



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:23 PM UTC

PDB ID : 9C97 / pdb_00009c97
Title : Yeast 20S proteasome soaked with BRA-346 fraction
Authors : Meneghello, R.; Rustiguel, J.K.
Deposited on : 2024-06-13
Resolution : 3.33 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

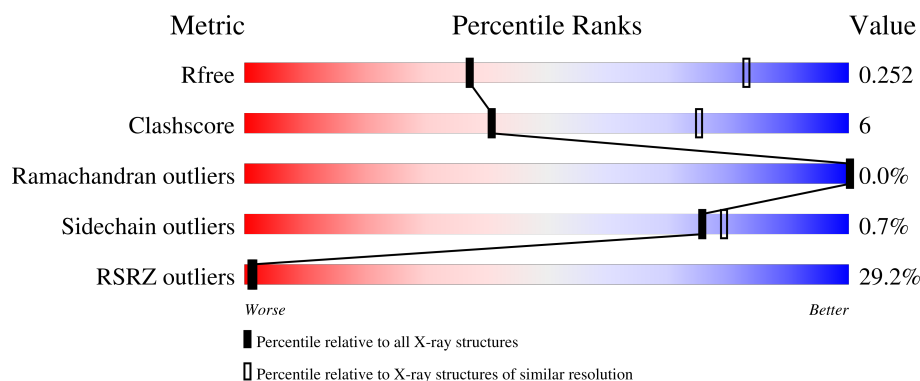
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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 $\leq 5\%$. 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	32% 86% 14%
1	O	250	29% 79% 20%
2	B	258	38% 79% 15% 6%
2	P	258	33% 79% 16% 5%
3	C	254	46% 74% 19% 7%

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Mol	Chain	Length	Quality of chain
3	Q	254	44% 77% 17% 6%
4	D	260	33% 78% 13% 9%
4	R	260	50% 74% 18% 8%
5	E	234	44% 82% 16% .
5	S	234	53% 79% 19% ..
6	F	287	32% 70% 15% 15%
6	T	287	34% 71% 14% 15%
7	G	252	30% 77% 18% .
7	U	252	29% 80% 16% .
8	H	232	22% 83% 12% ..
8	V	232	20% 79% 16% .
9	I	205	19% 76% 24%
9	W	205	12% 80% 20%
10	J	198	13% 77% 22% .
10	X	198	12% 78% 20% .
11	K	212	13% 91% 9%
11	Y	212	20% 85% 15%
12	L	222	11% 84% 16%
12	Z	222	22% 82% 18%
13	M	233	16% 80% 19% .
13	a	233	23% 80% 20%
14	N	196	15% 88% 12%
14	b	196	15% 80% 19% .

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49866 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 PRE8 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- Molecule 2 is a protein called PRE9 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1894	1197	319	375	3			
2	P	244	Total	C	N	O	S	0	0	0
			1909	1206	322	378	3			

- Molecule 3 is a protein called PRE6 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	236	Total	C	N	O	S	0	0	0
			1848	1156	324	364	4			
3	Q	239	Total	C	N	O	S	0	0	0
			1875	1171	329	371	4			

- Molecule 4 is a protein called PUP2 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	237	Total	C	N	O	S	0	0	0
			1836	1151	309	369	7			
4	R	239	Total	C	N	O	S	0	0	0
			1850	1159	311	373	7			

- Molecule 5 is a protein called PRE5 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1770	1113	307	346	4			
5	S	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

- Molecule 6 is a protein called PRE10 isoform 1.

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
			1894	1204	330	356	4			

- Molecule 7 is a protein called SCL1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	242	Total	C	N	O	S	0	0	0
			1913	1217	321	367	8			

- Molecule 8 is a protein called proteasome endopeptidase complex.

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
			1680	1060	293	321	6			

- Molecule 9 is a protein called PUP3 isoform 1.

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 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called proteasome endopeptidase complex.

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 PRE7 isoform 1.

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 subunit beta.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	O	S	0	0
			5	4	1		
15	C	1	Total	O	S	0	0
			5	4	1		
15	D	1	Total	O	S	0	0
			5	4	1		
15	E	1	Total	O	S	0	0
			5	4	1		
15	E	1	Total	O	S	0	0
			5	4	1		
15	E	1	Total	O	S	0	0
			5	4	1		
15	F	1	Total	O	S	0	0
			5	4	1		
15	F	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	P	1	Total	O	S	0	0
			5	4	1		
15	P	1	Total	O	S	0	0
			5	4	1		
15	Q	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	R	1	Total	O	S	0	0
			5	4	1		
15	S	1	Total	O	S	0	0
			5	4	1		
15	S	1	Total	O	S	0	0
			5	4	1		
15	T	1	Total	O	S	0	0
			5	4	1		
15	U	1	Total	O	S	0	0
			5	4	1		
15	H	1	Total	O	S	0	0
			5	4	1		
15	H	1	Total	O	S	0	0
			5	4	1		
15	I	1	Total	O	S	0	0
			5	4	1		
15	J	1	Total	O	S	0	0
			5	4	1		
15	J	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		
15	L	1	Total	O	S	0	0
			5	4	1		
15	L	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	M	1	Total	O	S	0	0
			5	4	1		
15	N	1	Total	O	S	0	0
			5	4	1		
15	N	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	V	1	Total	O	S	0	0
			5	4	1		
15	X	1	Total	O	S	0	0
			5	4	1		
15	Z	1	Total	O	S	0	0
			5	4	1		
15	Z	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	a	1	Total	O	S	0	0
			5	4	1		
15	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	L	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	W	1	Total	Mg	0	0
			1	1		
16	Y	1	Total	Mg	0	0
			1	1		
16	Z	1	Total	Mg	0	0
			1	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	7	Total O 7 7	0	0
17	B	12	Total O 12 12	0	0
17	C	5	Total O 5 5	0	0
17	D	11	Total O 11 11	0	0
17	E	5	Total O 5 5	0	0
17	F	11	Total O 11 11	0	0
17	G	14	Total O 14 14	0	0
17	O	9	Total O 9 9	0	0
17	P	9	Total O 9 9	0	0
17	Q	2	Total O 2 2	0	0
17	R	9	Total O 9 9	0	0
17	S	12	Total O 12 12	0	0
17	T	10	Total O 10 10	0	0
17	U	11	Total O 11 11	0	0
17	H	19	Total O 19 19	0	0
17	I	8	Total O 8 8	0	0
17	J	19	Total O 19 19	0	0
17	K	7	Total O 7 7	0	0
17	L	11	Total O 11 11	0	0
17	M	11	Total O 11 11	0	0
17	N	7	Total O 7 7	0	0
17	V	8	Total O 8 8	0	0

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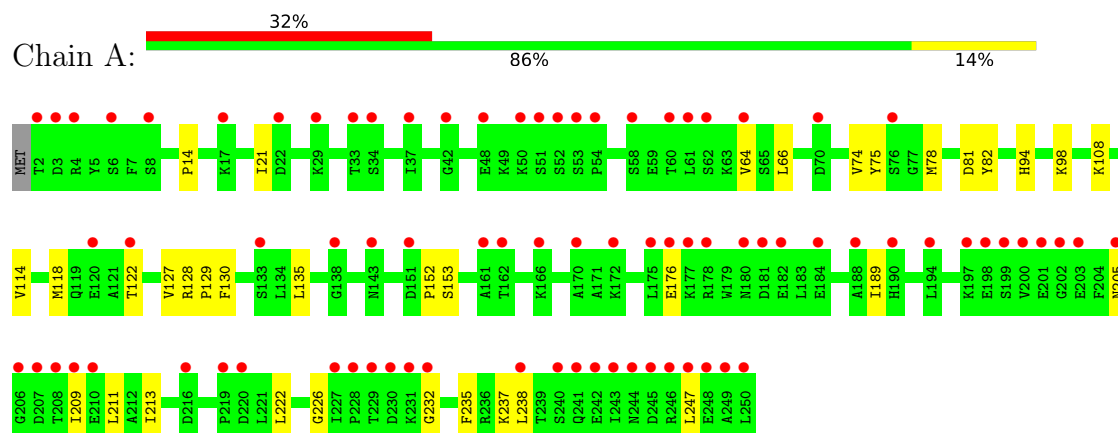
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	16	Total 16	O 16	0	0
17	X	13	Total 13	O 13	0	0
17	Y	7	Total 7	O 7	0	0
17	Z	21	Total 21	O 21	0	0
17	a	27	Total 27	O 27	0	0
17	b	15	Total 15	O 15	0	0

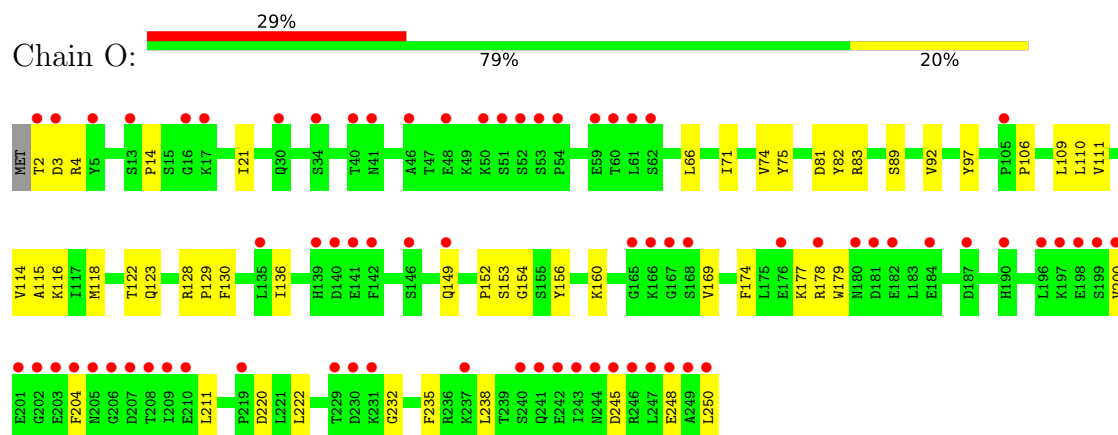
3 Residue-property plots [i](#)

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

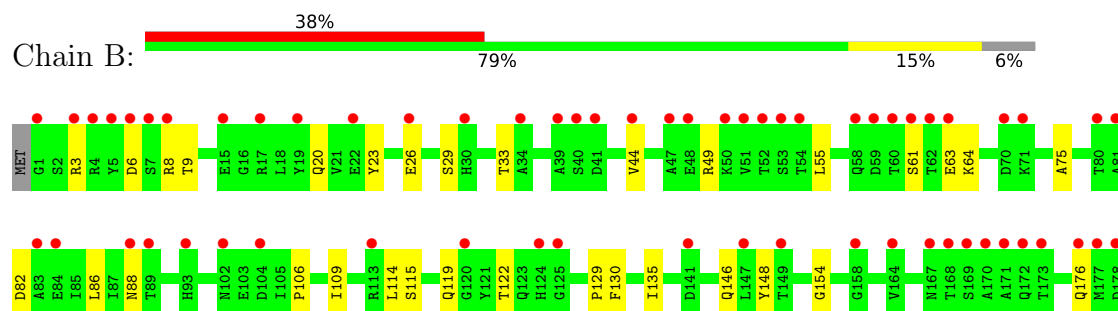
• Molecule 1: PRE8 isoform 1

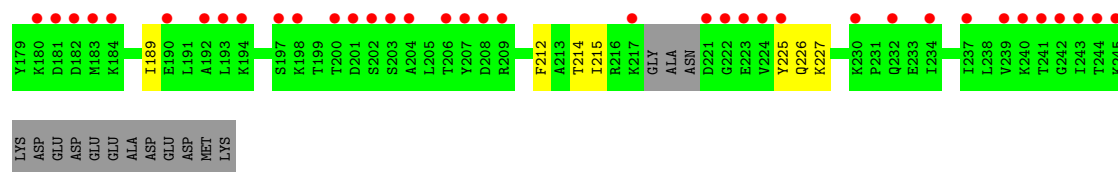


• Molecule 1: PRE8 isoform 1

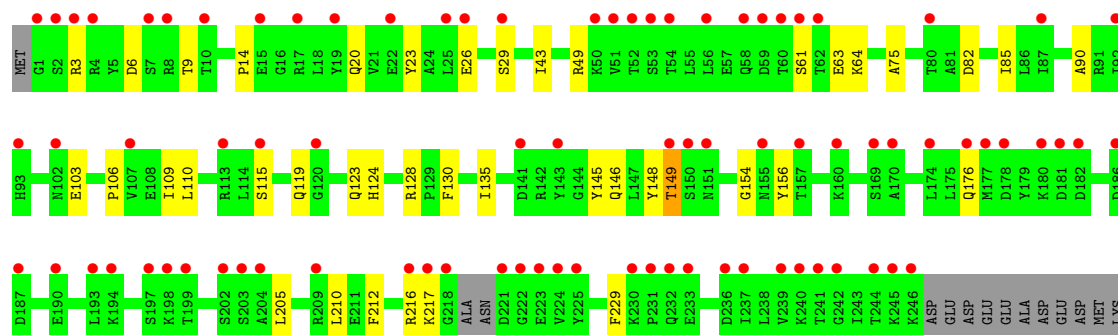


• Molecule 2: PRE9 isoform 1

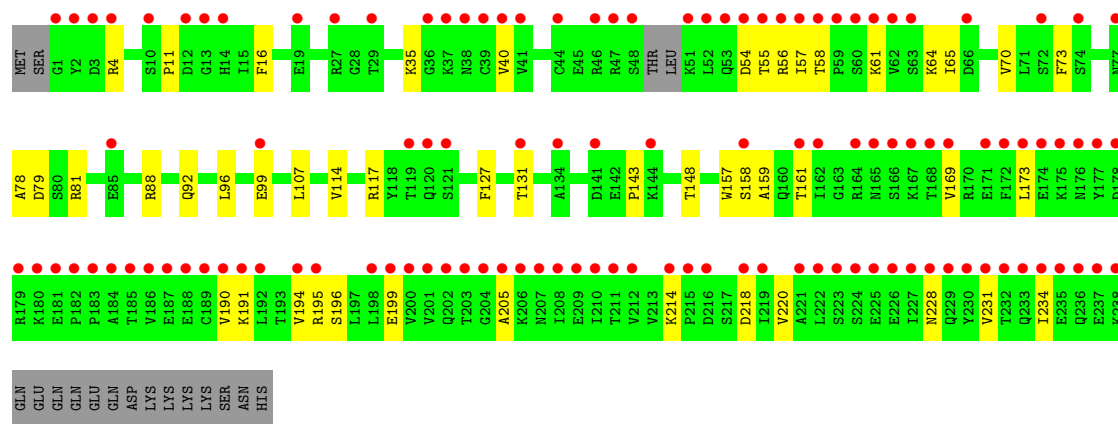
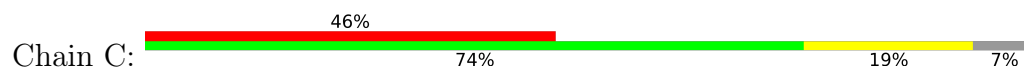




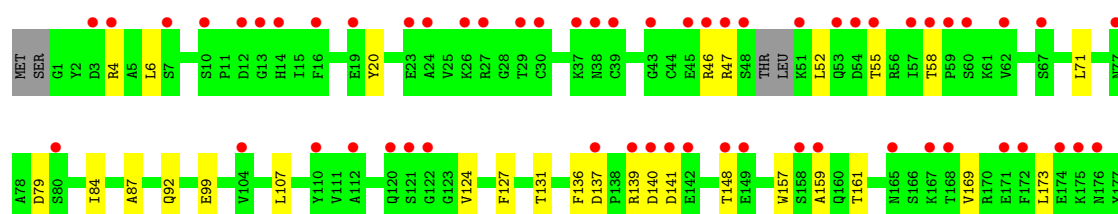
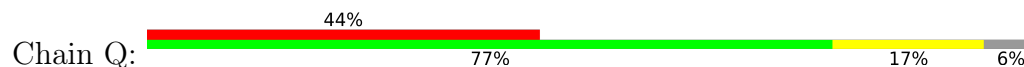
• Molecule 2: PRE9 isoform 1

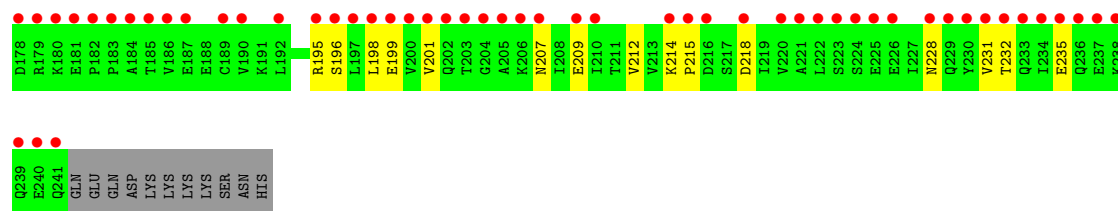


• Molecule 3: PRE6 isoform 1

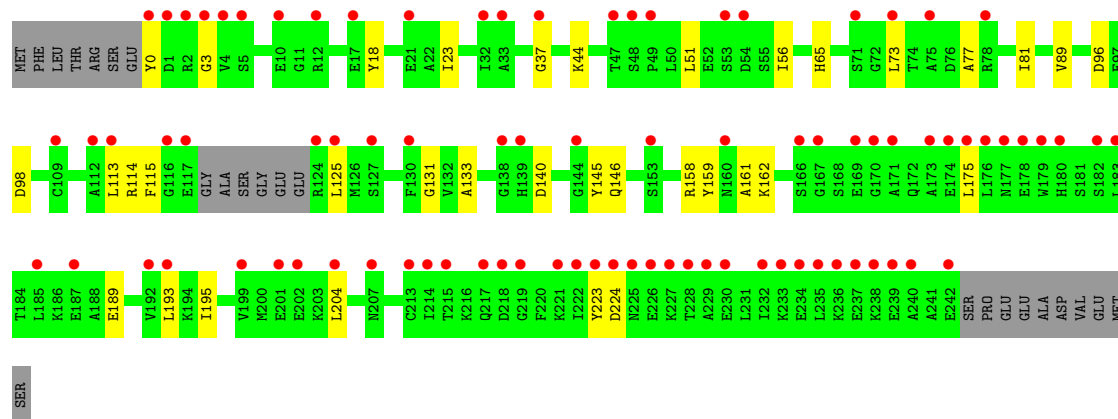
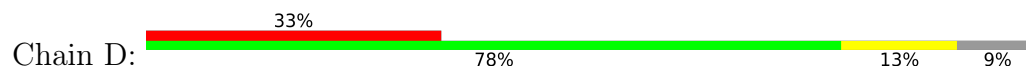


• Molecule 3: PRE6 isoform 1

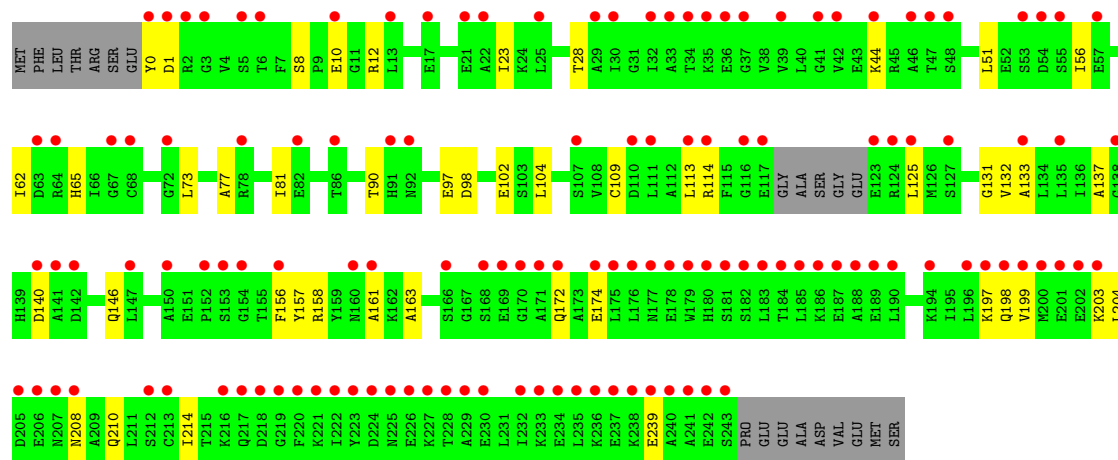
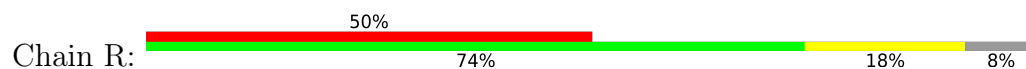




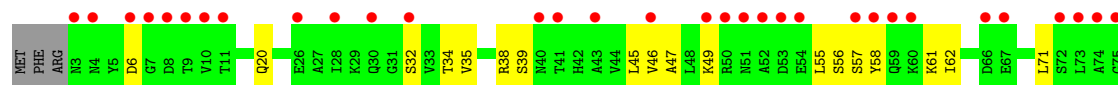
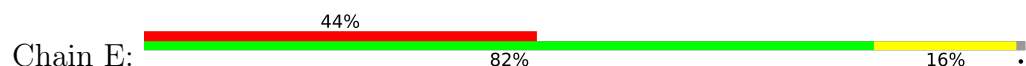
● Molecule 4: PUP2 isoform 1

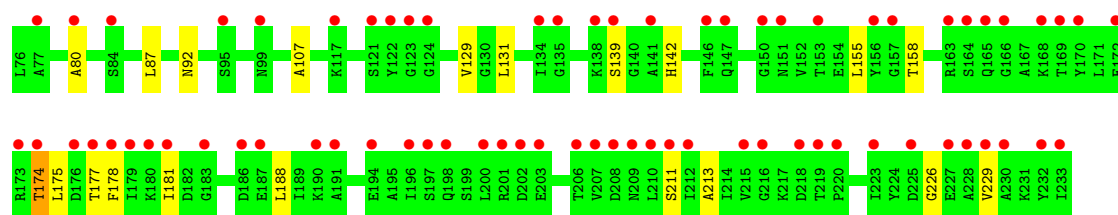


● Molecule 4: PUP2 isoform 1

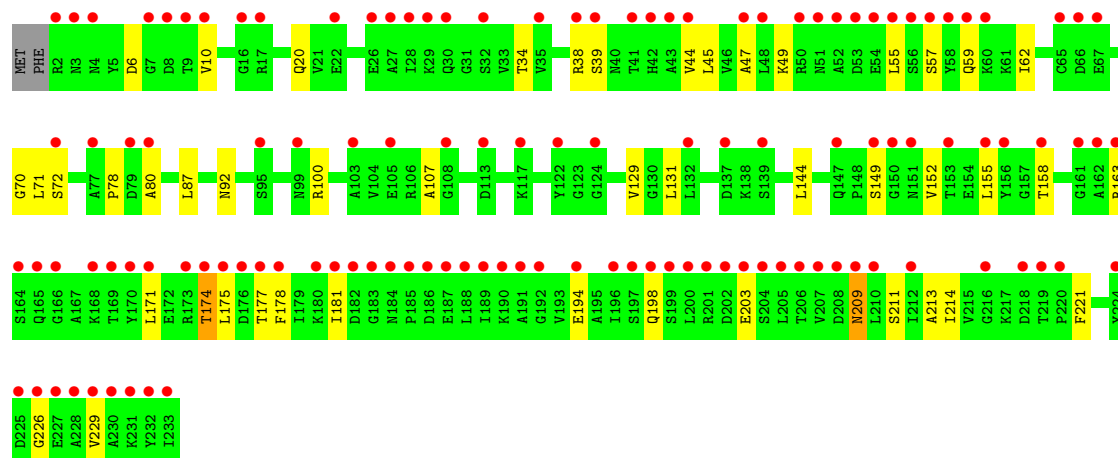


● Molecule 5: PRE5 isoform 1

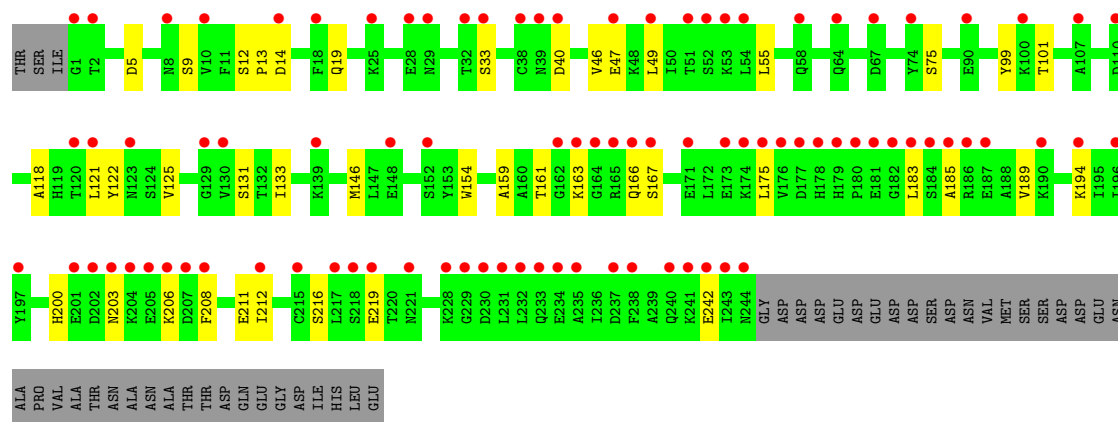




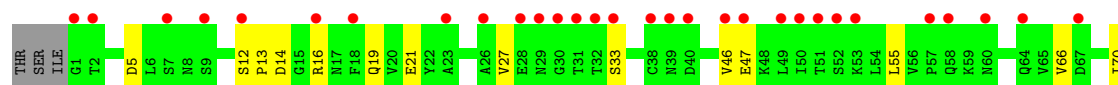
- Molecule 5: PRE5 isoform 1

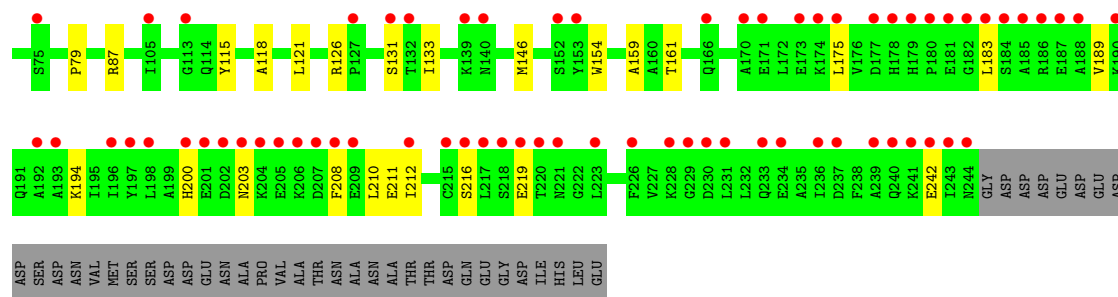


- Molecule 6: PRE10 isoform 1



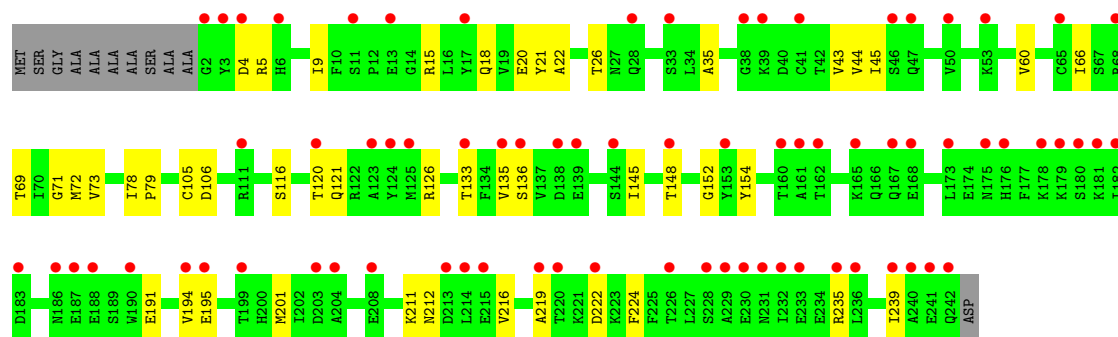
- Molecule 6: PRE10 isoform 1





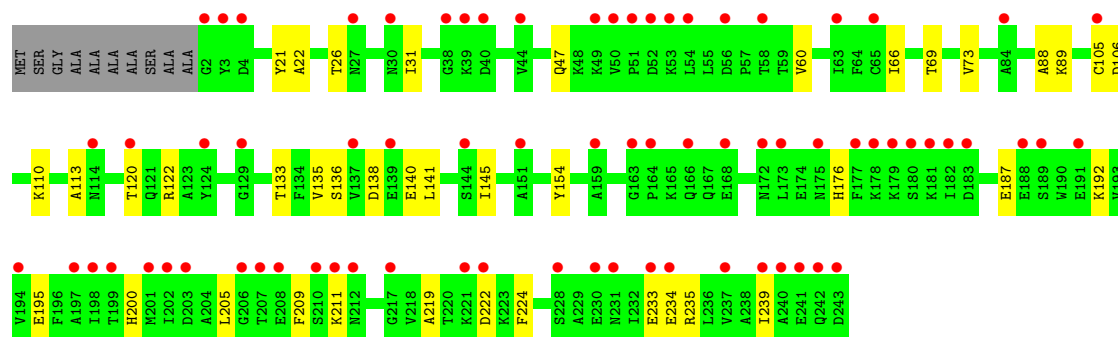
• Molecule 7: SCL1 isoform 1

Chain G: 30% 77% 18% .



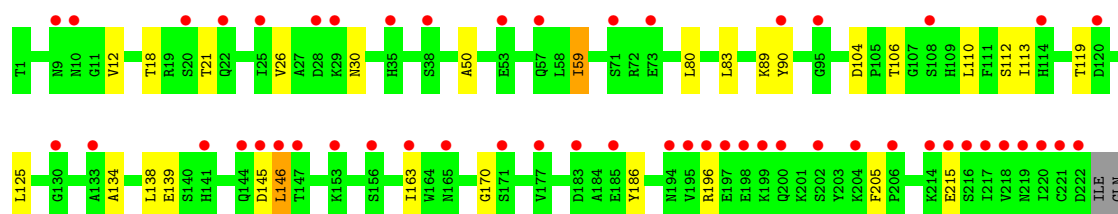
• Molecule 7: SCL1 isoform 1

Chain U: 29% 80% 16% .



• Molecule 8: proteasome endopeptidase complex

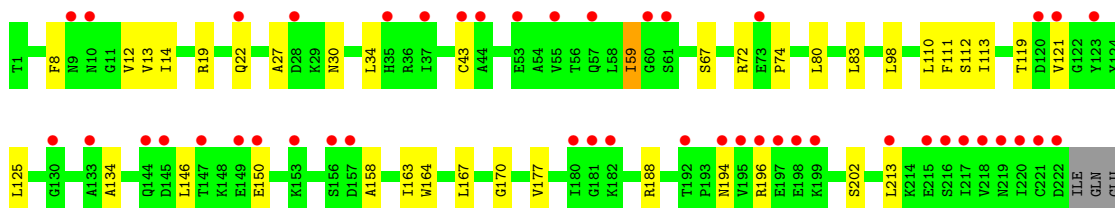
Chain H: 22% 83% 12% . .



GLU
GLN
VAL
ASP
ILE
THR
ALA

• Molecule 8: proteasome endopeptidase complex

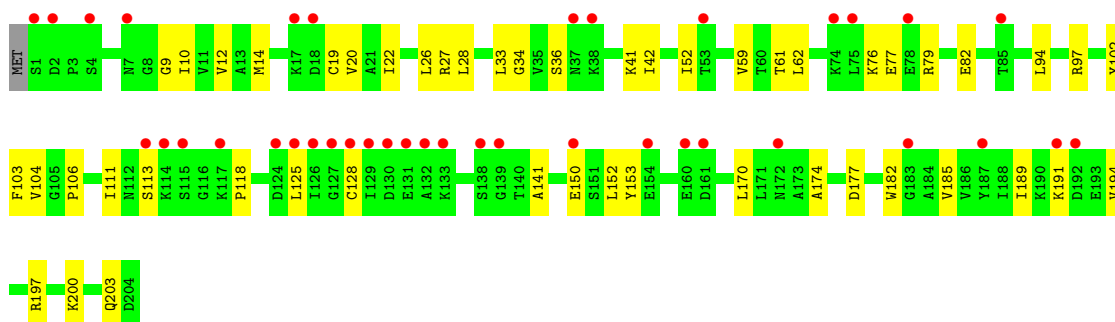
Chain V: 



GLU
GLN
VAL
ASP
ILE
THR
ALA

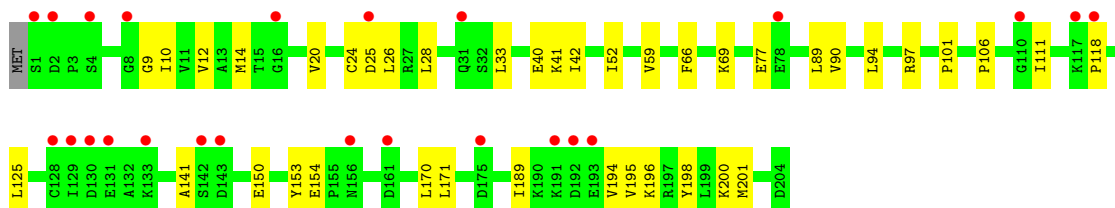
• Molecule 9: PUP3 isoform 1

Chain I: 



• Molecule 9: PUP3 isoform 1

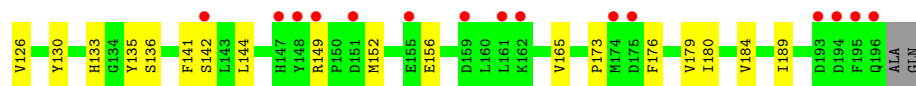
Chain W: 



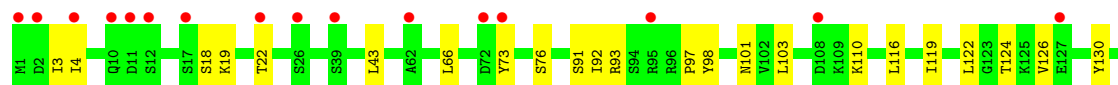
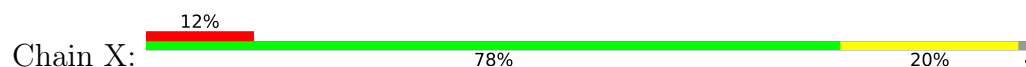
• Molecule 10: Proteasome subunit beta

Chain J: 





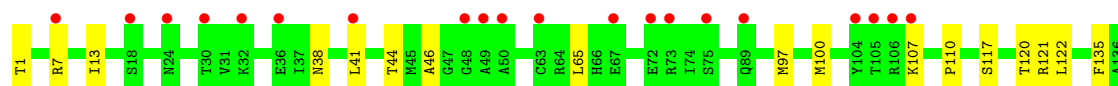
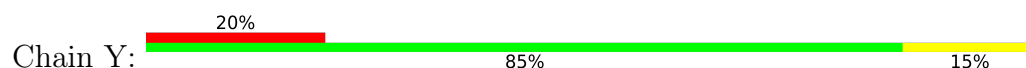
- Molecule 10: Proteasome subunit beta



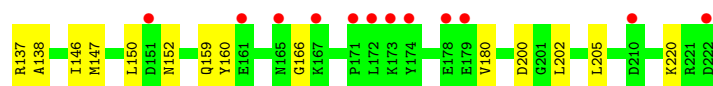
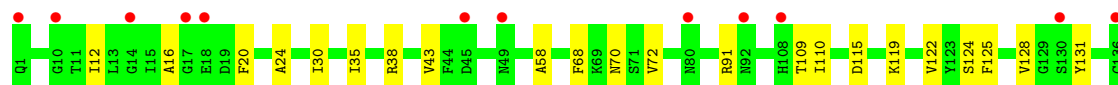
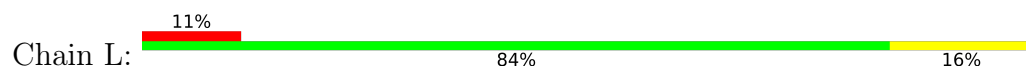
- Molecule 11: proteasome endopeptidase complex



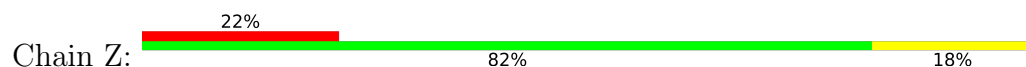
- Molecule 11: proteasome endopeptidase complex

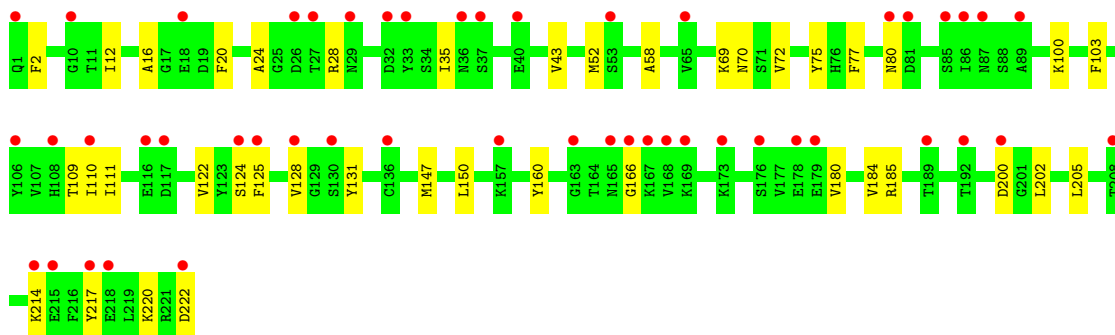


- Molecule 12: PRE7 isoform 1

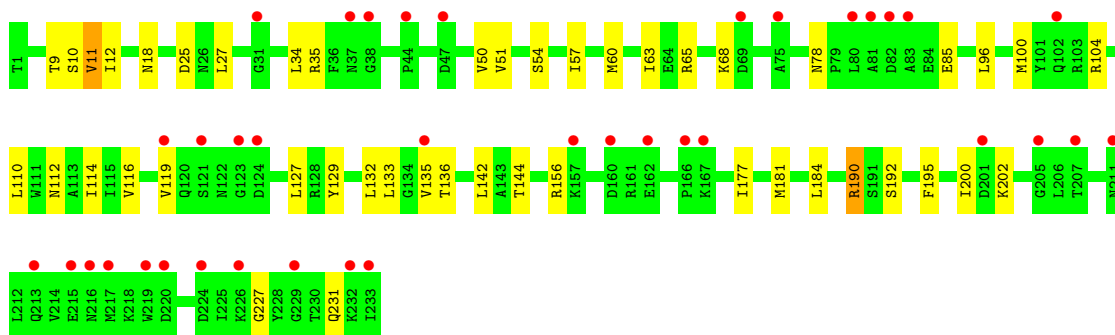
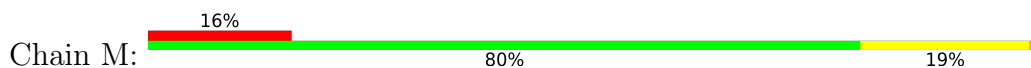


- Molecule 12: PRE7 isoform 1

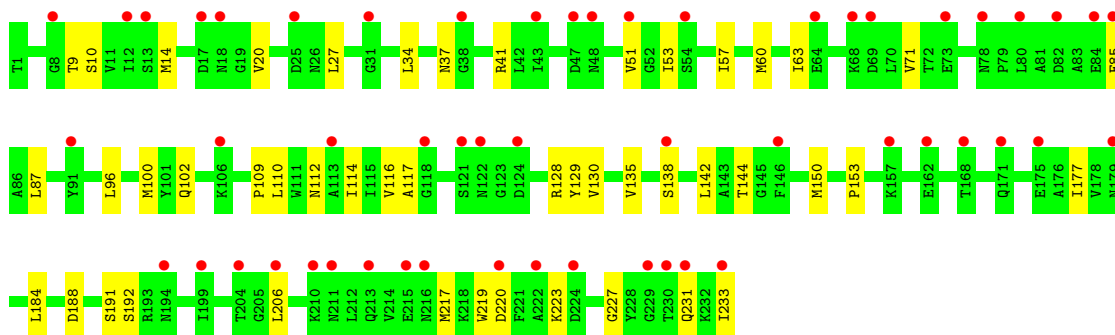
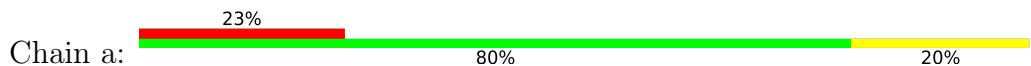




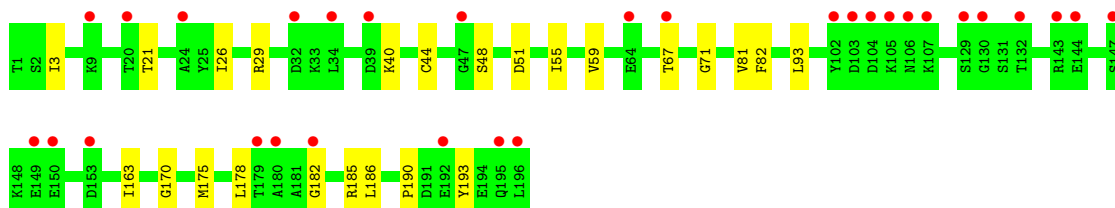
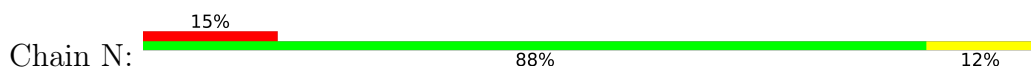
• Molecule 13: Proteasome subunit beta



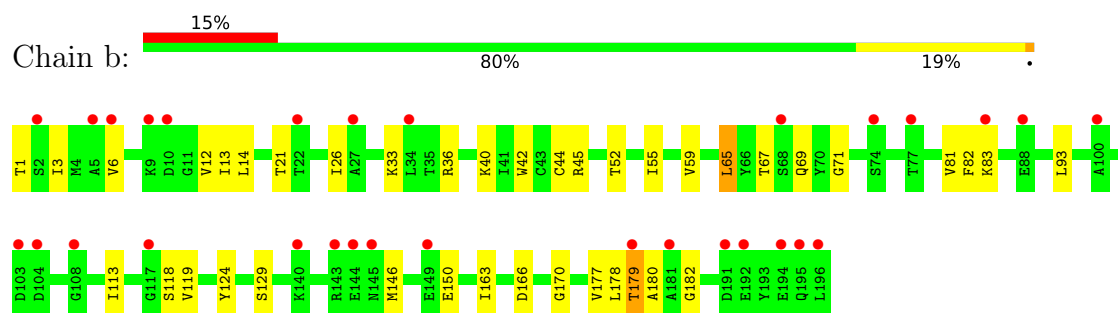
• Molecule 13: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta type-1



● Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.51Å 299.92Å 143.91Å 90.00° 108.46° 90.00°	Depositor
Resolution (Å)	49.11 – 3.33 49.11 – 3.33	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.11-3.33) 86.4 (49.11-3.33)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.200 , 0.252 0.201 , 0.252	Depositor DCC
R_{free} test set	6630 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	-19.1	Xtriage
Anisotropy	-2.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	49866	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG

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	0.10	0/1944	0.28	0/2632
1	O	0.10	0/1944	0.27	0/2632
2	B	0.10	0/1923	0.26	0/2600
2	P	0.10	0/1938	0.26	0/2619
3	C	0.11	0/1876	0.28	0/2538
3	Q	0.10	0/1903	0.29	0/2574
4	D	0.09	0/1861	0.27	0/2507
4	R	0.09	0/1875	0.25	0/2526
5	E	0.10	0/1797	0.28	0/2429
5	S	0.10	0/1811	0.28	0/2447
6	F	0.11	0/1936	0.27	0/2614
6	T	0.10	0/1934	0.27	0/2611
7	G	0.10	0/1945	0.26	0/2634
7	U	0.10	0/1951	0.26	0/2641
8	H	0.10	0/1715	0.27	0/2326
8	V	0.10	0/1711	0.27	0/2321
9	I	0.10	0/1611	0.29	0/2174
9	W	0.10	0/1611	0.29	0/2174
10	J	0.10	0/1598	0.29	0/2154
10	X	0.10	0/1589	0.29	0/2142
11	K	0.11	0/1681	0.28	0/2274
11	Y	0.10	0/1681	0.27	0/2274
12	L	0.10	0/1795	0.28	0/2420
12	Z	0.10	0/1795	0.29	0/2420
13	M	0.10	0/1855	0.28	0/2514
13	a	0.11	0/1855	0.30	0/2514
14	N	0.10	0/1541	0.26	0/2087
14	b	0.11	0/1541	0.29	0/2087
All	All	0.10	0/50217	0.28	0/67885

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1907	0	1917	25	0
1	O	1907	0	1917	32	0
2	B	1894	0	1897	26	0
2	P	1909	0	1918	26	0
3	C	1848	0	1862	35	0
3	Q	1875	0	1884	28	0
4	D	1836	0	1819	27	0
4	R	1850	0	1827	32	0
5	E	1770	0	1773	25	0
5	S	1784	0	1788	30	0
6	F	1896	0	1889	26	0
6	T	1894	0	1884	25	0
7	G	1907	0	1901	29	0
7	U	1913	0	1903	28	0
8	H	1684	0	1688	18	0
8	V	1680	0	1683	28	0
9	I	1581	0	1574	35	0
9	W	1581	0	1574	28	0
10	J	1570	0	1577	36	0
10	X	1561	0	1569	27	0
11	K	1644	0	1595	15	0
11	Y	1644	0	1595	19	0
12	L	1757	0	1711	23	0
12	Z	1757	0	1710	25	0
13	M	1824	0	1832	28	0
13	a	1824	0	1832	31	0
14	N	1512	0	1481	14	0
14	b	1512	0	1481	21	0
15	B	5	0	0	0	0
15	C	5	0	0	0	0
15	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	20	0	0	0	0
15	F	10	0	0	0	0
15	G	10	0	0	0	0
15	H	10	0	0	0	0
15	I	5	0	0	0	0
15	J	10	0	0	0	0
15	K	15	0	0	0	0
15	L	10	0	0	0	0
15	M	20	0	0	0	0
15	N	10	0	0	1	0
15	P	10	0	0	0	0
15	Q	5	0	0	0	0
15	R	5	0	0	1	0
15	S	10	0	0	0	0
15	T	5	0	0	0	0
15	U	5	0	0	0	0
15	V	5	0	0	0	0
15	X	5	0	0	0	0
15	Z	10	0	0	0	0
15	a	20	0	0	0	0
15	b	5	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	A	7	0	0	1	0
17	B	12	0	0	1	0
17	C	5	0	0	0	0
17	D	11	0	0	0	0
17	E	5	0	0	0	0
17	F	11	0	0	0	0
17	G	14	0	0	0	0
17	H	19	0	0	0	0
17	I	8	0	0	0	0
17	J	19	0	0	0	0
17	K	7	0	0	0	0
17	L	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	M	11	0	0	1	0
17	N	7	0	0	0	0
17	O	9	0	0	0	0
17	P	9	0	0	0	0
17	Q	2	0	0	0	0
17	R	9	0	0	0	0
17	S	12	0	0	0	0
17	T	10	0	0	0	0
17	U	11	0	0	0	0
17	V	8	0	0	0	0
17	W	16	0	0	0	0
17	X	13	0	0	0	0
17	Y	7	0	0	0	0
17	Z	21	0	0	0	0
17	a	27	0	0	0	0
17	b	15	0	0	0	0
All	All	49866	0	49081	639	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 6.

All (639) 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)
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.66	0.75
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.69	0.75
10:J:173:PRO:HB3	10:X:22:THR:HG21	1.69	0.75
3:C:79:ASP:HB3	3:C:127:PHE:HD1	1.55	0.71
4:D:96:ASP:HB2	12:L:91:ARG:HG3	1.72	0.71
14:b:40:LYS:HE2	14:b:182:GLY:HA2	1.72	0.71
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.74	0.70
4:R:161:ALA:HB3	5:S:55:LEU:HD13	1.73	0.69
4:R:140:ASP:OD2	4:R:146:GLN:NE2	2.26	0.69
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.74	0.69
10:J:1:MET:HE1	10:J:135:TYR:H	1.58	0.68
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.77	0.66
10:J:22:THR:HG21	10:X:173:PRO:HB3	1.76	0.66
8:V:19:ARG:HH11	8:V:170:GLY:HA3	1.61	0.66
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.77	0.66
10:J:19:LYS:HG2	10:J:180:ILE:HG13	1.78	0.65
6:F:194:LYS:HD2	6:F:242:GLU:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	1.80	0.64
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.81	0.63
10:J:152:MET:HE2	10:J:156:GLU:HB3	1.81	0.63
12:L:38:ARG:NH1	12:L:200:ASP:OD1	2.31	0.62
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.80	0.62
10:J:101:ASN:HB3	10:J:133:HIS:CE1	2.34	0.62
10:X:92:ILE:HG21	10:X:122:LEU:HA	1.81	0.62
3:C:131:THR:HG1	3:C:148:THR:HG1	1.47	0.62
13:M:35:ARG:NH1	15:N:201:SO4:O2	2.33	0.62
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.82	0.61
8:H:89:LYS:HE3	8:H:90:TYR:HE1	1.66	0.61
6:T:189:VAL:HG13	6:T:212:ILE:HG21	1.83	0.61
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.82	0.61
8:H:196:ARG:NH1	9:I:150:GLU:OE2	2.34	0.60
14:N:185:ARG:NH1	13:a:233:ILE:OXT	2.33	0.60
8:V:13:VAL:HG22	8:V:177:VAL:HG13	1.82	0.60
7:U:140:GLU:HB2	8:V:72:ARG:HH12	1.66	0.60
10:J:43:LEU:HB2	10:J:189:ILE:HD13	1.83	0.60
10:J:92:ILE:HG21	10:J:122:LEU:HA	1.82	0.60
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.82	0.60
13:a:9:THR:OG1	13:a:10:SER:N	2.32	0.60
3:C:169:VAL:HG13	3:C:196:SER:HB3	1.83	0.60
5:E:92:ASN:ND2	12:L:70:ASN:OD1	2.33	0.60
3:Q:87:ALA:HB1	3:Q:107:LEU:HD11	1.82	0.60
13:M:129:TYR:HE2	13:M:144:THR:HG22	1.67	0.60
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.83	0.60
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.84	0.60
12:Z:109:THR:HB	12:Z:125:PHE:HB2	1.82	0.60
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.84	0.59
3:Q:137:ASP:HB2	3:Q:140:ASP:HB3	1.83	0.59
9:I:61:THR:HG22	10:J:85:ARG:HH22	1.67	0.59
14:b:146:MET:HB3	14:b:150:GLU:HG3	1.85	0.59
4:R:174:GLU:OE1	4:R:198:GLN:NE2	2.33	0.59
6:T:175:LEU:HD12	6:T:183:LEU:HD11	1.84	0.59
6:F:40:ASP:OD2	6:F:216:SER:OG	2.21	0.59
11:K:1:THR:HG21	11:K:46:ALA:HA	1.85	0.59
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.85	0.59
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.85	0.59
12:L:109:THR:HB	12:L:125:PHE:HB2	1.85	0.59
3:Q:79:ASP:HB3	3:Q:127:PHE:HD1	1.68	0.58
7:U:31:ILE:HG23	7:U:47:GLN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:9:THR:OG1	13:M:10:SER:N	2.37	0.58
2:B:88:ASN:OD1	9:I:76:LYS:NZ	2.37	0.58
1:O:97:TYR:OH	9:W:77:GLU:OE2	2.15	0.58
9:W:97:ARG:HH22	10:X:93:ARG:HD3	1.68	0.58
10:X:3:ILE:HD12	10:X:136:SER:HB3	1.85	0.58
11:Y:1:THR:HG21	11:Y:46:ALA:HA	1.86	0.58
6:F:33:SER:HG	6:F:75:SER:HG	1.51	0.58
2:B:82:ASP:HB3	2:B:130:PHE:HD1	1.68	0.58
5:E:6:ASP:O	5:E:20:GLN:NE2	2.37	0.58
10:J:86:GLN:HG2	10:J:90:LYS:HE3	1.86	0.58
2:P:176:GLN:HG2	3:Q:52:LEU:HD13	1.86	0.58
8:V:213:LEU:HD21	9:W:200:LYS:HE3	1.84	0.57
13:a:227:GLY:HA3	13:a:231:GLN:HB3	1.85	0.57
2:P:205:LEU:HD11	2:P:210:LEU:HD21	1.86	0.57
12:L:24:ALA:HB1	12:L:202:LEU:HD11	1.86	0.57
6:F:189:VAL:HG13	6:F:212:ILE:HG21	1.87	0.57
2:B:3:ARG:HH12	4:D:3:GLY:HA2	1.70	0.57
9:W:14:MET:HE3	9:W:153:TYR:HD1	1.70	0.57
7:G:148:THR:HG22	7:G:154:TYR:HB2	1.85	0.57
3:Q:198:LEU:HA	3:Q:201:VAL:HG22	1.87	0.57
10:X:184:VAL:HG22	10:X:189:ILE:HG12	1.87	0.57
3:C:35:LYS:HD2	3:C:158:SER:HA	1.86	0.57
3:Q:161:THR:HG21	3:Q:169:VAL:HB	1.87	0.57
8:H:104:ASP:OD1	8:H:106:THR:OG1	2.18	0.56
13:a:96:LEU:O	13:a:100:MET:HG2	2.05	0.56
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.87	0.56
3:Q:6:LEU:O	4:R:0:TYR:OH	2.15	0.56
5:S:71:LEU:HD13	5:S:131:LEU:HD22	1.88	0.56
11:Y:97:MET:N	11:Y:117:SER:OG	2.37	0.56
1:A:122:THR:HG22	1:A:129:PRO:HB3	1.87	0.56
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.70	0.56
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.88	0.56
5:S:144:LEU:HD22	5:S:152:VAL:HG12	1.88	0.56
3:Q:169:VAL:HG13	3:Q:196:SER:HB2	1.89	0.55
5:E:38:ARG:NH1	5:E:39:SER:O	2.40	0.55
1:O:81:ASP:HB3	1:O:130:PHE:HD1	1.71	0.55
10:J:4:ILE:HG22	10:J:103:LEU:HD12	1.88	0.55
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.89	0.55
6:F:146:MET:HE2	6:F:159:ALA:HB1	1.88	0.55
5:E:174:THR:HG22	5:E:177:THR:HB	1.88	0.55
10:J:1:MET:HE1	10:J:135:TYR:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HG	1:A:232:GLY:HA2	1.89	0.55
7:U:69:THR:HG22	7:U:222:ASP:HA	1.89	0.55
4:D:193:LEU:HD22	4:D:204:LEU:HD21	1.89	0.55
1:A:118:MET:HE2	1:A:152:PRO:HA	1.89	0.54
5:E:47:ALA:HB3	5:E:211:SER:HB3	1.89	0.54
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.90	0.54
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.89	0.54
2:P:212:PHE:HB3	2:P:229:PHE:HB2	1.90	0.54
11:Y:44:THR:HG21	11:Y:100:MET:HE3	1.90	0.54
5:E:49:LYS:HB3	5:E:58:TYR:O	2.07	0.54
7:G:135:VAL:HG12	7:G:145:ILE:HG12	1.89	0.54
2:P:119:GLN:NE2	2:P:123:GLN:OE1	2.40	0.54
11:Y:159:ARG:HH12	11:Y:163:ALA:HB2	1.73	0.54
13:a:41:ARG:NH1	13:a:53:ILE:O	2.41	0.54
4:D:158:ARG:O	5:E:57:SER:N	2.41	0.54
7:U:205:LEU:HD12	7:U:209:PHE:HZ	1.72	0.54
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.90	0.54
1:A:211:LEU:HD22	1:A:238:LEU:HD22	1.90	0.54
4:D:140:ASP:OD2	4:D:146:GLN:NE2	2.40	0.54
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.89	0.53
4:D:89:VAL:HG21	11:K:65:LEU:HG	1.91	0.53
14:b:59:VAL:HG22	14:b:81:VAL:HG12	1.89	0.53
14:b:65:LEU:O	14:b:69:GLN:HG2	2.09	0.53
1:O:21:ILE:HD12	1:O:153:SER:HA	1.90	0.53
9:I:113:SER:HA	9:I:191:LYS:HE3	1.90	0.53
1:O:211:LEU:HD22	1:O:238:LEU:HD22	1.89	0.53
12:L:152:ASN:O	12:L:159:GLN:NE2	2.39	0.53
11:K:18:SER:OG	11:K:174:SER:N	2.42	0.53
10:X:92:ILE:HG21	10:X:122:LEU:HD23	1.90	0.53
6:F:5:ASP:O	6:F:19:GLN:NE2	2.41	0.53
1:O:122:THR:HG22	1:O:129:PRO:HB3	1.90	0.53
6:F:133:ILE:HG12	6:F:146:MET:HG3	1.89	0.53
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.90	0.53
3:C:92:GLN:HG3	10:J:66:LEU:HB2	1.91	0.53
5:S:174:THR:HG22	5:S:177:THR:HB	1.91	0.53
11:Y:38:ASN:ND2	11:Y:41:LEU:HB2	2.24	0.52
2:P:63:GLU:HG3	2:P:64:LYS:HG2	1.90	0.52
10:J:29:LYS:HD3	11:K:122:LEU:HD22	1.90	0.52
3:C:40:VAL:HG22	3:C:143:PRO:HB3	1.91	0.52
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.44	0.52
4:R:44:LYS:HB2	4:R:208:ASN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:92:ILE:HA	10:X:97:PRO:HB3	1.91	0.52
2:B:63:GLU:HG3	2:B:64:LYS:HG2	1.91	0.52
3:C:96:LEU:HD11	10:J:58:GLU:HB3	1.91	0.52
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.45	0.52
9:W:12:VAL:HG12	9:W:170:LEU:HD12	1.92	0.52
6:F:12:SER:OG	6:F:14:ASP:OD1	2.26	0.52
2:P:6:ASP:HB3	3:Q:4:ARG:HH11	1.75	0.52
2:P:49:ARG:NH1	2:P:61:SER:OG	2.42	0.52
3:Q:47:ARG:O	3:Q:207:ASN:ND2	2.42	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.52
9:I:189:ILE:HG23	9:I:194:VAL:HG22	1.91	0.52
12:L:38:ARG:NH2	8:V:164:TRP:O	2.41	0.52
1:O:118:MET:O	1:O:122:THR:HG23	2.09	0.52
2:P:106:PRO:HD2	2:P:109:ILE:HD12	1.92	0.52
6:T:118:ALA:HA	6:T:121:LEU:HD12	1.92	0.52
10:J:184:VAL:HG22	10:J:189:ILE:HG12	1.92	0.52
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.91	0.52
9:I:33:LEU:HD11	10:J:141:PHE:HD2	1.75	0.51
11:K:200:VAL:O	11:K:204:GLU:HB2	2.10	0.51
14:N:21:THR:HG22	14:N:26:ILE:HA	1.92	0.51
3:C:55:THR:HA	3:C:58:THR:HG22	1.91	0.51
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.76	0.51
3:Q:198:LEU:HD11	3:Q:231:VAL:HG23	1.91	0.51
5:S:49:LYS:O	5:S:209:ASN:ND2	2.42	0.51
13:M:96:LEU:O	13:M:100:MET:HG2	2.09	0.51
13:a:27:LEU:HB2	13:a:192:SER:HB2	1.91	0.51
1:O:149:GLN:O	1:O:156:TYR:HA	2.11	0.51
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.92	0.51
4:R:203:LYS:O	4:R:208:ASN:ND2	2.39	0.51
10:J:142:SER:OG	11:Y:135:PHE:HB3	2.10	0.51
7:G:69:THR:HG22	7:G:222:ASP:HA	1.92	0.51
3:C:64:LYS:HA	3:C:70:VAL:HG23	1.93	0.51
11:K:38:ASN:ND2	11:K:41:LEU:HB2	2.26	0.51
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.92	0.51
14:b:179:THR:HG22	14:b:180:ALA:H	1.76	0.51
5:E:71:LEU:HD13	5:E:131:LEU:HD22	1.93	0.51
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.92	0.51
12:L:147:MET:HA	12:L:150:LEU:HD12	1.93	0.51
6:F:47:GLU:HG3	6:F:208:PHE:HB2	1.93	0.51
7:G:15:ARG:NH2	7:G:20:GLU:OE1	2.37	0.51
7:U:138:ASP:OD2	8:V:72:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:160:TYR:CG	12:L:166:GLY:HA2	2.46	0.51
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.93	0.51
4:D:23:ILE:HD13	4:D:133:ALA:HB2	1.93	0.51
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.93	0.51
13:M:63:ILE:HD13	13:M:114:ILE:HD11	1.93	0.51
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.92	0.51
11:Y:200:VAL:O	11:Y:204:GLU:HB2	2.10	0.51
5:E:139:SER:HB2	5:E:142:HIS:NE2	2.25	0.51
11:Y:7:ARG:HD2	11:Y:110:PRO:HG2	1.92	0.51
14:b:163:ILE:HG23	14:b:170:GLY:HA2	1.93	0.51
5:S:100:ARG:NH2	13:a:85:GLU:O	2.43	0.50
10:J:165:VAL:HG21	10:J:179:VAL:HG21	1.93	0.50
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.93	0.50
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.93	0.50
6:F:118:ALA:HA	6:F:121:LEU:HD12	1.93	0.50
3:Q:195:ARG:O	3:Q:199:GLU:HG2	2.11	0.50
4:R:23:ILE:HD13	4:R:133:ALA:HB2	1.92	0.50
10:X:19:LYS:HG2	10:X:180:ILE:HG13	1.93	0.50
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.47	0.50
2:B:176:GLN:NE2	17:B:401:HOH:O	2.37	0.50
6:F:163:LYS:HD3	6:F:203:ASN:HD21	1.75	0.50
10:J:58:GLU:OE1	11:K:81:LYS:NZ	2.43	0.50
5:S:92:ASN:ND2	12:Z:70:ASN:OD1	2.44	0.50
9:I:19:CYS:HA	9:I:111:ILE:HD11	1.93	0.50
12:L:124:SER:O	12:L:131:TYR:HA	2.12	0.50
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.93	0.50
5:E:45:LEU:HB2	5:E:213:ALA:HB3	1.94	0.50
12:Z:58:ALA:HB3	13:a:135:VAL:HG13	1.93	0.50
4:D:175:LEU:HD13	4:D:195:ILE:HD12	1.93	0.50
12:L:20:PHE:HE2	12:L:180:VAL:HG21	1.75	0.50
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.93	0.50
1:A:176:GLU:HG2	2:B:55:LEU:HG	1.93	0.50
6:T:146:MET:HE2	6:T:159:ALA:HB1	1.93	0.50
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.94	0.49
8:V:134:ALA:HB1	8:V:158:ALA:HB1	1.92	0.49
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.94	0.49
1:O:111:VAL:HG22	1:O:136:ILE:HD12	1.94	0.49
7:U:211:LYS:HB3	7:U:233:GLU:HB2	1.94	0.49
8:H:59:ILE:HG12	8:H:83:LEU:HG	1.94	0.49
8:H:89:LYS:HE3	8:H:90:TYR:CE1	2.47	0.49
9:I:26:LEU:HD11	9:I:185:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:58:ALA:HB3	13:M:135:VAL:HG13	1.94	0.49
6:F:200:HIS:CE1	6:F:208:PHE:HB3	2.47	0.49
7:G:195:GLU:HA	7:G:239:ILE:HD11	1.95	0.49
5:S:47:ALA:HB3	5:S:211:SER:HB2	1.94	0.49
6:T:133:ILE:HG12	6:T:146:MET:HG3	1.95	0.49
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.94	0.49
10:J:46:PHE:HD2	10:J:53:THR:HB	1.76	0.49
3:C:99:GLU:OE2	11:K:121:ARG:NH1	2.39	0.49
7:G:4:ASP:HA	7:G:9:ILE:HD11	1.95	0.49
7:U:195:GLU:OE2	7:U:235:ARG:NH1	2.44	0.49
14:N:59:VAL:HG22	14:N:81:VAL:HG12	1.95	0.49
10:X:91:SER:HB3	10:X:98:TYR:H	1.78	0.49
4:D:114:ARG:HE	4:D:125:LEU:HD22	1.77	0.49
11:K:13:ILE:HG13	11:K:153:ALA:HB1	1.94	0.49
13:M:57:ILE:HG23	13:M:60:MET:HE2	1.94	0.49
2:B:44:VAL:HG22	2:B:214:THR:HG22	1.94	0.49
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.94	0.49
10:X:43:LEU:HB2	10:X:189:ILE:HD13	1.94	0.49
11:Y:165:ALA:HB1	11:Y:172:GLY:HA2	1.95	0.49
12:Z:20:PHE:HE2	12:Z:180:VAL:HG21	1.77	0.49
10:J:37:GLN:HG3	10:J:189:ILE:HD12	1.94	0.49
10:X:152:MET:HE2	10:X:156:GLU:HB3	1.93	0.49
3:C:16:PHE:HB2	4:D:0:TYR:OH	2.13	0.48
3:Q:228:ASN:HA	3:Q:231:VAL:HG12	1.95	0.48
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.48	0.48
12:L:43:VAL:HG12	12:L:205:LEU:HD12	1.93	0.48
9:W:125:LEU:H	9:W:125:LEU:HD23	1.78	0.48
13:a:53:ILE:HD12	13:a:60:MET:HG3	1.95	0.48
6:T:194:LYS:HD2	6:T:242:GLU:HG3	1.94	0.48
8:V:59:ILE:HG12	8:V:83:LEU:HG	1.95	0.48
3:C:61:LYS:NZ	3:C:73:PHE:O	2.46	0.48
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.95	0.48
6:T:14:ASP:CG	6:T:16:ARG:HD3	2.38	0.48
13:M:18:ASN:HA	13:M:202:LYS:HE2	1.95	0.48
3:C:195:ARG:HG2	3:C:234:ILE:HG21	1.95	0.48
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.94	0.48
2:B:8:ARG:HD3	3:C:4:ARG:CZ	2.44	0.48
6:F:131:SER:HB3	6:F:161:THR:HG21	1.95	0.48
5:S:194:GLU:O	5:S:198:GLN:HG2	2.14	0.48
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.95	0.48
12:L:220:LYS:HE3	8:V:194:ASN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:ALA:HB1	3:C:173:LEU:HD13	1.96	0.48
7:G:45:ILE:HG22	7:G:216:VAL:HG22	1.95	0.48
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.95	0.48
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.94	0.48
9:W:171:LEU:HD22	9:W:201:MET:HB3	1.96	0.48
7:G:5:ARG:O	7:G:18:GLN:NE2	2.43	0.48
9:W:28:LEU:HD22	10:X:126:VAL:HG11	1.96	0.48
7:G:195:GLU:OE2	7:G:235:ARG:NH1	2.47	0.48
4:R:77:ALA:O	4:R:81:ILE:HG12	2.14	0.48
6:T:46:VAL:HG12	6:T:211:GLU:HB3	1.95	0.48
14:N:67:THR:HA	14:N:71:GLY:O	2.14	0.48
14:N:190:PRO:HB2	13:a:217:MET:HE1	1.95	0.48
2:P:3:ARG:NH2	4:R:1:ASP:O	2.46	0.48
8:H:139:GLU:OE1	14:N:29:ARG:NH2	2.47	0.48
1:A:114:VAL:O	1:A:118:MET:HG3	2.14	0.48
3:C:4:ARG:NH2	4:D:0:TYR:O	2.44	0.48
3:C:191:LYS:HG3	3:C:234:ILE:HD11	1.95	0.48
7:U:219:ALA:HB2	7:U:224:PHE:HD1	1.79	0.48
8:V:14:ILE:HD12	8:V:34:LEU:HD22	1.96	0.48
10:X:101:ASN:HB3	10:X:133:HIS:CE1	2.48	0.48
4:R:158:ARG:O	5:S:57:SER:N	2.47	0.47
1:A:74:VAL:HG12	1:A:135:LEU:HB2	1.94	0.47
5:S:155:LEU:HD13	5:S:158:THR:HB	1.95	0.47
6:T:16:ARG:NH2	6:T:21:GLU:OE1	2.47	0.47
9:I:14:MET:HE3	9:I:153:TYR:HD1	1.79	0.47
2:P:124:HIS:HB3	3:Q:124:VAL:HG23	1.95	0.47
6:T:47:GLU:HG3	6:T:208:PHE:HB2	1.95	0.47
10:J:130:TYR:HB2	10:J:144:LEU:HD13	1.96	0.47
2:B:154:GLY:O	3:C:81:ARG:NH2	2.42	0.47
3:C:65:ILE:HG21	3:C:107:LEU:HD21	1.96	0.47
12:L:115:ASP:OD1	12:L:119:LYS:N	2.47	0.47
4:D:113:LEU:HD12	4:D:115:PHE:HE1	1.80	0.47
1:O:2:THR:HG21	1:O:4:ARG:HH11	1.80	0.47
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.50	0.47
2:P:26:GLU:O	2:P:29:SER:OG	2.23	0.47
4:R:97:GLU:OE2	12:Z:75:TYR:OH	2.26	0.47
4:R:163:ALA:N	4:R:172:GLN:OE1	2.47	0.47
9:I:103:PHE:HA	9:I:125:LEU:HD22	1.96	0.47
14:N:40:LYS:HE2	14:N:182:GLY:HA2	1.97	0.47
8:V:111:PHE:HD1	8:V:121:VAL:HG12	1.79	0.47
9:W:14:MET:HE3	9:W:153:TYR:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:2:PHE:CD1	13:a:109:PRO:HG3	2.50	0.47
13:a:51:VAL:HG13	13:a:114:ILE:HG23	1.96	0.47
1:A:118:MET:O	1:A:122:THR:HG23	2.14	0.47
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.97	0.47
8:H:12:VAL:HG21	8:H:110:LEU:HB2	1.97	0.47
1:A:108:LYS:NZ	17:A:301:HOH:O	2.47	0.47
1:A:189:ILE:HD11	1:A:213:ILE:HG21	1.95	0.47
3:Q:92:GLN:HG3	10:X:66:LEU:HB2	1.97	0.47
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.96	0.47
9:I:33:LEU:HD11	10:J:141:PHE:CD2	2.50	0.47
12:L:35:ILE:O	13:M:156:ARG:NH2	2.44	0.47
9:W:189:ILE:HG23	9:W:194:VAL:HG22	1.96	0.47
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.97	0.47
13:a:220:ASP:OD2	13:a:223:LYS:NZ	2.45	0.47
1:O:106:PRO:HG2	1:O:109:LEU:HD23	1.97	0.46
2:P:216:ARG:HG2	2:P:217:LYS:H	1.80	0.46
7:U:140:GLU:HB2	8:V:72:ARG:NH1	2.30	0.46
10:J:9:VAL:O	10:J:11:ASP:N	2.41	0.46
1:A:64:VAL:HB	1:A:237:LYS:HZ1	1.80	0.46
12:Z:12:ILE:HG13	12:Z:110:ILE:HD12	1.97	0.46
2:B:86:LEU:HB3	2:B:114:LEU:HD11	1.97	0.46
1:O:3:ASP:OD2	7:U:122:ARG:NH2	2.45	0.46
4:R:157:TYR:CE2	5:S:59:GLN:HG3	2.51	0.46
8:V:202:SER:OG	9:W:154:GLU:OE2	2.30	0.46
5:E:181:ILE:HB	5:E:188:LEU:HD13	1.97	0.46
7:G:191:GLU:HB3	7:G:235:ARG:NH1	2.30	0.46
7:U:106:ASP:OD1	7:U:106:ASP:N	2.48	0.46
12:L:124:SER:HB2	12:L:137:ARG:HG2	1.98	0.46
13:M:12:ILE:HD11	13:M:177:ILE:HG23	1.96	0.46
9:I:77:GLU:HG2	9:I:79:ARG:HG2	1.98	0.46
9:I:203:GLN:HG3	11:Y:197:PHE:CE1	2.51	0.46
12:Z:184:VAL:HG12	12:Z:202:LEU:HD21	1.98	0.46
4:D:159:TYR:CG	4:D:162:LYS:HB2	2.51	0.46
5:E:35:VAL:HG22	5:E:46:VAL:HB	1.97	0.46
4:R:109:CYS:SG	4:R:156:PHE:HB3	2.56	0.46
7:U:195:GLU:HA	7:U:239:ILE:HD11	1.97	0.46
10:J:3:ILE:HB	10:J:18:SER:HB3	1.97	0.46
13:M:50:VAL:HG23	13:M:200:ILE:HD11	1.97	0.46
14:b:3:ILE:HB	14:b:44:CYS:HB3	1.96	0.46
14:b:12:VAL:HG12	14:b:178:LEU:HB2	1.97	0.46
1:A:21:ILE:HD12	1:A:153:SER:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:SER:HB3	2:B:154:GLY:O	2.15	0.46
5:E:155:LEU:HD23	6:F:55:LEU:HA	1.97	0.46
14:b:59:VAL:HG11	14:b:82:PHE:CE2	2.50	0.46
4:R:28:THR:HG21	4:R:199:VAL:HG21	1.97	0.46
5:S:149:SER:O	6:T:79:PRO:HG2	2.15	0.46
14:b:21:THR:HG22	14:b:26:ILE:HA	1.98	0.46
2:B:75:ALA:HB3	2:B:135:ILE:HB	1.97	0.46
4:D:159:TYR:CE2	4:D:162:LYS:HD3	2.51	0.46
7:U:66:ILE:HA	7:U:89:LYS:HG2	1.98	0.46
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.97	0.46
1:O:222:LEU:HG	1:O:232:GLY:HA2	1.97	0.45
5:S:163:ARG:NH1	5:S:203:GLU:OE2	2.49	0.45
13:a:128:ARG:HG3	13:a:138:SER:HB3	1.97	0.45
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.51	0.45
7:G:211:LYS:HG3	7:G:212:ASN:OD1	2.16	0.45
2:P:90:ALA:HB1	2:P:110:LEU:HD21	1.97	0.45
11:Y:159:ARG:NH1	11:Y:163:ALA:HB2	2.30	0.45
13:a:110:LEU:O	13:a:112:ASN:N	2.49	0.45
4:D:73:LEU:HD12	4:D:131:GLY:HA3	1.98	0.45
8:V:111:PHE:CD1	8:V:121:VAL:HG12	2.51	0.45
2:B:9:THR:HB	2:B:20:GLN:HG3	1.99	0.45
13:M:129:TYR:CE2	13:M:144:THR:HG22	2.50	0.45
13:a:57:ILE:HG23	13:a:60:MET:HE2	1.99	0.45
3:C:190:VAL:O	3:C:194:VAL:HG22	2.16	0.45
4:R:146:GLN:HG2	4:R:158:ARG:CZ	2.47	0.45
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.98	0.45
5:S:155:LEU:HD23	6:T:55:LEU:HA	1.98	0.45
4:D:44:LYS:HB3	4:D:56:ILE:HD12	1.99	0.45
5:E:226:GLY:O	5:E:229:VAL:HG22	2.17	0.45
1:O:71:ILE:HG21	1:O:110:LEU:HD23	1.99	0.45
7:U:135:VAL:HG12	7:U:145:ILE:HG12	1.98	0.45
14:b:67:THR:HA	14:b:71:GLY:O	2.17	0.45
14:b:83:LYS:HE3	14:b:83:LYS:HB3	1.84	0.45
6:F:46:VAL:HG12	6:F:211:GLU:HB3	1.98	0.45
1:O:83:ARG:HD2	7:U:110:LYS:HE3	1.98	0.45
5:S:6:ASP:O	5:S:20:GLN:NE2	2.49	0.45
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.52	0.45
10:J:46:PHE:CD2	10:J:53:THR:HB	2.52	0.45
10:J:96:ARG:NH1	11:K:91:LYS:HD3	2.32	0.45
1:A:64:VAL:HB	1:A:237:LYS:NZ	2.31	0.45
13:M:78:ASN:HD21	13:M:85:GLU:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:24:CYS:HB3	9:W:42:ILE:HD11	1.97	0.45
3:Q:232:THR:O	3:Q:235:GLU:HG3	2.17	0.45
8:V:196:ARG:NH1	9:W:150:GLU:OE2	2.50	0.45
4:R:114:ARG:HG2	4:R:125:LEU:HD22	1.99	0.44
7:U:22:ALA:O	7:U:26:THR:HG23	2.18	0.44
8:H:215:GLU:HG3	9:I:197:ARG:HG2	1.99	0.44
13:M:25:ASP:HA	13:M:195:PHE:HA	1.99	0.44
12:Z:43:VAL:HG12	12:Z:205:LEU:HD12	1.99	0.44
14:b:13:ILE:HG12	14:b:177:VAL:HG13	1.99	0.44
2:B:225:TYR:CE2	2:B:227:LYS:HB2	2.52	0.44
7:G:73:VAL:HG13	7:G:133:THR:HB	1.98	0.44
8:H:21:THR:HG22	8:H:26:VAL:HA	1.99	0.44
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.99	0.44
9:W:69:LYS:HD3	9:W:89:LEU:HD11	1.99	0.44
2:B:6:ASP:HB3	3:C:4:ARG:HH11	1.83	0.44
2:B:49:ARG:NH1	2:B:61:SER:OG	2.48	0.44
2:B:146:GLN:HB3	2:B:148:TYR:CE1	2.52	0.44
2:B:215:ILE:HG12	2:B:226:GLN:HG3	1.99	0.44
5:S:62:ILE:HA	5:S:72:SER:HA	1.98	0.44
7:U:73:VAL:HG13	7:U:133:THR:HB	1.99	0.44
9:I:200:LYS:HE3	11:Y:198:TRP:CD1	2.52	0.44
10:X:165:VAL:HG21	10:X:179:VAL:HG21	2.00	0.44
6:F:154:TRP:CZ3	7:G:60:VAL:HA	2.52	0.44
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.53	0.44
4:R:8:SER:N	4:R:12:ARG:O	2.42	0.44
4:R:44:LYS:HB3	4:R:56:ILE:HD12	2.00	0.44
9:W:196:LYS:HE2	9:W:198:TYR:CE1	2.53	0.44
1:A:226:GLY:HA3	8:H:186:TYR:HB3	1.99	0.44
4:D:77:ALA:O	4:D:81:ILE:HG12	2.17	0.44
4:D:158:ARG:HB3	5:E:57:SER:HB3	2.00	0.44
7:G:45:ILE:HD12	7:G:201:MET:HE2	1.99	0.44
4:R:102:GLU:OE1	12:Z:80:ASN:ND2	2.51	0.44
6:F:175:LEU:HD22	6:F:183:LEU:HD21	2.00	0.44
1:O:66:LEU:HD12	1:O:235:PHE:CD1	2.53	0.44
1:O:174:PHE:O	1:O:177:LYS:HG2	2.18	0.44
3:Q:159:ALA:HB1	3:Q:173:LEU:HD13	1.99	0.44
11:K:44:THR:HG21	11:K:100:MET:HE3	2.00	0.44
12:L:138:ALA:HB3	12:L:147:MET:HG2	1.99	0.44
13:M:190:ARG:HG3	17:M:408:HOH:O	2.17	0.44
2:B:122:THR:HG22	2:B:129:PRO:HB3	1.99	0.44
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:129:TYR:HE2	13:a:144:THR:HG22	1.82	0.44
1:A:94:HIS:HA	1:A:98:LYS:HB3	1.99	0.44
3:Q:99:GLU:OE2	11:Y:121:ARG:NH1	2.44	0.44
4:R:90:THR:OG1	15:R:301:SO4:O1	2.36	0.44
9:I:28:LEU:HD22	10:J:126:VAL:HG11	1.98	0.44
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.99	0.44
8:V:30:ASN:O	8:V:188:ARG:NH2	2.48	0.44
12:Z:28:ARG:NE	12:Z:200:ASP:OD1	2.51	0.44
13:a:71:VAL:HG22	13:a:87:LEU:HD12	2.00	0.44
13:a:217:MET:HB3	13:a:219:TRP:CD1	2.52	0.44
6:F:185:ALA:HB3	6:F:219:GLU:HG3	1.99	0.43
3:Q:55:THR:HA	3:Q:58:THR:HG22	1.99	0.43
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.43
12:Z:100:LYS:HB3	12:Z:103:PHE:O	2.18	0.43
3:C:161:THR:HG21	3:C:169:VAL:HB	1.99	0.43
5:E:155:LEU:HD13	5:E:158:THR:HB	1.99	0.43
1:O:114:VAL:O	1:O:118:MET:HG3	2.17	0.43
2:P:14:PRO:HA	3:Q:20:TYR:CD1	2.54	0.43
2:P:149:THR:O	2:P:156:TYR:HA	2.17	0.43
4:R:8:SER:OG	4:R:10:GLU:OE1	2.36	0.43
10:J:92:ILE:HA	10:J:97:PRO:HB3	2.00	0.43
9:W:111:ILE:HD13	9:W:118:PRO:HA	2.00	0.43
11:Y:13:ILE:HG13	11:Y:153:ALA:HB1	1.99	0.43
12:Z:28:ARG:HH21	12:Z:35:ILE:HD11	1.83	0.43
13:a:63:ILE:HD11	13:a:110:LEU:HD13	2.00	0.43
4:D:189:GLU:OE2	4:D:223:TYR:OH	2.31	0.43
3:Q:46:ARG:NH2	3:Q:209:GLU:OE2	2.51	0.43
9:I:97:ARG:HD3	9:I:102:TYR:CE2	2.54	0.43
14:b:6:VAL:HG22	14:b:124:TYR:HB2	2.00	0.43
3:C:228:ASN:HA	3:C:231:VAL:HG22	2.00	0.43
7:G:219:ALA:HB2	7:G:224:PHE:HD1	1.83	0.43
4:R:197:LYS:NZ	4:R:239:GLU:OE1	2.37	0.43
6:T:12:SER:OG	6:T:14:ASP:OD1	2.22	0.43
14:N:59:VAL:HG11	14:N:82:PHE:CE2	2.53	0.43
8:V:12:VAL:HG21	8:V:110:LEU:HB2	2.00	0.43
2:P:146:GLN:HB3	2:P:148:TYR:CE1	2.53	0.43
12:Z:28:ARG:HH22	12:Z:222:ASP:C	2.27	0.43
14:b:55:ILE:HD11	14:b:93:LEU:HD13	1.99	0.43
14:b:113:ILE:HA	14:b:118:SER:O	2.18	0.43
6:F:166:GLN:HG3	6:F:167:SER:H	1.84	0.43
6:T:131:SER:HB3	6:T:161:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.53	0.43
1:O:74:VAL:HG22	1:O:75:TYR:H	1.82	0.43
1:O:116:LYS:HG3	2:P:85:ILE:HD11	2.00	0.43
7:U:113:ALA:HB2	7:U:154:TYR:HB3	2.00	0.43
11:K:97:MET:HG2	11:K:99:THR:HG23	2.00	0.43
8:V:146:LEU:HD22	8:V:150:GLU:HB3	2.01	0.43
1:O:118:MET:HE2	1:O:152:PRO:HA	2.01	0.43
6:T:200:HIS:CE1	6:T:208:PHE:HB3	2.53	0.43
13:M:110:LEU:O	13:M:112:ASN:N	2.51	0.43
8:V:22:GLN:HG2	8:V:27:ALA:HB2	2.00	0.43
5:S:38:ARG:NH1	5:S:39:SER:O	2.52	0.43
7:U:105:CYS:HB2	7:U:136:SER:OG	2.18	0.43
14:N:190:PRO:HA	14:N:193:TYR:CE2	2.54	0.43
12:Z:124:SER:O	12:Z:131:TYR:HA	2.19	0.43
13:a:150:MET:HE3	13:a:184:LEU:HD23	2.00	0.43
4:R:77:ALA:HB2	4:R:132:VAL:HG21	2.01	0.43
13:a:27:LEU:HD11	13:a:34:LEU:HB3	2.00	0.43
13:a:51:VAL:HG22	13:a:116:VAL:HG22	2.01	0.43
7:G:71:GLY:HA3	7:G:224:PHE:CZ	2.54	0.42
7:G:116:SER:HB2	7:G:152:GLY:HA2	2.00	0.42
1:O:245:ASP:O	1:O:248:GLU:HG2	2.18	0.42
8:V:8:PHE:HB2	8:V:146:LEU:O	2.19	0.42
9:W:52:ILE:HG22	9:W:59:VAL:HG22	1.99	0.42
13:a:10:SER:O	13:a:41:ARG:NH2	2.52	0.42
13:a:20:VAL:HG21	13:a:117:ALA:HB1	2.01	0.42
1:A:127:VAL:HG23	7:G:121:GLN:HG2	2.00	0.42
4:D:161:ALA:HB3	5:E:55:LEU:HD13	2.00	0.42
2:P:9:THR:HB	2:P:20:GLN:HG3	2.00	0.42
2:P:43:ILE:HD11	2:P:145:TYR:HB3	2.01	0.42
4:R:197:LYS:HB2	4:R:204:LEU:HD22	2.01	0.42
13:M:129:TYR:HB2	13:M:142:LEU:HD13	2.00	0.42
5:E:49:LYS:HB3	5:E:58:TYR:HB3	2.01	0.42
1:O:160:LYS:HD3	1:O:179:TRP:CH2	2.54	0.42
9:W:33:LEU:HD11	10:X:141:PHE:HD2	1.84	0.42
12:Z:147:MET:HA	12:Z:150:LEU:HD12	2.00	0.42
2:P:82:ASP:HB3	2:P:130:PHE:HD1	1.85	0.42
12:Z:185:ARG:HD3	12:Z:217:TYR:CD2	2.54	0.42
1:A:209:ILE:HD11	1:A:247:LEU:HD11	2.01	0.42
2:B:106:PRO:HD2	2:B:109:ILE:HD12	2.02	0.42
6:T:66:VAL:HB	6:T:70:ILE:HB	2.01	0.42
9:I:27:ARG:HB2	9:I:182:TRP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:68:PHE:O	12:L:72:VAL:HG23	2.20	0.42
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.00	0.42
1:A:78:MET:HE2	1:A:78:MET:HB3	1.93	0.42
1:A:81:ASP:HB3	1:A:130:PHE:HD1	1.84	0.42
2:P:6:ASP:HB3	3:Q:4:ARG:NH1	2.34	0.42
3:Q:157:TRP:CZ2	4:R:51:LEU:HD12	2.55	0.42
5:S:10:VAL:HA	6:T:126:ARG:HB2	2.00	0.42
6:T:27:VAL:HG11	6:T:131:SER:HB2	2.02	0.42
6:T:87:ARG:HG2	6:T:115:TYR:CD2	2.54	0.42
9:I:22:ILE:HG12	9:I:42:ILE:HD13	2.00	0.42
13:M:119:VAL:HG23	13:M:200:ILE:HG22	2.02	0.42
8:V:67:SER:HB3	8:V:74:PRO:HG3	2.01	0.42
9:W:26:LEU:HD21	9:W:40:GLU:HG2	2.01	0.42
1:A:74:VAL:HG22	1:A:75:TYR:H	1.85	0.42
7:U:234:GLU:OE2	7:U:235:ARG:NH2	2.49	0.42
11:Y:120:THR:HG22	11:Y:122:LEU:HG	2.01	0.42
13:a:129:TYR:HB2	13:a:142:LEU:HD13	2.02	0.42
6:F:99:TYR:O	6:F:101:THR:N	2.46	0.42
3:Q:141:ASP:OD1	3:Q:141:ASP:N	2.51	0.42
10:X:4:ILE:HG22	10:X:103:LEU:HD22	2.01	0.42
12:Z:160:TYR:CG	12:Z:166:GLY:HA2	2.55	0.42
13:a:188:ASP:HB3	13:a:191:SER:HB3	2.01	0.42
4:D:65:HIS:CE1	4:D:98:ASP:HB3	2.55	0.42
5:S:45:LEU:HB2	5:S:213:ALA:HB3	2.02	0.42
13:M:104:ARG:HD2	13:M:133:LEU:O	2.20	0.42
3:C:88:ARG:NH1	10:J:70:ARG:HA	2.35	0.42
3:C:114:VAL:HG22	3:C:117:ARG:HH12	1.85	0.42
1:O:89:SER:HA	1:O:92:VAL:HG12	2.01	0.42
5:S:44:VAL:HG22	5:S:214:ILE:HD13	2.02	0.42
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.49	0.42
6:F:9:SER:HB2	7:G:126:ARG:HD3	2.02	0.41
7:G:72:MET:HE2	7:G:72:MET:HB3	1.83	0.41
3:Q:136:PHE:CE2	3:Q:215:PRO:HG3	2.54	0.41
6:T:5:ASP:O	6:T:19:GLN:NE2	2.52	0.41
6:T:13:PRO:HA	7:U:21:TYR:CD1	2.55	0.41
6:T:216:SER:OG	6:T:219:GLU:HB2	2.20	0.41
8:H:18:THR:HB	8:H:30:ASN:HA	2.02	0.41
9:I:79:ARG:HH12	9:I:82:GLU:HG2	1.84	0.41
10:X:130:TYR:HB2	10:X:144:LEU:HD13	2.02	0.41
3:C:54:ASP:OD2	3:C:56:ARG:NH2	2.52	0.41
5:S:226:GLY:O	5:S:229:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:92:ILE:HG21	10:J:122:LEU:HD23	2.03	0.41
13:a:14:MET:HG2	13:a:177:ILE:HD11	2.02	0.41
14:b:14:LEU:HB3	14:b:44:CYS:SG	2.60	0.41
6:F:163:LYS:HD3	6:F:203:ASN:ND2	2.34	0.41
6:F:200:HIS:NE2	6:F:206:LYS:O	2.53	0.41
7:G:105:CYS:HB2	7:G:136:SER:OG	2.20	0.41
1:O:220:ASP:OD1	1:O:220:ASP:N	2.52	0.41
2:P:75:ALA:HB3	2:P:135:ILE:HB	2.02	0.41
12:L:146:ILE:HG22	12:L:150:LEU:HD11	2.03	0.41
9:W:66:PHE:CZ	9:W:90:VAL:HG22	2.55	0.41
10:X:103:LEU:HG	10:X:116:LEU:HD11	2.01	0.41
13:a:130:VAL:HA	13:a:135:VAL:O	2.20	0.41
14:b:129:SER:OG	14:b:166:ASP:OD2	2.27	0.41
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.02	0.41
4:R:137:ALA:HB3	4:R:214:ILE:HD13	2.02	0.41
8:H:205:PHE:HE2	9:I:152:LEU:HD13	1.86	0.41
12:L:12:ILE:HG13	12:L:110:ILE:HD12	2.02	0.41
10:X:73:TYR:OH	10:X:110:LYS:NZ	2.28	0.41
1:A:205:ASN:O	1:A:209:ILE:HG12	2.21	0.41
9:I:10:ILE:HD11	9:I:174:ALA:HB2	2.02	0.41
12:Z:52:MET:HG3	12:Z:111:ILE:HG22	2.03	0.41
2:B:6:ASP:HB3	3:C:4:ARG:NH1	2.36	0.41
7:U:138:ASP:HB3	7:U:141:LEU:HB2	2.03	0.41
9:I:28:LEU:HB3	9:I:36:SER:HB3	2.02	0.41
13:M:132:LEU:HD23	13:M:132:LEU:H	1.86	0.41
9:W:40:GLU:OE2	9:W:198:TYR:OH	2.26	0.41
12:Z:214:LYS:HB2	12:Z:214:LYS:HE3	1.87	0.41
4:D:146:GLN:HG2	4:D:158:ARG:CZ	2.51	0.41
2:P:115:SER:HB3	2:P:154:GLY:O	2.21	0.41
13:M:65:ARG:HA	13:M:68:LYS:HG2	2.02	0.41
8:V:19:ARG:NH1	8:V:170:GLY:HA3	2.31	0.41
3:C:195:ARG:O	3:C:199:GLU:HG2	2.21	0.41
3:C:205:ALA:HB2	3:C:231:VAL:HG21	2.03	0.41
1:O:200:VAL:HG11	1:O:204:PHE:CD1	2.56	0.41
4:R:62:ILE:HG21	4:R:104:LEU:HD11	2.03	0.41
4:R:73:LEU:HD12	4:R:131:GLY:HA3	2.02	0.41
4:R:113:LEU:HD12	5:S:78:PRO:HB2	2.03	0.41
5:S:87:LEU:HD12	5:S:87:LEU:HA	1.87	0.41
7:U:176:HIS:HB2	7:U:200:HIS:HE1	1.85	0.41
9:I:12:VAL:HG12	9:I:170:LEU:HD12	2.02	0.41
10:J:103:LEU:HD23	10:J:103:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ILE:HG21	8:V:167:LEU:HD11	2.02	0.41
13:M:51:VAL:HG22	13:M:116:VAL:HG22	2.03	0.41
8:V:43:CYS:SG	8:V:98:LEU:HB3	2.61	0.41
13:a:150:MET:C	13:a:153:PRO:HD2	2.45	0.41
1:A:14:PRO:HA	2:B:23:TYR:CD1	2.56	0.41
2:B:26:GLU:O	2:B:29:SER:OG	2.26	0.41
2:B:189:ILE:HG23	2:B:212:PHE:CZ	2.55	0.41
3:Q:71:LEU:HD22	3:Q:84:ILE:HG12	2.03	0.41
3:Q:139:ARG:NH2	11:Y:107:LYS:HG3	2.36	0.41
4:R:65:HIS:CE1	4:R:98:ASP:HB3	2.56	0.41
9:I:62:LEU:HD12	9:I:104:VAL:HG21	2.01	0.41
13:M:129:TYR:O	13:M:136:THR:HA	2.21	0.41
9:W:9:GLY:HA2	9:W:25:ASP:OD2	2.21	0.41
4:D:159:TYR:CE2	5:E:56:SER:HB3	2.57	0.40
7:G:66:ILE:HD11	7:G:72:MET:HE2	2.01	0.40
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.03	0.40
1:O:250:LEU:HD23	1:O:250:LEU:HA	1.96	0.40
6:F:122:TYR:HB2	6:F:125:VAL:HG22	2.02	0.40
7:G:22:ALA:O	7:G:26:THR:HG23	2.21	0.40
7:G:35:ALA:HB2	7:G:44:VAL:HG12	2.03	0.40
7:G:106:ASP:OD1	7:G:106:ASP:N	2.49	0.40
8:H:134:ALA:O	8:H:138:LEU:HG	2.21	0.40
9:I:62:LEU:HD23	9:I:62:LEU:HA	1.88	0.40
13:M:181:MET:HE2	13:M:184:LEU:HD12	2.03	0.40
10:X:193:ASP:OD1	10:X:194:ASP:N	2.51	0.40
11:Y:147:ASP:OD1	11:Y:147:ASP:N	2.45	0.40
12:Z:220:LYS:HE3	12:Z:222:ASP:OD2	2.21	0.40
3:C:99:GLU:HG3	11:K:81:LYS:HD3	2.02	0.40
5:E:32:SER:HB3	5:E:61:LYS:HE3	2.03	0.40
6:F:13:PRO:HA	7:G:21:TYR:CD1	2.56	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.20	0.40
1:O:123:GLN:HG3	2:P:128:ARG:HG2	2.03	0.40
13:M:11:VAL:HG12	13:M:54:SER:HB3	2.02	0.40
9:W:101:PRO:O	10:X:93:ARG:NH2	2.50	0.40
10:X:119:ILE:HA	10:X:124:THR:O	2.22	0.40
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.57	0.40
4:D:223:TYR:O	4:D:224:ASP:HB3	2.21	0.40
2:P:103:GLU:OE2	10:X:76:SER:OG	2.30	0.40
10:J:18:SER:HB2	10:J:176:PHE:HB2	2.03	0.40
1:A:66:LEU:HD12	1:A:235:PHE:CD1	2.57	0.40
3:C:157:TRP:CZ2	4:D:51:LEU:HD12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:178:ARG:HD2	1:O:178:ARG:HA	1.77	0.40
7:U:66:ILE:HD12	7:U:88:ALA:HB3	2.03	0.40
9:I:34:GLY:O	11:Y:167:ARG:NH1	2.48	0.40
12:Z:69:LYS:O	12:Z:72:VAL:HG12	2.22	0.40
12:Z:77:PHE:HD1	12:Z:77:PHE:HA	1.79	0.40
14:b:1:THR:HG23	14:b:33:LYS:HD3	2.04	0.40
14:b:45:ARG:HB2	14:b:52:THR:HB	2.03	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	247/250 (99%)	235 (95%)	12 (5%)	0	100	100
1	O	247/250 (99%)	237 (96%)	10 (4%)	0	100	100
2	B	238/258 (92%)	232 (98%)	6 (2%)	0	100	100
2	P	240/258 (93%)	235 (98%)	5 (2%)	0	100	100
3	C	232/254 (91%)	226 (97%)	6 (3%)	0	100	100
3	Q	235/254 (92%)	227 (97%)	8 (3%)	0	100	100
4	D	233/260 (90%)	227 (97%)	6 (3%)	0	100	100
4	R	235/260 (90%)	229 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	230/234 (98%)	225 (98%)	5 (2%)	0	100	100
6	F	242/287 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	242/287 (84%)	232 (96%)	10 (4%)	0	100	100
7	G	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
7	U	240/252 (95%)	230 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	220/232 (95%)	209 (95%)	9 (4%)	2 (1%)	14	43
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	J	194/198 (98%)	186 (96%)	8 (4%)	0	100	100
10	X	193/198 (98%)	185 (96%)	8 (4%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6270/6586 (95%)	6050 (96%)	218 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	145	ASP
8	H	146	LEU

5.3.2 Protein sidechains ⓘ

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	208/209 (100%)	208 (100%)	0	100	100
1	O	208/209 (100%)	207 (100%)	1 (0%)	81	82
2	B	202/216 (94%)	201 (100%)	1 (0%)	81	82
2	P	204/216 (94%)	203 (100%)	1 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	208/226 (92%)	207 (100%)	1 (0%)	81	82
3	Q	211/226 (93%)	208 (99%)	3 (1%)	59	72
4	D	196/215 (91%)	196 (100%)	0	100	100
4	R	197/215 (92%)	197 (100%)	0	100	100
5	E	189/193 (98%)	187 (99%)	2 (1%)	65	75
5	S	191/193 (99%)	187 (98%)	4 (2%)	47	66
6	F	201/238 (84%)	200 (100%)	1 (0%)	81	82
6	T	200/238 (84%)	199 (100%)	1 (0%)	81	82
7	G	206/210 (98%)	206 (100%)	0	100	100
7	U	206/210 (98%)	206 (100%)	0	100	100
8	H	181/190 (95%)	179 (99%)	2 (1%)	65	75
8	V	179/190 (94%)	178 (99%)	1 (1%)	78	81
9	I	172/173 (99%)	172 (100%)	0	100	100
9	W	172/173 (99%)	171 (99%)	1 (1%)	78	81
10	J	174/175 (99%)	173 (99%)	1 (1%)	78	81
10	X	173/175 (99%)	172 (99%)	1 (1%)	78	81
11	K	169/169 (100%)	169 (100%)	0	100	100
11	Y	169/169 (100%)	167 (99%)	2 (1%)	63	74
12	L	185/185 (100%)	184 (100%)	1 (0%)	81	82
12	Z	185/185 (100%)	184 (100%)	1 (0%)	81	82
13	M	199/199 (100%)	196 (98%)	3 (2%)	57	71
13	a	199/199 (100%)	196 (98%)	3 (2%)	57	71
14	N	162/162 (100%)	161 (99%)	1 (1%)	78	81
14	b	162/162 (100%)	159 (98%)	3 (2%)	50	68
All	All	5308/5520 (96%)	5273 (99%)	35 (1%)	76	79

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	33	THR
3	C	220	VAL
5	E	34	THR
5	E	174	THR
6	F	49	LEU

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Mol	Chain	Res	Type
1	O	169	VAL
2	P	149	THR
3	Q	131	THR
3	Q	148	THR
3	Q	212	VAL
5	S	34	THR
5	S	171	LEU
5	S	174	THR
5	S	209	ASN
6	T	203	ASN
8	H	59	ILE
8	H	146	LEU
10	J	136	SER
12	L	128	VAL
13	M	11	VAL
13	M	127	LEU
13	M	190	ARG
14	N	178	LEU
8	V	59	ILE
9	W	195	VAL
10	X	174	MET
11	Y	65	LEU
11	Y	137	TYR
12	Z	128	VAL
13	a	37	ASN
13	a	102	GLN
13	a	206	LEU
14	b	65	LEU
14	b	119	VAL
14	b	179	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
3	C	116	GLN
3	C	176	ASN
4	D	149	HIS
5	E	90	GLN
7	G	6	HIS
1	O	218	ASN
2	P	88	ASN

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Mol	Chain	Res	Type
2	P	95	GLN
3	Q	116	GLN
4	R	149	HIS
4	R	210	GLN
5	S	30	GLN
7	U	6	HIS
7	U	212	ASN
8	H	22	GLN
8	H	86	HIS
9	I	37	ASN
9	I	168	GLN
10	J	118	GLN
11	K	62	GLN
11	K	133	GLN
11	K	179	HIS
12	L	80	ASN
12	L	158	ASN
12	L	197	GLN
13	M	26	ASN
13	M	211	ASN
8	V	144	GLN
9	W	37	ASN
9	W	47	HIS
9	W	63	ASN
9	W	168	GLN
10	X	63	ASN
11	Y	62	GLN
11	Y	190	ASN
11	Y	209	ASN
12	Z	158	ASN
14	b	106	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 9 are monoatomic - leaving 44 for Mogul analysis.

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	SO4	K	303	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	P	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	B	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	a	304	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	L	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Q	301	-	4,4,4	0.67	0	6,6,6	0.11	0
15	SO4	M	303	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	N	203	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	G	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	J	201	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Z	303	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	F	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	K	304	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	S	301	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	E	301	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	a	303	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	R	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	F	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	J	202	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	U	301	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	D	301	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	L	303	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	M	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	Z	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	K	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	I	302	-	4,4,4	0.67	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	SO4	N	201	-	4,4,4	0.66	0	6,6,6	0.09	0
15	SO4	E	303	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	H	302	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	S	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	G	301	-	4,4,4	0.68	0	6,6,6	0.11	0
15	SO4	P	302	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	X	201	-	4,4,4	0.67	0	6,6,6	0.11	0
15	SO4	H	303	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	E	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	b	201	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	M	304	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	E	304	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	V	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	M	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	T	301	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	a	301	-	4,4,4	0.68	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	R	301	SO4	1	0
15	N	201	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/250 (99%)	1.75	81 (32%) 1 1	18, 38, 73, 97	0
1	O	249/250 (99%)	1.61	72 (28%) 1 1	11, 34, 71, 96	0
2	B	242/258 (93%)	2.09	98 (40%) 0 0	19, 45, 77, 104	0
2	P	244/258 (94%)	1.75	84 (34%) 1 1	15, 35, 73, 97	0
3	C	236/254 (92%)	2.24	118 (50%) 0 0	17, 50, 94, 112	0
3	Q	239/254 (94%)	2.17	111 (46%) 0 0	19, 48, 90, 116	0
4	D	237/260 (91%)	1.89	86 (36%) 1 1	14, 40, 65, 105	0
4	R	239/260 (91%)	2.30	131 (54%) 0 0	20, 52, 79, 103	0
5	E	231/234 (98%)	2.02	103 (44%) 0 0	21, 41, 70, 89	0
5	S	232/234 (99%)	2.40	123 (53%) 0 0	24, 46, 80, 93	0
6	F	244/287 (85%)	1.88	91 (37%) 1 1	18, 39, 75, 83	0
6	T	244/287 (85%)	2.05	98 (40%) 0 0	18, 40, 78, 107	0
7	G	241/252 (95%)	1.63	75 (31%) 1 1	15, 35, 60, 93	0
7	U	242/252 (96%)	1.64	74 (30%) 1 1	15, 35, 62, 92	0
8	H	222/232 (95%)	1.45	52 (23%) 2 2	12, 31, 55, 95	0
8	V	222/232 (95%)	1.31	46 (20%) 2 3	16, 28, 53, 87	0
9	I	204/205 (99%)	1.28	38 (18%) 3 4	14, 29, 55, 80	0
9	W	204/205 (99%)	1.13	24 (11%) 9 9	12, 23, 48, 76	0
10	J	196/198 (98%)	1.17	26 (13%) 7 7	15, 30, 50, 102	0
10	X	195/198 (98%)	1.15	24 (12%) 8 8	12, 27, 52, 106	0
11	K	212/212 (100%)	1.18	27 (12%) 8 7	12, 25, 45, 83	0
11	Y	212/212 (100%)	1.32	43 (20%) 3 3	15, 31, 51, 69	0
12	L	222/222 (100%)	1.06	24 (10%) 11 10	11, 23, 42, 60	0
12	Z	222/222 (100%)	1.42	49 (22%) 2 2	11, 31, 53, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	1.11	37 (15%) 5 5	12, 26, 47, 66	0
13	a	233/233 (100%)	1.43	53 (22%) 2 2	15, 30, 52, 74	0
14	N	196/196 (100%)	1.12	30 (15%) 5 5	16, 28, 54, 83	0
14	b	196/196 (100%)	1.16	30 (15%) 5 5	13, 27, 54, 69	0
All	All	6338/6586 (96%)	1.62	1848 (29%) 1 1	11, 34, 72, 116	0

All (1848) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	40	ASP	7.5
2	P	218	GLY	7.4
3	Q	241	GLN	7.3
5	S	187	GLU	7.2
6	F	244	ASN	7.2
3	C	236	GLN	7.1
2	B	54	THR	7.0
2	B	59	ASP	6.9
4	D	117	GLU	6.9
4	D	0	TYR	6.9
9	W	131	GLU	6.8
2	P	222	GLY	6.8
6	T	51	THR	6.8
5	S	54	GLU	6.7
10	X	193	ASP	6.6
2	B	244	THR	6.5
6	T	181	GLU	6.4
3	C	168	THR	6.2
9	I	192	ASP	6.2
7	G	188	GLU	6.2
2	P	54	THR	6.1
2	B	7	SER	6.1
3	C	58	THR	6.0
3	Q	234	ILE	5.9
2	B	223	GLU	5.9
4	R	0	TYR	5.9
3	Q	237	GLU	5.9
3	C	171	GLU	5.8
3	C	228	ASN	5.8
5	E	203	GLU	5.7
3	Q	58	THR	5.7
5	E	123	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
6	T	207	ASP	5.7
4	R	1	ASP	5.6
3	C	204	GLY	5.6
1	O	249	ALA	5.6
1	A	52	SER	5.6
7	U	222	ASP	5.6
5	S	200	LEU	5.6
8	H	221	CYS	5.6
4	D	224	ASP	5.6
2	B	40	SER	5.6
4	R	201	GLU	5.5
5	S	51	ASN	5.5
10	J	194	ASP	5.5
9	I	131	GLU	5.5
6	F	242	GLU	5.5
3	Q	48	SER	5.5
3	C	38	ASN	5.4
5	E	3	ASN	5.4
4	D	1	ASP	5.4
2	P	1	GLY	5.4
7	G	2	GLY	5.4
3	C	237	GLU	5.4
3	Q	225	GLU	5.4
5	E	227	GLU	5.4
5	S	203	GLU	5.4
5	E	177	THR	5.4
5	S	233	ILE	5.4
8	V	222	ASP	5.3
4	R	243	SER	5.3
3	C	175	LYS	5.3
10	J	196	GLN	5.3
5	S	124	GLY	5.3
8	H	108	SER	5.3
5	S	186	ASP	5.3
10	X	194	ASP	5.2
5	S	226	GLY	5.2
7	G	180	SER	5.2
5	S	229	VAL	5.2
1	A	248	GLU	5.2
2	P	61	SER	5.2
3	Q	240	GLU	5.2
3	C	184	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
3	Q	229	GLN	5.1
5	S	32	SER	5.1
4	D	2	ARG	5.1
2	P	221	ASP	5.1
3	Q	239	GLN	5.1
5	S	207	VAL	5.1
5	S	173	ARG	5.1
3	Q	55	THR	5.1
6	T	2	THR	5.1
5	S	56	SER	5.1
2	B	62	THR	5.0
6	F	182	GLY	5.0
1	O	62	SER	5.0
6	F	184	SER	5.0
4	D	54	ASP	5.0
3	Q	167	LYS	5.0
6	T	204	LYS	5.0
4	R	202	GLU	5.0
7	U	243	ASP	5.0
5	S	205	LEU	5.0
6	T	178	HIS	5.0
7	G	3	TYR	5.0
3	C	48	SER	5.0
4	D	177	ASN	5.0
6	T	241	LYS	5.0
5	E	174	THR	5.0
7	G	179	LYS	4.9
4	R	242	GLU	4.9
1	A	2	THR	4.9
7	G	124	TYR	4.9
7	G	242	GLN	4.9
13	a	85	GLU	4.9
1	O	167	GLY	4.9
4	D	226	GLU	4.9
2	P	245	LYS	4.9
1	A	250	LEU	4.9
3	C	223	SER	4.8
6	T	205	GLU	4.8
3	Q	236	GLN	4.8
6	T	39	ASN	4.8
4	R	234	GLU	4.8
5	S	202	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
6	F	237	ASP	4.8
4	D	242	GLU	4.8
6	T	166	GLN	4.8
6	T	237	ASP	4.8
6	T	180	PRO	4.8
3	C	37	LYS	4.8
8	H	218	VAL	4.8
2	B	202	SER	4.8
3	C	60	SER	4.8
6	T	206	LYS	4.8
5	S	52	ALA	4.7
2	P	203	SER	4.7
13	a	211	ASN	4.7
1	O	250	LEU	4.7
4	R	123	GLU	4.7
9	W	133	LYS	4.7
7	U	242	GLN	4.7
5	S	58	TYR	4.7
3	Q	238	LYS	4.7
8	V	198	GLU	4.7
3	Q	202	GLN	4.7
2	B	168	THR	4.7
6	T	184	SER	4.7
3	Q	232	THR	4.7
6	F	230	ASP	4.7
9	I	133	LYS	4.7
6	T	187	GLU	4.7
2	P	242	GLY	4.6
6	T	230	ASP	4.6
5	E	121	SER	4.6
1	O	244	ASN	4.6
4	R	169	GLU	4.6
5	E	190	LYS	4.6
1	A	202	GLY	4.6
2	P	59	ASP	4.6
4	R	3	GLY	4.6
13	a	82	ASP	4.6
2	B	51	VAL	4.6
1	O	52	SER	4.6
3	C	203	THR	4.6
1	A	200	VAL	4.6
8	V	120	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
6	F	181	GLU	4.5
2	B	171	ALA	4.5
6	T	173	GLU	4.5
6	T	218	SER	4.5
4	D	180	HIS	4.5
1	A	4	ARG	4.5
3	Q	230	TYR	4.5
3	Q	59	PRO	4.5
14	b	191	ASP	4.5
6	F	1	GLY	4.5
4	R	226	GLU	4.5
7	U	203	ASP	4.5
5	S	204	SER	4.5
1	A	198	GLU	4.5
5	E	77	ALA	4.4
11	K	212	GLY	4.4
5	S	169	THR	4.4
3	C	185	THR	4.4
3	C	232	THR	4.4
2	B	3	ARG	4.4
1	O	141	GLU	4.4
2	B	201	ASP	4.4
3	Q	218	ASP	4.4
4	R	224	ASP	4.4
5	E	95	SER	4.4
5	S	209	ASN	4.4
3	C	235	GLU	4.4
4	R	178	GLU	4.4
2	B	245	LYS	4.4
7	G	181	LYS	4.4
3	Q	207	ASN	4.4
5	E	209	ASN	4.4
13	a	216	ASN	4.4
4	R	217	GLN	4.4
2	B	173	THR	4.4
2	P	182	ASP	4.4
6	F	40	ASP	4.4
14	b	104	ASP	4.4
4	R	177	ASN	4.4
7	G	228	SER	4.4
3	Q	235	GLU	4.3
12	Z	169	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
3	Q	185	THR	4.3
8	H	28	ASP	4.3
7	U	124	TYR	4.3
3	C	221	ALA	4.3
5	S	181	ILE	4.3
3	C	186	VAL	4.3
5	E	202	ASP	4.3
3	C	180	LYS	4.3
13	a	215	GLU	4.3
5	S	231	LYS	4.3
5	S	198	GLN	4.3
3	C	238	LYS	4.3
3	Q	180	LYS	4.3
5	S	117	LYS	4.3
5	S	206	THR	4.3
2	P	236	ASP	4.3
5	S	227	GLU	4.3
2	B	221	ASP	4.2
3	Q	10	SER	4.2
4	R	216	LYS	4.2
3	Q	199	GLU	4.2
3	C	167	LYS	4.2
1	A	249	ALA	4.2
2	B	222	GLY	4.2
1	A	177	LYS	4.2
5	S	57	SER	4.2
1	O	203	GLU	4.2
3	C	209	GLU	4.2
4	R	239	GLU	4.2
2	B	208	ASP	4.2
2	B	232	GLN	4.2
3	Q	38	ASN	4.2
6	T	240	GLN	4.2
2	B	204	ALA	4.2
1	A	54	PRO	4.2
8	V	182	LYS	4.2
3	C	199	GLU	4.1
6	F	202	ASP	4.1
6	T	200	HIS	4.1
3	Q	204	GLY	4.1
2	B	225	TYR	4.1
3	C	201	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
10	X	1	MET	4.1
4	D	214	ILE	4.1
4	R	46	ALA	4.1
5	S	230	ALA	4.1
1	O	245	ASP	4.1
3	Q	203	THR	4.1
6	F	234	GLU	4.1
10	J	195	PHE	4.1
2	B	176	GLN	4.1
3	Q	233	GLN	4.1
4	R	2	ARG	4.1
3	Q	137	ASP	4.1
6	T	202	ASP	4.1
7	G	178	LYS	4.1
3	C	234	ILE	4.1
2	B	34	ALA	4.1
2	B	88	ASN	4.0
1	A	220	ASP	4.0
2	B	217	LYS	4.0
3	C	225	GLU	4.0
4	D	169	GLU	4.0
3	Q	53	GLN	4.0
6	F	178	HIS	4.0
6	T	242	GLU	4.0
2	B	242	GLY	4.0
4	D	4	VAL	4.0
7	U	181	LYS	4.0
2	B	182	ASP	4.0
2	P	178	ASP	4.0
5	E	8	ASP	4.0
5	E	225	ASP	4.0
5	S	196	ILE	4.0
11	Y	72	GLU	4.0
1	A	231	LYS	4.0
2	P	239	VAL	4.0
6	T	244	ASN	4.0
5	S	197	SER	4.0
7	U	240	ALA	4.0
1	A	3	ASP	4.0
2	B	53	SER	4.0
3	C	187	GLU	4.0
6	T	177	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
3	Q	51	LYS	4.0
5	S	59	GLN	3.9
5	S	77	ALA	3.9
4	R	221	LYS	3.9
8	V	219	ASN	3.9
2	B	52	THR	3.9
3	C	174	GLU	3.9
1	O	181	ASP	3.9
6	F	207	ASP	3.9
2	B	113	ARG	3.9
6	F	179	HIS	3.9
1	A	240	SER	3.9
1	O	207	ASP	3.9
5	S	218	ASP	3.9
8	H	222	ASP	3.9
3	C	55	THR	3.9
5	S	201	ARG	3.9
3	Q	165	ASN	3.9
6	F	29	ASN	3.9
6	F	180	PRO	3.9
2	B	178	ASP	3.9
5	S	225	ASP	3.9
10	X	10	GLN	3.9
8	V	43	CYS	3.9
3	C	46	ARG	3.9
1	O	200	VAL	3.9
13	M	38	GLY	3.9
4	R	236	LYS	3.9
5	S	53	ASP	3.9
9	W	192	ASP	3.9
10	X	11	ASP	3.9
4	R	179	TRP	3.9
4	R	124	ARG	3.8
14	N	149	GLU	3.8
4	D	116	GLY	3.8
5	E	233	ILE	3.8
6	T	53	LYS	3.8
3	C	216	ASP	3.8
5	E	59	GLN	3.8
5	E	218	ASP	3.8
5	S	2	ARG	3.8
4	R	187	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
5	E	122	TYR	3.8
6	T	171	GLU	3.8
7	U	178	LYS	3.8
1	O	61	LEU	3.8
3	C	10	SER	3.8
9	I	130	ASP	3.8
7	U	53	LYS	3.8
3	C	13	GLY	3.8
4	R	225	ASN	3.8
5	S	165	GLN	3.8
4	D	182	SER	3.8
11	Y	147	ASP	3.8
2	B	207	TYR	3.8
2	B	60	THR	3.8
4	D	229	ALA	3.8
1	O	53	SER	3.8
7	G	222	ASP	3.8
9	I	18	ASP	3.8
3	C	230	TYR	3.8
4	R	114	ARG	3.8
5	E	187	GLU	3.8
8	V	221	CYS	3.8
5	E	191	ALA	3.7
4	R	194	LYS	3.7
5	S	190	LYS	3.7
8	V	195	VAL	3.7
6	F	177	ASP	3.7
3	C	227	ILE	3.7
1	O	201	GLU	3.7
1	O	2	THR	3.7
3	C	233	GLN	3.7
8	V	10	ASN	3.7
3	C	141	ASP	3.7
4	R	218	ASP	3.7
8	H	145	ASP	3.7
5	S	232	TYR	3.7
6	T	221	ASN	3.7
9	W	1	SER	3.7
4	R	205	ASP	3.7
10	X	135	TYR	3.7
3	C	39	CYS	3.7
2	B	237	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
6	T	175	LEU	3.7
4	R	203	LYS	3.7
2	P	202	SER	3.7
9	W	130	ASP	3.7
5	E	219	THR	3.7
6	F	2	THR	3.7
11	Y	210	VAL	3.7
3	C	53	GLN	3.7
8	H	217	ILE	3.7
3	C	56	ARG	3.6
5	E	169	THR	3.6
4	D	221	LYS	3.6
2	B	167	ASN	3.6
5	S	192	GLY	3.6
3	Q	171	GLU	3.6
7	U	233	GLU	3.6
3	C	12	ASP	3.6
7	U	52	ASP	3.6
9	I	2	ASP	3.6
6	F	162	GLY	3.6
6	T	1	GLY	3.6
4	R	33	ALA	3.6
5	E	207	VAL	3.6
7	G	241	GLU	3.6
1	O	51	SER	3.6
3	Q	60	SER	3.6
4	D	48	SER	3.6
5	S	176	ASP	3.6
9	W	143	ASP	3.6
12	Z	214	LYS	3.6
5	S	151	ASN	3.6
8	H	9	ASN	3.6
13	a	78	ASN	3.6
5	S	132	LEU	3.6
8	H	216	SER	3.6
1	A	206	GLY	3.6
2	B	125	GLY	3.6
7	U	2	GLY	3.6
3	C	226	GLU	3.6
14	b	192	GLU	3.6
4	R	47	THR	3.6
5	S	30	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
6	F	58	GLN	3.5
11	Y	157	GLY	3.5
4	D	113	LEU	3.5
2	B	15	GLU	3.5
2	P	151	ASN	3.5
4	R	207	ASN	3.5
7	U	241	GLU	3.5
3	C	44	CYS	3.5
2	B	4	ARG	3.5
2	P	197	SER	3.5
3	Q	47	ARG	3.5
11	K	106	ARG	3.5
5	S	66	ASP	3.5
7	U	183	ASP	3.5
1	O	197	LYS	3.5
3	Q	37	LYS	3.5
3	Q	220	VAL	3.5
6	F	163	LYS	3.5
6	F	241	LYS	3.5
8	V	218	VAL	3.5
1	O	247	LEU	3.5
6	F	231	LEU	3.5
14	N	196	LEU	3.5
2	P	237	ILE	3.5
4	R	21	GLU	3.5
7	U	212	ASN	3.5
5	S	9	THR	3.5
6	T	52	SER	3.5
5	E	186	ASP	3.5
6	T	174	LYS	3.5
13	M	47	ASP	3.5
4	D	112	ALA	3.5
3	C	52	LEU	3.5
5	S	185	PRO	3.5
2	B	8	ARG	3.5
1	O	190	HIS	3.5
3	Q	43	GLY	3.5
5	S	161	GLY	3.5
8	V	22	GLN	3.5
8	V	144	GLN	3.5
10	J	10	GLN	3.5
3	Q	158	SER	3.5

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Mol	Chain	Res	Type	RSRZ
5	E	73	LEU	3.5
4	D	201	GLU	3.5
14	b	194	GLU	3.5
3	C	176	ASN	3.5
4	R	35	LYS	3.5
6	F	221	ASN	3.5
8	H	10	ASN	3.5
3	C	202	GLN	3.5
8	H	202	SER	3.5
11	Y	75	SER	3.5
6	F	243	ILE	3.5
7	G	183	ASP	3.5
13	a	69	ASP	3.5
5	E	201	ARG	3.5
1	A	203	GLU	3.4
3	C	181	GLU	3.4
5	S	178	PHE	3.4
2	B	193	LEU	3.4
5	S	177	THR	3.4
6	T	57	PRO	3.4
14	b	68	SER	3.4
2	P	246	LYS	3.4
3	C	144	LYS	3.4
1	O	204	PHE	3.4
10	X	195	PHE	3.4
3	C	200	VAL	3.4
7	G	194	VAL	3.4
6	T	203	ASN	3.4
11	K	124	GLY	3.4
7	G	240	ALA	3.4
7	U	182	ILE	3.4
7	U	105	CYS	3.4
8	H	38	SER	3.4
13	M	69	ASP	3.4
5	S	122	TYR	3.4
12	L	172	LEU	3.4
7	G	229	ALA	3.4
1	A	208	THR	3.4
3	Q	206	LYS	3.4
1	O	240	SER	3.4
3	Q	7	SER	3.4
5	E	57	SER	3.4

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Mol	Chain	Res	Type	RSRZ
10	J	193	ASP	3.4
11	Y	152	ASP	3.4
14	N	103	ASP	3.4
7	G	230	GLU	3.4
7	U	168	GLU	3.4
13	M	215	GLU	3.4
2	P	10	THR	3.4
1	A	50	LYS	3.4
2	B	184	LYS	3.4
3	C	51	LYS	3.4
3	Q	26	LYS	3.4
4	R	238	LYS	3.4
6	F	139	LYS	3.4
7	U	231	ASN	3.4
3	C	121	SER	3.4
3	C	166	SER	3.4
3	Q	189	CYS	3.4
3	Q	223	SER	3.4
6	T	226	PHE	3.4
1	A	245	ASP	3.4
4	D	219	GLY	3.4
4	R	171	ALA	3.4
1	O	231	LYS	3.4
6	F	206	LYS	3.4
2	P	232	GLN	3.4
2	P	241	THR	3.4
7	U	207	THR	3.4
11	Y	30	THR	3.4
4	D	225	ASN	3.3
1	A	120	GLU	3.3
2	P	223	GLU	3.3
4	D	5	SER	3.3
4	D	127	SER	3.3
4	R	42	VAL	3.3
4	R	111	LEU	3.3
6	F	201	GLU	3.3
8	H	197	GLU	3.3
3	Q	140	ASP	3.3
1	A	241	GLN	3.3
3	Q	183	PRO	3.3
4	R	180	HIS	3.3
1	A	242	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	242	GLU	3.3
2	B	63	GLU	3.3
5	S	194	GLU	3.3
4	D	153	SER	3.3
4	R	241	ALA	3.3
9	I	128	CYS	3.3
10	J	1	MET	3.3
3	C	218	ASP	3.3
8	V	35	HIS	3.3
2	B	102	ASN	3.3
6	F	217	LEU	3.3
6	F	187	GLU	3.3
7	G	139	GLU	3.3
8	H	215	GLU	3.3
2	B	1	GLY	3.3
2	B	203	SER	3.3
2	P	204	ALA	3.3
6	T	182	GLY	3.3
3	Q	3	ASP	3.3
4	R	140	ASP	3.3
7	G	4	ASP	3.3
3	C	229	GLN	3.3
5	E	165	GLN	3.3
6	T	231	LEU	3.3
1	A	201	GLU	3.3
8	V	220	ILE	3.3
13	a	229	GLY	3.3
1	A	199	SER	3.3
6	T	216	SER	3.3
12	L	174	TYR	3.3
2	P	8	ARG	3.3
5	E	176	ASP	3.3
4	D	179	TRP	3.3
3	Q	187	GLU	3.3
6	T	50	ILE	3.3
7	U	206	GLY	3.3
3	C	179	ARG	3.2
1	A	8	SER	3.2
3	C	59	PRO	3.2
4	R	233	LYS	3.2
5	S	208	ASP	3.2
13	a	47	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	30	GLN	3.2
4	R	228	THR	3.2
7	U	50	VAL	3.2
1	O	206	GLY	3.2
1	O	248	GLU	3.2
4	R	36	GLU	3.2
6	F	129	GLY	3.2
10	J	155	GLU	3.2
13	a	84	GLU	3.2
2	B	240	LYS	3.2
5	S	180	LYS	3.2
11	Y	199	LYS	3.2
3	C	3	ASP	3.2
3	Q	141	ASP	3.2
5	E	179	ILE	3.2
13	M	233	ILE	3.2
11	Y	203	GLU	3.2
4	R	186	LYS	3.2
6	T	190	LYS	3.2
9	W	191	LYS	3.2
3	C	215	PRO	3.2
4	R	182	SER	3.2
5	S	139	SER	3.2
14	N	153	ASP	3.2
1	A	209	ILE	3.2
5	E	52	ALA	3.2
4	R	237	GLU	3.2
1	O	17	LYS	3.2
7	G	186	ASN	3.2
5	E	232	TYR	3.2
3	Q	172	PHE	3.2
5	E	198	GLN	3.2
6	F	166	GLN	3.2
11	K	96	SER	3.2
13	a	121	SER	3.2
2	P	194	LYS	3.2
5	E	49	LYS	3.2
5	S	166	GLY	3.2
4	R	25	LEU	3.2
3	C	207	ASN	3.2
4	R	208	ASN	3.2
5	E	170	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	6	SER	3.2
1	O	243	ILE	3.2
3	Q	4	ARG	3.2
6	F	233	GLN	3.2
10	J	142	SER	3.2
5	S	219	THR	3.2
5	S	228	ALA	3.2
1	A	181	ASP	3.1
4	R	37	GLY	3.1
4	R	230	GLU	3.1
6	F	203	ASN	3.1
2	B	172	GLN	3.1
1	A	51	SER	3.1
2	B	47	ALA	3.1
2	B	180	LYS	3.1
3	C	206	LYS	3.1
6	T	228	LYS	3.1
2	P	62	THR	3.1
3	Q	121	SER	3.1
4	D	47	THR	3.1
4	D	53	SER	3.1
4	R	5	SER	3.1
7	U	120	THR	3.1
12	Z	124	SER	3.1
1	A	61	LEU	3.1
1	A	230	ASP	3.1
4	D	37	GLY	3.1
4	R	190	LEU	3.1
5	S	55	LEU	3.1
7	U	217	GLY	3.1
9	I	124	ASP	3.1
14	N	104	ASP	3.1
4	D	174	GLU	3.1
4	D	213	CYS	3.1
4	D	239	GLU	3.1
4	R	174	GLU	3.1
7	G	233	GLU	3.1
8	V	197	GLU	3.1
11	Y	151	GLU	3.1
2	B	239	VAL	3.1
3	C	47	ARG	3.1
5	S	170	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
4	R	227	LYS	3.1
13	a	233	ILE	3.1
8	H	22	GLN	3.1
8	H	133	ALA	3.1
3	Q	197	LEU	3.1
5	S	41	THR	3.1
5	S	164	SER	3.1
8	V	156	SER	3.1
3	Q	19	GLU	3.1
5	E	58	TYR	3.1
12	Z	80	ASN	3.1
13	M	216	ASN	3.1
4	R	188	ALA	3.1
6	T	58	GLN	3.1
10	J	161	LEU	3.1
9	I	115	SER	3.1
1	A	48	GLU	3.1
1	A	178	ARG	3.1
4	D	187	GLU	3.1
12	Z	215	GLU	3.1
1	A	228	PRO	3.1
10	J	113	LYS	3.1
3	C	210	ILE	3.1
5	E	141	ALA	3.1
6	T	185	ALA	3.1
1	A	247	LEU	3.1
7	G	167	GLN	3.1
3	C	211	THR	3.1
6	T	31	THR	3.1
8	H	147	THR	3.1
2	B	61	SER	3.1
4	R	48	SER	3.1
4	D	21	GLU	3.1
13	M	219	TRP	3.1
1	A	22	ASP	3.1
2	B	181	ASP	3.1
3	Q	54	ASP	3.1
11	Y	155	TYR	3.1
3	C	222	LEU	3.0
5	E	99	ASN	3.0
6	T	179	HIS	3.0
3	Q	122	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
12	Z	166	GLY	3.0
3	Q	168	THR	3.0
3	C	190	VAL	3.0
5	E	26	GLU	3.0
7	U	188	GLU	3.0
4	R	200	MET	3.0
8	V	217	ILE	3.0
6	F	197	TYR	3.0
4	D	175	LEU	3.0
4	R	235	LEU	3.0
2	B	17	ARG	3.0
1	O	202	GLY	3.0
6	F	64	GLN	3.0
2	B	198	LYS	3.0
6	F	32	THR	3.0
7	G	133	THR	3.0
1	O	199	SER	3.0
3	Q	182	PRO	3.0
6	F	14	ASP	3.0
8	V	145	ASP	3.0
11	K	118	ASP	3.0
3	Q	27	ARG	3.0
3	C	214	LYS	3.0
4	R	154	GLY	3.0
5	S	4	ASN	3.0
1	O	198	GLU	3.0
2	P	233	GLU	3.0
4	D	178	GLU	3.0
4	D	237	GLU	3.0
4	R	117	GLU	3.0
12	L	18	GLU	3.0
13	a	162	GLU	3.0
5	S	48	LEU	3.0
5	S	199	SER	3.0
7	U	180	SER	3.0
3	C	27	ARG	3.0
5	S	50	ARG	3.0
9	I	132	ALA	3.0
1	O	3	ASP	3.0
2	B	6	ASP	3.0
9	W	25	ASP	3.0
10	J	175	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	60	LYS	3.0
12	L	173	LYS	3.0
7	G	65	CYS	3.0
12	Z	10	GLY	3.0
7	U	58	THR	3.0
2	B	243	ILE	3.0
4	D	232	ILE	3.0
6	F	186	ARG	3.0
1	O	46	ALA	3.0
9	I	113	SER	3.0
10	J	76	SER	3.0
13	a	54	SER	3.0
2	B	230	LYS	3.0
2	P	224	VAL	3.0
2	P	155	ASN	3.0
4	D	228	THR	3.0
6	T	201	GLU	2.9
11	K	182	GLU	2.9
1	O	237	LYS	2.9
5	E	180	LYS	2.9
14	b	100	ALA	2.9
3	C	2	TYR	2.9
5	S	44	VAL	2.9
3	C	178	ASP	2.9
12	Z	163	GLY	2.9
5	S	189	ILE	2.9
6	F	49	LEU	2.9
6	F	215	CYS	2.9
12	L	165	ASN	2.9
1	A	60	THR	2.9
4	D	223	TYR	2.9
6	T	75	SER	2.9
6	F	164	GLY	2.9
5	E	208	ASP	2.9
5	E	212	ILE	2.9
5	E	200	LEU	2.9
5	S	163	ARG	2.9
2	B	149	THR	2.9
5	E	9	THR	2.9
5	S	3	ASN	2.9
8	H	194	ASN	2.9
11	Y	107	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
4	R	22	ALA	2.9
5	E	10	VAL	2.9
4	R	41	GLY	2.9
4	R	212	SER	2.9
6	T	229	GLY	2.9
11	K	142	SER	2.9
13	M	123	GLY	2.9
3	Q	195	ARG	2.9
5	E	181	ILE	2.9
13	M	102	GLN	2.9
13	a	171	GLN	2.9
1	A	229	THR	2.9
7	G	160	THR	2.9
6	F	235	ALA	2.9
11	K	67	GLU	2.9
11	Y	202	GLU	2.9
12	L	171	PRO	2.9
1	A	64	VAL	2.9
3	Q	201	VAL	2.9
11	Y	144	TYR	2.9
6	T	18	PHE	2.9
1	A	58	SER	2.9
2	P	150	SER	2.9
13	M	121	SER	2.9
14	b	2	SER	2.9
1	O	241	GLN	2.9
2	P	176	GLN	2.9
12	Z	32	ASP	2.9
3	Q	221	ALA	2.9
8	H	206	PRO	2.9
1	A	176	GLU	2.9
5	E	54	GLU	2.9
6	T	47	GLU	2.9
8	H	219	ASN	2.9
9	W	8	GLY	2.9
12	L	17	GLY	2.9
1	A	29	LYS	2.9
2	B	183	MET	2.9
4	D	176	LEU	2.9
4	D	235	LEU	2.9
4	R	113	LEU	2.9
5	S	60	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
6	F	54	LEU	2.9
3	C	14	HIS	2.8
5	E	32	SER	2.8
6	F	240	GLN	2.8
6	T	12	SER	2.8
7	G	28	GLN	2.8
3	Q	12	ASP	2.8
5	E	53	ASP	2.8
2	P	60	THR	2.8
2	B	48	GLU	2.8
3	Q	23	GLU	2.8
5	S	99	ASN	2.8
4	D	170	GLY	2.8
4	R	44	LYS	2.8
4	R	223	TYR	2.8
10	X	174	MET	2.8
11	Y	211	ILE	2.8
13	M	213	GLN	2.8
4	D	33	ALA	2.8
7	G	161	ALA	2.8
11	Y	49	ALA	2.8
5	S	220	PRO	2.8
1	A	216	ASP	2.8
2	B	141	ASP	2.8
2	B	206	THR	2.8
4	R	6	THR	2.8
10	X	151	ASP	2.8
9	I	150	GLU	2.8
11	Y	67	GLU	2.8
3	Q	176	ASN	2.8
8	V	153	LYS	2.8
14	N	106	ASN	2.8
2	B	147	LEU	2.8
9	W	128	CYS	2.8
8	V	57	GLN	2.8
12	L	1	GLN	2.8
4	D	166	SER	2.8
4	R	229	ALA	2.8
7	G	46	SER	2.8
7	U	151	ALA	2.8
13	a	113	ALA	2.8
1	O	229	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	52	THR	2.8
3	C	231	VAL	2.8
2	B	70	ASP	2.8
3	Q	29	THR	2.8
6	T	132	THR	2.8
6	T	219	GLU	2.8
6	T	234	GLU	2.8
1	O	196	LEU	2.8
2	P	177	MET	2.8
6	T	212	ILE	2.8
13	M	211	ASN	2.8
6	T	197	TYR	2.8
3	C	189	CYS	2.8
4	D	75	ALA	2.8
4	R	161	ALA	2.8
5	S	43	ALA	2.8
7	G	204	ALA	2.8
13	M	75	ALA	2.8
8	H	196	ARG	2.8
4	R	199	VAL	2.8
7	G	33	SER	2.8
12	Z	167	LYS	2.8
2	B	241	THR	2.8
2	P	244	THR	2.8
8	H	73	GLU	2.8
11	K	151	GLU	2.8
11	Y	182	GLU	2.8
12	Z	27	THR	2.8
1	O	230	ASP	2.8
4	R	63	ASP	2.8
5	E	6	ASP	2.8
6	T	236	ILE	2.8
7	G	182	ILE	2.8
7	U	3	TYR	2.8
2	B	30	HIS	2.8
2	B	192	ALA	2.8
4	R	64	ARG	2.8
6	T	192	ALA	2.8
1	A	76	SER	2.8
2	P	169	SER	2.8
4	R	107	SER	2.8
5	S	72	SER	2.8

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Mol	Chain	Res	Type	RSRZ
6	F	175	LEU	2.8
7	G	136	SER	2.8
1	A	184	GLU	2.8
2	B	84	GLU	2.8
3	Q	209	GLU	2.8
6	F	173	GLU	2.8
8	H	185	GLU	2.8
7	G	190	TRP	2.7
11	Y	146	TRP	2.7
5	S	113	ASP	2.7
13	a	224	ASP	2.7
6	T	60	ASN	2.7
6	F	74	TYR	2.7
14	N	102	TYR	2.7
1	A	17	LYS	2.7
3	C	205	ALA	2.7
14	N	180	ALA	2.7
2	B	58	GLN	2.7
4	R	213	CYS	2.7
3	C	169	VAL	2.7
4	D	185	LEU	2.7
1	A	37	ILE	2.7
2	B	169	SER	2.7
1	A	33	THR	2.7
3	Q	181	GLU	2.7
6	F	219	GLU	2.7
9	I	78	GLU	2.7
9	I	126	ILE	2.7
9	I	129	ILE	2.7
4	R	34	THR	2.7
1	A	42	GLY	2.7
14	N	182	GLY	2.7
3	Q	178	ASP	2.7
3	C	4	ARG	2.7
10	J	95	ARG	2.7
4	D	233	LYS	2.7
5	E	40	ASN	2.7
5	E	168	LYS	2.7
11	Y	145	LYS	2.7
3	Q	186	VAL	2.7
1	A	238	LEU	2.7
1	O	105	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	Q	39	CYS	2.7
7	G	232	ILE	2.7
7	U	63	ILE	2.7
12	Z	86	ILE	2.7
3	C	188	GLU	2.7
8	H	198	GLU	2.7
12	Z	179	GLU	2.7
5	S	7	GLY	2.7
13	a	138	SER	2.7
14	b	179	THR	2.7
2	P	4	ARG	2.7
3	Q	46	ARG	2.7
6	T	16	ARG	2.7
2	B	19	TYR	2.7
5	S	155	LEU	2.7
4	R	152	PRO	2.7
8	H	220	ILE	2.7
2	B	26	GLU	2.7
3	Q	174	GLU	2.7
4	D	202	GLU	2.7
4	R	189	GLU	2.7
5	E	7	GLY	2.7
5	E	166	GLY	2.7
6	T	113	GLY	2.7
8	V	73	GLU	2.7
1	O	40	THR	2.7
1	O	60	THR	2.7
5	E	173	ARG	2.7
11	Y	48	GLY	2.7
1	O	146	SER	2.7
4	D	238	LYS	2.7
4	R	197	LYS	2.7
9	W	4	SER	2.7
5	S	8	ASP	2.7
7	U	40	ASP	2.7
10	J	73	TYR	2.7
2	B	164	VAL	2.7
5	E	46	VAL	2.7
6	F	232	LEU	2.7
6	T	49	LEU	2.7
7	U	137	VAL	2.7
12	Z	108	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
7	U	172	ASN	2.7
6	F	212	ILE	2.7
7	U	166	GLN	2.7
2	B	50	LYS	2.7
3	C	85	GLU	2.7
6	T	30	GLY	2.7
10	J	110	LYS	2.7
2	B	89	THR	2.7
2	P	80	THR	2.7
3	C	29	THR	2.7
2	P	53	SER	2.7
5	S	149	SER	2.7
6	T	152	SER	2.7
10	X	26	SER	2.7
4	R	133	ALA	2.7
5	S	191	ALA	2.7
14	b	181	ALA	2.7
4	D	204	LEU	2.7
11	Y	200	VAL	2.7
4	R	142	ASP	2.7
10	X	72	ASP	2.7
7	U	114	ASN	2.7
7	U	175	ASN	2.7
3	Q	16	PHE	2.6
1	A	166	LYS	2.6
3	Q	175	LYS	2.6
2	P	15	GLU	2.6
7	G	168	GLU	2.6
7	U	38	GLY	2.6
14	N	192	GLU	2.6
6	T	38	CYS	2.6
3	Q	231	VAL	2.6
4	R	185	LEU	2.6
6	T	170	ALA	2.6
8	V	61	SER	2.6
14	b	27	ALA	2.6
10	X	108	ASP	2.6
11	K	147	ASP	2.6
12	Z	26	ASP	2.6
13	M	124	ASP	2.6
12	Z	1	GLN	2.6
14	b	195	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
13	a	38	GLY	2.6
1	O	184	GLU	2.6
3	C	19	GLU	2.6
7	G	208	GLU	2.6
4	D	215	THR	2.6
6	T	220	THR	2.6
12	Z	136	CYS	2.6
2	B	170	ALA	2.6
3	C	62	VAL	2.6
8	H	195	VAL	2.6
14	b	34	LEU	2.6
3	C	158	SER	2.6
7	G	144	SER	2.6
9	I	4	SER	2.6
10	X	17	SER	2.6
2	B	5	TYR	2.6
1	O	246	ARG	2.6
2	B	124	HIS	2.6
4	D	12	ARG	2.6
4	R	222	ILE	2.6
5	S	212	ILE	2.6
6	F	228	LYS	2.6
8	H	153	LYS	2.6
2	P	141	ASP	2.6
4	R	54	ASP	2.6
10	J	72	ASP	2.6
12	L	210	ASP	2.6
12	Z	117	ASP	2.6
2	P	120	GLY	2.6
5	S	16	GLY	2.6
6	F	229	GLY	2.6
9	I	127	GLY	2.6
1	O	176	GLU	2.6
4	R	10	GLU	2.6
12	Z	218	GLU	2.6
2	P	51	VAL	2.6
7	U	199	THR	2.6
1	A	246	ARG	2.6
2	B	194	LYS	2.6
2	P	217	LYS	2.6
4	D	236	LYS	2.6
4	R	78	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
6	T	139	LYS	2.6
7	G	165	LYS	2.6
7	U	49	LYS	2.6
1	A	133	SER	2.6
2	P	7	SER	2.6
3	C	74	SER	2.6
9	W	142	SER	2.6
1	O	187	ASP	2.6
2	P	187	ASP	2.6
14	b	103	ASP	2.6
1	A	244	ASN	2.6
1	O	16	GLY	2.6
6	F	39	ASN	2.6
8	V	194	ASN	2.6
9	W	156	ASN	2.6
12	L	10	GLY	2.6
2	P	26	GLU	2.6
6	F	28	GLU	2.6
7	U	191	GLU	2.6
1	A	161	ALA	2.6
5	E	230	ALA	2.6
5	E	50	ARG	2.6
7	G	226	THR	2.6
12	Z	192	THR	2.6
3	Q	30	CYS	2.6
11	K	211	ILE	2.6
1	A	62	SER	2.6
1	O	219	PRO	2.6
4	D	71	SER	2.6
4	R	53	SER	2.6
4	R	220	PHE	2.6
7	G	11	SER	2.6
2	P	58	GLN	2.6
3	Q	120	GLN	2.6
1	A	70	ASP	2.6
4	R	170	GLY	2.6
1	A	180	ASN	2.6
3	C	66	ASP	2.6
3	Q	77	ASN	2.6
9	I	172	ASN	2.6
13	a	48	ASN	2.6
6	T	183	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	190	GLU	2.6
13	a	73	GLU	2.6
13	a	175	GLU	2.6
6	T	186	ARG	2.6
14	b	143	ARG	2.6
7	G	199	THR	2.6
13	M	207	THR	2.6
7	G	239	ILE	2.5
3	C	177	TYR	2.5
2	P	29	SER	2.5
3	Q	224	SER	2.5
7	U	210	SER	2.5
8	H	156	SER	2.5
13	a	13	SER	2.5
3	C	198	LEU	2.5
1	O	205	ASN	2.5
3	C	54	ASP	2.5
3	Q	139	ARG	2.5
2	B	22	GLU	2.5
3	Q	190	VAL	2.5
4	D	218	ASP	2.5
6	F	25	LYS	2.5
7	U	194	VAL	2.5
11	K	143	ASN	2.5
12	Z	165	ASN	2.5
5	E	194	GLU	2.5
8	V	53	GLU	2.5
13	a	64	GLU	2.5
13	a	210	LYS	2.5
14	N	105	LYS	2.5
5	S	162	ALA	2.5
7	U	198	ILE	2.5
5	E	139	SER	2.5
5	S	150	GLY	2.5
6	F	33	SER	2.5
10	X	12	SER	2.5
14	N	195	GLN	2.5
1	O	166	LYS	2.5
2	B	44	VAL	2.5
6	F	176	VAL	2.5
7	G	135	VAL	2.5
1	A	143	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	184	ALA	2.5
4	D	230	GLU	2.5
6	F	47	GLU	2.5
9	I	160	GLU	2.5
10	J	159	ASP	2.5
14	b	149	GLU	2.5
4	R	30	ILE	2.5
2	B	200	THR	2.5
11	K	30	THR	2.5
6	F	208	PHE	2.5
5	S	42	HIS	2.5
4	D	3	GLY	2.5
5	E	163	ARG	2.5
8	H	204	LYS	2.5
9	I	125	LEU	2.5
14	N	107	LYS	2.5
4	R	68	CYS	2.5
8	H	144	GLN	2.5
11	Y	63	CYS	2.5
4	R	181	SER	2.5
14	N	129	SER	2.5
14	N	147	SER	2.5
4	D	192	VAL	2.5
6	F	130	VAL	2.5
2	B	81	ALA	2.5
3	C	165	ASN	2.5
4	R	160	ASN	2.5
6	T	29	ASN	2.5
12	L	80	ASN	2.5
12	Z	36	ASN	2.5
13	a	199	ILE	2.5
6	F	51	THR	2.5
8	V	192	THR	2.5
13	a	168	THR	2.5
1	O	5	TYR	2.5
3	C	61	LYS	2.5
3	Q	222	LEU	2.5
5	S	17	ARG	2.5
6	F	53	LYS	2.5
8	H	114	HIS	2.5
13	M	226	LYS	2.5
4	R	116	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
13	a	118	GLY	2.5
1	A	188	ALA	2.5
3	C	224	SER	2.5
13	M	81	ALA	2.5
7	U	139	GLU	2.5
10	X	4	ILE	2.5
2	B	177	MET	2.5
4	D	207	ASN	2.5
5	E	4	ASN	2.5
10	J	151	ASP	2.5
12	Z	200	ASP	2.5
3	C	131	THR	2.5
8	H	214	LYS	2.5
9	I	117	LYS	2.5
7	G	173	LEU	2.5
12	Z	33	TYR	2.5
1	O	165	GLY	2.5
14	N	130	GLY	2.5
4	D	32	ILE	2.4
12	Z	37	SER	2.4
5	S	105	GLU	2.4
7	G	13	GLU	2.4
8	V	215	GLU	2.4
14	N	144	GLU	2.4
2	P	17	ARG	2.4
3	C	77	ASN	2.4
3	C	191	LYS	2.4
3	Q	216	ASP	2.4
7	G	111	ARG	2.4
12	L	222	ASP	2.4
13	M	37	ASN	2.4
6	F	120	THR	2.4
13	a	220	ASP	2.4
13	a	206	LEU	2.4
12	L	108	HIS	2.4
3	C	212	VAL	2.4
7	G	38	GLY	2.4
1	A	170	ALA	2.4
4	D	217	GLN	2.4
2	P	190	GLU	2.4
5	E	72	SER	2.4
8	H	53	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
11	Y	18	SER	2.4
12	Z	116	GLU	2.4
4	R	156	PHE	2.4
3	C	164	ARG	2.4
6	F	174	LYS	2.4
7	U	221	LYS	2.4
3	Q	192	LEU	2.4
3	Q	198	LEU	2.4
5	S	184	ASN	2.4
2	B	41	ASP	2.4
7	G	120	THR	2.4
8	H	120	ASP	2.4
13	a	17	ASP	2.4
14	N	39	ASP	2.4
14	N	67	THR	2.4
9	W	118	PRO	2.4
1	O	139	HIS	2.4
13	a	31	GLY	2.4
3	C	134	ALA	2.4
5	S	103	ALA	2.4
6	F	185	ALA	2.4
4	R	198	GLN	2.4
11	Y	89	GLN	2.4
13	a	231	GLN	2.4
11	Y	32	LYS	2.4
3	C	99	GLU	2.4
3	Q	45	GLU	2.4
4	R	17	GLU	2.4
5	E	146	PHE	2.4
6	T	209	GLU	2.4
8	V	150	GLU	2.4
4	R	168	SER	2.4
5	E	211	SER	2.4
10	X	39	SER	2.4
3	C	192	LEU	2.4
11	Y	41	LEU	2.4
1	A	162	THR	2.4
11	K	146	TRP	2.4
7	G	175	ASN	2.4
7	U	30	ASN	2.4
8	V	9	ASN	2.4
9	I	37	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	181	ASP	2.4
1	A	232	GLY	2.4
4	R	91	HIS	2.4
5	S	216	GLY	2.4
7	G	153	TYR	2.4
9	W	16	GLY	2.4
13	M	31	GLY	2.4
3	Q	112	ALA	2.4
6	T	239	ALA	2.4
5	E	147	GLN	2.4
6	F	190	LYS	2.4
3	C	172	PHE	2.4
1	A	210	GLU	2.4
4	D	183	LEU	2.4
5	E	210	LEU	2.4
5	S	26	GLU	2.4
1	A	53	SER	2.4
4	R	55	SER	2.4
6	T	215	CYS	2.4
3	Q	62	VAL	2.4
4	R	39	VAL	2.4
5	S	10	VAL	2.4
7	G	148	THR	2.4
1	O	41	ASN	2.4
3	Q	13	GLY	2.4
9	W	2	ASP	2.4
9	W	175	ASP	2.4
13	M	220	ASP	2.4
4	R	150	ALA	2.4
5	S	28	ILE	2.4
8	V	37	ILE	2.4
8	V	133	ALA	2.4
9	W	129	ILE	2.4
2	P	50	LYS	2.4
2	P	240	LYS	2.4
7	U	179	LYS	2.4
9	I	17	LYS	2.4
9	W	117	LYS	2.4
12	L	167	LYS	2.4
5	S	38	ARG	2.4
2	P	174	LEU	2.4
5	S	210	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	171	GLU	2.4
7	G	195	GLU	2.4
11	K	72	GLU	2.4
6	T	131	SER	2.4
7	U	51	PRO	2.4
12	Z	128	VAL	2.4
5	E	206	THR	2.3
5	S	183	GLY	2.3
1	A	227	ILE	2.3
1	O	209	ILE	2.3
2	B	234	ILE	2.3
2	P	19	TYR	2.3
3	C	195	ARG	2.3
3	Q	205	ALA	2.3
4	D	222	ILE	2.3
6	F	100	LYS	2.3
7	G	231	ASN	2.3
10	X	62	ALA	2.3
12	L	49	ASN	2.3
7	G	17	TYR	2.3
13	a	124	ASP	2.3
1	O	30	GLN	2.3
3	C	120	GLN	2.3
4	R	196	LEU	2.3
6	F	238	PHE	2.3
8	H	200	GLN	2.3
1	O	59	GLU	2.3
12	Z	178	GLU	2.3
6	F	10	VAL	2.3
6	T	46	VAL	2.3
5	E	164	SER	2.3
6	F	167	SER	2.3
7	U	228	SER	2.3
3	C	36	GLY	2.3
4	D	167	GLY	2.3
9	I	53	THR	2.3
13	M	232	LYS	2.3
3	Q	57	ILE	2.3
10	X	95	ARG	2.3
1	A	190	HIS	2.3
5	E	80	ALA	2.3
6	T	188	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	Q	110	TYR	2.3
11	Y	143	ASN	2.3
11	Y	208	ASN	2.3
6	F	110	ASP	2.3
14	N	32	ASP	2.3
1	A	194	LEU	2.3
4	D	130	PHE	2.3
4	R	13	LEU	2.3
7	G	236	LEU	2.3
13	a	146	PHE	2.3
1	O	182	GLU	2.3
7	G	187	GLU	2.3
9	W	193	GLU	2.3
11	Y	195	GLU	2.3
3	C	41	VAL	2.3
7	G	50	VAL	2.3
14	N	9	LYS	2.3
1	A	34	SER	2.3
2	P	115	SER	2.3
3	C	57	ILE	2.3
5	S	108	GLY	2.3
7	U	163	GLY	2.3
8	V	60	GLY	2.3
12	L	130	SER	2.3
13	M	229	GLY	2.3
3	C	119	THR	2.3
4	D	240	ALA	2.3
7	G	219	ALA	2.3
13	a	230	THR	2.3
10	J	147	HIS	2.3
10	J	174	MET	2.3
12	L	136	CYS	2.3
4	R	147	LEU	2.3
5	E	151	ASN	2.3
6	F	123	ASN	2.3
6	T	223	LEU	2.3
9	I	75	LEU	2.3
1	A	151	ASP	2.3
5	S	137	ASP	2.3
8	H	183	ASP	2.3
13	M	82	ASP	2.3
2	P	198	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
5	S	35	VAL	2.3
12	Z	168	VAL	2.3
13	a	106	LYS	2.3
2	P	209	ARG	2.3
2	P	231	PRO	2.3
4	D	49	PRO	2.3
5	E	28	ILE	2.3
6	T	196	ILE	2.3
8	V	180	ILE	2.3
4	R	166	SER	2.3
5	S	174	THR	2.3
6	T	7	SER	2.3
13	a	80	LEU	2.3
2	P	102	ASN	2.3
4	D	160	ASN	2.3
14	b	145	ASN	2.3
2	P	186	ASP	2.3
7	G	203	ASP	2.3
12	L	45	ASP	2.3
12	Z	81	ASP	2.3
1	O	50	LYS	2.3
12	Z	173	LYS	2.3
2	B	209	ARG	2.3
2	P	3	ARG	2.3
3	Q	142	GLU	2.3
11	Y	73	ARG	2.3
12	Z	18	GLU	2.3
2	P	92	ILE	2.3
3	C	182	PRO	2.3
3	C	219	ILE	2.3
7	U	202	ILE	2.3
1	A	138	GLY	2.3
5	E	75	GLY	2.3
5	E	157	GLY	2.3
6	T	23	ALA	2.3
6	T	26	ALA	2.3
7	G	123	ALA	2.3
3	Q	148	THR	2.3
4	D	125	LEU	2.3
5	S	158	THR	2.3
5	S	188	LEU	2.3
7	G	162	THR	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	220	THR	2.3
14	b	77	THR	2.3
1	O	34	SER	2.3
3	Q	80	SER	2.3
14	b	74	SER	2.3
2	P	225	TYR	2.3
12	Z	106	TYR	2.3
1	O	149	GLN	2.3
2	P	230	LYS	2.3
5	E	138	LYS	2.3
5	S	29	LYS	2.3
6	F	8	ASN	2.3
8	H	29	LYS	2.3
12	Z	29	ASN	2.3
7	G	235	ARG	2.3
11	K	9	GLN	2.3
1	A	207	ASP	2.3
7	U	44	VAL	2.3
9	I	161	ASP	2.3
9	W	161	ASP	2.3
10	X	2	ASP	2.3
14	b	10	ASP	2.3
7	U	230	GLU	2.2
7	U	234	GLU	2.2
7	U	239	ILE	2.2
1	O	54	PRO	2.2
4	R	67	GLY	2.2
4	R	72	GLY	2.2
4	R	141	ALA	2.2
5	E	150	GLY	2.2
6	T	127	PRO	2.2
5	S	47	ALA	2.2
5	S	80	ALA	2.2
7	G	125	MET	2.2
14	b	5	ALA	2.2
3	C	173	LEU	2.2
4	R	125	LEU	2.2
5	S	171	LEU	2.2
5	S	175	LEU	2.2
2	B	80	THR	2.2
3	Q	14	HIS	2.2
8	H	35	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
10	X	22	THR	2.2
6	T	9	SER	2.2
7	G	53	LYS	2.2
7	U	39	LYS	2.2
8	V	199	LYS	2.2
8	V	216	SER	2.2
9	I	1	SER	2.2
9	I	187	TYR	2.2
10	X	73	TYR	2.2
11	Y	104	TYR	2.2
1	A	205	ASN	2.2
1	O	180	ASN	2.2
3	Q	104	VAL	2.2
3	Q	228	ASN	2.2
6	T	233	GLN	2.2
8	H	165	ASN	2.2
5	S	67	GLU	2.2
5	S	182	ASP	2.2
7	U	4	ASP	2.2
13	M	201	ASP	2.2
5	E	134	ILE	2.2
8	H	25	ILE	2.2
5	E	228	ALA	2.2
8	V	181	GLY	2.2
8	V	213	LEU	2.2
14	b	117	GLY	2.2
4	D	227	LYS	2.2
6	F	194	LYS	2.2
7	U	177	PHE	2.2
7	U	211	LYS	2.2
12	Z	125	PHE	2.2
9	I	85	THR	2.2
11	Y	105	THR	2.2
12	Z	157	LYS	2.2
14	b	140	LYS	2.2
4	D	124	ARG	2.2
5	E	156	TYR	2.2
6	F	165	ARG	2.2
7	G	68	ARG	2.2
11	K	144	TYR	2.2
6	F	52	SER	2.2
7	U	144	SER	2.2

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Mol	Chain	Res	Type	RSRZ
8	H	20	SER	2.2
3	Q	200	VAL	2.2
5	E	215	VAL	2.2
8	V	55	VAL	2.2
13	M	119	VAL	2.2
13	a	213	GLN	2.2
12	Z	87	ASN	2.2
4	D	10	GLU	2.2
5	E	172	GLU	2.2
6	F	90	GLU	2.2
6	F	196	ILE	2.2
4	R	175	LEU	2.2
8	V	28	ASP	2.2
13	M	224	ASP	2.2
5	E	74	ALA	2.2
7	U	129	GLY	2.2
9	I	183	GLY	2.2
13	M	83	ALA	2.2
2	B	71	LYS	2.2
9	I	191	LYS	2.2
13	M	157	LYS	2.2
6	F	18	PHE	2.2
2	P	216	ARG	2.2
4	R	184	THR	2.2
7	G	176	HIS	2.2
13	a	204	THR	2.2
2	P	143	TYR	2.2
8	H	177	VAL	2.2
13	a	51	VAL	2.2
8	H	171	SER	2.2
7	G	47	GLN	2.2
8	V	149	GLU	2.2
10	X	127	GLU	2.2
13	a	122	ASN	2.2
8	H	146	LEU	2.2
14	N	150	GLU	2.2
14	b	144	GLU	2.2
3	C	183	PRO	2.2
11	Y	212	GLY	2.2
13	a	8	GLY	2.2
1	A	197	LYS	2.2
11	K	183	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
12	Z	222	ASP	2.2
13	M	167	LYS	2.2
14	b	83	LYS	2.2
3	Q	179	ARG	2.2
4	D	78	ARG	2.2
10	J	149	ARG	2.2
10	X	154	THR	2.2
2	P	107	VAL	2.2
8	H	90	TYR	2.2
13	a	91	TYR	2.2
14	b	6	VAL	2.2
3	Q	196	SER	2.2
3	Q	210	ILE	2.2
4	R	232	ILE	2.2
5	E	197	SER	2.2
6	T	33	SER	2.2
13	a	12	ILE	2.2
3	Q	149	GLU	2.2
4	D	17	GLU	2.2
4	D	234	GLU	2.2
5	E	67	GLU	2.2
1	A	172	LYS	2.2
5	S	27	ALA	2.2
6	F	107	ALA	2.2
6	T	140	ASN	2.2
7	U	197	ALA	2.2
11	Y	24	ASN	2.2
5	E	124	GLY	2.2
12	L	14	GLY	2.2
14	N	47	GLY	2.2
14	b	108	GLY	2.2
13	a	25	ASP	2.2
2	B	93	HIS	2.2
4	D	139	HIS	2.2
1	A	122	THR	2.1
5	E	41	THR	2.1
5	E	153	THR	2.1
4	R	32	ILE	2.1
8	H	163	ILE	2.1
5	S	147	GLN	2.1
2	B	197	SER	2.1
4	R	153	SER	2.1

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Mol	Chain	Res	Type	RSRZ
7	U	201	MET	2.1
12	Z	85	SER	2.1
13	a	68	LYS	2.1
1	O	178	ARG	2.1
2	P	22	GLU	2.1
3	Q	226	GLU	2.1
4	R	206	GLU	2.1
7	U	159	ALA	2.1
12	L	161	GLU	2.1
12	Z	40	GLU	2.1
14	b	88	GLU	2.1
2	B	120	GLY	2.1
3	Q	215	PRO	2.1
4	R	219	GLY	2.1
8	H	130	GLY	2.1
11	K	205	GLY	2.1
4	R	92	ASN	2.1
7	U	27	ASN	2.1
4	R	110	ASP	2.1
8	V	157	ASP	2.1
7	U	237	VAL	2.1
8	H	141	HIS	2.1
11	K	210	VAL	2.1
11	Y	150	VAL	2.1
5	E	11	THR	2.1
8	V	147	THR	2.1
11	Y	181	THR	2.1
1	A	243	ILE	2.1
3	C	162	ILE	2.1
8	V	123	TYR	2.1
3	Q	214	LYS	2.1
4	R	183	LEU	2.1
9	I	114	LYS	2.1
11	K	145	LYS	2.1
2	B	83	ALA	2.1
3	Q	159	ALA	2.1
1	O	210	GLU	2.1
3	C	1	GLY	2.1
3	C	63	SER	2.1
6	F	152	SER	2.1
11	Y	194	GLY	2.1
12	Z	130	SER	2.1

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Mol	Chain	Res	Type	RSRZ
13	M	44	PRO	2.1
5	E	51	ASN	2.1
9	I	7	ASN	2.1
11	Y	176	ASN	2.1
12	L	92	ASN	2.1
13	a	194	ASN	2.1
3	C	194	VAL	2.1
4	D	109	CYS	2.1
7	G	41	CYS	2.1
7	G	6	HIS	2.1
1	O	135	LEU	2.1
2	P	149	THR	2.1
2	P	157	THR	2.1
2	P	199	THR	2.1
4	R	135	LEU	2.1
5	S	224	TYR	2.1
6	F	183	LEU	2.1
6	F	204	LYS	2.1
6	T	105	ILE	2.1
6	T	153	TYR	2.1
7	U	54	LEU	2.1
10	J	162	LYS	2.1
13	a	43	ILE	2.1
2	B	39	ALA	2.1
2	P	170	ALA	2.1
3	Q	24	ALA	2.1
5	E	43	ALA	2.1
11	Y	50	ALA	2.1
14	N	24	ALA	2.1
2	B	158	GLY	2.1
4	R	57	GLU	2.1
4	R	82	GLU	2.1
6	F	205	GLU	2.1
7	U	208	GLU	2.1
9	I	139	GLY	2.1
11	K	195	GLU	2.1
11	Y	36	GLU	2.1
13	M	162	GLU	2.1
1	O	142	PHE	2.1
3	C	72	SER	2.1
5	E	178	PHE	2.1
5	S	39	SER	2.1

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Mol	Chain	Res	Type	RSRZ
5	S	95	SER	2.1
9	I	138	SER	2.1
12	Z	176	SER	2.1
11	K	115	VAL	2.1
2	P	180	LYS	2.1
2	P	56	LEU	2.1
2	P	93	HIS	2.1
8	H	199	LYS	2.1
7	U	173	LEU	2.1
1	O	208	THR	2.1
3	C	161	THR	2.1
14	N	143	ARG	2.1
12	Z	217	TYR	2.1
4	D	171	ALA	2.1
8	V	44	ALA	2.1
12	Z	89	ALA	2.1
13	a	222	ALA	2.1
4	R	172	GLN	2.1
5	E	135	GLY	2.1
9	W	110	GLY	2.1
10	J	24	GLY	2.1
13	M	205	GLY	2.1
1	A	182	GLU	2.1
6	F	148	GLU	2.1
7	U	164	PRO	2.1
12	L	178	GLU	2.1
1	O	168	SER	2.1
2	P	2	SER	2.1
4	R	127	SER	2.1
12	Z	53	SER	2.1
5	E	117	LYS	2.1
9	I	74	LYS	2.1
4	D	73	LEU	2.1
4	D	193	LEU	2.1
6	T	198	LEU	2.1
12	Z	110	ILE	2.1
13	M	80	LEU	2.1
14	b	196	LEU	2.1
2	B	104	ASP	2.1
6	F	67	ASP	2.1
6	T	67	ASP	2.1
6	F	38	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
10	J	148	TYR	2.1
12	Z	189	THR	2.1
4	R	29	ALA	2.1
4	R	240	ALA	2.1
7	U	84	ALA	2.1
4	D	138	GLY	2.1
6	T	64	GLN	2.1
9	W	31	GLN	2.1
1	O	48	GLU	2.1
6	T	28	GLU	2.1
8	V	121	VAL	2.0
9	I	38	LYS	2.0
13	a	157	LYS	2.0
14	b	9	LYS	2.0
3	Q	67	SER	2.0
5	E	84	SER	2.0
7	U	189	SER	2.0
4	R	176	LEU	2.0
5	E	223	ILE	2.0
6	F	121	LEU	2.0
8	V	196	ARG	2.0
4	D	173	ALA	2.0
5	E	66	ASP	2.0
5	S	79	ASP	2.0
5	S	156	TYR	2.0
6	T	32	THR	2.0
10	J	22	THR	2.0
10	J	30	ASP	2.0
11	K	22	ALA	2.0
12	L	151	ASP	2.0
12	Z	208	THR	2.0
13	M	160	ASP	2.0
14	N	20	THR	2.0
14	N	132	THR	2.0
14	b	22	THR	2.0
5	E	183	GLY	2.0
8	V	130	GLY	2.0
1	A	219	PRO	2.0
5	E	220	PRO	2.0
13	M	166	PRO	2.0
5	S	22	GLU	2.0
7	G	39	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
9	W	78	GLU	2.0
11	K	202	GLU	2.0
2	B	224	VAL	2.0
11	K	150	VAL	2.0
12	Z	65	VAL	2.0
13	M	135	VAL	2.0
1	A	175	LEU	2.0
2	P	25	LEU	2.0
2	P	193	LEU	2.0
11	Y	7	ARG	2.0
14	N	34	LEU	2.0
1	O	13	SER	2.0
3	C	208	ILE	2.0
6	F	218	SER	2.0
6	T	243	ILE	2.0
8	H	71	SER	2.0
10	X	136	SER	2.0
13	M	217	MET	2.0
13	a	18	ASN	2.0
13	a	179	ASN	2.0
4	R	86	THR	2.0
5	S	153	THR	2.0
6	T	193	ALA	2.0
11	K	155	TYR	2.0
14	N	179	THR	2.0
1	O	140	ASP	2.0
7	G	138	ASP	2.0
7	G	213	ASP	2.0
7	U	56	ASP	2.0
4	D	144	GLY	2.0
4	R	138	GLY	2.0
5	E	216	GLY	2.0
2	P	160	LYS	2.0
5	S	65	CYS	2.0
6	T	208	PHE	2.0
5	S	168	LYS	2.0
7	U	65	CYS	2.0
8	H	95	GLY	2.0
8	H	57	GLN	2.0
2	P	113	ARG	2.0
3	C	40	VAL	2.0
4	D	199	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
5	E	229	VAL	2.0
7	G	215	GLU	2.0
9	I	154	GLU	2.0
12	L	179	GLU	2.0
14	N	64	GLU	2.0
11	Y	106	ARG	2.0
6	T	217	LEU	2.0
7	G	214	LEU	2.0
2	P	87	ILE	2.0
5	E	196	ILE	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 oligosaccharides in this entry.

6.4 Ligands [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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
15	SO4	S	301	5/5	0.71	0.36	40,45,49,58	5
15	SO4	Q	301	5/5	0.72	0.28	36,43,48,57	5
15	SO4	K	304	5/5	0.74	0.30	77,93,132,139	0
15	SO4	a	301	5/5	0.74	0.29	43,44,51,68	5
15	SO4	E	301	5/5	0.75	0.26	37,44,50,67	5
15	SO4	M	303	5/5	0.75	0.22	64,65,72,107	0
15	SO4	J	202	5/5	0.75	0.31	40,47,70,79	5
15	SO4	T	301	5/5	0.79	0.27	73,86,101,122	0
15	SO4	X	201	5/5	0.79	0.26	31,41,47,65	5
15	SO4	L	303	5/5	0.79	0.32	54,60,108,123	0
15	SO4	a	304	5/5	0.79	0.29	48,65,90,91	0
15	SO4	F	302	5/5	0.80	0.29	64,86,111,139	0
15	SO4	C	301	5/5	0.82	0.18	45,46,57,71	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	SO4	Z	303	5/5	0.82	0.28	72,77,103,114	0
16	MG	Z	301	1/1	0.82	0.43	67,67,67,67	0
15	SO4	a	302	5/5	0.83	0.22	30,40,42,55	5
15	SO4	a	303	5/5	0.83	0.22	55,55,70,97	0
15	SO4	J	201	5/5	0.83	0.28	22,26,28,32	5
15	SO4	E	304	5/5	0.83	0.20	43,44,60,80	5
15	SO4	E	303	5/5	0.84	0.19	28,43,56,60	5
15	SO4	K	303	5/5	0.85	0.22	46,48,89,106	0
15	SO4	D	301	5/5	0.86	0.24	55,60,61,85	0
15	SO4	Z	302	5/5	0.86	0.28	66,76,100,119	0
15	SO4	M	301	5/5	0.86	0.22	25,26,48,50	5
15	SO4	F	301	5/5	0.86	0.24	52,57,84,92	0
15	SO4	L	302	5/5	0.87	0.16	38,48,65,92	0
15	SO4	H	302	5/5	0.88	0.22	32,34,40,54	5
15	SO4	S	302	5/5	0.88	0.22	32,33,44,48	5
15	SO4	P	301	5/5	0.88	0.24	33,36,54,60	5
15	SO4	V	302	5/5	0.88	0.24	32,38,42,65	5
15	SO4	N	203	5/5	0.89	0.20	23,35,52,61	5
16	MG	Y	301	1/1	0.89	0.20	29,29,29,29	1
15	SO4	G	301	5/5	0.89	0.19	23,30,59,65	5
15	SO4	I	302	5/5	0.90	0.19	37,41,69,73	5
15	SO4	U	301	5/5	0.90	0.17	41,54,65,105	0
15	SO4	M	302	5/5	0.90	0.23	63,63,93,95	0
15	SO4	P	302	5/5	0.91	0.20	47,66,92,95	0
15	SO4	B	301	5/5	0.91	0.21	46,49,83,97	0
15	SO4	M	304	5/5	0.92	0.24	52,54,57,71	0
15	SO4	G	302	5/5	0.92	0.18	69,69,118,122	0
16	MG	H	301	1/1	0.92	0.16	47,47,47,47	0
15	SO4	E	302	5/5	0.92	0.19	20,23,32,38	5
15	SO4	R	301	5/5	0.92	0.19	37,62,69,80	0
16	MG	L	301	1/1	0.93	0.10	17,17,17,17	0
16	MG	V	301	1/1	0.93	0.18	40,40,40,40	0
15	SO4	b	201	5/5	0.93	0.15	14,17,35,43	5
15	SO4	K	302	5/5	0.93	0.17	28,35,37,41	5
16	MG	W	301	1/1	0.94	0.14	23,23,23,23	0
15	SO4	N	201	5/5	0.94	0.15	18,19,21,29	5
16	MG	I	301	1/1	0.94	0.10	27,27,27,27	0
16	MG	K	301	1/1	0.95	0.09	27,27,27,27	0
15	SO4	H	303	5/5	0.95	0.16	36,37,51,53	5
16	MG	N	202	1/1	0.98	0.12	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.