Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 01:56 AM EDT

PDB ID	:	3WXR
Title	:	Yeast 20S proteasome with a mutation of alpha7 subunit
Authors	:	Yashiroda, H.; Toda, Y.; Otsu, S.; Takagi, K.; Mizushima, T.; Murata, S.
Deposited on	:	2014-08-06
Resolution	:	3.15 Å(reported)

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

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

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

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

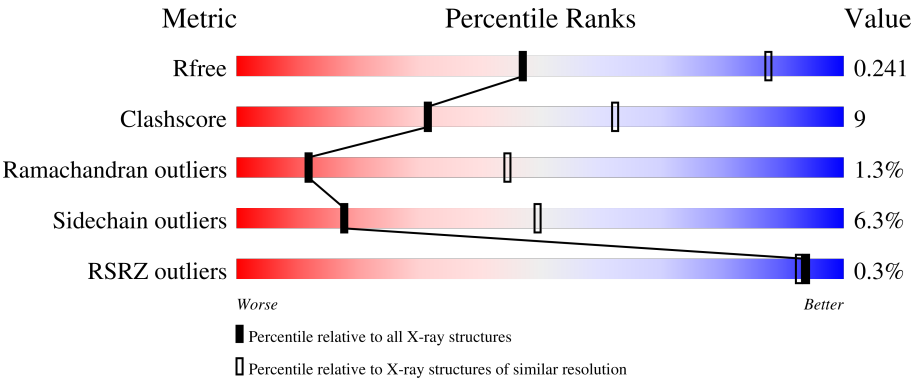
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	252	% 77% 16%
1	O	252	75% 18%
2	B	250	78% 20%
2	P	250	80% 18%
3	C	258	66% 24% 6%

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Mol	Chain	Length	Quality of chain
3	Q	258	% 68% 22% 5%
4	D	254	70% 20% 5%
4	R	254	% 69% 21% 5%
5	E	260	% 67% 23% 8%
5	S	260	72% 18% 8%
6	F	234	68% 26% 5%
6	T	234	69% 25%
7	G	277	65% 19% 14%
7	U	277	65% 17% 14%
8	H	215	74% 14% 9%
8	V	215	% 71% 20% 7%
9	I	261	70% 15% 15%
9	W	261	70% 13% 15%
10	J	205	83% 15%
10	X	205	79% 19%
11	K	238	% 65% 17% 17%
11	Y	238	58% 21% 17%
12	L	287	56% 17% 26%
12	Z	287	61% 12% 26%
13	1	241	68% 22% 8%
13	M	241	67% 21% 5% 8%
14	2	266	68% 18% 12%
14	N	266	70% 15% 12%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 49360 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 subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	O	243	Total	C	N	O	S	0	0	0
			1920	1221	322	369	8			

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
2	P	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	242	Total	C	N	O	S	0	0	0
			1895	1196	319	377	3			
3	Q	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	239	Total	C	N	O	S	0	0	0
			1842	1152	311	372	7			
5	S	238	Total	C	N	O	S	0	0	0
			1842	1152	310	373	7			

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			
6	T	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	237	Total	C	N	O	S	0	0	0
			1847	1176	322	344	5			
7	U	237	Total	C	N	O	S	0	0	0
			1847	1176	322	344	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	11	MET	-	expression tag	UNP P21242
U	11	MET	-	expression tag	UNP P21242

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
8	V	199	Total	C	N	O	S	0	0	0
			1528	965	253	303	7			

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
9	W	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
10	X	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	197	Total	C	N	O	S	0	0	0
			1576	1000	268	303	5			
11	Y	198	Total	C	N	O	S	0	0	0
			1584	1005	269	304	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	198	GLY	-	expression tag	UNP P22141
K	199	SER	-	expression tag	UNP P22141
K	200	GLY	-	expression tag	UNP P22141
K	201	SER	-	expression tag	UNP P22141
K	202	LEU	-	expression tag	UNP P22141
K	203	GLU	-	expression tag	UNP P22141
K	204	VAL	-	expression tag	UNP P22141
K	205	LEU	-	expression tag	UNP P22141
K	206	PHE	-	expression tag	UNP P22141
K	207	GLN	-	expression tag	UNP P22141
K	208	GLY	-	expression tag	UNP P22141
K	209	PRO	-	expression tag	UNP P22141
K	210	GLY	-	expression tag	UNP P22141
K	211	SER	-	expression tag	UNP P22141
K	212	GLY	-	expression tag	UNP P22141
K	213	SER	-	expression tag	UNP P22141
K	214	THR	-	expression tag	UNP P22141
K	215	MET	-	expression tag	UNP P22141
K	216	ASP	-	expression tag	UNP P22141
K	217	TYR	-	expression tag	UNP P22141
K	218	LYS	-	expression tag	UNP P22141
K	219	ASP	-	expression tag	UNP P22141
K	220	HIS	-	expression tag	UNP P22141
K	221	ASP	-	expression tag	UNP P22141
K	222	GLY	-	expression tag	UNP P22141

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Chain	Residue	Modelled	Actual	Comment	Reference
K	223	ASP	-	expression tag	UNP P22141
K	224	TYR	-	expression tag	UNP P22141
K	225	LYS	-	expression tag	UNP P22141
K	226	ASP	-	expression tag	UNP P22141
K	227	HIS	-	expression tag	UNP P22141
K	228	ASP	-	expression tag	UNP P22141
K	229	ILE	-	expression tag	UNP P22141
K	230	ASP	-	expression tag	UNP P22141
K	231	TYR	-	expression tag	UNP P22141
K	232	LYS	-	expression tag	UNP P22141
K	233	ASP	-	expression tag	UNP P22141
K	234	ASP	-	expression tag	UNP P22141
K	235	ASP	-	expression tag	UNP P22141
K	236	ASP	-	expression tag	UNP P22141
K	237	LYS	-	expression tag	UNP P22141
Y	198	GLY	-	expression tag	UNP P22141
Y	199	SER	-	expression tag	UNP P22141
Y	200	GLY	-	expression tag	UNP P22141
Y	201	SER	-	expression tag	UNP P22141
Y	202	LEU	-	expression tag	UNP P22141
Y	203	GLU	-	expression tag	UNP P22141
Y	204	VAL	-	expression tag	UNP P22141
Y	205	LEU	-	expression tag	UNP P22141
Y	206	PHE	-	expression tag	UNP P22141
Y	207	GLN	-	expression tag	UNP P22141
Y	208	GLY	-	expression tag	UNP P22141
Y	209	PRO	-	expression tag	UNP P22141
Y	210	GLY	-	expression tag	UNP P22141
Y	211	SER	-	expression tag	UNP P22141
Y	212	GLY	-	expression tag	UNP P22141
Y	213	SER	-	expression tag	UNP P22141
Y	214	THR	-	expression tag	UNP P22141
Y	215	MET	-	expression tag	UNP P22141
Y	216	ASP	-	expression tag	UNP P22141
Y	217	TYR	-	expression tag	UNP P22141
Y	218	LYS	-	expression tag	UNP P22141
Y	219	ASP	-	expression tag	UNP P22141
Y	220	HIS	-	expression tag	UNP P22141
Y	221	ASP	-	expression tag	UNP P22141
Y	222	GLY	-	expression tag	UNP P22141
Y	223	ASP	-	expression tag	UNP P22141
Y	224	TYR	-	expression tag	UNP P22141

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	225	LYS	-	expression tag	UNP P22141
Y	226	ASP	-	expression tag	UNP P22141
Y	227	HIS	-	expression tag	UNP P22141
Y	228	ASP	-	expression tag	UNP P22141
Y	229	ILE	-	expression tag	UNP P22141
Y	230	ASP	-	expression tag	UNP P22141
Y	231	TYR	-	expression tag	UNP P22141
Y	232	LYS	-	expression tag	UNP P22141
Y	233	ASP	-	expression tag	UNP P22141
Y	234	ASP	-	expression tag	UNP P22141
Y	235	ASP	-	expression tag	UNP P22141
Y	236	ASP	-	expression tag	UNP P22141
Y	237	LYS	-	expression tag	UNP P22141

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	1	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called Proteasome subunit beta type-7.

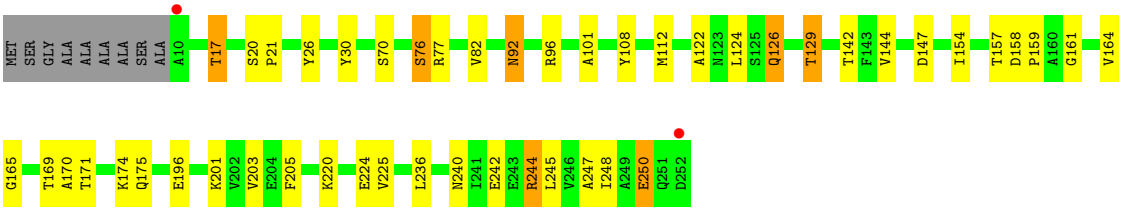
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	2	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

3 Residue-property plots (i)

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

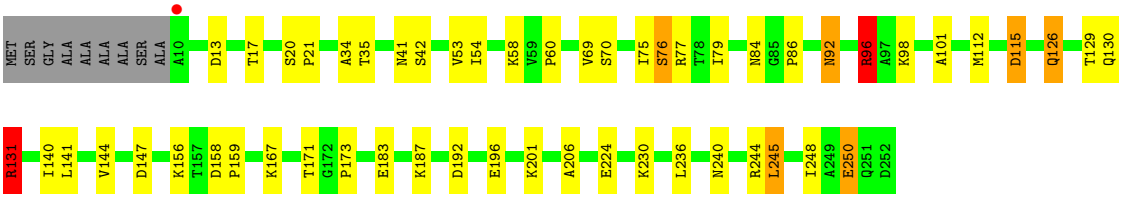
• Molecule 1: Proteasome subunit alpha type-1

Chain A:



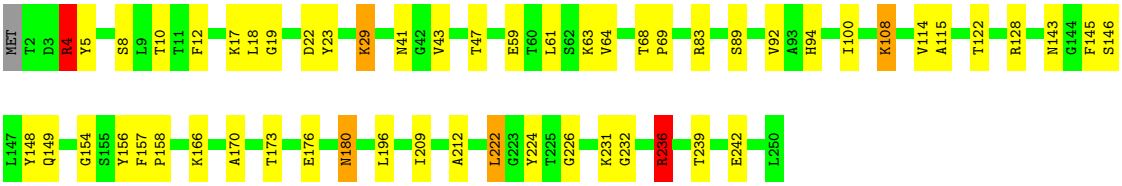
• Molecule 1: Proteasome subunit alpha type-1

Chain O:



• Molecule 2: Proteasome subunit alpha type-2

Chain B:

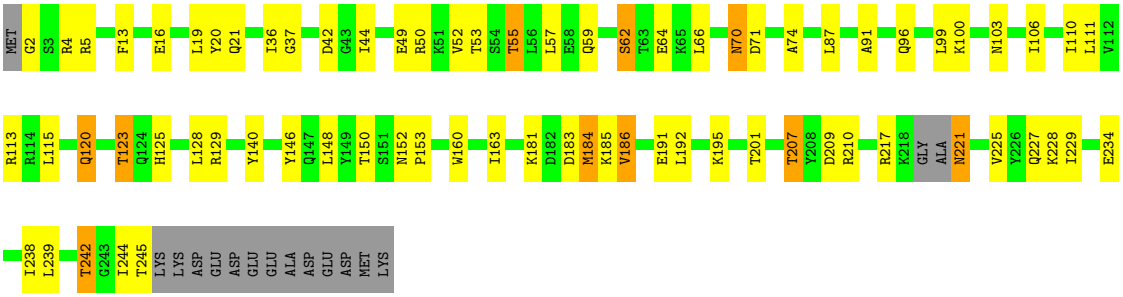


• Molecule 2: Proteasome subunit alpha type-2

Chain P:

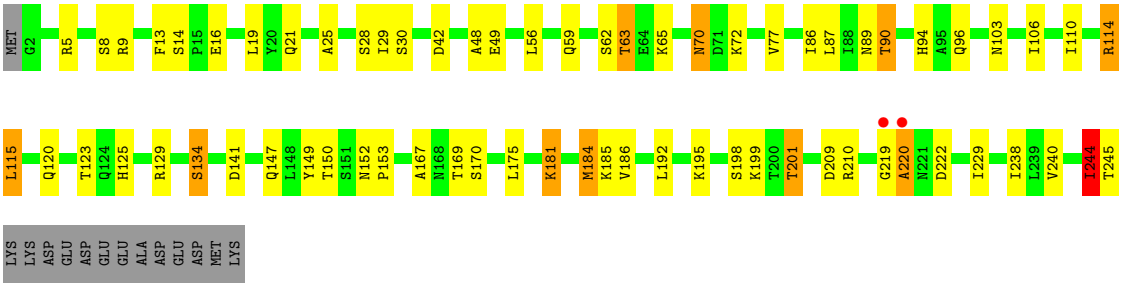
• Molecule 3: Proteasome subunit alpha type-3

Chain C:



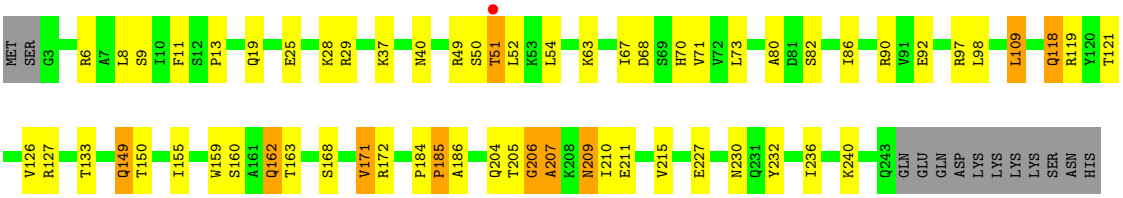
• Molecule 3: Proteasome subunit alpha type-3

Chain Q:



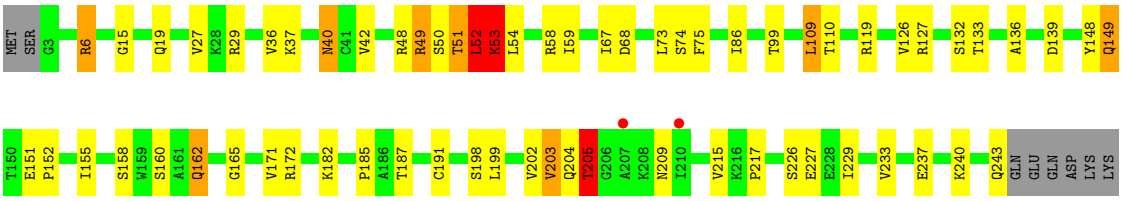
• Molecule 4: Proteasome subunit alpha type-4

Chain D:



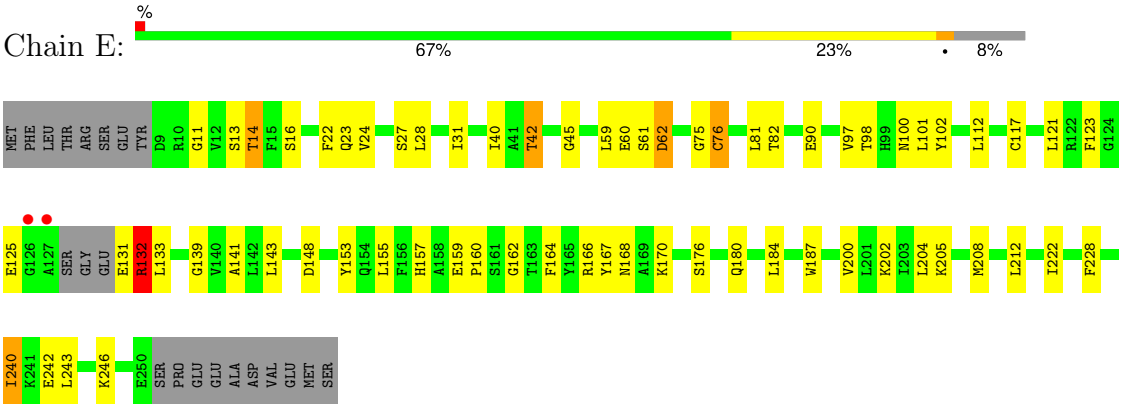
• Molecule 4: Proteasome subunit alpha type-4

Chain R:



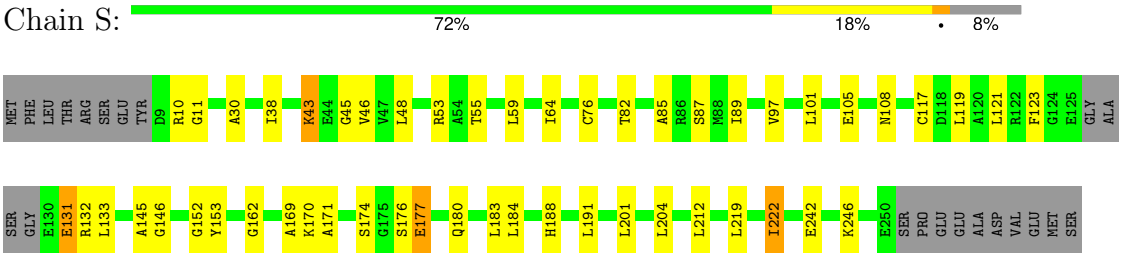
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



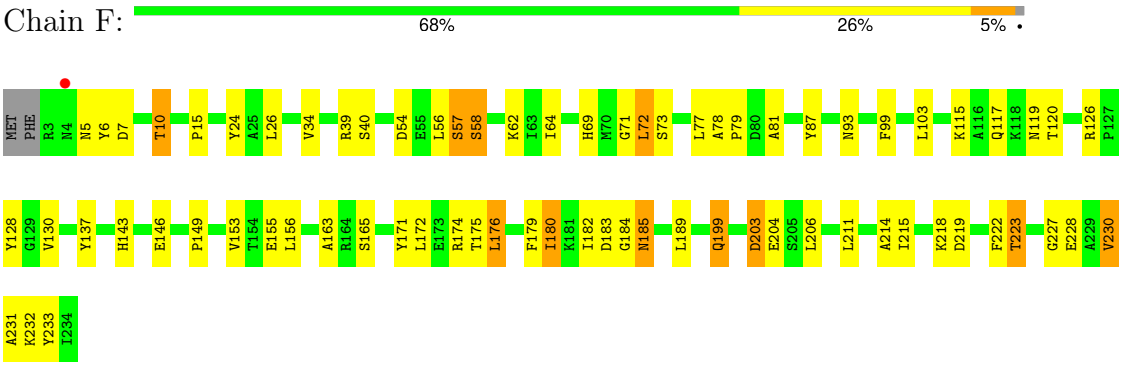
• Molecule 5: Proteasome subunit alpha type-5

Chain S:



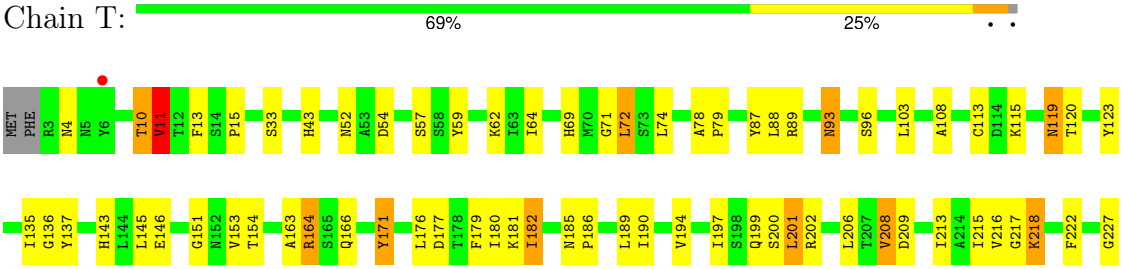
• Molecule 6: Proteasome subunit alpha type-6

Chain F:



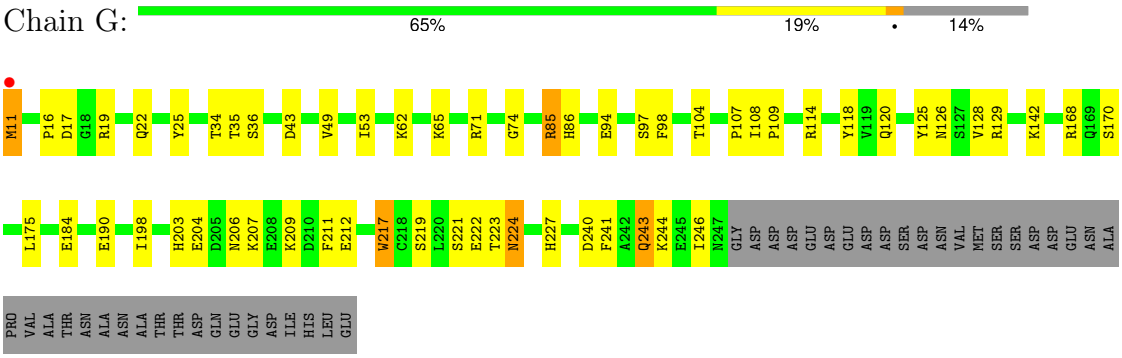
• Molecule 6: Proteasome subunit alpha type-6

Chain T:



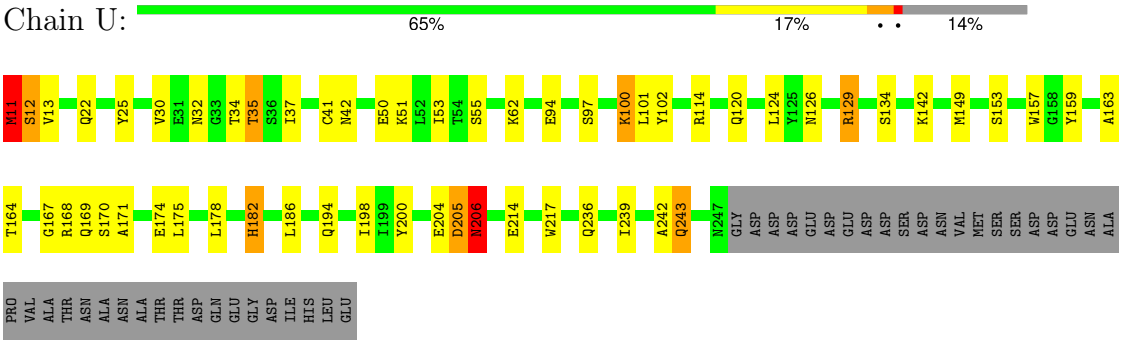
• Molecule 7: Probable proteasome subunit alpha type-7

Chain G:



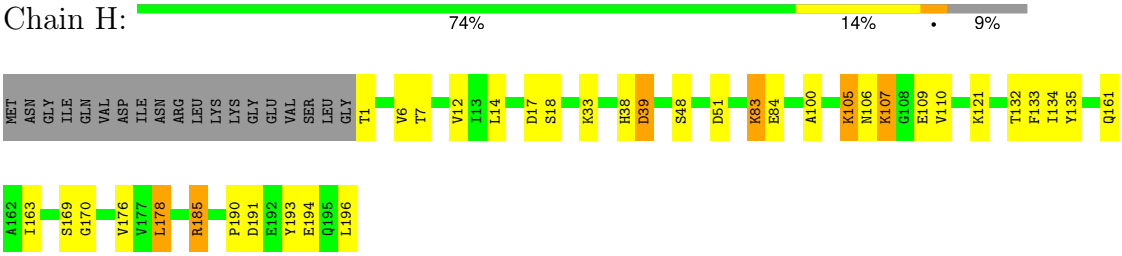
• Molecule 7: Probable proteasome subunit alpha type-7

Chain U:



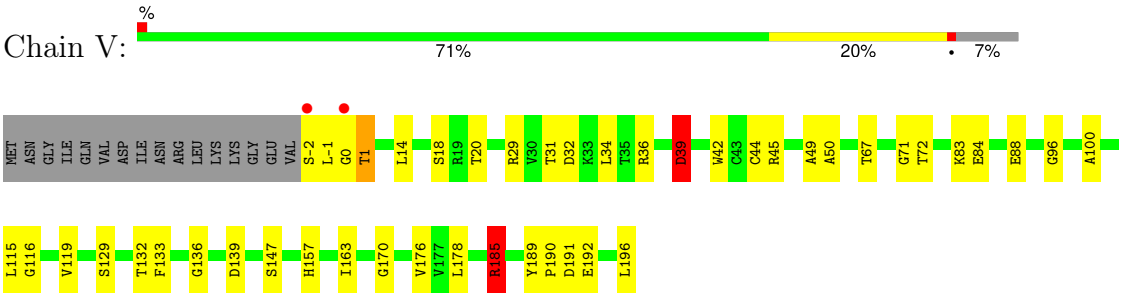
• Molecule 8: Proteasome subunit beta type-1

Chain H:



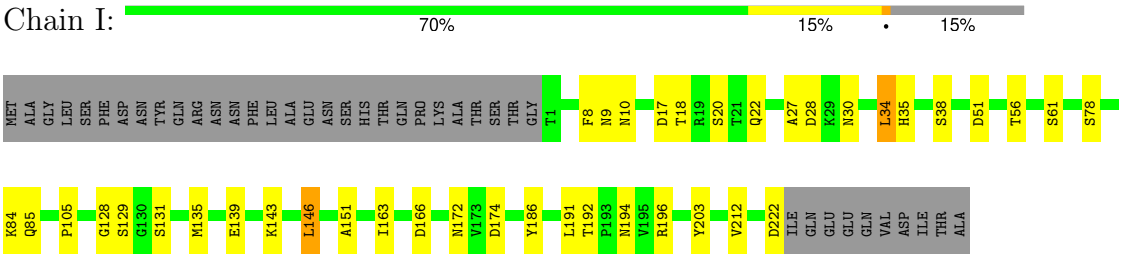
• Molecule 8: Proteasome subunit beta type-1

Chain V:



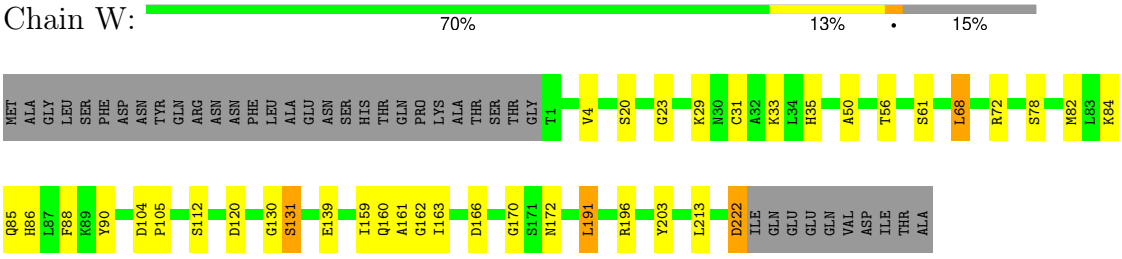
• Molecule 9: Proteasome subunit beta type-2

Chain I:



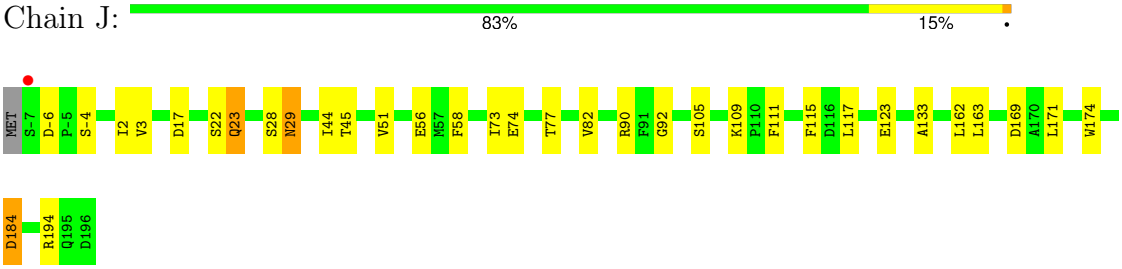
• Molecule 9: Proteasome subunit beta type-2

Chain W:



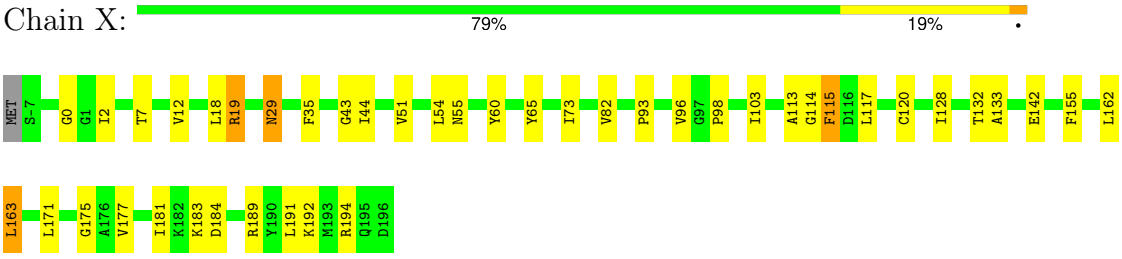
• Molecule 10: Proteasome subunit beta type-3

Chain J:



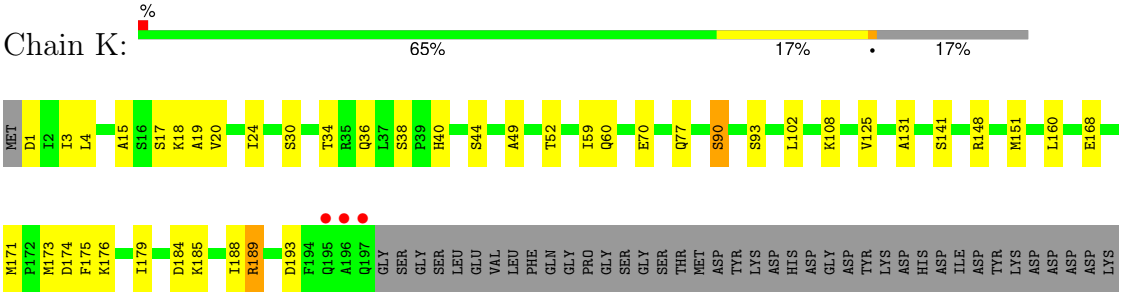
• Molecule 10: Proteasome subunit beta type-3

Chain X:



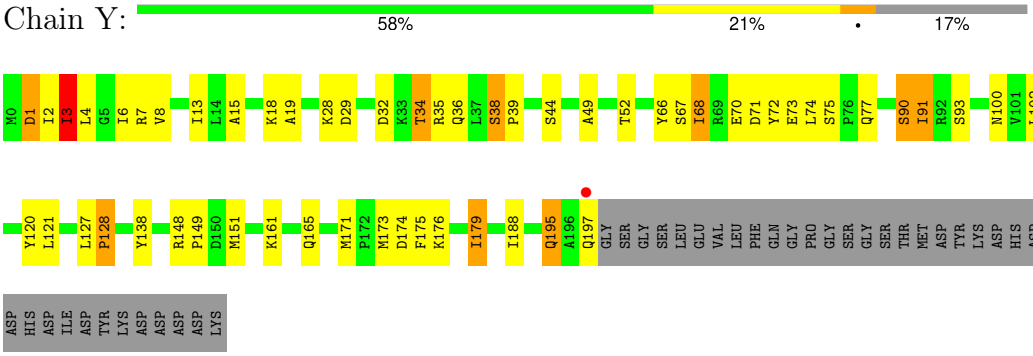
• Molecule 11: Proteasome subunit beta type-4

Chain K:



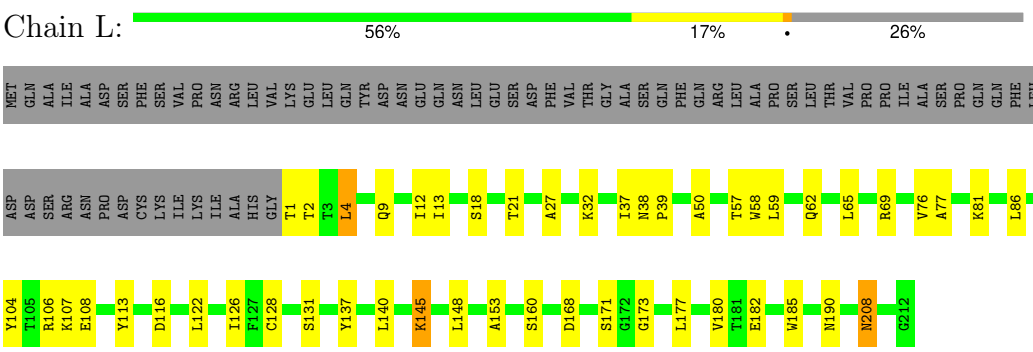
• Molecule 11: Proteasome subunit beta type-4

Chain Y:



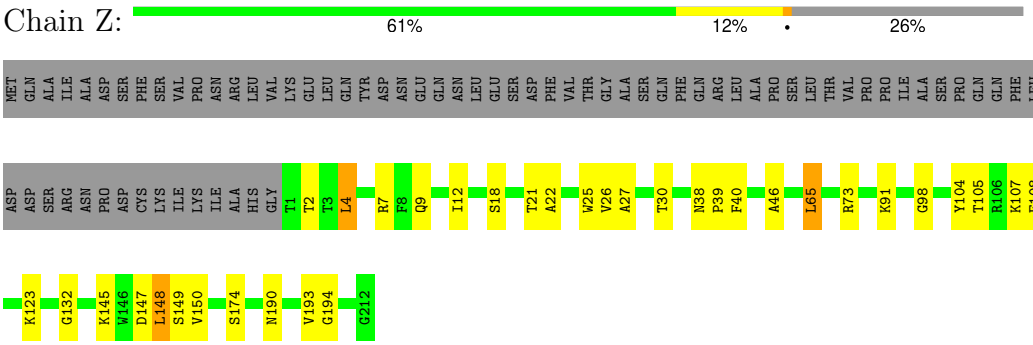
• Molecule 12: Proteasome subunit beta type-5

Chain L:



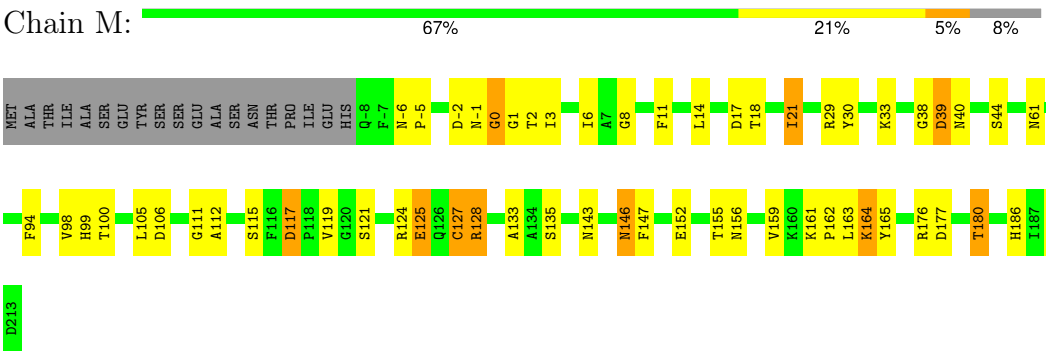
• Molecule 12: Proteasome subunit beta type-5

Chain Z:



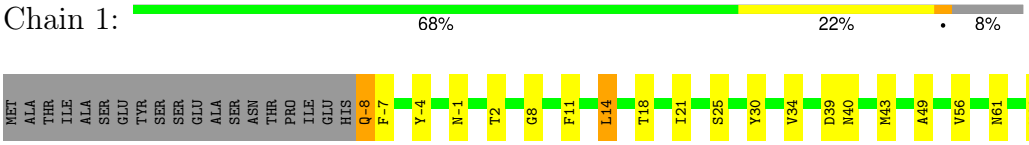
• Molecule 13: Proteasome subunit beta type-6

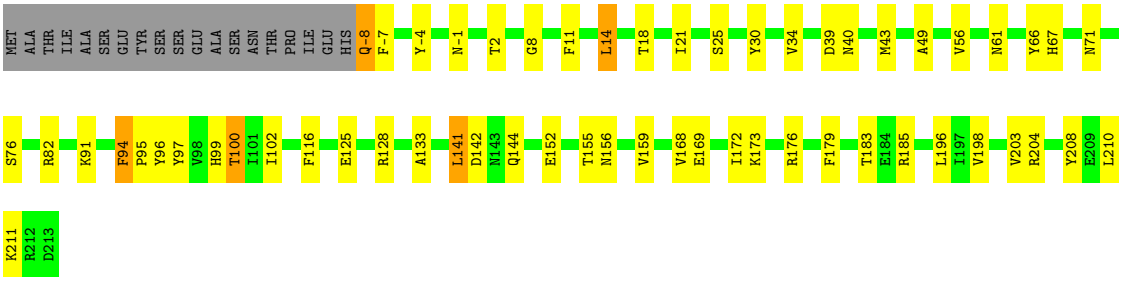
Chain M:



• Molecule 13: Proteasome subunit beta type-6

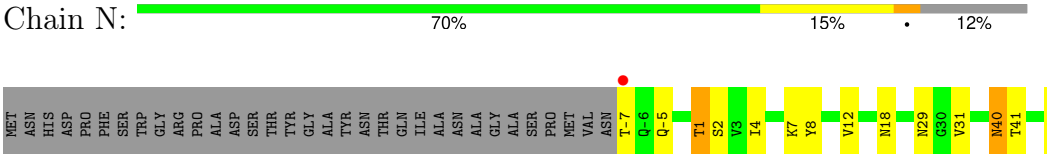
Chain 1:

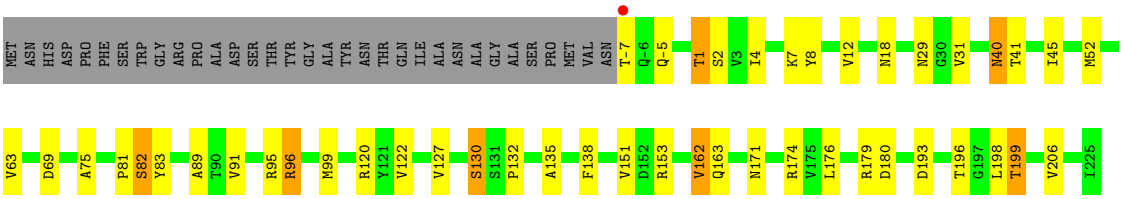




• Molecule 14: Proteasome subunit beta type-7

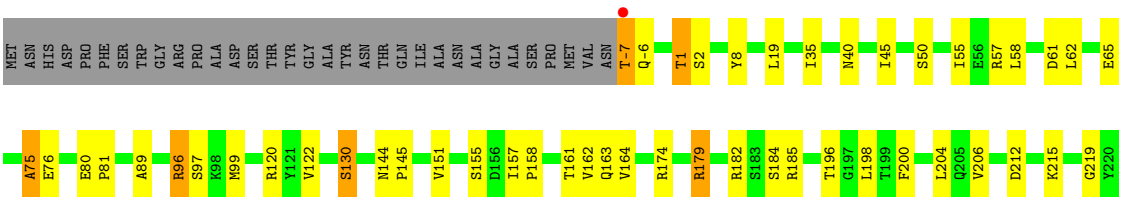
Chain N:





• Molecule 14: Proteasome subunit beta type-7

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.25Å 298.62Å 145.40Å 90.00° 113.13° 90.00°	Depositor
Resolution (Å)	48.20 – 3.15 48.20 – 3.15	Depositor EDS
% Data completeness (in resolution range)	86.6 (48.20-3.15) 86.7 (48.20-3.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.174 , 0.242 0.176 , 0.241	Depositor DCC
R_{free} test set	8012 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49360	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.59	0/1959	0.87	0/2652
1	O	0.57	0/1958	0.88	2/2652 (0.1%)
2	B	0.57	0/1944	0.85	2/2632 (0.1%)
2	P	0.52	0/1944	0.80	0/2632
3	C	0.55	0/1924	0.87	1/2603 (0.0%)
3	Q	0.56	0/1934	0.85	0/2618
4	D	0.53	0/1919	0.88	1/2598 (0.0%)
4	R	0.55	0/1919	0.88	3/2598 (0.1%)
5	E	0.57	0/1866	0.89	1/2513 (0.0%)
5	S	0.53	0/1866	0.85	0/2513
6	F	0.53	0/1811	0.83	0/2447
6	T	0.52	0/1811	0.85	0/2447
7	G	0.55	0/1886	0.81	0/2545
7	U	0.55	0/1886	0.84	1/2545 (0.0%)
8	H	0.59	0/1541	0.88	0/2087
8	V	0.61	0/1557	0.90	3/2108 (0.1%)
9	I	0.58	0/1715	0.87	0/2326
9	W	0.54	0/1715	0.84	1/2326 (0.0%)
10	J	0.59	0/1611	0.85	0/2174
10	X	0.59	0/1611	0.83	0/2174
11	K	0.60	0/1604	0.91	0/2163
11	Y	0.57	0/1612	0.90	1/2173 (0.0%)
12	L	0.60	0/1681	0.86	0/2274
12	Z	0.60	0/1681	0.86	0/2274
13	1	0.57	0/1795	0.88	0/2420
13	M	0.61	0/1795	0.91	1/2420 (0.0%)
14	2	0.61	0/1855	0.90	0/2514
14	N	0.58	0/1855	0.89	1/2514 (0.0%)
All	All	0.57	0/50255	0.87	18/67942 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	71	ASP	CB-CG-OD1	-7.67	111.39	118.30
1	O	131	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	B	236	ARG	NE-CZ-NH2	7.41	124.00	120.30
7	U	11	MET	CG-SD-CE	7.20	111.72	100.20
4	R	52	LEU	CA-CB-CG	7.18	131.82	115.30
1	O	96	ARG	NE-CZ-NH1	7.12	123.86	120.30
8	V	1	THR	N-CA-C	6.97	129.82	111.00
2	B	4	ARG	NE-CZ-NH1	6.83	123.71	120.30
8	V	185	ARG	NE-CZ-NH1	6.71	123.66	120.30
13	M	117	ASP	CB-CA-C	-6.70	97.00	110.40
4	R	119	ARG	NE-CZ-NH1	5.49	123.04	120.30
9	W	23	GLY	N-CA-C	-5.45	99.47	113.10
11	Y	3	ILE	CG1-CB-CG2	-5.11	100.16	111.40
8	V	96	GLY	N-CA-C	-5.10	100.36	113.10
14	N	162	VAL	CB-CA-C	-5.08	101.74	111.40
4	R	139	ASP	CB-CG-OD1	5.06	122.86	118.30
4	D	119	ARG	NE-CZ-NH1	5.05	122.82	120.30
5	E	184	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1921	0	1910	32	0
1	O	1920	0	1910	42	0
2	B	1907	0	1917	46	0
2	P	1907	0	1917	35	0
3	C	1895	0	1892	50	0
3	Q	1904	0	1901	42	0
4	D	1890	0	1900	42	0
4	R	1890	0	1900	42	0
5	E	1842	0	1821	45	0
5	S	1842	0	1819	26	0
6	F	1784	0	1788	49	0
6	T	1784	0	1788	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1847	0	1847	25	0
7	U	1847	0	1847	43	0
8	H	1512	0	1481	26	0
8	V	1528	0	1495	28	0
9	I	1684	0	1688	25	0
9	W	1684	0	1688	28	0
10	J	1581	0	1574	19	0
10	X	1581	0	1574	32	0
11	K	1576	0	1581	19	0
11	Y	1584	0	1590	36	0
12	L	1644	0	1595	35	0
12	Z	1644	0	1595	20	0
13	1	1757	0	1711	46	0
13	M	1757	0	1711	50	0
14	2	1824	0	1832	31	0
14	N	1824	0	1832	31	0
All	All	49360	0	49104	890	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 9.

All (890) 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)
13:M:155:THR:HG21	13:M:159:VAL:HG12	1.35	1.05
13:M:18:THR:CG2	13:M:30:TYR:HA	1.90	1.01
8:H:1:THR:HG22	8:H:33:LYS:HZ3	1.26	0.99
7:U:11:MET:O	7:U:13:VAL:N	1.96	0.98
11:K:184:ASP:OD2	11:K:189:ARG:NH1	1.99	0.94
13:1:18:THR:CG2	13:1:30:TYR:HA	2.01	0.90
12:Z:105:THR:OG1	12:Z:108:GLU:HG2	1.71	0.89
3:C:181:LYS:O	3:C:184:MET:HG3	1.73	0.89
4:R:204:GLN:O	4:R:205:THR:OG1	1.90	0.88
14:2:-7:THR:CG2	14:2:99:MET:O	2.22	0.87
7:G:94:GLU:HG2	7:G:114:ARG:HB3	1.54	0.87
13:1:18:THR:HG22	13:1:30:TYR:HA	1.56	0.87
1:O:92:ASN:C	1:O:92:ASN:HD22	1.77	0.87
8:V:36:ARG:HG3	8:V:42:TRP:CE2	2.12	0.85
13:M:155:THR:O	13:M:156:ASN:HB3	1.77	0.84
1:O:101:ALA:HA	1:O:112:MET:HE2	1.59	0.83
8:H:1:THR:CG2	8:H:33:LYS:HZ3	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:ALA:O	13:M:128:ARG:NH2	2.13	0.81
6:F:227:GLY:O	6:F:230:VAL:HG23	1.82	0.80
4:R:51:THR:HG23	4:R:52:LEU:HA	1.65	0.79
2:B:5:TYR:OH	7:G:126:ASN:ND2	2.16	0.79
13:M:152:GLU:HB2	13:M:155:THR:OG1	1.83	0.78
7:U:11:MET:O	7:U:13:VAL:HG22	1.83	0.77
8:V:-1:LEU:O	8:V:1:THR:N	2.18	0.77
13:M:155:THR:CG2	13:M:159:VAL:HG12	2.16	0.75
8:H:1:THR:HG22	8:H:33:LYS:NZ	2.01	0.75
12:L:128:CYS:HB2	12:L:137:TYR:CE2	2.22	0.75
14:2:96:ARG:HG3	14:2:97:SER:N	1.99	0.74
14:N:8:TYR:CE2	14:N:162:VAL:HG22	2.21	0.74
9:W:35:HIS:HB3	9:W:56:THR:HG21	1.68	0.74
6:F:183:ASP:O	6:F:185:ASN:N	2.21	0.74
6:F:10:THR:HG21	6:F:120:THR:HA	1.70	0.73
11:Y:148:ARG:O	11:Y:151:MET:HG3	1.88	0.73
2:P:194:LEU:HD21	2:P:250:LEU:HD13	1.70	0.73
7:U:169:GLN:OE1	7:U:169:GLN:N	2.20	0.73
3:C:50:ARG:NH1	3:C:62:SER:OG	2.21	0.73
13:1:43:MET:HE2	13:1:56:VAL:HA	1.70	0.73
13:M:18:THR:HG22	13:M:30:TYR:HA	1.70	0.72
12:Z:145:LYS:HB3	12:Z:148:LEU:HD13	1.71	0.72
4:D:159:TRP:CD2	4:D:162:GLN:HG2	2.25	0.72
12:Z:107:LYS:H	12:Z:107:LYS:HD2	1.54	0.72
13:1:155:THR:O	13:1:156:ASN:HB3	1.89	0.72
9:I:129:SER:HB2	9:I:166:ASP:OD2	1.90	0.71
12:L:13:ILE:HD12	12:L:153:ALA:HB1	1.73	0.70
6:F:93:ASN:HD21	13:M:61:ASN:HD21	1.39	0.70
1:O:126:GLN:O	1:O:129:THR:HB	1.91	0.70
6:T:208:VAL:HG13	6:T:227:GLY:HA2	1.73	0.70
4:D:37:LYS:HG2	4:D:160:SER:O	1.90	0.70
1:A:196:GLU:HG2	1:A:201:LYS:HB2	1.73	0.70
14:N:-7:THR:N	14:N:99:MET:O	2.24	0.70
13:M:6:ILE:HG12	13:M:127:CYS:HB2	1.74	0.70
2:B:115:ALA:HB1	2:B:154:GLY:O	1.92	0.70
11:Y:1:ASP:OD2	11:Y:1:ASP:N	2.24	0.69
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.74	0.69
10:X:2:ILE:HG21	10:X:133:ALA:HB3	1.74	0.69
13:M:155:THR:O	13:M:156:ASN:CB	2.40	0.69
11:Y:161:LYS:O	11:Y:165:GLN:HG3	1.93	0.69
7:G:34:THR:HG21	7:G:65:LYS:NZ	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:129:THR:HG22	2:P:128:ARG:NH2	2.08	0.69
7:G:53:ILE:HD11	7:G:212:GLU:HB2	1.74	0.69
13:1:155:THR:HG21	13:1:159:VAL:HB	1.74	0.68
4:D:163:THR:HG21	4:D:171:VAL:HG22	1.76	0.68
3:Q:65:LYS:NZ	3:Q:77:VAL:O	2.27	0.68
13:1:14:LEU:HD13	13:1:34:VAL:HG13	1.75	0.68
9:W:78:SER:O	9:W:82:MET:HG3	1.94	0.68
14:2:-7:THR:HG21	14:2:99:MET:O	1.93	0.68
1:A:164:VAL:HG23	2:B:61:LEU:HG	1.76	0.67
3:Q:123:THR:HG22	4:R:127:ARG:HH21	1.57	0.67
3:C:207:THR:HB	3:C:209:ASP:OD1	1.95	0.67
3:Q:48:ALA:HB1	3:Q:65:LYS:HD3	1.78	0.66
7:U:94:GLU:HG2	7:U:114:ARG:HB3	1.78	0.66
1:A:129:THR:HG22	2:B:128:ARG:HH21	1.60	0.66
4:R:53:LYS:HE2	4:R:53:LYS:H	1.60	0.66
4:R:67:ILE:HG21	4:R:109:LEU:HD11	1.77	0.66
8:H:105:LYS:HD2	8:H:105:LYS:C	2.16	0.66
13:M:186:HIS:HD2	13:M:188:GLN:H	1.43	0.66
1:A:17:THR:HG21	1:A:129:THR:HA	1.78	0.66
5:S:97:VAL:HG21	12:Z:65:LEU:HD13	1.78	0.66
5:S:45:GLY:HA2	5:S:153:TYR:CE1	2.31	0.66
2:B:222:LEU:HD11	2:B:224:TYR:CE1	2.30	0.65
12:L:86:LEU:O	12:L:89:GLN:HB2	1.96	0.65
12:L:106:ARG:CD	12:L:182:GLU:OE2	2.44	0.65
10:X:117:LEU:HD23	10:X:117:LEU:H	1.60	0.65
8:V:176:VAL:HG12	8:V:178:LEU:HD13	1.78	0.65
13:M:3:ILE:HG21	13:M:44:SER:OG	1.97	0.65
11:K:148:ARG:O	11:K:151:MET:HG3	1.97	0.64
9:I:35:HIS:HB3	9:I:56:THR:HG21	1.78	0.64
1:O:129:THR:HG22	2:P:128:ARG:HH21	1.62	0.64
7:U:35:THR:HG22	7:U:167:GLY:H	1.62	0.64
1:A:92:ASN:C	1:A:92:ASN:HD22	2.01	0.64
9:I:128:GLY:O	9:I:131:SER:HB2	1.97	0.64
1:O:92:ASN:C	1:O:92:ASN:ND2	2.46	0.64
4:D:159:TRP:CE3	4:D:162:GLN:HG2	2.32	0.64
13:M:2:THR:HG21	13:M:133:ALA:HB3	1.79	0.64
11:Y:138:TYR:CE2	11:Y:171:MET:HG3	2.33	0.64
3:C:113:ARG:NH2	11:K:70:GLU:OE1	2.26	0.64
3:Q:16:GLU:O	4:R:29:ARG:NH1	2.30	0.64
6:T:119:ASN:N	6:T:119:ASN:HD22	1.95	0.64
14:N:151:VAL:HG23	14:N:151:VAL:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:194:VAL:O	6:T:197:ILE:HG22	1.98	0.63
9:W:213:LEU:HD21	10:X:192:LYS:HD2	1.80	0.63
3:C:181:LYS:O	3:C:184:MET:CG	2.47	0.63
6:T:88:LEU:HD11	6:T:108:ALA:HB1	1.79	0.63
3:Q:49:GLU:OE2	3:Q:201:THR:HG22	1.98	0.63
5:S:170:LYS:HG3	5:S:171:ALA:N	2.13	0.63
14:N:120:ARG:HH11	14:N:130:SER:HB2	1.64	0.63
7:U:205:ASP:O	7:U:206:ASN:CB	2.46	0.63
2:B:236:ARG:CG	2:B:236:ARG:HH21	2.12	0.62
6:F:128:TYR:O	6:F:149:PRO:HB3	1.97	0.62
2:B:222:LEU:CD1	2:B:224:TYR:CE1	2.82	0.62
8:H:161:GLN:HE21	8:V:136:GLY:HA2	1.64	0.62
14:2:19:LEU:HB2	14:2:184:SER:HB2	1.81	0.62
1:O:96:ARG:CG	1:O:96:ARG:HH11	2.11	0.62
4:R:199:LEU:O	4:R:203:VAL:HG23	1.97	0.62
11:Y:171:MET:CE	11:Y:173:MET:HB3	2.29	0.62
12:L:106:ARG:HD3	12:L:182:GLU:OE2	1.99	0.62
5:E:242:GLU:O	5:E:246:LYS:HG2	1.99	0.62
4:R:53:LYS:H	4:R:53:LYS:CE	2.12	0.62
13:M:18:THR:HG22	13:M:29:ARG:O	1.99	0.61
14:2:151:VAL:HG23	14:2:151:VAL:O	2.00	0.61
11:Y:28:LYS:HE3	12:Z:123:LYS:O	2.00	0.61
3:C:44:ILE:HD11	3:C:146:TYR:HB3	1.82	0.61
3:C:87:LEU:HB3	3:C:115:LEU:HD21	1.82	0.61
8:H:14:LEU:HD11	8:H:100:ALA:HB3	1.83	0.61
11:Y:66:TYR:CZ	11:Y:74:LEU:HD21	2.36	0.61
6:F:69:HIS:HE1	6:F:103:LEU:O	1.84	0.60
7:U:34:THR:OG1	7:U:50:GLU:HG2	2.01	0.60
3:Q:86:ILE:O	3:Q:90:THR:HG23	2.01	0.60
5:S:105:GLU:OE2	13:1:66:TYR:OH	2.17	0.60
10:X:82:VAL:HG11	10:X:115:PHE:CZ	2.36	0.60
6:F:39:ARG:NH1	6:F:40:SER:O	2.35	0.60
6:T:171:TYR:C	6:T:171:TYR:CD2	2.74	0.60
1:O:250:GLU:OE2	1:O:250:GLU:N	2.34	0.60
11:Y:36:GLN:HG3	11:Y:188:ILE:HD12	1.83	0.60
2:B:122:THR:HG22	3:C:129:ARG:HE	1.66	0.60
5:E:97:VAL:HG11	12:L:65:LEU:CD2	2.32	0.60
1:O:131:ARG:HH11	1:O:131:ARG:HG2	1.67	0.60
13:M:155:THR:HG21	13:M:159:VAL:CG1	2.23	0.60
4:R:162:GLN:HE22	4:R:172:ARG:HE	1.47	0.60
11:Y:4:LEU:HB2	11:Y:15:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:19:ARG:HD3	10:X:171:LEU:O	2.02	0.60
5:S:121:LEU:HD23	5:S:123:PHE:CE1	2.37	0.59
5:E:40:ILE:HG13	5:E:200:VAL:HG23	1.84	0.59
13:1:-8:GLN:HE21	13:1:-7:PHE:H	1.50	0.59
2:B:236:ARG:HH21	2:B:236:ARG:HG2	1.67	0.59
10:J:74:GLU:OE2	10:J:105:SER:OG	2.20	0.59
1:O:131:ARG:HH11	1:O:131:ARG:CG	2.16	0.59
2:B:59:GLU:H	2:B:59:GLU:CD	2.06	0.59
10:X:44:ILE:HB	10:X:51:VAL:HG13	1.85	0.59
1:O:196:GLU:HG2	1:O:201:LYS:CB	2.33	0.59
4:D:51:THR:HG22	4:D:52:LEU:HD13	1.84	0.58
11:K:20:VAL:HG11	12:L:122:LEU:HD11	1.85	0.58
2:P:122:THR:HG22	3:Q:129:ARG:HH21	1.67	0.58
4:R:37:LYS:HD3	4:R:160:SER:HA	1.85	0.58
4:D:118:GLN:O	4:D:121:THR:OG1	2.20	0.58
7:G:94:GLU:HG3	7:G:114:ARG:HH11	1.67	0.58
1:O:101:ALA:CA	1:O:112:MET:HE2	2.31	0.58
3:Q:19:LEU:HD13	3:Q:123:THR:HG23	1.85	0.58
1:A:126:GLN:O	1:A:129:THR:HB	2.03	0.58
12:Z:46:ALA:HB3	12:Z:98:GLY:O	2.04	0.58
11:Y:6:ILE:HG23	11:Y:13:ILE:HB	1.85	0.57
11:Y:18:LYS:HD3	11:Y:179:ILE:HG13	1.84	0.57
1:A:247:ALA:O	1:A:250:GLU:HG2	2.05	0.57
2:P:241:GLN:HA	2:P:241:GLN:OE1	2.05	0.57
9:I:30:ASN:ND2	9:I:172:ASN:OD1	2.36	0.57
13:M:18:THR:HG23	13:M:30:TYR:HA	1.81	0.57
1:A:196:GLU:HG2	1:A:201:LYS:CB	2.34	0.57
2:B:4:ARG:HG2	2:B:4:ARG:HH11	1.69	0.57
3:C:152:ASN:HB2	3:C:153:PRO:CD	2.35	0.57
14:2:8:TYR:CE2	14:2:162:VAL:HG22	2.39	0.57
7:U:194:GLN:O	7:U:198:ILE:HG13	2.05	0.57
8:V:-1:LEU:HD11	8:V:45:ARG:NH1	2.20	0.57
3:C:96:GLN:HE22	3:C:99:LEU:HD23	1.68	0.57
5:E:121:LEU:HD23	5:E:123:PHE:CE2	2.39	0.57
1:A:129:THR:CG2	2:B:128:ARG:HH21	2.17	0.56
3:C:70:ASN:C	3:C:70:ASN:HD22	2.07	0.56
11:Y:138:TYR:CZ	11:Y:171:MET:HG3	2.40	0.56
11:Y:7:ARG:HH11	11:Y:7:ARG:HG2	1.70	0.56
12:L:76:VAL:N	12:L:108:GLU:OE1	2.38	0.56
4:R:162:GLN:HA	4:R:162:GLN:HE21	1.70	0.56
5:S:121:LEU:HD23	5:S:123:PHE:HE1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:42:VAL:HG11	4:R:136:ALA:HB1	1.87	0.56
6:T:43:HIS:CD2	6:T:215:ILE:HD11	2.41	0.56
2:P:218:ASN:HD22	2:P:218:ASN:N	2.03	0.56
14:N:1:THR:OG1	14:N:2:SER:N	2.36	0.56
7:G:71:ARG:NH2	14:N:63:VAL:HG11	2.21	0.56
6:T:11:VAL:HG22	6:T:11:VAL:O	2.06	0.56
13:1:11:PHE:CE2	13:1:168:VAL:HA	2.41	0.56
5:S:177:GLU:N	5:S:177:GLU:OE2	2.39	0.56
10:X:103:ILE:CD1	10:X:181:ILE:HG22	2.36	0.56
12:Z:4:LEU:C	12:Z:4:LEU:HD23	2.27	0.56
5:E:45:GLY:HA2	5:E:153:TYR:CE1	2.41	0.55
8:H:185:ARG:NE	14:2:225:ILE:OXT	2.36	0.55
11:K:90:SER:O	11:K:93:SER:HB3	2.05	0.55
12:L:4:LEU:C	12:L:4:LEU:HD23	2.26	0.55
2:P:116:LYS:O	2:P:120:GLU:HG3	2.05	0.55
2:P:250:LEU:HD12	2:P:250:LEU:C	2.27	0.55
9:I:143:LYS:O	9:I:146:LEU:HD22	2.07	0.55
14:N:45:ILE:HG21	14:N:52:MET:HG3	1.87	0.55
7:U:129:ARG:HG3	7:U:129:ARG:HH11	1.71	0.55
3:C:49:GLU:OE2	3:C:201:THR:HG23	2.07	0.55
14:N:8:TYR:HE2	14:N:162:VAL:HG22	1.69	0.55
2:P:12:PHE:H	3:Q:21:GLN:HE22	1.55	0.55
9:W:35:HIS:CB	9:W:56:THR:HG21	2.35	0.55
3:C:191:GLU:O	3:C:195:LYS:HG2	2.07	0.55
2:P:64:VAL:HG11	2:P:212:ALA:HB3	1.88	0.55
4:D:67:ILE:HG21	4:D:109:LEU:HD11	1.89	0.55
5:E:45:GLY:HA2	5:E:153:TYR:CD1	2.42	0.55
1:O:196:GLU:HG2	1:O:201:LYS:HB2	1.88	0.55
6:T:137:TYR:CE2	6:T:218:LYS:HA	2.41	0.55
13:1:100:THR:HG23	13:1:116:PHE:HB2	1.89	0.55
2:B:4:ARG:HH11	2:B:4:ARG:CG	2.20	0.55
3:C:91:ALA:HB2	3:C:115:LEU:HD12	1.89	0.55
6:F:62:LYS:O	6:F:73:SER:HA	2.07	0.55
2:P:46:ALA:CB	2:P:211:LEU:HD12	2.36	0.55
7:U:30:VAL:HG11	7:U:134:SER:HB2	1.88	0.55
14:2:1:THR:HG21	14:2:182:ARG:O	2.07	0.54
4:D:133:THR:O	4:D:149:GLN:HA	2.08	0.54
11:Y:2:ILE:HD13	11:Y:175:PHE:CG	2.42	0.54
13:1:155:THR:O	13:1:156:ASN:CB	2.52	0.54
2:P:49:LYS:HG3	2:P:210:GLU:HB2	1.89	0.54
10:X:7:THR:HG22	10:X:12:VAL:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:125:HIS:HB3	4:R:126:VAL:HG12	1.88	0.54
9:W:222:ASP:OD1	9:W:222:ASP:N	2.40	0.54
11:Y:19:ALA:HB2	11:Y:176:LYS:HB2	1.88	0.54
5:E:131:GLU:O	5:E:133:LEU:HA	2.07	0.54
13:M:29:ARG:HA	13:M:191:ASP:OD2	2.08	0.54
4:D:25:GLU:OE2	4:D:28:LYS:HE2	2.07	0.54
6:F:87:TYR:CD2	6:F:115:LYS:HD2	2.43	0.54
13:M:39:ASP:OD2	13:M:67:HIS:HE1	1.91	0.54
3:C:228:LYS:NZ	3:C:234:GLU:OE2	2.33	0.54
4:R:155:ILE:HD11	5:S:82:THR:OG1	2.07	0.54
4:D:50:SER:HA	4:D:209:ASN:ND2	2.22	0.53
8:H:1:THR:CG2	8:H:33:LYS:NZ	2.67	0.53
7:G:203:HIS:CE1	7:G:211:PHE:HB3	2.42	0.53
8:V:189:TYR:HB3	8:V:190:PRO:CD	2.39	0.53
2:B:226:GLY:HA3	9:I:186:TYR:O	2.08	0.53
6:F:171:TYR:C	6:F:171:TYR:CD2	2.82	0.53
13:M:112:ALA:HB2	13:M:124:ARG:NH2	2.24	0.53
5:S:45:GLY:HA2	5:S:153:TYR:CD1	2.44	0.53
13:1:-4:TYR:CD1	13:1:97:TYR:HB2	2.44	0.53
5:E:204:LEU:O	5:E:208:MET:HG3	2.08	0.53
4:R:50:SER:O	4:R:209:ASN:ND2	2.42	0.53
6:T:10:THR:HG21	6:T:120:THR:HA	1.91	0.53
3:C:140:TYR:CD1	3:C:225:VAL:HG21	2.44	0.53
3:C:238:ILE:O	3:C:242:THR:OG1	2.25	0.53
10:J:117:LEU:N	10:J:117:LEU:HD23	2.24	0.53
14:N:18:ASN:HA	14:N:31:VAL:O	2.08	0.53
7:U:34:THR:OG1	7:U:50:GLU:CG	2.56	0.53
13:1:91:LYS:HE3	13:1:94:PHE:O	2.08	0.53
1:A:205:PHE:CD1	1:A:205:PHE:C	2.82	0.53
10:J:28:SER:HB2	11:K:125:VAL:HG21	1.89	0.53
11:Y:2:ILE:O	11:Y:3:ILE:HD12	2.09	0.53
1:A:76:SER:OG	1:A:77:ARG:N	2.42	0.53
1:O:236:LEU:HB3	1:O:240:ASN:HB2	1.91	0.53
6:T:11:VAL:CG1	6:T:123:TYR:HD1	2.22	0.53
8:V:67:THR:HA	8:V:71:GLY:O	2.09	0.53
12:Z:30:THR:O	12:Z:30:THR:OG1	2.24	0.53
3:C:123:THR:HG22	4:D:127:ARG:HH21	1.73	0.52
10:J:44:ILE:HG22	10:J:51:VAL:HG22	1.92	0.52
2:P:239:THR:OG1	2:P:242:GLU:HG3	2.09	0.52
1:O:131:ARG:HG2	1:O:131:ARG:NH1	2.21	0.52
8:V:18:SER:OG	8:V:29:ARG:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HG12	1:A:154:ILE:HG12	1.91	0.52
2:P:26:THR:O	2:P:30:GLN:HG3	2.10	0.52
14:2:89:ALA:HA	14:2:122:VAL:HG21	1.91	0.52
14:2:144:ASN:O	14:2:145:PRO:C	2.47	0.52
12:L:4:LEU:HD23	12:L:4:LEU:O	2.09	0.52
7:U:12:SER:HB3	7:U:124:LEU:C	2.30	0.52
13:1:43:MET:CE	13:1:56:VAL:HA	2.40	0.52
14:2:212:ASP:O	14:2:215:LYS:HG2	2.10	0.52
13:M:-1:ASN:O	13:M:21:ILE:HD13	2.10	0.52
13:M:117:ASP:HB3	13:M:119:VAL:H	1.75	0.52
3:C:221:ASN:N	3:C:221:ASN:HD22	2.06	0.52
7:G:11:MET:HG3	7:G:22:GLN:HG3	1.92	0.52
4:R:36:VAL:HG23	4:R:191:CYS:SG	2.50	0.52
5:S:117:CYS:HB3	5:S:162:GLY:O	2.10	0.51
12:L:58:TRP:O	12:L:62:GLN:HG2	2.09	0.51
1:A:21:PRO:HA	2:B:23:TYR:CD1	2.45	0.51
3:C:181:LYS:HG3	3:C:184:MET:HG2	1.91	0.51
5:E:167:TYR:CE1	6:F:57:SER:HB2	2.45	0.51
3:Q:70:ASN:C	3:Q:70:ASN:HD22	2.13	0.51
13:1:155:THR:HG21	13:1:159:VAL:CB	2.40	0.51
2:B:10:THR:HB	2:B:122:THR:O	2.10	0.51
6:F:71:GLY:HA3	6:F:222:PHE:CE1	2.46	0.51
1:A:158:ASP:HB2	1:A:159:PRO:CD	2.40	0.51
2:B:180:ASN:C	2:B:180:ASN:HD22	2.11	0.51
10:X:0:GLY:HA2	10:X:132:THR:HG21	1.92	0.51
5:E:167:TYR:CE1	5:E:170:LYS:HD3	2.46	0.51
2:P:66:LEU:C	2:P:66:LEU:HD23	2.31	0.51
6:T:13:PHE:H	7:U:22:GLN:HE22	1.59	0.51
6:T:87:TYR:CD2	6:T:115:LYS:HD2	2.46	0.51
6:F:119:ASN:N	6:F:119:ASN:HD22	2.09	0.51
7:U:41:CYS:HB2	7:U:186:LEU:O	2.11	0.51
7:U:100:LYS:HE2	14:2:57:ARG:HH22	1.76	0.51
7:U:178:LEU:HD11	7:U:194:GLN:HG3	1.93	0.51
9:W:112:SER:OG	9:W:120:ASP:HB2	2.11	0.51
2:B:89:SER:O	2:B:92:VAL:HG12	2.11	0.51
5:E:90:GLU:OE2	12:L:69:ARG:NH1	2.44	0.51
11:K:24:ILE:O	11:Y:138:TYR:OH	2.23	0.51
7:U:94:GLU:HG3	7:U:114:ARG:HH11	1.76	0.51
11:Y:44:SER:OG	11:Y:102:LEU:HB2	2.11	0.51
2:B:29:LYS:HE2	2:B:29:LYS:HA	1.93	0.50
4:R:233:VAL:O	4:R:237:GLU:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:OG	1:A:224:GLU:OE2	2.11	0.50
13:M:-2:ASP:OD1	13:M:-2:ASP:C	2.48	0.50
13:M:1:GLY:HA3	13:M:33:LYS:HZ2	1.76	0.50
13:1:152:GLU:C	13:1:155:THR:HG1	2.10	0.50
5:E:40:ILE:HG13	5:E:200:VAL:CG2	2.41	0.50
9:I:172:ASN:ND2	9:I:192:THR:HA	2.26	0.50
13:M:-6:ASN:HD22	13:M:-5:PRO:HD2	1.75	0.50
8:V:20:THR:HG23	8:V:31:THR:OG1	2.11	0.50
12:Z:7:ARG:HD2	12:Z:110:PRO:O	2.11	0.50
13:1:169:GLU:O	13:1:173:LYS:HG3	2.10	0.50
1:A:92:ASN:C	1:A:92:ASN:ND2	2.64	0.50
4:D:37:LYS:HD3	4:D:160:SER:HA	1.93	0.50
4:D:133:THR:OG1	4:D:150:THR:OG1	2.28	0.50
8:H:133:PHE:HA	8:V:132:THR:O	2.11	0.50
11:K:15:ALA:HB2	11:K:160:LEU:HD11	1.94	0.50
3:C:13:PHE:H	4:D:19:GLN:HE22	1.59	0.50
11:Y:90:SER:O	11:Y:93:SER:HB3	2.12	0.50
2:B:68:THR:HB	2:B:69:PRO:HD2	1.93	0.50
12:L:86:LEU:HD13	12:L:86:LEU:C	2.32	0.50
2:B:196:LEU:HD23	2:B:209:ILE:HD12	1.94	0.50
12:L:77:ALA:HA	12:L:113:TYR:CE2	2.47	0.50
2:P:10:THR:HG23	2:P:20:GLN:HB2	1.93	0.50
13:1:8:GLY:HA3	13:1:11:PHE:CE1	2.47	0.50
5:E:112:LEU:C	5:E:112:LEU:HD13	2.33	0.50
13:M:8:GLY:HA3	13:M:11:PHE:CE1	2.47	0.50
4:R:203:VAL:CG1	4:R:209:ASN:HB2	2.42	0.50
1:O:21:PRO:HA	2:P:23:TYR:CD1	2.47	0.49
7:U:149:MET:HB3	7:U:159:TYR:CE1	2.47	0.49
14:2:-7:THR:HG22	14:2:99:MET:O	2.10	0.49
7:G:240:ASP:O	7:G:241:PHE:C	2.50	0.49
14:N:91:VAL:O	14:N:95:ARG:HG2	2.12	0.49
6:F:203:ASP:OD1	6:F:204:GLU:OE1	2.30	0.49
6:T:54:ASP:H	6:T:57:SER:HB3	1.76	0.49
3:Q:106:ILE:HD11	3:Q:110:ILE:HG22	1.94	0.49
13:1:43:MET:HB2	13:1:102:ILE:HG22	1.93	0.49
14:2:120:ARG:HH11	14:2:130:SER:HB2	1.76	0.49
2:B:94:HIS:HD2	9:I:61:SER:OG	1.95	0.49
8:H:194:GLU:OE1	14:2:185:ARG:NH1	2.43	0.49
6:T:69:HIS:HE1	6:T:103:LEU:O	1.96	0.49
8:V:49:ALA:O	8:V:50:ALA:C	2.51	0.49
13:1:34:VAL:HG12	13:1:196:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:55:ILE:HA	14:2:58:LEU:HD12	1.93	0.49
4:D:86:ILE:HG22	4:D:90:ARG:HD2	1.94	0.49
3:Q:141:ASP:OD2	3:Q:147:GLN:NE2	2.46	0.49
8:H:83:LYS:HD3	8:H:84:GLU:N	2.28	0.49
12:L:107:LYS:H	12:L:107:LYS:HD2	1.77	0.49
1:A:101:ALA:HA	1:A:112:MET:HE2	1.95	0.49
2:B:12:PHE:H	3:C:21:GLN:HE22	1.61	0.49
3:C:59:GLN:OE1	3:C:209:ASP:HA	2.12	0.49
12:L:37:ILE:HD13	12:L:59:LEU:HD23	1.94	0.49
13:1:91:LYS:HD3	13:1:96:TYR:CE2	2.48	0.49
13:M:18:THR:CG2	13:M:29:ARG:O	2.60	0.49
13:M:177:ASP:OD2	9:W:203:TYR:OH	2.24	0.49
14:N:174:ARG:HB2	14:N:206:VAL:HG13	1.94	0.49
8:V:83:LYS:HG3	8:V:119:VAL:CG2	2.43	0.49
12:L:1:THR:HG22	12:L:2:THR:N	2.27	0.48
1:O:53:VAL:CG1	1:O:144:VAL:HG11	2.43	0.48
3:Q:13:PHE:H	4:R:19:GLN:HE22	1.61	0.48
5:S:188:HIS:O	5:S:191:LEU:HD12	2.13	0.48
8:V:157:HIS:CD2	8:V:196:LEU:HD23	2.48	0.48
10:X:35:PHE:CD1	10:X:55:ASN:ND2	2.81	0.48
3:C:191:GLU:HG3	3:C:242:THR:HG23	1.95	0.48
3:Q:5:ARG:HB2	3:Q:5:ARG:CZ	2.42	0.48
6:T:164:ARG:O	6:T:200:SER:CB	2.61	0.48
13:1:18:THR:HG21	13:1:30:TYR:CD1	2.47	0.48
5:E:121:LEU:HD23	5:E:123:PHE:HE2	1.76	0.48
6:F:137:TYR:CE2	6:F:218:LYS:HA	2.49	0.48
13:M:106:ASP:OD1	13:M:106:ASP:C	2.52	0.48
8:V:-2:SER:HA	8:V:49:ALA:H	1.77	0.48
5:E:202:LYS:O	5:E:205:LYS:HB2	2.14	0.48
13:M:-1:ASN:HA	13:M:21:ILE:O	2.13	0.48
7:U:205:ASP:O	7:U:206:ASN:HB2	2.13	0.48
8:V:14:LEU:HD11	8:V:100:ALA:HB3	1.95	0.48
14:2:-7:THR:OG1	14:2:-6:GLN:N	2.45	0.48
2:B:222:LEU:HD11	2:B:224:TYR:CZ	2.48	0.48
5:E:59:LEU:HD12	5:E:60:GLU:N	2.29	0.48
9:W:31:CYS:SG	9:W:33:LYS:HE3	2.54	0.48
10:X:155:PHE:CE1	10:X:189:ARG:HD2	2.48	0.48
10:X:163:LEU:CD2	10:X:191:LEU:HD13	2.44	0.48
13:1:91:LYS:HD3	13:1:96:TYR:CZ	2.48	0.48
14:2:155:SER:O	14:2:158:PRO:HD2	2.14	0.48
4:D:51:THR:HG22	4:D:52:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:36:GLN:HG3	11:K:188:ILE:CD1	2.44	0.48
5:S:53:ARG:HG2	5:S:53:ARG:O	2.14	0.48
1:A:82:VAL:CG1	1:A:142:THR:HB	2.43	0.48
6:F:231:ALA:O	6:F:233:TYR:N	2.46	0.48
13:M:161:LYS:HG3	13:M:162:PRO:HD2	1.95	0.48
6:T:33:SER:HB3	6:T:62:LYS:HE3	1.96	0.48
6:T:177:ASP:O	6:T:181:LYS:HE2	2.14	0.48
7:U:205:ASP:OD1	7:U:205:ASP:N	2.47	0.48
14:2:1:THR:OG1	14:2:2:SER:N	2.47	0.48
4:D:206:GLY:O	4:D:207:ALA:C	2.52	0.48
3:Q:59:GLN:OE1	3:Q:209:ASP:HA	2.14	0.48
3:Q:229:ILE:HD12	3:Q:229:ILE:N	2.29	0.48
9:W:139:GLU:HA	9:W:139:GLU:OE1	2.13	0.48
2:B:29:LYS:HA	2:B:29:LYS:CE	2.44	0.48
4:D:52:LEU:C	4:D:54:LEU:H	2.17	0.48
4:D:163:THR:HG23	4:D:168:SER:HB2	1.96	0.48
14:N:120:ARG:NH1	14:N:130:SER:HB2	2.28	0.48
1:O:115:ASP:OD2	9:W:72:ARG:NH1	2.47	0.48
14:2:157:ILE:HB	14:2:158:PRO:HD3	1.96	0.48
2:B:222:LEU:HD12	2:B:224:TYR:CE1	2.49	0.47
5:E:132:ARG:HE	5:E:132:ARG:N	2.12	0.47
1:O:96:ARG:HH11	1:O:96:ARG:HG2	1.78	0.47
9:W:88:PHE:CD2	9:W:88:PHE:C	2.88	0.47
12:Z:40:PHE:CD2	12:Z:73:ARG:NH1	2.82	0.47
5:E:76:CYS:HB2	5:E:143:LEU:O	2.14	0.47
9:I:9:ASN:OD1	9:I:10:ASN:N	2.48	0.47
12:L:13:ILE:HD12	12:L:153:ALA:CB	2.44	0.47
2:B:239:THR:OG1	2:B:242:GLU:HG3	2.15	0.47
6:F:6:TYR:CE2	6:F:15:PRO:HD3	2.49	0.47
4:R:203:VAL:HG11	4:R:209:ASN:HB2	1.96	0.47
13:1:172:ILE:O	13:1:176:ARG:HG3	2.13	0.47
4:D:8:LEU:O	4:D:19:GLN:HG3	2.14	0.47
4:D:9:SER:HB2	4:D:121:THR:O	2.14	0.47
13:M:146:ASN:OD1	13:M:146:ASN:N	2.47	0.47
6:T:190:ILE:HG23	6:T:213:ILE:HD13	1.96	0.47
14:2:174:ARG:HA	14:2:206:VAL:HG11	1.94	0.47
2:B:64:VAL:HG11	2:B:212:ALA:CB	2.44	0.47
13:M:1:GLY:HA3	13:M:33:LYS:NZ	2.30	0.47
1:O:141:LEU:O	1:O:156:LYS:HA	2.14	0.47
4:R:151:GLU:HB3	4:R:152:PRO:CD	2.44	0.47
11:Y:91:ILE:HG12	11:Y:121:LEU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:OG1	1:A:170:ALA:N	2.47	0.47
3:C:106:ILE:HD11	3:C:110:ILE:HG22	1.97	0.47
3:C:244:ILE:HG22	3:C:244:ILE:O	2.15	0.47
5:E:62:ASP:OD1	5:E:62:ASP:N	2.43	0.47
7:G:108:ILE:N	7:G:109:PRO:CD	2.78	0.47
14:N:89:ALA:HA	14:N:122:VAL:HG21	1.95	0.47
2:P:235:PHE:C	2:P:235:PHE:CD1	2.88	0.47
3:Q:14:SER:OG	3:Q:16:GLU:OE1	2.33	0.47
6:T:179:PHE:HA	6:T:182:ILE:HG13	1.97	0.47
9:W:20:SER:HB2	9:W:31:CYS:SG	2.54	0.47
12:Z:27:ALA:O	13:1:128:ARG:NH1	2.48	0.47
5:E:159:GLU:HB3	5:E:160:PRO:CD	2.45	0.47
7:G:86:HIS:HE2	7:G:118:TYR:HH	1.62	0.47
1:O:167:LYS:HD3	1:O:192:ASP:HA	1.97	0.47
6:T:119:ASN:N	6:T:119:ASN:ND2	2.63	0.47
2:B:64:VAL:HG11	2:B:212:ALA:HB3	1.97	0.47
1:O:41:ASN:ND2	1:O:173:PRO:HD2	2.30	0.47
2:P:46:ALA:HB2	2:P:211:LEU:HD12	1.95	0.47
13:1:198:VAL:HG22	13:1:203:VAL:HG22	1.97	0.47
12:L:12:ILE:HB	12:L:180:VAL:HB	1.96	0.47
8:V:14:LEU:HD23	8:V:44:CYS:SG	2.55	0.47
5:E:208:MET:HE1	5:E:212:LEU:HA	1.96	0.46
6:F:180:ILE:HD13	6:F:180:ILE:O	2.15	0.46
2:P:12:PHE:N	3:Q:21:GLN:HE22	2.13	0.46
1:A:164:VAL:HG22	1:A:165:GLY:H	1.80	0.46
4:D:70:HIS:CD2	4:D:71:VAL:CG2	2.98	0.46
1:O:58:LYS:O	1:O:60:PRO:HD3	2.16	0.46
1:A:245:LEU:O	1:A:248:ILE:HG13	2.15	0.46
6:F:215:ILE:O	6:F:222:PHE:HA	2.16	0.46
13:M:155:THR:O	13:M:155:THR:HG22	2.15	0.46
3:Q:25:ALA:O	3:Q:28:SER:HB3	2.15	0.46
4:R:52:LEU:HD12	4:R:54:LEU:H	1.81	0.46
6:T:217:GLY:O	6:T:218:LYS:C	2.53	0.46
9:W:213:LEU:HG	10:X:192:LYS:HB2	1.98	0.46
13:1:43:MET:CB	13:1:102:ILE:HG22	2.45	0.46
7:G:36:SER:HB3	7:G:49:VAL:HG23	1.97	0.46
9:I:139:GLU:OE2	14:2:179:ARG:NH1	2.48	0.46
12:L:140:LEU:CD1	12:L:160:SER:OG	2.64	0.46
3:Q:9:ARG:HD2	4:R:6:ARG:NH2	2.29	0.46
3:Q:30:SER:O	3:Q:167:ALA:HA	2.16	0.46
6:T:136:GLY:HA2	6:T:216:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:132:THR:O	8:V:133:PHE:HA	2.16	0.46
1:O:77:ARG:NH2	8:V:39:ASP:OD2	2.48	0.46
6:T:59:TYR:CE1	6:T:209:ASP:HB3	2.50	0.46
8:V:83:LYS:HD3	8:V:84:GLU:N	2.30	0.46
10:X:162:LEU:HD23	10:X:162:LEU:C	2.35	0.46
13:1:141:LEU:O	13:1:142:ASP:C	2.52	0.46
2:B:176:GLU:OE2	3:C:55:THR:HG23	2.15	0.46
5:E:168:ASN:HB3	5:E:187:TRP:CE2	2.50	0.46
9:I:51:ASP:OD2	10:J:90:ARG:NH2	2.41	0.46
12:L:97:MET:O	12:L:116:ASP:HA	2.16	0.46
1:O:54:ILE:HD12	1:O:206:ALA:HB1	1.98	0.46
3:Q:152:ASN:HB2	3:Q:153:PRO:HD2	1.98	0.46
6:T:113:CYS:SG	6:T:151:GLY:O	2.74	0.46
14:2:219:GLY:HA3	14:2:223:GLN:HB3	1.97	0.46
1:A:161:GLY:O	2:B:83:ARG:NH2	2.48	0.46
2:B:43:VAL:HG23	2:B:145:PHE:HB3	1.97	0.46
8:H:6:VAL:O	8:H:12:VAL:HG23	2.16	0.46
10:J:2:ILE:HG21	10:J:133:ALA:HB3	1.97	0.46
3:Q:70:ASN:ND2	3:Q:72:LYS:H	2.13	0.46
6:T:171:TYR:HB2	6:T:199:GLN:HG3	1.97	0.46
2:B:222:LEU:HD22	2:B:232:GLY:HA2	1.98	0.46
10:J:29:ASN:HB3	10:J:174:TRP:CE3	2.51	0.46
2:P:194:LEU:CD2	2:P:250:LEU:HD13	2.42	0.46
5:S:169:ALA:HB1	5:S:183:LEU:HD22	1.97	0.46
6:T:15:PRO:HA	7:U:25:TYR:CD1	2.50	0.46
10:X:29:ASN:H	10:X:29:ASN:ND2	2.13	0.46
11:Y:70:GLU:O	11:Y:71:ASP:C	2.53	0.46
1:A:101:ALA:HA	1:A:112:MET:CE	2.45	0.46
13:M:18:THR:HG21	13:M:30:TYR:HD1	1.81	0.46
14:N:81:PRO:O	14:N:82:SER:C	2.55	0.46
3:Q:181:LYS:HG3	3:Q:184:MET:HG3	1.98	0.46
7:U:129:ARG:HH11	7:U:129:ARG:CG	2.29	0.46
2:B:17:LYS:HD3	2:B:22:ASP:OD2	2.15	0.46
3:C:4:ARG:NH1	5:E:125:GLU:OE1	2.49	0.46
3:C:183:ASP:O	3:C:184:MET:O	2.34	0.46
6:F:5:ASN:HB2	6:F:6:TYR:CE2	2.51	0.46
6:F:64:ILE:HB	6:F:72:LEU:CD2	2.46	0.46
6:F:171:TYR:HB2	6:F:199:GLN:HG2	1.98	0.46
4:R:229:ILE:O	4:R:233:VAL:HG23	2.16	0.46
5:S:101:LEU:O	13:1:82:ARG:NH1	2.46	0.46
6:T:146:GLU:O	6:T:153:VAL:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:179:PHE:O	6:T:180:ILE:C	2.54	0.46
7:U:236:GLN:HA	7:U:236:GLN:NE2	2.29	0.46
11:Y:32:ASP:OD1	11:Y:34:THR:HG22	2.16	0.46
13:1:39:ASP:OD2	13:1:67:HIS:HE1	1.99	0.46
3:C:152:ASN:HB2	3:C:153:PRO:HD2	1.98	0.45
8:H:190:PRO:O	8:H:191:ASP:C	2.53	0.45
12:L:128:CYS:HB2	12:L:137:TYR:CD2	2.50	0.45
1:O:196:GLU:HG2	1:O:201:LYS:HB3	1.97	0.45
6:T:93:ASN:HD21	13:1:61:ASN:HD21	1.64	0.45
11:Y:36:GLN:HG3	11:Y:188:ILE:CD1	2.46	0.45
4:D:92:GLU:HA	4:D:92:GLU:OE1	2.16	0.45
5:E:81:LEU:HD12	5:E:139:GLY:HA3	1.98	0.45
13:M:-1:ASN:O	13:M:0:GLY:O	2.34	0.45
2:P:74:VAL:CG1	2:P:75:TYR:N	2.79	0.45
6:T:74:LEU:C	6:T:74:LEU:HD12	2.37	0.45
12:Z:21:THR:HG22	12:Z:26:VAL:HA	1.97	0.45
13:1:91:LYS:O	13:1:95:PRO:HA	2.16	0.45
3:C:19:LEU:O	3:C:20:TYR:C	2.54	0.45
3:C:52:VAL:HG12	3:C:64:GLU:OE1	2.17	0.45
9:I:8:PHE:HB3	9:I:151:ALA:HB2	1.98	0.45
13:M:38:GLY:O	13:M:40:ASN:N	2.50	0.45
3:Q:195:LYS:O	3:Q:198:SER:HB3	2.16	0.45
5:S:43:LYS:N	5:S:43:LYS:HD2	2.31	0.45
11:Y:6:ILE:CG2	11:Y:13:ILE:HB	2.47	0.45
4:D:98:LEU:O	12:L:81:LYS:HE2	2.17	0.45
11:K:193:ASP:OD2	11:K:193:ASP:N	2.50	0.45
13:M:17:ASP:OD1	13:M:33:LYS:NZ	2.49	0.45
1:O:183:GLU:OE2	2:P:54:PRO:HD2	2.16	0.45
4:R:133:THR:O	4:R:149:GLN:HA	2.16	0.45
6:T:71:GLY:HA3	6:T:222:PHE:CE2	2.52	0.45
6:T:164:ARG:O	6:T:200:SER:HB2	2.16	0.45
13:1:94:PHE:N	13:1:95:PRO:HD3	2.30	0.45
3:C:120:GLN:O	3:C:123:THR:HB	2.17	0.45
12:L:168:ASP:HB3	12:L:171:SER:HB2	1.99	0.45
1:O:35:THR:HG21	1:O:140:ILE:HG13	1.99	0.45
2:P:64:VAL:HG11	2:P:212:ALA:CB	2.46	0.45
4:R:27:VAL:O	4:R:165:GLY:HA2	2.17	0.45
8:V:32:ASP:OD2	8:V:185:ARG:NH2	2.50	0.45
11:Y:103:ILE:HB	11:Y:116:TYR:HB2	1.98	0.45
13:1:-4:TYR:CE1	13:1:97:TYR:HB2	2.51	0.45
1:A:236:LEU:HB3	1:A:240:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:LEU:HD23	3:C:111:LEU:C	2.36	0.45
9:I:17:ASP:HA	9:I:172:ASN:O	2.17	0.45
4:R:73:LEU:HD23	4:R:74:SER:N	2.31	0.45
5:S:85:ALA:O	5:S:89:ILE:HG12	2.17	0.45
11:K:4:LEU:HD23	11:K:131:ALA:HB2	1.98	0.45
1:O:250:GLU:OE2	1:O:250:GLU:CA	2.65	0.45
2:P:94:HIS:CD2	9:W:61:SER:OG	2.70	0.45
10:X:163:LEU:HD21	10:X:191:LEU:HD13	1.99	0.45
11:Y:171:MET:HE3	11:Y:173:MET:HB3	1.97	0.45
3:C:120:GLN:CG	4:D:80:ALA:HB1	2.47	0.45
6:F:182:ILE:HG22	6:F:182:ILE:O	2.17	0.45
5:S:212:LEU:C	5:S:212:LEU:HD23	2.37	0.45
7:U:171:ALA:O	7:U:175:LEU:HD23	2.17	0.45
5:E:40:ILE:CG1	5:E:200:VAL:CG2	2.94	0.45
5:E:132:ARG:HB2	5:E:133:LEU:HA	1.99	0.45
1:O:245:LEU:HA	1:O:248:ILE:HG12	1.99	0.45
2:P:119:GLN:O	2:P:122:THR:HB	2.16	0.45
4:R:40:ASN:HD22	4:R:40:ASN:H	1.64	0.45
13:M:152:GLU:CG	13:M:159:VAL:HG13	2.46	0.45
3:Q:96:GLN:NE2	10:X:60:TYR:HA	2.32	0.45
4:R:68:ASP:HA	11:Y:68:ILE:CD1	2.46	0.45
11:Y:49:ALA:O	12:Z:91:LYS:NZ	2.50	0.45
1:A:158:ASP:HB2	1:A:159:PRO:HD2	1.99	0.44
1:A:220:LYS:HB3	1:A:242:GLU:HB2	1.98	0.44
5:E:180:GLN:NE2	6:F:54:ASP:OD1	2.39	0.44
6:F:175:THR:O	6:F:176:LEU:C	2.55	0.44
6:F:214:ALA:HA	6:F:223:THR:O	2.17	0.44
8:H:7:THR:HG23	8:H:110:VAL:HG23	1.99	0.44
9:I:194:ASN:HB3	13:1:211:LYS:HE2	1.99	0.44
6:T:11:VAL:HG11	6:T:123:TYR:HD1	1.82	0.44
14:N:198:LEU:HD23	14:N:199:THR:N	2.33	0.44
1:O:101:ALA:HA	1:O:112:MET:CE	2.37	0.44
4:R:148:TYR:CE2	4:R:158:SER:HB2	2.52	0.44
6:T:71:GLY:HA3	6:T:222:PHE:CZ	2.52	0.44
7:U:200:TYR:OH	7:U:239:ILE:HG23	2.16	0.44
8:V:36:ARG:HG3	8:V:42:TRP:CZ2	2.51	0.44
4:D:82:SER:O	4:D:86:ILE:HD12	2.18	0.44
5:E:11:GLY:O	5:E:14:THR:OG1	2.34	0.44
10:J:111:PHE:CD1	10:J:111:PHE:C	2.90	0.44
12:L:50:ALA:CB	13:M:119:VAL:HG23	2.47	0.44
12:L:145:LYS:HB3	12:L:148:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:176:ARG:HD2	13:1:208:TYR:CD2	2.52	0.44
2:B:41:ASN:OD1	2:B:41:ASN:N	2.50	0.44
7:G:175:LEU:HD13	7:G:198:ILE:HD13	1.99	0.44
10:J:115:PHE:CD1	10:J:115:PHE:N	2.85	0.44
5:S:146:GLY:HA2	5:S:222:ILE:HG12	1.98	0.44
5:S:242:GLU:O	5:S:246:LYS:HG2	2.17	0.44
7:U:200:TYR:CD1	7:U:242:ALA:HB1	2.52	0.44
7:G:85:ARG:NH1	14:N:69:ASP:OD2	2.46	0.44
9:I:20:SER:HB3	9:I:28:ASP:HB3	1.99	0.44
11:K:59:ILE:O	11:K:60:GLN:C	2.55	0.44
14:N:40:ASN:HD22	14:N:40:ASN:H	1.64	0.44
2:P:106:PRO:CG	2:P:109:LEU:HD12	2.48	0.44
7:U:178:LEU:HD11	7:U:194:GLN:CG	2.47	0.44
13:1:-1:ASN:OD1	13:1:49:ALA:HB3	2.18	0.44
6:F:143:HIS:ND1	6:F:155:GLU:OE2	2.40	0.44
8:H:176:VAL:HG12	8:H:178:LEU:HD13	2.00	0.44
9:I:22:GLN:HG3	9:I:27:ALA:HB2	2.00	0.44
1:A:122:ALA:HB1	1:A:161:GLY:O	2.18	0.44
3:C:19:LEU:HD13	3:C:123:THR:HG23	1.99	0.44
4:D:210:ILE:HG22	4:D:211:GLU:N	2.32	0.44
7:U:51:LYS:HD2	7:U:214:GLU:OE2	2.18	0.44
2:B:94:HIS:CD2	9:I:61:SER:OG	2.70	0.44
6:F:176:LEU:HA	6:F:179:PHE:CE2	2.53	0.44
3:Q:175:LEU:HD13	3:Q:199:LYS:HD2	2.00	0.44
6:T:52:ASN:ND2	6:T:54:ASP:O	2.51	0.44
10:X:117:LEU:HD23	10:X:117:LEU:N	2.30	0.44
2:B:170:ALA:O	2:B:173:THR:HB	2.18	0.44
7:G:243:GLN:O	7:G:246:ILE:HG22	2.18	0.44
10:J:-6:ASP:OD1	10:J:-4:SER:N	2.48	0.44
3:Q:169:THR:O	3:Q:170:SER:C	2.56	0.44
10:X:65:TYR:CD1	10:X:73:ILE:HB	2.53	0.44
12:Z:174:SER:HA	12:Z:193:VAL:HG23	1.99	0.44
3:C:191:GLU:HG3	3:C:242:THR:CG2	2.47	0.43
5:E:13:SER:HB2	6:F:126:ARG:HD3	1.98	0.43
7:G:97:SER:OG	7:G:98:PHE:N	2.51	0.43
4:R:202:VAL:O	4:R:202:VAL:HG12	2.17	0.43
9:W:163:ILE:HG23	9:W:170:GLY:HA2	2.00	0.43
13:1:-1:ASN:HA	13:1:21:ILE:O	2.18	0.43
13:1:176:ARG:NH1	13:1:208:TYR:CD1	2.86	0.43
1:A:225:VAL:HG11	1:A:236:LEU:HD12	1.99	0.43
4:D:210:ILE:CG2	4:D:211:GLU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:101:LEU:HD12	12:L:57:THR:HG22	2.00	0.43
9:I:18:THR:HB	9:I:30:ASN:HA	1.99	0.43
10:J:169:ASP:OD1	10:J:171:LEU:N	2.48	0.43
3:Q:219:GLY:O	3:Q:220:ALA:HB3	2.17	0.43
10:X:113:ALA:CA	10:X:128:ILE:HD12	2.48	0.43
10:X:115:PHE:N	10:X:115:PHE:CD1	2.86	0.43
4:D:82:SER:O	4:D:86:ILE:CD1	2.66	0.43
5:E:42:THR:HG23	5:E:45:GLY:O	2.18	0.43
8:H:109:GLU:OE2	8:H:121:LYS:HE2	2.18	0.43
1:O:76:SER:HB3	1:O:79:ILE:HB	2.00	0.43
4:R:171:VAL:HG23	4:R:198:SER:HB2	2.00	0.43
5:S:121:LEU:HD12	6:T:79:PRO:HG2	2.00	0.43
3:C:160:TRP:CD2	3:C:163:ILE:HD13	2.52	0.43
4:D:184:PRO:O	4:D:186:ALA:N	2.50	0.43
5:E:157:HIS:O	5:E:164:PHE:HA	2.18	0.43
6:F:218:LYS:HG3	6:F:219:ASP:N	2.34	0.43
4:R:73:LEU:HD22	4:R:86:ILE:HD11	2.00	0.43
6:T:163:ALA:O	6:T:164:ARG:HB2	2.17	0.43
3:C:16:GLU:O	4:D:29:ARG:NH1	2.51	0.43
14:N:176:LEU:O	14:N:180:ASP:HB3	2.18	0.43
1:O:42:SER:HA	1:O:54:ILE:O	2.19	0.43
3:Q:42:ASP:CG	3:Q:186:VAL:HG23	2.39	0.43
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.00	0.43
1:A:30:TYR:CD1	7:G:16:PRO:HA	2.53	0.43
2:B:158:PRO:O	3:C:57:LEU:HD12	2.19	0.43
5:E:155:LEU:HB3	5:E:167:TYR:O	2.19	0.43
7:G:125:TYR:HB2	7:G:128:VAL:HG22	1.99	0.43
10:J:58:PHE:CZ	10:J:82:VAL:HG22	2.53	0.43
1:O:84:ASN:OD1	1:O:171:THR:HB	2.19	0.43
6:T:11:VAL:O	6:T:11:VAL:CG2	2.67	0.43
9:W:29:LYS:NZ	10:X:142:GLU:OE2	2.51	0.43
12:Z:149:SER:O	12:Z:150:VAL:C	2.57	0.43
14:2:80:GLU:O	14:2:81:PRO:C	2.57	0.43
14:2:174:ARG:HB2	14:2:206:VAL:HG13	2.01	0.43
2:B:148:TYR:CE2	2:B:158:PRO:HB3	2.54	0.43
2:B:236:ARG:CG	2:B:236:ARG:NH2	2.76	0.43
8:H:38:HIS:O	8:H:39:ASP:C	2.56	0.43
8:H:163:ILE:HG23	8:H:170:GLY:HA2	2.00	0.43
13:M:152:GLU:CB	13:M:155:THR:OG1	2.62	0.43
2:P:246:ARG:HD3	2:P:246:ARG:HA	1.94	0.43
3:Q:96:GLN:HB3	10:X:60:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:115:LEU:O	8:V:116:GLY:C	2.56	0.43
10:X:117:LEU:H	10:X:117:LEU:CD2	2.30	0.43
11:Y:66:TYR:CE1	11:Y:74:LEU:HD21	2.54	0.43
5:E:75:GLY:HA3	5:E:228:PHE:CE1	2.53	0.43
6:F:5:ASN:HB2	6:F:6:TYR:CD2	2.54	0.43
13:M:143:ASN:O	13:M:147:PHE:HA	2.19	0.43
3:Q:125:HIS:CB	4:R:126:VAL:HG12	2.48	0.43
6:T:201:LEU:CD1	6:T:206:LEU:HD22	2.49	0.43
4:D:155:ILE:HD11	5:E:82:THR:OG1	2.19	0.43
7:U:37:ILE:HG22	7:U:163:ALA:CB	2.49	0.43
10:X:18:LEU:HD12	10:X:175:GLY:HA3	2.01	0.43
2:B:47:THR:HG21	2:B:63:LYS:HE3	2.00	0.43
4:D:29:ARG:O	4:D:29:ARG:CG	2.67	0.43
6:F:130:VAL:O	6:F:149:PRO:HG3	2.19	0.43
8:H:193:TYR:O	8:H:196:LEU:HG	2.19	0.43
11:K:171:MET:CE	11:K:173:MET:HB2	2.48	0.43
9:W:130:GLY:O	9:W:131:SER:C	2.57	0.43
10:X:93:PRO:CG	10:X:117:LEU:HD12	2.49	0.43
8:H:48:SER:OG	8:H:51:ASP:HB2	2.19	0.42
9:I:84:LYS:HG3	9:I:85:GLN:N	2.34	0.42
12:L:39:PRO:O	12:L:185:TRP:CD1	2.72	0.42
14:N:7:LYS:HB3	14:N:12:VAL:HG12	2.00	0.42
14:N:163:GLN:OE1	14:N:163:GLN:N	2.50	0.42
2:P:9:LEU:HD12	2:P:127:VAL:N	2.33	0.42
4:R:48:ARG:O	4:R:49:ARG:C	2.58	0.42
10:X:82:VAL:HG11	10:X:115:PHE:CE1	2.54	0.42
10:X:114:GLY:N	10:X:128:ILE:HD13	2.34	0.42
13:1:18:THR:HG22	13:1:18:THR:O	2.19	0.42
3:C:185:LYS:O	3:C:186:VAL:C	2.58	0.42
6:F:146:GLU:O	6:F:153:VAL:HA	2.18	0.42
10:J:22:SER:O	10:J:23:GLN:HB2	2.19	0.42
13:M:117:ASP:HB3	13:M:119:VAL:N	2.34	0.42
14:N:179:ARG:NH1	9:W:139:GLU:OE2	2.52	0.42
14:2:35:ILE:HD12	14:2:45:ILE:HD12	2.00	0.42
14:2:161:THR:OG1	14:2:164:VAL:HG23	2.19	0.42
2:B:89:SER:OG	2:B:114:VAL:HG22	2.19	0.42
6:F:15:PRO:HA	7:G:25:TYR:CD1	2.53	0.42
6:F:78:ALA:HB3	6:F:79:PRO:HD3	2.01	0.42
7:G:219:SER:HB3	7:G:222:GLU:HB2	2.00	0.42
8:H:106:ASN:O	8:H:107:LYS:CB	2.67	0.42
9:I:203:TYR:HD1	13:1:144:GLN:OE1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:73:ILE:HD11	10:J:77:THR:HG22	2.02	0.42
11:K:17:SER:HB2	11:K:175:PHE:HB2	2.01	0.42
3:Q:219:GLY:O	3:Q:220:ALA:CB	2.66	0.42
12:Z:2:THR:OG1	12:Z:132:GLY:HA3	2.18	0.42
3:C:42:ASP:OD1	3:C:186:VAL:HG23	2.19	0.42
3:C:125:HIS:HB3	4:D:126:VAL:HG12	2.01	0.42
9:I:146:LEU:HD23	9:I:146:LEU:N	2.34	0.42
12:L:38:ASN:HB2	12:L:39:PRO:CD	2.49	0.42
14:N:4:ILE:HG22	14:N:135:ALA:HB1	2.00	0.42
1:O:34:ALA:O	1:O:86:PRO:HD3	2.19	0.42
4:R:110:THR:HG21	4:R:148:TYR:HB3	2.01	0.42
7:G:74:GLY:HA3	7:G:227:HIS:CD2	2.55	0.42
9:I:135:MET:SD	14:2:179:ARG:NH1	2.93	0.42
11:K:19:ALA:HB2	11:K:176:LYS:HG2	2.02	0.42
2:P:196:LEU:HD23	2:P:209:ILE:HD12	2.01	0.42
7:U:53:ILE:HG23	7:U:55:SER:O	2.20	0.42
7:U:206:ASN:O	7:U:206:ASN:ND2	2.41	0.42
9:W:84:LYS:HG3	9:W:85:GLN:N	2.35	0.42
12:Z:38:ASN:HB2	12:Z:39:PRO:CD	2.49	0.42
2:B:180:ASN:C	2:B:180:ASN:ND2	2.72	0.42
3:C:239:LEU:HB3	3:C:245:THR:HG21	2.01	0.42
4:D:29:ARG:O	4:D:29:ARG:HG3	2.18	0.42
12:L:126:ILE:CG2	12:L:140:LEU:HD23	2.50	0.42
2:P:197:LYS:HA	2:P:204:PHE:CE1	2.54	0.42
5:S:48:LEU:HD11	5:S:145:ALA:HB2	2.01	0.42
5:S:64:ILE:HG22	5:S:64:ILE:O	2.20	0.42
11:Y:67:SER:HA	11:Y:72:TYR:O	2.20	0.42
11:Y:127:LEU:HB3	11:Y:128:PRO:HD2	2.00	0.42
4:D:68:ASP:OD2	4:D:97:ARG:NH1	2.52	0.42
14:N:132:PRO:HB2	14:N:151:VAL:HG23	2.01	0.42
1:O:75:ILE:HA	1:O:98:LYS:HG2	2.02	0.42
14:2:198:LEU:C	14:2:198:LEU:HD23	2.40	0.42
6:F:69:HIS:CE1	6:F:103:LEU:O	2.69	0.42
1:O:70:SER:OG	1:O:224:GLU:OE2	2.26	0.42
4:R:51:THR:CG2	4:R:52:LEU:HA	2.45	0.42
6:T:78:ALA:N	6:T:79:PRO:CD	2.83	0.42
6:T:89:ARG:O	6:T:93:ASN:HB2	2.20	0.42
12:Z:193:VAL:O	12:Z:194:GLY:C	2.58	0.42
13:1:176:ARG:NH1	13:1:208:TYR:CE1	2.88	0.42
14:2:75:ALA:O	14:2:76:GLU:C	2.57	0.42
4:D:25:GLU:CD	4:D:28:LYS:HE2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:24:VAL:O	5:E:27:SER:HB3	2.20	0.42
6:F:99:PHE:O	14:N:83:TYR:HA	2.19	0.42
10:J:90:ARG:HD2	10:J:90:ARG:O	2.20	0.42
12:L:107:LYS:H	12:L:107:LYS:CD	2.32	0.42
3:Q:94:HIS:CE1	3:Q:114:ARG:HD3	2.55	0.42
3:Q:244:ILE:O	3:Q:245:THR:C	2.58	0.42
4:R:27:VAL:HG11	4:R:132:SER:HB3	2.01	0.42
7:U:170:SER:O	7:U:174:GLU:HG2	2.20	0.42
10:X:103:ILE:HD12	10:X:181:ILE:HG22	2.01	0.42
6:F:163:ALA:O	6:F:165:SER:N	2.53	0.42
10:J:123:GLU:O	10:J:123:GLU:HG2	2.20	0.42
13:M:163:LEU:O	13:M:164:LYS:O	2.38	0.42
14:N:193:ASP:HB3	14:N:196:THR:OG1	2.19	0.42
3:Q:62:SER:OG	3:Q:63:THR:N	2.53	0.42
6:T:10:THR:CG2	6:T:120:THR:HA	2.50	0.42
9:W:4:VAL:HG22	9:W:159:ILE:HD11	2.02	0.42
12:Z:22:ALA:HB3	12:Z:25:TRP:HD1	1.84	0.42
6:F:54:ASP:CB	6:F:56:LEU:H	2.33	0.41
11:K:18:LYS:HD3	11:K:179:ILE:HG13	2.02	0.41
3:Q:149:TYR:CZ	4:R:59:ILE:HD12	2.55	0.41
5:S:38:ILE:HD13	5:S:204:LEU:HG	2.01	0.41
4:D:11:PHE:H	5:E:23:GLN:HE22	1.67	0.41
5:E:133:LEU:O	5:E:133:LEU:CD2	2.68	0.41
6:F:171:TYR:CD2	6:F:172:LEU:N	2.88	0.41
7:G:43:ASP:OD1	7:G:221:SER:OG	2.17	0.41
11:K:44:SER:OG	11:K:102:LEU:HB2	2.20	0.41
13:M:117:ASP:HB2	13:M:121:SER:H	1.85	0.41
2:P:68:THR:HB	2:P:69:PRO:CD	2.49	0.41
9:W:162:GLY:O	9:W:166:ASP:HB3	2.19	0.41
10:X:54:LEU:CD1	10:X:96:VAL:HG21	2.50	0.41
5:S:176:SER:O	5:S:180:GLN:HB2	2.20	0.41
9:W:104:ASP:HB2	9:W:105:PRO:HD2	2.01	0.41
9:W:160:GLN:O	9:W:161:ALA:C	2.57	0.41
7:G:223:THR:O	7:G:224:ASN:HB2	2.19	0.41
13:M:105:LEU:HD23	13:M:111:GLY:HA2	2.03	0.41
14:N:41:THR:OG1	14:N:81:PRO:HG3	2.20	0.41
1:O:13:ASP:OD2	1:O:20:SER:HA	2.21	0.41
4:R:75:PHE:CD2	4:R:75:PHE:C	2.94	0.41
7:U:178:LEU:O	7:U:182:HIS:HB2	2.20	0.41
8:V:39:ASP:OD1	8:V:39:ASP:N	2.42	0.41
4:D:118:GLN:NE2	4:D:118:GLN:C	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:212:LEU:CD2	5:E:240:ILE:HD11	2.51	0.41
6:F:171:TYR:HD2	6:F:172:LEU:N	2.18	0.41
12:L:131:SER:OG	12:L:168:ASP:OD2	2.33	0.41
1:O:92:ASN:ND2	1:O:92:ASN:O	2.54	0.41
2:P:177:LYS:HE2	2:P:177:LYS:HB3	1.96	0.41
6:T:11:VAL:HG23	7:U:129:ARG:N	2.35	0.41
2:B:8:SER:OG	3:C:128:LEU:HA	2.19	0.41
7:G:217:TRP:CH2	7:G:222:GLU:HB3	2.55	0.41
8:H:17:ASP:OD2	8:H:169:SER:HA	2.20	0.41
9:I:35:HIS:CB	9:I:56:THR:HG21	2.47	0.41
10:J:3:VAL:HG23	10:J:45:THR:HG22	2.01	0.41
14:N:151:VAL:O	14:N:151:VAL:CG2	2.64	0.41
5:S:46:VAL:HG11	5:S:145:ALA:HB1	2.02	0.41
3:C:244:ILE:O	3:C:244:ILE:CG2	2.68	0.41
5:E:117:CYS:HB3	5:E:162:GLY:O	2.21	0.41
6:F:119:ASN:N	6:F:119:ASN:ND2	2.68	0.41
12:L:208:ASN:OD1	11:Y:149:PRO:HD2	2.21	0.41
14:N:-5:GLN:HG3	14:N:-5:GLN:O	2.20	0.41
1:O:69:VAL:HA	7:U:157:TRP:CZ3	2.56	0.41
8:V:34:LEU:HD13	8:V:176:VAL:HG23	2.01	0.41
9:W:50:ALA:HB2	10:X:120:CYS:HB2	2.02	0.41
1:A:108:TYR:O	9:I:78:SER:HA	2.21	0.41
3:C:37:GLY:C	3:C:148:LEU:HD21	2.40	0.41
5:E:98:THR:CG2	5:E:102:TYR:CE2	3.04	0.41
14:N:122:VAL:HA	14:N:127:VAL:O	2.20	0.41
3:Q:29:ILE:HG12	3:Q:134:SER:HB2	2.03	0.41
3:Q:42:ASP:OD1	3:Q:42:ASP:N	2.50	0.41
7:U:94:GLU:HG2	7:U:114:ARG:CB	2.49	0.41
7:U:169:GLN:O	7:U:170:SER:C	2.57	0.41
10:X:43:GLY:O	10:X:98:PRO:HA	2.21	0.41
13:1:2:THR:HG21	13:1:133:ALA:HB3	2.02	0.41
14:2:204:LEU:HD12	14:2:204:LEU:N	2.35	0.41
1:A:20:SER:HB3	1:A:26:TYR:HE2	1.85	0.41
2:B:149:GLN:O	2:B:156:TYR:HA	2.21	0.41
5:E:60:GLU:O	5:E:62:ASP:N	2.54	0.41
6:F:230:VAL:O	6:F:231:ALA:C	2.60	0.41
8:H:106:ASN:O	8:H:107:LYS:HB2	2.20	0.41
8:H:134:ILE:O	8:H:135:TYR:C	2.57	0.41
13:M:98:VAL:O	13:M:98:VAL:HG23	2.21	0.41
13:M:176:ARG:O	13:M:180:THR:OG1	2.23	0.41
4:R:227:GLU:OE2	4:R:227:GLU:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:37:ILE:HG22	7:U:163:ALA:HB2	2.03	0.41
7:U:101:LEU:HD23	7:U:102:TYR:CZ	2.56	0.41
7:U:205:ASP:O	7:U:206:ASN:HB3	2.20	0.41
7:U:243:GLN:HE21	7:U:243:GLN:HA	1.86	0.41
12:Z:12:ILE:HG23	12:Z:112:ILE:HD11	2.03	0.41
6:F:7:ASP:OD2	6:F:24:TYR:OH	2.31	0.41
6:F:211:LEU:HG	6:F:230:VAL:HG11	2.03	0.41
9:I:34:LEU:HD22	9:I:174:ASP:HB3	2.03	0.41
10:J:184:ASP:OD1	10:J:184:ASP:N	2.51	0.41
3:Q:62:SER:O	3:Q:63:THR:HG23	2.21	0.41
8:V:84:GLU:O	8:V:88:GLU:HB2	2.20	0.41
9:W:172:ASN:HB3	9:W:191:LEU:O	2.22	0.41
13:1:179:PHE:O	13:1:183:THR:OG1	2.27	0.41
1:A:203:VAL:HB	1:A:244:ARG:HD3	2.03	0.40
5:E:31:ILE:HD13	5:E:141:ALA:HB2	2.03	0.40
6:F:204:GLU:OE1	6:F:204:GLU:N	2.53	0.40
12:L:4:LEU:C	12:L:4:LEU:CD2	2.90	0.40
1:O:147:ASP:OD2	9:W:72:ARG:NH2	2.53	0.40
1:O:158:ASP:HB2	1:O:159:PRO:CD	2.51	0.40
3:Q:87:LEU:HD22	3:Q:115:LEU:HD21	2.01	0.40
11:Y:38:SER:OG	11:Y:73:GLU:OE2	2.38	0.40
6:F:54:ASP:C	6:F:56:LEU:H	2.24	0.40
13:M:163:LEU:O	13:M:164:LYS:C	2.60	0.40
6:T:135:ILE:HA	6:T:143:HIS:O	2.21	0.40
7:U:149:MET:HE1	7:U:164:THR:HB	2.02	0.40
9:W:86:HIS:O	9:W:90:TYR:HD2	2.04	0.40
2:B:108:LYS:HE2	2:B:143:ASN:HD21	1.86	0.40
3:C:2:GLY:O	3:C:5:ARG:HG3	2.22	0.40
3:C:74:ALA:HB2	3:C:227:GLN:HE21	1.85	0.40
4:D:73:LEU:HD23	4:D:73:LEU:C	2.42	0.40
4:D:232:TYR:O	4:D:236:ILE:HD13	2.21	0.40
5:E:16:SER:HA	5:E:22:PHE:CZ	2.56	0.40
5:E:166:ARG:HB3	6:F:58:SER:OG	2.21	0.40
8:H:14:LEU:HD12	8:H:14:LEU:N	2.36	0.40
13:M:-5:PRO:HB2	14:N:96:ARG:NH1	2.36	0.40
4:R:15:GLY:O	5:S:30:ALA:HB2	2.22	0.40
11:Y:100:ASN:OD1	11:Y:120:TYR:N	2.53	0.40
3:C:100:LYS:HG3	10:J:56:GLU:HB3	2.04	0.40
4:D:184:PRO:O	4:D:185:PRO:C	2.59	0.40
11:K:40:HIS:CD2	11:K:108:LYS:HD3	2.56	0.40
13:M:115:SER:HB3	13:M:125:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:90:ARG:NH1	9:W:68:LEU:HB3	2.36	0.40
2:P:203:GLU:OE1	2:P:203:GLU:HA	2.22	0.40
6:T:11:VAL:HG22	7:U:11:MET:SD	2.61	0.40
13:1:-8:GLN:NE2	13:1:-7:PHE:H	2.16	0.40
13:1:183:THR:OG1	13:1:210:LEU:HD22	2.21	0.40
7:G:17:ASP:HB2	7:G:19:ARG:HD3	2.04	0.40
11:K:174:ASP:HB2	11:Y:174:ASP:HB2	2.04	0.40
14:N:171:ASN:HD22	14:N:174:ARG:HH21	1.69	0.40
6:T:64:ILE:HB	6:T:72:LEU:CD2	2.51	0.40
8:V:1:THR:O	8:V:129:SER:N	2.54	0.40
8:V:190:PRO:O	8:V:192:GLU:N	2.54	0.40
11:Y:29:ASP:C	11:Y:29:ASP:OD1	2.60	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	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
1	O	241/252 (96%)	229 (95%)	12 (5%)	0	100	100
2	B	247/250 (99%)	240 (97%)	5 (2%)	2 (1%)	19	55
2	P	247/250 (99%)	229 (93%)	16 (6%)	2 (1%)	19	55
3	C	238/258 (92%)	227 (95%)	8 (3%)	3 (1%)	12	44
3	Q	242/258 (94%)	219 (90%)	18 (7%)	5 (2%)	7	33
4	D	239/254 (94%)	227 (95%)	5 (2%)	7 (3%)	4	25
4	R	239/254 (94%)	217 (91%)	16 (7%)	6 (2%)	5	29
5	E	235/260 (90%)	217 (92%)	15 (6%)	3 (1%)	12	44
5	S	234/260 (90%)	215 (92%)	12 (5%)	7 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	230/234 (98%)	201 (87%)	23 (10%)	6 (3%)	5 28
6	T	230/234 (98%)	204 (89%)	18 (8%)	8 (4%)	3 21
7	G	235/277 (85%)	216 (92%)	18 (8%)	1 (0%)	34 68
7	U	235/277 (85%)	214 (91%)	17 (7%)	4 (2%)	9 38
8	H	194/215 (90%)	177 (91%)	15 (8%)	2 (1%)	15 51
8	V	197/215 (92%)	179 (91%)	15 (8%)	3 (2%)	10 41
9	I	220/261 (84%)	209 (95%)	9 (4%)	2 (1%)	17 53
9	W	220/261 (84%)	206 (94%)	13 (6%)	1 (0%)	29 65
10	J	202/205 (98%)	187 (93%)	13 (6%)	2 (1%)	15 51
10	X	202/205 (98%)	185 (92%)	17 (8%)	0	100 100
11	K	195/238 (82%)	183 (94%)	10 (5%)	2 (1%)	15 51
11	Y	196/238 (82%)	174 (89%)	18 (9%)	4 (2%)	7 34
12	L	210/287 (73%)	197 (94%)	12 (6%)	1 (0%)	29 65
12	Z	210/287 (73%)	198 (94%)	12 (6%)	0	100 100
13	1	220/241 (91%)	206 (94%)	14 (6%)	0	100 100
13	M	220/241 (91%)	204 (93%)	12 (6%)	4 (2%)	8 37
14	2	231/266 (87%)	210 (91%)	19 (8%)	2 (1%)	17 53
14	N	231/266 (87%)	212 (92%)	17 (7%)	2 (1%)	17 53
All	All	6281/6996 (90%)	5816 (93%)	386 (6%)	79 (1%)	12 44

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	184	MET
5	E	132	ARG
6	F	176	LEU
6	F	203	ASP
11	K	49	ALA
13	M	0	GLY
13	M	39	ASP
13	M	164	LYS
2	P	185	LEU
3	Q	63	THR
3	Q	220	ALA
4	R	49	ARG
4	R	226	SER

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Mol	Chain	Res	Type
5	S	10	ARG
5	S	131	GLU
6	T	4	ASN
7	U	12	SER
7	U	206	ASN
8	V	0	GLY
11	Y	195	GLN
3	C	62	SER
4	D	185	PRO
4	D	206	GLY
5	E	61	SER
6	F	184	GLY
6	F	232	LYS
12	L	173	GLY
14	N	1	THR
4	R	53	LYS
4	R	185	PRO
4	R	205	THR
5	S	11	GLY
5	S	152	GLY
6	T	176	LEU
7	U	142	LYS
8	V	191	ASP
4	D	51	THR
4	D	205	THR
5	E	176	SER
7	G	142	LYS
8	H	39	ASP
11	K	185	LYS
13	M	191	ASP
3	Q	184	MET
3	Q	222	ASP
5	S	55	THR
5	S	132	ARG
6	T	186	PRO
4	D	207	ALA
2	P	249	ALA
6	T	202	ARG
8	V	39	ASP
2	B	19	GLY
2	B	166	LYS
3	C	186	VAL

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Mol	Chain	Res	Type
6	F	228	GLU
10	J	23	GLN
4	R	217	PRO
5	S	174	SER
6	T	218	LYS
7	U	182	HIS
9	W	131	SER
14	2	75	ALA
4	D	13	PRO
4	D	204	GLN
8	H	107	LYS
14	N	75	ALA
6	T	11	VAL
11	Y	128	PRO
10	J	92	GLY
3	Q	244	ILE
11	Y	8	VAL
11	Y	39	PRO
6	F	34	VAL
14	2	221	GLY
6	T	182	ILE
9	I	105	PRO
9	I	163	ILE
6	T	208	VAL

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	207/210 (99%)	193 (93%)	14 (7%)	16	46
1	O	207/210 (99%)	194 (94%)	13 (6%)	18	49
2	B	208/209 (100%)	197 (95%)	11 (5%)	22	55
2	P	208/209 (100%)	198 (95%)	10 (5%)	25	59
3	C	203/216 (94%)	187 (92%)	16 (8%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	Q	203/216 (94%)	184 (91%)	19 (9%)	8 30
4	D	213/226 (94%)	198 (93%)	15 (7%)	15 45
4	R	213/226 (94%)	196 (92%)	17 (8%)	12 39
5	E	196/215 (91%)	185 (94%)	11 (6%)	21 53
5	S	197/215 (92%)	184 (93%)	13 (7%)	16 47
6	F	191/193 (99%)	175 (92%)	16 (8%)	11 37
6	T	191/193 (99%)	177 (93%)	14 (7%)	14 43
7	G	196/230 (85%)	176 (90%)	20 (10%)	7 27
7	U	196/230 (85%)	179 (91%)	17 (9%)	10 34
8	H	162/178 (91%)	157 (97%)	5 (3%)	40 70
8	V	163/178 (92%)	158 (97%)	5 (3%)	40 70
9	I	181/214 (85%)	174 (96%)	7 (4%)	32 64
9	W	181/214 (85%)	177 (98%)	4 (2%)	52 77
10	J	172/173 (99%)	165 (96%)	7 (4%)	30 63
10	X	172/173 (99%)	164 (95%)	8 (5%)	26 60
11	K	174/209 (83%)	163 (94%)	11 (6%)	18 49
11	Y	175/209 (84%)	160 (91%)	15 (9%)	10 35
12	L	169/235 (72%)	159 (94%)	10 (6%)	19 51
12	Z	169/235 (72%)	161 (95%)	8 (5%)	26 60
13	1	185/201 (92%)	172 (93%)	13 (7%)	15 45
13	M	185/201 (92%)	172 (93%)	13 (7%)	15 45
14	2	199/224 (89%)	186 (94%)	13 (6%)	17 48
14	N	199/224 (89%)	191 (96%)	8 (4%)	31 64
All	All	5315/5866 (91%)	4982 (94%)	333 (6%)	18 49

All (333) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	76	SER
1	A	92	ASN
1	A	96	ARG
1	A	124	LEU
1	A	126	GLN

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Mol	Chain	Res	Type
1	A	129	THR
1	A	147	ASP
1	A	157	THR
1	A	171	THR
1	A	174	LYS
1	A	175	GLN
1	A	244	ARG
1	A	250	GLU
2	B	4	ARG
2	B	18	LEU
2	B	29	LYS
2	B	100	ILE
2	B	108	LYS
2	B	146	SER
2	B	157	PHE
2	B	180	ASN
2	B	222	LEU
2	B	231	LYS
2	B	236	ARG
3	C	36	ILE
3	C	53	THR
3	C	55	THR
3	C	66	LEU
3	C	70	ASN
3	C	103	ASN
3	C	120	GLN
3	C	123	THR
3	C	150	THR
3	C	192	LEU
3	C	207	THR
3	C	210	ARG
3	C	217	ARG
3	C	221	ASN
3	C	229	ILE
3	C	242	THR
4	D	6	ARG
4	D	40	ASN
4	D	49	ARG
4	D	63	LYS
4	D	109	LEU
4	D	118	GLN
4	D	149	GLN

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Mol	Chain	Res	Type
4	D	162	GLN
4	D	171	VAL
4	D	172	ARG
4	D	209	ASN
4	D	215	VAL
4	D	227	GLU
4	D	230	ASN
4	D	240	LYS
5	E	14	THR
5	E	28	LEU
5	E	42	THR
5	E	62	ASP
5	E	76	CYS
5	E	100	ASN
5	E	132	ARG
5	E	148	ASP
5	E	222	ILE
5	E	240	ILE
5	E	243	LEU
6	F	10	THR
6	F	26	LEU
6	F	57	SER
6	F	58	SER
6	F	72	LEU
6	F	77	LEU
6	F	117	GLN
6	F	156	LEU
6	F	174	ARG
6	F	180	ILE
6	F	185	ASN
6	F	189	LEU
6	F	199	GLN
6	F	206	LEU
6	F	223	THR
6	F	230	VAL
7	G	11	MET
7	G	35	THR
7	G	62	LYS
7	G	85	ARG
7	G	104	THR
7	G	107	PRO
7	G	120	GLN

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Mol	Chain	Res	Type
7	G	129	ARG
7	G	168	ARG
7	G	170	SER
7	G	184	GLU
7	G	190	GLU
7	G	204	GLU
7	G	206	ASN
7	G	207	LYS
7	G	209	LYS
7	G	217	TRP
7	G	224	ASN
7	G	243	GLN
7	G	244	LYS
8	H	18	SER
8	H	83	LYS
8	H	105	LYS
8	H	178	LEU
8	H	185	ARG
9	I	34	LEU
9	I	38	SER
9	I	146	LEU
9	I	191	LEU
9	I	196	ARG
9	I	212	VAL
9	I	222	ASP
10	J	17	ASP
10	J	29	ASN
10	J	109	LYS
10	J	162	LEU
10	J	163	LEU
10	J	184	ASP
10	J	194	ARG
11	K	1	ASP
11	K	3	ILE
11	K	30	SER
11	K	34	THR
11	K	38	SER
11	K	52	THR
11	K	77	GLN
11	K	90	SER
11	K	141	SER
11	K	168	GLU

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Mol	Chain	Res	Type
11	K	189	ARG
12	L	4	LEU
12	L	9	GLN
12	L	18	SER
12	L	21	THR
12	L	32	LYS
12	L	104	TYR
12	L	145	LYS
12	L	177	LEU
12	L	190	ASN
12	L	208	ASN
13	M	14	LEU
13	M	21	ILE
13	M	76	SER
13	M	94	PHE
13	M	99	HIS
13	M	100	THR
13	M	125	GLU
13	M	127	CYS
13	M	128	ARG
13	M	135	SER
13	M	146	ASN
13	M	165	TYR
13	M	180	THR
14	N	29	ASN
14	N	40	ASN
14	N	82	SER
14	N	96	ARG
14	N	130	SER
14	N	138	PHE
14	N	153	ARG
14	N	199	THR
1	O	17	THR
1	O	76	SER
1	O	92	ASN
1	O	96	ARG
1	O	115	ASP
1	O	126	GLN
1	O	130	GLN
1	O	131	ARG
1	O	187	LYS
1	O	230	LYS

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Mol	Chain	Res	Type
1	O	244	ARG
1	O	245	LEU
1	O	250	GLU
2	P	29	LYS
2	P	107	THR
2	P	157	PHE
2	P	174	PHE
2	P	211	LEU
2	P	218	ASN
2	P	229	THR
2	P	241	GLN
2	P	246	ARG
2	P	250	LEU
3	Q	8	SER
3	Q	56	LEU
3	Q	70	ASN
3	Q	89	ASN
3	Q	90	THR
3	Q	103	ASN
3	Q	114	ARG
3	Q	115	LEU
3	Q	120	GLN
3	Q	134	SER
3	Q	150	THR
3	Q	181	LYS
3	Q	185	LYS
3	Q	192	LEU
3	Q	201	THR
3	Q	210	ARG
3	Q	238	ILE
3	Q	240	VAL
3	Q	244	ILE
4	R	6	ARG
4	R	40	ASN
4	R	51	THR
4	R	52	LEU
4	R	53	LYS
4	R	58	ARG
4	R	99	THR
4	R	109	LEU
4	R	149	GLN
4	R	162	GLN

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Mol	Chain	Res	Type
4	R	182	LYS
4	R	187	THR
4	R	203	VAL
4	R	205	THR
4	R	215	VAL
4	R	240	LYS
4	R	243	GLN
5	S	43	LYS
5	S	59	LEU
5	S	76	CYS
5	S	87	SER
5	S	108	ASN
5	S	119	LEU
5	S	131	GLU
5	S	133	LEU
5	S	177	GLU
5	S	184	LEU
5	S	201	LEU
5	S	219	LEU
5	S	222	ILE
6	T	10	THR
6	T	11	VAL
6	T	72	LEU
6	T	93	ASN
6	T	96	SER
6	T	119	ASN
6	T	145	LEU
6	T	154	THR
6	T	164	ARG
6	T	166	GLN
6	T	171	TYR
6	T	185	ASN
6	T	189	LEU
6	T	201	LEU
7	U	11	MET
7	U	32	ASN
7	U	35	THR
7	U	42	ASN
7	U	62	LYS
7	U	97	SER
7	U	100	LYS
7	U	120	GLN

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Mol	Chain	Res	Type
7	U	126	ASN
7	U	129	ARG
7	U	153	SER
7	U	168	ARG
7	U	204	GLU
7	U	205	ASP
7	U	206	ASN
7	U	217	TRP
7	U	243	GLN
8	V	39	ASP
8	V	72	THR
8	V	139	ASP
8	V	147	SER
8	V	185	ARG
9	W	68	LEU
9	W	191	LEU
9	W	196	ARG
9	W	222	ASP
10	X	19	ARG
10	X	29	ASN
10	X	115	PHE
10	X	163	LEU
10	X	177	VAL
10	X	183	LYS
10	X	184	ASP
10	X	194	ARG
11	Y	1	ASP
11	Y	3	ILE
11	Y	34	THR
11	Y	35	ARG
11	Y	38	SER
11	Y	52	THR
11	Y	68	ILE
11	Y	75	SER
11	Y	77	GLN
11	Y	90	SER
11	Y	91	ILE
11	Y	117	GLN
11	Y	179	ILE
11	Y	195	GLN
11	Y	197	GLN
12	Z	4	LEU

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Mol	Chain	Res	Type
12	Z	9	GLN
12	Z	18	SER
12	Z	65	LEU
12	Z	104	TYR
12	Z	147	ASP
12	Z	148	LEU
12	Z	190	ASN
13	1	-8	GLN
13	1	14	LEU
13	1	25	SER
13	1	40	ASN
13	1	71	ASN
13	1	76	SER
13	1	94	PHE
13	1	99	HIS
13	1	100	THR
13	1	125	GLU
13	1	141	LEU
13	1	185	ARG
13	1	204	ARG
14	2	-7	THR
14	2	1	THR
14	2	40	ASN
14	2	50	SER
14	2	61	ASP
14	2	62	LEU
14	2	65	GLU
14	2	96	ARG
14	2	130	SER
14	2	163	GLN
14	2	179	ARG
14	2	196	THR
14	2	200	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	123	ASN
1	A	126	GLN
1	A	130	GLN
1	A	184	ASN

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Mol	Chain	Res	Type
1	A	195	ASN
2	B	94	HIS
2	B	143	ASN
2	B	180	ASN
3	C	21	GLN
3	C	70	ASN
3	C	96	GLN
3	C	120	GLN
3	C	124	GLN
3	C	156	ASN
3	C	227	GLN
3	C	233	GLN
4	D	16	HIS
4	D	19	GLN
4	D	40	ASN
4	D	79	ASN
4	D	118	GLN
4	D	149	GLN
4	D	230	ASN
5	E	23	GLN
5	E	99	HIS
5	E	233	ASN
6	F	60	GLN
6	F	69	HIS
6	F	100	ASN
6	F	117	GLN
6	F	119	ASN
6	F	121	GLN
6	F	199	GLN
7	G	120	GLN
7	G	243	GLN
7	G	247	ASN
8	H	38	HIS
8	H	161	GLN
9	I	30	ASN
9	I	66	HIS
9	I	144	GLN
9	I	172	ASN
10	J	29	ASN
10	J	63	ASN
11	K	54	GLN
11	K	77	GLN

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Mol	Chain	Res	Type
11	K	85	GLN
12	L	9	GLN
12	L	85	ASN
12	L	176	ASN
12	L	190	ASN
13	M	-6	ASN
13	M	40	ASN
13	M	61	ASN
13	M	67	HIS
13	M	70	HIS
13	M	186	HIS
14	N	10	ASN
14	N	18	ASN
14	N	40	ASN
14	N	94	GLN
14	N	100	ASN
14	N	171	ASN
14	N	186	ASN
14	N	205	GLN
1	O	92	ASN
1	O	123	ASN
1	O	126	GLN
1	O	130	GLN
1	O	195	ASN
1	O	240	ASN
1	O	251	GLN
2	P	94	HIS
2	P	218	ASN
3	Q	21	GLN
3	Q	70	ASN
3	Q	96	GLN
3	Q	120	GLN
3	Q	124	GLN
3	Q	156	ASN
4	R	19	GLN
4	R	40	ASN
4	R	55	GLN
4	R	162	GLN
4	R	238	GLN
4	R	243	GLN
5	S	23	GLN
5	S	108	ASN

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Mol	Chain	Res	Type
5	S	157	HIS
5	S	168	ASN
5	S	233	ASN
6	T	69	HIS
6	T	117	GLN
6	T	119	ASN
6	T	121	GLN
7	U	22	GLN
7	U	89	ASN
7	U	120	GLN
7	U	126	ASN
7	U	236	GLN
7	U	243	GLN
8	V	38	HIS
8	V	161	GLN
9	W	30	ASN
9	W	144	GLN
9	W	172	ASN
10	X	29	ASN
10	X	63	ASN
11	Y	54	GLN
11	Y	62	ASN
11	Y	77	GLN
11	Y	85	GLN
11	Y	117	GLN
11	Y	145	HIS
11	Y	190	GLN
12	Z	85	ASN
12	Z	176	ASN
12	Z	208	ASN
12	Z	209	ASN
13	1	-8	GLN
13	1	-6	ASN
13	1	40	ASN
13	1	61	ASN
13	1	67	HIS
13	1	71	ASN
13	1	144	GLN
14	2	10	ASN
14	2	40	ASN
14	2	94	GLN
14	2	163	GLN

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Mol	Chain	Res	Type
14	2	171	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	243/252 (96%)	-0.66	2 (0%) 86 78	29, 46, 74, 113	0
1	O	243/252 (96%)	-0.66	1 (0%) 92 89	32, 48, 72, 104	0
2	B	249/250 (99%)	-0.63	0 100 100	31, 49, 79, 105	0
2	P	249/250 (99%)	-0.55	0 100 100	36, 54, 81, 114	0
3	C	242/258 (93%)	-0.60	0 100 100	30, 50, 83, 106	0
3	Q	244/258 (94%)	-0.42	2 (0%) 86 78	31, 53, 96, 132	0
4	D	241/254 (94%)	-0.37	1 (0%) 92 89	33, 59, 106, 126	0
4	R	241/254 (94%)	-0.29	2 (0%) 86 78	38, 62, 108, 128	0
5	E	239/260 (91%)	-0.48	2 (0%) 86 78	31, 55, 80, 106	0
5	S	238/260 (91%)	-0.53	0 100 100	33, 57, 85, 121	0
6	F	232/234 (99%)	-0.41	1 (0%) 92 89	39, 60, 91, 121	0
6	T	232/234 (99%)	-0.43	1 (0%) 92 89	39, 60, 91, 123	0
7	G	237/277 (85%)	-0.57	1 (0%) 92 89	32, 55, 89, 119	0
7	U	237/277 (85%)	-0.51	0 100 100	34, 53, 89, 106	0
8	H	196/215 (91%)	-0.76	0 100 100	26, 40, 59, 80	0
8	V	199/215 (92%)	-0.70	2 (1%) 82 73	27, 40, 64, 130	0
9	I	222/261 (85%)	-0.70	0 100 100	31, 41, 62, 102	0
9	W	222/261 (85%)	-0.73	0 100 100	34, 47, 67, 106	0
10	J	204/205 (99%)	-0.74	1 (0%) 91 86	27, 43, 59, 84	0
10	X	204/205 (99%)	-0.71	0 100 100	29, 42, 66, 93	0
11	K	197/238 (82%)	-0.69	3 (1%) 73 61	26, 43, 65, 139	0
11	Y	198/238 (83%)	-0.70	1 (0%) 91 86	28, 44, 65, 125	0
12	L	212/287 (73%)	-0.71	0 100 100	26, 42, 58, 70	0
12	Z	212/287 (73%)	-0.75	0 100 100	27, 43, 62, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	222/241 (92%)	-0.68	0 100 100	29, 44, 62, 90	0
13	M	222/241 (92%)	-0.72	0 100 100	28, 45, 67, 95	0
14	2	233/266 (87%)	-0.68	1 (0%) 92 89	27, 40, 55, 68	0
14	N	233/266 (87%)	-0.71	1 (0%) 92 89	30, 44, 63, 73	0
All	All	6343/6996 (90%)	-0.60	22 (0%) 94 92	26, 48, 82, 139	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	Y	197	GLN	3.9
8	V	-2	SER	3.8
5	E	127	ALA	3.3
6	T	6	TYR	3.2
4	R	207	ALA	3.2
7	G	11	MET	3.0
3	Q	219	GLY	3.0
1	A	10	ALA	2.9
14	N	-7	THR	2.9
11	K	195	GLN	2.8
1	A	252	ASP	2.7
11	K	196	ALA	2.6
5	E	126	GLY	2.6
14	2	-7	THR	2.4
8	V	0	GLY	2.4
11	K	197	GLN	2.3
1	O	10	ALA	2.3
4	D	51	THR	2.2
3	Q	220	ALA	2.1
10	J	-7	SER	2.1
4	R	210	ILE	2.1
6	F	4	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.