Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 06:01 PM EDT

PDB ID	:	5D2L
Title	:	Crystal structure of TCR C7 in complex with HCMV NLV epitope presented by HLA-A2
Authors	:	Gao, M.; Mariuzza, R.A.
Deposited on	:	2015-08-05
Resolution	:	3.51 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:

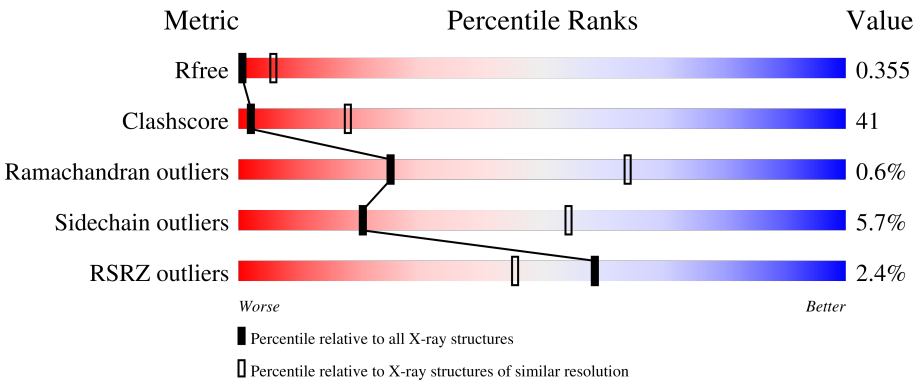
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.51 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	276	58% 40%
1	C	276	61% 35%
1	G	276	2% 46% 47%
1	M	276	% 48% 48%
2	B	100	3% 48% 50%

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Mol	Chain	Length	Quality of chain
2	D	100	55% 41%
2	H	100	2% 49% 42% 5%
2	N	100	2% 44% 54%
3	E	205	% 51% 35% 5% 9%
3	I	205	% 46% 40% 10%
3	K	205	7% 35% 48% 10% 6%
3	O	205	4% 47% 37% 7% 9%
4	F	245	% 44% 46% 7%
4	J	245	3% 43% 44% 8%
4	L	245	% 38% 48% 5% 8%
4	P	245	8% 51% 42%
5	Q	9	22% 78%
5	R	9	11% 89%
5	T	9	22% 67% 11%
5	U	9	11% 89%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25272 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2242	1401	408	424	9	0	0	0
1	G	270	2199	1379	395	416	9	0	0	0
1	M	273	2210	1379	401	421	9	0	0	0
1	C	274	2242	1401	408	424	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892
G	0	MET	-	initiating methionine	UNP P01892
M	0	MET	-	initiating methionine	UNP P01892
C	0	MET	-	initiating methionine	UNP P01892

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	823	522	140	158	3	0	0	0
2	H	96	777	494	128	152	3	0	0	0
2	N	100	825	524	138	159	4	0	0	0
2	D	100	827	527	137	159	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called C7 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	185	1404	878	227	293	6	0	0	0
3	K	192	1452	912	237	296	7	0	0	0
3	O	187	1435	900	234	294	7	0	0	0
3	E	187	1432	897	234	294	7	0	0	0

- Molecule 4 is a protein called C7 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	J	226	1759	1108	303	343	5	0	0	0
4	L	226	1699	1064	299	331	5	0	0	0
4	P	235	1784	1122	306	351	5	0	0	0
4	F	238	1852	1163	323	361	5	0	0	0

- Molecule 5 is a protein called ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	Q	9	64	42	10	11	1	0	0	0
5	U	9	64	42	10	11	1	0	0	0
5	T	9	64	42	10	11	1	0	0	0
5	R	9	64	42	10	11	1	0	0	0

- Molecule 6 is water.

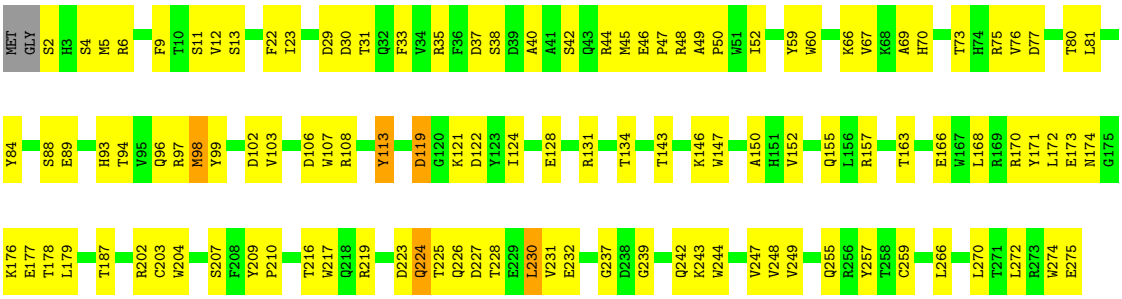
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total O 9 9	0	0
6	B	1	Total O 1 1	0	0
6	I	3	Total O 3 3	0	0
6	J	2	Total O 2 2	0	0
6	G	7	Total O 7 7	0	0
6	K	2	Total O 2 2	0	0
6	M	3	Total O 3 3	0	0
6	N	5	Total O 5 5	0	0
6	O	5	Total O 5 5	0	0
6	P	5	Total O 5 5	0	0
6	C	8	Total O 8 8	0	0
6	D	2	Total O 2 2	0	0
6	E	2	Total O 2 2	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.

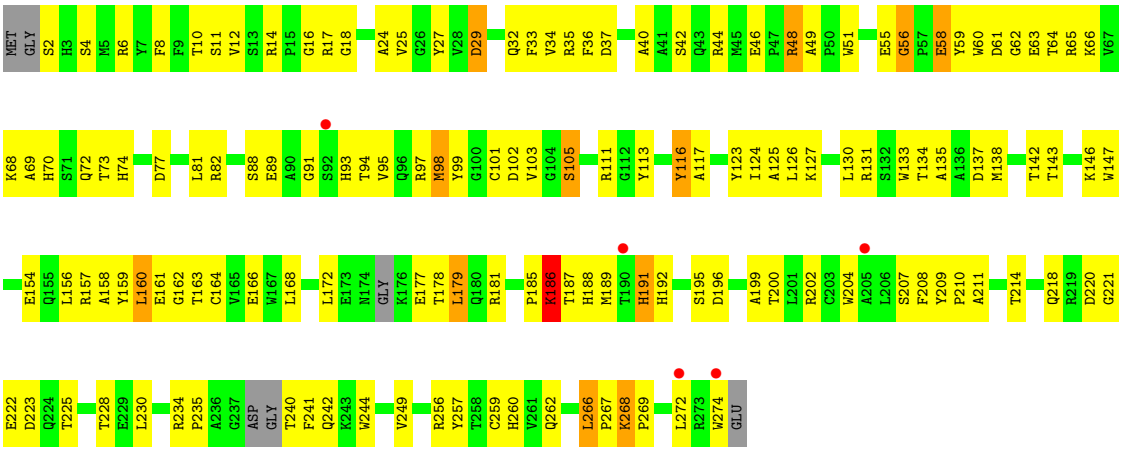
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



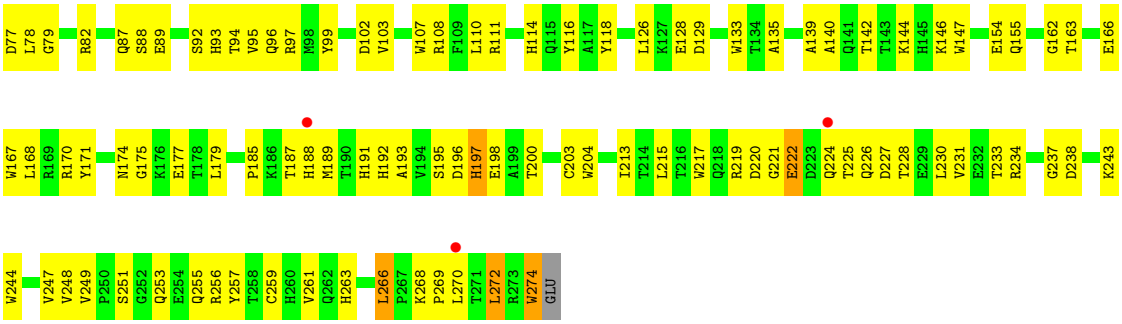
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain G:



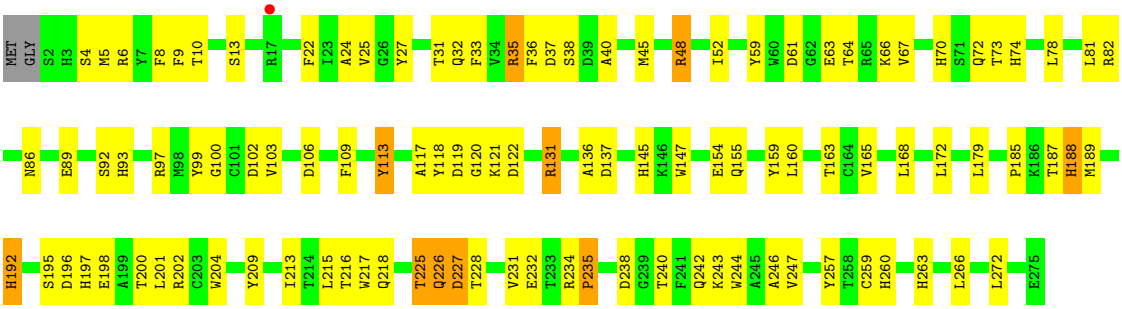
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain M:



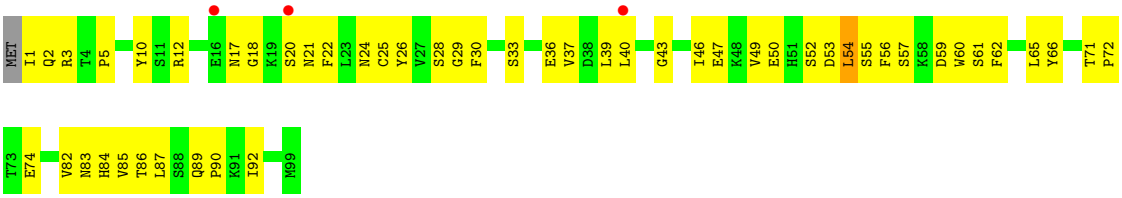
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain C:



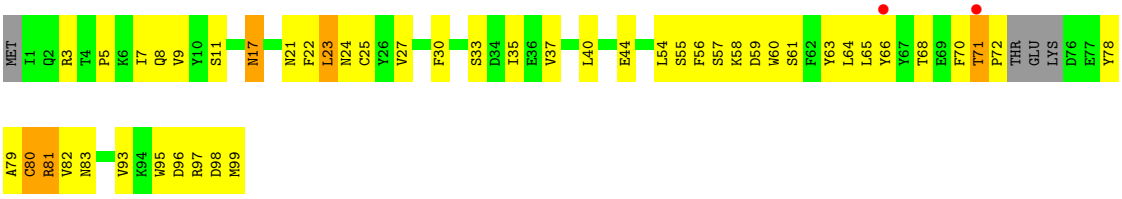
- Molecule 2: Beta-2-microglobulin

Chain B:



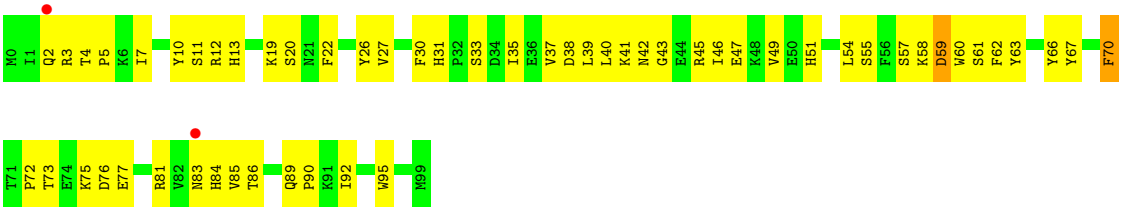
- Molecule 2: Beta-2-microglobulin

Chain H:



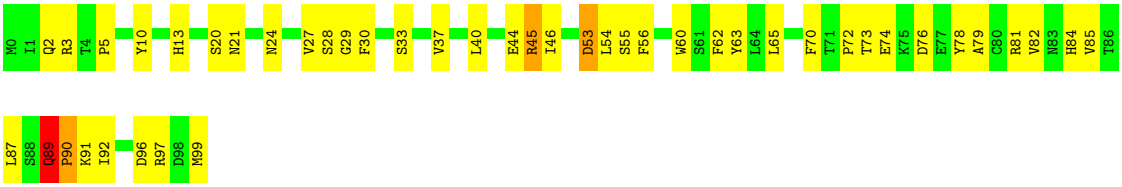
- Molecule 2: Beta-2-microglobulin

Chain N:



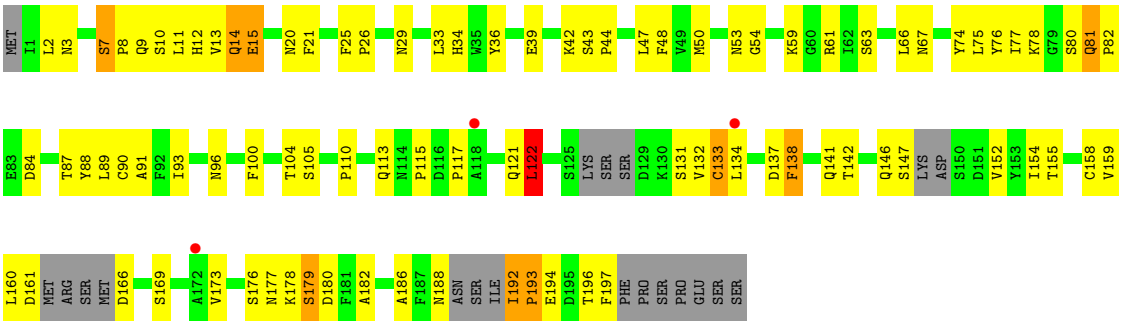
- Molecule 2: Beta-2-microglobulin

Chain D:



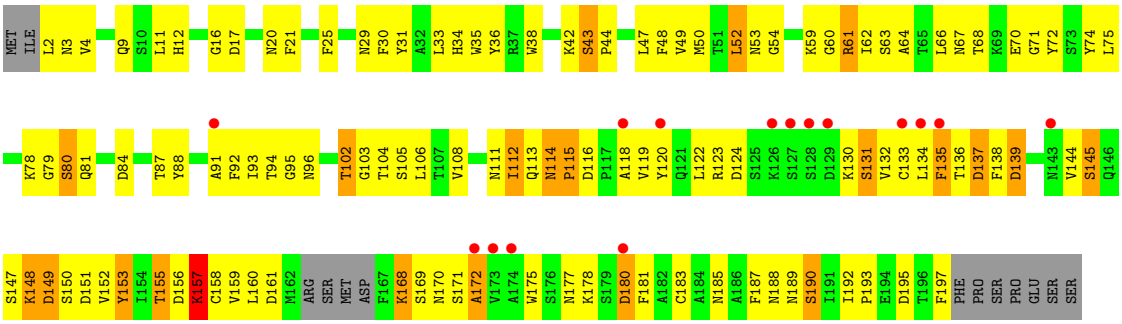
- Molecule 3: C7 TCR alpha chain

Chain I:



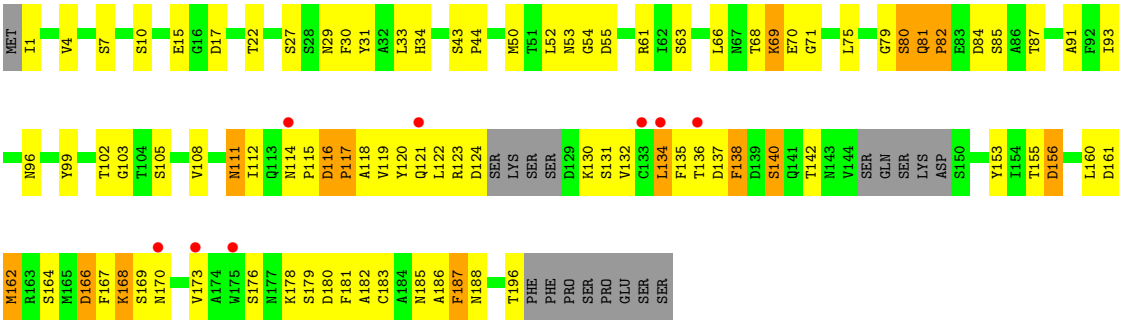
- Molecule 3: C7 TCR alpha chain

Chain K:



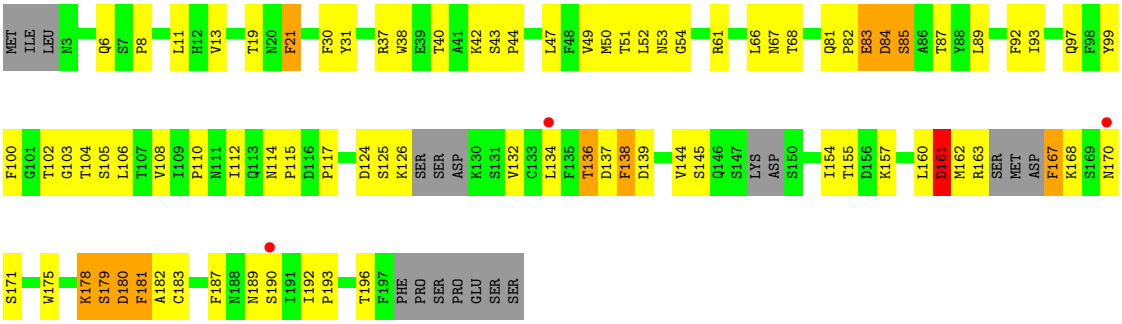
- Molecule 3: C7 TCR alpha chain

Chain O:



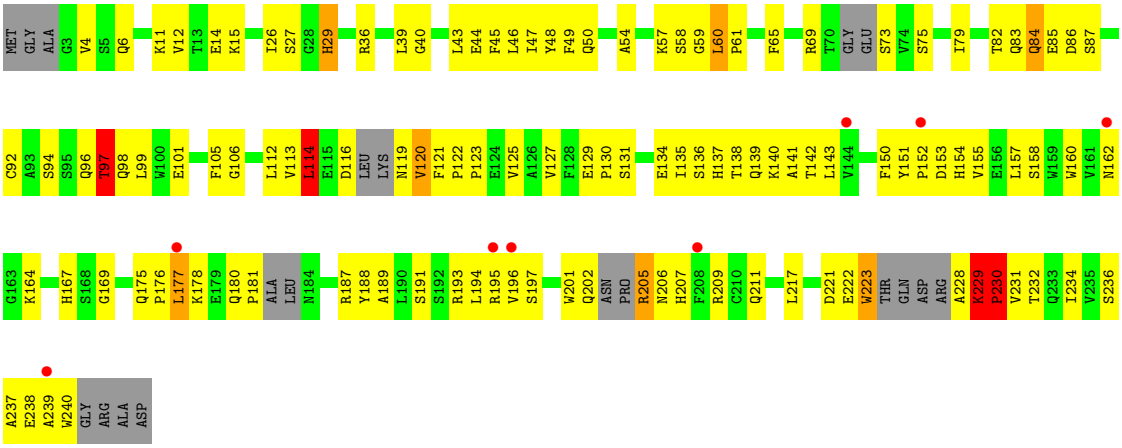
- Molecule 3: C7 TCR alpha chain

Chain E:



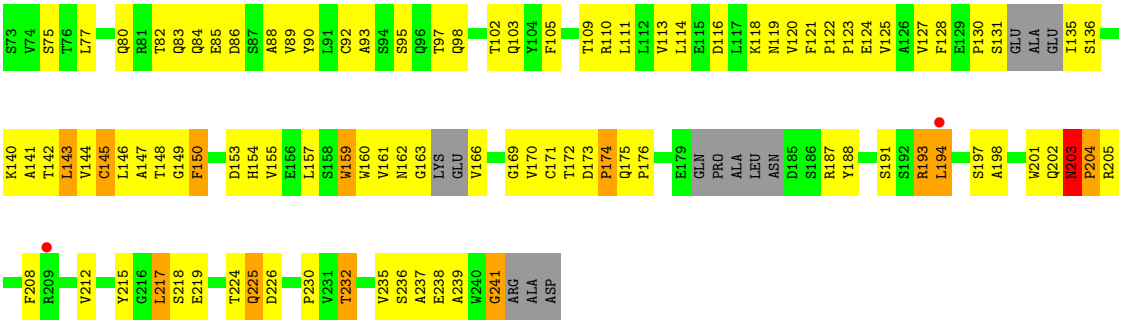
- Molecule 4: C7 TCR beta chain

Chain J:



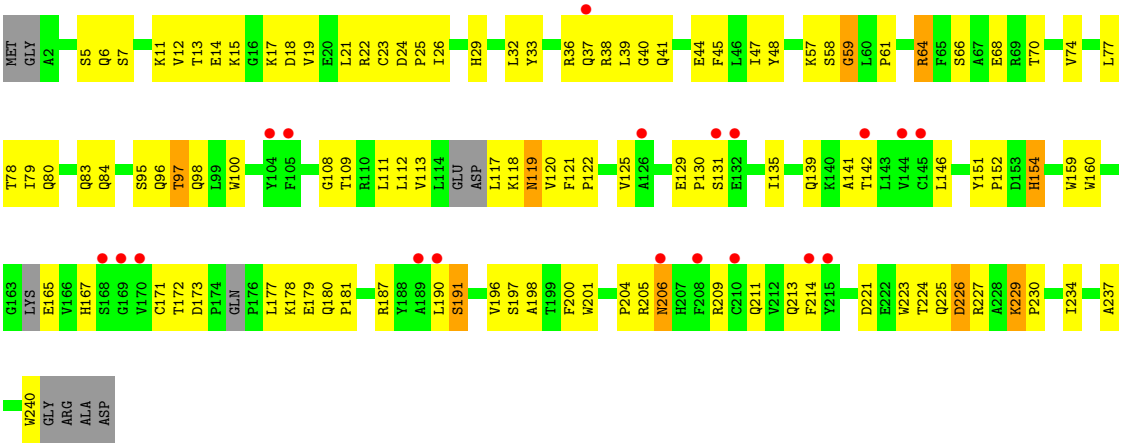
- Molecule 4: C7 TCR beta chain

Chain L:



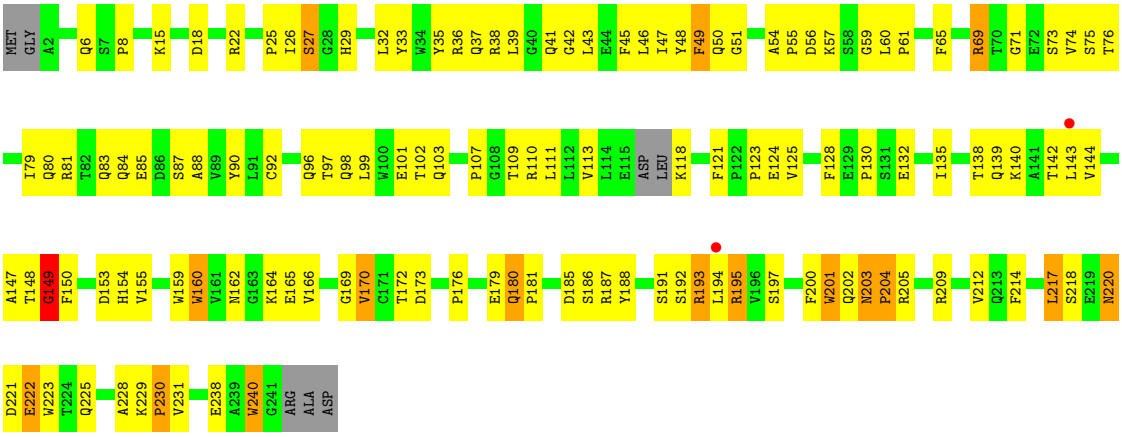
- Molecule 4: C7 TCR beta chain

Chain P:



- Molecule 4: C7 TCR beta chain

Chain F:

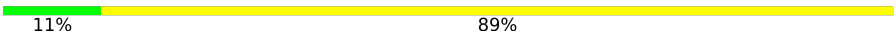


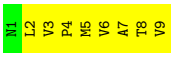
- Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL

Chain Q:

- Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL

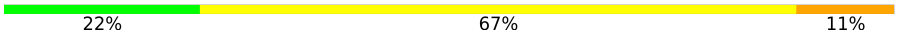
Chain U:

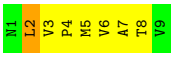




- Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL

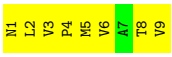
Chain T:





- Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	151.76Å 366.64Å 151.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 3.51 49.84 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.51-3.51) 91.4 (49.84-3.51)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.270 , 0.355 0.274 , 0.355	Depositor DCC
R_{free} test set	2702 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	79.4	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 60.1	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	0.86	EDS
Total number of atoms	25272	wwPDB-VP
Average B, all atoms (Å^2)	80.0	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 26.44 % 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 2.6340e-03. 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	0.47	0/2307	0.61	1/3132 (0.0%)
1	C	0.46	0/2307	0.59	1/3132 (0.0%)
1	G	0.53	1/2262 (0.0%)	0.72	2/3072 (0.1%)
1	M	0.42	0/2272	0.69	2/3085 (0.1%)
2	B	0.43	0/845	0.66	0/1143
2	D	0.53	0/850	0.68	2/1151 (0.2%)
2	H	0.44	0/798	0.64	0/1083
2	N	0.52	0/848	0.80	0/1150
3	E	0.46	0/1463	0.70	0/1987
3	I	0.54	0/1433	0.80	4/1946 (0.2%)
3	K	0.56	1/1486 (0.1%)	0.85	4/2018 (0.2%)
3	O	0.54	2/1466 (0.1%)	0.82	4/1992 (0.2%)
4	F	0.54	1/1900 (0.1%)	0.77	3/2586 (0.1%)
4	J	0.50	2/1801 (0.1%)	0.76	2/2448 (0.1%)
4	L	0.52	0/1737	0.95	11/2362 (0.5%)
4	P	0.43	0/1829	0.73	2/2494 (0.1%)
5	Q	0.45	0/64	0.72	0/88
5	R	0.42	0/64	0.67	0/88
5	T	0.55	0/64	0.78	0/88
5	U	0.30	0/64	0.50	0/88
All	All	0.49	7/25860 (0.0%)	0.74	38/35133 (0.1%)

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	1
1	C	0	1
1	G	0	4
2	H	0	1
2	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	3
3	K	0	5
3	O	0	3
4	F	0	3
4	J	0	2
4	L	0	5
4	P	0	3
All	All	0	32

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	230	PRO	N-CD	5.28	1.55	1.47
1	G	267	PRO	N-CD	5.25	1.55	1.47
3	K	172	ALA	CA-CB	-5.25	1.41	1.52
3	O	82	PRO	N-CD	5.13	1.55	1.47
3	O	117	PRO	N-CD	5.13	1.55	1.47
4	F	230	PRO	N-CD	5.08	1.54	1.47
4	J	61	PRO	N-CD	5.00	1.54	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	241	GLY	N-CA-C	12.45	144.23	113.10
3	I	7	SER	C-N-CD	-11.91	94.40	120.60
4	L	149	GLY	N-CA-C	10.65	139.73	113.10
1	G	179	LEU	N-CA-C	8.08	132.81	111.00
3	I	192	ILE	C-N-CD	6.94	142.98	128.40
3	K	114	ASN	C-N-CD	-6.57	106.14	120.60
4	P	146	LEU	CA-CB-CG	6.29	129.77	115.30
3	K	190	SER	N-CA-C	-6.21	94.22	111.00
4	L	203	ASN	C-N-CD	6.09	141.20	128.40
2	D	2	GLN	CA-CB-CG	6.07	126.74	113.40
4	L	54	ALA	C-N-CD	6.06	141.13	128.40
4	L	174	PRO	N-CA-CB	6.04	110.55	103.30
3	O	162	MET	CA-CB-CG	6.02	123.54	113.30
3	O	43	SER	C-N-CD	6.00	141.01	128.40
2	D	89	GLN	C-N-CD	6.00	141.00	128.40
3	I	122	LEU	N-CA-C	-5.97	94.88	111.00
4	L	194	LEU	CA-CB-CG	5.97	129.03	115.30
4	J	138	THR	N-CA-C	5.95	127.05	111.00
4	L	56	ASP	N-CA-C	-5.94	94.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	180	GLN	C-N-CD	5.93	140.85	128.40
4	L	157	LEU	CA-CB-CG	5.90	128.87	115.30
3	I	193	PRO	CA-N-CD	-5.88	103.27	111.50
1	M	19	GLU	C-N-CD	5.81	140.61	128.40
4	F	229	LYS	C-N-CD	5.80	140.57	128.40
1	M	50	PRO	N-CA-CB	5.71	110.15	103.30
3	O	81	GLN	C-N-CD	5.69	140.35	128.40
3	O	116	ASP	C-N-CD	5.69	140.34	128.40
1	G	266	LEU	C-N-CD	5.65	140.27	128.40
4	F	149	GLY	N-CA-C	-5.58	99.14	113.10
4	L	4	VAL	N-CA-C	5.55	125.99	111.00
3	K	43	SER	C-N-CD	5.47	139.89	128.40
4	F	204	PRO	N-CA-C	5.38	126.08	112.10
1	A	224	GLN	CA-C-N	-5.38	105.37	117.20
4	L	225	GLN	CA-CB-CG	5.35	125.17	113.40
1	C	215	LEU	CA-CB-CG	5.07	126.95	115.30
3	K	157	LYS	N-CA-C	5.06	124.66	111.00
4	J	230	PRO	CA-N-CD	-5.01	104.48	111.50
4	L	86	ASP	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	GLN	Mainchain
1	C	225	THR	Peptide
3	E	161	ASP	Peptide
3	E	181	PHE	Peptide
3	E	84	ASP	Peptide
4	F	149	GLY	Peptide
4	F	27	SER	Peptide
4	F	69	ARG	Peptide
1	G	105	SER	Peptide
1	G	160	LEU	Mainchain
1	G	186	LYS	Peptide
1	G	56	GLY	Peptide
2	H	17	ASN	Peptide
4	J	229	LYS	Peptide
4	J	97	THR	Peptide
3	K	130	LYS	Peptide
3	K	131	SER	Peptide
3	K	139	ASP	Peptide

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Mol	Chain	Res	Type	Group
3	K	145	SER	Peptide
3	K	54	GLY	Peptide
4	L	136	SER	Peptide
4	L	204	PRO	Peptide
4	L	232	THR	Peptide
4	L	58	SER	Peptide
4	L	9	SER	Peptide
2	N	19	LYS	Peptide
3	O	111	ASN	Peptide
3	O	136	THR	Peptide
3	O	156	ASP	Peptide
4	P	206	ASN	Peptide
4	P	224	THR	Peptide
4	P	59	GLY	Peptide

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	2242	0	2090	131	0
1	C	2242	0	2090	122	0
1	G	2199	0	2039	220	0
1	M	2210	0	2042	163	0
2	B	823	0	787	47	0
2	D	827	0	781	51	0
2	H	777	0	715	63	0
2	N	825	0	770	78	0
3	E	1432	0	1307	102	0
3	I	1404	0	1269	125	1
3	K	1452	0	1320	213	4
3	O	1435	0	1323	107	2
4	F	1852	0	1726	181	0
4	J	1759	0	1634	156	0
4	L	1699	0	1542	201	0
4	P	1784	0	1638	134	2
5	Q	64	0	74	12	0
5	R	64	0	74	12	0
5	T	64	0	74	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	U	64	0	74	27	0
6	A	9	0	0	4	0
6	B	1	0	0	0	0
6	C	8	0	0	1	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	G	7	0	0	3	0
6	I	3	0	0	1	0
6	J	2	0	0	1	0
6	K	2	0	0	0	0
6	M	3	0	0	3	0
6	N	5	0	0	2	0
6	O	5	0	0	0	0
6	P	5	0	0	1	0
All	All	25272	0	23369	1971	5

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 41.

All (1971) 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)
3:I:192:ILE:HG23	3:I:193:PRO:CD	1.42	1.46
1:A:230:LEU:HD21	1:A:243:LYS:NZ	1.27	1.43
3:K:175:TRP:CZ2	4:L:146:LEU:HD22	1.53	1.42
4:L:88:ALA:CB	4:L:110:ARG:HG3	1.46	1.41
3:K:112:ILE:CG2	3:K:139:ASP:HB3	1.48	1.41
3:K:175:TRP:CZ2	4:L:146:LEU:HD13	1.57	1.38
4:L:170:VAL:HA	4:L:194:LEU:CD2	1.51	1.38
3:K:38:TRP:CE3	3:K:44:PRO:HG3	1.59	1.38
4:P:112:LEU:CD1	4:P:154:HIS:CE1	2.05	1.38
1:C:202:ARG:CD	1:C:244:TRP:HE1	1.37	1.35
3:I:192:ILE:CG2	3:I:193:PRO:HD3	1.57	1.35
1:G:98:MET:HE2	1:G:113:TYR:CD1	1.59	1.34
4:J:29:HIS:HD2	4:J:94:SER:CB	1.40	1.34
3:K:61:ARG:HD2	3:K:78:LYS:O	1.25	1.32
4:P:14:GLU:OE2	4:P:117:LEU:CD2	1.76	1.31
1:G:98:MET:CE	1:G:113:TYR:CE1	2.15	1.30
2:N:13:HIS:CE1	4:F:81:ARG:NH2	1.99	1.29
2:D:44:GLU:OE2	2:D:46:ILE:HD11	1.28	1.28
3:K:138:PHE:HE1	3:K:157:LYS:CE	1.45	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:8:PRO:O	3:I:104:THR:HG23	1.23	1.27
1:A:102:ASP:CG	1:A:113:TYR:OH	1.73	1.26
1:G:192:HIS:CD2	1:G:202:ARG:HH21	1.51	1.26
1:G:98:MET:CE	1:G:113:TYR:CD1	2.19	1.26
4:F:170:VAL:CG1	4:F:194:LEU:HD13	1.64	1.26
1:A:4:SER:HB2	1:A:102:ASP:OD1	1.36	1.25
3:K:175:TRP:CZ2	4:L:146:LEU:CD2	2.19	1.25
4:P:7:SER:OG	4:P:22:ARG:HB3	1.35	1.25
1:A:230:LEU:CD2	1:A:243:LYS:NZ	1.98	1.24
4:J:47:ILE:HD11	4:J:60:LEU:CD2	1.66	1.24
3:K:175:TRP:HZ2	4:L:146:LEU:CG	1.52	1.21
1:G:97:ARG:NH1	5:U:6:VAL:CG1	2.01	1.21
4:L:88:ALA:HB3	4:L:110:ARG:CG	1.70	1.20
3:K:175:TRP:CZ2	4:L:146:LEU:CD1	2.23	1.20
3:E:167:PHE:HD2	3:E:168:LYS:N	1.39	1.20
1:G:97:ARG:HH11	5:U:6:VAL:CG1	1.52	1.19
3:O:138:PHE:CE1	3:O:142:THR:HG21	1.75	1.19
1:G:98:MET:HE1	1:G:113:TYR:CE1	1.76	1.19
1:G:97:ARG:HH11	5:U:6:VAL:HG11	1.08	1.19
3:K:136:THR:HG22	3:K:171:SER:HA	1.23	1.19
3:K:112:ILE:CG2	3:K:139:ASP:CB	2.21	1.17
4:J:29:HIS:CD2	4:J:94:SER:CB	2.27	1.17
3:K:138:PHE:CE1	3:K:157:LYS:CE	2.27	1.17
4:P:112:LEU:HD11	4:P:154:HIS:CE1	1.74	1.16
1:G:97:ARG:NE	1:G:116:TYR:HE1	1.41	1.16
1:G:98:MET:HE2	1:G:113:TYR:CE1	1.80	1.16
3:I:122:LEU:CA	3:I:132:VAL:O	1.93	1.15
3:K:161:ASP:CG	3:K:168:LYS:HD3	1.65	1.15
1:A:230:LEU:HD21	1:A:243:LYS:CE	1.77	1.14
3:O:182:ALA:HB1	3:O:185:ASN:HB3	1.24	1.14
4:L:89:VAL:HG12	4:L:110:ARG:CB	1.75	1.14
3:K:148:LYS:HB3	3:K:149:ASP:O	1.46	1.14
4:L:89:VAL:HG12	4:L:110:ARG:HB2	1.27	1.14
3:K:138:PHE:CE1	3:K:157:LYS:HE2	1.84	1.13
1:G:16:GLY:HA3	1:G:17:ARG:HB2	1.29	1.12
1:C:202:ARG:HD3	1:C:244:TRP:HE1	1.01	1.12
4:L:83:GLN:HG3	4:L:84:GLN:H	0.98	1.12
2:N:40:LEU:HD23	2:N:43:GLY:HA3	1.13	1.12
3:K:175:TRP:CE2	4:L:146:LEU:HD22	1.82	1.12
1:A:230:LEU:CD2	1:A:243:LYS:CE	2.28	1.12
4:F:170:VAL:HG13	4:F:194:LEU:CD1	1.78	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:175:TRP:HZ2	4:L:146:LEU:CD2	1.58	1.11
4:J:29:HIS:HD2	4:J:94:SER:HB2	1.07	1.10
4:L:88:ALA:HB1	4:L:89:VAL:HA	1.31	1.09
4:P:112:LEU:HD12	4:P:154:HIS:CE1	1.83	1.09
3:O:53:ASN:HB2	3:O:68:THR:HG23	1.33	1.09
4:F:54:ALA:HB1	4:F:57:LYS:HE3	1.27	1.09
3:K:175:TRP:HZ2	4:L:146:LEU:CD1	1.64	1.09
3:K:138:PHE:HE1	3:K:157:LYS:HE2	0.97	1.08
1:G:192:HIS:CD2	1:G:202:ARG:NH2	2.22	1.08
3:K:138:PHE:CE1	3:K:157:LYS:HE3	1.89	1.08
3:O:138:PHE:CE1	3:O:142:THR:CG2	2.35	1.07
4:J:47:ILE:HD11	4:J:60:LEU:HD21	1.12	1.07
2:N:73:THR:CG2	2:N:76:ASP:OD1	2.01	1.07
4:F:218:SER:OG	4:F:221:ASP:HB2	1.55	1.07
3:E:136:THR:HG23	3:E:171:SER:HB2	1.14	1.07
1:G:2:SER:N	1:G:105:SER:HG	1.52	1.07
3:O:138:PHE:HE1	3:O:142:THR:CG2	1.68	1.07
1:A:4:SER:HB3	1:A:102:ASP:CG	1.75	1.07
4:P:97:THR:HG22	4:P:98:GLN:HG2	1.37	1.07
4:J:141:ALA:HB3	4:J:196:VAL:O	1.55	1.06
1:M:78:LEU:HD23	1:M:95:VAL:CG2	1.86	1.06
3:I:146:GLN:CD	3:I:154:ILE:HG12	1.75	1.06
4:P:223:TRP:CH2	4:P:229:LYS:O	2.09	1.06
1:G:97:ARG:NE	1:G:116:TYR:CE1	2.15	1.06
3:K:112:ILE:HG23	3:K:139:ASP:HB3	1.10	1.05
1:C:202:ARG:HD3	1:C:244:TRP:NE1	1.69	1.05
1:C:202:ARG:CG	1:C:244:TRP:HE1	1.68	1.05
4:L:88:ALA:CB	4:L:110:ARG:CG	2.27	1.05
4:J:29:HIS:CD2	4:J:94:SER:HB2	1.87	1.05
4:P:14:GLU:HG2	4:P:117:LEU:HG	1.06	1.05
3:K:61:ARG:CD	3:K:78:LYS:O	2.04	1.05
2:B:37:VAL:HG12	2:B:82:VAL:HG22	1.10	1.05
1:M:19:GLU:OE1	1:M:19:GLU:N	1.88	1.04
4:J:29:HIS:CD2	4:J:94:SER:OG	2.09	1.04
2:N:73:THR:HG22	2:N:76:ASP:OD1	1.56	1.04
4:P:14:GLU:HG2	4:P:117:LEU:CG	1.87	1.04
1:A:102:ASP:CG	1:A:113:TYR:HH	1.53	1.04
3:I:33:LEU:HD12	3:I:91:ALA:O	1.58	1.04
4:P:112:LEU:HD11	4:P:154:HIS:HE1	1.10	1.04
4:J:113:VAL:O	4:J:114:LEU:HG	1.57	1.03
4:L:170:VAL:CA	4:L:194:LEU:CD2	2.35	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:14:GLU:OE2	4:P:117:LEU:HD21	0.87	1.03
4:P:14:GLU:CG	4:P:117:LEU:HG	1.89	1.03
3:K:185:ASN:O	3:K:188:ASN:ND2	1.91	1.03
1:M:20:PRO:HD2	1:M:75:ARG:CD	1.89	1.03
4:J:136:SER:HA	4:J:139:GLN:OE1	1.58	1.03
4:P:14:GLU:CD	4:P:117:LEU:HD21	1.77	1.03
4:L:170:VAL:CA	4:L:194:LEU:HD23	1.89	1.02
1:C:226:GLN:NE2	1:C:227:ASP:OD1	1.92	1.02
4:J:47:ILE:CD1	4:J:60:LEU:CD2	2.37	1.02
3:K:148:LYS:HB3	3:K:149:ASP:C	1.79	1.01
4:L:204:PRO:HG3	4:L:241:GLY:HA3	1.42	1.01
1:C:202:ARG:CD	1:C:244:TRP:NE1	2.21	1.01
4:J:194:LEU:HD23	4:J:195:ARG:N	1.75	1.01
4:F:218:SER:OG	4:F:221:ASP:CB	2.07	1.01
4:P:223:TRP:CZ2	4:P:229:LYS:O	2.13	1.01
1:M:82:ARG:NH1	1:M:93:HIS:HD2	1.56	1.01
3:E:136:THR:HG23	3:E:171:SER:CB	1.89	1.01
3:E:136:THR:CG2	3:E:171:SER:CB	2.40	1.00
1:A:4:SER:CB	1:A:102:ASP:OD1	2.08	1.00
1:M:78:LEU:HD23	1:M:95:VAL:HG23	1.41	1.00
4:P:196:VAL:HG22	4:P:197:SER:H	1.23	1.00
3:O:53:ASN:HB2	3:O:68:THR:CG2	1.89	1.00
4:J:47:ILE:CD1	4:J:60:LEU:HD23	1.91	0.99
3:E:181:PHE:HB2	3:E:182:ALA:HA	1.44	0.99
1:M:66:LYS:HZ1	3:O:29:ASN:CG	1.66	0.99
1:G:35:ARG:HH21	1:G:48:ARG:CG	1.76	0.99
1:G:116:TYR:HD2	1:G:117:ALA:N	1.61	0.98
3:K:175:TRP:HE1	4:L:146:LEU:HD21	1.25	0.98
4:P:112:LEU:HD12	4:P:154:HIS:NE2	1.78	0.97
1:A:4:SER:CB	1:A:102:ASP:CG	2.32	0.97
2:D:44:GLU:OE2	2:D:46:ILE:CD1	2.10	0.97
3:E:167:PHE:CD2	3:E:168:LYS:N	2.18	0.97
3:E:192:ILE:HG22	3:E:193:PRO:CD	1.94	0.97
1:G:82:ARG:HH21	1:G:89:GLU:N	1.61	0.97
4:L:170:VAL:HG22	4:L:194:LEU:HD21	1.44	0.97
4:L:89:VAL:CG1	4:L:110:ARG:HB2	1.93	0.97
1:M:82:ARG:HH11	1:M:93:HIS:HD2	1.03	0.97
3:E:83:GLU:HA	3:E:84:ASP:OD1	1.64	0.96
1:G:98:MET:CE	1:G:113:TYR:HE1	1.67	0.96
3:K:175:TRP:CH2	4:L:146:LEU:HD13	2.00	0.96
4:F:149:GLY:H	4:F:150:PHE:HD2	1.14	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ALA:O	1:G:134:THR:HG22	1.64	0.95
1:A:227:ASP:OD2	1:A:248:VAL:HG22	1.65	0.95
3:E:136:THR:CG2	3:E:171:SER:HB2	1.93	0.95
1:M:73:THR:HG21	5:T:6:VAL:HG23	1.44	0.95
4:F:54:ALA:HB1	4:F:57:LYS:CE	1.96	0.95
1:A:230:LEU:CD2	1:A:243:LYS:HZ3	1.72	0.95
3:K:49:VAL:HG21	4:L:102:THR:HG22	1.47	0.95
1:G:97:ARG:HG2	1:G:116:TYR:CD1	2.02	0.95
4:F:159:TRP:HE1	4:F:192:SER:HG	1.15	0.95
3:K:185:ASN:CG	3:K:188:ASN:ND2	2.20	0.95
4:L:83:GLN:HG3	4:L:84:GLN:N	1.82	0.95
2:H:22:PHE:CD2	2:H:68:THR:O	2.20	0.95
4:L:97:THR:CB	4:L:98:GLN:OE1	2.15	0.95
4:P:97:THR:CG2	4:P:98:GLN:HG2	1.96	0.94
1:G:2:SER:N	1:G:105:SER:OG	1.98	0.94
1:G:97:ARG:NH1	5:U:6:VAL:HG13	1.81	0.94
2:N:42:ASN:H	2:N:43:GLY:HA2	1.32	0.94
1:G:187:THR:HB	1:G:272:LEU:HD21	1.49	0.94
4:P:223:TRP:CZ2	4:P:225:GLN:NE2	2.34	0.94
3:I:14:GLN:OE1	3:I:14:GLN:N	2.00	0.94
3:K:112:ILE:HG21	3:K:139:ASP:HB3	1.47	0.94
3:K:148:LYS:HB2	3:K:149:ASP:HA	1.48	0.93
2:N:13:HIS:HE1	4:F:81:ARG:NH2	1.60	0.93
3:O:81:GLN:HB3	3:O:82:PRO:HD2	1.48	0.93
1:A:35:ARG:HD3	1:A:48:ARG:HE	1.32	0.93
4:F:160:TRP:NE1	4:F:165:GLU:HA	1.81	0.93
2:N:13:HIS:CE1	4:F:81:ARG:HH22	1.75	0.93
4:P:223:TRP:CH2	4:P:225:GLN:NE2	2.35	0.93
4:L:83:GLN:CG	4:L:84:GLN:H	1.80	0.93
3:K:192:ILE:HG13	3:K:193:PRO:HD2	1.50	0.93
4:L:191:SER:OG	4:L:193:ARG:NH2	2.02	0.93
2:N:13:HIS:CE1	4:F:81:ARG:HH21	1.74	0.93
1:C:231:VAL:HG11	1:C:244:TRP:HE3	1.33	0.92
1:G:16:GLY:CA	1:G:17:ARG:HB2	1.99	0.92
1:M:20:PRO:HD2	1:M:75:ARG:HD3	1.47	0.92
3:I:8:PRO:O	3:I:104:THR:CG2	2.15	0.92
3:K:136:THR:HB	3:K:170:ASN:O	1.69	0.92
1:G:98:MET:HE2	1:G:113:TYR:HD1	1.29	0.91
1:M:219:ARG:HD3	1:M:224:GLN:NE2	1.86	0.91
4:P:160:TRP:HE3	4:P:209:ARG:HD2	1.34	0.91
1:C:4:SER:HB3	1:C:102:ASP:OD1	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:170:VAL:HA	4:L:194:LEU:HD23	0.93	0.91
4:F:223:TRP:HH2	4:F:228:ALA:O	1.54	0.91
3:K:112:ILE:HG23	3:K:139:ASP:CB	1.95	0.91
4:J:135:ILE:HA	4:J:140:LYS:O	1.71	0.91
3:K:53:ASN:HA	3:K:66:LEU:HD22	1.53	0.91
4:F:170:VAL:HG13	4:F:194:LEU:HD13	0.94	0.91
1:G:98:MET:HE1	1:G:113:TYR:HE1	1.11	0.91
3:K:136:THR:HG22	3:K:171:SER:CA	2.00	0.91
1:C:131:ARG:HH11	1:C:131:ARG:HG3	1.35	0.90
1:G:35:ARG:HH21	1:G:48:ARG:HG2	1.36	0.90
2:N:4:THR:HG23	2:N:86:THR:HG21	1.51	0.90
3:K:175:TRP:CE2	4:L:146:LEU:CD2	2.49	0.90
4:L:202:GLN:CA	4:L:204:PRO:HD2	2.01	0.90
4:F:149:GLY:HA3	4:F:150:PHE:HB3	1.53	0.90
3:O:138:PHE:CD1	3:O:142:THR:HG21	2.06	0.90
3:I:178:LYS:CG	3:I:179:SER:OG	2.19	0.90
1:C:102:ASP:CG	1:C:113:TYR:OH	2.10	0.90
3:K:161:ASP:CG	3:K:168:LYS:CD	2.39	0.90
1:G:162:GLY:O	1:G:166:GLU:HG2	1.72	0.90
4:L:89:VAL:HG12	4:L:110:ARG:CG	1.99	0.89
4:P:112:LEU:CD1	4:P:154:HIS:NE2	2.33	0.89
1:G:17:ARG:HG3	1:G:17:ARG:HH11	1.37	0.89
3:K:38:TRP:HE3	3:K:44:PRO:HG3	1.35	0.89
1:M:10:THR:HG21	2:N:54:LEU:HD22	1.53	0.89
1:C:100:GLY:O	1:C:113:TYR:HD2	1.56	0.89
4:F:160:TRP:O	4:F:209:ARG:HG2	1.73	0.89
2:H:24:ASN:HD21	2:H:65:LEU:HG	1.38	0.89
1:M:188:HIS:HB2	1:M:204:TRP:HB2	1.55	0.89
4:F:193:ARG:HH11	4:F:193:ARG:HG3	1.38	0.89
3:I:138:PHE:HE1	3:I:142:THR:HG1	1.18	0.89
3:K:156:ASP:OD1	3:K:157:LYS:N	2.06	0.88
1:A:230:LEU:HD21	1:A:243:LYS:HZ3	0.84	0.88
3:K:175:TRP:CZ2	4:L:146:LEU:CG	2.45	0.88
1:M:82:ARG:NH1	1:M:93:HIS:CD2	2.41	0.88
2:N:40:LEU:CD2	2:N:43:GLY:HA3	2.02	0.88
3:K:161:ASP:OD1	3:K:168:LYS:CD	2.20	0.88
3:K:144:VAL:HG23	3:K:157:LYS:NZ	1.89	0.88
4:L:88:ALA:HB3	4:L:110:ARG:HG3	0.88	0.87
2:N:54:LEU:HD21	2:N:62:PHE:CD1	2.09	0.87
1:G:98:MET:CE	1:G:113:TYR:HD1	1.75	0.87
1:C:202:ARG:CG	1:C:244:TRP:NE1	2.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:88:ALA:HB1	4:L:110:ARG:HG3	1.57	0.87
3:O:138:PHE:CE1	3:O:142:THR:CB	2.56	0.87
1:A:102:ASP:OD2	1:A:113:TYR:OH	1.93	0.86
3:K:112:ILE:HG22	3:K:139:ASP:OD2	1.75	0.86
4:P:151:TYR:O	4:P:214:PHE:CE1	2.27	0.86
3:K:135:PHE:HZ	3:K:192:ILE:CD1	1.88	0.86
2:N:13:HIS:HE1	4:F:81:ARG:HH22	1.12	0.86
1:G:116:TYR:CD2	1:G:117:ALA:N	2.43	0.86
3:I:146:GLN:OE1	3:I:154:ILE:CD1	2.24	0.86
1:G:16:GLY:HA3	1:G:17:ARG:CB	2.05	0.86
3:K:175:TRP:NE1	4:L:146:LEU:HD21	1.90	0.86
1:M:215:LEU:HD21	1:M:261:VAL:HG22	1.55	0.86
1:M:82:ARG:HH11	1:M:93:HIS:CD2	1.93	0.85
1:A:230:LEU:HD23	1:A:243:LYS:CE	2.03	0.85
4:P:7:SER:OG	4:P:22:ARG:CB	2.22	0.85
3:O:61:ARG:NH1	3:O:84:ASP:OD2	2.09	0.85
3:O:80:SER:O	3:O:81:GLN:NE2	2.09	0.85
4:F:121:PHE:CE2	4:F:187:ARG:NH2	2.44	0.85
3:E:178:LYS:O	3:E:179:SER:OG	1.95	0.85
3:I:146:GLN:OE1	3:I:154:ILE:HD11	1.75	0.85
3:E:38:TRP:HD1	3:E:44:PRO:HG3	1.41	0.85
4:F:110:ARG:NH2	4:F:154:HIS:CD2	2.45	0.85
2:N:2:GLN:NE2	2:N:85:VAL:HB	1.91	0.85
4:L:127:VAL:HG11	4:L:239:ALA:HB2	1.57	0.84
1:C:226:GLN:OE1	1:C:227:ASP:N	2.09	0.84
3:E:136:THR:CG2	3:E:171:SER:HB3	2.06	0.84
1:G:225:THR:O	6:G:301:HOH:O	1.95	0.84
1:A:42:SER:OG	1:A:44:ARG:HG2	1.77	0.84
4:F:96:GLN:O	4:F:97:THR:OG1	1.94	0.84
4:F:201:TRP:C	4:F:204:PRO:HD3	1.97	0.84
3:I:15:GLU:OE2	6:I:301:HOH:O	1.94	0.84
3:O:119:VAL:HA	3:O:134:LEU:O	1.77	0.84
1:M:9:PHE:HB2	1:M:97:ARG:HB3	1.60	0.84
3:K:175:TRP:NE1	4:L:146:LEU:CD2	2.40	0.84
4:J:223:TRP:HA	4:J:223:TRP:CE3	2.13	0.83
3:K:120:TYR:HH	4:L:135:ILE:N	1.76	0.83
4:L:161:VAL:HG23	4:L:166:VAL:HG11	1.59	0.83
4:F:54:ALA:CB	4:F:57:LYS:HE3	2.07	0.83
3:O:53:ASN:CB	3:O:68:THR:HG23	2.06	0.83
4:F:160:TRP:HE1	4:F:165:GLU:HA	1.37	0.83
4:P:39:LEU:HD12	4:P:39:LEU:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:MET:H	1:C:64:THR:HG22	1.41	0.83
2:D:79:ALA:HB1	2:D:92:ILE:HD11	1.59	0.83
4:F:26:ILE:O	4:F:27:SER:OG	1.96	0.83
1:G:125:ALA:HB3	1:G:134:THR:CG2	2.08	0.83
1:G:218:GLN:HB3	1:G:223:ASP:HA	1.59	0.83
4:F:197:SER:HB3	4:F:200:PHE:HB2	1.60	0.83
4:J:84:GLN:NE2	1:G:177:GLU:OE1	2.11	0.83
4:J:129:GLU:HG3	4:J:130:PRO:HD2	1.59	0.83
3:E:192:ILE:HG22	3:E:193:PRO:HD2	1.60	0.83
4:J:194:LEU:CD2	4:J:196:VAL:HG23	2.08	0.82
1:G:58:GLU:O	1:G:62:GLY:N	2.13	0.82
4:L:150:PHE:CE1	4:L:188:TYR:O	2.33	0.82
3:I:178:LYS:HG2	3:I:179:SER:HG	1.44	0.82
2:N:12:ARG:O	2:N:13:HIS:CG	2.32	0.82
3:O:138:PHE:CE1	3:O:142:THR:HB	2.14	0.82
1:M:66:LYS:NZ	3:O:29:ASN:CG	2.32	0.82
3:E:30:PHE:HD2	3:E:92:PHE:CE2	1.98	0.82
4:F:46:LEU:O	4:F:59:GLY:HA3	1.80	0.82
3:K:38:TRP:CE3	3:K:44:PRO:CG	2.55	0.82
1:C:100:GLY:O	1:C:113:TYR:CD2	2.32	0.82
2:D:54:LEU:HD21	2:D:62:PHE:CD1	2.13	0.82
3:E:136:THR:HA	3:E:138:PHE:HE1	1.45	0.82
4:P:160:TRP:HD1	4:P:165:GLU:HG3	1.44	0.82
1:A:230:LEU:CD2	1:A:243:LYS:HZ1	1.90	0.81
4:L:123:PRO:HG3	4:L:150:PHE:HD2	1.43	0.81
3:K:148:LYS:CB	3:K:149:ASP:C	2.49	0.81
3:I:194:GLU:O	3:I:196:THR:CG2	2.28	0.81
3:E:178:LYS:C	3:E:179:SER:OG	2.11	0.81
3:K:161:ASP:OD1	3:K:168:LYS:HD2	1.81	0.81
1:C:192:HIS:CE1	1:C:202:ARG:HH12	1.98	0.81
1:C:225:THR:O	1:C:228:THR:HG22	1.79	0.81
3:I:178:LYS:C	3:I:179:SER:OG	2.16	0.81
2:B:17:ASN:ND2	2:B:74:GLU:OE1	2.14	0.81
2:B:37:VAL:CG1	2:B:82:VAL:HG22	2.04	0.81
3:I:178:LYS:HG2	3:I:179:SER:OG	1.79	0.80
4:J:160:TRP:CZ3	4:J:211:GLN:CB	2.64	0.80
4:P:112:LEU:CG	4:P:154:HIS:CE1	2.63	0.80
4:P:19:VAL:HG22	4:P:79:ILE:HG12	1.63	0.80
3:E:136:THR:HG22	3:E:171:SER:HB3	1.63	0.80
1:G:14:ARG:O	1:G:18:GLY:HA3	1.80	0.80
3:O:122:LEU:HD22	4:P:130:PRO:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:SER:CB	1:C:102:ASP:OD1	2.29	0.80
3:E:138:PHE:O	3:E:139:ASP:C	2.16	0.79
1:G:192:HIS:HD2	1:G:202:ARG:NH2	1.69	0.79
1:A:223:ASP:O	1:A:225:THR:HG23	1.82	0.79
3:I:138:PHE:CD1	3:I:142:THR:OG1	2.35	0.79
2:H:70:PHE:HE1	2:H:78:TYR:CD1	2.00	0.79
1:M:220:ASP:OD1	6:M:301:HOH:O	2.01	0.79
1:C:234:ARG:NH2	1:C:242:GLN:OE1	2.12	0.79
4:F:223:TRP:CZ3	4:F:230:PRO:HD2	2.18	0.79
3:K:49:VAL:HG21	4:L:102:THR:CG2	2.13	0.79
3:O:81:GLN:HB3	3:O:82:PRO:CD	2.12	0.78
4:F:110:ARG:NH2	4:F:154:HIS:HD2	1.80	0.78
3:I:146:GLN:CD	3:I:154:ILE:CG1	2.52	0.78
1:G:125:ALA:HB3	1:G:134:THR:HG21	1.64	0.78
4:J:27:SER:OG	6:J:301:HOH:O	2.00	0.78
4:P:178:LYS:HA	4:P:187:ARG:O	1.81	0.78
3:I:192:ILE:HG23	3:I:193:PRO:HD3	0.78	0.78
3:K:38:TRP:CZ3	3:K:42:LYS:O	2.35	0.78
3:K:112:ILE:HG22	3:K:139:ASP:CG	2.05	0.78
4:L:25:PRO:HG3	4:L:32:LEU:HD13	1.65	0.78
4:L:64:ARG:O	4:L:80:GLN:NE2	2.17	0.78
4:F:149:GLY:N	4:F:150:PHE:HD2	1.81	0.78
3:K:175:TRP:HE1	4:L:146:LEU:CD2	1.96	0.78
1:G:133:TRP:CZ3	1:G:147:TRP:CZ3	2.72	0.78
3:K:144:VAL:HG23	3:K:157:LYS:HZ1	1.46	0.78
2:N:73:THR:HG21	2:N:76:ASP:OD1	1.81	0.78
3:E:49:VAL:CG2	4:F:102:THR:HG22	2.13	0.78
3:I:115:PRO:CB	3:I:137:ASP:OD2	2.32	0.77
3:K:148:LYS:CB	3:K:149:ASP:CA	2.61	0.77
3:K:49:VAL:CG2	4:L:102:THR:HG22	2.15	0.77
1:C:93:HIS:ND1	1:C:118:TYR:OH	2.14	0.77
2:B:37:VAL:HG21	2:B:66:TYR:CE1	2.19	0.77
3:I:178:LYS:HG3	3:I:179:SER:OG	1.83	0.77
4:J:60:LEU:HD12	4:J:60:LEU:O	1.83	0.77
1:C:72:GLN:HG3	4:F:55:PRO:HB2	1.66	0.77
1:M:192:HIS:O	1:M:200:THR:OG1	2.02	0.77
1:C:66:LYS:NZ	5:R:1:ASN:OD1	2.18	0.77
1:M:87:GLN:OE1	1:M:93:HIS:NE2	2.17	0.77
2:N:42:ASN:O	6:N:101:HOH:O	2.01	0.77
3:O:138:PHE:HD1	3:O:142:THR:OG1	1.67	0.77
2:N:42:ASN:N	2:N:43:GLY:HA2	1.96	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:97:THR:OG1	4:F:98:GLN:HG2	1.85	0.77
4:J:217:LEU:HD13	4:J:221:ASP:HB3	1.67	0.77
4:L:170:VAL:CG2	4:L:194:LEU:HD21	2.15	0.77
1:A:187:THR:HB	1:A:272:LEU:HD11	1.67	0.77
1:G:188:HIS:HB3	1:G:204:TRP:HB2	1.66	0.77
1:G:220:ASP:OD2	1:G:256:ARG:CZ	2.32	0.77
3:K:138:PHE:CZ	3:K:157:LYS:HE3	2.19	0.77
1:M:78:LEU:CD2	1:M:95:VAL:HG23	2.13	0.77
2:D:87:LEU:HD13	2:D:90:PRO:HA	1.66	0.77
4:F:217:LEU:CD1	4:F:218:SER:H	1.97	0.77
4:J:84:GLN:HA	4:J:113:VAL:HG21	1.67	0.77
3:I:138:PHE:CE1	3:I:142:THR:OG1	2.38	0.76
4:P:14:GLU:H	4:P:17:LYS:HZ1	1.33	0.76
1:G:218:GLN:HB2	1:G:222:GLU:O	1.86	0.76
1:A:4:SER:HB3	1:A:102:ASP:OD2	1.84	0.76
4:P:7:SER:HG	4:P:22:ARG:HB3	1.51	0.76
4:F:132:GLU:HG3	4:F:135:ILE:HG21	1.68	0.76
2:N:30:PHE:CE1	2:N:62:PHE:HB2	2.20	0.76
4:F:159:TRP:O	4:F:166:VAL:HB	1.84	0.76
1:G:133:TRP:CZ3	1:G:147:TRP:CE3	2.72	0.76
4:L:143:LEU:HD12	4:L:144:VAL:N	2.00	0.76
1:C:235:PRO:O	2:D:10:TYR:OH	2.01	0.76
3:K:161:ASP:OD1	3:K:168:LYS:HD3	1.83	0.76
1:A:230:LEU:HD21	1:A:243:LYS:HE2	1.68	0.76
3:K:185:ASN:CG	3:K:188:ASN:HD22	1.89	0.76
4:L:143:LEU:HD12	4:L:144:VAL:H	1.50	0.76
2:N:54:LEU:HD21	2:N:62:PHE:HD1	1.51	0.76
2:D:76:ASP:HB3	2:D:78:TYR:HE1	1.50	0.76
3:O:53:ASN:CB	3:O:68:THR:CG2	2.62	0.75
2:B:89:GLN:HB2	2:B:90:PRO:HD2	1.68	0.75
2:H:24:ASN:OD1	2:H:65:LEU:HD23	1.86	0.75
3:K:17:ASP:O	3:K:80:SER:OG	2.04	0.75
4:P:223:TRP:HZ2	4:P:225:GLN:HE21	1.30	0.75
1:G:97:ARG:NH1	5:U:6:VAL:HG11	1.84	0.75
3:K:135:PHE:CZ	3:K:192:ILE:CD1	2.70	0.75
2:D:44:GLU:HG2	2:D:46:ILE:HG12	1.67	0.75
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.20	0.75
4:J:223:TRP:HA	4:J:223:TRP:HE3	1.47	0.75
3:K:59:LYS:HD2	3:K:60:GLY:H	1.50	0.75
4:J:113:VAL:O	4:J:114:LEU:CG	2.35	0.75
1:G:17:ARG:HG3	1:G:17:ARG:NH1	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:151:TYR:O	4:P:214:PHE:CZ	2.40	0.75
4:J:57:LYS:O	4:J:59:GLY:N	2.17	0.75
1:M:20:PRO:HD2	1:M:75:ARG:HD2	1.67	0.75
4:P:122:PRO:HD3	4:P:230:PRO:HG3	1.69	0.75
1:G:97:ARG:HH12	5:U:6:VAL:CG1	1.99	0.75
3:K:31:TYR:HD1	5:U:4:PRO:HB2	1.52	0.75
4:P:14:GLU:HB2	4:P:17:LYS:HE3	1.69	0.75
3:E:84:ASP:HB3	3:E:85:SER:HB2	1.69	0.75
4:F:142:THR:HA	4:F:195:ARG:HB2	1.66	0.75
1:A:96:GLN:OE1	2:B:60:TRP:CE3	2.39	0.75
4:J:29:HIS:CD2	4:J:94:SER:C	2.59	0.75
1:G:192:HIS:CD2	1:G:202:ARG:HD2	2.21	0.75
3:K:185:ASN:C	3:K:188:ASN:HD22	1.90	0.75
3:E:49:VAL:HG21	4:F:102:THR:HG22	1.67	0.75
1:A:230:LEU:CD2	1:A:243:LYS:HE2	2.13	0.74
4:P:112:LEU:CG	4:P:154:HIS:NE2	2.50	0.74
1:A:102:ASP:OD1	1:A:113:TYR:OH	1.93	0.74
4:L:153:ASP:HB2	4:L:188:TYR:CD2	2.22	0.74
3:K:148:LYS:HB2	3:K:149:ASP:CA	2.17	0.74
1:C:192:HIS:ND1	1:C:202:ARG:NH1	2.30	0.74
4:P:112:LEU:HG	4:P:154:HIS:NE2	2.02	0.74
1:C:131:ARG:HG3	1:C:131:ARG:NH1	1.98	0.74
3:E:136:THR:CA	3:E:138:PHE:HE1	2.00	0.74
3:O:53:ASN:HB2	3:O:68:THR:CB	2.17	0.74
3:K:135:PHE:CZ	3:K:192:ILE:HG12	2.23	0.74
4:P:112:LEU:CD1	4:P:154:HIS:HE1	1.71	0.74
3:E:97:GLN:NE2	3:E:99:TYR:OH	2.20	0.74
4:F:218:SER:OG	4:F:221:ASP:HB3	1.86	0.74
4:F:223:TRP:CH2	4:F:228:ALA:O	2.39	0.74
1:A:93:HIS:ND1	1:A:119:ASP:OD1	2.20	0.74
4:J:47:ILE:CG1	4:J:60:LEU:HD23	2.18	0.74
4:L:88:ALA:CB	4:L:89:VAL:HA	2.03	0.74
1:C:66:LYS:HD2	5:R:4:PRO:HA	1.67	0.74
3:K:25:PHE:CZ	3:K:71:GLY:HA2	2.22	0.74
3:K:93:ILE:HG22	5:U:5:MET:HE1	1.70	0.74
3:K:192:ILE:HG13	3:K:193:PRO:CD	2.17	0.74
1:A:33:PHE:HD1	1:A:52:ILE:HD12	1.52	0.73
3:O:138:PHE:CD1	3:O:142:THR:CB	2.71	0.73
3:I:48:PHE:HE1	3:I:59:LYS:HG3	1.52	0.73
4:F:205:ARG:HA	4:F:240:TRP:CH2	2.23	0.73
4:J:178:LYS:HD2	4:J:188:TYR:CE1	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:138:PHE:HE1	3:O:142:THR:CB	1.96	0.73
1:C:35:ARG:HD2	2:D:53:ASP:CG	2.08	0.73
3:E:192:ILE:CG2	3:E:193:PRO:HD3	2.17	0.73
1:A:202:ARG:HG3	1:A:244:TRP:HE1	1.53	0.73
4:F:201:TRP:O	4:F:204:PRO:CD	2.36	0.73
1:G:186:LYS:HG3	1:G:186:LYS:O	1.87	0.73
1:G:192:HIS:HD2	1:G:202:ARG:HH21	0.87	0.73
1:M:259:CYS:HB3	1:M:272:LEU:HB2	1.70	0.73
3:I:194:GLU:O	3:I:196:THR:HG23	1.89	0.73
1:G:214:THR:HG23	1:G:214:THR:O	1.89	0.73
2:H:21:ASN:OD1	2:H:22:PHE:N	2.22	0.73
2:B:36:GLU:HB2	2:B:83:ASN:HB3	1.71	0.73
3:I:192:ILE:CG2	3:I:193:PRO:CD	2.36	0.73
4:J:129:GLU:CG	4:J:130:PRO:HD2	2.18	0.73
4:P:159:TRP:CD1	4:P:209:ARG:O	2.41	0.73
3:E:192:ILE:CG2	3:E:193:PRO:CD	2.66	0.73
1:G:191:HIS:ND1	1:G:191:HIS:O	2.20	0.72
4:L:10:ASN:HB2	4:L:154:HIS:NE2	2.04	0.72
1:C:202:ARG:HE	1:C:244:TRP:HZ2	1.33	0.72
3:I:146:GLN:NE2	3:I:154:ILE:HG12	2.04	0.72
4:J:116:ASP:HB3	4:J:119:ASN:N	2.05	0.72
2:H:37:VAL:HG23	2:H:81:ARG:O	1.88	0.72
3:K:138:PHE:O	3:K:139:ASP:OD1	2.07	0.72
4:L:173:ASP:OD2	4:L:191:SER:OG	2.07	0.72
1:C:225:THR:O	1:C:228:THR:N	2.16	0.72
1:A:99:TYR:OH	5:Q:3:VAL:HG12	1.90	0.72
4:L:202:GLN:C	4:L:204:PRO:HD2	2.09	0.72
4:P:18:ASP:OD2	2:D:20:SER:OG	2.08	0.72
3:E:42:LYS:HD2	3:E:43:SER:H	1.55	0.72
4:J:194:LEU:HD22	4:J:196:VAL:HG23	1.70	0.72
3:K:34:HIS:HB2	3:K:91:ALA:HB3	1.71	0.72
4:F:160:TRP:O	4:F:209:ARG:CG	2.37	0.72
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.70	0.72
4:F:150:PHE:CE1	4:F:155:VAL:HG11	2.23	0.72
3:K:2:LEU:HB3	3:K:3:ASN:HA	1.70	0.72
4:L:88:ALA:HB1	4:L:89:VAL:CA	2.15	0.72
1:C:235:PRO:HD2	2:D:10:TYR:OH	1.89	0.72
3:I:117:PRO:HB2	3:I:196:THR:HB	1.71	0.72
3:K:9:GLN:HA	3:K:104:THR:HA	1.70	0.72
4:L:202:GLN:HA	4:L:204:PRO:HD2	1.70	0.72
4:P:196:VAL:HG22	4:P:197:SER:N	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:98:GLN:HB2	4:J:101:GLU:OE1	1.90	0.72
1:M:96:GLN:NE2	2:N:31:HIS:HE1	1.87	0.72
2:D:89:GLN:HG3	2:D:90:PRO:HD2	1.72	0.72
1:M:59:TYR:OH	1:M:171:TYR:OH	2.06	0.71
4:J:114:LEU:N	4:J:114:LEU:HD12	2.03	0.71
1:M:197:HIS:O	1:M:198:GLU:HG2	1.90	0.71
1:M:224:GLN:OE1	1:M:227:ASP:HB3	1.90	0.71
3:O:70:GLU:N	3:O:71:GLY:HA2	2.05	0.71
4:P:160:TRP:CE3	4:P:209:ARG:HD2	2.22	0.71
4:J:29:HIS:NE2	4:J:94:SER:O	2.22	0.71
3:E:30:PHE:HD2	3:E:92:PHE:HE2	1.39	0.71
4:J:178:LYS:HD2	4:J:188:TYR:HE1	1.55	0.71
1:M:89:GLU:HG2	1:M:89:GLU:O	1.90	0.71
1:M:87:GLN:OE1	1:M:93:HIS:CE1	2.44	0.71
4:F:170:VAL:HA	4:F:194:LEU:HD12	1.72	0.71
1:A:223:ASP:O	1:A:225:THR:CG2	2.38	0.71
2:N:12:ARG:O	2:N:13:HIS:ND1	2.23	0.71
2:H:24:ASN:HD21	2:H:65:LEU:CG	2.03	0.70
2:H:24:ASN:OD1	2:H:65:LEU:CD2	2.39	0.70
3:K:102:THR:OG1	3:K:103:GLY:N	2.23	0.70
3:E:112:ILE:HG22	3:E:115:PRO:HD3	1.73	0.70
4:F:84:GLN:CD	4:F:85:GLU:H	1.93	0.70
3:I:194:GLU:O	3:I:196:THR:HG22	1.91	0.70
4:P:112:LEU:HG	4:P:154:HIS:CE1	2.26	0.70
3:E:178:LYS:O	3:E:180:ASP:N	2.21	0.70
1:A:230:LEU:HD23	1:A:243:LYS:HE3	1.71	0.70
4:P:151:TYR:O	4:P:214:PHE:HE1	1.75	0.70
4:L:160:TRP:NE1	4:L:163:GLY:O	2.23	0.70
2:D:33:SER:HB3	2:D:62:PHE:CD2	2.25	0.70
4:F:217:LEU:HD13	4:F:218:SER:H	1.54	0.70
1:G:192:HIS:CG	1:G:202:ARG:NH2	2.60	0.70
4:F:121:PHE:HE2	4:F:187:ARG:HH21	1.37	0.70
3:K:112:ILE:CG2	3:K:139:ASP:CG	2.59	0.70
1:M:66:LYS:CE	3:O:29:ASN:ND2	2.54	0.70
1:M:95:VAL:CG1	1:M:116:TYR:CE1	2.74	0.70
1:A:59:TYR:HH	1:A:171:TYR:HH	1.40	0.70
4:L:89:VAL:HG12	4:L:110:ARG:HG3	1.73	0.70
3:O:155:THR:HG23	4:P:173:ASP:OD2	1.91	0.70
1:C:218:GLN:HG2	1:C:260:HIS:CD2	2.27	0.70
4:P:119:ASN:HB3	4:P:151:TYR:CD2	2.27	0.70
4:L:204:PRO:CG	4:L:241:GLY:HA3	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4:THR:CG2	2:N:86:THR:HG21	2.22	0.69
1:C:231:VAL:HG11	1:C:244:TRP:CE3	2.24	0.69
3:K:50:MET:HB3	3:K:66:LEU:HD12	1.73	0.69
2:N:57:SER:O	2:N:59:ASP:N	2.24	0.69
4:P:25:PRO:HD3	4:P:32:LEU:HD21	1.74	0.69
3:E:136:THR:HA	3:E:138:PHE:CE1	2.27	0.69
4:J:160:TRP:HB2	4:J:209:ARG:CB	2.23	0.69
3:K:35:TRP:HE1	3:K:75:LEU:HD22	1.56	0.69
3:K:59:LYS:HD2	3:K:60:GLY:N	2.07	0.69
4:L:202:GLN:HA	4:L:202:GLN:OE1	1.90	0.69
3:O:34:HIS:HB2	3:O:91:ALA:HB3	1.72	0.69
4:L:9:SER:O	4:L:10:ASN:OD1	2.09	0.69
4:L:127:VAL:CG1	4:L:239:ALA:HB2	2.22	0.69
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.73	0.69
3:I:122:LEU:CA	3:I:132:VAL:H	2.05	0.69
1:G:24:ALA:HB3	1:G:36:PHE:HB3	1.74	0.69
3:K:148:LYS:CB	3:K:149:ASP:HA	2.20	0.69
4:L:33:TYR:HB2	4:L:93:ALA:HB3	1.73	0.69
4:L:88:ALA:HB1	4:L:110:ARG:HA	1.75	0.69
4:L:170:VAL:HA	4:L:194:LEU:HD21	1.69	0.69
4:F:201:TRP:O	4:F:204:PRO:HD3	1.93	0.69
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.74	0.69
4:L:125:VAL:HB	4:L:237:ALA:HB2	1.73	0.69
1:A:99:TYR:CZ	5:Q:3:VAL:HG12	2.26	0.69
3:I:161:ASP:OD2	3:I:166:ASP:N	2.25	0.69
3:O:138:PHE:HD1	3:O:142:THR:HG1	1.37	0.69
4:P:160:TRP:CD1	4:P:165:GLU:HG3	2.27	0.69
2:H:71:THR:OG1	2:H:72:PRO:HD3	1.92	0.68
4:J:47:ILE:HG13	4:J:60:LEU:HD23	1.74	0.68
1:M:219:ARG:NH2	1:M:222:GLU:OE1	2.26	0.68
3:I:146:GLN:NE2	3:I:154:ILE:CG1	2.57	0.68
4:J:85:GLU:O	4:J:87:SER:N	2.27	0.68
1:G:35:ARG:HE	1:G:48:ARG:HG3	1.56	0.68
1:G:159:TYR:CD1	1:G:163:THR:OG1	2.46	0.68
4:F:98:GLN:NE2	4:F:98:GLN:HA	2.08	0.68
1:G:192:HIS:HB2	1:G:202:ARG:HH22	1.57	0.68
1:M:22:PHE:H	1:M:38:SER:HB2	1.56	0.68
3:I:117:PRO:O	3:I:196:THR:O	2.12	0.68
2:H:22:PHE:HD2	2:H:68:THR:O	1.75	0.68
3:I:34:HIS:HB2	3:I:91:ALA:HB3	1.73	0.68
1:G:162:GLY:O	1:G:166:GLU:CG	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:5:MET:HB3	1:M:168:LEU:HD13	1.75	0.68
3:K:112:ILE:HG22	3:K:139:ASP:CB	2.21	0.68
4:L:10:ASN:HB2	4:L:154:HIS:CE1	2.28	0.68
4:L:36:ARG:HB3	4:L:89:VAL:O	1.94	0.68
4:L:114:LEU:HD23	4:L:116:ASP:H	1.59	0.68
1:G:98:MET:HE3	1:G:99:TYR:HA	1.76	0.68
4:L:90:TYR:N	4:L:109:THR:O	2.22	0.68
1:M:200:THR:HG22	1:M:248:VAL:HA	1.75	0.68
3:K:131:SER:HG	4:L:128:PHE:HD1	1.41	0.68
1:C:27:TYR:CE2	1:C:32:GLN:HB2	2.28	0.68
4:J:153:ASP:O	4:J:155:VAL:N	2.26	0.67
3:O:53:ASN:CB	3:O:68:THR:OG1	2.43	0.67
3:I:146:GLN:HE22	3:I:154:ILE:HD13	1.57	0.67
4:L:123:PRO:HG3	4:L:150:PHE:CD2	2.27	0.67
1:M:21:ARG:HG3	1:M:38:SER:HB3	1.76	0.67
1:G:6:ARG:HB3	1:G:8:PHE:HE2	1.60	0.67
4:L:62:SER:CA	4:L:65:PHE:CE2	2.78	0.67
1:C:10:THR:HG21	2:D:54:LEU:HD22	1.75	0.67
3:E:50:MET:HB3	3:E:66:LEU:HD12	1.75	0.67
3:K:148:LYS:CB	3:K:149:ASP:O	2.34	0.67
4:J:113:VAL:C	4:J:114:LEU:HG	2.14	0.67
4:L:47:ILE:HD11	4:L:67:ALA:HB3	1.77	0.67
3:O:117:PRO:HB2	3:O:196:THR:HA	1.77	0.67
1:A:121:LYS:HE3	2:B:1:ILE:HD13	1.77	0.67
1:G:55:GLU:O	1:G:59:TYR:HB3	1.95	0.67
3:K:123:ARG:HA	3:K:131:SER:OG	1.94	0.67
3:O:134:LEU:HD13	3:O:173:VAL:HG12	1.75	0.67
4:F:98:GLN:HB2	4:F:101:GLU:OE1	1.95	0.67
3:K:11:LEU:HB3	3:K:106:LEU:HD13	1.76	0.67
3:O:160:LEU:O	3:O:168:LYS:HA	1.95	0.67
3:E:132:VAL:HG22	3:E:175:TRP:HB3	1.75	0.67
1:A:42:SER:OG	1:A:44:ARG:CG	2.42	0.67
4:P:14:GLU:OE2	4:P:117:LEU:CG	2.40	0.67
1:G:143:THR:HB	5:U:9:VAL:HG23	1.76	0.66
3:K:112:ILE:HG21	3:K:139:ASP:CB	2.13	0.66
2:N:47:GLU:HG3	2:N:47:GLU:O	1.94	0.66
1:G:66:LYS:HD2	5:U:4:PRO:HA	1.76	0.66
1:M:66:LYS:HZ2	3:O:29:ASN:HB2	1.60	0.66
4:P:204:PRO:HB2	4:P:205:ARG:HA	1.78	0.66
1:M:78:LEU:HD23	1:M:95:VAL:HG21	1.74	0.66
4:F:170:VAL:CG1	4:F:194:LEU:CD1	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:135:PHE:HZ	3:K:192:ILE:CG1	2.08	0.66
3:K:144:VAL:CG2	3:K:157:LYS:NZ	2.57	0.66
1:M:133:TRP:HB2	1:M:144:LYS:HG3	1.77	0.66
3:O:138:PHE:CD1	3:O:142:THR:OG1	2.48	0.66
4:P:26:ILE:HB	4:P:29:HIS:CD2	2.30	0.66
3:I:178:LYS:C	3:I:179:SER:HG	1.98	0.66
4:J:206:ASN:OD1	4:J:207:HIS:N	2.28	0.66
3:E:181:PHE:CB	3:E:182:ALA:HA	2.20	0.66
3:O:53:ASN:HB2	3:O:68:THR:OG1	1.96	0.66
3:E:84:ASP:HA	3:E:85:SER:OG	1.95	0.66
4:F:79:ILE:O	4:F:79:ILE:HG13	1.96	0.66
4:J:223:TRP:CZ2	4:J:228:ALA:O	2.49	0.66
3:E:84:ASP:HB3	3:E:85:SER:O	1.95	0.66
3:I:13:VAL:C	3:I:14:GLN:OE1	2.33	0.65
1:G:35:ARG:CG	1:G:46:GLU:HB3	2.26	0.65
4:F:165:GLU:O	4:F:166:VAL:HG23	1.95	0.65
1:A:255:GLN:NE2	6:A:301:HOH:O	2.11	0.65
3:K:135:PHE:HZ	3:K:192:ILE:HD11	1.62	0.65
4:L:170:VAL:HG22	4:L:194:LEU:CD2	2.21	0.65
3:E:124:ASP:HB3	4:F:128:PHE:HA	1.75	0.65
4:F:98:GLN:HA	4:F:98:GLN:HE21	1.61	0.65
3:I:160:LEU:HD12	3:I:169:SER:HB2	1.77	0.65
4:J:65:PHE:HA	4:J:79:ILE:HG22	1.78	0.65
3:K:151:ASP:CG	3:K:177:ASN:H	1.99	0.65
1:M:77:ASP:OD2	5:T:8:THR:HB	1.97	0.65
3:O:15:GLU:OE1	3:O:168:LYS:NZ	2.29	0.65
4:P:100:TRP:HH2	5:T:7:ALA:HB2	1.61	0.65
4:F:6:GLN:HB3	4:F:107:PRO:HD2	1.77	0.65
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.79	0.65
3:K:185:ASN:O	3:K:188:ASN:CB	2.44	0.65
1:M:237:GLY:O	1:M:238:ASP:HB2	1.94	0.65
3:O:17:ASP:O	3:O:80:SER:OG	2.15	0.65
3:E:82:PRO:O	3:E:85:SER:OG	2.08	0.65
1:G:97:ARG:CG	1:G:116:TYR:CD1	2.80	0.65
1:M:87:GLN:OE1	1:M:93:HIS:CD2	2.50	0.65
2:N:81:ARG:HG3	2:N:92:ILE:HG13	1.76	0.65
3:O:138:PHE:CD1	3:O:142:THR:CG2	2.75	0.65
4:L:159:TRP:CZ2	4:L:194:LEU:HG	2.32	0.65
4:F:195:ARG:HG2	4:F:195:ARG:HH11	1.61	0.65
4:F:160:TRP:CD1	4:F:165:GLU:HA	2.31	0.65
1:C:202:ARG:NE	1:C:244:TRP:HZ2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:5:SER:HB2	4:L:24:ASP:HB3	1.79	0.65
2:N:2:GLN:NE2	2:N:85:VAL:CG2	2.60	0.65
1:G:98:MET:HE1	1:G:99:TYR:C	2.18	0.64
1:G:137:ASP:OD1	1:G:138:MET:N	2.25	0.64
2:H:17:ASN:OD1	2:H:97:ARG:NH1	2.30	0.64
3:I:192:ILE:HG23	3:I:193:PRO:N	2.13	0.64
3:I:178:LYS:O	3:I:180:ASP:N	2.25	0.64
4:J:26:ILE:HG22	4:J:27:SER:H	1.63	0.64
1:M:35:ARG:HD3	1:M:48:ARG:HH11	1.61	0.64
1:M:95:VAL:CG1	1:M:116:TYR:HE1	2.10	0.64
3:O:118:ALA:HB1	3:O:120:TYR:CE1	2.32	0.64
4:P:11:LYS:NZ	4:P:19:VAL:HB	2.12	0.64
1:M:37:ASP:HB3	1:M:40:ALA:HB2	1.80	0.64
1:C:187:THR:C	1:C:188:HIS:ND1	2.50	0.64
2:B:37:VAL:HG21	2:B:66:TYR:CZ	2.32	0.64
3:I:132:VAL:CG1	3:I:173:VAL:HG13	2.28	0.64
3:I:160:LEU:CD2	4:J:169:GLY:O	2.46	0.64
4:J:194:LEU:HD23	4:J:195:ARG:H	1.61	0.64
2:H:72:PRO:HB2	2:H:78:TYR:OH	1.98	0.64
4:L:90:TYR:HB2	4:L:109:THR:HG23	1.79	0.64
1:M:58:GLU:HA	1:M:61:ASP:HB3	1.79	0.64
1:M:219:ARG:HG3	1:M:257:TYR:CE2	2.32	0.64
3:E:82:PRO:HA	3:E:108:VAL:HG21	1.78	0.64
3:I:146:GLN:CD	3:I:154:ILE:CD1	2.66	0.64
1:G:27:TYR:OH	2:H:63:TYR:OH	2.12	0.64
4:L:103:GLN:HG2	4:L:105:PHE:HE1	1.63	0.64
3:I:7:SER:CB	3:I:8:PRO:HD3	2.28	0.64
4:L:97:THR:CB	4:L:98:GLN:CD	2.66	0.64
1:A:81:LEU:HG	5:Q:9:VAL:HG21	1.80	0.64
4:J:127:VAL:HG11	4:J:239:ALA:HB2	1.79	0.64
4:L:161:VAL:HG23	4:L:166:VAL:CG1	2.27	0.64
4:F:170:VAL:HG12	4:F:194:LEU:HD13	1.76	0.64
3:I:138:PHE:HE1	3:I:142:THR:O	1.81	0.64
3:K:16:GLY:N	3:K:80:SER:O	2.31	0.64
4:L:161:VAL:CG2	4:L:166:VAL:HG11	2.27	0.64
3:E:53:ASN:HB2	3:E:68:THR:HB	1.79	0.64
1:A:35:ARG:HD2	2:B:53:ASP:OD1	1.98	0.63
3:K:135:PHE:CE1	3:K:138:PHE:HB3	2.33	0.63
4:F:121:PHE:CD2	4:F:187:ARG:NH2	2.66	0.63
3:I:141:GLN:HG3	3:I:141:GLN:O	1.98	0.63
1:G:234:ARG:HG3	1:G:242:GLN:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:PHE:CE1	2:H:78:TYR:CE1	2.86	0.63
1:C:120:GLY:O	2:D:3:ARG:NH2	2.32	0.63
4:J:129:GLU:CD	4:J:130:PRO:CD	2.66	0.63
1:C:202:ARG:NE	1:C:244:TRP:CZ2	2.66	0.63
1:A:80:THR:HG23	5:Q:9:VAL:HG23	1.79	0.63
3:I:194:GLU:C	3:I:196:THR:HG23	2.18	0.63
4:J:97:THR:HB	4:J:98:GLN:HG2	1.80	0.63
1:G:97:ARG:NH1	5:U:6:VAL:HG12	2.10	0.63
4:L:150:PHE:CE1	4:L:188:TYR:C	2.72	0.63
4:L:191:SER:CB	4:L:193:ARG:HH21	2.12	0.63
3:O:138:PHE:HE1	3:O:142:THR:HB	1.58	0.63
3:O:140:SER:C	3:O:142:THR:H	2.02	0.63
4:F:159:TRP:NE1	4:F:192:SER:OG	2.19	0.63
4:F:173:ASP:OD2	4:F:191:SER:OG	2.17	0.63
4:F:200:PHE:O	4:F:204:PRO:HB3	1.99	0.63
4:J:83:GLN:HG2	4:J:84:GLN:H	1.63	0.63
2:H:5:PRO:HB3	2:H:30:PHE:HB3	1.78	0.63
4:L:218:SER:O	4:L:218:SER:OG	2.12	0.63
1:M:146:LYS:HZ2	4:P:97:THR:HG1	1.47	0.63
2:N:2:GLN:NE2	2:N:85:VAL:CB	2.60	0.63
3:I:196:THR:OG1	3:I:197:PHE:N	2.32	0.63
4:J:238:GLU:HG3	4:J:239:ALA:N	2.14	0.63
1:G:77:ASP:OD1	1:G:97:ARG:NH2	2.32	0.63
4:L:201:TRP:C	4:L:204:PRO:CD	2.67	0.63
1:G:192:HIS:HB2	1:G:202:ARG:NH2	2.12	0.62
2:H:11:SER:HB2	2:H:95:TRP:HZ2	1.63	0.62
1:M:12:VAL:HG22	1:M:94:THR:HG23	1.81	0.62
3:O:123:ARG:HG2	3:O:124:ASP:H	1.64	0.62
3:O:180:ASP:OD1	3:O:182:ALA:HB2	1.98	0.62
4:F:230:PRO:O	4:F:231:VAL:CG2	2.47	0.62
3:I:10:SER:O	3:I:11:LEU:HD23	1.99	0.62
3:K:38:TRP:HZ3	3:K:42:LYS:O	1.81	0.62
3:I:33:LEU:CD1	3:I:91:ALA:O	2.42	0.62
2:H:70:PHE:CE1	2:H:78:TYR:CD1	2.87	0.62
3:O:33:LEU:HB3	3:O:50:MET:HB2	1.81	0.62
4:F:165:GLU:O	4:F:166:VAL:CG2	2.46	0.62
4:F:193:ARG:HH11	4:F:193:ARG:CG	2.09	0.62
4:F:195:ARG:HH11	4:F:195:ARG:CG	2.13	0.62
1:G:126:LEU:HD11	1:G:130:LEU:HA	1.82	0.62
3:K:161:ASP:CB	3:K:168:LYS:HD3	2.29	0.62
4:P:21:LEU:HB2	4:P:77:LEU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:20:PRO:CD	1:M:75:ARG:HD2	2.29	0.62
4:F:47:ILE:HG22	4:F:48:TYR:N	2.13	0.62
1:A:96:GLN:OE1	2:B:60:TRP:HE3	1.83	0.62
3:K:115:PRO:HB3	3:K:139:ASP:OD2	2.00	0.62
1:C:102:ASP:OD1	1:C:113:TYR:OH	2.10	0.62
3:E:38:TRP:CD1	3:E:44:PRO:HG3	2.29	0.62
2:H:24:ASN:CG	2:H:65:LEU:HD21	2.20	0.62
3:I:146:GLN:NE2	3:I:154:ILE:HD13	2.15	0.62
1:G:73:THR:HG21	5:U:6:VAL:HG12	1.82	0.62
4:L:119:ASN:OD1	4:L:187:ARG:NH2	2.33	0.62
3:I:15:GLU:HG3	3:I:15:GLU:O	1.99	0.61
4:L:161:VAL:HG13	4:L:208:PHE:HA	1.81	0.61
1:G:133:TRP:CE3	1:G:147:TRP:HE3	2.18	0.61
4:L:153:ASP:HB2	4:L:188:TYR:HD2	1.64	0.61
3:O:183:CYS:O	3:O:186:ALA:HB2	2.00	0.61
4:P:64:ARG:HH11	4:P:64:ARG:CG	2.13	0.61
1:C:213:ILE:HG13	1:C:263:HIS:HB2	1.82	0.61
1:A:22:PHE:H	1:A:38:SER:HB3	1.65	0.61
4:J:234:ILE:HD12	4:J:234:ILE:O	1.99	0.61
3:K:185:ASN:ND2	3:K:188:ASN:ND2	2.48	0.61
2:N:73:THR:HG23	2:N:75:LYS:H	1.64	0.61
4:F:132:GLU:CG	4:F:135:ILE:HG21	2.31	0.61
3:K:185:ASN:O	3:K:188:ASN:N	2.30	0.61
1:M:103:VAL:HA	1:M:108:ARG:O	2.01	0.61
3:E:181:PHE:HB2	3:E:182:ALA:CA	2.25	0.61
3:K:185:ASN:O	3:K:188:ASN:HB3	2.01	0.61
1:C:197:HIS:ND1	1:C:198:GLU:HG3	2.16	0.61
2:N:59:ASP:HB3	2:N:61:SER:OG	2.01	0.61
2:B:36:GLU:CB	2:B:83:ASN:HB3	2.29	0.61
2:N:81:ARG:HD3	2:N:92:ILE:HG12	1.83	0.61
4:P:14:GLU:CD	4:P:117:LEU:CD2	2.53	0.61
1:M:47:PRO:HB3	1:M:60:TRP:CH2	2.36	0.61
2:D:89:GLN:HG3	2:D:90:PRO:CD	2.31	0.61
3:E:126:LYS:HD2	3:E:126:LYS:N	2.16	0.61
4:F:25:PRO:HG2	4:F:73:SER:HB2	1.81	0.60
4:L:161:VAL:HG12	4:L:162:ASN:N	2.16	0.60
1:G:27:TYR:CD1	1:G:32:GLN:NE2	2.66	0.60
2:H:44:GLU:OE1	4:F:71:GLY:HA2	2.00	0.60
2:N:81:ARG:HD3	2:N:92:ILE:CG1	2.30	0.60
1:A:73:THR:HG23	3:I:96:ASN:HD21	1.67	0.60
1:G:218:GLN:OE1	1:G:221:GLY:HA2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:LEU:HD13	2:D:89:GLN:O	2.01	0.60
3:I:13:VAL:HG23	3:I:15:GLU:H	1.66	0.60
3:I:87:THR:HA	3:I:105:SER:HA	1.83	0.60
1:G:99:TYR:CZ	5:U:3:VAL:HG12	2.37	0.60
1:G:207:SER:HA	1:G:240:THR:HB	1.83	0.60
4:L:150:PHE:O	4:L:150:PHE:HD1	1.84	0.60
2:D:82:VAL:O	2:D:90:PRO:HB2	2.02	0.60
1:A:231:VAL:HG23	1:A:231:VAL:O	2.00	0.60
1:M:195:SER:O	1:M:197:HIS:ND1	2.34	0.60
1:C:187:THR:HB	1:C:272:LEU:HD11	1.81	0.60
1:G:6:ARG:HB2	1:G:27:TYR:HB2	1.83	0.60
1:G:56:GLY:HA2	1:G:60:TRP:CE2	2.36	0.60
1:M:95:VAL:HG13	1:M:116:TYR:CE1	2.37	0.60
2:D:30:PHE:HE1	2:D:62:PHE:HB2	1.66	0.60
1:A:93:HIS:HB3	1:A:119:ASP:OD1	2.02	0.60
4:J:129:GLU:CG	4:J:130:PRO:CD	2.79	0.60
1:G:35:ARG:NH2	1:G:48:ARG:CG	2.58	0.60
1:G:159:TYR:HD1	1:G:163:THR:OG1	1.84	0.60
3:K:68:THR:O	3:K:68:THR:HG22	2.02	0.60
1:G:123:TYR:CE2	1:G:143:THR:HG21	2.37	0.60
4:F:222:GLU:HG2	4:F:223:TRP:N	2.15	0.60
4:J:12:VAL:HG22	4:J:154:HIS:CE1	2.37	0.59
4:J:129:GLU:CD	4:J:130:PRO:HD2	2.22	0.59
1:G:195:SER:CB	1:G:196:ASP:HA	2.32	0.59
2:H:70:PHE:CZ	2:H:78:TYR:CE2	2.90	0.59
2:N:2:GLN:HE21	2:N:85:VAL:HB	1.65	0.59
4:F:88:ALA:HB3	4:F:90:TYR:CE1	2.37	0.59
4:F:125:VAL:HG22	4:F:147:ALA:HA	1.84	0.59
4:F:170:VAL:CA	4:F:194:LEU:HD12	2.32	0.59
4:F:197:SER:CB	4:F:200:PHE:HB2	2.30	0.59
1:G:97:ARG:CG	1:G:116:TYR:CE1	2.85	0.59
1:C:81:LEU:HG	5:R:9:VAL:HG21	1.83	0.59
2:D:45:ARG:O	2:D:45:ARG:HG2	2.00	0.59
3:I:74:TYR:HB3	3:I:76:TYR:HE1	1.66	0.59
4:J:223:TRP:HZ2	4:J:228:ALA:O	1.86	0.59
3:K:135:PHE:CZ	3:K:192:ILE:CG1	2.85	0.59
2:N:41:LYS:O	2:N:42:ASN:OD1	2.20	0.59
1:A:37:ASP:HB3	1:A:40:ALA:HB2	1.84	0.59
4:J:113:VAL:C	4:J:114:LEU:CG	2.69	0.59
1:G:209:TYR:CD1	1:G:210:PRO:HA	2.37	0.59
1:G:220:ASP:OD2	1:G:256:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:135:PHE:HE1	3:K:138:PHE:HB3	1.66	0.59
1:M:146:LYS:NZ	4:P:97:THR:OG1	2.31	0.59
1:A:203:CYS:HB2	1:A:217:TRP:CZ3	2.38	0.59
1:G:192:HIS:CE1	2:H:98:ASP:HB3	2.37	0.59
1:G:259:CYS:HB3	1:G:272:LEU:HB2	1.84	0.59
1:M:103:VAL:HB	1:M:107:TRP:HA	1.83	0.59
4:J:129:GLU:CD	4:J:130:PRO:HD3	2.23	0.59
4:J:194:LEU:HD21	4:J:196:VAL:CG2	2.33	0.59
4:L:201:TRP:C	4:L:204:PRO:HD3	2.23	0.59
3:K:136:THR:CG2	3:K:171:SER:CB	2.80	0.59
3:K:192:ILE:CG1	3:K:193:PRO:HD2	2.29	0.59
1:C:35:ARG:HH11	2:D:53:ASP:CG	2.06	0.59
4:F:223:TRP:CE3	4:F:230:PRO:HD2	2.37	0.59
1:A:170:ARG:O	1:A:174:ASN:ND2	2.32	0.59
3:I:115:PRO:HB3	3:I:137:ASP:OD2	2.01	0.59
3:K:21:PHE:HB2	3:K:75:LEU:HB3	1.85	0.59
1:M:197:HIS:N	1:M:197:HIS:HD1	2.01	0.59
1:M:213:ILE:HG13	1:M:263:HIS:HB2	1.85	0.59
4:P:66:SER:HG	4:P:78:THR:HG1	1.49	0.59
4:J:69:ARG:HA	4:J:75:SER:HB2	1.84	0.59
3:K:20:ASN:HA	3:K:75:LEU:O	2.03	0.59
3:K:144:VAL:HG23	3:K:157:LYS:HZ2	1.67	0.59
1:M:255:GLN:NE2	1:M:255:GLN:O	2.35	0.59
4:P:23:CYS:SG	4:P:24:ASP:N	2.76	0.59
2:B:92:ILE:HG23	2:B:92:ILE:O	2.03	0.58
1:G:133:TRP:CE3	1:G:147:TRP:CE3	2.90	0.58
1:M:270:LEU:HD13	1:M:272:LEU:CD2	2.32	0.58
4:F:110:ARG:HH21	4:F:154:HIS:CD2	2.20	0.58
4:J:26:ILE:HG22	4:J:27:SER:N	2.18	0.58
3:K:136:THR:HG21	3:K:171:SER:CB	2.33	0.58
1:M:197:HIS:O	1:M:198:GLU:CG	2.50	0.58
2:H:35:ILE:HG13	2:H:83:ASN:O	2.03	0.58
1:M:198:GLU:HA	1:M:251:SER:H	1.67	0.58
1:M:203:CYS:HB2	1:M:217:TRP:HE1	1.68	0.58
3:K:138:PHE:HZ	3:K:157:LYS:HG2	1.68	0.58
3:O:118:ALA:HB1	3:O:120:TYR:CZ	2.39	0.58
4:P:47:ILE:HG22	4:P:57:LYS:HA	1.85	0.58
4:P:160:TRP:CH2	4:P:211:GLN:HG3	2.38	0.58
1:C:238:ASP:HB3	1:C:240:THR:HG22	1.84	0.58
4:J:229:LYS:CB	4:J:230:PRO:HA	2.33	0.58
4:L:204:PRO:HG3	4:L:241:GLY:CA	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:253:GLN:HG3	1:M:256:ARG:HE	1.68	0.58
1:G:178:THR:O	1:G:181:ARG:HB3	2.02	0.58
1:M:13:SER:HB3	1:M:78:LEU:HD13	1.85	0.58
2:N:81:ARG:CG	2:N:92:ILE:HG13	2.33	0.58
1:C:216:THR:HG23	1:C:260:HIS:HB2	1.85	0.58
1:G:73:THR:HG23	5:U:8:THR:HG22	1.85	0.58
4:L:147:ALA:HB2	4:L:212:VAL:HG21	1.84	0.58
1:C:35:ARG:HD2	2:D:53:ASP:OD2	2.04	0.58
1:C:72:GLN:CG	4:F:55:PRO:HB2	2.34	0.58
1:A:89:GLU:OE2	1:C:86:ASN:ND2	2.32	0.58
4:J:135:ILE:O	4:J:139:GLN:OE1	2.20	0.58
4:J:162:ASN:HA	4:J:207:HIS:CE1	2.39	0.58
4:F:153:ASP:O	4:F:155:VAL:N	2.37	0.58
1:M:10:THR:HG21	2:N:54:LEU:CD2	2.29	0.58
4:P:14:GLU:CG	4:P:117:LEU:CG	2.66	0.58
3:E:82:PRO:HA	3:E:108:VAL:CG2	2.33	0.58
4:F:97:THR:OG1	4:F:98:GLN:N	2.35	0.58
1:G:35:ARG:HH21	1:G:48:ARG:CD	2.17	0.58
1:G:133:TRP:CZ3	1:G:147:TRP:HZ3	2.20	0.58
3:K:61:ARG:CB	3:K:78:LYS:O	2.51	0.58
3:O:182:ALA:CB	3:O:185:ASN:HB3	2.15	0.58
4:P:211:GLN:HE21	4:P:234:ILE:HG13	1.68	0.58
4:F:50:GLN:NE2	4:F:97:THR:O	2.36	0.58
1:G:123:TYR:CE2	5:U:9:VAL:HG21	2.39	0.57
1:M:170:ARG:O	1:M:174:ASN:ND2	2.37	0.57
3:E:82:PRO:O	3:E:84:ASP:HA	2.03	0.57
3:E:134:LEU:HD11	4:F:144:VAL:HG21	1.86	0.57
1:A:66:LYS:HE2	3:I:29:ASN:CG	2.25	0.57
4:J:83:GLN:CG	4:J:84:GLN:H	2.17	0.57
3:K:175:TRP:HZ2	4:L:146:LEU:CB	2.15	0.57
4:L:147:ALA:CB	4:L:212:VAL:HG21	2.35	0.57
4:L:201:TRP:O	4:L:204:PRO:CD	2.52	0.57
3:E:84:ASP:CB	3:E:85:SER:HB2	2.34	0.57
3:E:145:SER:HB2	3:E:189:ASN:HB3	1.86	0.57
3:E:192:ILE:HG23	3:E:193:PRO:HD3	1.84	0.57
2:N:70:PHE:CZ	2:N:72:PRO:HB3	2.39	0.57
3:I:121:GLN:O	3:I:132:VAL:O	2.23	0.57
4:J:217:LEU:HD13	4:J:221:ASP:CB	2.34	0.57
1:M:74:HIS:O	1:M:77:ASP:N	2.36	0.57
1:A:266:LEU:HD13	1:A:270:LEU:HD13	1.87	0.57
4:L:95:SER:OG	4:L:103:GLN:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:121:PHE:O	4:L:150:PHE:HA	2.04	0.57
3:O:27:SER:HB2	3:O:69:LYS:HD2	1.86	0.57
3:O:140:SER:C	3:O:142:THR:N	2.56	0.57
4:F:143:LEU:HB2	4:F:194:LEU:O	2.03	0.57
1:A:163:THR:HA	1:A:166:GLU:HB2	1.86	0.57
3:I:122:LEU:N	3:I:132:VAL:O	2.37	0.57
4:J:194:LEU:HD21	4:J:196:VAL:HG23	1.84	0.57
1:G:35:ARG:HG2	1:G:46:GLU:HB3	1.86	0.57
4:P:226:ASP:N	4:P:226:ASP:OD1	2.36	0.57
2:D:5:PRO:HB3	2:D:30:PHE:HB3	1.86	0.57
4:F:118:LYS:CD	4:F:217:LEU:HD21	2.35	0.57
3:I:2:LEU:HD21	3:I:26:PRO:HB3	1.87	0.57
4:J:14:GLU:HB2	4:J:114:LEU:O	2.04	0.57
1:G:220:ASP:OD1	1:G:256:ARG:HG3	2.05	0.57
1:M:139:ALA:O	1:M:142:THR:OG1	2.22	0.57
3:I:2:LEU:HD13	3:I:26:PRO:HG3	1.87	0.57
4:J:6:GLN:NE2	4:J:92:CYS:HB3	2.20	0.57
1:G:35:ARG:NH2	1:G:48:ARG:NE	2.53	0.57
1:M:58:GLU:O	1:M:62:GLY:N	2.30	0.57
3:O:53:ASN:ND2	3:O:68:THR:OG1	2.38	0.57
3:O:187:PHE:N	3:O:187:PHE:CD2	2.73	0.57
1:C:113:TYR:CD2	1:C:113:TYR:N	2.73	0.57
1:G:12:VAL:HG11	2:H:33:SER:HB3	1.86	0.56
1:M:5:MET:HB2	1:M:28:VAL:HG12	1.87	0.56
4:P:197:SER:HB3	4:P:200:PHE:CD2	2.40	0.56
2:B:84:HIS:ND1	2:B:85:VAL:O	2.39	0.56
3:K:35:TRP:O	3:K:47:LEU:HB3	2.05	0.56
3:K:135:PHE:CE1	3:K:138:PHE:CD2	2.93	0.56
4:F:87:SER:HB3	4:F:113:VAL:HG12	1.87	0.56
1:A:204:TRP:CZ3	1:A:244:TRP:HB2	2.41	0.56
3:I:146:GLN:NE2	3:I:154:ILE:CD1	2.69	0.56
4:P:7:SER:OG	4:P:22:ARG:HD3	2.05	0.56
4:P:37:GLN:HG3	4:P:41:GLN:OE1	2.05	0.56
1:C:73:THR:HG21	5:R:6:VAL:HG23	1.86	0.56
3:E:157:LYS:NZ	3:E:170:ASN:HD21	2.03	0.56
2:B:20:SER:OG	4:L:18:ASP:OD2	2.23	0.56
4:L:170:VAL:CA	4:L:194:LEU:HD21	2.30	0.56
1:A:96:GLN:NE2	2:B:62:PHE:CE1	2.67	0.56
1:G:124:ILE:HD12	1:G:143:THR:HG23	1.87	0.56
1:C:10:THR:HG21	2:D:54:LEU:CD2	2.35	0.56
4:L:145:CYS:SG	4:L:146:LEU:N	2.77	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LYS:HG2	1:C:244:TRP:H	1.70	0.56
3:I:50:MET:HB3	3:I:66:LEU:HD22	1.88	0.56
3:K:185:ASN:CB	3:K:188:ASN:HD22	2.18	0.56
1:M:133:TRP:HB2	1:M:144:LYS:CG	2.36	0.56
1:C:5:MET:HB2	1:C:168:LEU:HD13	1.88	0.56
1:G:234:ARG:HB3	2:H:8:GLN:HE21	1.71	0.56
4:P:223:TRP:CZ3	4:P:229:LYS:O	2.57	0.56
4:F:150:PHE:CD1	4:F:155:VAL:HG11	2.40	0.56
3:K:62:ILE:HG22	3:K:75:LEU:HD11	1.88	0.56
4:J:29:HIS:HD2	4:J:94:SER:CA	2.13	0.56
1:G:199:ALA:N	1:G:249:VAL:O	2.39	0.56
4:F:179:GLU:HB2	4:F:187:ARG:O	2.06	0.56
4:F:230:PRO:O	4:F:231:VAL:HG22	2.06	0.56
1:A:89:GLU:HG2	1:C:86:ASN:OD1	2.05	0.55
1:C:122:ASP:OD1	2:D:60:TRP:NE1	2.36	0.55
2:D:74:GLU:HA	2:D:97:ARG:NH2	2.21	0.55
1:A:33:PHE:CD1	1:A:52:ILE:HD12	2.38	0.55
1:G:133:TRP:CZ3	1:G:147:TRP:HE3	2.21	0.55
3:K:138:PHE:CZ	3:K:157:LYS:CE	2.82	0.55
1:M:256:ARG:HD3	6:M:301:HOH:O	2.05	0.55
2:D:76:ASP:HB3	2:D:78:TYR:CE1	2.36	0.55
1:A:131:ARG:NH2	1:A:157:ARG:NH2	2.54	0.55
4:J:160:TRP:CE3	4:J:211:GLN:CB	2.90	0.55
4:J:207:HIS:HB3	4:J:240:TRP:CZ3	2.41	0.55
2:H:24:ASN:ND2	2:H:65:LEU:HD21	2.21	0.55
3:K:180:ASP:N	3:K:180:ASP:OD1	2.38	0.55
1:M:253:GLN:O	1:M:256:ARG:HG3	2.06	0.55
4:J:129:GLU:HG3	4:J:130:PRO:CD	2.34	0.55
1:M:14:ARG:NH2	1:M:21:ARG:HB2	2.21	0.55
1:C:131:ARG:HH11	1:C:131:ARG:CG	2.12	0.55
2:D:56:PHE:HA	2:D:62:PHE:HA	1.86	0.55
3:I:42:LYS:NZ	3:I:43:SER:OG	2.40	0.55
4:F:150:PHE:CE1	4:F:155:VAL:CG1	2.90	0.55
4:J:157:LEU:HD23	4:J:158:SER:N	2.22	0.55
3:K:136:THR:CB	3:K:170:ASN:O	2.51	0.55
4:L:82:THR:HG22	4:L:83:GLN:N	2.21	0.55
4:L:88:ALA:HB1	4:L:89:VAL:HG12	1.89	0.55
4:L:170:VAL:CB	4:L:194:LEU:HD21	2.35	0.55
1:M:66:LYS:HE3	3:O:29:ASN:ND2	2.21	0.55
2:N:83:ASN:OD1	2:N:84:HIS:N	2.40	0.55
3:E:93:ILE:HG22	5:R:5:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:VAL:CG2	2:H:82:VAL:HG12	2.36	0.55
4:L:124:GLU:HA	4:L:235:VAL:HG11	1.87	0.55
1:M:219:ARG:O	1:M:222:GLU:N	2.40	0.55
3:O:138:PHE:CD2	3:O:138:PHE:N	2.74	0.55
4:P:17:LYS:NZ	4:P:221:ASP:OD1	2.29	0.55
3:I:34:HIS:CE1	3:I:93:ILE:HD11	2.42	0.55
4:J:127:VAL:HG23	4:J:237:ALA:HB3	1.89	0.55
4:J:131:SER:HB2	4:J:134:GLU:HB3	1.89	0.55
1:G:192:HIS:CB	1:G:202:ARG:NH2	2.70	0.55
3:K:122:LEU:HD13	4:L:144:VAL:HG23	1.88	0.55
4:L:59:GLY:O	4:L:61:PRO:HD3	2.06	0.55
1:M:133:TRP:CB	1:M:144:LYS:HG3	2.36	0.55
3:O:123:ARG:HG2	3:O:124:ASP:N	2.22	0.55
4:P:83:GLN:O	4:P:113:VAL:HG11	2.06	0.55
1:C:231:VAL:HG23	1:C:232:GLU:O	2.06	0.55
2:B:18:GLY:HA2	2:B:71:THR:HG22	1.88	0.55
2:D:90:PRO:O	2:D:90:PRO:HG2	2.07	0.55
1:G:81:LEU:HG	5:U:9:VAL:HG11	1.88	0.54
3:I:14:GLN:O	3:I:15:GLU:HB3	2.07	0.54
1:M:163:THR:HA	1:M:166:GLU:HB2	1.89	0.54
1:M:268:LYS:HB2	1:M:269:PRO:HD2	1.89	0.54
5:T:7:ALA:O	5:T:8:THR:HG23	2.06	0.54
1:A:88:SER:OG	1:A:89:GLU:N	2.40	0.54
1:G:98:MET:CE	1:G:99:TYR:CA	2.85	0.54
3:K:185:ASN:CB	3:K:188:ASN:ND2	2.69	0.54
4:L:201:TRP:C	4:L:204:PRO:HD2	2.28	0.54
4:F:36:ARG:HB3	4:F:46:LEU:HD11	1.89	0.54
4:F:125:VAL:HG21	4:F:212:VAL:HG21	1.89	0.54
2:N:83:ASN:HB2	2:N:90:PRO:HG3	1.89	0.54
4:P:141:ALA:HB2	4:P:198:ALA:HA	1.89	0.54
3:E:136:THR:HG22	3:E:171:SER:CB	2.24	0.54
1:A:103:VAL:HG12	1:A:108:ARG:C	2.28	0.54
4:J:221:ASP:CG	4:J:222:GLU:H	2.11	0.54
2:H:11:SER:HB2	2:H:95:TRP:CZ2	2.42	0.54
3:K:52:LEU:HD12	3:K:52:LEU:O	2.07	0.54
3:E:138:PHE:N	3:E:138:PHE:CD1	2.72	0.54
1:G:82:ARG:HH21	1:G:88:SER:C	2.08	0.54
3:K:66:LEU:HD23	3:K:67:ASN:N	2.23	0.54
3:K:144:VAL:CG2	3:K:157:LYS:HZ1	2.15	0.54
4:L:7:SER:O	4:L:22:ARG:HB3	2.08	0.54
3:O:87:THR:HA	3:O:105:SER:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:54:ALA:CB	4:F:57:LYS:CE	2.78	0.54
4:F:98:GLN:HE21	4:F:98:GLN:CA	2.19	0.54
4:J:123:PRO:HA	4:J:150:PHE:HB3	1.88	0.54
1:M:128:GLU:OE1	1:M:128:GLU:N	2.36	0.54
1:A:12:VAL:HG22	1:A:94:THR:HG22	1.90	0.54
1:G:143:THR:CB	5:U:9:VAL:HG23	2.38	0.54
3:K:47:LEU:O	3:K:48:PHE:HD1	1.91	0.54
4:P:223:TRP:CE2	4:P:229:LYS:O	2.61	0.54
4:F:155:VAL:HG12	4:F:214:PHE:HD1	1.71	0.54
3:I:160:LEU:HD22	4:J:169:GLY:O	2.07	0.54
1:G:91:GLY:HA3	1:G:93:HIS:CE1	2.43	0.54
1:M:66:LYS:NZ	3:O:29:ASN:CB	2.71	0.54
1:G:218:GLN:CD	1:G:221:GLY:HA2	2.27	0.54
2:H:71:THR:O	2:H:72:PRO:O	2.26	0.54
4:L:7:SER:OG	4:L:8:PRO:HA	2.08	0.54
4:L:13:THR:OG1	4:L:14:GLU:N	2.40	0.54
2:N:46:ILE:O	2:N:49:VAL:HG23	2.08	0.54
1:C:159:TYR:CD1	1:C:163:THR:HB	2.43	0.54
2:H:24:ASN:CG	2:H:65:LEU:CD2	2.77	0.53
1:M:175:GLY:O	1:M:179:LEU:N	2.41	0.53
3:I:9:GLN:HA	3:I:104:THR:HA	1.90	0.53
4:J:98:GLN:HA	4:J:98:GLN:NE2	2.23	0.53
4:J:177:LEU:HB3	4:J:189:ALA:HB3	1.91	0.53
2:H:70:PHE:HE1	2:H:78:TYR:CG	2.26	0.53
1:C:195:SER:OG	1:C:196:ASP:N	2.39	0.53
2:B:21:ASN:OD1	2:B:22:PHE:N	2.33	0.53
1:G:138:MET:N	1:G:138:MET:SD	2.82	0.53
4:L:203:ASN:N	4:L:204:PRO:HD2	2.22	0.53
1:M:219:ARG:O	1:M:220:ASP:C	2.46	0.53
3:E:8:PRO:O	3:E:104:THR:HB	2.08	0.53
4:F:160:TRP:CD1	4:F:165:GLU:CA	2.91	0.53
4:J:160:TRP:CH2	4:J:211:GLN:CB	2.91	0.53
1:M:110:LEU:HD23	1:M:111:ARG:HG2	1.91	0.53
2:D:30:PHE:CE1	2:D:62:PHE:HB2	2.44	0.53
4:J:122:PRO:HG3	4:J:230:PRO:HB2	1.90	0.53
1:G:58:GLU:O	1:G:61:ASP:N	2.42	0.53
1:M:191:HIS:NE2	1:M:193:ALA:HB2	2.24	0.53
2:B:57:SER:O	2:B:60:TRP:N	2.41	0.53
2:B:85:VAL:O	2:B:86:THR:OG1	2.19	0.53
4:J:130:PRO:HG3	4:J:142:THR:O	2.09	0.53
1:M:154:GLU:HB3	3:O:52:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:4:VAL:HG21	3:O:99:TYR:O	2.08	0.53
4:P:159:TRP:O	4:P:165:GLU:HB2	2.07	0.53
3:E:84:ASP:HB3	3:E:85:SER:CB	2.39	0.53
1:A:2:SER:HB3	1:A:103:VAL:O	2.08	0.53
4:L:191:SER:CB	4:L:193:ARG:NH2	2.70	0.53
2:N:58:LYS:NZ	6:N:102:HOH:O	2.40	0.53
3:E:136:THR:CA	3:E:138:PHE:CE1	2.86	0.53
1:A:4:SER:CB	1:A:102:ASP:OD2	2.53	0.53
3:I:160:LEU:HD23	4:J:169:GLY:O	2.09	0.53
3:K:52:LEU:HD12	3:K:52:LEU:H	1.73	0.53
3:K:185:ASN:O	3:K:188:ASN:CG	2.46	0.53
1:C:59:TYR:O	1:C:63:GLU:HG2	2.09	0.53
4:F:26:ILE:O	4:F:26:ILE:HG22	2.09	0.53
3:K:59:LYS:CD	3:K:60:GLY:H	2.21	0.53
3:O:182:ALA:O	3:O:186:ALA:N	2.40	0.53
4:F:123:PRO:HB3	4:F:150:PHE:CD2	2.43	0.53
1:A:131:ARG:NH1	6:A:302:HOH:O	2.31	0.53
3:I:115:PRO:CA	3:I:137:ASP:OD2	2.56	0.53
3:I:74:TYR:HB3	3:I:76:TYR:CE1	2.44	0.52
1:G:99:TYR:OH	5:U:3:VAL:HG12	2.09	0.52
1:G:218:GLN:CB	1:G:223:ASP:HA	2.37	0.52
4:L:191:SER:HB2	4:L:193:ARG:HH21	1.74	0.52
1:M:63:GLU:OE1	5:T:2:LEU:HD12	2.08	0.52
3:O:29:ASN:HB2	5:T:4:PRO:HG3	1.91	0.52
4:F:118:LYS:HD2	4:F:217:LEU:HD21	1.91	0.52
4:F:217:LEU:HD12	4:F:218:SER:H	1.73	0.52
2:H:70:PHE:CZ	2:H:78:TYR:CD2	2.97	0.52
3:K:25:PHE:CE1	3:K:71:GLY:HA2	2.44	0.52
1:M:67:VAL:O	1:M:70:HIS:HB2	2.09	0.52
3:E:157:LYS:HZ2	3:E:170:ASN:HD21	1.56	0.52
3:I:117:PRO:O	3:I:196:THR:C	2.48	0.52
4:P:11:LYS:HZ3	4:P:19:VAL:HB	1.72	0.52
4:P:70:THR:O	4:P:74:VAL:HB	2.09	0.52
4:F:140:LYS:CD	4:F:197:SER:HA	2.39	0.52
4:J:135:ILE:CA	4:J:140:LYS:O	2.52	0.52
4:L:203:ASN:N	4:L:204:PRO:CD	2.72	0.52
1:M:97:ARG:HH22	1:M:147:TRP:HH2	1.56	0.52
1:G:192:HIS:HD2	1:G:202:ARG:HD2	1.73	0.52
3:O:44:PRO:HG2	3:O:44:PRO:O	2.10	0.52
4:P:15:LYS:HZ2	4:P:83:GLN:HG3	1.75	0.52
2:D:37:VAL:HG22	2:D:82:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:49:VAL:HG21	4:F:102:THR:CG2	2.36	0.52
4:F:193:ARG:HG3	4:F:193:ARG:NH1	2.18	0.52
4:L:125:VAL:HG21	4:L:236:SER:O	2.10	0.52
4:L:217:LEU:HB2	4:L:230:PRO:O	2.09	0.52
4:P:61:PRO:O	6:P:301:HOH:O	2.19	0.52
1:C:74:HIS:CD2	1:C:97:ARG:HH21	2.27	0.52
2:D:74:GLU:HA	2:D:97:ARG:HH22	1.75	0.52
3:E:89:LEU:HD21	3:E:100:PHE:CD1	2.43	0.52
3:I:155:THR:HG21	4:J:191:SER:OG	2.09	0.52
4:J:11:LYS:NZ	4:J:217:LEU:CD2	2.73	0.52
2:N:60:TRP:HA	2:N:60:TRP:CE3	2.42	0.52
4:J:36:ARG:HB3	4:J:46:LEU:HD11	1.92	0.52
4:J:96:GLN:O	4:J:98:GLN:N	2.40	0.52
1:G:12:VAL:HA	1:G:94:THR:HA	1.92	0.52
2:H:55:SER:OG	2:H:56:PHE:N	2.43	0.52
3:I:146:GLN:CG	3:I:154:ILE:HG12	2.40	0.52
1:M:219:ARG:N	1:M:222:GLU:O	2.41	0.52
2:N:41:LYS:O	2:N:77:GLU:O	2.27	0.52
3:E:181:PHE:CB	3:E:182:ALA:CA	2.86	0.52
4:F:6:GLN:HG3	4:F:22:ARG:O	2.10	0.52
3:I:182:ALA:O	3:I:186:ALA:HB2	2.10	0.52
1:C:155:GLN:HE21	3:E:51:THR:HG21	1.75	0.52
3:I:158:CYS:SG	4:J:193:ARG:NH1	2.83	0.51
1:G:131:ARG:NH2	6:G:303:HOH:O	2.27	0.51
2:H:37:VAL:HG21	2:H:82:VAL:HG12	1.93	0.51
4:L:36:ARG:HD2	4:L:90:TYR:CG	2.45	0.51
4:L:130:PRO:HG2	4:L:201:TRP:CE2	2.45	0.51
1:M:230:LEU:C	1:M:230:LEU:HD12	2.30	0.51
3:O:61:ARG:NH1	3:O:81:GLN:HB2	2.25	0.51
3:E:157:LYS:CE	3:E:170:ASN:OD1	2.58	0.51
4:J:6:GLN:HE21	4:J:92:CYS:HB3	1.74	0.51
4:J:141:ALA:CB	4:J:196:VAL:O	2.45	0.51
1:G:168:LEU:O	1:G:172:LEU:HG	2.11	0.51
1:G:200:THR:HG21	1:G:202:ARG:NH2	2.26	0.51
2:N:12:ARG:O	2:N:12:ARG:HG2	2.09	0.51
4:P:97:THR:CG2	4:P:98:GLN:N	2.73	0.51
2:D:73:THR:HG22	2:D:74:GLU:H	1.74	0.51
3:O:52:LEU:O	3:O:55:ASP:N	2.42	0.51
3:E:30:PHE:CD2	3:E:92:PHE:HE2	2.23	0.51
3:K:50:MET:HB3	3:K:66:LEU:CD1	2.40	0.51
3:O:134:LEU:HD12	3:O:135:PHE:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:140:SER:O	3:O:142:THR:N	2.43	0.51
2:D:54:LEU:HD21	2:D:62:PHE:HD1	1.72	0.51
4:F:37:GLN:NE2	4:F:38:ARG:O	2.44	0.51
3:I:81:GLN:HG2	3:I:82:PRO:HD2	1.92	0.51
4:J:113:VAL:HG22	4:J:114:LEU:N	2.26	0.51
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.46	0.51
2:H:24:ASN:OD1	2:H:66:TYR:O	2.28	0.51
4:L:62:SER:CA	4:L:65:PHE:HE2	2.24	0.51
4:F:121:PHE:HE2	4:F:187:ARG:NH2	1.92	0.51
2:B:37:VAL:CG2	2:B:66:TYR:CZ	2.94	0.51
3:K:21:PHE:HE1	3:K:88:TYR:CD2	2.28	0.51
3:K:59:LYS:CD	3:K:60:GLY:N	2.73	0.51
3:K:152:VAL:HG13	3:K:153:TYR:N	2.26	0.51
4:L:161:VAL:O	4:L:162:ASN:CB	2.59	0.51
2:N:11:SER:C	2:N:13:HIS:H	2.13	0.51
3:O:181:PHE:O	3:O:182:ALA:HB3	2.11	0.51
3:E:157:LYS:NZ	3:E:170:ASN:OD1	2.44	0.51
3:E:161:ASP:OD1	3:E:161:ASP:N	2.43	0.51
4:F:73:SER:OG	4:F:74:VAL:N	2.43	0.51
3:I:34:HIS:O	3:I:90:CYS:HA	2.10	0.51
1:G:101:CYS:N	1:G:164:CYS:SG	2.84	0.51
3:K:185:ASN:HB2	3:K:188:ASN:HB3	1.92	0.51
1:M:188:HIS:HD2	1:M:204:TRP:HE3	1.59	0.51
1:C:226:GLN:OE1	1:C:227:ASP:HB2	2.10	0.51
2:B:1:ILE:HG13	2:B:2:GLN:N	2.26	0.51
3:O:134:LEU:HD12	3:O:135:PHE:N	2.26	0.51
1:C:6:ARG:HA	1:C:100:GLY:HA3	1.92	0.51
2:D:70:PHE:HE1	2:D:72:PRO:HB3	1.75	0.51
3:E:21:PHE:CD2	3:E:21:PHE:N	2.79	0.51
3:I:113:GLN:OE1	3:I:113:GLN:N	2.24	0.51
1:M:9:PHE:HE2	1:M:99:TYR:CE2	2.28	0.51
4:P:135:ILE:HG13	4:P:141:ALA:HA	1.92	0.51
4:F:29:HIS:ND1	4:F:96:GLN:HG2	2.26	0.51
1:A:143:THR:HG21	5:Q:9:VAL:HG12	1.92	0.51
3:I:81:GLN:N	3:I:84:ASP:OD2	2.40	0.51
4:L:123:PRO:CG	4:L:150:PHE:HD2	2.18	0.51
4:L:215:TYR:HA	4:L:232:THR:OG1	2.11	0.51
3:E:83:GLU:OE1	3:E:162:MET:CE	2.58	0.51
3:E:187:PHE:O	3:E:192:ILE:HD12	2.11	0.51
3:I:44:PRO:HG2	4:J:105:PHE:CD2	2.47	0.50
4:F:35:TYR:OH	4:F:103:GLN:OE1	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:47:ILE:CG2	4:F:48:TYR:N	2.73	0.50
1:A:207:SER:O	1:A:207:SER:OG	2.22	0.50
2:B:1:ILE:HG13	2:B:2:GLN:H	1.75	0.50
4:P:160:TRP:HA	4:P:165:GLU:HB3	1.92	0.50
4:F:83:GLN:HA	4:F:113:VAL:HG21	1.93	0.50
4:F:135:ILE:CD1	4:F:201:TRP:HZ3	2.24	0.50
3:I:2:LEU:HD23	3:I:3:ASN:H	1.77	0.50
1:G:37:ASP:HB3	1:G:40:ALA:HB2	1.93	0.50
4:L:150:PHE:CD1	4:L:150:PHE:C	2.85	0.50
2:N:2:GLN:HE22	2:N:85:VAL:HB	1.76	0.50
2:N:33:SER:O	2:N:35:ILE:HD12	2.11	0.50
2:N:38:ASP:OD2	2:N:45:ARG:HB3	2.12	0.50
3:O:96:ASN:H	5:T:5:MET:HE2	1.75	0.50
4:F:123:PRO:HA	4:F:149:GLY:HA3	1.92	0.50
4:F:170:VAL:HA	4:F:194:LEU:CD1	2.40	0.50
1:G:98:MET:CE	1:G:99:TYR:HA	2.41	0.50
3:K:30:PHE:HD1	3:K:92:PHE:HE1	1.57	0.50
4:L:46:LEU:O	4:L:47:ILE:HG22	2.12	0.50
4:P:130:PRO:HB3	4:P:142:THR:O	2.11	0.50
3:I:154:ILE:HD12	3:I:155:THR:N	2.26	0.50
1:G:102:ASP:HB2	1:G:111:ARG:HG3	1.93	0.50
1:M:66:LYS:NZ	3:O:29:ASN:HB2	2.25	0.50
1:M:249:VAL:HG22	1:M:257:TYR:CD1	2.46	0.50
4:P:64:ARG:CG	4:P:64:ARG:NH1	2.73	0.50
1:C:13:SER:HB3	1:C:78:LEU:HD13	1.93	0.50
4:F:203:ASN:N	4:F:204:PRO:CD	2.75	0.50
4:J:29:HIS:CD2	4:J:94:SER:O	2.64	0.50
3:K:144:VAL:CG2	3:K:157:LYS:HZ2	2.23	0.50
3:K:161:ASP:HA	3:K:168:LYS:HB3	1.93	0.50
4:L:10:ASN:OD1	4:L:109:THR:HA	2.12	0.50
4:L:89:VAL:CG1	4:L:110:ARG:CG	2.83	0.50
4:L:204:PRO:HB2	4:L:205:ARG:HA	1.93	0.50
3:E:84:ASP:HA	3:E:85:SER:HG	1.76	0.50
4:F:170:VAL:CA	4:F:194:LEU:CD1	2.90	0.50
4:L:67:ALA:HB2	4:L:77:LEU:HD13	1.93	0.50
2:N:20:SER:HB3	4:F:18:ASP:CG	2.32	0.50
4:F:110:ARG:HH21	4:F:154:HIS:HA	1.77	0.50
1:A:131:ARG:NH2	6:A:302:HOH:O	2.19	0.50
1:G:189:MET:CE	1:G:274:TRP:N	2.75	0.50
4:J:150:PHE:O	4:J:187:ARG:HB2	2.12	0.50
2:H:70:PHE:CE1	2:H:78:TYR:CZ	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:146:LEU:HD12	4:L:146:LEU:O	2.12	0.50
4:P:37:GLN:HG3	4:P:41:GLN:CD	2.32	0.50
1:C:188:HIS:ND1	1:C:188:HIS:N	2.60	0.50
1:A:147:TRP:HB3	1:A:152:VAL:HB	1.92	0.49
2:B:18:GLY:N	2:B:72:PRO:O	2.37	0.49
3:I:36:TYR:O	3:I:88:TYR:HA	2.12	0.49
2:H:96:ASP:HB3	2:H:99:MET:HB2	1.94	0.49
3:K:135:PHE:CZ	3:K:192:ILE:HD11	2.44	0.49
4:L:150:PHE:CD1	4:L:188:TYR:O	2.65	0.49
1:M:227:ASP:OD1	1:M:248:VAL:HG12	2.12	0.49
1:G:97:ARG:HH22	5:U:8:THR:HA	1.77	0.49
3:K:61:ARG:HH21	3:K:84:ASP:CG	2.15	0.49
4:P:11:LYS:O	4:P:111:LEU:HD12	2.13	0.49
1:A:98:MET:C	1:A:98:MET:HE2	2.33	0.49
1:G:195:SER:HB2	1:G:196:ASP:HA	1.93	0.49
3:K:135:PHE:CD1	3:K:135:PHE:C	2.85	0.49
2:B:89:GLN:CB	2:B:90:PRO:HD2	2.42	0.49
3:K:48:PHE:HD2	3:K:64:ALA:HB2	1.77	0.49
1:C:99:TYR:OH	5:R:3:VAL:HG12	2.12	0.49
1:C:202:ARG:HG3	1:C:244:TRP:NE1	2.26	0.49
3:E:6:GLN:OE1	3:E:103:GLY:HA2	2.11	0.49
4:F:69:ARG:HB2	4:F:75:SER:HB2	1.94	0.49
4:F:162:ASN:O	4:F:164:LYS:HG3	2.13	0.49
1:A:203:CYS:HB2	1:A:217:TRP:HZ3	1.75	0.49
2:B:52:SER:OG	2:B:65:LEU:N	2.43	0.49
4:J:131:SER:HB2	4:J:134:GLU:CB	2.42	0.49
1:G:185:PRO:HB3	1:G:208:PHE:HB3	1.93	0.49
3:K:35:TRP:C	3:K:36:TYR:HD1	2.16	0.49
4:L:202:GLN:N	4:L:204:PRO:HD2	2.27	0.49
1:M:8:PHE:HB2	1:M:25:VAL:HG13	1.92	0.49
1:C:25:VAL:HG21	1:C:32:GLN:HE21	1.77	0.49
4:J:162:ASN:HB2	4:J:164:LYS:NZ	2.28	0.49
1:G:142:THR:O	1:G:146:LYS:HG3	2.13	0.49
3:K:72:TYR:CD1	3:K:72:TYR:C	2.85	0.49
3:K:119:VAL:HA	3:K:134:LEU:O	2.13	0.49
4:L:170:VAL:CG2	4:L:194:LEU:CD2	2.87	0.49
4:P:21:LEU:HD22	4:P:109:THR:HG21	1.95	0.49
4:P:38:ARG:O	4:P:40:GLY:HA2	2.12	0.49
4:P:129:GLU:HG3	4:P:201:TRP:CZ2	2.48	0.49
4:L:36:ARG:HD2	4:L:90:TYR:HA	1.94	0.49
4:L:150:PHE:HD1	4:L:150:PHE:C	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:HB2	1:A:97:ARG:HB3	1.95	0.49
2:H:54:LEU:HA	2:H:64:LEU:HD21	1.93	0.49
4:L:11:LYS:O	4:L:111:LEU:HA	2.13	0.49
1:M:49:ALA:HB3	1:M:52:ILE:HG22	1.94	0.49
1:M:73:THR:HG22	5:T:8:THR:HG21	1.95	0.49
4:J:113:VAL:O	4:J:114:LEU:CB	2.60	0.49
1:G:142:THR:OG1	6:G:302:HOH:O	2.20	0.49
3:K:133:CYS:SG	3:K:183:CYS:N	2.86	0.49
3:K:159:VAL:N	4:L:171:CYS:SG	2.85	0.49
1:M:21:ARG:NH2	1:M:37:ASP:OD2	2.38	0.49
1:A:219:ARG:HD2	1:A:257:TYR:CZ	2.47	0.49
4:J:49:PHE:CE1	4:J:54:ALA:HB2	2.47	0.49
4:J:154:HIS:N	4:J:154:HIS:CD2	2.80	0.49
4:F:218:SER:HG	4:F:221:ASP:CB	2.22	0.49
4:J:153:ASP:OD2	4:J:176:PRO:HG3	2.12	0.48
1:G:98:MET:HE3	1:G:99:TYR:CA	2.40	0.48
3:K:2:LEU:CB	3:K:3:ASN:HA	2.39	0.48
3:K:175:TRP:CZ2	4:L:146:LEU:CB	2.95	0.48
4:L:125:VAL:HG22	4:L:235:VAL:HG12	1.95	0.48
1:M:37:ASP:OD1	1:M:38:SER:N	2.46	0.48
2:N:3:ARG:O	2:N:30:PHE:HA	2.13	0.48
4:P:196:VAL:CG2	4:P:197:SER:H	2.06	0.48
4:F:35:TYR:CD1	4:F:43:LEU:HD21	2.48	0.48
4:F:217:LEU:CD1	4:F:218:SER:N	2.72	0.48
2:H:7:ILE:HG23	2:H:93:VAL:HG21	1.95	0.48
3:K:63:SER:O	3:K:75:LEU:HA	2.12	0.48
1:M:197:HIS:ND1	1:M:197:HIS:N	2.60	0.48
2:D:89:GLN:HG3	2:D:90:PRO:N	2.28	0.48
3:E:31:TYR:C	3:E:31:TYR:CD2	2.86	0.48
3:I:7:SER:HB2	3:I:8:PRO:HD3	1.96	0.48
3:I:134:LEU:HB3	3:I:173:VAL:HA	1.94	0.48
3:K:48:PHE:HE2	3:K:63:SER:HA	1.77	0.48
4:L:141:ALA:H	4:L:198:ALA:H	1.61	0.48
1:M:259:CYS:HB3	1:M:272:LEU:CB	2.43	0.48
1:M:270:LEU:HD13	1:M:272:LEU:HD21	1.95	0.48
1:C:102:ASP:OD2	1:C:113:TYR:OH	2.29	0.48
2:N:12:ARG:O	2:N:13:HIS:CE1	2.67	0.48
1:G:35:ARG:NH2	1:G:48:ARG:CD	2.76	0.48
1:G:192:HIS:CB	1:G:202:ARG:HH22	2.23	0.48
2:H:24:ASN:ND2	2:H:65:LEU:CD2	2.76	0.48
4:L:62:SER:CA	4:L:65:PHE:CD2	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:73:THR:HG22	5:T:8:THR:CG2	2.43	0.48
1:M:203:CYS:HB2	1:M:217:TRP:NE1	2.28	0.48
1:M:225:THR:OG1	1:M:226:GLN:N	2.47	0.48
1:C:24:ALA:HB3	1:C:36:PHE:HB3	1.96	0.48
1:C:145:HIS:HD2	6:C:305:HOH:O	1.95	0.48
3:E:178:LYS:HG2	3:E:179:SER:OG	2.13	0.48
2:B:10:TYR:HE2	2:B:26:TYR:HB3	1.79	0.48
2:B:37:VAL:HG21	2:B:66:TYR:CD1	2.49	0.48
3:K:136:THR:HG21	3:K:171:SER:HB3	1.95	0.48
4:L:88:ALA:CB	4:L:110:ARG:HA	2.42	0.48
2:N:54:LEU:HD23	2:N:54:LEU:C	2.34	0.48
2:N:63:TYR:CD1	2:N:63:TYR:C	2.87	0.48
4:P:14:GLU:OE2	4:P:117:LEU:HD11	2.13	0.48
4:F:160:TRP:H	4:F:209:ARG:HG3	1.78	0.48
1:A:70:HIS:HD2	5:Q:6:VAL:HG22	1.77	0.48
3:I:152:VAL:HA	3:I:176:SER:OG	2.13	0.48
2:H:70:PHE:HZ	2:H:78:TYR:CD2	2.31	0.48
3:O:120:TYR:HB3	4:P:131:SER:OG	2.14	0.48
3:O:123:ARG:HB2	3:O:131:SER:HB3	1.95	0.48
3:E:87:THR:HA	3:E:105:SER:HA	1.96	0.48
1:A:59:TYR:OH	1:A:171:TYR:OH	2.16	0.48
1:A:225:THR:OG1	1:A:226:GLN:HB2	2.14	0.48
3:I:121:GLN:HG3	4:J:131:SER:HA	1.95	0.48
1:G:163:THR:HA	1:G:166:GLU:HG2	1.95	0.48
3:K:138:PHE:H	3:K:138:PHE:HD2	1.61	0.48
1:M:102:ASP:HB2	1:M:111:ARG:HG2	1.95	0.48
3:O:79:GLY:C	3:O:81:GLN:OE1	2.51	0.48
4:J:45:PHE:HZ	4:J:48:TYR:HB3	1.78	0.48
1:G:10:THR:HG22	2:H:56:PHE:CE2	2.48	0.48
4:L:82:THR:CG2	4:L:83:GLN:N	2.77	0.48
4:L:130:PRO:HD2	4:L:201:TRP:CZ2	2.49	0.48
2:N:30:PHE:CE1	2:N:35:ILE:HD11	2.48	0.48
4:P:160:TRP:HH2	4:P:234:ILE:HD11	1.78	0.48
1:C:22:PHE:H	1:C:38:SER:HB3	1.78	0.48
3:E:84:ASP:CA	3:E:85:SER:CB	2.91	0.48
4:F:123:PRO:HA	4:F:149:GLY:CA	2.44	0.48
4:F:201:TRP:O	4:F:204:PRO:CG	2.62	0.48
1:A:177:GLU:CG	1:A:178:THR:N	2.77	0.48
3:K:118:ALA:HB2	3:K:197:PHE:HB3	1.96	0.48
3:O:131:SER:OG	3:O:181:PHE:HE2	1.97	0.48
2:D:74:GLU:OE1	2:D:74:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:33:TYR:O	4:F:92:CYS:HA	2.14	0.48
4:F:130:PRO:HB3	4:F:142:THR:O	2.14	0.48
3:I:33:LEU:O	3:I:50:MET:N	2.41	0.47
4:L:150:PHE:HE1	4:L:188:TYR:C	2.15	0.47
4:L:161:VAL:HG12	4:L:162:ASN:H	1.78	0.47
1:C:103:VAL:HG12	1:C:109:PHE:HA	1.96	0.47
4:J:14:GLU:HA	4:J:114:LEU:O	2.14	0.47
1:G:234:ARG:CG	1:G:242:GLN:HB2	2.43	0.47
2:H:3:ARG:HH21	2:H:61:SER:HB2	1.78	0.47
3:K:124:ASP:CA	4:L:128:PHE:HA	2.45	0.47
4:L:150:PHE:CZ	4:L:155:VAL:HG11	2.49	0.47
1:M:11:SER:HA	1:M:21:ARG:O	2.14	0.47
1:M:217:TRP:HZ3	1:M:247:VAL:HG22	1.79	0.47
1:C:159:TYR:HD1	1:C:163:THR:HB	1.78	0.47
2:B:49:VAL:HG12	2:B:50:GLU:O	2.15	0.47
1:G:98:MET:SD	1:G:99:TYR:N	2.87	0.47
3:O:155:THR:CG2	4:P:173:ASP:OD2	2.60	0.47
4:P:173:ASP:N	4:P:173:ASP:OD1	2.47	0.47
1:C:66:LYS:HE3	5:R:2:LEU:HB2	1.95	0.47
4:F:60:LEU:HD22	4:F:65:PHE:HB3	1.94	0.47
4:F:201:TRP:O	4:F:204:PRO:HG3	2.14	0.47
1:A:66:LYS:HE2	3:I:29:ASN:OD1	2.14	0.47
1:G:66:LYS:NZ	5:U:2:LEU:O	2.45	0.47
4:L:103:GLN:OE1	4:L:103:GLN:N	2.48	0.47
4:L:131:SER:HB2	4:L:135:ILE:HG21	1.96	0.47
1:C:27:TYR:CD2	1:C:32:GLN:HB2	2.49	0.47
1:A:202:ARG:HG3	1:A:244:TRP:NE1	2.26	0.47
1:G:68:LYS:O	1:G:72:GLN:HG2	2.15	0.47
1:M:14:ARG:HH21	1:M:21:ARG:HB2	1.78	0.47
2:D:55:SER:O	2:D:63:TYR:N	2.46	0.47
4:F:84:GLN:CG	4:F:85:GLU:H	2.27	0.47
2:B:40:LEU:HD23	2:B:43:GLY:HA2	1.96	0.47
4:J:191:SER:OG	4:J:191:SER:O	2.33	0.47
3:K:135:PHE:HZ	3:K:192:ILE:HG12	1.67	0.47
4:L:140:LYS:HA	4:L:197:SER:HA	1.95	0.47
1:M:203:CYS:HB2	1:M:217:TRP:CZ2	2.50	0.47
1:M:213:ILE:HD11	1:M:261:VAL:CG1	2.44	0.47
1:C:155:GLN:HG2	3:E:51:THR:HG21	1.96	0.47
1:A:49:ALA:O	1:A:52:ILE:HG22	2.15	0.47
3:I:61:ARG:NH1	3:I:84:ASP:OD2	2.48	0.47
3:I:89:LEU:HD22	3:I:100:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:86:ASP:N	4:J:86:ASP:OD1	2.48	0.47
4:J:223:TRP:NE1	4:J:228:ALA:O	2.47	0.47
1:G:42:SER:HB3	1:G:44:ARG:HG3	1.97	0.47
1:G:98:MET:SD	1:G:98:MET:C	2.93	0.47
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.50	0.47
1:G:218:GLN:HB2	1:G:222:GLU:C	2.35	0.47
4:L:36:ARG:HB2	4:L:44:GLU:OE2	2.15	0.47
3:O:118:ALA:CB	3:O:120:TYR:CZ	2.98	0.47
3:O:153:TYR:HB3	4:P:177:LEU:HD21	1.97	0.47
4:P:118:LYS:O	4:P:120:VAL:N	2.48	0.47
4:P:154:HIS:ND1	4:P:154:HIS:N	2.60	0.47
4:P:172:THR:HG22	4:P:173:ASP:H	1.80	0.47
1:C:9:PHE:HE2	1:C:99:TYR:CE2	2.33	0.47
3:E:138:PHE:CE1	3:E:170:ASN:O	2.68	0.47
4:J:175:GLN:HG3	4:J:176:PRO:HD2	1.96	0.47
3:K:115:PRO:HG3	3:K:139:ASP:OD2	2.14	0.47
4:L:224:THR:OG1	4:L:225:GLN:N	2.48	0.47
3:O:137:ASP:HB3	3:O:169:SER:HA	1.97	0.47
3:O:168:LYS:HB3	3:O:168:LYS:HE2	1.67	0.47
4:P:84:GLN:HA	4:P:113:VAL:HG13	1.96	0.47
4:P:190:LEU:HD12	4:P:191:SER:H	1.80	0.47
4:P:223:TRP:CZ2	4:P:225:GLN:CG	2.97	0.47
4:F:83:GLN:CA	4:F:113:VAL:HG21	2.45	0.47
1:A:35:ARG:HD3	1:A:48:ARG:NE	2.14	0.47
3:I:42:LYS:HG2	3:I:43:SER:N	2.30	0.47
4:J:123:PRO:CA	4:J:150:PHE:HB3	2.45	0.47
3:K:33:LEU:HD23	3:K:91:ALA:O	2.15	0.47
3:O:112:ILE:HG22	3:O:114:ASN:H	1.80	0.47
1:C:22:PHE:H	1:C:38:SER:CB	2.27	0.47
1:C:172:LEU:HD23	1:C:179:LEU:HD13	1.97	0.47
1:C:231:VAL:CG1	1:C:244:TRP:HE3	2.17	0.47
4:F:155:VAL:HG12	4:F:214:PHE:CD1	2.50	0.47
4:F:201:TRP:HA	4:F:204:PRO:HG3	1.96	0.47
1:G:125:ALA:C	1:G:134:THR:HG22	2.34	0.47
3:K:137:ASP:N	3:K:137:ASP:OD1	2.47	0.47
3:K:175:TRP:NE1	4:L:146:LEU:HD22	2.12	0.47
4:P:33:TYR:OH	4:P:95:SER:OG	2.13	0.47
3:E:13:VAL:O	3:E:108:VAL:HA	2.15	0.47
2:B:26:TYR:CE2	2:B:28:SER:HB2	2.51	0.46
1:G:187:THR:HB	1:G:272:LEU:CD2	2.32	0.46
3:E:84:ASP:HB3	3:E:85:SER:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:138:PHE:O	3:E:139:ASP:O	2.33	0.46
1:G:159:TYR:CE1	1:G:163:THR:OG1	2.68	0.46
1:G:163:THR:HA	1:G:166:GLU:CG	2.45	0.46
4:L:150:PHE:CE2	4:L:155:VAL:HG11	2.50	0.46
2:N:22:PHE:HD2	2:N:67:TYR:HB2	1.80	0.46
1:C:147:TRP:N	1:C:147:TRP:CD1	2.83	0.46
4:F:56:ASP:OD1	4:F:57:LYS:N	2.48	0.46
2:H:7:ILE:HD11	2:H:25:CYS:SG	2.56	0.46
3:K:38:TRP:CZ3	3:K:44:PRO:HG3	2.38	0.46
3:K:151:ASP:OD2	3:K:181:PHE:HB3	2.15	0.46
4:L:89:VAL:HG11	4:L:110:ARG:HB2	1.91	0.46
4:P:196:VAL:CG2	4:P:197:SER:N	2.73	0.46
3:E:114:ASN:HA	3:E:115:PRO:HD2	1.57	0.46
4:F:15:LYS:NZ	4:F:83:GLN:HE21	2.14	0.46
4:F:36:ARG:HE	4:F:38:ARG:NH1	2.13	0.46
2:H:3:ARG:NH2	2:H:59:ASP:O	2.43	0.46
1:M:266:LEU:HD12	1:M:266:LEU:N	2.31	0.46
1:C:243:LYS:CG	1:C:244:TRP:H	2.28	0.46
4:J:11:LYS:HZ1	4:J:217:LEU:CD2	2.29	0.46
3:O:7:SER:HB3	3:O:22:THR:HB	1.98	0.46
1:C:136:ALA:O	1:C:137:ASP:HB3	2.16	0.46
1:A:93:HIS:CG	1:A:119:ASP:OD1	2.68	0.46
4:J:217:LEU:CD1	4:J:221:ASP:HB3	2.41	0.46
1:G:97:ARG:HH12	5:U:6:VAL:HG12	1.74	0.46
1:G:234:ARG:HB3	2:H:8:GLN:NE2	2.31	0.46
4:L:159:TRP:CE3	4:L:170:VAL:HG13	2.50	0.46
1:M:188:HIS:CD2	1:M:204:TRP:HE3	2.33	0.46
3:O:53:ASN:CA	3:O:68:THR:HG23	2.46	0.46
4:P:24:ASP:HA	4:P:25:PRO:HD2	1.76	0.46
2:D:96:ASP:HB3	2:D:99:MET:HB3	1.97	0.46
1:A:84:TYR:OH	1:A:146:LYS:NZ	2.26	0.46
3:I:15:GLU:OE1	3:I:110:PRO:HA	2.15	0.46
1:M:187:THR:HB	1:M:272:LEU:HD11	1.98	0.46
4:P:130:PRO:HD2	4:P:201:TRP:CZ2	2.51	0.46
1:C:33:PHE:O	1:C:52:ILE:HG21	2.15	0.46
4:F:176:PRO:HB2	4:F:188:TYR:HB3	1.97	0.46
1:A:106:ASP:N	1:A:106:ASP:OD1	2.48	0.46
4:J:202:GLN:O	4:J:205:ARG:N	2.49	0.46
1:G:97:ARG:CD	1:G:116:TYR:CE1	2.98	0.46
1:G:154:GLU:O	1:G:157:ARG:HG2	2.16	0.46
1:M:129:ASP:OD1	1:M:129:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ASP:N	1:C:106:ASP:OD1	2.47	0.46
1:C:189:MET:HG3	1:C:202:ARG:O	2.16	0.46
4:F:165:GLU:C	4:F:166:VAL:HG23	2.36	0.46
1:A:217:TRP:CD1	1:A:247:VAL:HG11	2.51	0.46
2:B:3:ARG:NH1	2:B:59:ASP:O	2.29	0.46
3:I:137:ASP:CG	3:I:138:PHE:H	2.19	0.46
3:I:159:VAL:HA	3:I:169:SER:O	2.15	0.46
1:M:78:LEU:CD2	1:M:95:VAL:CG2	2.74	0.46
1:M:135:ALA:HB1	1:M:140:ALA:HB1	1.97	0.46
1:M:198:GLU:HB3	1:M:249:VAL:O	2.16	0.46
4:F:202:GLN:C	4:F:204:PRO:HD3	2.36	0.46
1:G:99:TYR:CE2	5:U:3:VAL:HG12	2.51	0.46
3:K:81:GLN:O	3:K:108:VAL:HG21	2.16	0.46
3:E:11:LEU:HD13	3:E:19:THR:HG21	1.97	0.46
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.97	0.45
4:J:84:GLN:O	4:J:87:SER:OG	2.33	0.45
2:H:21:ASN:OD1	2:H:22:PHE:O	2.34	0.45
2:H:70:PHE:CE1	2:H:78:TYR:CG	3.04	0.45
3:K:158:CYS:SG	4:L:172:THR:N	2.84	0.45
1:M:14:ARG:HB3	1:M:17:ARG:HB2	1.98	0.45
1:M:96:GLN:HE22	2:N:31:HIS:HE1	1.62	0.45
3:O:50:MET:HB3	3:O:66:LEU:HD22	1.98	0.45
4:P:14:GLU:OE2	4:P:117:LEU:CD1	2.63	0.45
1:C:35:ARG:HD3	1:C:48:ARG:HD3	1.98	0.45
4:F:180:GLN:CA	4:F:186:SER:OG	2.63	0.45
4:F:195:ARG:CG	4:F:195:ARG:NH1	2.73	0.45
4:J:180:GLN:HA	4:J:181:PRO:HA	1.72	0.45
1:G:6:ARG:CB	1:G:8:PHE:HE2	2.27	0.45
1:G:98:MET:HE3	1:G:113:TYR:HD1	1.73	0.45
2:H:7:ILE:HD12	2:H:82:VAL:HG11	1.97	0.45
2:H:40:LEU:HD12	2:H:79:ALA:HB3	1.98	0.45
2:N:59:ASP:O	2:N:60:TRP:HB2	2.17	0.45
4:P:38:ARG:HG2	4:P:38:ARG:HH11	1.81	0.45
3:E:154:ILE:HG22	3:E:155:THR:N	2.31	0.45
3:I:21:PHE:CE2	3:I:77:ILE:HD11	2.51	0.45
3:I:138:PHE:CD1	3:I:138:PHE:O	2.70	0.45
1:G:59:TYR:O	1:G:63:GLU:HG2	2.17	0.45
3:K:124:ASP:H	3:K:131:SER:CB	2.29	0.45
3:E:82:PRO:HG3	3:E:110:PRO:HB3	1.98	0.45
3:E:157:LYS:HE2	3:E:170:ASN:OD1	2.16	0.45
4:J:151:TYR:HB2	4:J:187:ARG:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:ALA:O	1:G:73:THR:OG1	2.26	0.45
3:K:31:TYR:CD1	5:U:4:PRO:HB2	2.42	0.45
3:K:190:SER:O	3:K:190:SER:OG	2.34	0.45
1:M:97:ARG:NH2	1:M:147:TRP:HH2	2.13	0.45
3:O:112:ILE:HB	3:O:115:PRO:HG3	1.98	0.45
4:F:202:GLN:C	4:F:204:PRO:CD	2.85	0.45
1:A:9:PHE:HZ	5:Q:2:LEU:HD23	1.82	0.45
1:A:22:PHE:H	1:A:38:SER:CB	2.29	0.45
1:A:98:MET:C	1:A:98:MET:CE	2.85	0.45
2:B:89:GLN:HB2	2:B:90:PRO:CD	2.44	0.45
1:G:102:ASP:HB2	1:G:111:ARG:CG	2.47	0.45
1:M:220:ASP:HB3	1:M:221:GLY:H	1.64	0.45
4:P:160:TRP:HA	4:P:165:GLU:CB	2.46	0.45
1:C:67:VAL:HA	1:C:70:HIS:HD2	1.82	0.45
1:G:124:ILE:HG12	1:G:135:ALA:HA	1.99	0.45
4:L:46:LEU:C	4:L:47:ILE:CG2	2.85	0.45
2:N:2:GLN:HE21	2:N:85:VAL:CB	2.27	0.45
3:O:102:THR:HA	3:O:103:GLY:HA3	1.74	0.45
4:F:138:THR:O	4:F:139:GLN:HB2	2.16	0.45
3:I:53:ASN:HA	3:I:54:GLY:HA2	1.57	0.45
2:H:7:ILE:HB	2:H:27:VAL:HG12	1.99	0.45
1:C:99:TYR:CZ	5:R:3:VAL:HG12	2.52	0.45
2:B:3:ARG:NH1	2:B:60:TRP:O	2.50	0.45
1:G:179:LEU:N	1:G:179:LEU:HD12	2.31	0.45
1:G:235:PRO:HA	1:G:241:PHE:HA	1.98	0.45
4:P:159:TRP:HD1	4:P:209:ARG:O	1.99	0.45
3:E:84:ASP:HA	3:E:85:SER:CB	2.47	0.45
4:J:29:HIS:HD2	4:J:94:SER:C	2.13	0.45
4:J:194:LEU:HD23	4:J:195:ARG:C	2.37	0.45
1:G:81:LEU:HG	5:U:9:VAL:CG1	2.47	0.45
1:G:179:LEU:N	1:G:179:LEU:CD1	2.80	0.45
3:K:38:TRP:CE3	3:K:42:LYS:O	2.69	0.45
3:K:136:THR:CG2	3:K:171:SER:CA	2.83	0.45
4:L:169:GLY:C	4:L:194:LEU:HD22	2.37	0.45
2:N:5:PRO:HD3	2:N:84:HIS:CD2	2.51	0.45
2:D:13:HIS:HB2	2:D:21:ASN:OD1	2.17	0.45
1:A:103:VAL:HG12	1:A:108:ARG:O	2.17	0.45
3:I:48:PHE:CE1	3:I:59:LYS:HG3	2.41	0.45
4:J:120:VAL:O	4:J:121:PHE:CG	2.70	0.45
1:G:81:LEU:CG	5:U:9:VAL:HG11	2.46	0.45
1:G:234:ARG:NH2	1:G:244:TRP:HE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:72:TYR:CD1	3:K:72:TYR:O	2.70	0.45
3:O:161:ASP:O	3:O:162:MET:HB3	2.16	0.45
1:C:8:PHE:HB2	1:C:25:VAL:HG13	1.99	0.45
2:D:70:PHE:CE1	2:D:72:PRO:HB3	2.52	0.45
1:A:259:CYS:HB3	1:A:272:LEU:HB2	2.00	0.44
2:B:46:ILE:HG13	2:B:47:GLU:N	2.31	0.44
3:I:138:PHE:HD1	3:I:142:THR:OG1	1.95	0.44
4:J:84:GLN:CD	1:G:177:GLU:OE1	2.56	0.44
1:G:185:PRO:CA	1:G:208:PHE:HB3	2.46	0.44
1:G:188:HIS:HB3	1:G:204:TRP:CB	2.41	0.44
4:L:70:THR:N	4:L:75:SER:OG	2.44	0.44
4:L:154:HIS:CD2	4:L:215:TYR:CB	3.01	0.44
2:N:2:GLN:HE21	2:N:85:VAL:CG2	2.30	0.44
2:N:39:LEU:HD23	2:N:39:LEU:HA	1.80	0.44
2:N:75:LYS:O	2:N:76:ASP:C	2.54	0.44
4:P:97:THR:HG22	4:P:98:GLN:N	2.32	0.44
4:F:26:ILE:HB	4:F:29:HIS:CD2	2.52	0.44
1:A:223:ASP:O	1:A:225:THR:HG22	2.16	0.44
4:J:48:TYR:CD1	4:J:99:LEU:HD11	2.52	0.44
2:H:3:ARG:NH2	2:H:61:SER:HB2	2.32	0.44
2:H:72:PRO:HB2	2:H:78:TYR:HH	1.81	0.44
3:K:175:TRP:CZ2	4:L:146:LEU:HB2	2.52	0.44
4:L:83:GLN:CG	4:L:84:GLN:N	2.54	0.44
3:O:1:ILE:HG13	3:O:1:ILE:O	2.17	0.44
1:C:66:LYS:CD	5:R:4:PRO:HA	2.42	0.44
4:F:29:HIS:CE1	4:F:96:GLN:HG2	2.52	0.44
3:I:146:GLN:OE1	3:I:154:ILE:HG12	2.14	0.44
4:J:119:ASN:N	4:J:119:ASN:OD1	2.50	0.44
4:J:177:LEU:C	4:J:177:LEU:CD1	2.86	0.44
1:G:82:ARG:NH2	1:G:89:GLU:N	2.46	0.44
1:G:157:ARG:HG3	1:G:158:ALA:N	2.31	0.44
3:K:47:LEU:O	3:K:48:PHE:CD1	2.70	0.44
4:L:130:PRO:HB3	4:L:142:THR:O	2.16	0.44
1:M:66:LYS:HZ1	3:O:29:ASN:ND2	2.14	0.44
2:N:22:PHE:CE1	4:F:80:GLN:NE2	2.85	0.44
4:P:211:GLN:HE22	4:P:213:GLN:HB2	1.83	0.44
4:F:41:GLN:O	4:F:42:GLY:C	2.55	0.44
1:A:274:TRP:CE3	1:A:275:GLU:HB2	2.53	0.44
2:H:24:ASN:ND2	2:H:65:LEU:CG	2.77	0.44
4:L:10:ASN:HB3	4:L:110:ARG:O	2.17	0.44
2:N:51:HIS:HB3	2:N:66:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:58:SER:HA	4:P:59:GLY:HA2	1.42	0.44
5:T:3:VAL:O	5:T:4:PRO:C	2.55	0.44
3:I:115:PRO:HA	3:I:137:ASP:CG	2.38	0.44
1:G:156:LEU:HA	1:G:156:LEU:HD23	1.77	0.44
1:G:204:TRP:CE3	1:G:244:TRP:HB3	2.51	0.44
2:H:9:VAL:CG2	2:H:80:CYS:HB2	2.47	0.44
4:L:171:CYS:HB2	4:L:193:ARG:O	2.17	0.44
1:M:189:MET:SD	1:M:274:TRP:CZ3	3.10	0.44
3:E:49:VAL:HG23	4:F:102:THR:HG22	1.97	0.44
3:E:102:THR:O	3:E:102:THR:OG1	2.34	0.44
1:A:49:ALA:HA	1:A:50:PRO:HD2	1.77	0.44
1:A:98:MET:HE2	1:A:98:MET:HB3	1.49	0.44
3:I:66:LEU:HD12	3:I:67:ASN:N	2.32	0.44
4:J:125:VAL:O	4:J:237:ALA:HB2	2.17	0.44
1:G:116:TYR:CD2	1:G:116:TYR:C	2.85	0.44
3:K:113:GLN:O	3:K:114:ASN:C	2.53	0.44
3:K:135:PHE:CZ	3:K:192:ILE:HD13	2.51	0.44
3:K:192:ILE:O	3:K:193:PRO:C	2.56	0.44
2:B:86:THR:O	2:B:87:LEU:HD23	2.18	0.44
3:I:137:ASP:O	3:I:138:PHE:CD2	2.70	0.44
4:L:37:GLN:HG2	4:L:89:VAL:H	1.82	0.44
1:M:195:SER:O	1:M:197:HIS:CE1	2.70	0.44
1:M:231:VAL:HG13	1:M:244:TRP:HE3	1.83	0.44
4:F:230:PRO:C	4:F:231:VAL:HG23	2.37	0.44
1:A:47:PRO:HB3	1:A:60:TRP:CH2	2.53	0.44
4:J:39:LEU:HA	4:J:40:GLY:HA2	1.68	0.44
4:J:196:VAL:HG12	4:J:197:SER:N	2.33	0.44
3:O:31:TYR:HB2	5:T:4:PRO:HB2	2.00	0.44
4:P:45:PHE:HZ	4:P:48:TYR:HB3	1.83	0.44
1:C:37:ASP:HB3	1:C:40:ALA:HB2	2.00	0.44
3:E:160:LEU:HD23	4:F:169:GLY:O	2.18	0.44
4:F:172:THR:HG22	4:F:192:SER:HB2	2.00	0.44
4:J:120:VAL:C	4:J:121:PHE:CG	2.91	0.43
1:G:16:GLY:CA	1:G:17:ARG:CB	2.77	0.43
1:G:133:TRP:HZ3	1:G:147:TRP:HZ3	1.65	0.43
1:G:189:MET:HE3	1:G:274:TRP:N	2.33	0.43
3:K:21:PHE:O	3:K:74:TYR:HA	2.17	0.43
3:K:136:THR:O	3:K:137:ASP:HB2	2.18	0.43
4:P:14:GLU:HG2	4:P:117:LEU:CD1	2.45	0.43
1:C:25:VAL:CG2	1:C:32:GLN:HE21	2.31	0.43
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:220:ASN:N	4:F:220:ASN:OD1	2.51	0.43
1:A:247:VAL:HG23	1:A:249:VAL:HG23	1.99	0.43
4:J:11:LYS:HZ1	4:J:217:LEU:HD22	1.83	0.43
4:J:49:PHE:CE2	4:J:69:ARG:HB2	2.53	0.43
4:J:84:GLN:O	4:J:113:VAL:HG11	2.18	0.43
3:K:131:SER:HA	4:L:128:PHE:HE1	1.83	0.43
3:K:160:LEU:O	3:K:168:LYS:HB3	2.18	0.43
4:L:130:PRO:HG2	4:L:201:TRP:NE1	2.32	0.43
1:M:59:TYR:O	1:M:63:GLU:HG2	2.18	0.43
3:E:124:ASP:CG	3:E:125:SER:HA	2.37	0.43
4:F:135:ILE:HD13	4:F:201:TRP:HZ3	1.83	0.43
4:J:120:VAL:O	4:J:121:PHE:CD1	2.70	0.43
1:G:127:LYS:HD2	1:G:127:LYS:HA	1.66	0.43
1:G:228:THR:HG23	1:G:228:THR:O	2.18	0.43
2:N:63:TYR:CD1	2:N:63:TYR:O	2.70	0.43
2:N:81:ARG:CD	2:N:92:ILE:CG1	2.96	0.43
3:O:123:ARG:O	4:P:129:GLU:HB3	2.19	0.43
3:O:176:SER:CB	3:O:181:PHE:O	2.66	0.43
2:D:40:LEU:HD13	2:D:81:ARG:H	1.83	0.43
4:F:33:TYR:OH	4:F:99:LEU:HA	2.19	0.43
1:A:73:THR:HB	5:Q:8:THR:HG22	2.01	0.43
4:J:131:SER:O	4:J:135:ILE:HG23	2.19	0.43
1:G:191:HIS:ND1	1:G:191:HIS:C	2.72	0.43
3:K:63:SER:O	3:K:75:LEU:HD12	2.19	0.43
4:L:39:LEU:HA	4:L:39:LEU:HD12	1.76	0.43
4:L:160:TRP:C	4:L:161:VAL:CG2	2.85	0.43
1:M:162:GLY:O	1:M:166:GLU:HG3	2.17	0.43
1:M:177:GLU:N	1:M:177:GLU:OE1	2.51	0.43
4:P:64:ARG:HH11	4:P:64:ARG:HG2	1.80	0.43
1:C:188:HIS:O	1:C:204:TRP:N	2.42	0.43
3:E:53:ASN:HA	3:E:54:GLY:HA2	1.63	0.43
4:F:149:GLY:CA	4:F:150:PHE:HB3	2.35	0.43
1:A:124:ILE:HG13	1:A:134:THR:O	2.19	0.43
4:J:223:TRP:CE2	4:J:228:ALA:O	2.72	0.43
3:O:131:SER:OG	3:O:181:PHE:CE2	2.72	0.43
4:P:223:TRP:CE2	4:P:225:GLN:HG2	2.52	0.43
4:F:218:SER:CB	4:F:221:ASP:HB2	2.44	0.43
2:H:23:LEU:HD13	2:H:70:PHE:CE1	2.53	0.43
3:K:11:LEU:O	3:K:12:HIS:ND1	2.51	0.43
4:L:34:TRP:CZ3	4:L:92:CYS:HB2	2.54	0.43
4:L:120:VAL:O	4:L:230:PRO:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:231:VAL:HG22	1:M:244:TRP:H	1.84	0.43
3:O:123:ARG:HG3	3:O:130:LYS:O	2.18	0.43
4:P:11:LYS:HG3	4:P:12:VAL:N	2.33	0.43
4:P:160:TRP:CH2	4:P:234:ILE:HD11	2.53	0.43
3:I:20:ASN:HA	3:I:75:LEU:O	2.19	0.43
4:J:164:LYS:HE2	4:J:164:LYS:HB2	1.87	0.43
1:G:58:GLU:HA	1:G:61:ASP:HB2	2.00	0.43
1:G:214:THR:O	1:G:214:THR:CG2	2.60	0.43
3:K:21:PHE:HZ	3:K:106:LEU:HD22	1.84	0.43
3:K:29:ASN:O	3:K:94:THR:OG1	2.21	0.43
4:L:88:ALA:CB	4:L:110:ARG:HG2	2.39	0.43
1:C:160:LEU:O	1:C:165:VAL:HG23	2.18	0.43
3:E:157:LYS:HE2	3:E:157:LYS:HB3	1.75	0.43
3:E:163:ARG:HD3	3:E:163:ARG:HA	1.63	0.43
4:F:22:ARG:HG2	4:F:76:THR:HG22	2.01	0.43
1:A:66:LYS:CD	5:Q:4:PRO:HA	2.48	0.43
1:A:237:GLY:C	1:A:239:GLY:H	2.22	0.43
4:J:84:GLN:OE1	1:G:177:GLU:OE1	2.37	0.43
1:G:17:ARG:HH11	1:G:17:ARG:CG	2.14	0.43
1:G:97:ARG:HE	1:G:116:TYR:HE1	0.61	0.43
3:K:47:LEU:HA	3:K:47:LEU:HD12	1.77	0.43
1:M:92:SER:O	1:M:92:SER:OG	2.25	0.43
2:N:89:GLN:O	2:N:90:PRO:C	2.56	0.43
3:E:37:ARG:HB2	3:E:47:LEU:HD11	2.01	0.43
3:I:2:LEU:HD23	3:I:3:ASN:N	2.33	0.43
3:I:25:PHE:HB2	3:I:26:PRO:HD2	2.01	0.43
3:I:34:HIS:ND1	3:I:93:ILE:HD11	2.34	0.43
1:G:97:ARG:NH1	5:U:7:ALA:O	2.46	0.43
4:L:159:TRP:CE2	4:L:194:LEU:HG	2.54	0.43
1:M:53:GLU:HA	1:M:60:TRP:HZ2	1.84	0.43
3:O:34:HIS:NE2	3:O:93:ILE:HD11	2.33	0.43
2:D:82:VAL:O	2:D:90:PRO:CB	2.65	0.43
4:F:153:ASP:CG	4:F:176:PRO:HG3	2.39	0.43
4:F:194:LEU:HD12	4:F:194:LEU:HA	1.81	0.43
1:A:172:LEU:HD23	1:A:179:LEU:HD13	2.01	0.43
1:A:231:VAL:O	1:A:232:GLU:C	2.57	0.43
3:K:4:VAL:HG11	3:K:92:PHE:HB3	2.00	0.43
4:L:82:THR:HG21	4:L:113:VAL:HG22	2.00	0.43
1:M:256:ARG:HB3	6:M:301:HOH:O	2.19	0.43
3:O:53:ASN:HA	3:O:54:GLY:HA2	1.66	0.43
4:F:32:LEU:O	4:F:49:PHE:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:193:ARG:CG	4:F:193:ARG:NH1	2.72	0.43
1:A:228:THR:HA	1:A:247:VAL:HG12	2.01	0.42
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.99	0.42
4:J:211:GLN:HA	4:J:236:SER:HB3	2.00	0.42
4:J:217:LEU:O	4:J:231:VAL:HG12	2.19	0.42
3:K:122:LEU:HG	4:L:130:PRO:HA	2.00	0.42
3:K:134:LEU:CD2	4:L:142:THR:HG21	2.49	0.42
1:M:59:TYR:HH	1:M:171:TYR:HH	1.36	0.42
1:M:78:LEU:HB3	1:M:82:ARG:NH2	2.33	0.42
1:M:233:THR:HG22	1:M:243:LYS:HD3	2.00	0.42
3:O:63:SER:O	3:O:75:LEU:HD12	2.19	0.42
3:O:111:ASN:OD1	3:O:112:ILE:N	2.43	0.42
1:C:154:GLU:HB3	3:E:52:LEU:HD11	2.01	0.42
1:A:46:GLU:HG3	1:A:47:PRO:HD2	2.00	0.42
1:A:77:ASP:OD1	5:Q:9:VAL:HG22	2.18	0.42
3:K:111:ASN:OD1	3:K:112:ILE:N	2.52	0.42
4:L:88:ALA:HB1	4:L:89:VAL:CG1	2.49	0.42
4:P:6:GLN:OE1	4:P:108:GLY:N	2.52	0.42
1:A:69:ALA:HB1	3:I:96:ASN:ND2	2.34	0.42
4:J:58:SER:O	4:J:58:SER:OG	2.32	0.42
4:J:231:VAL:O	4:J:232:THR:C	2.57	0.42
1:G:49:ALA:HB1	1:G:51:TRP:NE1	2.35	0.42
1:G:162:GLY:O	1:G:166:GLU:CD	2.58	0.42
1:G:162:GLY:C	1:G:166:GLU:OE2	2.58	0.42
1:G:218:GLN:CB	1:G:222:GLU:O	2.62	0.42
3:K:96:ASN:ND2	4:L:48:TYR:OH	2.52	0.42
4:L:175:GLN:H	4:L:175:GLN:HG2	1.59	0.42
1:C:31:THR:HG23	1:C:209:TYR:CE1	2.54	0.42
1:C:63:GLU:OE2	1:C:66:LYS:NZ	2.49	0.42
4:F:217:LEU:HD12	4:F:218:SER:N	2.34	0.42
4:J:4:VAL:HG11	4:J:105:PHE:O	2.19	0.42
4:J:151:TYR:HA	4:J:152:PRO:HA	1.84	0.42
1:G:32:GLN:O	1:G:49:ALA:HB2	2.19	0.42
1:M:25:VAL:HG11	2:N:55:SER:OG	2.20	0.42
2:N:57:SER:C	2:N:59:ASP:H	2.15	0.42
1:C:201:LEU:O	1:C:246:ALA:HA	2.19	0.42
1:A:107:TRP:CZ2	1:A:172:LEU:HD13	2.54	0.42
1:A:128:GLU:H	1:A:128:GLU:HG2	1.39	0.42
3:I:11:LEU:HD12	3:I:21:PHE:CE1	2.55	0.42
3:I:36:TYR:N	3:I:89:LEU:O	2.48	0.42
3:I:146:GLN:HB3	3:I:147:SER:H	1.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:177:ASN:OD1	3:I:178:LYS:N	2.51	0.42
4:L:83:GLN:O	4:L:84:GLN:C	2.57	0.42
4:L:170:VAL:CB	4:L:194:LEU:CD2	2.95	0.42
1:M:4:SER:OG	1:M:6:ARG:NH1	2.52	0.42
1:M:225:THR:O	1:M:228:THR:HG22	2.20	0.42
3:E:11:LEU:HD12	3:E:106:LEU:HD13	2.01	0.42
1:A:76:VAL:O	1:A:80:THR:HG22	2.20	0.42
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.54	0.42
4:J:43:LEU:HD23	4:J:44:GLU:N	2.34	0.42
1:G:70:HIS:O	1:G:74:HIS:N	2.49	0.42
1:M:73:THR:HG21	5:T:6:VAL:CG2	2.32	0.42
2:N:30:PHE:CE2	2:N:63:TYR:HA	2.55	0.42
3:O:187:PHE:H	3:O:187:PHE:HD2	1.66	0.42
4:P:26:ILE:HB	4:P:29:HIS:HD2	1.82	0.42
3:E:167:PHE:HD2	3:E:168:LYS:H	0.61	0.42
1:A:75:ARG:HE	1:A:75:ARG:HB2	1.74	0.42
1:A:150:ALA:HB3	1:A:152:VAL:HG23	2.01	0.42
4:J:15:LYS:HA	4:J:82:THR:O	2.19	0.42
1:G:64:THR:O	1:G:68:LYS:HG3	2.20	0.42
3:K:94:THR:HG23	3:K:95:GLY:N	2.35	0.42
3:K:115:PRO:CG	3:K:139:ASP:OD2	2.68	0.42
3:K:193:PRO:C	3:K:195:ASP:N	2.72	0.42
1:C:35:ARG:HD2	2:D:53:ASP:OD1	2.19	0.42
1:C:73:THR:HG23	5:R:8:THR:CG2	2.49	0.42
1:C:192:HIS:CE1	1:C:202:ARG:NH1	2.78	0.42
1:C:259:CYS:HB3	1:C:272:LEU:HB2	2.00	0.42
1:A:66:LYS:HD3	5:Q:4:PRO:HA	2.02	0.42
1:A:152:VAL:HA	1:A:155:GLN:OE1	2.19	0.42
2:B:17:ASN:HD22	2:B:74:GLU:CD	2.23	0.42
3:K:61:ARG:CG	3:K:78:LYS:O	2.65	0.42
1:M:114:HIS:HB3	1:M:126:LEU:HB3	2.02	0.42
2:N:11:SER:O	2:N:13:HIS:N	2.53	0.42
2:N:40:LEU:HB3	2:N:43:GLY:CA	2.49	0.42
4:P:38:ARG:O	4:P:41:GLN:NE2	2.52	0.42
4:P:64:ARG:HB3	4:P:80:GLN:O	2.20	0.42
1:C:217:TRP:HZ3	1:C:257:TYR:HB3	1.85	0.42
1:A:173:GLU:HA	1:A:176:LYS:HD3	2.02	0.42
3:I:47:LEU:HD12	3:I:47:LEU:HA	1.90	0.42
4:J:47:ILE:CD1	4:J:60:LEU:HD21	2.05	0.42
4:J:238:GLU:HG3	4:J:239:ALA:H	1.80	0.42
1:G:61:ASP:O	1:G:65:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:52:LEU:HD23	3:O:52:LEU:HA	1.85	0.42
3:O:80:SER:N	3:O:81:GLN:NE2	2.68	0.42
3:E:117:PRO:HB2	3:E:196:THR:HA	2.02	0.42
2:B:55:SER:OG	2:B:56:PHE:N	2.52	0.42
3:I:63:SER:OG	3:I:76:TYR:HB2	2.19	0.42
4:J:46:LEU:HD22	4:J:60:LEU:HA	2.02	0.42
1:G:218:GLN:HB3	1:G:223:ASP:OD1	2.20	0.42
3:K:152:VAL:CG1	3:K:153:TYR:N	2.83	0.42
4:L:122:PRO:HA	4:L:123:PRO:HD3	1.87	0.42
4:L:218:SER:O	4:L:219:GLU:HB2	2.20	0.42
1:M:69:ALA:O	1:M:73:THR:OG1	2.29	0.42
1:M:142:THR:O	1:M:146:LYS:HG3	2.19	0.42
3:O:176:SER:HB2	3:O:181:PHE:O	2.20	0.42
4:P:121:PHE:HA	4:P:122:PRO:HD3	1.81	0.42
4:F:45:PHE:HZ	4:F:48:TYR:HD2	1.67	0.42
4:J:143:LEU:HB3	4:J:194:LEU:HB3	2.02	0.41
1:G:8:PHE:HB2	1:G:25:VAL:HG13	2.01	0.41
1:G:200:THR:HG21	1:G:202:ARG:CZ	2.49	0.41
3:K:115:PRO:CB	3:K:139:ASP:OD2	2.67	0.41
3:K:131:SER:OG	3:K:132:VAL:N	2.47	0.41
3:K:158:CYS:SG	3:K:159:VAL:N	2.93	0.41
4:L:6:GLN:HE21	4:L:6:GLN:HB2	1.64	0.41
4:L:141:ALA:N	4:L:198:ALA:H	2.18	0.41
1:M:219:ARG:CD	1:M:224:GLN:NE2	2.70	0.41
1:C:202:ARG:HG2	1:C:244:TRP:NE1	2.28	0.41
2:D:84:HIS:CG	2:D:85:VAL:H	2.38	0.41
2:B:74:GLU:OE1	2:B:74:GLU:HA	2.20	0.41
3:I:132:VAL:HG12	3:I:173:VAL:HG13	2.01	0.41
1:G:70:HIS:CD2	5:U:2:LEU:HD23	2.55	0.41
4:L:88:ALA:HB1	4:L:110:ARG:CA	2.46	0.41
1:M:197:HIS:C	1:M:198:GLU:CG	2.89	0.41
4:P:119:ASN:HB3	4:P:151:TYR:CE2	2.55	0.41
2:D:28:SER:OG	2:D:29:GLY:N	2.53	0.41
4:F:203:ASN:N	4:F:204:PRO:HD3	2.35	0.41
4:F:230:PRO:O	4:F:231:VAL:HG23	2.19	0.41
1:A:11:SER:HA	1:A:22:PHE:HA	2.02	0.41
1:A:73:THR:HG23	3:I:96:ASN:ND2	2.35	0.41
4:J:112:LEU:HG	4:J:113:VAL:O	2.20	0.41
1:G:72:GLN:HG2	1:G:72:GLN:H	1.57	0.41
3:K:135:PHE:C	3:K:135:PHE:HD1	2.23	0.41
4:L:175:GLN:HA	4:L:176:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:36:ARG:O	4:P:44:GLU:HB2	2.21	0.41
4:P:125:VAL:HG12	4:P:237:ALA:HB2	2.01	0.41
1:C:52:ILE:HD12	1:C:52:ILE:HA	1.89	0.41
1:A:13:SER:HB3	1:A:93:HIS:H	1.85	0.41
1:G:98:MET:CE	1:G:99:TYR:N	2.84	0.41
1:G:211:ALA:HB2	1:G:241:PHE:HE2	1.84	0.41
3:K:135:PHE:CE1	3:K:138:PHE:CG	3.08	0.41
3:K:188:ASN:O	3:K:189:ASN:HB2	2.19	0.41
4:L:21:LEU:HD12	4:L:21:LEU:N	2.35	0.41
1:M:99:TYR:OH	5:T:3:VAL:HG12	2.20	0.41
2:N:10:TYR:HE2	2:N:26:TYR:HB3	1.85	0.41
4:P:160:TRP:HD1	4:P:165:GLU:CG	2.23	0.41
1:C:218:GLN:HG2	1:C:260:HIS:HD2	1.79	0.41
1:C:243:LYS:HG2	1:C:244:TRP:N	2.33	0.41
4:J:134:GLU:HA	4:J:137:HIS:HB2	2.01	0.41
1:G:11:SER:O	1:G:95:VAL:N	2.53	0.41
1:G:266:LEU:HD23	1:G:266:LEU:HA	1.77	0.41
1:G:268:LYS:O	1:G:269:PRO:C	2.58	0.41
3:K:193:PRO:C	3:K:195:ASP:H	2.23	0.41
4:L:33:TYR:O	4:L:92:CYS:HA	2.21	0.41
1:M:128:GLU:H	1:M:128:GLU:CD	2.15	0.41
1:M:203:CYS:CB	1:M:217:TRP:HE1	2.31	0.41
1:M:234:ARG:HE	1:M:234:ARG:HB2	1.62	0.41
3:O:30:PHE:CD2	3:O:68:THR:HG22	2.55	0.41
3:O:80:SER:C	3:O:81:GLN:NE2	2.73	0.41
3:O:85:SER:OG	3:O:108:VAL:HG22	2.20	0.41
3:E:144:VAL:HG21	3:E:155:THR:O	2.19	0.41
4:F:51:GLY:O	4:F:69:ARG:NH1	2.52	0.41
4:F:96:GLN:C	4:F:97:THR:HG1	2.11	0.41
4:F:230:PRO:C	4:F:231:VAL:CG2	2.88	0.41
1:A:52:ILE:HD13	1:A:60:TRP:CH2	2.55	0.41
1:A:242:GLN:NE2	2:B:12:ARG:O	2.46	0.41
1:G:64:THR:HG22	1:G:68:LYS:CE	2.51	0.41
1:G:157:ARG:CG	1:G:158:ALA:N	2.83	0.41
1:G:262:GLN:HA	1:G:269:PRO:HB3	2.01	0.41
4:L:154:HIS:O	4:L:215:TYR:HD2	2.02	0.41
1:M:96:GLN:HE21	2:N:31:HIS:HE1	1.66	0.41
1:C:185:PRO:HD2	1:C:266:LEU:HG	2.03	0.41
3:E:125:SER:HB3	3:E:126:LYS:HD2	2.03	0.41
3:E:136:THR:N	3:E:138:PHE:HE1	2.18	0.41
4:F:140:LYS:HD3	4:F:197:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:ARG:O	2:H:30:PHE:HA	2.20	0.41
3:K:95:GLY:O	3:K:96:ASN:HB3	2.20	0.41
3:K:155:THR:O	3:K:172:ALA:HB1	2.20	0.41
1:M:95:VAL:HG22	1:M:118:TYR:HD1	1.84	0.41
1:M:102:ASP:HB2	1:M:111:ARG:CG	2.51	0.41
2:N:7:ILE:HA	2:N:27:VAL:HG12	2.03	0.41
4:P:13:THR:HB	4:P:17:LYS:HZ2	1.85	0.41
4:P:29:HIS:ND1	4:P:96:GLN:HA	2.36	0.41
3:I:76:TYR:N	3:I:76:TYR:CD1	2.88	0.41
3:I:188:ASN:ND2	3:I:192:ILE:CD1	2.83	0.41
1:G:33:PHE:CD1	1:G:34:VAL:HG13	2.56	0.41
3:K:11:LEU:HG	3:K:21:PHE:HE2	1.85	0.41
3:K:136:THR:HA	3:K:138:PHE:CE2	2.55	0.41
4:L:225:GLN:HB3	4:L:226:ASP:H	1.67	0.41
1:C:82:ARG:HD3	1:C:89:GLU:HA	2.03	0.41
1:C:92:SER:O	1:C:93:HIS:HD2	2.04	0.41
4:F:60:LEU:HA	4:F:61:PRO:HD3	1.97	0.41
4:F:124:GLU:N	4:F:148:THR:O	2.48	0.41
1:A:23:ILE:HD12	2:B:54:LEU:HB3	2.02	0.41
1:A:248:VAL:HG21	6:A:303:HOH:O	2.21	0.41
3:I:121:GLN:C	3:I:132:VAL:O	2.59	0.41
4:J:4:VAL:CG1	4:J:106:GLY:HA2	2.51	0.41
1:G:82:ARG:HH21	1:G:89:GLU:CA	2.31	0.41
1:G:97:ARG:CZ	1:G:116:TYR:HE1	2.21	0.41
1:G:134:THR:O	1:G:134:THR:HG23	2.20	0.41
1:G:192:HIS:HD2	1:G:202:ARG:CD	2.34	0.41
1:G:230:LEU:HD12	1:G:230:LEU:HA	1.83	0.41
1:G:259:CYS:C	1:G:260:HIS:HD1	2.23	0.41
3:K:35:TRP:O	3:K:47:LEU:CB	2.69	0.41
3:K:79:GLY:O	3:K:81:GLN:HG2	2.21	0.41
3:K:116:ASP:OD1	3:K:137:ASP:OD2	2.39	0.41
4:L:90:TYR:HB2	4:L:109:THR:CG2	2.49	0.41
1:M:49:ALA:HB1	1:M:51:TRP:NE1	2.36	0.41
2:N:22:PHE:HE1	4:F:80:GLN:NE2	2.19	0.41
4:P:45:PHE:CZ	4:P:48:TYR:HB3	2.56	0.41
1:C:200:THR:HA	1:C:247:VAL:O	2.21	0.41
4:F:154:HIS:CD2	4:F:154:HIS:N	2.88	0.41
5:R:2:LEU:HD12	5:R:2:LEU:N	2.36	0.41
1:A:45:MET:HG2	1:A:67:VAL:HG11	2.03	0.41
1:A:93:HIS:CB	1:A:119:ASP:OD1	2.67	0.41
3:I:133:CYS:SG	3:I:182:ALA:O	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:PRO:HG2	2:H:65:LEU:HD12	2.03	0.41
1:M:22:PHE:CD1	1:M:71:SER:HA	2.56	0.41
1:M:66:LYS:CE	3:O:29:ASN:CG	2.88	0.41
1:M:222:GLU:H	1:M:222:GLU:HG3	1.70	0.41
4:P:200:PHE:HD1	4:P:200:PHE:HA	1.74	0.41
4:P:206:ASN:HD22	4:P:240:TRP:C	2.24	0.41
4:F:8:PRO:O	4:F:109:THR:HG22	2.20	0.41
4:F:35:TYR:HB3	4:F:43:LEU:HD21	2.02	0.41
1:A:31:THR:HG23	1:A:209:TYR:CE1	2.56	0.40
4:J:50:GLN:NE2	4:J:97:THR:O	2.54	0.40
4:J:69:ARG:NH1	4:J:73:SER:O	2.55	0.40
4:J:129:GLU:HA	4:J:130:PRO:HD3	1.89	0.40
1:G:35:ARG:HH21	1:G:48:ARG:NE	2.18	0.40
2:H:7:ILE:HD12	2:H:82:VAL:CG1	2.51	0.40
2:H:65:LEU:HD23	2:H:66:TYR:N	2.36	0.40
3:K:185:ASN:HB2	3:K:188:ASN:CB	2.50	0.40
4:L:97:THR:CB	4:L:98:GLN:NE2	2.84	0.40
1:M:167:TRP:CZ3	1:M:170:ARG:HD3	2.56	0.40
2:N:37:VAL:HG21	2:N:66:TYR:CD2	2.56	0.40
3:O:121:GLN:HA	3:O:132:VAL:O	2.21	0.40
1:C:231:VAL:O	1:C:243:LYS:HE2	2.22	0.40
2:D:27:VAL:HG23	2:D:30:PHE:HE2	1.86	0.40
4:F:87:SER:HA	4:F:111:LEU:O	2.21	0.40
1:A:177:GLU:HG2	1:A:178:THR:N	2.36	0.40
3:I:146:GLN:NE2	3:I:154:ILE:HG21	2.37	0.40
3:K:87:THR:HA	3:K:105:SER:HA	2.03	0.40
3:K:161:ASP:OD1	3:K:168:LYS:HB3	2.21	0.40
4:L:88:ALA:HB2	4:L:111:LEU:N	2.37	0.40
4:L:124:GLU:O	4:L:147:ALA:HA	2.20	0.40
3:O:166:ASP:O	3:O:167:PHE:C	2.58	0.40
1:C:35:ARG:NH1	2:D:53:ASP:OD1	2.45	0.40
1:C:121:LYS:HD2	1:C:121:LYS:HA	1.73	0.40
1:C:202:ARG:HG2	1:C:244:TRP:CD1	2.56	0.40
1:A:9:PHE:N	1:A:97:ARG:O	2.48	0.40
1:A:70:HIS:NE2	5:Q:6:VAL:HG13	2.35	0.40
1:G:2:SER:HA	1:G:103:VAL:O	2.21	0.40
2:H:71:THR:OG1	2:H:72:PRO:CD	2.66	0.40
3:K:187:PHE:O	3:K:190:SER:OG	2.37	0.40
4:L:161:VAL:CG1	4:L:162:ASN:N	2.84	0.40
1:M:79:GLY:O	1:M:82:ARG:HB2	2.22	0.40
2:N:11:SER:HB3	2:N:95:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:53:ASN:HB2	3:O:68:THR:H	1.87	0.40
1:C:73:THR:HG23	5:R:8:THR:HG22	2.03	0.40
2:D:54:LEU:C	2:D:54:LEU:HD23	2.41	0.40
1:A:13:SER:HB3	1:A:93:HIS:N	2.36	0.40
1:A:29:ASP:HB3	1:A:30:ASP:H	1.61	0.40
1:A:69:ALA:O	3:I:96:ASN:ND2	2.54	0.40
1:A:216:THR:OG1	1:A:217:TRP:N	2.54	0.40
2:B:33:SER:HB3	2:B:62:PHE:CD2	2.56	0.40
4:J:98:GLN:NE2	4:J:98:GLN:CA	2.82	0.40
2:H:57:SER:O	2:H:58:LYS:C	2.60	0.40
3:K:35:TRP:O	3:K:36:TYR:HD1	2.04	0.40
3:K:136:THR:HG22	3:K:171:SER:CB	2.43	0.40
1:M:185:PRO:HD2	1:M:266:LEU:HD11	2.03	0.40
1:M:217:TRP:CZ3	1:M:247:VAL:HG22	2.56	0.40
3:E:61:ARG:HH12	3:E:81:GLN:HB3	1.86	0.40
3:E:136:THR:C	3:E:138:PHE:CD1	2.95	0.40
1:G:4:SER:O	1:G:29:ASP:N	2.42	0.40
1:G:27:TYR:HE2	2:H:55:SER:HG	1.64	0.40
1:G:187:THR:CB	1:G:272:LEU:HD21	2.35	0.40
3:K:136:THR:CG2	3:K:171:SER:HB3	2.50	0.40
4:P:151:TYR:CD1	4:P:152:PRO:HA	2.57	0.40
1:C:231:VAL:CG1	1:C:244:TRP:CE3	3.00	0.40
3:E:66:LEU:HD23	3:E:67:ASN:N	2.36	0.40
4:F:36:ARG:HD2	4:F:90:TYR:CZ	2.56	0.40
4:F:36:ARG:HH11	4:F:46:LEU:HD21	1.87	0.40

All (5) 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)
3:K:12:HIS:ND1	3:O:10:SER:OG[1_556]	1.92	0.28
3:K:12:HIS:CG	3:O:10:SER:OG[1_556]	2.00	0.20
3:K:189:ASN:OD1	4:P:181:PRO:CG[1_556]	2.09	0.11
3:I:10:SER:OG	3:I:12:HIS:ND1[3_655]	2.14	0.06
3:K:189:ASN:OD1	4:P:181:PRO:CD[1_556]	2.17	0.03

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	272/276 (99%)	255 (94%)	17 (6%)	0	100	100
1	C	272/276 (99%)	248 (91%)	23 (8%)	1 (0%)	34	71
1	G	264/276 (96%)	239 (90%)	25 (10%)	0	100	100
1	M	271/276 (98%)	242 (89%)	29 (11%)	0	100	100
2	B	97/100 (97%)	84 (87%)	13 (13%)	0	100	100
2	D	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
2	H	92/100 (92%)	82 (89%)	9 (10%)	1 (1%)	14	53
2	N	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
3	E	179/205 (87%)	152 (85%)	26 (14%)	1 (1%)	25	64
3	I	175/205 (85%)	137 (78%)	37 (21%)	1 (1%)	25	64
3	K	188/205 (92%)	158 (84%)	26 (14%)	4 (2%)	7	39
3	O	181/205 (88%)	160 (88%)	20 (11%)	1 (1%)	25	64
4	F	234/245 (96%)	197 (84%)	34 (14%)	3 (1%)	12	49
4	J	214/245 (87%)	185 (86%)	28 (13%)	1 (0%)	29	67
4	L	214/245 (87%)	183 (86%)	29 (14%)	2 (1%)	17	57
4	P	227/245 (93%)	192 (85%)	32 (14%)	3 (1%)	12	49
5	Q	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	T	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	U	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	3104/3340 (93%)	2707 (87%)	379 (12%)	18 (1%)	25	64

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	122	LEU

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Mol	Chain	Res	Type
4	J	114	LEU
3	K	147	SER
3	K	150	SER
4	L	174	PRO
4	P	229	LYS
4	F	181	PRO
3	K	153	TYR
3	O	178	LYS
3	E	190	SER
4	P	139	GLN
2	H	71	THR
3	K	115	PRO
4	P	119	ASN
4	L	203	ASN
1	C	235	PRO
4	F	203	ASN
4	F	180	GLN

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	231/232 (100%)	226 (98%)	5 (2%)	52	77
1	C	231/232 (100%)	221 (96%)	10 (4%)	29	62
1	G	226/232 (97%)	216 (96%)	10 (4%)	28	62
1	M	225/232 (97%)	216 (96%)	9 (4%)	31	64
2	B	93/95 (98%)	92 (99%)	1 (1%)	73	87
2	D	93/95 (98%)	88 (95%)	5 (5%)	22	56
2	H	86/95 (90%)	83 (96%)	3 (4%)	36	67
2	N	92/95 (97%)	90 (98%)	2 (2%)	52	77
3	E	158/185 (85%)	145 (92%)	13 (8%)	11	41
3	I	155/185 (84%)	145 (94%)	10 (6%)	17	50
3	K	158/185 (85%)	140 (89%)	18 (11%)	5	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	159/185 (86%)	145 (91%)	14 (9%)	10	39
4	F	198/212 (93%)	184 (93%)	14 (7%)	14	47
4	J	189/212 (89%)	176 (93%)	13 (7%)	15	48
4	L	174/212 (82%)	162 (93%)	12 (7%)	15	48
4	P	189/212 (89%)	178 (94%)	11 (6%)	20	54
5	Q	8/8 (100%)	7 (88%)	1 (12%)	4	24
5	R	8/8 (100%)	8 (100%)	0	100	100
5	T	8/8 (100%)	7 (88%)	1 (12%)	4	24
5	U	8/8 (100%)	8 (100%)	0	100	100
All	All	2689/2928 (92%)	2537 (94%)	152 (6%)	20	54

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	98	MET
1	A	113	TYR
1	A	119	ASP
1	A	230	LEU
2	B	54	LEU
3	I	14	GLN
3	I	15	GLU
3	I	39	GLU
3	I	78	LYS
3	I	80	SER
3	I	81	GLN
3	I	131	SER
3	I	133	CYS
3	I	138	PHE
3	I	179	SER
4	J	29	HIS
4	J	60	LEU
4	J	84	GLN
4	J	97	THR
4	J	114	LEU
4	J	120	VAL
4	J	167	HIS
4	J	177	LEU
4	J	201	TRP

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Mol	Chain	Res	Type
4	J	205	ARG
4	J	223	TRP
4	J	229	LYS
4	J	230	PRO
5	Q	5	MET
1	G	29	ASP
1	G	48	ARG
1	G	58	GLU
1	G	98	MET
1	G	116	TYR
1	G	160	LEU
1	G	161	GLU
1	G	186	LYS
1	G	191	HIS
1	G	268	LYS
2	H	23	LEU
2	H	80	CYS
2	H	81	ARG
3	K	43	SER
3	K	52	LEU
3	K	61	ARG
3	K	70	GLU
3	K	80	SER
3	K	102	THR
3	K	112	ILE
3	K	135	PHE
3	K	137	ASP
3	K	145	SER
3	K	148	LYS
3	K	149	ASP
3	K	155	THR
3	K	157	LYS
3	K	168	LYS
3	K	169	SER
3	K	178	LYS
3	K	180	ASP
4	L	6	GLN
4	L	9	SER
4	L	85	GLU
4	L	118	LYS
4	L	143	LEU
4	L	145	CYS

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Mol	Chain	Res	Type
4	L	148	THR
4	L	150	PHE
4	L	159	TRP
4	L	193	ARG
4	L	217	LEU
4	L	238	GLU
1	M	17	ARG
1	M	88	SER
1	M	155	GLN
1	M	196	ASP
1	M	197	HIS
1	M	222	GLU
1	M	266	LEU
1	M	272	LEU
1	M	274	TRP
2	N	59	ASP
2	N	70	PHE
3	O	69	LYS
3	O	80	SER
3	O	116	ASP
3	O	134	LEU
3	O	138	PHE
3	O	140	SER
3	O	156	ASP
3	O	164	SER
3	O	166	ASP
3	O	168	LYS
3	O	170	ASN
3	O	179	SER
3	O	187	PHE
3	O	188	ASN
4	P	5	SER
4	P	64	ARG
4	P	68	GLU
4	P	97	THR
4	P	154	HIS
4	P	167	HIS
4	P	171	CYS
4	P	179	GLU
4	P	191	SER
4	P	226	ASP
4	P	227	ARG

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Mol	Chain	Res	Type
5	T	2	LEU
1	C	35	ARG
1	C	48	ARG
1	C	61	ASP
1	C	113	TYR
1	C	119	ASP
1	C	131	ARG
1	C	188	HIS
1	C	192	HIS
1	C	226	GLN
1	C	227	ASP
2	D	45	ARG
2	D	53	ASP
2	D	89	GLN
2	D	90	PRO
2	D	91	LYS
3	E	21	PHE
3	E	40	THR
3	E	83	GLU
3	E	85	SER
3	E	136	THR
3	E	137	ASP
3	E	138	PHE
3	E	161	ASP
3	E	167	PHE
3	E	178	LYS
3	E	179	SER
3	E	180	ASP
3	E	183	CYS
4	F	39	LEU
4	F	49	PHE
4	F	160	TRP
4	F	170	VAL
4	F	185	ASP
4	F	193	ARG
4	F	195	ARG
4	F	201	TRP
4	F	217	LEU
4	F	220	ASN
4	F	222	GLU
4	F	225	GLN
4	F	238	GLU

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Mol	Chain	Res	Type
4	F	240	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
3	I	96	ASN
3	I	188	ASN
4	J	29	HIS
4	J	119	ASN
4	J	154	HIS
1	G	93	HIS
1	G	192	HIS
3	K	188	ASN
4	L	220	ASN
1	M	93	HIS
1	M	96	GLN
2	N	2	GLN
2	N	13	HIS
2	N	31	HIS
4	P	83	GLN
4	P	225	GLN
1	C	70	HIS
3	E	97	GLN
4	F	29	HIS
4	F	83	GLN
4	F	98	GLN
4	F	154	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	274/276 (99%)	-0.18	0	100	100	33, 56, 82, 107	0
1	C	274/276 (99%)	-0.20	1 (0%)	92	87	35, 51, 83, 100	0
1	G	270/276 (97%)	0.06	5 (1%)	66	53	57, 80, 102, 122	0
1	M	273/276 (98%)	0.06	3 (1%)	80	69	51, 77, 111, 119	0
2	B	99/100 (99%)	0.05	3 (3%)	50	37	45, 72, 108, 123	0
2	D	100/100 (100%)	-0.06	0	100	100	40, 66, 90, 113	0
2	H	96/100 (96%)	0.19	2 (2%)	63	50	59, 88, 110, 115	0
2	N	100/100 (100%)	0.18	2 (2%)	65	52	57, 87, 107, 116	0
3	E	187/205 (91%)	-0.05	3 (1%)	72	59	36, 63, 114, 131	0
3	I	185/205 (90%)	-0.04	3 (1%)	72	59	41, 72, 115, 126	0
3	K	192/205 (93%)	0.37	15 (7%)	13	10	55, 89, 129, 140	0
3	O	187/205 (91%)	0.15	8 (4%)	35	26	58, 91, 134, 151	0
4	F	238/245 (97%)	0.06	2 (0%)	86	75	38, 80, 125, 132	0
4	J	226/245 (92%)	0.17	8 (3%)	44	33	25, 88, 129, 141	0
4	L	226/245 (92%)	0.31	3 (1%)	77	65	74, 106, 127, 136	0
4	P	235/245 (95%)	0.33	19 (8%)	12	10	50, 95, 133, 154	0
5	Q	9/9 (100%)	0.07	0	100	100	43, 48, 51, 53	0
5	R	9/9 (100%)	-0.17	0	100	100	40, 41, 44, 46	0
5	T	9/9 (100%)	0.04	0	100	100	59, 63, 71, 72	0
5	U	9/9 (100%)	0.17	0	100	100	63, 67, 72, 73	0
All	All	3198/3340 (95%)	0.08	77 (2%)	59	45	25, 79, 122, 154	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	134	LEU	6.5
3	K	127	SER	6.3
3	K	128	SER	5.2
3	K	172	ALA	5.0
4	P	190	LEU	4.6
3	K	129	ASP	4.3
4	P	206	ASN	4.2
4	L	194	LEU	3.8
4	P	144	VAL	3.7
4	J	239	ALA	3.7
3	K	143	ASN	3.6
3	K	133	CYS	3.6
4	P	215	TYR	3.5
3	K	135	PHE	3.5
3	K	173	VAL	3.5
3	E	190	SER	3.4
4	P	169	GLY	3.4
3	O	136	THR	3.4
3	O	173	VAL	3.3
2	H	71	THR	3.3
4	J	162	ASN	3.3
3	O	114	ASN	3.2
1	M	188	HIS	3.2
3	I	118	ALA	3.2
4	J	144	VAL	3.1
4	P	131	SER	3.0
3	K	174	ALA	3.0
4	P	126	ALA	3.0
3	K	118	ALA	2.9
3	O	134	LEU	2.9
4	P	142	THR	2.9
4	J	208	PHE	2.9
3	K	126	LYS	2.9
1	G	190	THR	2.8
2	B	40	LEU	2.7
4	P	208	PHE	2.6
3	O	121	GLN	2.6
4	F	194	LEU	2.6
4	P	210	CYS	2.6
3	I	134	LEU	2.6
4	P	37	GLN	2.5
4	J	195	ARG	2.5
1	G	92	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	134	LEU	2.5
3	O	133	CYS	2.5
1	M	270	LEU	2.4
4	P	104	TYR	2.4
4	P	132	GLU	2.4
4	P	214	PHE	2.4
1	G	205	ALA	2.4
3	I	172	ALA	2.3
2	N	83	ASN	2.3
4	L	209	ARG	2.3
1	M	224	GLN	2.3
4	P	145	CYS	2.3
1	G	274	TRP	2.3
3	E	170	ASN	2.2
4	P	189	ALA	2.2
1	G	272	LEU	2.2
4	J	177	LEU	2.2
4	J	152	PRO	2.2
4	F	143	LEU	2.2
3	K	180	ASP	2.1
3	K	91	ALA	2.1
2	H	66	TYR	2.1
1	C	17	ARG	2.1
3	O	175	TRP	2.1
4	P	168	SER	2.1
4	P	170	VAL	2.1
3	O	170	ASN	2.1
4	P	105	PHE	2.1
2	N	2	GLN	2.0
2	B	20	SER	2.0
2	B	16	GLU	2.0
3	K	120	TYR	2.0
4	J	196	VAL	2.0
4	L	21	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.