Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:08 AM GMT

PDB ID	:	3NZX
Title	:	Crystal structure of the yeast 20S proteasome in complex with ligand 2c
Authors	:	Groll, M.; Gallastegui, N.; Marechal, X.; Le Ravalec, V.; Basse, N.; Richy, N.; Genin, E.; Huber, R.; Moroder, M.; Vidal, V.; Reboud-Ravaux, M.
Deposited on	:	2010-07-17
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

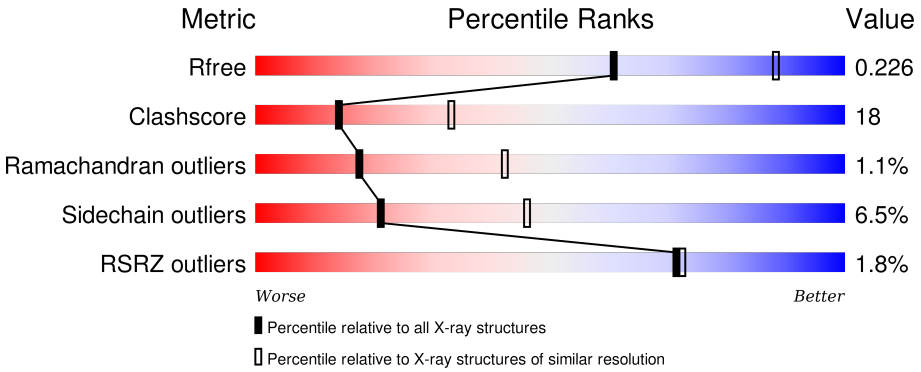
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	250	73% 24% •
1	O	250	73% 24% •
2	B	258	58% 32% • 5%
2	P	258	58% 32% 5% 5%
3	C	254	57% 35% • 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	8% 55% 37% 5%
4	D	260	3% 68% 22% 7%
4	R	260	3% 66% 24% 7%
5	E	234	2% 56% 38% 6%
5	S	234	5% 53% 41% 6%
6	F	288	% 52% 28% 5% 15%
6	T	288	2% 49% 31% 5% 15%
7	G	252	% 69% 23%
7	U	252	% 66% 26%
8	H	261	55% 29% 15%
8	V	261	55% 29% 15%
9	I	205	65% 31%
9	W	205	68% 29%
10	J	198	2% 63% 33%
10	X	198	3% 65% 31%
11	K	287	% 47% 23% 26%
11	Y	287	% 46% 24% 26%
12	L	241	% 59% 28% 5% 8%
12	Z	241	2% 60% 27% 5% 8%
13	1	266	59% 26% 12%
13	M	266	62% 23% 12%
14	2	215	66% 24% 9%
14	N	215	67% 23% 9%
15	3	5	60% 40%
15	4	5	60% 40%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50982 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 Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called TMC-95A mimic ligand 2c.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	5	Total	C	N	O	0	0	0
			55	42	5	8			
15	4	5	Total	C	N	O	0	0	0
			55	42	5	8			

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	57	Total O 57 57	0	0
16	B	36	Total O 36 36	0	0
16	C	44	Total O 44 44	0	0
16	D	41	Total O 41 41	0	0
16	E	23	Total O 23 23	0	0
16	F	45	Total O 45 45	0	0
16	G	64	Total O 64 64	0	0
16	H	51	Total O 51 51	0	0
16	I	69	Total O 69 69	0	0
16	J	51	Total O 51 51	0	0
16	K	40	Total O 40 40	0	0
16	L	56	Total O 56 56	0	0
16	M	73	Total O 73 73	0	0
16	N	54	Total O 54 54	0	0
16	O	34	Total O 34 34	0	0
16	P	29	Total O 29 29	0	0
16	Q	27	Total O 27 27	0	0
16	R	31	Total O 31 31	0	0
16	S	20	Total O 20 20	0	0
16	T	38	Total O 38 38	0	0
16	U	64	Total O 64 64	0	0

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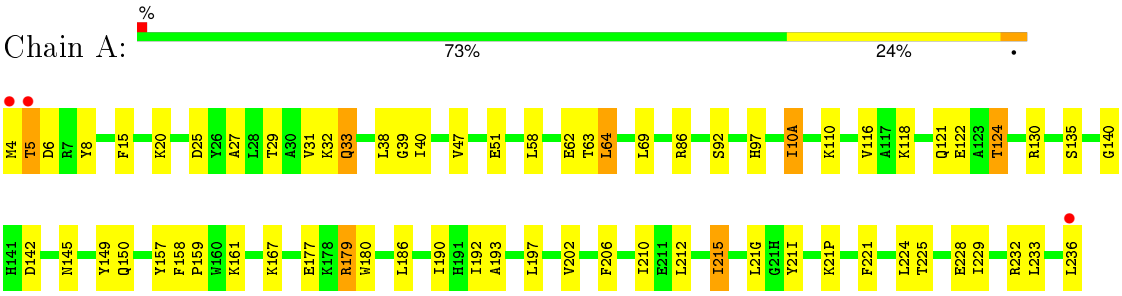
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	V	47	Total O 47 47	0	0
16	W	61	Total O 61 61	0	0
16	X	48	Total O 48 48	0	0
16	Y	47	Total O 47 47	0	0
16	Z	48	Total O 48 48	0	0
16	1	78	Total O 78 78	0	0
16	2	58	Total O 58 58	0	0

3 Residue-property plots (i)

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

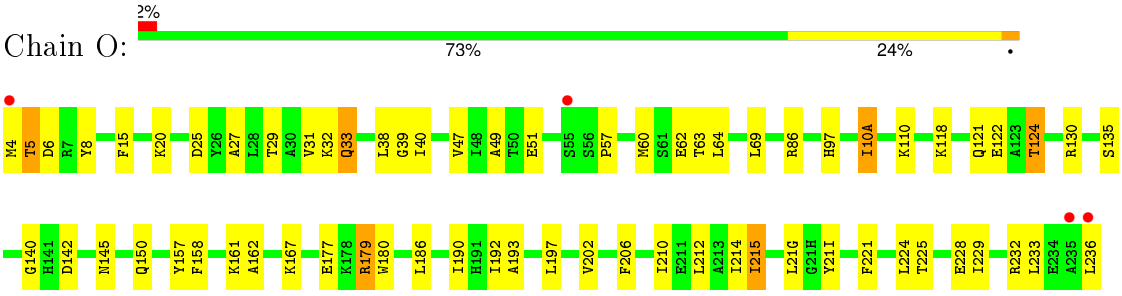
- Molecule 1: Proteasome component Y7

Chain A:



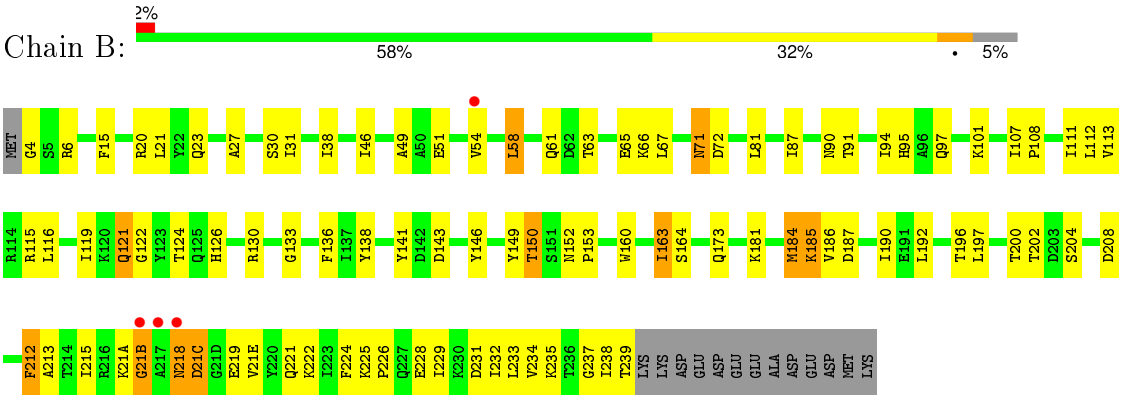
- Molecule 1: Proteasome component Y7

Chain O:



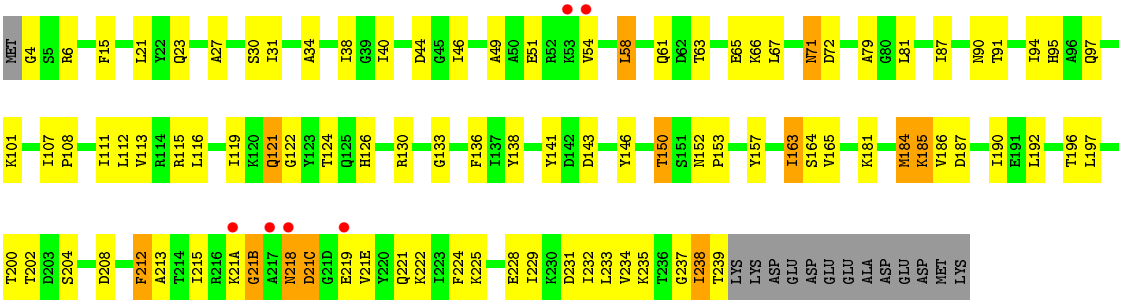
- Molecule 2: Proteasome component Y13

Chain B:



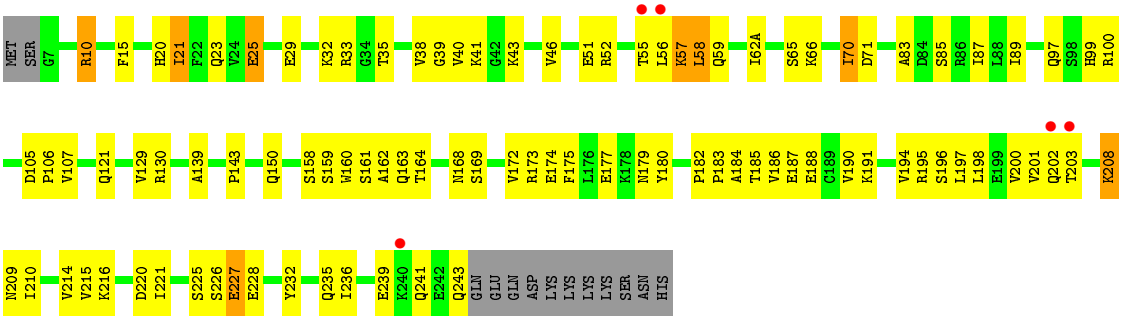
- Molecule 2: Proteasome component Y13

Chain P:



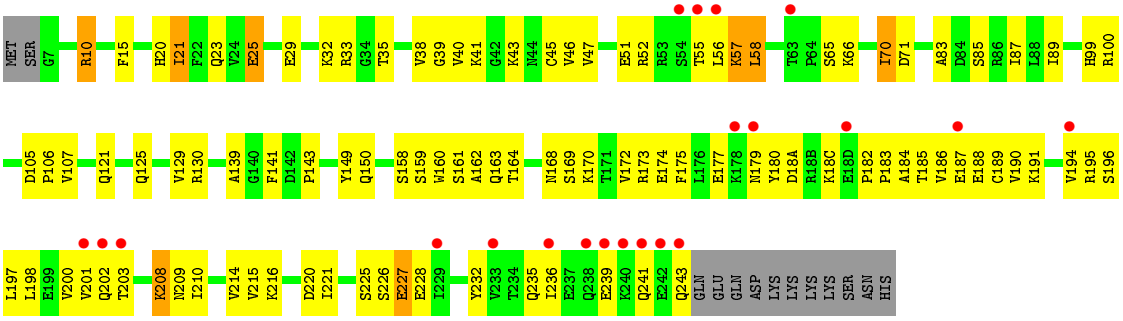
• Molecule 3: Proteasome component PRE6

Chain C:



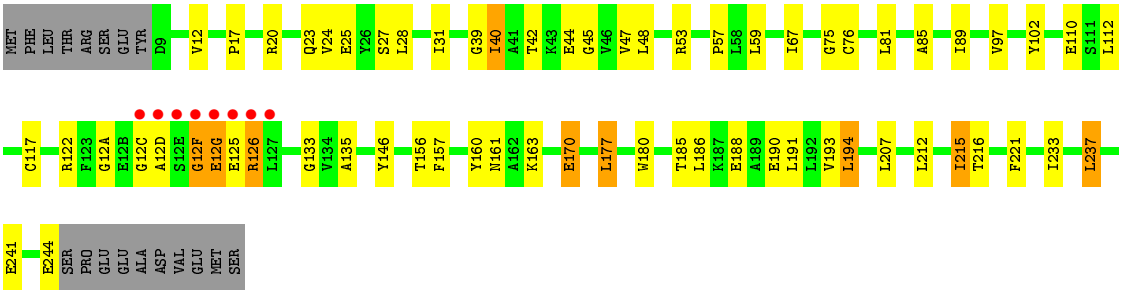
• Molecule 3: Proteasome component PRE6

Chain Q:



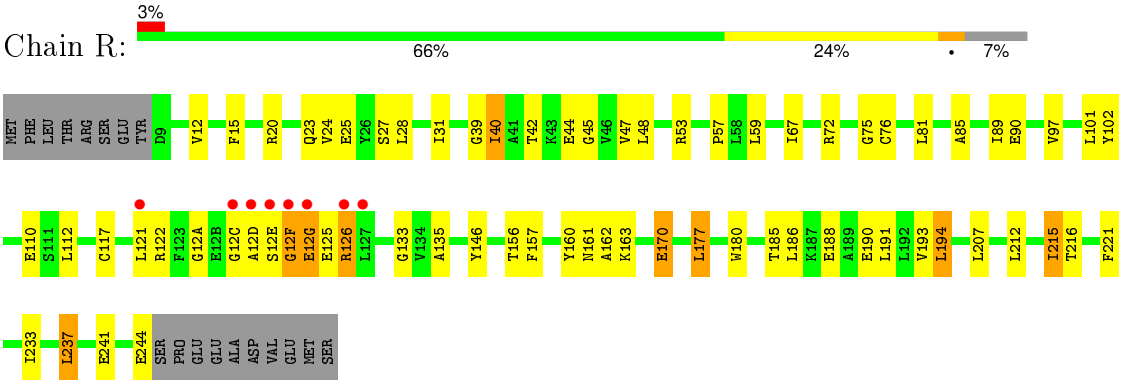
• Molecule 4: Proteasome component PUP2

Chain D:



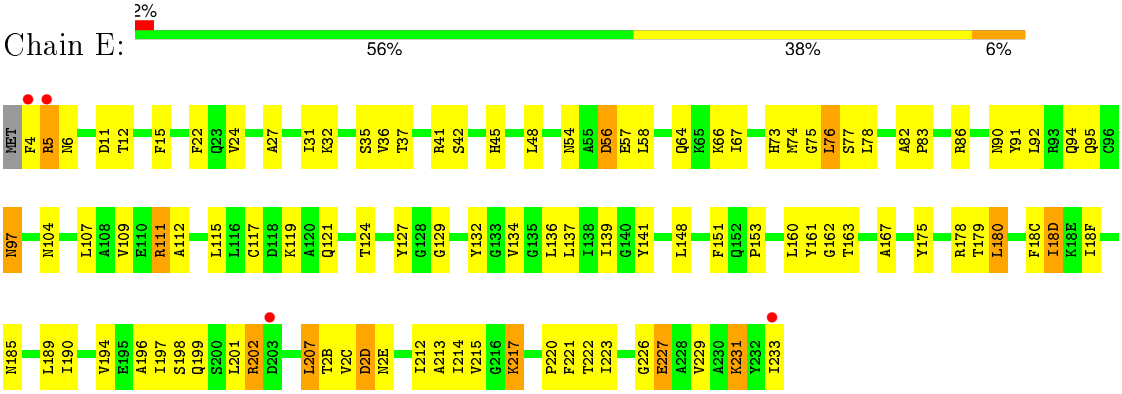
• Molecule 4: Proteasome component PUP2

Chain R:



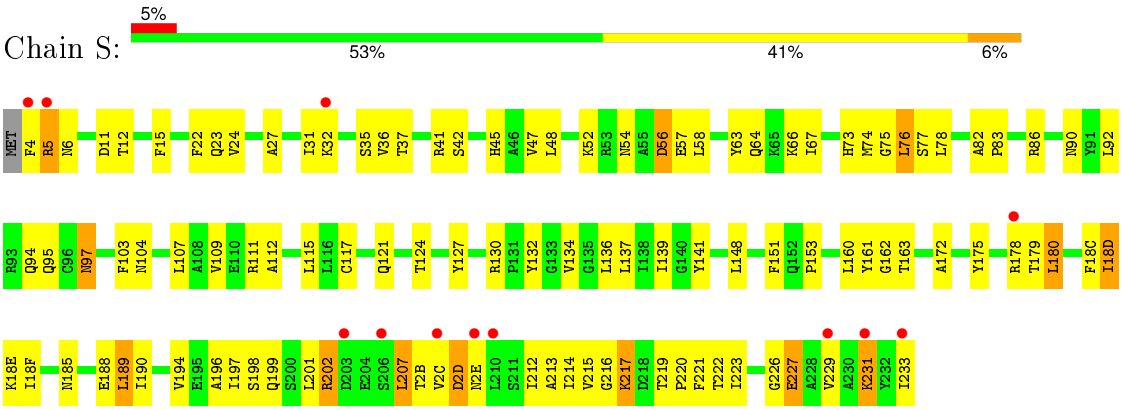
• Molecule 5: Proteasome component PRE5

Chain E:



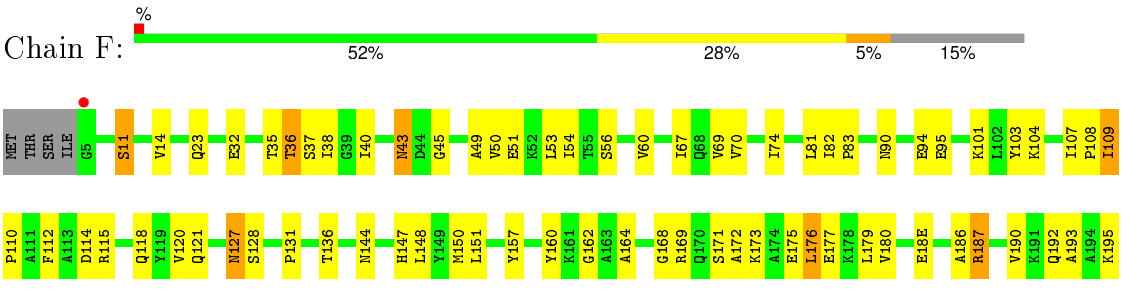
• Molecule 5: Proteasome component PRE5

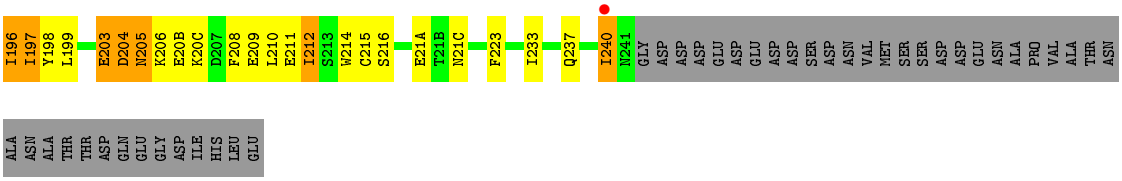
Chain S:



• Molecule 6: Proteasome component C1

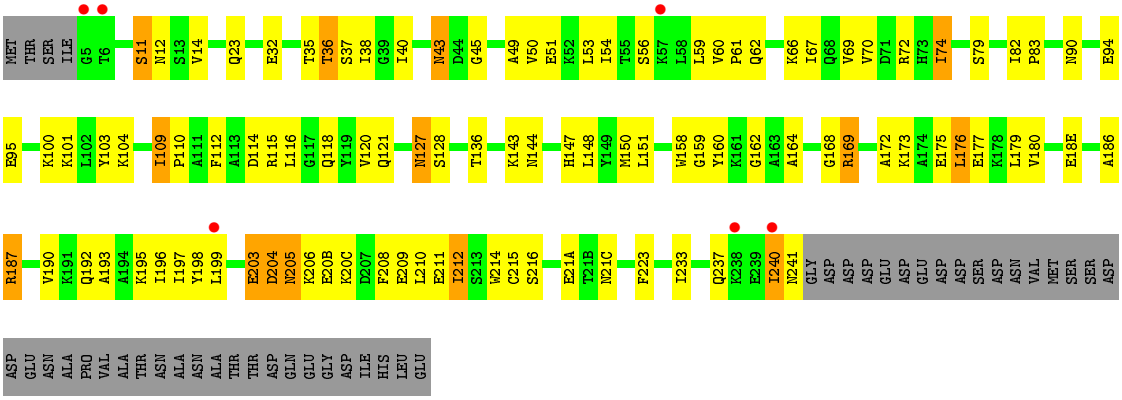
Chain F:





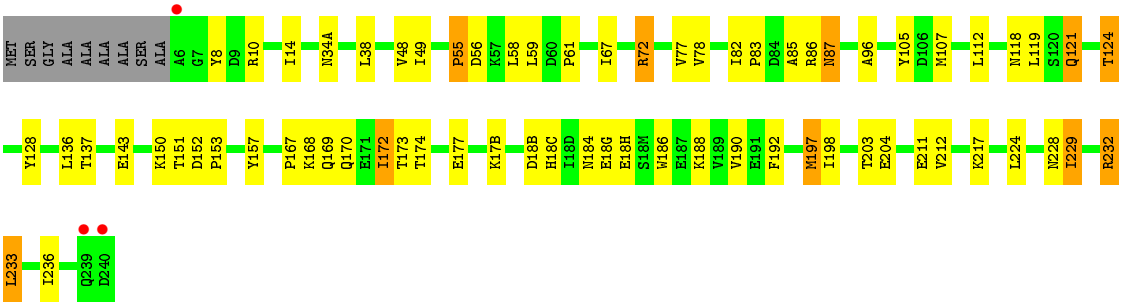
• Molecule 6: Proteasome component C1

Chain T:



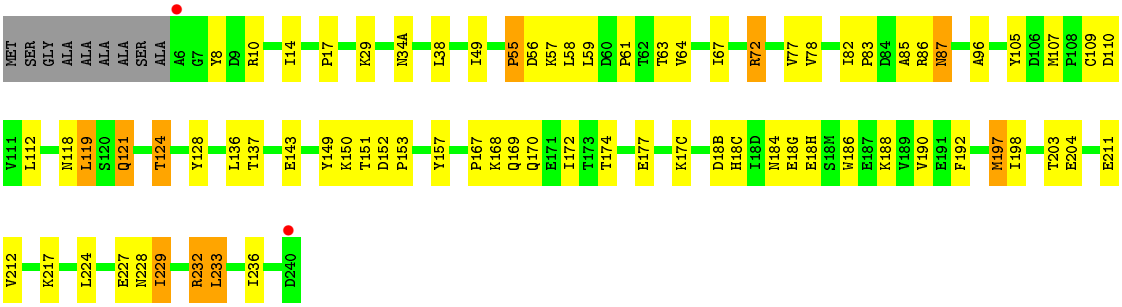
• Molecule 7: Proteasome component C7-alpha

Chain G:



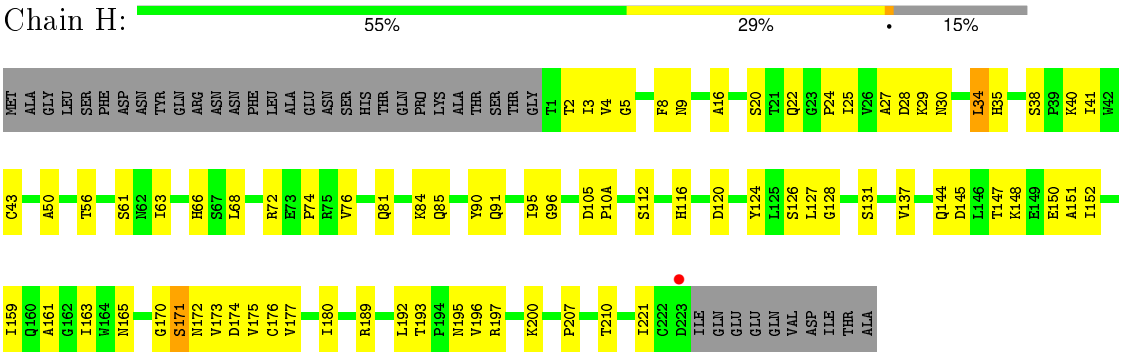
• Molecule 7: Proteasome component C7-alpha

Chain U:



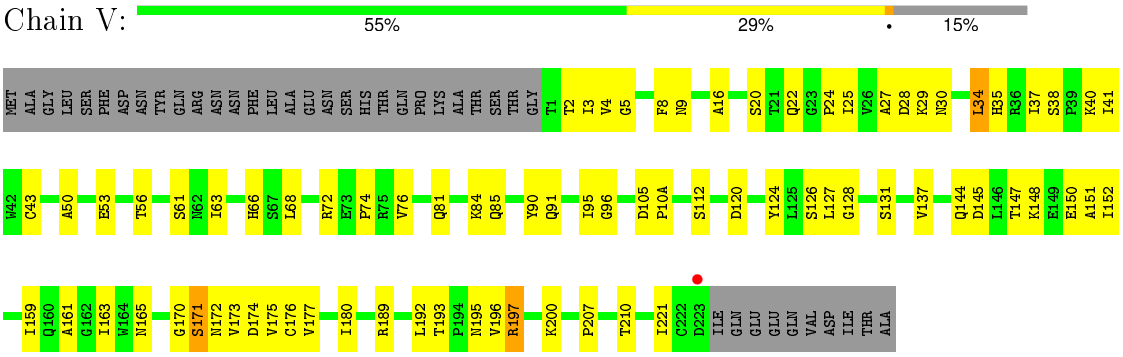
• Molecule 8: Proteasome component PUP1

Chain H:



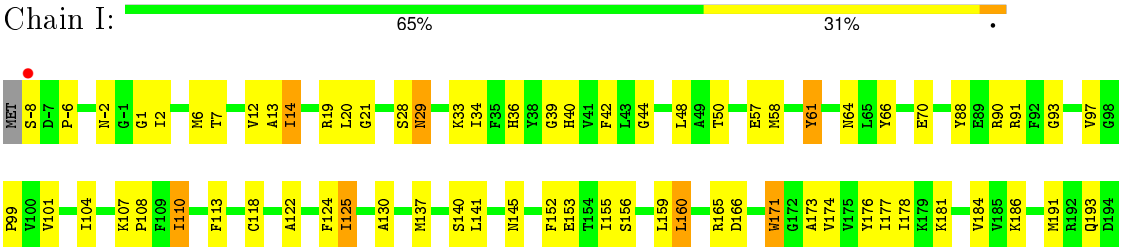
• Molecule 8: Proteasome component PUP1

Chain V:



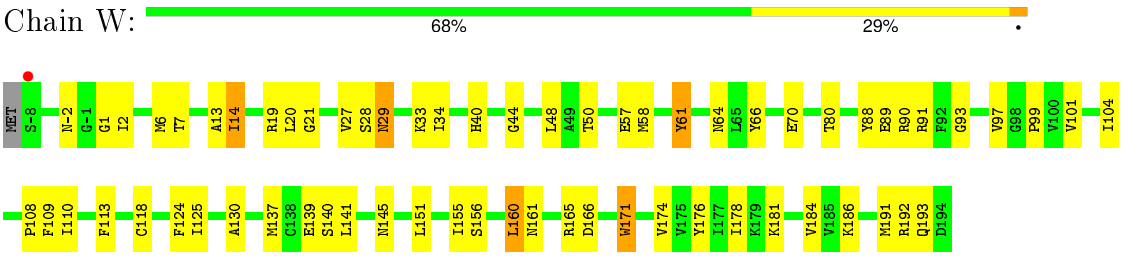
• Molecule 9: Proteasome component PUP3

Chain I:



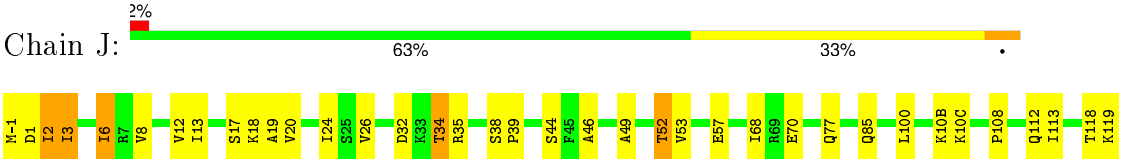
• Molecule 9: Proteasome component PUP3

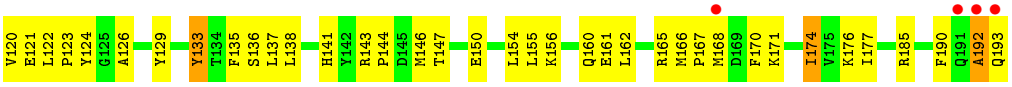
Chain W:



• Molecule 10: Proteasome component C11

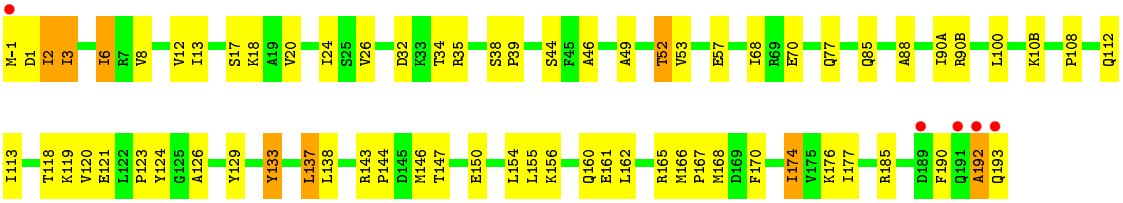
Chain J:





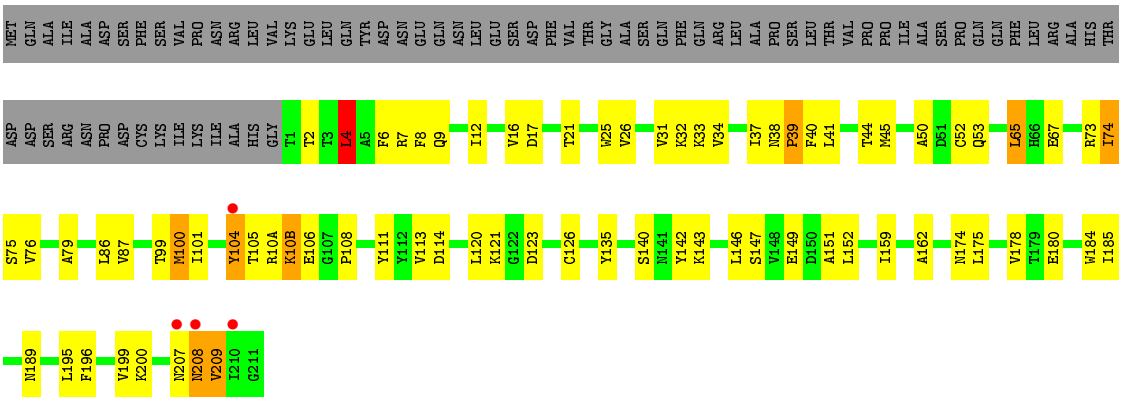
• Molecule 10: Proteasome component C11

Chain X:



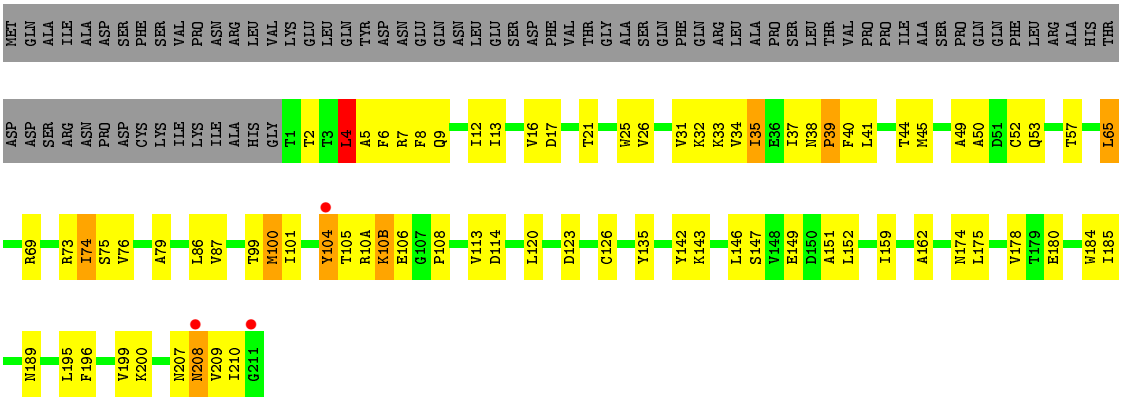
• Molecule 11: Proteasome component PRE2

Chain K:



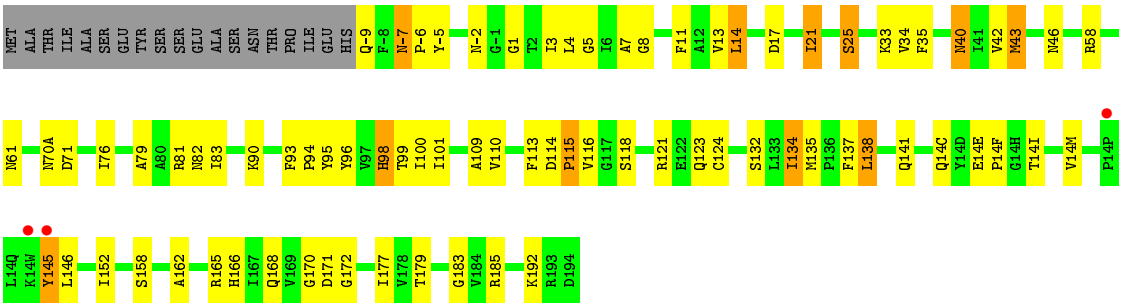
• Molecule 11: Proteasome component PRE2

Chain Y:



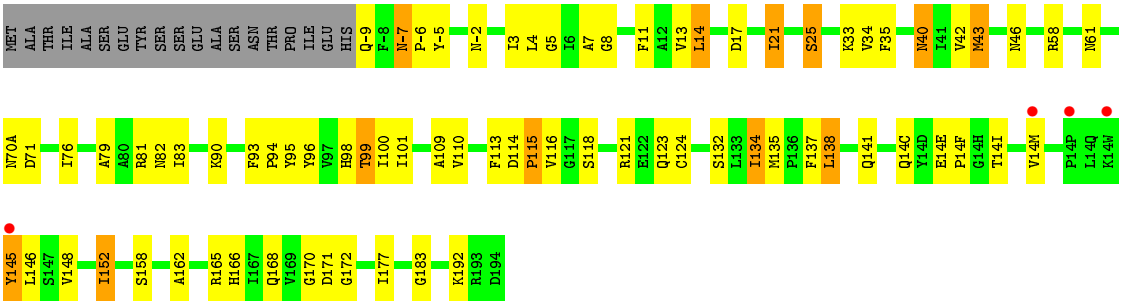
• Molecule 12: Proteasome component C5

Chain L:



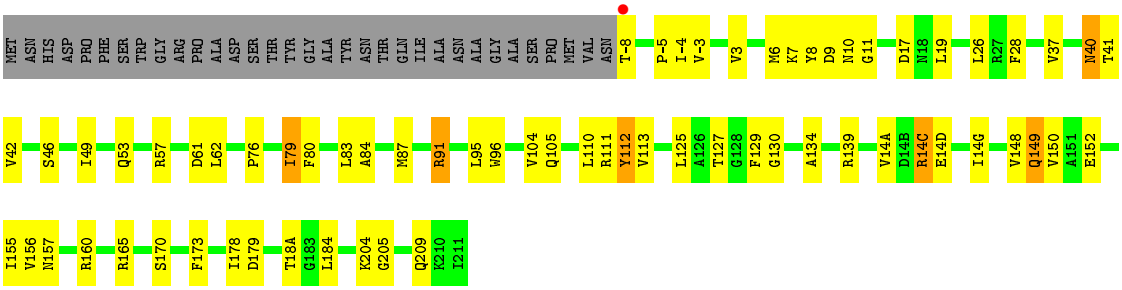
• Molecule 12: Proteasome component C5

Chain Z:



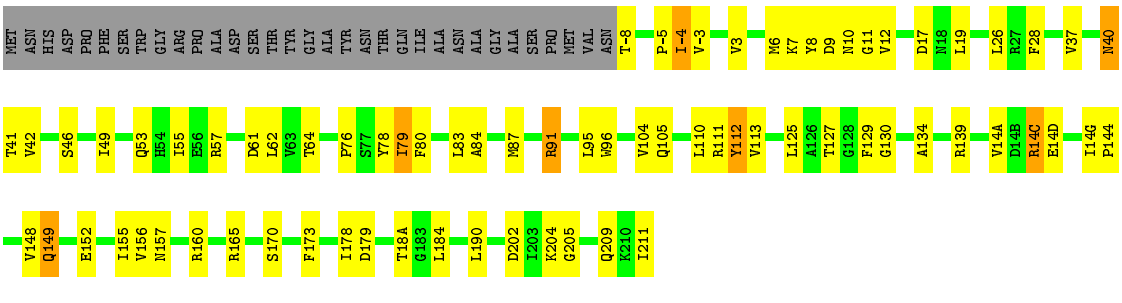
• Molecule 13: Proteasome component PRE4

Chain M:



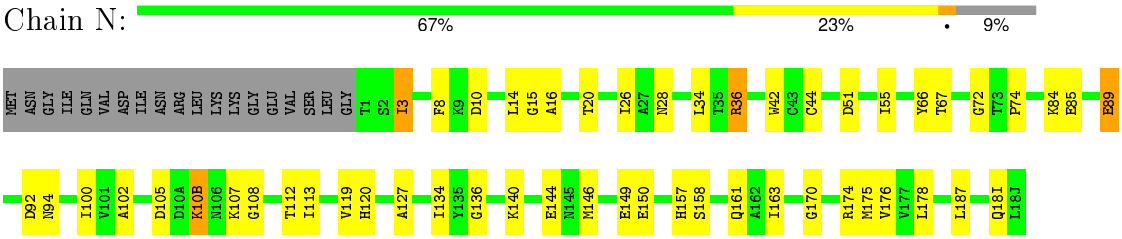
• Molecule 13: Proteasome component PRE4

Chain 1:



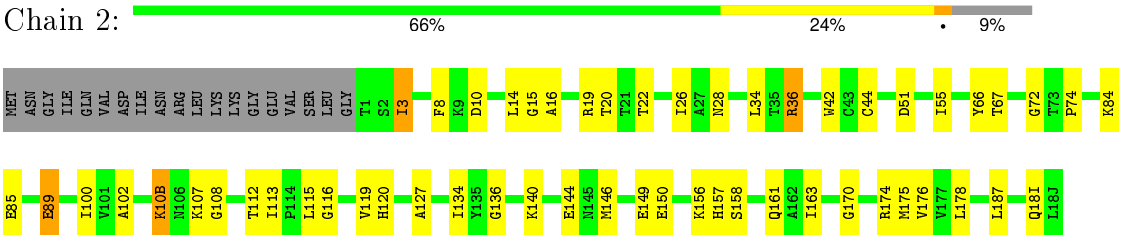
• Molecule 14: Proteasome component PRE3

Chain N:



- Molecule 14: Proteasome component PRE3

Chain 2:



- Molecule 15: TMC-95A mimic ligand 2c

Chain 3:

- Molecule 15: TMC-95A mimic ligand 2c

Chain 4:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.20Å 300.11Å 143.63Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 49.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.70) 99.7 (49.68-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.226 , 0.248 0.225 , 0.226	Depositor DCC
R_{free} test set	14176 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.902	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 359106 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	50982	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TY5, BOC, ABN, RE3

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	0.38	0/1952	0.64	0/2642
1	O	0.38	0/1952	0.64	0/2642
2	B	0.37	0/1934	0.64	0/2618
2	P	0.39	0/1934	0.64	0/2618
3	C	0.36	0/1919	0.62	0/2598
3	Q	0.38	0/1919	0.62	0/2598
4	D	0.37	0/1886	0.63	0/2541
4	R	0.38	0/1886	0.63	0/2541
5	E	0.36	0/1823	0.62	0/2463
5	S	0.38	0/1823	0.62	0/2463
6	F	0.38	0/1936	0.62	0/2614
6	T	0.39	0/1936	0.63	0/2614
7	G	0.41	0/1959	0.64	0/2652
7	U	0.40	0/1959	0.64	0/2652
8	H	0.37	0/1715	0.66	0/2326
8	V	0.36	0/1715	0.66	0/2326
9	I	0.40	0/1611	0.68	0/2174
9	W	0.41	0/1611	0.68	0/2174
10	J	0.40	0/1613	0.66	0/2173
10	X	0.40	0/1613	0.67	0/2173
11	K	0.46	0/1681	0.67	1/2274 (0.0%)
11	Y	0.46	0/1681	0.68	1/2274 (0.0%)
12	L	0.41	0/1795	0.68	0/2420
12	Z	0.41	0/1795	0.68	0/2420
13	1	0.40	0/1855	0.68	1/2514 (0.0%)
13	M	0.39	0/1855	0.67	1/2514 (0.0%)
14	2	0.40	0/1541	0.64	1/2087 (0.0%)
14	N	0.40	0/1541	0.64	0/2087
15	3	0.78	0/4	2.03	0/4
15	4	0.90	0/4	2.10	0/4
All	All	0.39	0/50448	0.65	5/68200 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	4	LEU	CA-CB-CG	5.65	128.30	115.30
11	K	4	LEU	CA-CB-CG	5.59	128.15	115.30
13	1	95	LEU	N-CA-C	-5.45	96.29	111.00
13	M	95	LEU	N-CA-C	-5.24	96.86	111.00
14	2	22	THR	N-CA-C	-5.18	97.01	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

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	1915	0	1926	54	0
1	O	1915	0	1926	58	0
2	B	1904	0	1901	92	0
2	P	1904	0	1901	89	0
3	C	1890	0	1900	97	0
3	Q	1890	0	1900	98	0
4	D	1861	0	1836	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	1861	0	1836	55	0
5	E	1795	0	1797	95	0
5	S	1795	0	1797	108	0
6	F	1896	0	1886	73	0
6	T	1896	0	1886	84	0
7	G	1921	0	1910	72	0
7	U	1921	0	1910	77	0
8	H	1684	0	1688	57	0
8	V	1684	0	1688	60	0
9	I	1581	0	1574	63	0
9	W	1581	0	1574	59	0
10	J	1585	0	1590	89	0
10	X	1585	0	1590	77	0
11	K	1644	0	1595	73	0
11	Y	1644	0	1595	79	0
12	L	1757	0	1711	70	0
12	Z	1757	0	1711	74	0
13	1	1824	0	1832	65	0
13	M	1824	0	1832	59	0
14	2	1512	0	1481	53	0
14	N	1512	0	1481	50	0
15	3	55	0	44	4	0
15	4	55	0	44	4	0
16	1	78	0	0	4	0
16	2	58	0	0	4	0
16	A	57	0	0	2	0
16	B	36	0	0	1	0
16	C	44	0	0	2	0
16	D	41	0	0	2	0
16	E	23	0	0	3	0
16	F	45	0	0	2	0
16	G	64	0	0	0	0
16	H	51	0	0	5	0
16	I	69	0	0	3	0
16	J	51	0	0	7	0
16	K	40	0	0	4	0
16	L	56	0	0	7	0
16	M	73	0	0	4	0
16	N	54	0	0	4	0
16	O	34	0	0	1	0
16	P	29	0	0	3	0
16	Q	27	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	R	31	0	0	2	0
16	S	20	0	0	1	0
16	T	38	0	0	3	0
16	U	64	0	0	8	0
16	V	47	0	0	4	0
16	W	61	0	0	1	0
16	X	48	0	0	3	0
16	Y	47	0	0	8	0
16	Z	48	0	0	4	0
All	All	50982	0	49342	1804	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1804) 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)
11:K:208:ASN:ND2	9:W:29:ASN:HD21	1.22	1.32
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	1.23	1.30
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.05	1.18
2:P:202:THR:HG22	2:P:204:SER:H	1.10	1.14
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.05	1.13
2:B:202:THR:HG22	2:B:204:SER:H	1.11	1.09
10:J:133:TYR:HD1	16:Y:593:HOH:O	1.38	1.05
11:K:208:ASN:ND2	9:W:29:ASN:ND2	2.05	1.04
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.37	1.04
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.37	1.03
10:J:133:TYR:HE1	16:X:876:HOH:O	1.43	1.01
9:I:29:ASN:ND2	11:Y:208:ASN:ND2	2.07	1.01
2:B:71:ASN:ND2	2:B:72:ASP:H	1.58	1.01
11:K:208:ASN:HD21	9:W:29:ASN:ND2	1.59	1.00
9:I:29:ASN:ND2	11:Y:208:ASN:HD21	1.59	1.00
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.41	1.00
2:B:15:PHE:H	3:C:23:GLN:HE22	1.08	0.98
2:P:71:ASN:ND2	2:P:72:ASP:H	1.60	0.97
11:K:207:ASN:ND2	10:X:144:PRO:HG3	1.79	0.96
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.30	0.96
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.29	0.96
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.29	0.95
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.46	0.94
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.93	0.93
3:C:163:GLN:NE2	3:C:164:THR:H	1.66	0.93
2:B:71:ASN:HD22	2:B:72:ASP:H	1.14	0.92
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.52	0.91
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.52	0.91
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.36	0.91
1:A:15:PHE:H	2:B:23:GLN:HE22	1.17	0.91
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.68	0.90
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.52	0.90
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.52	0.90
1:O:15:PHE:H	2:P:23:GLN:HE22	1.13	0.89
3:C:163:GLN:HE21	3:C:164:THR:N	1.69	0.89
3:C:163:GLN:HE21	3:C:164:THR:H	0.91	0.89
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.69	0.89
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.18	0.89
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.71	0.89
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.55	0.88
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.38	0.88
13:M:157:ASN:HD22	13:M:160:ARG:HH11	0.89	0.88
2:P:71:ASN:HD22	2:P:72:ASP:H	1.15	0.88
9:W:14:ILE:HG12	9:W:34:ILE:HD12	1.55	0.88
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	1.89	0.88
9:I:29:ASN:HD21	11:Y:208:ASN:HD21	0.91	0.87
11:K:208:ASN:HD21	9:W:29:ASN:HD21	0.91	0.87
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.72	0.87
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.38	0.87
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.73	0.87
5:S:207:LEU:HD23	5:S:207:LEU:H	1.39	0.86
3:C:185:THR:HG22	3:C:187:GLU:H	1.38	0.86
11:K:73:ARG:NH2	11:K:104:TYR:O	2.09	0.86
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.72	0.86
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.92	0.86
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.89	0.85
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.09	0.85
5:E:207:LEU:HD23	5:E:207:LEU:H	1.40	0.85
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.90	0.85
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.87	0.85
11:K:99:THR:HG22	11:K:113:VAL:O	1.76	0.85
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.56	0.85
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.59	0.85
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.92	0.85
9:I:14:ILE:HG12	9:I:34:ILE:HD12	1.58	0.84
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.56	0.84
3:C:185:THR:HB	3:C:188:GLU:HG2	1.58	0.83
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.93	0.83
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.58	0.83
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.43	0.83
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.59	0.83
11:K:142:TYR:O	11:K:143:LYS:HD2	1.79	0.82
10:J:-1:MET:HG2	10:J:1:ASP:H	1.44	0.82
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.58	0.82
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.28	0.82
11:K:208:ASN:HB3	16:K:776:HOH:O	1.79	0.82
2:B:71:ASN:HD22	2:B:72:ASP:N	1.78	0.82
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	1.94	0.82
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.26	0.81
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	1.95	0.81
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.09	0.81
2:P:71:ASN:HD22	2:P:72:ASP:N	1.78	0.81
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.28	0.81
10:J:168:MET:HE3	10:X:168:MET:HE3	1.64	0.80
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.81	0.80
2:P:202:THR:HG22	2:P:204:SER:N	1.95	0.80
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.64	0.80
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.87	0.80
6:T:109:ILE:HD13	6:T:109:ILE:N	1.97	0.79
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.62	0.79
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.12	0.79
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.48	0.79
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.31	0.79
6:F:35:THR:HG21	6:F:51:GLU:O	1.82	0.79
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.48	0.79
10:X:-1:MET:HG2	10:X:1:ASP:H	1.46	0.79
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.65	0.78
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.47	0.78
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.65	0.78
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.19	0.78
3:C:232:TYR:O	3:C:236:ILE:HG12	1.83	0.78
6:T:35:THR:HG21	6:T:51:GLU:O	1.82	0.77
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.82	0.77
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.97	0.77
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.65	0.77
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.49	0.77
12:L:166:HIS:HD2	12:L:168:GLN:H	1.33	0.77
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.31	0.77
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.15	0.77
14:N:3:ILE:HD13	14:N:3:ILE:O	1.84	0.77
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.66	0.77
3:Q:232:TYR:O	3:Q:236:ILE:HG12	1.84	0.77
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.66	0.76
5:E:167:ALA:HB3	16:E:1131:HOH:O	1.85	0.76
6:F:109:ILE:HD13	6:F:109:ILE:N	2.00	0.76
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.68	0.76
7:U:87:ASN:HD22	7:U:87:ASN:C	1.88	0.76
2:B:202:THR:HG22	2:B:204:SER:N	1.95	0.75
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.86	0.75
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.52	0.75
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.51	0.75
11:K:208:ASN:HD22	9:W:29:ASN:HD21	1.28	0.75
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.67	0.75
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.99	0.75
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.15	0.75
3:Q:65:SER:HB2	16:Q:303:HOH:O	1.86	0.75
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.69	0.75
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.69	0.75
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.21	0.75
7:G:87:ASN:HD22	7:G:87:ASN:C	1.90	0.74
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.33	0.74
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.68	0.74
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.69	0.74
9:I:29:ASN:HD21	11:Y:208:ASN:HD22	1.30	0.74
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.85	0.74
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	1.86	0.74
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.69	0.74
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.52	0.74
2:P:71:ASN:ND2	2:P:72:ASP:N	2.36	0.74
10:J:2:ILE:O	10:J:3:ILE:HD13	1.87	0.74
10:X:2:ILE:O	10:X:3:ILE:HD13	1.87	0.74
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.01	0.73
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.68	0.73
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.22	0.73
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.24	0.73
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.71	0.73
2:B:71:ASN:ND2	2:B:72:ASP:N	2.34	0.73
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.18	0.73
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.70	0.73
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.18	0.73
7:G:59:LEU:O	7:G:61:PRO:HD3	1.88	0.73
5:S:15:PHE:H	6:T:23:GLN:HE22	1.36	0.72
7:U:59:LEU:O	7:U:61:PRO:HD3	1.89	0.72
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.38	0.72
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.54	0.72
9:W:27:VAL:HG13	16:X:622:HOH:O	1.88	0.72
10:J:24:ILE:O	10:X:133:TYR:OH	2.08	0.72
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.70	0.72
7:U:172:ILE:HD13	7:U:197:MET:HE1	1.71	0.72
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	1.87	0.72
8:V:53:GLU:HB2	16:V:1327:HOH:O	1.88	0.72
5:E:97:ASN:HD21	12:L:61:ASN:ND2	1.88	0.71
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.89	0.71
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.54	0.71
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.55	0.71
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.90	0.71
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.03	0.71
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.71	0.71
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.72	0.71
11:Y:180:GLU:N	16:Y:812:HOH:O	2.06	0.71
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.70	0.71
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.72	0.71
12:L:21:ILE:C	12:L:21:ILE:HD13	2.11	0.71
3:C:71:ASP:HA	10:J:68:ILE:HD13	1.71	0.71
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.55	0.70
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.72	0.70
6:T:237:GLN:O	6:T:240:ILE:HG22	1.91	0.70
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.55	0.70
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.72	0.70
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.74	0.70
5:E:12:THR:HG21	5:E:124:THR:HA	1.74	0.70
6:T:79:SER:HA	16:T:1238:HOH:O	1.92	0.70
12:Z:21:ILE:C	12:Z:21:ILE:HD13	2.11	0.70
7:U:86:ARG:HD2	16:U:248:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.72	0.70
7:U:17:PRO:HD3	16:U:584:HOH:O	1.91	0.70
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.73	0.70
3:Q:191:LYS:HG3	3:Q:236:ILE:HD11	1.74	0.70
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.92	0.70
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.74	0.69
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.27	0.69
12:L:98:HIS:HD2	16:L:199:HOH:O	1.76	0.69
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.22	0.69
5:E:207:LEU:CD2	5:E:207:LEU:H	2.06	0.69
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.74	0.69
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.73	0.69
5:S:207:LEU:H	5:S:207:LEU:CD2	2.05	0.69
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.27	0.69
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.74	0.69
14:2:3:ILE:HD11	14:2:127:ALA:HB3	1.74	0.69
2:P:163:ILE:HG12	2:P:164:SER:H	1.57	0.69
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.75	0.69
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.41	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.69
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.39	0.68
9:I:6:MET:CE	9:I:155:ILE:HA	2.22	0.68
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.93	0.68
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.39	0.68
12:Z:114:ASP:HB3	12:Z:118:SER:H	1.58	0.68
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.91	0.68
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.75	0.68
13:1:-3:VAL:HG12	13:1:49:ILE:HG13	1.75	0.68
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.59	0.68
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.08	0.68
14:N:3:ILE:H	14:N:3:ILE:HD12	1.58	0.68
7:U:67:ILE:HD13	7:U:211:GLU:HG2	1.76	0.68
12:L:96:TYR:CD1	15:3:2:TY5:H49	2.28	0.68
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.04	0.68
6:T:54:ILE:HG12	6:T:208:PHE:HA	1.74	0.68
14:2:51:ASP:O	14:2:55:ILE:HG12	1.94	0.68
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.74	0.68
1:O:121:GLN:O	1:O:124:THR:HB	1.94	0.68
1:O:118:LYS:HE2	1:O:122:GLU:OE1	1.94	0.68
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	1.75	0.68
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.56	0.68
12:Z:96:TYR:CD1	15:4:2:TY5:H49	2.28	0.68
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.24	0.67
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.75	0.67
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.76	0.67
3:C:186:VAL:O	3:C:190:VAL:HG23	1.95	0.67
3:C:191:LYS:HG3	3:C:236:ILE:HD11	1.74	0.67
9:W:6:MET:CE	9:W:155:ILE:HA	2.24	0.67
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.24	0.67
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.77	0.67
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.10	0.67
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.95	0.67
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.07	0.67
5:S:198:SER:HA	5:S:201:LEU:HG	1.76	0.67
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.39	0.67
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.30	0.67
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.76	0.67
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.09	0.67
12:L:114:ASP:HB3	12:L:118:SER:H	1.60	0.67
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.58	0.67
5:S:12:THR:HG21	5:S:124:THR:HA	1.75	0.67
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.58	0.67
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.25	0.67
7:U:67:ILE:HD13	7:U:211:GLU:CD	2.15	0.67
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.59	0.67
2:B:15:PHE:H	3:C:23:GLN:NE2	1.89	0.67
11:K:40:PHE:CB	11:K:73:ARG:NH2	2.58	0.67
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.77	0.67
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.92	0.67
10:J:133:TYR:OH	10:X:24:ILE:O	2.12	0.66
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.75	0.66
7:G:172:ILE:HD13	7:G:197:MET:CE	2.26	0.66
9:W:6:MET:HE1	9:W:155:ILE:HA	1.75	0.66
4:R:72:ARG:HG3	16:R:1302:HOH:O	1.95	0.66
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.78	0.66
7:G:67:ILE:HD13	7:G:211:GLU:CD	2.15	0.66
8:V:148:LYS:O	8:V:152:ILE:HG12	1.95	0.66
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.77	0.66
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.95	0.66
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.59	0.66
5:E:198:SER:HA	5:E:201:LEU:HG	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:121:GLN:O	2:P:124:THR:HB	1.94	0.66
8:V:128:GLY:O	8:V:131:SER:HB2	1.94	0.66
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.09	0.66
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	1.96	0.66
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.42	0.66
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.78	0.66
6:F:237:GLN:O	6:F:240:ILE:HG22	1.94	0.66
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.09	0.66
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.08	0.66
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.77	0.66
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.96	0.66
5:E:15:PHE:H	6:F:23:GLN:HE22	1.43	0.66
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.77	0.66
8:H:148:LYS:O	8:H:152:ILE:HG12	1.95	0.66
2:P:101:LYS:NZ	10:X:85:GLN:HE22	1.93	0.66
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.31	0.66
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.60	0.66
14:N:51:ASP:O	14:N:55:ILE:HG12	1.94	0.66
1:A:118:LYS:HE2	1:A:122:GLU:OE1	1.96	0.66
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.57	0.65
7:U:121:GLN:O	7:U:124:THR:HB	1.95	0.65
7:G:67:ILE:HD13	7:G:211:GLU:HG2	1.77	0.65
5:S:201:LEU:O	5:S:202:ARG:HB2	1.96	0.65
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.11	0.65
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.76	0.65
3:C:41:LYS:HG2	3:C:161:SER:O	1.95	0.65
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.61	0.65
13:1:149:GLN:H	13:1:149:GLN:NE2	1.94	0.65
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.60	0.65
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.44	0.65
6:F:54:ILE:HG12	6:F:208:PHE:HA	1.77	0.65
13:M:149:GLN:NE2	13:M:149:GLN:H	1.95	0.65
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.79	0.65
6:T:54:ILE:HD11	6:T:209:GLU:HB2	1.77	0.65
7:G:121:GLN:O	7:G:124:THR:HB	1.97	0.65
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.78	0.65
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.43	0.65
8:H:128:GLY:O	8:H:131:SER:HB2	1.96	0.65
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.61	0.65
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.78	0.65
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.78	0.65
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.79	0.64
4:D:215:ILE:HD13	4:D:215:ILE:C	2.18	0.64
12:L:114:ASP:CB	12:L:118:SER:HB3	2.26	0.64
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.01	0.64
3:Q:21:ILE:N	3:Q:21:ILE:HD13	2.12	0.64
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.32	0.64
5:E:221:PHE:HE1	5:E:223:ILE:HD11	1.61	0.64
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.97	0.64
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.79	0.64
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.78	0.64
11:Y:31:VAL:HG11	15:4:5:ABN:H3	1.79	0.64
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.61	0.64
12:L:135:MET:CE	9:W:165:ARG:NH2	2.61	0.64
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.79	0.64
1:A:121:GLN:O	1:A:124:THR:HB	1.97	0.64
9:I:6:MET:HE1	9:I:155:ILE:HA	1.78	0.64
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.80	0.64
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.13	0.64
5:E:201:LEU:O	5:E:202:ARG:HB2	1.97	0.64
11:K:31:VAL:HG11	15:3:5:ABN:H3	1.80	0.64
8:H:172:ASN:HD22	8:H:193:THR:HA	1.63	0.64
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.63	0.64
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.97	0.64
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.12	0.64
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	1.97	0.64
7:U:172:ILE:HD13	7:U:197:MET:CE	2.28	0.63
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.46	0.63
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.80	0.63
8:V:196:VAL:HG23	16:V:652:HOH:O	1.96	0.63
14:2:107:LYS:HG2	14:2:108:GLY:H	1.63	0.63
4:R:53:ARG:HG2	4:R:53:ARG:O	1.97	0.63
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.81	0.63
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.80	0.63
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.80	0.63
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.80	0.63
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.64	0.63
5:S:221:PHE:HE1	5:S:223:ILE:HD11	1.61	0.63
6:T:177:GLU:OE2	7:U:57:LYS:HE2	1.99	0.63
2:B:163:ILE:HG12	2:B:164:SER:H	1.63	0.63
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:HD23	5:E:207:LEU:N	2.14	0.63
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	1.97	0.63
6:T:109:ILE:CD1	6:T:109:ILE:N	2.62	0.63
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.81	0.63
12:Z:114:ASP:CB	12:Z:118:SER:HB3	2.29	0.62
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.99	0.62
5:E:73:HIS:HE1	5:E:107:LEU:O	1.81	0.62
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.81	0.62
5:S:214:ILE:HG12	5:S:215:VAL:N	2.13	0.62
7:U:67:ILE:HD13	7:U:211:GLU:CG	2.30	0.62
11:Y:40:PHE:CB	11:Y:73:ARG:NH2	2.62	0.62
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.80	0.62
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.82	0.62
5:S:132:TYR:O	5:S:153:PRO:HB3	1.99	0.62
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.35	0.62
14:N:107:LYS:HG2	14:N:108:GLY:H	1.64	0.62
10:X:-1:MET:HG2	10:X:1:ASP:N	2.15	0.62
7:G:172:ILE:HD13	7:G:197:MET:HE1	1.81	0.62
8:H:90:TYR:CB	8:H:95:ILE:HD13	2.30	0.62
8:V:90:TYR:CB	8:V:95:ILE:HD13	2.30	0.62
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.14	0.62
2:P:185:LYS:HD3	2:P:186:VAL:N	2.15	0.62
8:V:221:ILE:HD12	9:W:40:HIS:HA	1.82	0.62
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.99	0.62
13:1:152:GLU:O	13:1:156:VAL:HG23	1.99	0.62
4:D:53:ARG:HG2	4:D:53:ARG:O	2.00	0.62
10:J:-1:MET:HG2	10:J:1:ASP:N	2.13	0.61
5:E:97:ASN:ND2	12:L:61:ASN:HD21	1.98	0.61
16:P:462:HOH:O	3:Q:87:ILE:HD11	2.00	0.61
11:K:184:TRP:O	11:K:185:ILE:HD13	2.00	0.61
10:X:44:SER:OG	10:X:100:LEU:HB2	2.00	0.61
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.63	0.61
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.81	0.61
13:1:37:VAL:HG11	13:1:79:ILE:CD1	2.30	0.61
2:P:163:ILE:HG12	2:P:164:SER:N	2.14	0.61
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.82	0.61
5:S:73:HIS:HE1	5:S:107:LEU:O	1.81	0.61
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.82	0.61
13:M:37:VAL:HG11	13:M:79:ILE:CD1	2.30	0.61
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.30	0.61
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:2:ILE:HD13	10:X:2:ILE:N	2.14	0.61
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.30	0.61
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.02	0.61
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.82	0.61
5:E:214:ILE:HG12	5:E:215:VAL:N	2.16	0.61
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.31	0.61
2:B:237:GLY:C	2:B:238:ILE:HD13	2.20	0.61
13:M:152:GLU:O	13:M:156:VAL:HG23	2.01	0.60
5:E:227:GLU:CD	5:E:227:GLU:H	2.04	0.60
4:R:24:VAL:O	4:R:27:SER:HB3	2.00	0.60
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.02	0.60
2:B:15:PHE:N	3:C:23:GLN:HE22	1.90	0.60
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.12	0.60
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.30	0.60
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.35	0.60
3:C:57:LYS:O	3:C:58:LEU:HB2	2.01	0.60
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.82	0.60
12:L:90:LYS:HE3	12:L:93:PHE:O	2.02	0.60
7:G:67:ILE:HD13	7:G:211:GLU:CG	2.31	0.60
8:V:81:GLN:O	8:V:85:GLN:HG3	2.00	0.60
2:P:237:GLY:C	2:P:238:ILE:HD13	2.22	0.60
13:M:40:ASN:H	13:M:40:ASN:HD22	1.49	0.60
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.17	0.60
4:D:102:TYR:O	12:L:81:ARG:HG3	2.02	0.60
3:C:15:PHE:H	4:D:23:GLN:HE22	1.47	0.60
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.15	0.60
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.84	0.60
3:Q:170:LYS:HB2	16:Q:833:HOH:O	2.00	0.60
8:V:172:ASN:HD22	8:V:193:THR:HA	1.66	0.60
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.02	0.60
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.17	0.60
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.37	0.60
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.37	0.60
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.15	0.60
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.16	0.60
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.83	0.60
2:B:185:LYS:HD3	2:B:186:VAL:N	2.16	0.60
4:R:186:LEU:O	4:R:190:GLU:HG3	2.02	0.59
8:V:34:LEU:HB2	16:V:578:HOH:O	2.00	0.59
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.84	0.59
2:P:143:ASP:OD2	10:X:10(B):LYS:HE2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:210:ILE:HB	16:Y:1226:HOH:O	2.01	0.59
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.15	0.59
3:C:185:THR:HG22	3:C:187:GLU:N	2.13	0.59
7:U:87:ASN:ND2	7:U:87:ASN:C	2.54	0.59
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.85	0.59
10:J:44:SER:OG	10:J:100:LEU:HB2	2.03	0.59
1:A:40:ILE:HD13	1:A:193:ALA:HB2	1.83	0.59
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.83	0.59
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.37	0.59
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.83	0.59
4:R:215:ILE:HD13	4:R:215:ILE:C	2.22	0.59
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.84	0.59
5:E:132:TYR:O	5:E:153:PRO:HB3	2.02	0.59
13:1:40:ASN:HD22	13:1:40:ASN:H	1.50	0.59
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.37	0.59
10:J:168:MET:CE	10:X:168:MET:HE3	2.32	0.59
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.83	0.59
5:S:207:LEU:N	5:S:207:LEU:HD23	2.13	0.59
7:G:87:ASN:ND2	7:G:87:ASN:C	2.56	0.59
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.84	0.59
5:S:227:GLU:CD	5:S:227:GLU:H	2.04	0.59
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.85	0.59
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.37	0.59
8:H:81:GLN:O	8:H:85:GLN:HG3	2.02	0.59
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.03	0.59
13:M:17:ASP:HA	13:M:173:PHE:CB	2.33	0.59
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.02	0.59
11:K:10(A):ARG:HB3	11:K:10(B):LYS:HE3	1.85	0.59
14:N:3:ILE:HD11	14:N:127:ALA:HB3	1.84	0.59
10:X:113:ILE:HA	10:X:118:THR:O	2.03	0.59
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.83	0.59
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.18	0.58
11:K:12:ILE:HB	11:K:178:VAL:HB	1.84	0.58
10:X:13:ILE:N	10:X:13:ILE:HD12	2.17	0.58
14:2:3:ILE:H	14:2:3:ILE:HD12	1.69	0.58
12:Z:3:ILE:HG13	12:Z:100:ILE:HD12	1.85	0.58
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.38	0.58
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.33	0.58
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.34	0.58
10:X:52:THR:CG2	10:X:53:VAL:N	2.66	0.58
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:19:LEU:HD12	13:1:28:PHE:O	2.04	0.58
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.84	0.58
9:I:39:GLY:HA3	16:I:416:HOH:O	2.02	0.58
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.84	0.58
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.18	0.58
5:E:54:ASN:ND2	5:E:56:ASP:O	2.35	0.58
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.39	0.58
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.84	0.58
4:D:24:VAL:O	4:D:27:SER:HB3	2.03	0.58
12:Z:21:ILE:CD1	12:Z:21:ILE:C	2.72	0.58
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.84	0.58
5:E:226:GLY:O	5:E:229:VAL:HG22	2.04	0.58
11:K:40:PHE:CG	11:K:73:ARG:CZ	2.87	0.58
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.19	0.58
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.33	0.58
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.86	0.58
7:G:233:LEU:O	7:G:236:ILE:HG13	2.04	0.58
10:J:52:THR:CG2	10:J:53:VAL:N	2.66	0.58
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.04	0.58
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.34	0.58
14:2:3:ILE:HG22	14:2:16:ALA:HB1	1.86	0.58
5:S:194:VAL:O	5:S:197:ILE:HG22	2.04	0.57
14:N:3:ILE:N	14:N:3:ILE:HD12	2.19	0.57
6:F:109:ILE:CD1	6:F:109:ILE:N	2.66	0.57
6:F:67:ILE:HB	6:F:223:PHE:CE2	2.39	0.57
1:A:186:LEU:O	1:A:190:ILE:HG13	2.04	0.57
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.86	0.57
4:R:102:TYR:O	12:Z:81:ARG:HG3	2.03	0.57
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.35	0.57
8:H:221:ILE:HD12	9:I:40:HIS:HA	1.86	0.57
11:Y:184:TRP:O	11:Y:185:ILE:HD13	2.03	0.57
5:S:226:GLY:O	5:S:229:VAL:HG22	2.05	0.57
3:C:185:THR:HG22	3:C:186:VAL:N	2.19	0.57
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.69	0.57
4:D:186:LEU:O	4:D:190:GLU:HG3	2.05	0.57
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.85	0.57
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.86	0.57
1:O:40:ILE:HD13	1:O:193:ALA:HB2	1.84	0.57
5:S:78:LEU:HD12	5:S:78:LEU:C	2.24	0.57
10:J:133:TYR:HE2	10:J:166:MET:SD	2.28	0.57
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:233:LEU:O	7:U:236:ILE:HG13	2.05	0.57
7:G:186:TRP:O	7:G:190:VAL:HG23	2.05	0.57
12:L:21:ILE:HB	12:L:25:SER:O	2.04	0.57
12:Z:21:ILE:HB	12:Z:25:SER:O	2.04	0.57
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.86	0.57
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.39	0.57
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.87	0.57
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.40	0.57
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.04	0.57
12:L:145:TYR:CD1	12:L:146:LEU:N	2.72	0.57
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.87	0.57
11:Y:40:PHE:CG	11:Y:73:ARG:CZ	2.88	0.57
14:N:3:ILE:C	14:N:3:ILE:HD13	2.25	0.57
12:L:96:TYR:CE1	15:3:2:TY5:H49	2.39	0.57
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.73	0.57
7:U:227:GLU:HG2	16:U:1255:HOH:O	2.04	0.57
6:T:172:ALA:O	6:T:176:LEU:HD22	2.05	0.57
13:1:17:ASP:HA	13:1:173:PHE:CB	2.35	0.57
10:X:90(B):ARG:NH1	16:X:266:HOH:O	2.33	0.57
8:H:112:SER:OG	8:H:120:ASP:HB2	2.05	0.57
12:L:21:ILE:CD1	12:L:21:ILE:C	2.73	0.56
5:S:54:ASN:ND2	5:S:56:ASP:O	2.38	0.56
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.19	0.56
5:E:160:LEU:HD13	5:E:163:THR:HB	1.87	0.56
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.20	0.56
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.53	0.56
3:C:46:VAL:O	3:C:215:VAL:HG12	2.05	0.56
10:J:52:THR:HG22	10:J:53:VAL:N	2.21	0.56
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.05	0.56
6:F:172:ALA:O	6:F:176:LEU:HD22	2.06	0.56
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.17	0.56
14:2:107:LYS:HG2	14:2:108:GLY:N	2.20	0.56
6:T:173:LYS:O	6:T:177:GLU:HG3	2.06	0.56
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.87	0.56
12:L:1:GLY:N	16:L:755:HOH:O	2.39	0.56
8:V:90:TYR:HB3	8:V:95:ILE:HD13	1.87	0.56
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.41	0.56
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.87	0.56
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.87	0.56
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	2.06	0.56
5:E:78:LEU:HD12	5:E:78:LEU:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:215:ILE:HD13	4:R:216:THR:N	2.21	0.56
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.41	0.56
11:K:44:THR:OG1	11:K:100:MET:HB2	2.05	0.56
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.87	0.56
7:U:186:TRP:O	7:U:190:VAL:HG23	2.05	0.56
11:Y:10(A):ARG:HB3	11:Y:10(B):LYS:HE3	1.87	0.56
5:E:194:VAL:O	5:E:197:ILE:HG22	2.06	0.56
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.21	0.56
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.70	0.56
13:M:19:LEU:HD12	13:M:28:PHE:O	2.05	0.56
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.88	0.56
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.88	0.56
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.88	0.56
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.87	0.56
1:A:97:HIS:HD2	8:H:61:SER:OG	1.89	0.56
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.06	0.56
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.27	0.55
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.87	0.55
10:X:52:THR:HG22	10:X:53:VAL:H	1.70	0.55
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.41	0.55
12:L:177:ILE:HD12	12:L:177:ILE:N	2.21	0.55
2:B:143:ASP:OD2	10:J:10(B):LYS:HE2	2.06	0.55
6:T:67:ILE:HB	6:T:223:PHE:CE2	2.40	0.55
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.88	0.55
10:J:13:ILE:HG22	10:J:155:LEU:HD11	1.88	0.55
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.88	0.55
11:K:10(B):LYS:CD	11:K:10(B):LYS:N	2.60	0.55
14:2:3:ILE:HD12	14:2:127:ALA:O	2.05	0.55
10:J:113:ILE:HA	10:J:118:THR:O	2.05	0.55
7:G:107:MET:HE3	7:G:112:LEU:CD1	2.32	0.55
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.07	0.55
8:H:90:TYR:HB3	8:H:95:ILE:HD13	1.89	0.55
2:P:234:VAL:HA	2:P:239:THR:HA	1.88	0.55
10:X:156:LYS:O	10:X:160:GLN:HG3	2.07	0.55
9:W:156:SER:O	9:W:160:LEU:HB2	2.06	0.55
12:Z:96:TYR:CE1	15:4:2:TY5:H49	2.42	0.55
14:N:107:LYS:HG2	14:N:108:GLY:N	2.21	0.55
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.88	0.55
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.22	0.55
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.36	0.55
10:X:52:THR:HG22	10:X:53:VAL:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.07	0.55
6:T:147:HIS:HD2	16:T:282:HOH:O	1.90	0.55
5:S:227:GLU:N	5:S:227:GLU:CD	2.60	0.55
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.41	0.55
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.72	0.55
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.07	0.55
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.89	0.55
1:O:186:LEU:O	1:O:190:ILE:HG13	2.07	0.55
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.35	0.55
10:J:135:PHE:HZ	16:J:898:HOH:O	1.89	0.55
6:F:173:LYS:O	6:F:177:GLU:HG3	2.07	0.55
5:S:160:LEU:HD13	5:S:163:THR:HB	1.88	0.55
9:I:101:VAL:O	9:I:110:ILE:HA	2.07	0.54
7:G:55:PRO:HG2	7:G:56:ASP:H	1.72	0.54
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.37	0.54
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.07	0.54
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.42	0.54
10:J:13:ILE:N	10:J:13:ILE:HD12	2.23	0.54
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.37	0.54
6:F:192:GLN:O	6:F:196:ILE:HG13	2.07	0.54
6:T:186:ALA:O	6:T:190:VAL:HG23	2.07	0.54
13:1:148:VAL:HG23	16:1:182:HOH:O	2.06	0.54
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.08	0.54
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.72	0.54
10:X:133:TYR:HE2	10:X:166:MET:SD	2.30	0.54
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.42	0.54
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.07	0.54
14:N:3:ILE:HD12	14:N:127:ALA:O	2.08	0.54
14:2:3:ILE:CD1	14:2:3:ILE:O	2.55	0.54
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.22	0.54
3:C:21:ILE:CD1	3:C:21:ILE:N	2.71	0.54
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.88	0.54
7:G:77:VAL:CG1	7:G:137:THR:HB	2.38	0.54
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.07	0.54
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.89	0.54
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.08	0.54
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.05	0.54
5:E:227:GLU:CD	5:E:227:GLU:N	2.60	0.54
10:J:52:THR:HG22	10:J:53:VAL:H	1.71	0.54
3:C:35:THR:HB	3:C:51:GLU:HG3	1.90	0.54
2:B:234:VAL:HA	2:B:239:THR:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:105:ASP:HB2	16:N:775:HOH:O	2.07	0.54
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.42	0.54
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.22	0.54
7:U:55:PRO:HG2	7:U:56:ASP:H	1.72	0.54
5:S:78:LEU:HD12	5:S:78:LEU:O	2.08	0.54
3:Q:159:SER:O	4:R:59:LEU:HD22	2.08	0.54
7:U:38:LEU:HD23	7:U:197:MET:HE3	1.90	0.54
2:B:108:PRO:HB2	2:B:111:ILE:HD12	1.89	0.54
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.08	0.54
7:U:77:VAL:CG1	7:U:137:THR:HB	2.37	0.54
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.38	0.54
11:Y:31:VAL:HG11	15:4:5:ABN:C3	2.38	0.53
11:K:31:VAL:HG11	15:3:5:ABN:C3	2.38	0.53
4:R:121:LEU:HB2	16:R:853:HOH:O	2.07	0.53
11:Y:200:LYS:HE2	16:Y:772:HOH:O	2.07	0.53
3:C:175:PHE:O	3:C:179:ASN:HB2	2.09	0.53
11:K:32:LYS:N	11:K:32:LYS:HD2	2.23	0.53
13:M:14(C):ARG:CG	13:M:14(C):ARG:HH11	2.20	0.53
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.89	0.53
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.89	0.53
9:I:156:SER:O	9:I:160:LEU:HB2	2.08	0.53
2:B:181:LYS:O	2:B:184:MET:HG3	2.09	0.53
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.74	0.53
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.23	0.53
11:Y:210:ILE:HB	16:Y:1150:HOH:O	2.08	0.53
9:W:28:SER:CB	10:X:120:VAL:HG21	2.39	0.53
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.08	0.53
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.91	0.53
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.09	0.53
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.44	0.53
1:O:142:ASP:OD1	1:O:145:ASN:HB2	2.08	0.53
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.89	0.53
11:K:67:GLU:OE2	16:K:959:HOH:O	2.18	0.53
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.89	0.53
2:B:163:ILE:HG12	2:B:164:SER:N	2.22	0.53
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.08	0.53
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.44	0.53
10:J:156:LYS:O	10:J:160:GLN:HG3	2.09	0.53
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.24	0.53
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.89	0.53
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.44	0.53
5:E:18(D):ILE:O	5:E:18(D):ILE:HG12	2.09	0.53
2:P:108:PRO:HB2	2:P:111:ILE:HD12	1.90	0.53
3:C:21:ILE:N	3:C:21:ILE:HD13	2.23	0.53
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.57	0.53
2:P:27:ALA:O	2:P:31:ILE:HG12	2.09	0.53
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.29	0.53
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.73	0.53
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.05	0.53
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.39	0.53
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.08	0.53
2:P:63:THR:HG22	2:P:63:THR:O	2.09	0.53
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.39	0.53
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.22	0.53
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.09	0.53
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.89	0.53
11:K:74:ILE:HG12	11:K:79:ALA:HB2	1.91	0.53
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.23	0.53
6:T:67:ILE:HG12	6:T:211:GLU:OE1	2.09	0.53
1:O:62:GLU:C	1:O:64:LEU:H	2.10	0.53
12:Z:134:ILE:HD11	12:Z:162:ALA:HB2	1.91	0.53
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.43	0.53
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.09	0.53
9:I:6:MET:HE3	9:I:155:ILE:HA	1.91	0.53
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.09	0.53
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.91	0.53
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.25	0.53
7:U:107:MET:HE3	7:U:112:LEU:CD1	2.32	0.52
7:U:228:ASN:HB3	16:U:242:HOH:O	2.09	0.52
3:C:235:GLN:O	3:C:239:GLU:HG2	2.09	0.52
5:S:74:MET:HE2	5:S:109:VAL:HG22	1.91	0.52
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.74	0.52
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.09	0.52
7:U:49:ILE:CD1	7:U:212:VAL:HG22	2.39	0.52
6:F:101:LYS:NZ	14:N:85:GLU:OE1	2.42	0.52
2:B:27:ALA:O	2:B:31:ILE:HG12	2.09	0.52
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.29	0.52
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.44	0.52
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.91	0.52
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.57	0.52
6:T:36:THR:CG2	6:T:51:GLU:OE2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:238:ILE:N	2:P:238:ILE:HD13	2.24	0.52
10:J:13:ILE:CG2	10:J:155:LEU:HD11	2.40	0.52
11:K:74:ILE:HG13	11:K:75:SER:N	2.24	0.52
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.91	0.52
1:A:4:MET:SD	1:A:5:THR:N	2.68	0.52
10:X:13:ILE:HG22	10:X:155:LEU:HD11	1.91	0.52
8:V:38:SER:OG	8:V:41:ILE:HD13	2.10	0.52
8:V:112:SER:OG	8:V:120:ASP:HB2	2.09	0.52
1:A:69:LEU:HD23	1:A:69:LEU:C	2.30	0.52
14:N:3:ILE:HG22	14:N:16:ALA:HB1	1.92	0.52
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.08	0.52
3:Q:182:PRO:O	3:Q:184:ALA:N	2.43	0.52
12:Z:14(I):THR:HB	12:Z:14(M):VAL:HG23	1.92	0.52
3:C:20:HIS:HB3	3:C:25:GLU:OE1	2.10	0.52
1:A:62:GLU:C	1:A:64:LEU:H	2.13	0.52
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.92	0.52
9:W:101:VAL:O	9:W:110:ILE:HA	2.10	0.52
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.73	0.52
5:E:78:LEU:HD12	5:E:78:LEU:O	2.10	0.52
12:L:3:ILE:HG13	12:L:100:ILE:HD12	1.92	0.52
1:O:150:GLN:O	1:O:157:TYR:HA	2.10	0.52
12:L:79:ALA:O	12:L:83:ILE:HG12	2.09	0.52
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.92	0.52
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.10	0.52
11:K:104:TYR:CE1	11:K:180:GLU:OE2	2.63	0.52
10:X:143:ARG:HB2	10:X:146:MET:HG3	1.91	0.52
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.44	0.52
1:A:150:GLN:O	1:A:157:TYR:HA	2.09	0.52
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.45	0.52
3:Q:85:SER:O	3:Q:89:ILE:HG13	2.10	0.52
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.92	0.52
10:J:133:TYR:CD1	16:Y:593:HOH:O	2.28	0.52
4:D:237:LEU:O	4:D:241:GLU:HG3	2.10	0.52
7:G:198:ILE:HG23	7:G:203:THR:O	2.10	0.52
3:C:43:LYS:O	3:C:43:LYS:HG2	2.10	0.52
11:K:180:GLU:HB2	16:K:924:HOH:O	2.09	0.51
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.91	0.51
9:I:28:SER:CB	10:J:120:VAL:HG21	2.40	0.51
7:U:198:ILE:HG23	7:U:203:THR:O	2.10	0.51
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.24	0.51
7:G:49:ILE:CD1	7:G:212:VAL:HG22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.92	0.51
2:P:87:ILE:O	2:P:91:THR:HG23	2.10	0.51
11:Y:38:ASN:ND2	16:Y:1288:HOH:O	2.14	0.51
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.38	0.51
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.45	0.51
2:P:186:VAL:O	2:P:190:ILE:HG13	2.10	0.51
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.91	0.51
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.45	0.51
13:M:83:LEU:O	13:M:87:MET:HG2	2.10	0.51
4:D:112:LEU:C	4:D:112:LEU:HD13	2.30	0.51
4:R:112:LEU:C	4:R:112:LEU:HD13	2.31	0.51
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.92	0.51
8:H:35:HIS:CB	8:H:56:THR:HG21	2.39	0.51
12:Z:79:ALA:O	12:Z:83:ILE:HG12	2.10	0.51
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.31	0.51
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.11	0.51
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.25	0.51
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.11	0.51
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.92	0.51
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.26	0.51
2:B:63:THR:HG22	2:B:63:THR:O	2.11	0.51
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.40	0.51
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.90	0.51
6:F:186:ALA:O	6:F:190:VAL:HG23	2.10	0.51
11:K:105:THR:OG1	11:K:106:GLU:HG3	2.10	0.51
5:E:74:MET:HE2	5:E:109:VAL:HG22	1.91	0.51
5:E:95:GLN:HG3	5:E:115:LEU:HD13	1.91	0.51
1:O:177:GLU:HG2	2:P:58:LEU:HD22	1.92	0.51
11:Y:74:ILE:HG12	11:Y:79:ALA:HB2	1.91	0.51
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.90	0.51
7:U:77:VAL:HG12	7:U:137:THR:HB	1.91	0.51
11:Y:74:ILE:HG13	11:Y:75:SER:N	2.26	0.51
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.93	0.51
12:Z:21:ILE:O	12:Z:21:ILE:HD13	2.10	0.51
3:C:227:GLU:OE1	3:C:227:GLU:N	2.42	0.51
3:C:182:PRO:O	3:C:184:ALA:N	2.43	0.51
9:W:-2:ASN:HA	9:W:21:GLY:O	2.11	0.51
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.09	0.51
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.40	0.51
4:R:20:ARG:HD3	4:R:25:GLU:CD	2.32	0.51
9:I:90:ARG:HD2	16:I:1159:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.91	0.51
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.25	0.51
13:1:37:VAL:HG11	13:1:79:ILE:HD13	1.92	0.51
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.11	0.51
6:T:159:GLY:HA3	7:U:63:THR:HG21	1.93	0.51
2:P:181:LYS:O	2:P:184:MET:HG3	2.10	0.51
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.11	0.51
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.93	0.51
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.93	0.51
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.46	0.51
9:I:19:ARG:HB2	9:I:171:TRP:HB2	1.93	0.51
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.93	0.50
3:C:159:SER:O	4:D:59:LEU:HD22	2.11	0.50
2:B:87:ILE:O	2:B:91:THR:HG23	2.11	0.50
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.92	0.50
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.09	0.50
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.93	0.50
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.12	0.50
10:J:168:MET:CE	10:X:168:MET:CE	2.89	0.50
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.60	0.50
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.21	0.50
3:Q:191:LYS:CG	3:Q:236:ILE:HD11	2.41	0.50
3:C:57:LYS:HD2	3:C:58:LEU:N	2.26	0.50
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.11	0.50
13:1:83:LEU:O	13:1:87:MET:HG2	2.11	0.50
4:D:89:ILE:HB	16:D:1044:HOH:O	2.10	0.50
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.25	0.50
7:G:8:TYR:C	7:G:10:ARG:H	2.14	0.50
7:U:8:TYR:C	7:U:10:ARG:H	2.14	0.50
10:X:146:MET:HE3	10:X:150:GLU:HB3	1.92	0.50
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.41	0.50
2:P:229:ILE:O	2:P:233:LEU:HB2	2.12	0.50
4:R:237:LEU:O	4:R:241:GLU:HG3	2.11	0.50
5:E:223:ILE:HD12	5:E:223:ILE:N	2.26	0.50
5:S:223:ILE:N	5:S:223:ILE:HD12	2.26	0.50
13:M:40:ASN:HD22	13:M:40:ASN:N	2.08	0.50
12:Z:3:ILE:HD13	12:Z:46:ASN:HB2	1.93	0.50
10:J:156:LYS:HE2	10:J:160:GLN:NE2	2.26	0.50
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.93	0.50
14:N:26:ILE:HG13	13:1:165:ARG:O	2.12	0.50
6:F:69:VAL:HG12	16:M:319:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:-2:ASN:HA	9:I:21:GLY:O	2.11	0.50
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.95	0.50
10:J:26:VAL:HG23	10:X:165:ARG:O	2.11	0.50
13:1:157:ASN:HB3	16:1:558:HOH:O	2.10	0.50
8:H:165:ASN:HD22	13:1:139:ARG:NH1	2.06	0.50
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.94	0.50
5:S:95:GLN:HG3	5:S:115:LEU:HD13	1.93	0.50
3:C:38:VAL:HG22	3:C:39:GLY:N	2.25	0.50
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.92	0.50
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.94	0.50
10:X:156:LYS:HE2	10:X:160:GLN:NE2	2.27	0.50
9:W:48:LEU:HG	9:W:50:THR:HG22	1.93	0.50
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.09	0.50
9:W:19:ARG:HB2	9:W:171:TRP:HB2	1.92	0.50
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.94	0.50
8:V:84:LYS:HG3	8:V:85:GLN:N	2.25	0.50
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.46	0.50
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.94	0.50
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.42	0.50
12:Z:114:ASP:OD2	12:Z:115:PRO:HD2	2.11	0.50
7:G:77:VAL:HG12	7:G:137:THR:HB	1.93	0.50
9:W:124:PHE:O	9:W:125:ILE:HD13	2.12	0.50
11:K:142:TYR:C	11:K:143:LYS:HD2	2.31	0.50
11:Y:37:ILE:HB	11:Y:41:LEU:CB	2.40	0.50
3:Q:20:HIS:HB3	3:Q:25:GLU:OE1	2.11	0.50
9:W:104:ILE:HD13	9:W:108:PRO:HA	1.94	0.50
12:L:134:ILE:HD13	12:L:158:SER:HB3	1.94	0.50
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.77	0.50
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.11	0.49
7:U:96:ALA:HA	7:U:107:MET:HE1	1.94	0.49
14:N:10(B):LYS:O	14:N:10(B):LYS:HD3	2.11	0.49
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.93	0.49
1:O:69:LEU:HD23	1:O:69:LEU:C	2.32	0.49
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.94	0.49
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.94	0.49
10:J:10(C):LYS:NZ	16:J:1133:HOH:O	2.45	0.49
6:T:203:GLU:O	6:T:206:LYS:HD2	2.13	0.49
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.93	0.49
10:X:112:GLN:NE2	10:X:126:ALA:H	2.10	0.49
10:J:112:GLN:NE2	16:J:898:HOH:O	2.39	0.49
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.77	0.49
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.56	0.49
5:E:48:LEU:HD13	5:E:77:SER:HB3	1.94	0.49
12:L:21:ILE:O	12:L:21:ILE:HD13	2.11	0.49
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.66	0.49
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.10	0.49
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.48	0.49
12:Z:35:PHE:O	12:Z:42:VAL:HA	2.11	0.49
11:Y:76:VAL:N	11:Y:106:GLU:OE2	2.43	0.49
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.94	0.49
11:Y:104:TYR:CE1	11:Y:180:GLU:OE2	2.65	0.49
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.37	0.49
13:M:37:VAL:HG11	13:M:79:ILE:HD13	1.94	0.49
4:D:20:ARG:HD3	4:D:25:GLU:CD	2.32	0.49
3:C:197:LEU:O	3:C:201:VAL:HG23	2.13	0.49
13:1:130:GLY:O	13:1:134:ALA:HB3	2.13	0.49
13:1:40:ASN:HD22	13:1:40:ASN:N	2.10	0.49
13:M:-5:PRO:C	13:M:-4:ILE:HD12	2.33	0.49
12:L:14(I):THR:HB	12:L:14(M):VAL:HG23	1.94	0.49
8:H:144:GLN:O	8:H:145:ASP:HB2	2.12	0.49
2:B:229:ILE:O	2:B:233:LEU:HB2	2.12	0.49
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.95	0.49
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.13	0.49
12:L:134:ILE:HD11	12:L:162:ALA:HB2	1.94	0.49
7:G:136:LEU:O	7:G:150:LYS:HA	2.12	0.49
3:Q:43:LYS:O	3:Q:43:LYS:HG2	2.12	0.49
12:L:166:HIS:CD2	12:L:168:GLN:H	2.22	0.49
9:W:160:LEU:HD11	9:W:191:MET:HB3	1.93	0.49
11:K:200:LYS:HE2	16:K:1088:HOH:O	2.12	0.49
10:J:133:TYR:C	16:J:198:HOH:O	2.51	0.49
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.66	0.49
6:F:49:ALA:HA	6:F:211:GLU:O	2.12	0.49
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.95	0.49
2:B:101:LYS:HG3	9:I:57:GLU:HB3	1.95	0.49
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.48	0.49
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.48	0.49
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.76	0.49
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.95	0.49
3:Q:21:ILE:N	3:Q:21:ILE:CD1	2.75	0.48
4:R:215:ILE:CD1	4:R:215:ILE:C	2.81	0.48
8:H:84:LYS:HG3	8:H:85:GLN:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:85:GLU:O	14:N:89:GLU:HB2	2.13	0.48
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.95	0.48
16:B:328:HOH:O	3:C:87:ILE:HD11	2.11	0.48
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.95	0.48
5:S:48:LEU:HD13	5:S:77:SER:HB3	1.95	0.48
12:Z:40:ASN:ND2	16:Z:799:HOH:O	2.46	0.48
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.28	0.48
11:Y:105:THR:OG1	11:Y:106:GLU:HG3	2.12	0.48
9:I:48:LEU:HG	9:I:50:THR:HG22	1.95	0.48
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.95	0.48
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.78	0.48
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.94	0.48
8:V:152:ILE:HD11	8:V:177:VAL:HG22	1.96	0.48
3:Q:99:HIS:CG	3:Q:107:VAL:HG12	2.48	0.48
3:Q:125:GLN:NE2	16:Q:872:HOH:O	2.45	0.48
5:S:35:SER:HB3	5:S:66:LYS:HZ3	1.78	0.48
6:T:176:LEU:O	6:T:180:VAL:HG23	2.13	0.48
1:O:60:MET:HE1	16:U:400:HOH:O	2.13	0.48
3:C:65:SER:HB2	16:C:274:HOH:O	2.13	0.48
14:N:14:LEU:O	14:N:175:MET:HA	2.13	0.48
1:A:233:LEU:O	1:A:236:LEU:HB2	2.13	0.48
3:C:241:GLN:C	3:C:243:GLN:H	2.17	0.48
13:1:184:LEU:C	13:1:184:LEU:HD23	2.34	0.48
14:2:3:ILE:CD1	14:2:3:ILE:C	2.81	0.48
14:N:67:THR:HA	14:N:72:GLY:O	2.13	0.48
7:U:136:LEU:O	7:U:150:LYS:HA	2.13	0.48
11:K:86:LEU:HD13	11:K:86:LEU:C	2.34	0.48
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.33	0.48
16:L:352:HOH:O	13:M:139:ARG:HD3	2.13	0.48
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.94	0.48
14:2:14:LEU:O	14:2:175:MET:HA	2.14	0.48
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.10	0.48
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.62	0.48
6:F:67:ILE:HG12	6:F:211:GLU:OE1	2.13	0.48
1:A:97:HIS:CD2	8:H:61:SER:OG	2.66	0.48
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.43	0.48
3:Q:241:GLN:C	3:Q:243:GLN:H	2.17	0.48
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.96	0.48
13:M:139:ARG:NH1	8:V:165:ASN:HD22	2.07	0.48
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.41	0.48
4:D:215:ILE:HD13	4:D:216:THR:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:35:HIS:CB	8:V:56:THR:HG21	2.42	0.48
9:I:160:LEU:HD11	9:I:191:MET:HB3	1.95	0.48
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.48	0.48
8:H:38:SER:OG	8:H:41:ILE:HD13	2.13	0.48
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.49	0.48
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.48	0.48
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.75	0.48
6:F:67:ILE:HB	6:F:223:PHE:HE2	1.77	0.48
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.29	0.48
8:H:175:VAL:HG12	8:H:176:CYS:N	2.28	0.48
2:P:136:PHE:O	2:P:150:THR:HA	2.14	0.48
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.97	0.47
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.94	0.47
2:P:231:ASP:O	2:P:235:LYS:HG2	2.14	0.47
1:O:86:ARG:NE	7:U:118:ASN:HD21	1.99	0.47
11:K:76:VAL:N	11:K:106:GLU:OE2	2.43	0.47
6:T:127:ASN:HD22	6:T:128:SER:N	2.12	0.47
1:O:110:LYS:HG2	16:O:376:HOH:O	2.14	0.47
5:S:190:ILE:HG23	5:S:212:ILE:HD13	1.96	0.47
14:2:85:GLU:O	14:2:89:GLU:HB2	2.14	0.47
6:T:109:ILE:HB	6:T:110:PRO:HD3	1.96	0.47
10:X:13:ILE:CG2	10:X:155:LEU:HD11	2.44	0.47
7:U:203:THR:HG22	7:U:204:GLU:O	2.14	0.47
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.49	0.47
2:B:90:ASN:O	2:B:94:ILE:HD12	2.14	0.47
4:R:85:ALA:O	4:R:89:ILE:HG12	2.13	0.47
11:K:10(A):ARG:NH1	11:K:10(A):ARG:HG2	2.28	0.47
3:C:173:ARG:O	3:C:177:GLU:HG3	2.13	0.47
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.95	0.47
10:J:18:LYS:HD3	10:J:174:ILE:HG12	1.96	0.47
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.80	0.47
14:2:89:GLU:HA	14:2:89:GLU:OE1	2.14	0.47
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.96	0.47
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.50	0.47
1:O:10(A):ILE:N	1:O:10(A):ILE:HD13	2.28	0.47
11:Y:38:ASN:O	11:Y:40:PHE:N	2.48	0.47
12:L:114:ASP:OD2	12:L:115:PRO:HD2	2.15	0.47
2:B:238:ILE:HD13	2:B:238:ILE:N	2.27	0.47
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.78	0.47
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.50	0.47
3:Q:197:LEU:HB3	3:Q:210:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.97	0.47
9:I:104:ILE:HG21	9:I:181:LYS:HG2	1.96	0.47
7:U:82:ILE:N	7:U:83:PRO:HD2	2.29	0.47
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.14	0.47
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.23	0.47
2:B:186:VAL:O	2:B:190:ILE:HG13	2.13	0.47
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.96	0.47
13:1:125:LEU:HA	16:1:219:HOH:O	2.14	0.47
12:L:3:ILE:HD13	12:L:46:ASN:HB2	1.96	0.47
5:E:2(C):VAL:HA	5:E:233:ILE:HD11	1.96	0.47
14:2:15:GLY:HA2	14:2:174:ARG:O	2.14	0.47
11:Y:35:ILE:HG13	16:Y:521:HOH:O	2.14	0.47
2:P:224:PHE:N	2:P:224:PHE:HD2	2.13	0.47
14:2:107:LYS:CG	14:2:108:GLY:H	2.25	0.47
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.30	0.47
10:J:112:GLN:NE2	10:J:126:ALA:H	2.12	0.47
8:H:126:SER:O	8:H:127:LEU:HD23	2.14	0.47
7:U:212:VAL:HG23	7:U:229:ILE:HD13	1.95	0.47
10:J:85:GLN:HB3	16:J:201:HOH:O	2.14	0.47
7:G:203:THR:HG22	7:G:204:GLU:O	2.15	0.47
7:G:49:ILE:HD12	7:G:212:VAL:HG22	1.96	0.47
5:S:2(C):VAL:HA	5:S:233:ILE:HD11	1.96	0.47
13:1:9:ASP:OD1	13:1:10:ASN:N	2.48	0.47
14:2:67:THR:HA	14:2:72:GLY:O	2.15	0.47
1:O:233:LEU:O	1:O:236:LEU:HB2	2.14	0.47
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.44	0.47
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.30	0.47
16:E:574:HOH:O	6:F:131:PRO:HD3	2.15	0.47
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.45	0.47
2:B:136:PHE:O	2:B:150:THR:HA	2.14	0.47
3:C:85:SER:O	3:C:89:ILE:HG13	2.14	0.47
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.97	0.47
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.49	0.47
3:C:163:GLN:HE22	3:C:173:ARG:NE	2.10	0.47
2:P:101:LYS:HG3	9:W:57:GLU:HB3	1.97	0.47
14:2:3:ILE:CD1	14:2:127:ALA:HB3	2.44	0.47
14:2:3:ILE:HD12	14:2:3:ILE:O	2.15	0.47
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.29	0.47
5:S:134:VAL:O	5:S:153:PRO:HG3	2.15	0.47
10:X:113:ILE:CG1	10:X:119:LYS:HG3	2.45	0.47
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:LYS:HZ2	10:J:85:GLN:NE2	2.13	0.47
6:T:69:VAL:HG12	16:T:811:HOH:O	2.14	0.47
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.49	0.47
7:G:82:ILE:N	7:G:83:PRO:HD2	2.29	0.47
8:V:175:VAL:HG12	8:V:176:CYS:N	2.30	0.47
4:D:170:GLU:N	4:D:170:GLU:OE1	2.48	0.47
1:A:10(A):ILE:N	1:A:10(A):ILE:HD13	2.29	0.47
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:N	2.61	0.47
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.62	0.47
3:Q:197:LEU:HB3	3:Q:210:ILE:CD1	2.45	0.47
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.30	0.47
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.45	0.47
9:I:104:ILE:HD13	9:I:108:PRO:HA	1.96	0.47
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.81	0.47
2:P:224:PHE:CD2	2:P:224:PHE:N	2.83	0.47
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.45	0.47
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.50	0.47
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.30	0.47
6:T:36:THR:HB	6:T:168:GLY:H	1.80	0.47
3:C:158:SER:CB	4:D:59:LEU:HD21	2.45	0.47
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.15	0.47
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.07	0.47
6:T:67:ILE:HB	6:T:223:PHE:HE2	1.79	0.47
10:X:18:LYS:HD3	10:X:174:ILE:HG12	1.97	0.47
1:O:97:HIS:HD2	8:V:61:SER:OG	1.97	0.47
5:E:190:ILE:HG23	5:E:212:ILE:HD13	1.97	0.47
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.96	0.47
1:A:58:LEU:HD12	7:G:173:THR:HG23	1.96	0.47
7:U:192:PHE:CD1	7:U:192:PHE:C	2.88	0.47
11:K:38:ASN:O	11:K:40:PHE:N	2.48	0.46
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.80	0.46
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.97	0.46
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.97	0.46
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.15	0.46
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.30	0.46
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.50	0.46
8:H:5:GLY:O	8:H:124:TYR:HA	2.15	0.46
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.31	0.46
6:F:36:THR:HB	6:F:168:GLY:H	1.79	0.46
3:C:191:LYS:CG	3:C:236:ILE:HD11	2.42	0.46
12:Z:-2:ASN:C	12:Z:21:ILE:HD12	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.29	0.46
4:D:156:THR:HG22	5:E:83:PRO:HD3	1.97	0.46
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.97	0.46
9:W:104:ILE:HG21	9:W:181:LYS:HG2	1.98	0.46
14:2:174:ARG:HD2	16:2:307:HOH:O	2.15	0.46
3:Q:29:GLU:OE2	3:Q:32:LYS:HE2	2.15	0.46
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.80	0.46
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.96	0.46
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.50	0.46
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.15	0.46
3:C:70:ILE:N	3:C:70:ILE:HD13	2.30	0.46
8:V:152:ILE:HD11	8:V:177:VAL:CG2	2.46	0.46
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.97	0.46
11:K:152:LEU:HD22	11:K:175:LEU:HD13	1.97	0.46
12:L:35:PHE:O	12:L:42:VAL:HA	2.16	0.46
6:F:127:ASN:HD22	6:F:128:SER:N	2.13	0.46
10:J:162:LEU:O	10:J:166:MET:HB2	2.15	0.46
13:1:6:MET:CG	13:1:155:ILE:HD11	2.36	0.46
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	2.09	0.46
1:A:40:ILE:N	1:A:40:ILE:HD12	2.31	0.46
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.30	0.46
6:F:127:ASN:HD22	6:F:127:ASN:C	2.19	0.46
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.14	0.46
5:E:4:PHE:CG	5:E:5:ARG:N	2.83	0.46
12:Z:99:THR:HG23	16:Z:231:HOH:O	2.15	0.46
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.15	0.46
8:V:144:GLN:O	8:V:145:ASP:HB2	2.15	0.46
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.30	0.46
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.50	0.46
5:S:4:PHE:CG	5:S:5:ARG:N	2.83	0.46
1:O:21(G):LEU:HD23	1:O:21(I):TYR:O	2.16	0.46
6:F:50:VAL:HG22	6:F:51:GLU:N	2.30	0.46
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.30	0.46
6:T:49:ALA:HA	6:T:211:GLU:O	2.16	0.46
6:T:101:LYS:NZ	14:2:85:GLU:OE1	2.46	0.46
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.45	0.46
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.80	0.46
6:T:162:GLY:O	7:U:58:LEU:HB3	2.16	0.46
16:H:953:HOH:O	9:I:153:GLU:HB2	2.16	0.46
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.16	0.46
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.97	0.46
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.16	0.46
2:B:107:ILE:HD13	2:B:112:LEU:HB2	1.98	0.46
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.50	0.46
6:T:101:LYS:HE2	13:1:57:ARG:NH2	2.30	0.46
6:F:162:GLY:O	7:G:58:LEU:HB3	2.15	0.46
14:N:92:ASP:HB2	16:N:197:HOH:O	2.16	0.46
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.98	0.46
3:C:97:GLN:NE2	16:C:255:HOH:O	2.46	0.46
11:K:209:VAL:HG13	16:W:348:HOH:O	2.16	0.46
13:M:184:LEU:HD23	13:M:184:LEU:C	2.36	0.46
3:Q:194:VAL:O	3:Q:198:LEU:HG	2.16	0.46
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.15	0.46
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.45	0.46
7:G:212:VAL:HB	7:G:224:LEU:HD12	1.96	0.46
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.81	0.46
11:K:140:SER:OG	10:X:137:LEU:HD21	2.15	0.46
10:J:168:MET:HE2	10:X:168:MET:HE2	1.98	0.46
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.98	0.46
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.98	0.46
10:X:100:LEU:CD2	10:X:112:GLN:HG3	2.46	0.46
6:T:127:ASN:HD22	6:T:127:ASN:C	2.19	0.46
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.81	0.46
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.16	0.46
6:F:103:TYR:O	6:F:104:LYS:HB3	2.16	0.46
2:B:224:PHE:CD2	2:B:224:PHE:N	2.83	0.46
2:P:202:THR:CG2	2:P:204:SER:HB2	2.46	0.46
7:U:96:ALA:HA	7:U:107:MET:CE	2.46	0.46
3:C:185:THR:CG2	3:C:186:VAL:N	2.79	0.46
13:1:14(C):ARG:CG	13:1:14(C):ARG:NH1	2.77	0.46
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.51	0.46
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.98	0.46
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.31	0.46
13:M:157:ASN:ND2	16:M:1332:HOH:O	2.48	0.46
3:C:194:VAL:O	3:C:198:LEU:HG	2.15	0.46
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.98	0.46
8:V:90:TYR:CG	8:V:95:ILE:HD13	2.51	0.46
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.98	0.46
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.98	0.46
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.16	0.46
6:T:50:VAL:HG22	6:T:51:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:74:ILE:CD1	6:F:109:ILE:HD12	2.46	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.52	0.45
5:S:76:LEU:O	5:S:76:LEU:HD23	2.16	0.45
2:P:122:GLY:C	2:P:124:THR:H	2.20	0.45
2:B:224:PHE:HD2	2:B:224:PHE:N	2.13	0.45
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.16	0.45
11:Y:2:THR:HG21	11:Y:162:ALA:CB	2.46	0.45
13:M:9:ASP:OD1	13:M:10:ASN:N	2.50	0.45
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.98	0.45
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.17	0.45
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.16	0.45
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.46	0.45
9:W:33:LYS:O	9:W:44:GLY:HA2	2.15	0.45
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.45	0.45
13:M:150:VAL:HG21	16:M:1069:HOH:O	2.16	0.45
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.57	0.45
16:S:656:HOH:O	6:T:12:ASN:HB2	2.16	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.97	0.45
6:F:203:GLU:C	6:F:205:ASN:H	2.18	0.45
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.46	0.45
5:S:67:ILE:HG21	5:S:213:ALA:HB2	1.99	0.45
7:G:96:ALA:HA	7:G:107:MET:CE	2.45	0.45
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.98	0.45
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.99	0.45
2:B:31:ILE:HD11	2:B:133:GLY:C	2.37	0.45
6:F:203:GLU:O	6:F:206:LYS:HD2	2.15	0.45
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.98	0.45
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.98	0.45
13:M:130:GLY:O	13:M:134:ALA:HB3	2.16	0.45
2:B:202:THR:CG2	2:B:204:SER:HB2	2.46	0.45
2:B:160:TRP:HA	3:C:59:GLN:HA	1.98	0.45
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.80	0.45
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.46	0.45
7:U:107:MET:CE	7:U:112:LEU:HD13	2.35	0.45
14:N:3:ILE:HG12	14:N:44:CYS:HB3	1.98	0.45
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.81	0.45
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.45
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.98	0.45
10:J:165:ARG:O	10:X:26:VAL:HG23	2.17	0.45
12:L:17:ASP:HA	12:L:172:GLY:O	2.16	0.45
5:S:36:VAL:HG22	5:S:37:THR:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.17	0.45
11:Y:7:ARG:HH11	11:Y:108:PRO:HB2	1.81	0.45
6:T:103:TYR:O	6:T:104:LYS:HB3	2.15	0.45
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.09	0.45
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.47	0.45
13:1:104:VAL:CG2	13:1:178:ILE:HG22	2.42	0.45
14:2:3:ILE:O	14:2:3:ILE:HD13	2.16	0.45
1:O:29:THR:O	1:O:33:GLN:HG2	2.15	0.45
13:M:40:ASN:ND2	13:M:40:ASN:H	2.14	0.45
6:T:49:ALA:CB	6:T:197:ILE:HD11	2.46	0.45
10:J:113:ILE:CG1	10:J:119:LYS:HG3	2.46	0.45
5:S:162:GLY:O	5:S:163:THR:HB	2.16	0.45
8:V:41:ILE:HG13	8:V:76:VAL:HG22	1.99	0.45
14:N:94:ASN:ND2	16:N:946:HOH:O	2.39	0.45
9:I:88:TYR:CE1	9:I:91:ARG:HD3	2.51	0.45
11:K:7:ARG:HH11	11:K:108:PRO:HB2	1.81	0.45
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.17	0.45
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.98	0.45
3:C:163:GLN:HG3	3:C:164:THR:N	2.31	0.45
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.52	0.45
13:1:104:VAL:HG23	13:1:178:ILE:CG2	2.43	0.45
8:H:90:TYR:CG	8:H:95:ILE:HD13	2.52	0.45
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.31	0.45
8:V:126:SER:O	8:V:127:LEU:HD23	2.17	0.45
7:G:212:VAL:HG23	7:G:229:ILE:HD13	1.98	0.45
4:D:85:ALA:O	4:D:89:ILE:HG12	2.16	0.45
8:H:41:ILE:HG13	8:H:76:VAL:HG22	1.99	0.45
1:O:39:GLY:HA2	1:O:47:VAL:O	2.16	0.45
9:I:58:MET:O	9:I:61:TYR:HB3	2.17	0.45
5:E:36:VAL:HG22	5:E:37:THR:N	2.32	0.45
1:A:39:GLY:HA2	1:A:47:VAL:O	2.17	0.45
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.55	0.45
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.97	0.45
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.16	0.45
3:Q:185:THR:CG2	3:Q:186:VAL:N	2.79	0.45
14:2:3:ILE:HD12	14:2:3:ILE:N	2.29	0.45
8:H:95:ILE:HB	16:H:234:HOH:O	2.16	0.45
10:J:146:MET:HE3	10:J:150:GLU:HB3	1.99	0.45
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.52	0.45
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.99	0.45
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:5:GLY:O	12:L:124:CYS:HA	2.17	0.45
7:G:192:PHE:CD1	7:G:192:PHE:C	2.89	0.45
5:E:231:LYS:HD2	5:E:231:LYS:H	1.81	0.45
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.16	0.45
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.17	0.45
4:D:215:ILE:CD1	4:D:215:ILE:C	2.85	0.45
1:O:40:ILE:N	1:O:40:ILE:HD12	2.31	0.45
6:T:49:ALA:HB1	6:T:197:ILE:CD1	2.47	0.45
2:P:31:ILE:HD11	2:P:133:GLY:C	2.37	0.45
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.17	0.45
6:T:45:GLY:HA3	6:T:215:CYS:O	2.16	0.45
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.97	0.45
11:K:2:THR:HG21	11:K:162:ALA:CB	2.46	0.45
2:P:67:LEU:HD23	2:P:213:ALA:HB2	1.98	0.45
2:P:90:ASN:O	2:P:94:ILE:HD12	2.17	0.45
9:I:14:ILE:CG1	9:I:34:ILE:HD12	2.40	0.45
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.52	0.45
2:P:121:GLN:NE2	16:P:462:HOH:O	2.48	0.45
9:I:165:ARG:HH21	12:Z:135:MET:HE3	1.82	0.45
1:A:29:THR:O	1:A:33:GLN:HG2	2.17	0.45
13:M:148:VAL:HG23	16:M:502:HOH:O	2.17	0.45
6:F:101:LYS:HE2	13:M:57:ARG:NH2	2.32	0.45
2:B:101:LYS:NZ	10:J:85:GLN:HE22	2.15	0.45
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.55	0.45
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.13	0.44
5:S:77:SER:OG	5:S:137:LEU:HB2	2.18	0.44
7:G:197:MET:HE3	7:G:197:MET:HA	1.99	0.44
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.52	0.44
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.52	0.44
13:1:202:ASP:HA	16:1:1172:HOH:O	2.16	0.44
11:Y:152:LEU:HD22	11:Y:175:LEU:HD13	1.99	0.44
4:R:42:THR:C	4:R:44:GLU:H	2.20	0.44
16:F:306:HOH:O	7:G:86:ARG:HD2	2.16	0.44
12:L:-2:ASN:C	12:L:21:ILE:HD12	2.38	0.44
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.99	0.44
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.99	0.44
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.51	0.44
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.17	0.44
5:E:35:SER:HB3	5:E:66:LYS:HZ3	1.83	0.44
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.16	0.44
12:Z:14(E):GLU:O	12:Z:14(F):PRO:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.47	0.44
4:D:17:PRO:HD2	16:D:1171:HOH:O	2.17	0.44
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.17	0.44
7:U:212:VAL:HB	7:U:224:LEU:HD12	2.00	0.44
3:Q:40:VAL:HG23	3:Q:189:CYS:SG	2.57	0.44
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.47	0.44
4:D:42:THR:C	4:D:44:GLU:H	2.20	0.44
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.33	0.44
5:E:220:PRO:O	5:E:222:THR:HG23	2.17	0.44
5:S:197:ILE:HG23	5:S:198:SER:N	2.33	0.44
6:T:35:THR:CG2	6:T:36:THR:N	2.81	0.44
5:E:223:ILE:CD1	5:E:223:ILE:N	2.80	0.44
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.46	0.44
6:F:49:ALA:CB	6:F:197:ILE:HD11	2.47	0.44
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.99	0.44
12:L:109:ALA:HA	16:L:975:HOH:O	2.16	0.44
10:X:6:ILE:HD13	10:X:154:LEU:HD23	2.00	0.44
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.98	0.44
11:K:99:THR:CG2	11:K:113:VAL:HB	2.48	0.44
6:T:203:GLU:C	6:T:205:ASN:H	2.20	0.44
10:X:162:LEU:O	10:X:166:MET:HB2	2.18	0.44
10:X:35:ARG:HH11	10:X:57:GLU:HG2	1.83	0.44
2:B:231:ASP:O	2:B:235:LYS:HG2	2.18	0.44
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.18	0.44
14:2:116:GLY:HA3	16:2:192:HOH:O	2.18	0.44
14:N:15:GLY:HA2	14:N:174:ARG:O	2.16	0.44
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.52	0.44
13:M:165:ARG:O	14:2:26:ILE:HG13	2.18	0.44
10:J:2:ILE:CD1	10:J:2:ILE:N	2.81	0.44
5:E:45:HIS:CD2	5:E:214:ILE:HD11	2.52	0.44
7:U:168:LYS:O	7:U:172:ILE:HG13	2.16	0.44
7:G:212:VAL:HG23	7:G:229:ILE:CD1	2.48	0.44
14:2:146:MET:HE3	16:2:774:HOH:O	2.17	0.44
1:A:92:SER:OG	1:A:116:VAL:HG22	2.17	0.44
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.38	0.44
4:D:207:LEU:HD23	4:D:233:ILE:HD13	1.99	0.44
11:K:6:PHE:HA	11:K:123:ASP:O	2.17	0.44
6:F:136:THR:O	6:F:150:MET:HA	2.18	0.44
7:G:107:MET:CE	7:G:112:LEU:HD13	2.36	0.44
3:Q:186:VAL:HG13	3:Q:214:VAL:HG11	1.99	0.44
9:I:6:MET:HE3	9:I:155:ILE:CG1	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:58:LEU:N	5:S:58:LEU:HD12	2.33	0.44
2:B:112:LEU:C	2:B:112:LEU:HD23	2.38	0.44
3:Q:41:LYS:HD3	3:Q:161:SER:HA	2.00	0.44
8:V:40:LYS:C	8:V:41:ILE:HD12	2.38	0.44
3:C:197:LEU:HB3	3:C:210:ILE:CD1	2.48	0.44
6:T:100:LYS:O	6:T:104:LYS:N	2.49	0.44
5:S:90:ASN:O	5:S:94:GLN:HG3	2.18	0.44
2:P:113:VAL:HG22	2:P:138:TYR:CG	2.53	0.44
7:U:151:THR:HG22	7:U:157:TYR:HB2	2.00	0.44
8:V:174:ASP:OD2	8:V:189:ARG:NH1	2.48	0.44
4:R:170:GLU:OE1	4:R:170:GLU:N	2.49	0.44
5:E:76:LEU:O	5:E:76:LEU:HD23	2.18	0.44
10:J:133:TYR:CE2	10:J:166:MET:SD	3.10	0.44
12:L:93:PHE:N	12:L:94:PRO:HD3	2.32	0.44
4:R:40:ILE:HG13	4:R:193:VAL:HG23	2.00	0.44
13:M:165:ARG:C	14:2:26:ILE:HG13	2.37	0.44
16:L:200:HOH:O	9:W:192:ARG:HG3	2.18	0.44
8:V:5:GLY:O	8:V:124:TYR:HA	2.17	0.44
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.00	0.44
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.00	0.44
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.52	0.44
10:J:136:SER:N	16:J:198:HOH:O	2.44	0.44
3:C:160:TRP:NE1	4:D:59:LEU:HD23	2.33	0.44
5:S:45:HIS:CD2	5:S:214:ILE:HD11	2.53	0.44
10:J:24:ILE:HD11	10:X:129:TYR:HB3	2.00	0.44
13:1:49:ILE:O	13:1:53:GLN:HG3	2.17	0.44
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.52	0.44
2:B:190:ILE:HG21	2:B:232:ILE:HD11	2.00	0.44
14:N:89:GLU:OE1	14:N:89:GLU:HA	2.17	0.44
10:J:12:VAL:HG23	10:J:108:PRO:HB2	2.00	0.44
2:B:213:ALA:HA	2:B:222:LYS:O	2.17	0.44
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.48	0.44
10:J:35:ARG:HH11	10:J:57:GLU:HG2	1.83	0.44
12:L:185:ARG:NH1	16:L:1161:HOH:O	2.46	0.44
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.99	0.44
14:N:3:ILE:CD1	14:N:3:ILE:N	2.81	0.43
2:P:141:TYR:C	2:P:141:TYR:CD1	2.90	0.43
6:T:136:THR:O	6:T:150:MET:HA	2.17	0.43
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.17	0.43
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.17	0.43
5:E:161:TYR:CE2	6:F:60:VAL:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:GLY:HA3	6:F:215:CYS:O	2.17	0.43
11:K:147:SER:C	11:K:149:GLU:N	2.72	0.43
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.57	0.43
9:W:6:MET:HE3	9:W:155:ILE:HA	1.96	0.43
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.82	0.43
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.31	0.43
7:G:151:THR:HG22	7:G:157:TYR:HB2	2.01	0.43
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.53	0.43
6:F:43:ASN:N	6:F:43:ASN:HD22	2.16	0.43
1:A:86:ARG:NE	7:G:118:ASN:HD21	2.00	0.43
2:B:122:GLY:C	2:B:124:THR:H	2.21	0.43
4:D:40:ILE:HG13	4:D:193:VAL:HG23	1.99	0.43
8:V:37:ILE:HB	8:V:41:ILE:HG22	1.99	0.43
1:A:140:GLY:HA2	1:A:215:ILE:HG13	2.00	0.43
9:W:13:ALA:HA	9:W:176:TYR:O	2.18	0.43
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.17	0.43
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.82	0.43
3:Q:70:ILE:HD13	3:Q:70:ILE:N	2.33	0.43
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.32	0.43
8:H:152:ILE:HD11	8:H:177:VAL:HG22	2.00	0.43
8:V:172:ASN:ND2	8:V:193:THR:HA	2.32	0.43
10:J:100:LEU:CD2	10:J:112:GLN:HG3	2.47	0.43
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.53	0.43
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.18	0.43
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.18	0.43
8:H:137:VAL:HG21	8:H:161:ALA:HB2	2.01	0.43
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.99	0.43
5:S:41:ARG:NH1	5:S:42:SER:O	2.52	0.43
7:U:18(H):GLU:N	7:U:18(H):GLU:CD	2.72	0.43
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.00	0.43
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.33	0.43
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.99	0.43
12:L:192:LYS:HE3	8:V:195:ASN:HB3	2.01	0.43
9:I:122:ALA:HB3	9:I:125:ILE:CD1	2.49	0.43
5:S:231:LYS:HD2	5:S:231:LYS:H	1.83	0.43
5:E:45:HIS:HD2	5:E:214:ILE:HD11	1.83	0.43
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.49	0.43
13:M:49:ILE:O	13:M:53:GLN:HG3	2.19	0.43
2:B:141:TYR:C	2:B:141:TYR:CD1	2.92	0.43
5:E:162:GLY:O	5:E:163:THR:HB	2.18	0.43
9:W:130:ALA:HB2	9:W:166:ASP:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:196:THR:O	2:P:200:THR:HG23	2.19	0.43
12:Z:170:GLY:O	12:Z:171:ASP:HB2	2.18	0.43
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	2.00	0.43
11:K:10(A):ARG:H	11:K:10(B):LYS:NZ	2.17	0.43
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.48	0.43
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.52	0.43
5:S:45:HIS:HD2	5:S:214:ILE:HD11	1.83	0.43
12:Z:40:ASN:HA	12:Z:40:ASN:HD22	1.67	0.43
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.01	0.43
2:P:181:LYS:HG3	2:P:184:MET:HG3	2.00	0.43
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.33	0.43
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.18	0.43
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.49	0.43
11:K:195:LEU:O	11:K:199:VAL:HG23	2.18	0.43
11:Y:50:ALA:CB	12:Z:116:VAL:HG23	2.49	0.43
3:C:29:GLU:OE2	3:C:32:LYS:HE2	2.19	0.43
9:I:13:ALA:HA	9:I:176:TYR:O	2.18	0.43
11:K:37:ILE:HB	11:K:41:LEU:CB	2.42	0.43
14:N:107:LYS:CG	14:N:108:GLY:H	2.26	0.43
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.82	0.43
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.82	0.43
2:B:113:VAL:HG22	2:B:138:TYR:CG	2.54	0.43
4:R:207:LEU:HD23	4:R:233:ILE:HD13	2.00	0.43
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.19	0.43
8:H:196:VAL:HG23	16:H:520:HOH:O	2.18	0.43
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.18	0.43
11:K:114:ASP:OD1	11:K:114:ASP:C	2.57	0.43
7:U:29:LYS:HD2	7:U:29:LYS:HA	1.79	0.43
6:T:43:ASN:HD22	6:T:43:ASN:N	2.17	0.43
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.18	0.43
5:S:201:LEU:O	5:S:202:ARG:CB	2.65	0.43
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.87	0.43
5:E:77:SER:OG	5:E:137:LEU:HB2	2.18	0.43
4:D:215:ILE:O	4:D:215:ILE:HG23	2.18	0.43
5:E:58:LEU:HD12	5:E:58:LEU:N	2.33	0.43
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.46	0.43
6:F:176:LEU:O	6:F:180:VAL:HG23	2.18	0.43
9:I:90:ARG:HH11	9:I:90:ARG:HA	1.84	0.43
14:N:26:ILE:HG13	13:1:165:ARG:C	2.39	0.43
14:N:26:ILE:HB	13:1:165:ARG:HA	2.01	0.43
1:O:49:ALA:HB2	1:O:212:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:19:ARG:NE	14:2:26:ILE:HD13	2.34	0.43
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	2.01	0.43
7:U:18(H):GLU:H	7:U:18(H):GLU:CD	2.21	0.43
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.43
9:W:58:MET:O	9:W:61:TYR:HB3	2.19	0.43
14:N:113:ILE:N	14:N:113:ILE:HD12	2.34	0.43
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.28	0.43
3:C:164:THR:HG21	3:C:172:VAL:HG13	2.00	0.43
10:X:133:TYR:CE2	10:X:166:MET:SD	3.12	0.43
2:P:112:LEU:HD23	2:P:112:LEU:C	2.39	0.43
13:M:40:ASN:ND2	13:M:40:ASN:N	2.66	0.43
12:Z:134:ILE:HD13	12:Z:158:SER:HB3	2.01	0.43
11:Y:4:LEU:CD1	11:Y:159:ILE:HG12	2.49	0.43
12:L:14(E):GLU:O	12:L:14(F):PRO:C	2.58	0.43
12:Z:148:VAL:O	12:Z:152:ILE:HG13	2.19	0.43
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.54	0.43
2:P:34:ALA:HB1	16:P:1134:HOH:O	2.17	0.43
12:L:113:PHE:CD1	12:L:113:PHE:N	2.86	0.43
10:J:52:THR:HG22	10:J:53:VAL:HG23	2.01	0.42
5:S:160:LEU:CD2	6:T:59:LEU:HD12	2.49	0.42
9:W:80:THR:HG1	9:W:109:PHE:HE2	1.65	0.42
7:G:232:ARG:NE	7:G:232:ARG:HA	2.33	0.42
8:H:116:HIS:HB2	16:H:324:HOH:O	2.19	0.42
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.84	0.42
3:C:186:VAL:HG13	3:C:214:VAL:HG11	2.00	0.42
5:E:197:ILE:HG23	5:E:198:SER:N	2.33	0.42
7:U:168:LYS:HE3	16:U:800:HOH:O	2.18	0.42
7:G:67:ILE:HD12	7:G:67:ILE:N	2.34	0.42
4:R:215:ILE:HG23	4:R:215:ILE:O	2.19	0.42
3:C:197:LEU:HB3	3:C:210:ILE:HD13	2.01	0.42
5:S:4:PHE:O	5:S:6:ASN:N	2.52	0.42
10:X:124:TYR:HB2	10:X:138:LEU:HD13	2.01	0.42
1:O:27:ALA:O	1:O:31:VAL:HG23	2.18	0.42
6:T:204:ASP:N	6:T:204:ASP:OD1	2.52	0.42
14:2:113:ILE:N	14:2:113:ILE:HD12	2.33	0.42
10:X:3:ILE:HG12	10:X:46:ALA:HB2	2.01	0.42
8:H:172:ASN:ND2	8:H:193:THR:HA	2.32	0.42
3:C:46:VAL:HG11	3:C:139:ALA:HB1	2.00	0.42
10:J:35:ARG:NH1	10:J:57:GLU:CG	2.82	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.19	0.42
5:E:201:LEU:O	5:E:202:ARG:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:97:VAL:HG11	11:K:65:LEU:HD22	2.01	0.42
8:H:40:LYS:C	8:H:41:ILE:HD12	2.39	0.42
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.49	0.42
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.55	0.42
5:S:103:PHE:O	13:1:78:TYR:HA	2.18	0.42
11:Y:21:THR:HG22	11:Y:26:VAL:HA	2.00	0.42
5:S:52:LYS:O	5:S:63:TYR:HD2	2.03	0.42
11:K:50:ALA:CB	12:L:116:VAL:HG23	2.49	0.42
1:A:110:LYS:HG2	16:A:285:HOH:O	2.20	0.42
1:A:221:PHE:C	1:A:221:PHE:CD2	2.92	0.42
1:A:38:LEU:HD12	1:A:38:LEU:C	2.39	0.42
1:O:38:LEU:HD12	1:O:38:LEU:C	2.40	0.42
7:G:8:TYR:C	7:G:10:ARG:N	2.73	0.42
10:X:137:LEU:HD23	10:X:137:LEU:HA	1.80	0.42
10:X:154:LEU:HA	10:X:154:LEU:HD12	1.88	0.42
6:F:90:ASN:O	6:F:94:GLU:HG3	2.20	0.42
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.20	0.42
8:V:50:ALA:HB2	9:W:118:CYS:HB2	2.02	0.42
6:T:90:ASN:O	6:T:94:GLU:HG3	2.18	0.42
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.54	0.42
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.20	0.42
3:Q:158:SER:CB	4:R:59:LEU:HD21	2.49	0.42
7:G:18(G):GLU:CG	7:G:188:LYS:HB2	2.44	0.42
4:R:121:LEU:HD13	5:S:130:ARG:NH2	2.35	0.42
9:W:137:MET:HE1	9:W:161:ASN:HB2	2.02	0.42
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.35	0.42
3:C:225:SER:OG	3:C:228:GLU:HG3	2.20	0.42
2:B:202:THR:HG21	2:B:204:SER:HB2	2.02	0.42
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.54	0.42
13:M:104:VAL:HG23	13:M:178:ILE:CG2	2.46	0.42
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.45	0.42
2:P:107:ILE:HD13	2:P:112:LEU:HB2	2.01	0.42
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	2.01	0.42
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.01	0.42
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.32	0.42
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.83	0.42
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.20	0.42
9:I:124:PHE:O	9:I:125:ILE:HD13	2.19	0.42
1:O:214:ILE:C	1:O:215:ILE:HD13	2.39	0.42
5:E:41:ARG:NH1	5:E:42:SER:O	2.53	0.42
13:1:-5:PRO:C	13:1:-4:ILE:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD22	1:A:224:LEU:HD12	2.00	0.42
9:W:90:ARG:HH11	9:W:90:ARG:HA	1.83	0.42
2:P:38:ILE:HD12	2:P:197:LEU:HG	2.01	0.42
5:S:216:GLY:O	5:S:219:THR:N	2.40	0.42
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.42
10:J:129:TYR:HB3	10:X:24:ILE:HD11	2.02	0.42
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.20	0.42
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.97	0.42
9:W:6:MET:HB3	9:W:151:LEU:HD11	2.02	0.42
3:C:41:LYS:HD3	3:C:161:SER:HA	2.00	0.42
4:D:177:LEU:HD13	5:E:58:LEU:HD11	2.01	0.42
14:2:176:VAL:HG12	14:2:178:LEU:CD1	2.48	0.42
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.54	0.42
10:X:100:LEU:HD23	10:X:112:GLN:HG3	2.02	0.42
2:B:185:LYS:CD	2:B:187:ASP:H	2.33	0.42
12:Z:33:LYS:NZ	16:Z:754:HOH:O	2.51	0.42
6:T:172:ALA:O	6:T:176:LEU:CD2	2.67	0.42
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	2.00	0.42
6:T:127:ASN:ND2	6:T:127:ASN:C	2.73	0.42
12:Z:109:ALA:HA	16:Z:375:HOH:O	2.19	0.42
1:O:97:HIS:CD2	8:V:61:SER:OG	2.72	0.42
7:G:18(B):ASP:O	7:G:18(C):HIS:HB3	2.19	0.42
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.55	0.42
1:A:21(P):LYS:HB2	16:A:1147:HOH:O	2.20	0.42
5:E:67:ILE:HG21	5:E:213:ALA:HB2	2.02	0.42
8:V:24:PRO:HG2	8:V:25:ILE:HD12	2.01	0.42
13:1:190:LEU:CD1	13:1:190:LEU:N	2.82	0.42
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	2.01	0.42
5:S:76:LEU:C	5:S:76:LEU:HD23	2.40	0.42
9:I:12:VAL:CG2	9:I:178:ILE:HB	2.50	0.42
12:L:33:LYS:HE2	12:L:33:LYS:HB3	1.74	0.42
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.20	0.42
2:B:67:LEU:HD23	2:B:213:ALA:HB2	2.02	0.42
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.55	0.42
5:S:220:PRO:O	5:S:222:THR:HG23	2.19	0.42
10:J:141:HIS:HB2	10:J:154:LEU:HD11	2.02	0.42
8:H:200:LYS:HE3	9:I:140:SER:O	2.19	0.42
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.87	0.42
2:P:44:ASP:N	2:P:44:ASP:OD2	2.52	0.42
10:X:185:ARG:HH11	10:X:185:ARG:HG2	1.84	0.42
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:ASN:OD1	11:K:38:ASN:C	2.57	0.42
9:I:130:ALA:HB2	9:I:166:ASP:CB	2.49	0.42
5:E:76:LEU:HD23	5:E:76:LEU:C	2.40	0.42
12:L:179:THR:HG21	16:L:1161:HOH:O	2.19	0.42
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.50	0.42
16:I:510:HOH:O	10:J:122:LEU:HD22	2.19	0.42
1:A:27:ALA:O	1:A:31:VAL:HG23	2.20	0.42
5:E:90:ASN:O	5:E:94:GLN:HG3	2.20	0.42
7:U:232:ARG:HA	7:U:232:ARG:NE	2.34	0.42
3:Q:208:LYS:HD2	3:Q:208:LYS:O	2.20	0.42
13:M:6:MET:CG	13:M:155:ILE:HD11	2.37	0.41
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.80	0.41
5:S:47:VAL:HG12	5:S:48:LEU:N	2.35	0.41
5:S:76:LEU:HA	5:S:137:LEU:O	2.20	0.41
14:2:3:ILE:HG22	14:2:16:ALA:HB2	2.01	0.41
8:V:128:GLY:O	8:V:131:SER:CB	2.64	0.41
9:I:124:PHE:C	9:I:125:ILE:HD13	2.40	0.41
8:H:174:ASP:OD2	8:H:189:ARG:NH1	2.48	0.41
14:2:156:LYS:HE3	16:2:1010:HOH:O	2.20	0.41
14:2:134:ILE:HG21	14:2:158:SER:O	2.19	0.41
1:O:221:PHE:C	1:O:221:PHE:CD2	2.92	0.41
6:F:35:THR:CG2	6:F:36:THR:N	2.82	0.41
3:C:195:ARG:CG	3:C:236:ILE:HD12	2.50	0.41
3:Q:195:ARG:CG	3:Q:236:ILE:HD12	2.49	0.41
6:F:70:VAL:HB	6:F:74:ILE:HB	2.02	0.41
12:Z:14:LEU:HA	12:Z:14:LEU:HD23	1.79	0.41
10:J:13:ILE:HG21	10:J:155:LEU:CD1	2.50	0.41
3:Q:39:GLY:O	3:Q:162:ALA:HA	2.20	0.41
1:O:140:GLY:HA2	1:O:215:ILE:HG13	2.02	0.41
11:K:21:THR:HG22	11:K:26:VAL:HA	2.00	0.41
9:I:-8:SER:O	9:I:-6:PRO:HD3	2.21	0.41
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.54	0.41
7:U:18(B):ASP:O	7:U:18(C):HIS:HB3	2.19	0.41
13:M:11:GLY:HA3	13:M:178:ILE:O	2.20	0.41
5:E:134:VAL:O	5:E:153:PRO:HG3	2.20	0.41
4:D:12(F):GLY:HA3	16:E:965:HOH:O	2.20	0.41
6:T:148:LEU:HB3	6:T:160:TYR:O	2.20	0.41
16:N:583:HOH:O	13:1:211:ILE:HD11	2.20	0.41
10:X:88:ALA:O	10:X:90(A):ILE:HG22	2.20	0.41
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	2.09	0.41
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:194:VAL:HG13	5:E:207:LEU:HD11	2.02	0.41
4:R:161:ASN:N	5:S:58:LEU:O	2.49	0.41
8:H:170:GLY:O	8:H:171:SER:HB2	2.21	0.41
14:N:176:VAL:HG12	14:N:178:LEU:CD1	2.48	0.41
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.86	0.41
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.51	0.41
11:K:4:LEU:C	11:K:4:LEU:HD22	2.41	0.41
11:Y:50:ALA:HB2	12:Z:116:VAL:HG23	2.02	0.41
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.02	0.41
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.02	0.41
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.86	0.41
13:M:112:TYR:C	13:M:112:TYR:CD2	2.94	0.41
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.35	0.41
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.82	0.41
2:P:202:THR:HG21	2:P:204:SER:HB2	2.03	0.41
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.80	0.41
11:K:146:LEU:HD23	11:K:151:ALA:HA	2.01	0.41
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.79	0.41
7:U:203:THR:HG22	7:U:204:GLU:N	2.35	0.41
5:E:4:PHE:O	5:E:6:ASN:N	2.54	0.41
2:B:225:LYS:O	2:B:226:PRO:C	2.59	0.41
1:O:197:LEU:O	1:O:202:VAL:HG23	2.20	0.41
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.35	0.41
3:Q:225:SER:OG	3:Q:228:GLU:HG3	2.20	0.41
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	2.03	0.41
9:I:14:ILE:HG23	9:I:176:TYR:HB2	2.02	0.41
5:S:45:HIS:HB2	5:S:189:LEU:HD12	2.02	0.41
7:G:168:LYS:O	7:G:172:ILE:HG13	2.20	0.41
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.51	0.41
12:L:135:MET:HE3	9:W:165:ARG:HH21	1.86	0.41
2:B:101:LYS:HZ1	10:J:85:GLN:HE22	1.67	0.41
4:R:207:LEU:C	4:R:207:LEU:HD23	2.41	0.41
1:O:31:VAL:HG11	1:O:135:SER:HB2	2.03	0.41
13:1:190:LEU:HD12	13:1:190:LEU:N	2.36	0.41
4:D:39:GLY:HA2	4:D:47:VAL:O	2.21	0.41
9:W:88:TYR:CE1	9:W:91:ARG:HD3	2.55	0.41
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.53	0.41
1:O:4:MET:SD	1:O:5:THR:N	2.71	0.41
10:J:2:ILE:N	10:J:2:ILE:HD13	2.36	0.41
7:U:18(G):GLU:CG	7:U:188:LYS:HB2	2.45	0.41
2:P:121:GLN:HG2	3:Q:83:ALA:HB1	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:68:ILE:HG13	16:J:810:HOH:O	2.20	0.41
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.79	0.41
2:B:232:ILE:O	2:B:232:ILE:HG13	2.21	0.41
2:B:113:VAL:HG22	2:B:138:TYR:CD2	2.56	0.41
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.86	0.41
5:S:24:VAL:O	5:S:27:ALA:HB3	2.21	0.41
1:A:21(G):LEU:HD23	1:A:21(I):TYR:O	2.20	0.41
5:E:179:THR:O	5:E:179:THR:HG22	2.21	0.41
5:S:194:VAL:HG13	5:S:207:LEU:HD11	2.02	0.41
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.84	0.41
10:J:3:ILE:HG12	10:J:46:ALA:HB2	2.03	0.41
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ3	1.86	0.41
2:P:27:ALA:O	2:P:30:SER:HB3	2.21	0.41
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.61	0.41
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.51	0.41
13:M:112:TYR:CE1	13:M:127:THR:HG22	2.56	0.41
5:E:24:VAL:O	5:E:27:ALA:HB3	2.20	0.41
11:Y:17:ASP:O	11:Y:33:LYS:HD2	2.21	0.41
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.20	0.41
8:H:24:PRO:HG2	8:H:25:ILE:HD12	2.03	0.41
8:H:34:LEU:HB2	16:H:540:HOH:O	2.20	0.41
6:F:157:TYR:C	6:F:157:TYR:CD1	2.94	0.41
1:O:122:GLU:C	1:O:124:THR:H	2.24	0.41
7:U:168:LYS:HG3	16:U:800:HOH:O	2.21	0.41
12:L:-2:ASN:HA	12:L:21:ILE:O	2.20	0.41
8:V:170:GLY:O	8:V:171:SER:HB2	2.21	0.41
13:1:7:LYS:HB3	13:1:12:VAL:HG12	2.03	0.41
8:H:128:GLY:O	8:H:131:SER:CB	2.68	0.41
10:J:100:LEU:HD23	10:J:112:GLN:HG3	2.03	0.41
10:X:13:ILE:HG21	10:X:155:LEU:HD12	2.03	0.41
5:S:172:ALA:CB	5:S:196:ALA:O	2.69	0.41
1:O:62:GLU:CD	1:O:62:GLU:H	2.24	0.41
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.84	0.41
3:C:39:GLY:O	3:C:162:ALA:HA	2.20	0.41
10:J:124:TYR:HB2	10:J:138:LEU:HD13	2.02	0.41
13:M:165:ARG:HA	14:2:26:ILE:HB	2.02	0.41
2:P:113:VAL:HG22	2:P:138:TYR:CD2	2.56	0.41
1:A:197:LEU:O	1:A:202:VAL:HG23	2.21	0.41
11:Y:147:SER:C	11:Y:149:GLU:N	2.71	0.41
5:S:161:TYR:CE2	6:T:60:VAL:HA	2.56	0.41
10:X:190:PHE:C	10:X:192:ALA:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:17:ASP:O	11:K:33:LYS:HD2	2.20	0.41
6:T:61:PRO:O	6:T:62:GLN:HB2	2.21	0.41
6:F:81:LEU:HA	16:F:313:HOH:O	2.21	0.41
7:U:109:CYS:HB3	16:U:1330:HOH:O	2.20	0.41
8:V:200:LYS:HE3	9:W:140:SER:O	2.21	0.41
13:M:3:VAL:HG23	13:M:46:SER:HB3	2.03	0.41
10:J:19:ALA:HB2	10:J:171:LYS:HG2	2.03	0.41
3:C:208:LYS:HD2	3:C:208:LYS:O	2.21	0.41
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.21	0.41
6:T:74:ILE:CD1	6:T:109:ILE:HD12	2.51	0.41
13:1:11:GLY:HA3	13:1:178:ILE:O	2.21	0.41
6:T:240:ILE:HG23	6:T:241:ASN:ND2	2.36	0.41
6:T:116:LEU:O	6:T:120:VAL:HG23	2.21	0.41
8:V:152:ILE:CD1	8:V:177:VAL:HG22	2.51	0.41
1:O:62:GLU:O	1:O:64:LEU:N	2.54	0.41
7:G:212:VAL:CG2	7:G:229:ILE:HD13	2.51	0.41
6:T:66:LYS:HE3	6:T:82:ILE:CD1	2.51	0.41
1:O:4:MET:CG	1:O:5:THR:H	2.31	0.41
12:L:170:GLY:O	12:L:171:ASP:HB2	2.21	0.41
14:N:134:ILE:HG21	14:N:158:SER:O	2.21	0.41
6:T:114:ASP:O	6:T:118:GLN:HG2	2.21	0.41
11:K:25:TRP:CH2	12:L:132:SER:HA	2.55	0.41
3:C:169:SER:HA	3:C:172:VAL:CG1	2.51	0.40
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.51	0.40
3:C:190:VAL:O	3:C:194:VAL:HG23	2.21	0.40
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.02	0.40
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.37	0.40
5:S:175:TYR:CE2	5:S:196:ALA:HB2	2.56	0.40
2:P:213:ALA:HA	2:P:222:LYS:O	2.21	0.40
8:V:25:ILE:HD13	16:V:1105:HOH:O	2.20	0.40
1:O:8:TYR:HD2	7:U:128:TYR:HB3	1.86	0.40
1:A:149:TYR:CE1	1:A:159:PRO:HB3	2.56	0.40
6:F:148:LEU:HB3	6:F:160:TYR:O	2.21	0.40
9:I:152:PHE:HB2	9:I:177:ILE:HD11	2.03	0.40
8:V:22:GLN:HG3	8:V:27:ALA:HB2	2.02	0.40
10:J:185:ARG:HH11	10:J:185:ARG:HG2	1.86	0.40
9:I:20:LEU:C	9:I:20:LEU:HD13	2.41	0.40
5:S:223:ILE:N	5:S:223:ILE:CD1	2.84	0.40
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	2.02	0.40
8:H:152:ILE:HD11	8:H:177:VAL:CG2	2.51	0.40
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:40:ASN:ND2	13:1:40:ASN:N	2.69	0.40
2:P:150:THR:O	2:P:157:TYR:HA	2.22	0.40
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.56	0.40
1:O:39:GLY:O	1:O:162:ALA:HA	2.21	0.40
11:K:4:LEU:CD1	11:K:159:ILE:HG12	2.52	0.40
7:G:151:THR:HG22	7:G:157:TYR:CB	2.51	0.40
9:W:61:TYR:C	9:W:61:TYR:CD1	2.94	0.40
9:W:89:GLU:O	9:W:90:ARG:NH1	2.53	0.40
4:R:39:GLY:HA2	4:R:47:VAL:O	2.21	0.40
6:F:114:ASP:O	6:F:118:GLN:HG2	2.22	0.40
8:V:2:THR:O	8:V:16:ALA:HA	2.22	0.40
2:P:79:ALA:HB2	2:P:165:VAL:HG23	2.03	0.40
7:G:48:VAL:HG23	7:G:48:VAL:O	2.21	0.40
11:Y:10(A):ARG:H	11:Y:10(B):LYS:NZ	2.18	0.40
5:S:18(F):ILE:HD13	5:S:188:GLU:HB3	2.03	0.40
5:S:214:ILE:O	5:S:221:PHE:HA	2.22	0.40
5:S:15:PHE:H	6:T:23:GLN:NE2	2.10	0.40
2:P:190:ILE:HG21	2:P:232:ILE:HD11	2.03	0.40
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.86	0.40
12:Z:33:LYS:HE2	12:Z:33:LYS:HB3	1.72	0.40
1:O:21(G):LEU:HG	1:O:21(I):TYR:CE1	2.56	0.40
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.21	0.40
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.04	0.40
10:J:190:PHE:C	10:J:192:ALA:H	2.24	0.40
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.86	0.40
7:G:18(H):GLU:N	7:G:18(H):GLU:CD	2.74	0.40
5:S:179:THR:O	5:S:179:THR:HG22	2.20	0.40
6:F:204:ASP:OD1	6:F:204:ASP:N	2.54	0.40
2:B:196:THR:O	2:B:200:THR:HG23	2.20	0.40
11:Y:49:ALA:HB1	12:Z:118:SER:OG	2.21	0.40
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.22	0.40
10:J:3:ILE:HA	10:J:3:ILE:HD12	1.90	0.40
12:Z:-7:ASN:HD22	12:Z:-5:TYR:H	1.68	0.40
5:S:12:THR:CG2	5:S:124:THR:HA	2.49	0.40
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.57	0.40
2:B:27:ALA:O	2:B:30:SER:HB3	2.22	0.40
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.56	0.40
10:J:6:ILE:CD1	10:J:154:LEU:HD23	2.52	0.40
7:U:119:LEU:HA	7:U:119:LEU:HD12	1.95	0.40
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.87	0.40
4:R:97:VAL:HG11	11:Y:65:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:3:ILE:CD1	14:N:3:ILE:C	2.88	0.40
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.29	0.40
5:E:214:ILE:O	5:E:221:PHE:HA	2.21	0.40
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.35	0.40
2:P:185:LYS:CD	2:P:187:ASP:H	2.34	0.40
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.36	0.40
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	2.03	0.40
9:W:130:ALA:HB2	9:W:166:ASP:OD1	2.21	0.40
7:G:203:THR:HG22	7:G:204:GLU:N	2.36	0.40
8:H:207:PRO:O	8:H:210:THR:OG1	2.28	0.40
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.90	0.40
13:1:112:TYR:CD2	13:1:112:TYR:C	2.93	0.40
13:1:3:VAL:HG23	13:1:46:SER:HB3	2.04	0.40
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.03	0.40
5:E:91:TYR:CD1	5:E:119:LYS:HD2	2.56	0.40
8:H:2:THR:O	8:H:16:ALA:HA	2.21	0.40
9:W:20:LEU:C	9:W:20:LEU:HD13	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	235 (95%)	10 (4%)	3 (1%)	16	39
1	O	248/250 (99%)	234 (94%)	11 (4%)	3 (1%)	16	39
2	B	242/258 (94%)	220 (91%)	18 (7%)	4 (2%)	11	29
2	P	242/258 (94%)	221 (91%)	17 (7%)	4 (2%)	11	29
3	C	239/254 (94%)	222 (93%)	13 (5%)	4 (2%)	11	29
3	Q	239/254 (94%)	221 (92%)	14 (6%)	4 (2%)	11	29
4	D	240/260 (92%)	217 (90%)	20 (8%)	3 (1%)	15	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	240/260 (92%)	216 (90%)	20 (8%)	4 (2%)	11	29
5	E	231/234 (99%)	207 (90%)	20 (9%)	4 (2%)	11	29
5	S	231/234 (99%)	208 (90%)	19 (8%)	4 (2%)	11	29
6	F	242/288 (84%)	228 (94%)	14 (6%)	0	100	100
6	T	242/288 (84%)	228 (94%)	13 (5%)	1 (0%)	39	69
7	G	241/252 (96%)	229 (95%)	11 (5%)	1 (0%)	39	69
7	U	241/252 (96%)	228 (95%)	12 (5%)	1 (0%)	39	69
8	H	220/261 (84%)	207 (94%)	9 (4%)	4 (2%)	11	27
8	V	220/261 (84%)	208 (94%)	8 (4%)	4 (2%)	11	27
9	I	202/205 (98%)	192 (95%)	8 (4%)	2 (1%)	19	45
9	W	202/205 (98%)	193 (96%)	7 (4%)	2 (1%)	19	45
10	J	196/198 (99%)	185 (94%)	8 (4%)	3 (2%)	13	32
10	X	196/198 (99%)	185 (94%)	8 (4%)	3 (2%)	13	32
11	K	210/287 (73%)	198 (94%)	9 (4%)	3 (1%)	14	35
11	Y	210/287 (73%)	199 (95%)	8 (4%)	3 (1%)	14	35
12	L	220/241 (91%)	202 (92%)	17 (8%)	1 (0%)	34	63
12	Z	220/241 (91%)	200 (91%)	19 (9%)	1 (0%)	34	63
13	1	231/266 (87%)	216 (94%)	14 (6%)	1 (0%)	39	69
13	M	231/266 (87%)	217 (94%)	13 (6%)	1 (0%)	39	69
14	2	194/215 (90%)	184 (95%)	10 (5%)	0	100	100
14	N	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
15	3	1/5 (20%)	1 (100%)	0	0	100	100
15	4	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6314/6948 (91%)	5887 (93%)	359 (6%)	68 (1%)	17	42

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
5	E	5	ARG
5	E	202	ARG
5	E	217	LYS

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Mol	Chain	Res	Type
3	Q	58	LEU
3	Q	203	THR
4	R	12(G)	GLU
5	S	5	ARG
5	S	202	ARG
5	S	217	LYS
1	A	5	THR
1	A	63	THR
1	A	167	LYS
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
8	H	91	GLN
9	I	145	ASN
10	J	49	ALA
10	J	192	ALA
11	K	209	VAL
12	L	71	ASP
1	O	5	THR
1	O	63	THR
1	O	167	LYS
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
8	V	91	GLN
9	W	145	ASN
10	X	49	ALA
10	X	192	ALA
11	Y	209	VAL
12	Z	71	ASP
2	B	184	MET
4	D	12(F)	GLY
5	E	180	LEU
11	K	39	PRO
4	R	12(F)	GLY
5	S	180	LEU
8	V	9	ASN
11	Y	39	PRO
13	1	96	TRP
3	C	202	GLN

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Mol	Chain	Res	Type
4	D	12(C)	GLY
8	H	9	ASN
8	H	171	SER
13	M	96	TRP
2	P	184	MET
3	Q	202	GLN
4	R	12(C)	GLY
8	H	96	GLY
11	K	208	ASN
6	T	143	LYS
8	V	171	SER
10	J	8	VAL
4	R	12(E)	SER
7	U	55	PRO
11	Y	208	ASN
7	G	55	PRO
8	V	96	GLY
10	X	8	VAL
9	I	93	GLY
9	W	93	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	198 (95%)	11 (5%)	28	57
1	O	209/209 (100%)	200 (96%)	9 (4%)	35	66
2	B	203/216 (94%)	191 (94%)	12 (6%)	24	51
2	P	203/216 (94%)	189 (93%)	14 (7%)	19	43
3	C	213/226 (94%)	202 (95%)	11 (5%)	29	58
3	Q	213/226 (94%)	202 (95%)	11 (5%)	29	58
4	D	198/215 (92%)	185 (93%)	13 (7%)	21	45
4	R	198/215 (92%)	185 (93%)	13 (7%)	21	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	192/193 (100%)	173 (90%)	19 (10%)	10	22
5	S	192/193 (100%)	174 (91%)	18 (9%)	11	25
6	F	201/239 (84%)	179 (89%)	22 (11%)	8	18
6	T	201/239 (84%)	179 (89%)	22 (11%)	8	18
7	G	207/210 (99%)	194 (94%)	13 (6%)	22	48
7	U	207/210 (99%)	195 (94%)	12 (6%)	25	52
8	H	181/214 (85%)	175 (97%)	6 (3%)	45	76
8	V	181/214 (85%)	175 (97%)	6 (3%)	45	76
9	I	172/173 (99%)	165 (96%)	7 (4%)	37	69
9	W	172/173 (99%)	167 (97%)	5 (3%)	50	80
10	J	175/175 (100%)	163 (93%)	12 (7%)	19	43
10	X	175/175 (100%)	164 (94%)	11 (6%)	22	48
11	K	169/235 (72%)	157 (93%)	12 (7%)	18	41
11	Y	169/235 (72%)	156 (92%)	13 (8%)	16	36
12	L	185/201 (92%)	169 (91%)	16 (9%)	13	29
12	Z	185/201 (92%)	169 (91%)	16 (9%)	13	29
13	1	199/224 (89%)	187 (94%)	12 (6%)	24	50
13	M	199/224 (89%)	189 (95%)	10 (5%)	30	60
14	2	162/178 (91%)	152 (94%)	10 (6%)	23	49
14	N	162/178 (91%)	153 (94%)	9 (6%)	26	54
All	All	5332/5816 (92%)	4987 (94%)	345 (6%)	21	46

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	33	GLN
1	A	64	LEU
1	A	10(A)	ILE
1	A	124	THR
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
1	A	192	ILE
1	A	215	ILE

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Mol	Chain	Res	Type
1	A	229	ILE
2	B	46	ILE
2	B	58	LEU
2	B	71	ASN
2	B	116	LEU
2	B	119	ILE
2	B	121	GLN
2	B	150	THR
2	B	163	ILE
2	B	185	LYS
2	B	192	LEU
2	B	212	PHE
2	B	218	ASN
3	C	10	ARG
3	C	21	ILE
3	C	25	GLU
3	C	57	LYS
3	C	66	LYS
3	C	70	ILE
3	C	121	GLN
3	C	150	GLN
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	28	LEU
4	D	40	ILE
4	D	48	LEU
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
4	D	244	GLU
5	E	11	ASP
5	E	32	LYS
5	E	56	ASP
5	E	57	GLU
5	E	76	LEU

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Mol	Chain	Res	Type
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	117	CYS
5	E	121	GLN
5	E	178	ARG
5	E	18(D)	ILE
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	2(D)	ASP
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	36	THR
6	F	43	ASN
6	F	56	SER
6	F	109	ILE
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	171	SER
6	F	176	LEU
6	F	18(E)	GLU
6	F	187	ARG
6	F	196	ILE
6	F	197	ILE
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	212	ILE
6	F	214	TRP
6	F	21(C)	ASN
6	F	233	ILE
6	F	240	ILE
7	G	14	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR

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Mol	Chain	Res	Type
7	G	169	GLN
7	G	172	ILE
7	G	184	ASN
7	G	197	MET
7	G	229	ILE
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	68	LEU
8	H	180	ILE
8	H	197	ARG
9	I	14	ILE
9	I	29	ASN
9	I	61	TYR
9	I	110	ILE
9	I	125	ILE
9	I	160	LEU
9	I	171	TRP
10	J	2	ILE
10	J	3	ILE
10	J	6	ILE
10	J	34	THR
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
10	J	133	TYR
10	J	137	LEU
10	J	174	ILE
10	J	177	ILE
11	K	4	LEU
11	K	8	PHE
11	K	9	GLN
11	K	39	PRO
11	K	53	GLN
11	K	65	LEU
11	K	74	ILE
11	K	87	VAL
11	K	100	MET
11	K	101	ILE

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Mol	Chain	Res	Type
11	K	104	TYR
11	K	10(B)	LYS
12	L	-7	ASN
12	L	14	LEU
12	L	21	ILE
12	L	25	SER
12	L	40	ASN
12	L	43	MET
12	L	58	ARG
12	L	70(A)	ASN
12	L	76	ILE
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	115	PRO
12	L	134	ILE
12	L	138	LEU
12	L	152	ILE
13	M	40	ASN
13	M	61	ASP
13	M	62	LEU
13	M	79	ILE
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
14	N	3	ILE
14	N	36	ARG
14	N	84	LYS
14	N	89	GLU
14	N	10(B)	LYS
14	N	119	VAL
14	N	144	GLU
14	N	149	GLU
14	N	18(I)	GLN
1	O	32	LYS
1	O	33	GLN
1	O	10(A)	ILE
1	O	124	THR
1	O	158	PHE

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Mol	Chain	Res	Type
1	O	179	ARG
1	O	192	ILE
1	O	215	ILE
1	O	229	ILE
2	P	40	ILE
2	P	46	ILE
2	P	58	LEU
2	P	71	ASN
2	P	116	LEU
2	P	119	ILE
2	P	121	GLN
2	P	150	THR
2	P	163	ILE
2	P	185	LYS
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
2	P	238	ILE
3	Q	10	ARG
3	Q	21	ILE
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	70	ILE
3	Q	121	GLN
3	Q	150	GLN
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	28	LEU
4	R	40	ILE
4	R	48	LEU
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
4	R	244	GLU

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Mol	Chain	Res	Type
5	S	11	ASP
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	117	CYS
5	S	121	GLN
5	S	178	ARG
5	S	18(D)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	2(D)	ASP
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	36	THR
6	T	43	ASN
6	T	56	SER
6	T	74	ILE
6	T	109	ILE
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	169	ARG
6	T	176	LEU
6	T	18(E)	GLU
6	T	187	ARG
6	T	196	ILE
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	212	ILE
6	T	214	TRP
6	T	21(C)	ASN
6	T	233	ILE
6	T	240	ILE
7	U	14	ILE
7	U	72	ARG

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Mol	Chain	Res	Type
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	229	ILE
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	43	CYS
8	V	68	LEU
8	V	180	ILE
8	V	197	ARG
9	W	14	ILE
9	W	29	ASN
9	W	61	TYR
9	W	160	LEU
9	W	171	TRP
10	X	2	ILE
10	X	3	ILE
10	X	6	ILE
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
10	X	133	TYR
10	X	137	LEU
10	X	174	ILE
10	X	177	ILE
11	Y	4	LEU
11	Y	8	PHE
11	Y	9	GLN
11	Y	35	ILE
11	Y	39	PRO
11	Y	53	GLN
11	Y	65	LEU
11	Y	74	ILE
11	Y	87	VAL
11	Y	100	MET

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Mol	Chain	Res	Type
11	Y	101	ILE
11	Y	104	TYR
11	Y	10(B)	LYS
12	Z	-7	ASN
12	Z	14	LEU
12	Z	21	ILE
12	Z	25	SER
12	Z	40	ASN
12	Z	43	MET
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	76	ILE
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	115	PRO
12	Z	134	ILE
12	Z	138	LEU
12	Z	152	ILE
13	1	-4	ILE
13	1	40	ASN
13	1	55	ILE
13	1	61	ASP
13	1	62	LEU
13	1	79	ILE
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
14	2	3	ILE
14	2	36	ARG
14	2	84	LYS
14	2	89	GLU
14	2	10(B)	LYS
14	2	115	LEU
14	2	119	VAL
14	2	144	GLU
14	2	149	GLU
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (193) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	161	ASN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	170	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	62	GLN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN

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Mol	Chain	Res	Type
6	F	241	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	81	GLN
9	I	145	ASN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	85	ASN
11	K	174	ASN
11	K	187	HIS
11	K	207	ASN
11	K	208	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	14(B)	ASN
12	L	1(I)	ASN
12	L	166	HIS

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Mol	Chain	Res	Type
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	191	GLN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	161	ASN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN

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Mol	Chain	Res	Type
5	S	170	GLN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	21	ASN
6	T	23	GLN
6	T	43	ASN
6	T	62	GLN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
6	T	241	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	81	GLN
9	W	145	ASN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	85	ASN

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Mol	Chain	Res	Type
11	Y	174	ASN
11	Y	187	HIS
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	85	HIS
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	191	GLN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	TY5	3	2	15	19,20,21	1.80	7 (36%)	22,25,27	0.96	2 (9%)
15	RE3	3	4	15	15,17,18	1.77	6 (40%)	21,25,27	2.18	6 (28%)
15	TY5	4	2	15	19,20,21	1.78	6 (31%)	22,25,27	0.97	1 (4%)
15	RE3	4	4	15	15,17,18	1.83	5 (33%)	21,25,27	2.18	7 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	TY5	3	2	15	-	0/9/11/13	0/2/2/2
15	RE3	3	4	15	-	0/5/23/25	0/2/2/2
15	TY5	4	2	15	-	0/9/11/13	0/2/2/2
15	RE3	4	4	15	-	0/5/23/25	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	4	RE3	CB-CA	-2.63	1.50	1.54
15	3	2	TY5	C53-C52	2.03	1.43	1.38
15	4	2	TY5	C53-C52	2.04	1.43	1.38
15	3	4	RE3	CZ3-CE3	2.04	1.43	1.38
15	3	2	TY5	C54-C55	2.05	1.43	1.38
15	3	2	TY5	CD2-CG	2.06	1.43	1.38
15	4	2	TY5	C51-C50	2.10	1.43	1.38
15	3	2	TY5	C54-C53	2.12	1.43	1.38
15	3	2	TY5	C51-C50	2.14	1.43	1.38
15	3	4	RE3	CH2-CZ2	2.14	1.43	1.38
15	4	4	RE3	CZ3-CH2	2.19	1.43	1.38
15	4	2	TY5	C54-C53	2.20	1.43	1.38
15	3	4	RE3	CE2-CD2	2.23	1.42	1.39
15	3	2	TY5	OH-CZ	2.25	1.43	1.37
15	4	4	RE3	CH2-CZ2	2.28	1.43	1.38
15	4	2	TY5	OH-CZ	2.30	1.43	1.37
15	3	4	RE3	CE3-CD2	2.36	1.42	1.39
15	4	4	RE3	CZ2-CE2	2.42	1.43	1.39
15	4	2	TY5	CD2-CG	2.44	1.44	1.38
15	4	4	RE3	CE3-CD2	2.73	1.43	1.39
15	3	4	RE3	OG-CG	2.82	1.45	1.42
15	4	4	RE3	CZ3-CE3	3.06	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	2	TY5	CE2-CZ	3.42	1.45	1.38
15	3	2	TY5	CE2-CZ	3.73	1.46	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3	4	RE3	CE2-NE1-CD1	-5.09	109.14	111.88
15	4	4	RE3	CE2-NE1-CD1	-5.02	109.17	111.88
15	3	4	RE3	CG-CD2-CE2	-4.14	106.97	108.80
15	4	4	RE3	CG-CD2-CE2	-3.98	107.04	108.80
15	3	4	RE3	O-C-CA	-2.64	118.62	125.49
15	4	4	RE3	CZ2-CE2-NE1	-2.56	125.79	131.02
15	4	4	RE3	OD1-CD1-CG	-2.55	122.55	124.71
15	4	4	RE3	O-C-CA	-2.51	118.94	125.49
15	3	4	RE3	CZ2-CE2-NE1	-2.49	125.92	131.02
15	3	2	TY5	O-C-CA	-2.19	119.79	125.49
15	3	2	TY5	C49-OH-CZ	2.69	124.93	117.70
15	4	2	TY5	C49-OH-CZ	2.95	125.61	117.70
15	4	4	RE3	CD2-CE2-NE1	3.01	111.59	109.61
15	3	4	RE3	CD2-CE2-NE1	3.67	112.02	109.61
15	3	4	RE3	CG-CD1-NE1	3.98	110.92	108.39
15	4	4	RE3	CG-CD1-NE1	4.36	111.16	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	2	TY5	2	0
15	4	2	TY5	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	250/250 (100%)	-0.46	3 (1%)	81	81	40, 54, 84, 107	0
1	O	250/250 (100%)	-0.41	4 (1%)	74	75	40, 56, 85, 107	0
2	B	244/258 (94%)	-0.29	4 (1%)	74	75	41, 58, 95, 120	0
2	P	244/258 (94%)	-0.24	6 (2%)	61	61	41, 59, 96, 120	0
3	C	241/254 (94%)	-0.11	5 (2%)	67	68	42, 63, 112, 129	0
3	Q	241/254 (94%)	0.18	21 (8%)	13	10	45, 65, 112, 129	0
4	D	242/260 (93%)	-0.22	8 (3%)	50	50	43, 61, 96, 127	0
4	R	242/260 (93%)	-0.17	8 (3%)	50	50	44, 62, 96, 127	0
5	E	233/234 (99%)	-0.20	4 (1%)	73	74	45, 65, 91, 113	0
5	S	233/234 (99%)	0.13	12 (5%)	31	30	45, 67, 93, 113	0
6	F	244/288 (84%)	-0.42	2 (0%)	87	88	42, 58, 91, 108	0
6	T	244/288 (84%)	-0.15	6 (2%)	61	61	43, 58, 92, 107	0
7	G	243/252 (96%)	-0.44	3 (1%)	81	81	38, 53, 79, 118	0
7	U	243/252 (96%)	-0.36	2 (0%)	87	88	39, 54, 79, 118	0
8	H	222/261 (85%)	-0.43	1 (0%)	91	93	37, 52, 70, 103	0
8	V	222/261 (85%)	-0.55	1 (0%)	91	93	38, 52, 70, 104	0
9	I	204/205 (99%)	-0.49	1 (0%)	91	93	37, 50, 68, 87	0
9	W	204/205 (99%)	-0.39	1 (0%)	91	93	37, 50, 68, 86	0
10	J	198/198 (100%)	-0.45	4 (2%)	68	69	37, 51, 69, 127	0
10	X	198/198 (100%)	-0.47	5 (2%)	61	61	39, 51, 69, 127	0
11	K	212/287 (73%)	-0.39	4 (1%)	70	70	36, 49, 76, 85	0
11	Y	212/287 (73%)	-0.43	3 (1%)	78	77	35, 51, 77, 86	0
12	L	222/241 (92%)	-0.47	3 (1%)	78	77	35, 51, 72, 100	0
12	Z	222/241 (92%)	-0.50	4 (1%)	71	72	35, 51, 72, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/266 (87%)	-0.59	0 100 100	37, 51, 64, 70	0
13	M	233/266 (87%)	-0.56	1 (0%) 93 94	37, 51, 64, 70	0
14	2	196/215 (91%)	-0.53	0 100 100	35, 48, 67, 81	0
14	N	196/215 (91%)	-0.58	0 100 100	37, 47, 67, 82	0
15	3	1/5 (20%)	-0.24	0 100 100	46, 46, 46, 46	0
15	4	1/5 (20%)	0.12	0 100 100	48, 48, 48, 48	0
All	All	6370/6948 (91%)	-0.35	116 (1%) 71 72	35, 54, 87, 129	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	12(F)	GLY	11.8
10	J	192	ALA	10.0
3	C	55	THR	8.9
7	U	6	ALA	8.7
4	D	12(E)	SER	8.3
10	X	192	ALA	8.1
4	D	12(F)	GLY	8.0
10	X	193	GLN	7.4
4	D	12(D)	ALA	7.4
4	D	12(C)	GLY	7.2
3	C	56	LEU	7.1
3	Q	236	ILE	6.5
4	R	12(E)	SER	6.0
10	J	193	GLN	5.9
2	B	218	ASN	5.9
4	D	126	ARG	5.8
7	G	6	ALA	5.6
5	S	5	ARG	5.6
4	R	12(D)	ALA	5.6
12	L	145	TYR	5.5
5	S	203	ASP	5.5
2	P	217	ALA	5.3
4	R	126	ARG	5.1
2	P	218	ASN	5.1
7	U	240	ASP	4.9
1	A	4	MET	4.9
4	R	12(C)	GLY	4.8
3	Q	56	LEU	4.4
3	Q	202	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
5	S	233	ILE	4.3
1	O	4	MET	4.3
2	B	217	ALA	4.3
10	X	189	ASP	4.3
12	Z	145	TYR	4.2
5	E	5	ARG	4.1
4	D	12(G)	GLU	4.1
3	Q	242	GLU	4.0
11	K	104	TYR	3.9
5	S	4	PHE	3.9
5	S	2(C)	VAL	3.8
5	E	203	ASP	3.7
3	Q	241	GLN	3.6
3	Q	203	THR	3.6
3	Q	243	GLN	3.6
5	S	178	ARG	3.5
12	Z	14(W)	LYS	3.5
3	Q	233	VAL	3.5
1	A	236	LEU	3.4
2	B	54	VAL	3.4
4	R	12(G)	GLU	3.4
3	C	203	THR	3.4
5	S	206	SER	3.4
5	E	4	PHE	3.3
3	Q	179	ASN	3.3
7	G	240	ASP	3.3
3	Q	55	THR	3.3
6	T	240	ILE	3.3
5	E	233	ILE	3.0
11	Y	208	ASN	2.9
3	Q	63	THR	2.9
13	M	-8	THR	2.9
5	S	210	LEU	2.8
10	X	191	GLN	2.8
6	T	238	LYS	2.7
9	I	-8	SER	2.7
3	Q	240	LYS	2.7
2	P	219	GLU	2.7
3	Q	54	SER	2.7
2	B	21(B)	GLY	2.7
4	R	127	LEU	2.7
6	F	5	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
10	J	191	GLN	2.6
11	Y	104	TYR	2.6
3	Q	239	GLU	2.6
1	O	236	LEU	2.6
10	X	-1	MET	2.6
8	V	223	ASP	2.6
3	Q	18(D)	GLU	2.6
11	K	208	ASN	2.6
6	T	57	LYS	2.6
2	P	54	VAL	2.6
3	Q	238	GLN	2.5
6	T	6	THR	2.5
4	D	127	LEU	2.4
6	T	5	GLY	2.4
11	K	207	ASN	2.4
5	S	231	LYS	2.4
1	O	55	SER	2.4
11	K	210	ILE	2.4
9	W	-8	SER	2.3
3	Q	194	VAL	2.3
5	S	229	VAL	2.3
1	A	5	THR	2.3
3	C	240	LYS	2.3
3	Q	178	LYS	2.3
8	H	223	ASP	2.3
3	Q	201	VAL	2.3
1	O	235	ALA	2.2
11	Y	211	GLY	2.2
2	P	21(A)	LYS	2.2
6	F	240	ILE	2.2
3	C	202	GLN	2.2
10	J	168	MET	2.2
5	S	2(E)	ASN	2.1
7	G	239	GLN	2.1
4	D	125	GLU	2.1
12	Z	14(M)	VAL	2.1
3	Q	229	ILE	2.1
2	P	53	LYS	2.1
3	Q	187	GLU	2.1
12	Z	14(P)	PRO	2.1
12	L	14(P)	PRO	2.1
4	R	121	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	S	32	LYS	2.1
12	L	14(W)	LYS	2.1
6	T	199	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	TY5	4	2	19/20	0.94	0.16	-	41,46,55,55	0
15	RE3	4	4	16/17	0.94	0.14	-	50,52,54,57	0
15	RE3	3	4	16/17	0.94	0.16	-	49,51,52,54	0
15	TY5	3	2	19/20	0.96	0.15	-	42,45,54,55	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.