecule 1: Probable bacterioferritin BfrB

Chain N:



• Molecule 1: Probable bacterioferritin BfrB

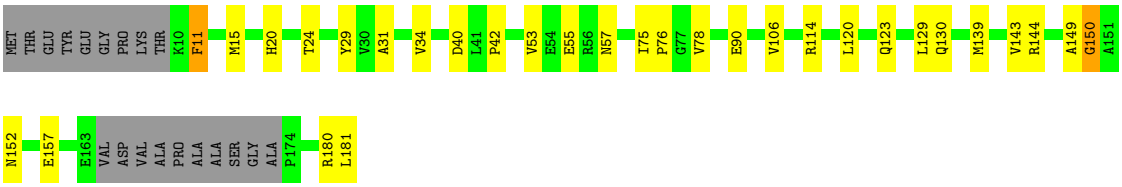
Chain O:

• Molecule 1: Probable bacterioferritin BfrB

Chain P:

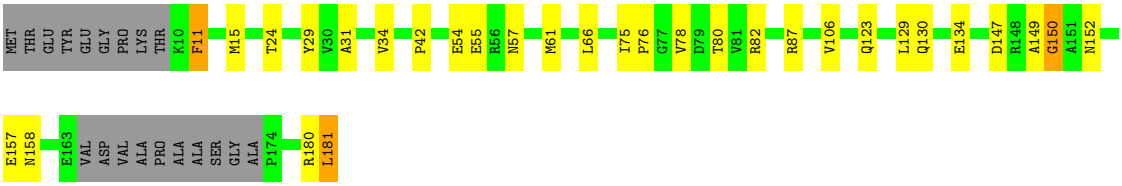
• Molecule 1: Probable bacterioferritin BfrB

Chain Q:



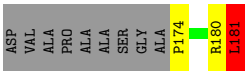
• Molecule 1: Probable bacterioferritin BfrB

Chain R:



• Molecule 1: Probable bacterioferritin BfrB

Chain S:

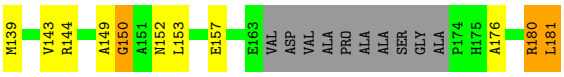


• Molecule 1: Probable bacterioferritin BfrB

Chain T:

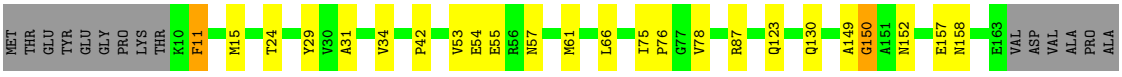
• Molecule 1: Probable bacterioferritin BfrB

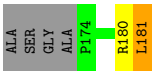
Chain U:



• Molecule 1: Probable bacterioferritin BfrB

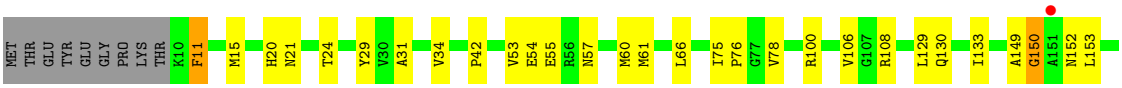
Chain V:

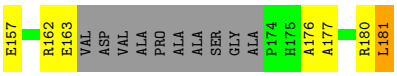




• Molecule 1: Probable bacterioferritin BfrB

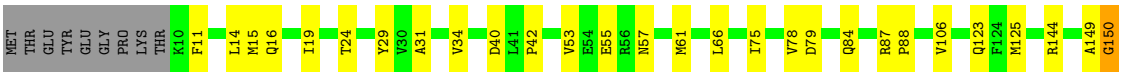
Chain W:





• Molecule 1: Probable bacterioferritin BfrB

Chain X:



A151
N152
E157
E163
VAL
ASP
VAL
ALA
PRO
ALA
ALA
SER
GLY
ALA
P174
R180
L181

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	226.07Å 226.18Å 113.69Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	31.98 – 3.00 31.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.2 (31.98-3.00) 81.2 (31.98-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.210 , 0.236 0.207 , 0.228	Depositor DCC
R_{free} test set	2009 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	31864	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2673e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.44	0/1382	0.60	1/1874 (0.1%)
1	B	0.42	0/1327	0.55	0/1794
1	C	0.46	0/1321	0.56	0/1787
1	D	0.45	0/1327	0.54	0/1794
1	E	0.45	0/1327	0.54	0/1794
1	F	0.45	0/1327	0.55	0/1794
1	G	0.44	0/1327	0.56	0/1794
1	H	0.44	0/1321	0.57	0/1787
1	I	0.48	0/1340	0.62	0/1809
1	J	0.46	0/1327	0.56	1/1794 (0.1%)
1	K	0.45	0/1327	0.53	0/1794
1	L	0.46	0/1327	0.55	0/1794
1	M	0.46	0/1327	0.56	1/1794 (0.1%)
1	N	0.44	0/1327	0.54	0/1794
1	O	0.43	0/1327	0.54	0/1794
1	P	0.43	0/1327	0.54	0/1794
1	Q	0.44	0/1327	0.54	0/1794
1	R	0.46	0/1327	0.54	0/1794
1	S	0.44	0/1327	0.56	1/1794 (0.1%)
1	T	0.45	0/1327	0.54	0/1794
1	U	0.46	0/1327	0.54	0/1794
1	V	0.46	0/1327	0.56	0/1794
1	W	0.44	0/1327	0.54	0/1794
1	X	0.44	0/1327	0.54	0/1794
All	All	0.45	0/31904	0.55	4/43137 (0.0%)

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	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	VAL	O-C-N	-9.72	107.15	122.70
1	M	181	LEU	CA-CB-CG	6.31	129.81	115.30
1	S	181	LEU	CA-CB-CG	5.85	128.76	115.30
1	J	181	LEU	CA-CB-CG	5.41	127.74	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	VAL	Peptide,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	1357	0	1298	48	0
1	B	1304	0	1253	28	0
1	C	1298	0	1242	24	0
1	D	1304	0	1253	31	0
1	E	1304	0	1253	31	0
1	F	1304	0	1253	27	0
1	G	1304	0	1253	24	3
1	H	1298	0	1242	25	0
1	I	1314	0	1276	42	0
1	J	1304	0	1253	27	0
1	K	1304	0	1253	39	0
1	L	1304	0	1253	25	5
1	M	1304	0	1253	30	5
1	N	1304	0	1253	30	5
1	O	1304	0	1253	30	0
1	P	1304	0	1253	24	0
1	Q	1304	0	1253	27	0
1	R	1304	0	1253	36	3
1	S	1304	0	1253	28	0
1	T	1304	0	1253	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1304	0	1253	37	0
1	V	1304	0	1253	23	5
1	W	1304	0	1253	42	0
1	X	1304	0	1253	31	0
2	A	21	0	0	4	0
2	B	27	0	0	2	0
2	C	23	0	0	4	0
2	D	20	0	0	2	0
2	E	31	0	0	9	0
2	F	24	0	0	5	0
2	G	19	0	0	5	0
2	H	22	0	0	3	0
2	I	19	0	0	4	0
2	J	32	0	0	6	0
2	K	21	0	0	9	0
2	L	19	0	0	3	0
2	M	22	0	0	2	0
2	N	21	0	0	3	0
2	O	18	0	0	1	0
2	P	15	0	0	2	0
2	Q	20	0	0	2	0
2	R	23	0	0	10	0
2	S	16	0	0	4	0
2	T	19	0	0	3	0
2	U	24	0	0	4	0
2	V	16	0	0	0	0
2	W	26	0	0	17	0
2	X	19	0	0	3	0
All	All	31864	0	30118	645	16

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 10.

All (645) 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:N:55:GLU:HG2	2:N:453:HOH:O	1.31	1.25
1:U:55:GLU:HG2	2:U:436:HOH:O	1.38	1.23
1:G:80:THR:HG23	2:G:501:HOH:O	1.47	1.15
1:X:144:ARG:HG3	2:X:493:HOH:O	1.52	1.09
1:E:55:GLU:HG2	2:E:431:HOH:O	1.53	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10[A]:LYS:HB3	1:I:12:HIS:HB3	1.39	1.05
1:C:70:ASP:HB3	2:C:458:HOH:O	1.62	1.00
1:K:17:GLU:HG3	2:K:507:HOH:O	1.60	0.99
1:L:144:ARG:HD2	2:L:441:HOH:O	1.66	0.95
1:A:180:ARG:O	1:A:181:LEU:HD23	1.66	0.95
1:I:10[B]:LYS:HB3	1:I:12:HIS:HB3	1.48	0.94
1:G:158:ASN:HB3	2:G:480:HOH:O	1.67	0.94
1:S:180:ARG:O	1:S:181:LEU:HD23	1.67	0.94
1:W:149:ALA:HB1	2:W:474:HOH:O	1.68	0.91
1:A:127:TRP:CD1	1:A:172:GLY:HA3	2.07	0.90
1:A:127:TRP:NE1	1:A:172:GLY:HA3	1.88	0.89
1:I:10[B]:LYS:CB	1:I:12:HIS:HB3	2.04	0.88
1:I:10[A]:LYS:CB	1:I:12:HIS:HB3	2.04	0.88
2:A:342:HOH:O	1:F:84:GLN:HG3	1.75	0.86
1:I:10[B]:LYS:HB3	1:I:12:HIS:H	1.43	0.83
1:I:10[A]:LYS:HB3	1:I:12:HIS:CB	2.09	0.82
1:T:180:ARG:O	1:T:181:LEU:HD23	1.78	0.82
1:M:180:ARG:O	1:M:181:LEU:HD23	1.78	0.82
1:D:144:ARG:HD2	2:D:419:HOH:O	1.81	0.81
1:I:10[B]:LYS:HB3	1:I:12:HIS:CB	2.13	0.78
1:W:149:ALA:C	2:W:474:HOH:O	2.21	0.78
1:D:180:ARG:O	1:D:181:LEU:HD23	1.84	0.77
1:M:53:VAL:CG1	1:M:181:LEU:HB2	2.14	0.77
1:A:181:LEU:C	2:A:432:HOH:O	2.23	0.77
1:D:57:ASN:HD21	1:D:181:LEU:H	1.32	0.77
1:A:127:TRP:HE1	1:A:172:GLY:H	1.32	0.76
1:C:162:ARG:NH2	2:C:299:HOH:O	2.14	0.76
1:W:157:GLU:CB	2:W:254:HOH:O	2.35	0.74
1:R:134:GLU:CG	2:R:420:HOH:O	2.34	0.74
1:K:155:GLU:CG	2:K:184:HOH:O	2.35	0.74
1:A:127:TRP:HE1	1:A:172:GLY:N	1.85	0.74
1:H:180:ARG:O	1:H:181:LEU:HD23	1.88	0.74
1:Q:57:ASN:HD21	1:Q:181:LEU:H	1.34	0.74
1:X:53:VAL:CG1	1:X:181:LEU:HB2	2.16	0.74
1:R:82:ARG:HD2	2:R:448:HOH:O	1.87	0.73
1:X:57:ASN:HD21	1:X:181:LEU:H	1.36	0.73
1:J:181:LEU:HD13	1:M:181:LEU:HD13	1.69	0.73
1:R:82:ARG:CD	2:R:448:HOH:O	2.36	0.73
2:W:234:HOH:O	1:X:84:GLN:HG3	1.89	0.73
1:X:42:PRO:HD2	1:X:157:GLU:OE1	1.88	0.73
1:K:155:GLU:HG2	2:K:184:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:42:PRO:HD2	1:U:157:GLU:OE1	1.88	0.73
1:W:157:GLU:CG	2:W:254:HOH:O	2.36	0.72
1:M:108:ARG:HD3	2:M:410:HOH:O	1.89	0.72
1:H:17:GLU:HG3	2:H:460:HOH:O	1.89	0.72
1:E:17:GLU:HG3	2:E:258:HOH:O	1.89	0.72
1:N:180:ARG:O	1:N:181:LEU:HD23	1.89	0.72
1:F:150:GLY:HA3	2:F:187:HOH:O	1.90	0.71
1:A:127:TRP:NE1	1:A:172:GLY:CA	2.53	0.71
1:R:180:ARG:C	1:R:181:LEU:HD23	2.10	0.71
1:N:61:MET:HG3	1:N:176:ALA:HB2	1.73	0.70
1:S:42:PRO:HD2	1:S:157:GLU:OE1	1.91	0.70
1:F:90:GLU:HB2	2:F:465:HOH:O	1.90	0.70
1:A:54:GLU:CD	1:A:169:ALA:HB2	2.12	0.70
1:I:10[B]:LYS:HB3	1:I:12:HIS:N	2.05	0.70
1:L:10:LYS:N	2:L:386:HOH:O	2.24	0.70
1:H:42:PRO:HD2	1:H:157:GLU:OE1	1.90	0.70
1:F:150:GLY:N	2:F:187:HOH:O	2.23	0.70
1:Q:180:ARG:O	1:Q:181:LEU:HD23	1.92	0.69
1:U:180:ARG:C	1:U:181:LEU:HD23	2.12	0.69
1:K:180:ARG:O	1:K:181:LEU:HD23	1.92	0.69
1:O:42:PRO:HD2	1:O:157:GLU:OE1	1.92	0.69
1:F:144:ARG:NE	1:K:40:ASP:OD2	2.26	0.69
1:I:10[A]:LYS:HB3	1:I:12:HIS:H	1.55	0.69
1:A:127:TRP:HE1	1:A:172:GLY:CA	2.06	0.68
1:R:80:THR:HG23	2:R:482:HOH:O	1.94	0.68
1:T:10:LYS:CB	2:T:415:HOH:O	2.42	0.67
1:I:10[A]:LYS:HB3	1:I:12:HIS:N	2.09	0.67
1:I:42:PRO:HD2	1:I:157:GLU:OE1	1.94	0.67
1:L:181:LEU:HD23	1:L:181:LEU:N	2.10	0.67
1:B:42:PRO:HD2	1:B:157:GLU:OE1	1.94	0.66
1:K:42:PRO:HD2	1:K:157:GLU:OE1	1.96	0.66
1:N:10:LYS:N	2:N:188:HOH:O	2.26	0.66
1:R:134:GLU:HG3	2:R:420:HOH:O	1.92	0.66
1:C:144:ARG:NE	1:H:40:ASP:OD2	2.28	0.66
1:R:61:MET:CE	1:R:180:ARG:HH11	2.09	0.66
1:O:180:ARG:O	1:O:181:LEU:HD23	1.96	0.66
1:Q:53:VAL:CG1	1:Q:181:LEU:HB2	2.26	0.66
2:A:342:HOH:O	1:F:84:GLN:CG	2.38	0.66
1:D:10:LYS:N	2:D:261:HOH:O	2.28	0.65
1:I:180:ARG:O	1:I:181:LEU:HD23	1.95	0.65
1:R:181:LEU:HD23	1:R:181:LEU:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:42:PRO:HD2	1:Q:157:GLU:OE1	1.96	0.65
1:M:42:PRO:HD2	1:M:157:GLU:OE1	1.96	0.65
1:N:42:PRO:HD2	1:N:157:GLU:OE1	1.96	0.65
1:F:150:GLY:CA	2:F:187:HOH:O	2.43	0.65
1:S:10:LYS:N	2:S:339:HOH:O	2.30	0.65
1:D:130:GLN:HB2	2:E:513:HOH:O	1.97	0.65
1:I:180:ARG:C	1:I:181:LEU:HD23	2.17	0.64
1:R:134:GLU:HG2	2:R:420:HOH:O	1.95	0.64
1:X:24:THR:HA	1:X:78:VAL:HG13	1.79	0.64
1:W:149:ALA:HA	2:W:405:HOH:O	1.97	0.64
1:B:180:ARG:O	1:B:181:LEU:HD23	1.98	0.64
1:N:57:ASN:HD21	1:N:181:LEU:H	1.46	0.64
1:Q:75:ILE:HD11	1:V:34:VAL:HG21	1.79	0.64
1:D:42:PRO:HD2	1:D:157:GLU:OE1	1.97	0.64
1:E:144:ARG:NE	1:Q:40:ASP:OD2	2.28	0.63
1:I:10[A]:LYS:HA	1:I:10[A]:LYS:HZ3	1.63	0.63
1:R:82:ARG:CZ	2:R:448:HOH:O	2.47	0.63
1:G:34:VAL:HG21	1:H:75:ILE:HD11	1.80	0.63
1:L:42:PRO:HD2	1:L:157:GLU:OE1	1.97	0.63
1:G:42:PRO:HD2	1:G:157:GLU:OE1	1.99	0.63
1:V:42:PRO:HD2	1:V:157:GLU:OE1	1.97	0.63
1:T:42:PRO:HD2	1:T:157:GLU:OE1	1.98	0.63
1:W:149:ALA:CB	2:W:474:HOH:O	2.36	0.62
1:J:144:ARG:NE	1:U:40:ASP:OD2	2.32	0.62
1:K:181:LEU:HD13	1:L:181:LEU:HD12	1.81	0.62
1:A:29:TYR:CE2	1:A:55:GLU:HG3	2.34	0.62
1:W:157:GLU:HB3	2:W:254:HOH:O	1.99	0.62
1:W:42:PRO:HD2	1:W:157:GLU:OE1	1.98	0.62
1:S:162:ARG:NH2	2:S:188:HOH:O	2.32	0.62
1:I:24:THR:HA	1:I:78:VAL:HG13	1.82	0.62
1:J:24:THR:HA	1:J:78:VAL:HG13	1.82	0.62
1:J:42:PRO:HD2	1:J:157:GLU:OE1	1.98	0.62
1:Q:24:THR:HA	1:Q:78:VAL:HG13	1.81	0.62
1:A:127:TRP:CD1	1:A:172:GLY:CA	2.82	0.61
1:A:166:VAL:O	1:A:167:ALA:CB	2.48	0.61
1:C:42:PRO:HD2	1:C:157:GLU:OE1	2.00	0.61
1:F:42:PRO:HD2	1:F:157:GLU:OE1	1.99	0.61
1:M:29:TYR:CE2	1:M:55:GLU:HG3	2.36	0.61
1:R:34:VAL:HG21	1:U:75:ILE:HD11	1.82	0.61
1:B:29:TYR:CE2	1:B:55:GLU:HG3	2.36	0.61
1:G:180:ARG:NH1	2:G:515:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:24:THR:HA	1:W:78:VAL:HG13	1.83	0.61
1:W:157:GLU:HG3	2:W:254:HOH:O	1.98	0.61
1:K:61:MET:HG3	1:K:176:ALA:HB2	1.82	0.61
1:O:24:THR:HA	1:O:78:VAL:HG13	1.82	0.61
1:A:42:PRO:HD2	1:A:157:GLU:OE1	2.01	0.61
1:B:34:VAL:HG21	1:E:75:ILE:HD11	1.82	0.61
1:B:180:ARG:C	1:B:181:LEU:HD23	2.20	0.60
1:N:24:THR:HA	1:N:78:VAL:HG13	1.82	0.60
1:D:130:GLN:CB	2:E:513:HOH:O	2.49	0.60
1:E:42:PRO:HD2	1:E:157:GLU:OE1	2.01	0.60
1:R:158:ASN:OD1	1:T:162:ARG:NH1	2.32	0.60
1:J:29:TYR:CE2	1:J:55:GLU:HG3	2.36	0.60
1:S:144:ARG:NE	1:X:40:ASP:OD2	2.31	0.60
1:A:53:VAL:HG13	1:A:181:LEU:HD12	1.83	0.60
1:A:24:THR:HA	1:A:78:VAL:HG13	1.82	0.60
1:C:24:THR:HA	1:C:78:VAL:HG13	1.84	0.60
1:F:24:THR:HA	1:F:78:VAL:HG13	1.84	0.60
1:G:24:THR:HA	1:G:78:VAL:HG13	1.82	0.60
1:S:24:THR:HA	1:S:78:VAL:HG13	1.82	0.60
1:C:29:TYR:CE2	1:C:55:GLU:HG3	2.36	0.60
1:P:42:PRO:HD2	1:P:157:GLU:OE1	2.01	0.60
1:M:24:THR:HA	1:M:78:VAL:HG13	1.84	0.60
1:V:24:THR:HA	1:V:78:VAL:HG13	1.84	0.59
1:R:75:ILE:HD11	1:U:34:VAL:HG21	1.85	0.59
1:H:57:ASN:HD21	1:H:181:LEU:H	1.49	0.59
1:I:29:TYR:CE2	1:I:55:GLU:HG3	2.37	0.59
1:T:29:TYR:CE2	1:T:55:GLU:HG3	2.38	0.59
1:Q:123:GLN:NE2	1:W:130:GLN:OE1	2.35	0.59
1:A:144:ARG:NE	1:D:40:ASP:OD2	2.34	0.59
1:O:53:VAL:CG1	1:O:181:LEU:HB2	2.32	0.59
1:U:24:THR:HA	1:U:78:VAL:HG13	1.84	0.59
1:A:167:ALA:HB1	1:A:168:PRO:CD	2.31	0.59
1:S:29:TYR:CE2	1:S:55:GLU:HG3	2.38	0.59
1:T:24:THR:HA	1:T:78:VAL:HG13	1.85	0.59
1:X:180:ARG:C	1:X:181:LEU:HD23	2.23	0.59
1:I:75:ILE:HD11	1:N:34:VAL:HG21	1.84	0.59
1:R:29:TYR:CE2	1:R:55:GLU:HG3	2.37	0.59
1:R:42:PRO:HD2	1:R:157:GLU:OE1	2.02	0.59
1:E:24:THR:HA	1:E:78:VAL:HG13	1.85	0.59
1:G:75:ILE:HD11	1:H:34:VAL:HG21	1.84	0.59
1:O:29:TYR:CE2	1:O:55:GLU:HG3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:24:THR:HA	1:P:78:VAL:HG13	1.85	0.59
1:X:180:ARG:O	1:X:181:LEU:HD23	2.02	0.59
1:K:24:THR:HA	1:K:78:VAL:HG13	1.84	0.58
1:Q:29:TYR:CE2	1:Q:55:GLU:HG3	2.38	0.58
1:F:29:TYR:CE2	1:F:55:GLU:HG3	2.38	0.58
1:V:29:TYR:CE2	1:V:55:GLU:HG3	2.38	0.58
2:W:234:HOH:O	1:X:84:GLN:CG	2.47	0.58
1:H:24:THR:HA	1:H:78:VAL:HG13	1.83	0.58
1:R:24:THR:HA	1:R:78:VAL:HG13	1.85	0.58
1:W:29:TYR:CE2	1:W:55:GLU:HG3	2.38	0.58
1:L:24:THR:HA	1:L:78:VAL:HG13	1.84	0.58
1:L:29:TYR:CE2	1:L:55:GLU:HG3	2.38	0.58
1:D:24:THR:HA	1:D:78:VAL:HG13	1.84	0.58
1:D:29:TYR:CE2	1:D:55:GLU:HG3	2.38	0.58
1:W:34:VAL:HG21	1:X:75:ILE:HD11	1.85	0.58
1:C:130:GLN:OE1	1:G:123:GLN:NE2	2.34	0.58
1:J:75:ILE:HD11	1:M:34:VAL:HG21	1.86	0.57
1:P:29:TYR:CE2	1:P:55:GLU:HG3	2.39	0.57
1:N:29:TYR:CE2	1:N:55:GLU:HG3	2.37	0.57
1:O:10:LYS:N	2:O:182:HOH:O	2.36	0.57
1:E:20:HIS:HB2	2:E:425:HOH:O	2.02	0.57
1:E:29:TYR:CE2	1:E:55:GLU:HG3	2.40	0.57
1:T:79:ASP:HA	2:T:188:HOH:O	2.03	0.57
1:I:34:VAL:HG21	1:N:75:ILE:HD11	1.86	0.57
1:M:53:VAL:HG11	1:M:181:LEU:HB2	1.86	0.57
1:E:87:ARG:NH2	2:E:192:HOH:O	2.31	0.57
1:C:75:ILE:HD11	1:D:34:VAL:HG21	1.87	0.57
1:W:163:GLU:HB3	2:W:503:HOH:O	2.04	0.57
1:B:24:THR:HA	1:B:78:VAL:HG13	1.85	0.57
1:W:61:MET:HG3	1:W:176:ALA:HB2	1.87	0.57
1:W:180:ARG:O	1:W:181:LEU:HD23	2.05	0.57
1:U:29:TYR:CE2	1:U:55:GLU:HG3	2.40	0.57
1:G:29:TYR:CE2	1:G:55:GLU:HG3	2.39	0.56
1:K:180:ARG:C	1:K:181:LEU:HD23	2.25	0.56
1:W:75:ILE:HD11	1:X:34:VAL:HG21	1.88	0.56
1:X:29:TYR:CE2	1:X:55:GLU:HG3	2.40	0.56
1:H:61:MET:HG3	1:H:176:ALA:HB2	1.87	0.56
1:S:75:ILE:HD11	1:T:34:VAL:HG21	1.87	0.56
1:P:149:ALA:O	1:P:150:GLY:O	2.24	0.56
1:K:53:VAL:CG1	1:K:181:LEU:HB2	2.35	0.56
1:E:130:GLN:OE1	1:V:123:GLN:NE2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:155:GLU:HG3	2:K:184:HOH:O	2.03	0.56
1:J:104:ASP:CB	2:J:428:HOH:O	2.53	0.56
1:H:29:TYR:CE2	1:H:55:GLU:HG3	2.41	0.56
1:E:17:GLU:CG	2:E:258:HOH:O	2.51	0.56
1:F:130:GLN:OE1	1:L:123:GLN:NE2	2.39	0.56
1:Q:34:VAL:HG21	1:V:75:ILE:HD11	1.88	0.56
1:O:34:VAL:HG21	1:P:75:ILE:HD11	1.88	0.55
1:K:34:VAL:HG21	1:L:75:ILE:HD11	1.87	0.55
1:K:29:TYR:CE2	1:K:55:GLU:HG3	2.41	0.55
1:K:75:ILE:HD11	1:L:34:VAL:HG21	1.89	0.55
1:P:180:ARG:O	1:P:181:LEU:HD23	2.06	0.55
1:U:57:ASN:HD21	1:U:181:LEU:H	1.54	0.55
1:C:20:HIS:HE1	2:C:497:HOH:O	1.90	0.55
1:R:61:MET:HE1	1:R:180:ARG:HH11	1.72	0.54
1:A:180:ARG:O	1:A:181:LEU:CD2	2.49	0.54
1:H:53:VAL:CG1	1:H:181:LEU:HB2	2.38	0.54
1:R:82:ARG:NE	2:R:448:HOH:O	2.40	0.54
1:B:149:ALA:O	1:B:150:GLY:O	2.26	0.54
1:W:149:ALA:O	1:W:150:GLY:O	2.24	0.54
1:I:162:ARG:NH1	1:L:158:ASN:OD1	2.34	0.53
1:J:130:GLN:OE1	1:R:123:GLN:NE2	2.41	0.53
1:W:53:VAL:HG11	1:W:181:LEU:C	2.28	0.53
1:R:31:ALA:HA	1:U:75:ILE:HG13	1.91	0.53
1:C:57:ASN:HD21	1:C:181:LEU:H	1.56	0.53
1:H:17:GLU:CG	2:H:460:HOH:O	2.53	0.53
1:O:54:GLU:OE2	1:O:180:ARG:NH1	2.42	0.53
1:O:75:ILE:HD11	1:P:34:VAL:HG21	1.89	0.53
1:S:34:VAL:HG21	1:T:75:ILE:HD11	1.90	0.53
1:F:61:MET:CE	1:F:180:ARG:HH11	2.21	0.53
1:B:116:GLU:CG	2:B:492:HOH:O	2.57	0.53
1:U:53:VAL:HG11	1:U:181:LEU:HB2	1.91	0.53
1:C:149:ALA:O	1:C:150:GLY:O	2.26	0.52
1:S:10:LYS:CB	2:S:467:HOH:O	2.57	0.52
1:A:149:ALA:O	1:A:150:GLY:O	2.27	0.52
1:I:130:GLN:OE1	1:K:123:GLN:NE2	2.43	0.52
1:G:10:LYS:N	2:G:214:HOH:O	2.42	0.52
1:T:149:ALA:O	1:T:150:GLY:O	2.28	0.52
1:K:57:ASN:HD21	1:K:181:LEU:H	1.58	0.52
1:G:158:ASN:OD1	1:P:162:ARG:NH1	2.36	0.52
1:K:17:GLU:CG	2:K:507:HOH:O	2.36	0.52
1:R:82:ARG:NH1	2:R:448:HOH:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:53:VAL:HG11	1:X:181:LEU:HB2	1.91	0.51
1:B:75:ILE:HD11	1:E:34:VAL:HG21	1.92	0.51
1:R:150:GLY:C	1:R:152:ASN:H	2.14	0.51
1:I:61:MET:HG3	1:I:176:ALA:HB2	1.92	0.51
1:I:149:ALA:O	1:I:150:GLY:O	2.28	0.51
1:X:53:VAL:HG13	1:X:181:LEU:HB2	1.92	0.51
1:A:61:MET:HG3	1:A:176:ALA:HB2	1.93	0.51
1:E:149:ALA:O	1:E:150:GLY:O	2.28	0.51
1:F:149:ALA:O	1:F:150:GLY:O	2.29	0.51
1:J:34:VAL:HG21	1:M:75:ILE:HD11	1.92	0.51
1:A:181:LEU:HD13	1:F:181:LEU:HD13	1.93	0.51
1:H:123:GLN:NE2	1:P:130:GLN:OE1	2.43	0.51
1:X:79:ASP:HB3	2:X:341:HOH:O	2.10	0.51
2:I:426:HOH:O	1:U:144:ARG:HD2	2.11	0.50
1:O:149:ALA:O	1:O:150:GLY:O	2.29	0.50
1:L:130:GLN:OE1	1:M:123:GLN:NE2	2.44	0.50
1:O:180:ARG:C	1:O:181:LEU:HD23	2.32	0.50
1:K:149:ALA:O	1:K:150:GLY:O	2.29	0.50
1:A:29:TYR:HE2	1:A:55:GLU:HG3	1.77	0.50
1:X:24:THR:HA	1:X:78:VAL:CG1	2.41	0.50
1:C:34:VAL:HG21	1:D:75:ILE:HD11	1.93	0.50
1:A:176:ALA:HB3	1:A:179:GLY:O	2.12	0.50
1:E:74:GLU:HG3	2:E:277:HOH:O	2.10	0.50
1:L:61:MET:HG3	1:L:176:ALA:HB2	1.92	0.50
1:A:171:SER:O	1:A:172:GLY:O	2.30	0.50
1:L:150:GLY:C	1:L:152:ASN:H	2.15	0.50
1:A:34:VAL:HG21	1:F:75:ILE:HD11	1.93	0.50
1:K:22:GLU:CD	2:K:260:HOH:O	2.50	0.49
1:S:74:GLU:HB3	2:S:274:HOH:O	2.12	0.49
1:E:150:GLY:C	1:E:152:ASN:H	2.14	0.49
1:H:53:VAL:HG11	1:H:181:LEU:HB2	1.93	0.49
1:K:181:LEU:CD1	1:L:181:LEU:HD12	2.42	0.49
1:I:10[A]:LYS:HB3	1:I:12:HIS:CA	2.41	0.49
1:R:149:ALA:O	1:R:150:GLY:O	2.30	0.49
1:F:180:ARG:O	1:F:181:LEU:HD23	2.12	0.49
1:I:75:ILE:HG13	1:N:31:ALA:HA	1.94	0.49
1:A:75:ILE:HD11	1:F:34:VAL:HG21	1.95	0.49
1:B:162:ARG:NH1	1:M:158:ASN:OD1	2.39	0.49
1:J:149:ALA:O	1:J:150:GLY:O	2.30	0.49
1:Q:114:ARG:NH2	2:Q:473:HOH:O	2.37	0.49
1:V:61:MET:CE	1:V:180:ARG:HH11	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:ALA:HA	1:H:75:ILE:HG13	1.95	0.49
1:J:104:ASP:HB2	2:J:428:HOH:O	2.11	0.49
1:L:180:ARG:C	1:L:181:LEU:HD23	2.34	0.49
1:W:21:ASN:ND2	2:W:346:HOH:O	2.30	0.49
1:I:86:ASP:O	2:I:230:HOH:O	2.20	0.48
1:E:10:LYS:N	2:E:351:HOH:O	2.46	0.48
1:M:149:ALA:O	1:M:150:GLY:O	2.32	0.48
1:A:179:GLY:O	1:A:180:ARG:HG2	2.13	0.48
1:F:97:ASP:HB2	2:F:469:HOH:O	2.12	0.48
1:Q:75:ILE:HG13	1:V:31:ALA:HA	1.96	0.48
1:V:15:MET:HG2	1:V:66:LEU:HD21	1.96	0.48
1:I:31:ALA:HA	1:N:75:ILE:HG13	1.96	0.48
1:Q:90:GLU:HG3	2:Q:424:HOH:O	2.13	0.48
1:S:75:ILE:HG13	1:T:31:ALA:HA	1.96	0.48
1:X:149:ALA:O	1:X:150:GLY:O	2.32	0.48
1:I:108:ARG:HD3	2:I:187:HOH:O	2.13	0.48
1:X:61:MET:CE	1:X:180:ARG:HH11	2.27	0.48
1:V:149:ALA:O	1:V:150:GLY:O	2.31	0.48
1:V:150:GLY:C	1:V:152:ASN:H	2.17	0.48
1:T:84:GLN:HB3	2:T:400:HOH:O	2.14	0.48
1:U:149:ALA:O	1:U:150:GLY:O	2.31	0.48
1:N:123:GLN:NE2	1:U:130:GLN:OE1	2.46	0.48
1:A:84:GLN:HB2	2:A:511:HOH:O	2.12	0.48
1:M:72:ARG:NH2	2:M:438:HOH:O	2.47	0.48
1:W:60:MET:CE	1:W:177:ALA:HB3	2.44	0.48
1:W:180:ARG:C	1:W:181:LEU:HD23	2.33	0.47
1:A:54:GLU:OE2	1:A:169:ALA:HB2	2.13	0.47
1:G:15:MET:HG2	1:G:66:LEU:HD21	1.95	0.47
1:K:150:GLY:C	1:K:152:ASN:H	2.17	0.47
1:O:31:ALA:HA	1:P:75:ILE:HG13	1.96	0.47
1:T:61:MET:HG3	1:T:176:ALA:HB2	1.96	0.47
1:D:29:TYR:HE2	1:D:55:GLU:HG3	1.80	0.47
1:A:172:GLY:CA	1:A:173:ALA:HB2	2.45	0.47
1:C:53:VAL:HG11	1:C:181:LEU:C	2.34	0.47
1:J:75:ILE:HG13	1:M:31:ALA:HA	1.95	0.47
1:O:75:ILE:HG13	1:P:31:ALA:HA	1.96	0.47
1:A:53:VAL:HG11	1:A:181:LEU:C	2.34	0.47
1:O:24:THR:HA	1:O:78:VAL:CG1	2.42	0.47
1:T:150:GLY:C	1:T:152:ASN:H	2.16	0.47
1:W:57:ASN:HD21	1:W:181:LEU:H	1.62	0.47
1:A:57:ASN:HD21	1:A:181:LEU:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:ALA:O	1:G:150:GLY:O	2.33	0.47
1:G:150:GLY:C	1:G:152:ASN:H	2.17	0.47
1:N:150:GLY:C	1:N:152:ASN:H	2.17	0.47
1:Q:144:ARG:NE	1:T:40:ASP:OD2	2.43	0.47
1:B:29:TYR:HE2	1:B:55:GLU:HG3	1.78	0.47
1:D:149:ALA:O	1:D:150:GLY:O	2.33	0.47
1:G:54:GLU:O	1:G:57:ASN:HB2	2.14	0.47
1:H:149:ALA:O	1:H:150:GLY:O	2.33	0.47
1:K:162:ARG:NH2	2:K:456:HOH:O	2.42	0.47
1:L:149:ALA:O	1:L:150:GLY:O	2.33	0.47
1:O:53:VAL:HG11	1:O:181:LEU:HB2	1.96	0.46
1:T:130:GLN:OE1	1:U:123:GLN:NE2	2.47	0.46
1:U:10:LYS:N	2:U:192:HOH:O	2.47	0.46
1:J:86:ASP:OD1	2:J:195:HOH:O	2.20	0.46
1:N:29:TYR:HE2	1:N:55:GLU:HG3	1.78	0.46
1:B:40:ASP:OD2	1:D:144:ARG:NE	2.42	0.46
1:J:57:ASN:HD21	1:J:181:LEU:H	1.63	0.46
1:N:53:VAL:CG1	1:N:181:LEU:HB2	2.45	0.46
1:O:29:TYR:HE2	1:O:55:GLU:HG3	1.80	0.46
1:O:40:ASP:OD2	1:X:144:ARG:NE	2.41	0.46
1:Q:130:GLN:OE1	1:S:123:GLN:NE2	2.45	0.46
1:S:61:MET:CE	1:S:180:ARG:HH11	2.28	0.46
1:W:31:ALA:HA	1:X:75:ILE:HG13	1.96	0.46
1:C:181:LEU:CD1	1:D:181:LEU:HD13	2.45	0.46
1:J:150:GLY:C	1:J:152:ASN:H	2.19	0.46
1:N:155:GLU:HG2	2:N:447:HOH:O	2.14	0.46
1:Q:57:ASN:ND2	1:Q:181:LEU:H	2.09	0.46
1:R:147:ASP:OD2	2:R:317:HOH:O	2.20	0.46
1:K:130:GLN:OE1	1:O:123:GLN:NE2	2.48	0.46
1:N:144:ARG:NE	1:S:40:ASP:OD2	2.39	0.46
1:S:15:MET:HG2	1:S:66:LEU:HD21	1.98	0.46
1:J:54:GLU:HB3	2:J:442:HOH:O	2.15	0.46
1:S:29:TYR:HE2	1:S:55:GLU:HG3	1.80	0.46
1:B:123:GLN:NE2	1:R:130:GLN:OE1	2.49	0.46
1:I:150:GLY:C	1:I:152:ASN:H	2.18	0.46
1:V:24:THR:HA	1:V:78:VAL:CG1	2.46	0.46
1:A:166:VAL:O	1:A:167:ALA:HB3	2.15	0.46
1:B:150:GLY:C	1:B:152:ASN:H	2.20	0.46
1:Q:150:GLY:C	1:Q:152:ASN:H	2.19	0.46
1:A:123:GLN:NE2	1:G:130:GLN:OE1	2.47	0.46
1:M:29:TYR:HE2	1:M:55:GLU:HG3	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:61:MET:HG3	1:U:176:ALA:HB2	1.98	0.46
1:A:11:PHE:CZ	1:A:15:MET:HE3	2.51	0.45
1:E:57:ASN:HD21	1:E:181:LEU:H	1.63	0.45
1:W:15:MET:HG2	1:W:66:LEU:HD21	1.98	0.45
1:W:60:MET:HE2	1:W:177:ALA:HB3	1.98	0.45
1:A:15:MET:HG2	1:A:66:LEU:HD21	1.98	0.45
1:K:106:VAL:HG12	1:K:129:LEU:HD23	1.99	0.45
1:Q:29:TYR:HE2	1:Q:55:GLU:HG3	1.81	0.45
1:K:11:PHE:CZ	1:K:15:MET:HE3	2.51	0.45
1:L:15:MET:HG2	1:L:66:LEU:HD21	1.98	0.45
1:M:24:THR:HA	1:M:78:VAL:CG1	2.45	0.45
1:R:29:TYR:HE2	1:R:55:GLU:HG3	1.79	0.45
1:T:29:TYR:HE2	1:T:55:GLU:HG3	1.81	0.45
1:K:144:ARG:NE	1:P:40:ASP:OD2	2.42	0.45
1:M:150:GLY:C	1:M:152:ASN:H	2.20	0.45
1:B:75:ILE:HG13	1:E:31:ALA:HA	1.99	0.45
1:D:53:VAL:HG11	1:D:181:LEU:HB2	1.99	0.45
1:O:15:MET:HG2	1:O:66:LEU:HD21	1.99	0.45
1:S:61:MET:HE3	1:S:180:ARG:HH11	1.82	0.45
1:A:24:THR:HA	1:A:78:VAL:CG1	2.45	0.45
1:A:172:GLY:HA3	1:A:173:ALA:HA	1.82	0.45
1:M:15:MET:HG2	1:M:66:LEU:HD21	1.99	0.45
1:U:86:ASP:HB2	2:U:468:HOH:O	2.16	0.45
1:A:172:GLY:N	1:A:173:ALA:HB2	2.32	0.45
1:I:10[B]:LYS:HB3	1:I:12:HIS:CA	2.47	0.45
1:N:75:ILE:HA	1:N:76:PRO:HD3	1.79	0.45
1:V:75:ILE:HA	1:V:76:PRO:HD3	1.81	0.45
1:C:29:TYR:HE2	1:C:55:GLU:HG3	1.79	0.45
1:M:53:VAL:HG13	1:M:181:LEU:HB2	1.92	0.45
1:P:150:GLY:C	1:P:152:ASN:H	2.20	0.45
1:S:149:ALA:O	1:S:150:GLY:O	2.35	0.45
1:V:158:ASN:OD1	1:W:162:ARG:NH1	2.42	0.45
1:H:162:ARG:NH2	2:W:254:HOH:O	2.49	0.45
1:K:75:ILE:HG13	1:L:31:ALA:HA	1.99	0.45
1:Q:139:MET:O	1:Q:143:VAL:HG23	2.17	0.45
1:W:150:GLY:N	2:W:474:HOH:O	2.45	0.45
1:X:144:ARG:NH1	2:X:493:HOH:O	2.50	0.45
1:B:106:VAL:HG12	1:B:129:LEU:CD2	2.46	0.45
1:J:29:TYR:HE2	1:J:55:GLU:HG3	1.80	0.45
1:D:150:GLY:C	1:D:152:ASN:H	2.19	0.44
1:O:106:VAL:HG12	1:O:129:LEU:CD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:THR:HA	1:D:78:VAL:CG1	2.48	0.44
1:B:31:ALA:HA	1:E:75:ILE:HG13	1.98	0.44
1:P:155:GLU:HG3	2:P:479:HOH:O	2.17	0.44
1:S:24:THR:HA	1:S:78:VAL:CG1	2.48	0.44
1:V:29:TYR:HE2	1:V:55:GLU:HG3	1.83	0.44
1:X:150:GLY:C	1:X:152:ASN:H	2.20	0.44
1:B:24:THR:HA	1:B:78:VAL:CG1	2.48	0.44
1:D:75:ILE:HA	1:D:76:PRO:HD3	1.80	0.44
1:F:29:TYR:HE2	1:F:55:GLU:HG3	1.81	0.44
1:K:106:VAL:HG12	1:K:129:LEU:CD2	2.47	0.44
1:R:11:PHE:CZ	1:R:15:MET:HE3	2.53	0.44
1:R:75:ILE:HG13	1:U:31:ALA:HA	2.00	0.44
1:S:106:VAL:HG13	1:S:125:MET:CE	2.47	0.44
1:U:180:ARG:O	1:U:181:LEU:HD23	2.17	0.44
1:U:11:PHE:CZ	1:U:15:MET:HE3	2.52	0.44
1:W:152:ASN:C	2:W:474:HOH:O	2.56	0.44
1:G:75:ILE:HG13	1:H:31:ALA:HA	1.98	0.44
1:N:15:MET:HG2	1:N:66:LEU:HD21	1.99	0.44
1:U:29:TYR:HE2	1:U:55:GLU:HG3	1.83	0.44
1:U:150:GLY:C	1:U:152:ASN:H	2.21	0.44
1:W:150:GLY:C	1:W:152:ASN:H	2.20	0.44
1:H:130:GLN:OE1	1:X:123:GLN:NE2	2.48	0.44
1:I:29:TYR:HE2	1:I:55:GLU:HG3	1.80	0.44
1:I:40:ASP:OD2	1:U:144:ARG:NE	2.43	0.44
1:O:65:HIS:HB2	1:O:124:PHE:CZ	2.53	0.44
1:N:106:VAL:HG12	1:N:129:LEU:HD23	2.00	0.44
1:N:149:ALA:O	1:N:150:GLY:O	2.36	0.44
1:N:158:ASN:OD1	1:O:162:ARG:NH1	2.41	0.44
1:O:66:LEU:HD12	1:O:73:VAL:HG23	2.00	0.44
1:F:150:GLY:C	1:F:152:ASN:H	2.22	0.43
1:J:29:TYR:CD2	1:J:55:GLU:HG3	2.53	0.43
1:J:54:GLU:CG	2:J:442:HOH:O	2.66	0.43
1:J:54:GLU:HG3	2:J:442:HOH:O	2.18	0.43
1:M:11:PHE:CZ	1:M:15:MET:HE3	2.52	0.43
1:R:15:MET:HG2	1:R:66:LEU:HD21	2.00	0.43
1:U:24:THR:HA	1:U:78:VAL:CG1	2.49	0.43
1:V:53:VAL:HG11	1:V:181:LEU:HB2	2.00	0.43
1:J:148:ARG:HD3	1:U:153:LEU:HD12	2.00	0.43
1:S:75:ILE:HA	1:S:76:PRO:HD3	1.81	0.43
1:A:54:GLU:O	1:A:57:ASN:HB2	2.19	0.43
1:H:22:GLU:CD	2:H:452:HOH:O	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:GLU:O	1:L:57:ASN:HB2	2.18	0.43
1:S:150:GLY:C	1:S:152:ASN:H	2.21	0.43
1:A:29:TYR:CD2	1:A:55:GLU:HG3	2.54	0.43
1:F:24:THR:HA	1:F:78:VAL:CG1	2.48	0.43
1:J:14:LEU:HD12	1:J:14:LEU:HA	1.81	0.43
1:A:106:VAL:HG13	1:A:125:MET:CE	2.48	0.43
1:D:130:GLN:OE1	1:E:123:GLN:NE2	2.51	0.43
1:G:40:ASP:OD2	1:P:144:ARG:NE	2.47	0.43
1:W:29:TYR:HE2	1:W:55:GLU:HG3	1.82	0.43
1:J:31:ALA:HA	1:M:75:ILE:HG13	1.99	0.43
1:K:11:PHE:CZ	1:K:15:MET:CE	3.00	0.43
1:P:29:TYR:HE2	1:P:55:GLU:HG3	1.82	0.43
1:S:57:ASN:HD21	1:S:181:LEU:H	1.67	0.43
1:G:75:ILE:HA	1:G:76:PRO:HD3	1.79	0.43
1:R:61:MET:HE3	1:R:180:ARG:HH11	1.82	0.43
1:U:54:GLU:O	1:U:57:ASN:HB2	2.19	0.43
1:W:106:VAL:HG12	1:W:129:LEU:CD2	2.49	0.43
1:O:29:TYR:HB3	1:O:52:ALA:HB2	2.00	0.43
1:O:57:ASN:ND2	1:O:180:ARG:HD2	2.34	0.43
1:P:53:VAL:HG11	1:P:181:LEU:C	2.40	0.43
1:T:75:ILE:HA	1:T:76:PRO:HD3	1.82	0.43
1:T:106:VAL:HG13	1:T:125:MET:CE	2.48	0.43
1:B:15:MET:HG2	1:B:66:LEU:HD21	2.00	0.43
1:B:116:GLU:HG3	2:B:492:HOH:O	2.19	0.43
1:C:29:TYR:CD2	1:C:55:GLU:HG3	2.54	0.43
1:E:127:TRP:CD2	1:E:174:PRO:HD3	2.54	0.43
1:E:150:GLY:C	1:E:152:ASN:N	2.71	0.43
1:O:54:GLU:O	1:O:57:ASN:HB2	2.19	0.43
1:O:150:GLY:C	1:O:152:ASN:H	2.20	0.43
1:Q:20:HIS:HA	1:Q:76:PRO:HG2	2.01	0.43
1:Q:106:VAL:HG12	1:Q:129:LEU:HD23	2.01	0.43
1:C:15:MET:HG2	1:C:66:LEU:HD21	2.01	0.42
1:E:29:TYR:HE2	1:E:55:GLU:HG3	1.84	0.42
1:U:66:LEU:HD12	1:U:73:VAL:HG23	2.00	0.42
1:D:54:GLU:O	1:D:57:ASN:HB2	2.19	0.42
1:D:123:GLN:NE2	1:V:130:GLN:OE1	2.51	0.42
1:L:29:TYR:HE2	1:L:55:GLU:HG3	1.81	0.42
1:N:106:VAL:HG12	1:N:129:LEU:CD2	2.48	0.42
1:T:140:ALA:HB2	2:U:518:HOH:O	2.18	0.42
1:B:65:HIS:HB2	1:B:124:PHE:CZ	2.54	0.42
1:W:11:PHE:CZ	1:W:15:MET:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:20:HIS:HA	1:W:76:PRO:HG2	2.01	0.42
1:H:148:ARG:HD3	1:W:153:LEU:HD12	2.02	0.42
1:W:54:GLU:O	1:W:57:ASN:HB2	2.20	0.42
1:Q:106:VAL:HG12	1:Q:129:LEU:CD2	2.50	0.42
1:A:130:GLN:OE1	1:C:123:GLN:NE2	2.49	0.42
1:I:75:ILE:HA	1:I:76:PRO:HD3	1.83	0.42
1:T:20:HIS:HA	1:T:76:PRO:HG2	2.02	0.42
1:E:106:VAL:HG12	1:E:129:LEU:HD23	2.02	0.42
1:I:10[A]:LYS:CG	1:I:12:HIS:HB3	2.47	0.42
1:N:24:THR:HA	1:N:78:VAL:CG1	2.47	0.42
1:P:24:THR:HA	1:P:78:VAL:CG1	2.49	0.42
1:U:106:VAL:HG12	1:U:129:LEU:HD23	2.02	0.42
1:U:139:MET:O	1:U:143:VAL:HG23	2.19	0.42
1:B:75:ILE:HA	1:B:76:PRO:HD3	1.83	0.42
1:G:180:ARG:O	1:G:181:LEU:HD23	2.20	0.42
1:I:11:PHE:CZ	1:I:15:MET:HE3	2.55	0.42
1:J:180:ARG:O	1:J:181:LEU:HD23	2.19	0.42
1:P:10:LYS:C	2:P:488:HOH:O	2.57	0.42
1:X:15:MET:HG2	1:X:66:LEU:HD21	2.01	0.42
1:B:106:VAL:HG12	1:B:129:LEU:HD23	2.02	0.42
1:C:150:GLY:C	1:C:152:ASN:H	2.23	0.42
1:I:29:TYR:CD2	1:I:55:GLU:HG3	2.55	0.42
1:K:84:GLN:NE2	2:L:417:HOH:O	2.53	0.42
1:M:54:GLU:O	1:M:57:ASN:HB2	2.20	0.42
1:Q:120:LEU:HD22	1:W:133:ILE:HG13	2.02	0.42
1:U:11:PHE:CZ	1:U:15:MET:CE	3.03	0.42
1:B:29:TYR:CD2	1:B:55:GLU:HG3	2.55	0.42
1:E:106:VAL:HG12	1:E:129:LEU:CD2	2.49	0.42
1:I:24:THR:HA	1:I:78:VAL:CG1	2.49	0.42
1:K:40:ASP:O	1:K:42:PRO:HD3	2.20	0.42
1:N:61:MET:CG	1:N:176:ALA:HB2	2.45	0.42
1:P:20:HIS:HA	1:P:76:PRO:HG2	2.02	0.42
1:Q:11:PHE:CZ	1:Q:15:MET:HE3	2.55	0.42
1:Q:75:ILE:HA	1:Q:76:PRO:HD3	1.81	0.42
1:Q:149:ALA:O	1:Q:150:GLY:O	2.38	0.42
1:C:180:ARG:O	1:C:181:LEU:HD23	2.20	0.41
1:F:123:GLN:NE2	1:M:130:GLN:OE1	2.48	0.41
1:M:106:VAL:HG12	1:M:129:LEU:HD23	2.02	0.41
1:Q:31:ALA:HA	1:V:75:ILE:HG13	2.02	0.41
1:T:11:PHE:CZ	1:T:15:MET:HE3	2.54	0.41
1:E:75:ILE:HA	1:E:76:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:MET:HG2	1:F:66:LEU:HD21	2.02	0.41
1:G:29:TYR:HE2	1:G:55:GLU:HG3	1.82	0.41
1:K:89:ARG:NH1	2:K:189:HOH:O	2.52	0.41
1:L:75:ILE:HA	1:L:76:PRO:HD3	1.84	0.41
1:N:150:GLY:C	1:N:152:ASN:N	2.73	0.41
1:W:75:ILE:HG13	1:X:31:ALA:HA	2.01	0.41
1:C:61:MET:HG3	1:C:176:ALA:HB2	2.03	0.41
1:R:24:THR:HA	1:R:78:VAL:CG1	2.50	0.41
1:R:150:GLY:C	1:R:152:ASN:N	2.73	0.41
1:T:54:GLU:O	1:T:57:ASN:HB2	2.21	0.41
1:T:57:ASN:HD21	1:T:181:LEU:H	1.68	0.41
1:X:106:VAL:HG13	1:X:125:MET:CE	2.50	0.41
1:B:96:LEU:HD22	1:B:140:ALA:HA	2.02	0.41
1:D:65:HIS:HB2	1:D:124:PHE:CZ	2.55	0.41
1:E:54:GLU:O	1:E:57:ASN:HB2	2.21	0.41
1:I:10[A]:LYS:HA	1:I:10[A]:LYS:NZ	2.31	0.41
1:K:22:GLU:OE2	2:K:260:HOH:O	2.21	0.41
1:M:29:TYR:CD2	1:M:55:GLU:HG3	2.55	0.41
1:P:29:TYR:CD2	1:P:55:GLU:HG3	2.55	0.41
1:R:106:VAL:HG12	1:R:129:LEU:CD2	2.51	0.41
1:U:20:HIS:HA	1:U:76:PRO:HG2	2.03	0.41
1:U:53:VAL:CG1	1:U:181:LEU:HB2	2.50	0.41
1:V:29:TYR:CD2	1:V:55:GLU:HG3	2.56	0.41
1:K:24:THR:HA	1:K:78:VAL:CG1	2.48	0.41
1:N:64:GLN:HG2	1:N:175:HIS:O	2.19	0.41
1:W:24:THR:HA	1:W:78:VAL:CG1	2.49	0.41
1:B:144:ARG:NE	1:M:40:ASP:OD2	2.47	0.41
2:C:391:HOH:O	1:D:83:ASN:HB3	2.21	0.41
1:D:66:LEU:HD12	1:D:73:VAL:HG23	2.02	0.41
1:F:20:HIS:HA	1:F:76:PRO:HG2	2.02	0.41
1:G:86:ASP:HB2	2:G:196:HOH:O	2.20	0.41
1:J:24:THR:HA	1:J:78:VAL:CG1	2.49	0.41
1:N:180:ARG:C	1:N:181:LEU:HD23	2.40	0.41
1:R:29:TYR:CD2	1:R:55:GLU:HG3	2.56	0.41
1:R:75:ILE:HA	1:R:76:PRO:HD3	1.80	0.41
1:T:29:TYR:CD2	1:T:55:GLU:HG3	2.56	0.41
1:A:150:GLY:C	1:A:152:ASN:H	2.22	0.41
1:B:54:GLU:O	1:B:57:ASN:HB2	2.20	0.41
1:C:31:ALA:HA	1:D:75:ILE:HG13	2.03	0.41
1:D:15:MET:HG2	1:D:66:LEU:HD21	2.03	0.41
1:L:11:PHE:CZ	1:L:15:MET:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:TYR:CD2	1:L:55:GLU:HG3	2.56	0.41
1:N:130:GLN:OE1	1:T:123:GLN:NE2	2.52	0.41
1:R:54:GLU:O	1:R:57:ASN:HB2	2.21	0.41
1:S:14:LEU:HD12	1:S:14:LEU:HA	1.88	0.41
1:S:29:TYR:CD2	1:S:55:GLU:HG3	2.56	0.41
1:V:53:VAL:CG1	1:V:181:LEU:HB2	2.51	0.41
1:A:89:ARG:O	1:A:89:ARG:HD2	2.20	0.41
1:E:15:MET:HG2	1:E:66:LEU:HD21	2.02	0.41
1:E:29:TYR:CD2	1:E:55:GLU:HG3	2.56	0.41
1:F:89:ARG:O	1:F:89:ARG:HD2	2.20	0.41
1:F:148:ARG:HD3	1:K:153:LEU:HD12	2.02	0.41
1:H:75:ILE:HA	1:H:76:PRO:HD3	1.81	0.41
1:I:20:HIS:HA	1:I:76:PRO:HG2	2.03	0.41
1:K:139:MET:O	1:K:143:VAL:HG23	2.21	0.41
1:K:148:ARG:HD3	1:P:153:LEU:HD12	2.02	0.41
1:M:106:VAL:HG12	1:M:129:LEU:CD2	2.50	0.41
1:O:106:VAL:HG12	1:O:129:LEU:HD23	2.02	0.41
1:T:24:THR:HA	1:T:78:VAL:CG1	2.49	0.41
1:T:150:GLY:C	1:T:152:ASN:N	2.74	0.41
1:U:65:HIS:HB2	1:U:124:PHE:CZ	2.55	0.41
1:X:29:TYR:HE2	1:X:55:GLU:HG3	1.82	0.41
1:A:11:PHE:CZ	1:A:15:MET:CE	3.03	0.41
1:C:75:ILE:HG13	1:D:31:ALA:HA	2.02	0.41
1:D:11:PHE:CZ	1:D:15:MET:HE3	2.56	0.41
1:E:14:LEU:HD12	1:E:14:LEU:HA	1.84	0.41
1:H:106:VAL:HG12	1:H:129:LEU:CD2	2.50	0.41
1:H:106:VAL:HG12	1:H:129:LEU:HD23	2.03	0.41
1:O:20:HIS:HA	1:O:76:PRO:HG2	2.03	0.41
1:U:47:HIS:O	1:U:50:SER:HB3	2.20	0.41
1:U:75:ILE:HA	1:U:76:PRO:HD3	1.83	0.41
1:U:106:VAL:HG12	1:U:129:LEU:CD2	2.51	0.41
1:X:16:GLN:O	1:X:19:ILE:HB	2.21	0.41
1:A:47:HIS:O	1:A:50:SER:HB3	2.21	0.40
1:A:65:HIS:HB2	1:A:124:PHE:CZ	2.56	0.40
1:E:139:MET:O	1:E:143:VAL:HG23	2.20	0.40
1:H:150:GLY:C	1:H:152:ASN:H	2.24	0.40
1:P:106:VAL:HG12	1:P:129:LEU:HD23	2.02	0.40
1:T:15:MET:HG2	1:T:66:LEU:HD21	2.02	0.40
1:W:29:TYR:CD2	1:W:55:GLU:HG3	2.56	0.40
1:X:87:ARG:HB2	1:X:88:PRO:HD2	2.03	0.40
1:B:14:LEU:HD12	1:B:14:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:MET:O	1:D:143:VAL:HG23	2.21	0.40
1:J:11:PHE:CZ	1:J:15:MET:HE3	2.56	0.40
1:M:47:HIS:O	1:M:50:SER:HB3	2.21	0.40
1:P:106:VAL:HG12	1:P:129:LEU:CD2	2.51	0.40
1:S:127:TRP:CD2	1:S:174:PRO:HD2	2.56	0.40
1:V:54:GLU:O	1:V:57:ASN:HB2	2.22	0.40
1:V:61:MET:HE1	1:V:180:ARG:HH11	1.86	0.40
1:C:24:THR:HA	1:C:78:VAL:CG1	2.51	0.40
1:K:65:HIS:HB2	1:K:124:PHE:CZ	2.56	0.40
1:O:29:TYR:CD2	1:O:55:GLU:HG3	2.56	0.40
1:S:54:GLU:O	1:S:57:ASN:HB2	2.21	0.40
1:W:100:ARG:HD2	2:W:183:HOH:O	2.21	0.40
1:F:29:TYR:CD2	1:F:55:GLU:HG3	2.56	0.40
1:G:150:GLY:C	1:G:152:ASN:N	2.75	0.40
1:I:131:GLU:OE2	2:I:421:HOH:O	2.22	0.40
1:J:15:MET:HG2	1:J:66:LEU:HD21	2.03	0.40
1:M:20:HIS:HA	1:M:76:PRO:HG2	2.03	0.40
1:W:108:ARG:HD3	2:W:496:HOH:O	2.22	0.40
1:L:106:VAL:HG13	1:L:125:MET:CE	2.51	0.40
1:T:180:ARG:C	1:T:181:LEU:HD23	2.40	0.40
1:V:11:PHE:CZ	1:V:15:MET:HE3	2.56	0.40
1:X:14:LEU:HD12	1:X:14:LEU:HA	1.91	0.40

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:ARG:CZ	1:V:87:ARG:NH2[4_555]	1.84	0.36
1:R:87:ARG:CZ	1:R:87:ARG:NH2[2_555]	1.84	0.36
1:L:87:ARG:NH2	1:V:87:ARG:CZ[4_555]	1.85	0.35
1:G:87:ARG:CZ	1:G:87:ARG:NH2[2_655]	1.86	0.34
1:G:87:ARG:NE	1:G:87:ARG:NH2[2_655]	2.00	0.20
1:L:87:ARG:NE	1:V:87:ARG:NH2[4_555]	2.00	0.20
1:M:87:ARG:CZ	1:N:87:ARG:NH2[1_554]	2.00	0.20
1:L:87:ARG:NH2	1:V:87:ARG:NE[4_555]	2.01	0.19
1:M:87:ARG:NH2	1:N:87:ARG:CZ[1_554]	2.01	0.19
1:R:87:ARG:NE	1:R:87:ARG:NH2[2_555]	2.03	0.17
1:G:87:ARG:CZ	1:G:87:ARG:CZ[2_655]	2.07	0.13
1:L:87:ARG:CZ	1:V:87:ARG:CZ[4_555]	2.09	0.11
1:R:87:ARG:CZ	1:R:87:ARG:CZ[2_555]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:87:ARG:NH2	1:N:87:ARG:NE[1_554]	2.13	0.07
1:M:87:ARG:NE	1:N:87:ARG:NH2[1_554]	2.15	0.05
1:M:87:ARG:CZ	1:N:87:ARG:CZ[1_554]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/181 (94%)	159 (94%)	4 (2%)	7 (4%)	3	16
1	B	158/181 (87%)	153 (97%)	4 (2%)	1 (1%)	25	64
1	C	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	D	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	E	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	F	158/181 (87%)	157 (99%)	0	1 (1%)	25	64
1	G	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	H	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	I	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	J	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	K	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	L	158/181 (87%)	155 (98%)	2 (1%)	1 (1%)	25	64
1	M	158/181 (87%)	155 (98%)	2 (1%)	1 (1%)	25	64
1	N	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	O	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	P	158/181 (87%)	155 (98%)	2 (1%)	1 (1%)	25	64
1	Q	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	R	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	S	158/181 (87%)	157 (99%)	0	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	U	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	V	158/181 (87%)	156 (99%)	1 (1%)	1 (1%)	25	64
1	W	158/181 (87%)	155 (98%)	2 (1%)	1 (1%)	25	64
1	X	158/181 (87%)	157 (99%)	0	1 (1%)	25	64
All	All	3804/4344 (88%)	3743 (98%)	31 (1%)	30 (1%)	19	57

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	VAL
1	A	167	ALA
1	A	171	SER
1	A	150	GLY
1	A	172	GLY
1	B	150	GLY
1	C	150	GLY
1	D	150	GLY
1	E	150	GLY
1	F	150	GLY
1	G	150	GLY
1	H	150	GLY
1	I	150	GLY
1	J	150	GLY
1	K	150	GLY
1	L	150	GLY
1	M	150	GLY
1	N	150	GLY
1	O	150	GLY
1	P	150	GLY
1	Q	150	GLY
1	R	150	GLY
1	S	150	GLY
1	T	150	GLY
1	U	150	GLY
1	V	150	GLY
1	W	150	GLY
1	X	150	GLY
1	A	168	PRO
1	A	170	ALA

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	135/147 (92%)	133 (98%)	2 (2%)	65	87
1	B	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	C	132/147 (90%)	130 (98%)	2 (2%)	65	87
1	D	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	E	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	F	133/147 (90%)	132 (99%)	1 (1%)	81	93
1	G	133/147 (90%)	132 (99%)	1 (1%)	81	93
1	H	132/147 (90%)	131 (99%)	1 (1%)	81	93
1	I	135/147 (92%)	131 (97%)	4 (3%)	41	75
1	J	133/147 (90%)	132 (99%)	1 (1%)	81	93
1	K	133/147 (90%)	132 (99%)	1 (1%)	81	93
1	L	133/147 (90%)	130 (98%)	3 (2%)	50	80
1	M	133/147 (90%)	132 (99%)	1 (1%)	81	93
1	N	133/147 (90%)	132 (99%)	1 (1%)	81	93
1	O	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	P	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	Q	133/147 (90%)	132 (99%)	1 (1%)	81	93
1	R	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	S	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	T	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	U	133/147 (90%)	130 (98%)	3 (2%)	50	80
1	V	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	W	133/147 (90%)	131 (98%)	2 (2%)	65	87
1	X	133/147 (90%)	132 (99%)	1 (1%)	81	93
All	All	3194/3528 (90%)	3151 (99%)	43 (1%)	69	89

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	181	LEU
1	B	11	PHE
1	B	181	LEU
1	C	11	PHE
1	C	181	LEU
1	D	11	PHE
1	D	181	LEU
1	E	11	PHE
1	E	181	LEU
1	F	11	PHE
1	G	11	PHE
1	H	11	PHE
1	I	10[A]	LYS
1	I	10[B]	LYS
1	I	11	PHE
1	I	181	LEU
1	J	11	PHE
1	K	11	PHE
1	L	11	PHE
1	L	180	ARG
1	L	181	LEU
1	M	11	PHE
1	N	11	PHE
1	O	11	PHE
1	O	180	ARG
1	P	11	PHE
1	P	181	LEU
1	Q	11	PHE
1	R	11	PHE
1	R	181	LEU
1	S	11	PHE
1	S	181	LEU
1	T	11	PHE
1	T	181	LEU
1	U	11	PHE
1	U	180	ARG
1	U	181	LEU
1	V	11	PHE
1	V	181	LEU
1	W	11	PHE
1	W	181	LEU
1	X	11	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	C	20	HIS
1	D	57	ASN
1	D	98	GLN
1	H	57	ASN
1	J	51	GLN
1	K	84	GLN
1	N	57	ASN
1	O	51	GLN
1	Q	57	ASN
1	X	57	ASN
1	X	175	HIS

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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	172/181 (95%)	-0.62	4 (2%)	60	31	3, 13, 46, 89	0
1	B	162/181 (89%)	-0.66	1 (0%)	89	72	4, 13, 34, 53	0
1	C	162/181 (89%)	-0.75	0	100	100	4, 12, 30, 46	0
1	D	162/181 (89%)	-0.70	0	100	100	4, 12, 32, 47	0
1	E	162/181 (89%)	-0.78	0	100	100	4, 13, 31, 46	0
1	F	162/181 (89%)	-0.79	0	100	100	4, 12, 31, 47	0
1	G	162/181 (89%)	-0.75	0	100	100	3, 12, 32, 41	0
1	H	162/181 (89%)	-0.68	0	100	100	4, 13, 33, 47	0
1	I	162/181 (89%)	-0.66	1 (0%)	89	72	4, 13, 33, 52	0
1	J	162/181 (89%)	-0.77	0	100	100	4, 12, 31, 47	0
1	K	162/181 (89%)	-0.67	0	100	100	4, 13, 33, 50	0
1	L	162/181 (89%)	-0.77	0	100	100	4, 12, 32, 44	0
1	M	162/181 (89%)	-0.77	0	100	100	5, 12, 32, 47	0
1	N	162/181 (89%)	-0.76	0	100	100	4, 13, 31, 44	0
1	O	162/181 (89%)	-0.66	1 (0%)	89	72	4, 14, 35, 50	0
1	P	162/181 (89%)	-0.70	1 (0%)	89	72	5, 13, 33, 51	0
1	Q	162/181 (89%)	-0.71	0	100	100	4, 12, 32, 47	0
1	R	162/181 (89%)	-0.73	0	100	100	4, 12, 32, 43	0
1	S	162/181 (89%)	-0.71	0	100	100	4, 13, 34, 49	0
1	T	162/181 (89%)	-0.66	1 (0%)	89	72	5, 14, 31, 50	0
1	U	162/181 (89%)	-0.69	0	100	100	4, 13, 32, 49	0
1	V	162/181 (89%)	-0.75	0	100	100	4, 13, 33, 49	0
1	W	162/181 (89%)	-0.69	1 (0%)	89	72	4, 13, 32, 53	0
1	X	162/181 (89%)	-0.65	0	100	100	4, 13, 33, 49	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3898/4344 (89%)	-0.71	10 (0%)	94	84	3, 13, 34, 89	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	151	ALA	4.9
1	A	166	VAL	4.0
1	W	151	ALA	3.5
1	P	151	ALA	3.4
1	A	171	SER	3.4
1	O	151	ALA	3.4
1	A	167	ALA	3.0
1	A	165	ASP	2.7
1	T	151	ALA	2.7
1	B	151	ALA	2.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.