Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2025 – 11:06 AM EDT

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 (i) symbol.

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

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

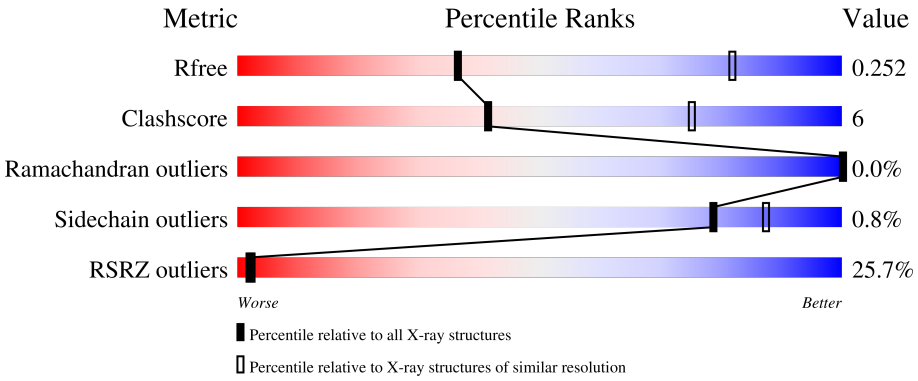
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.33 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}	164625	1325 (3.38-3.30)
Clashscore	180529	1376 (3.38-3.30)
Ramachandran outliers	177936	1376 (3.38-3.30)
Sidechain outliers	177891	1375 (3.38-3.30)
RSRZ outliers	164620	1325 (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 <=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	30% 85% 14%
1	O	250	26% 80% 20%
2	B	258	35% 79% 15% 6%
2	P	258	28% 78% 16% 5%
3	C	254	43% 74% 19% 7%

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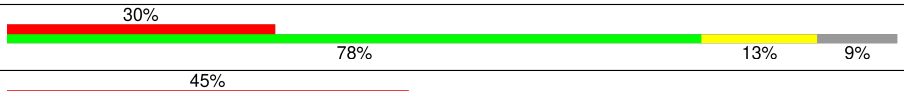
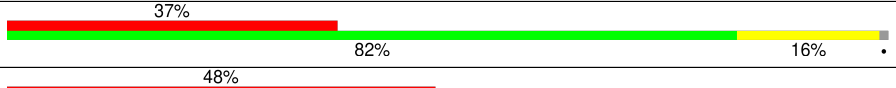
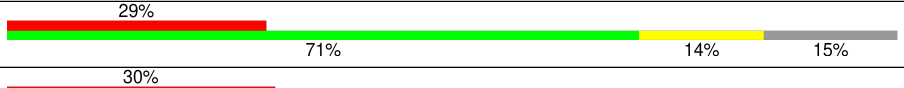
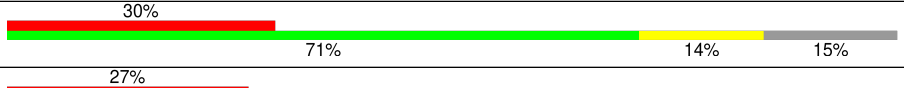
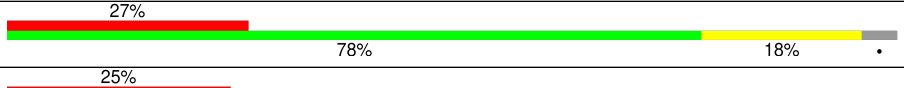
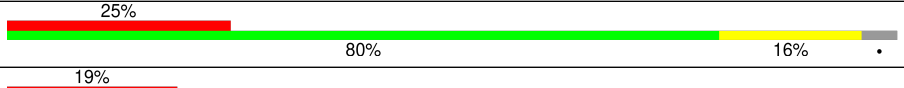
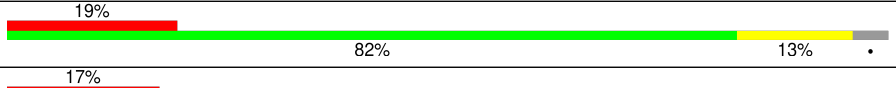
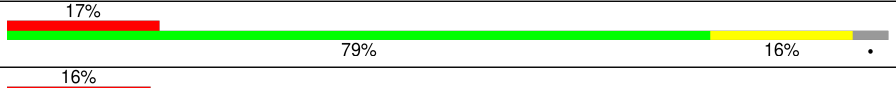
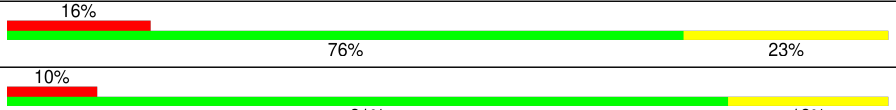
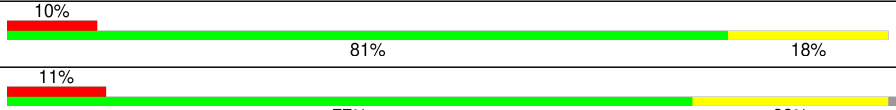
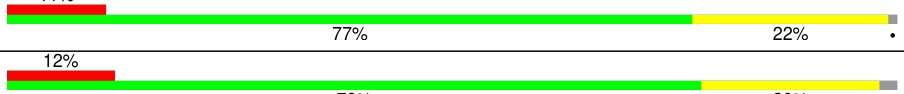
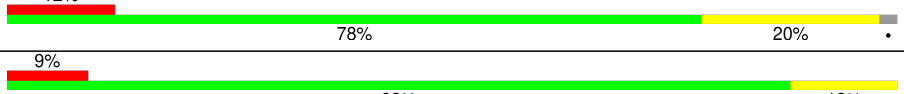
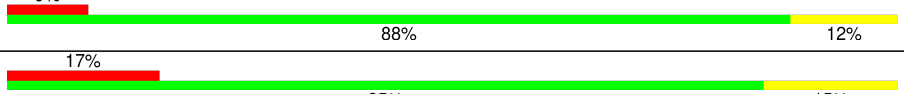
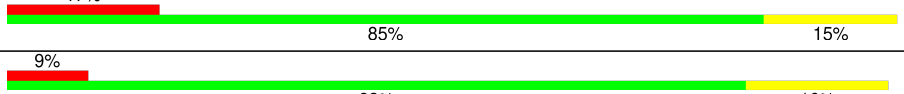
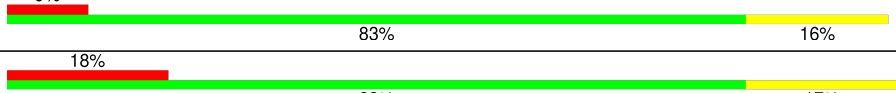
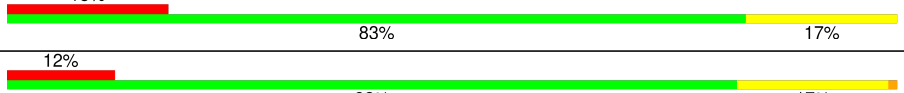
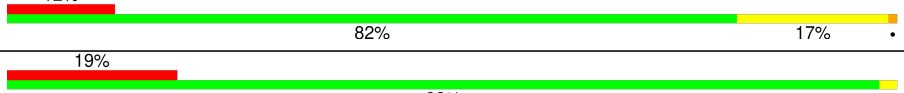
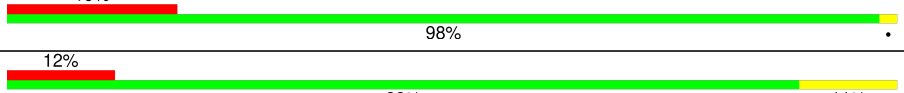
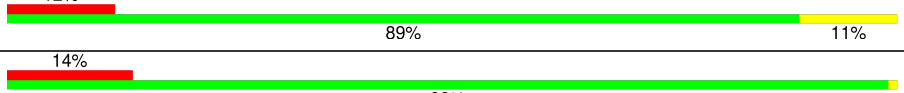
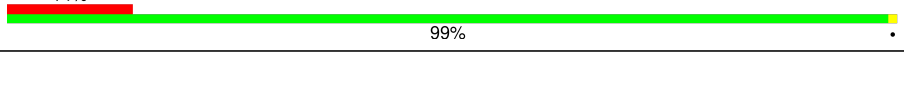
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	287	
6	T	287	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	

2 Entry composition (i)

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			

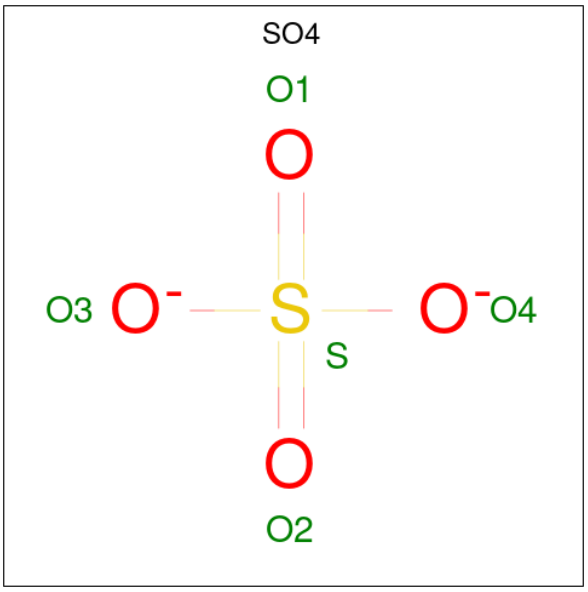
- Molecule 13 is a protein called Proteasome subunit beta.

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: O_4S).



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	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 5 4 1	0	0
15	S	1	Total O S 5 4 1	0	0
15	S	1	Total O S 5 4 1	0	0
15	T	1	Total O S 5 4 1	0	0
15	U	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	I	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	L	1	Total O S 5 4 1	0	0
15	L	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	N	1	Total O S 5 4 1	0	0
15	N	1	Total O S 5 4 1	0	0

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

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

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

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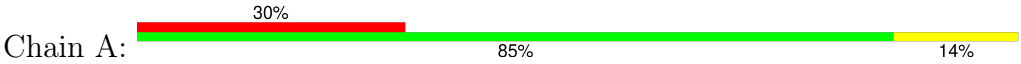
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	W	16	Total O 16 16	0	0
17	X	13	Total O 13 13	0	0
17	Y	7	Total O 7 7	0	0
17	Z	21	Total O 21 21	0	0
17	a	27	Total O 27 27	0	0
17	b	15	Total O 15 15	0	0

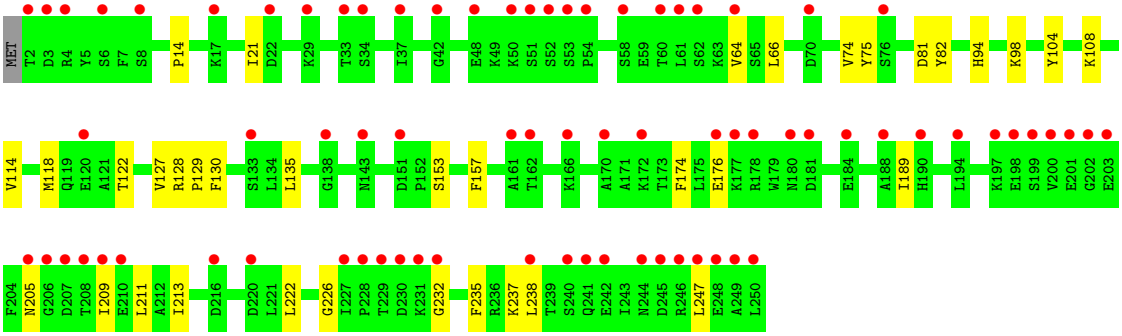
3 Residue-property plots (i)

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

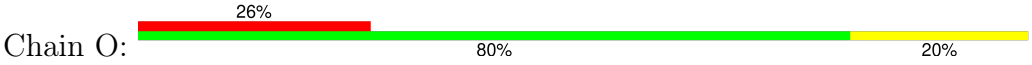
Chain A:

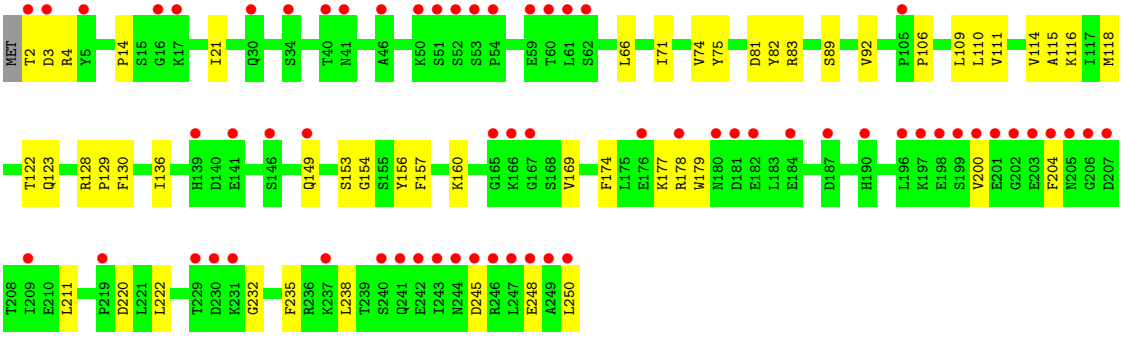




• Molecule 1: PRE8 isoform 1

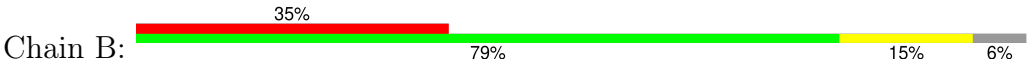
Chain O:

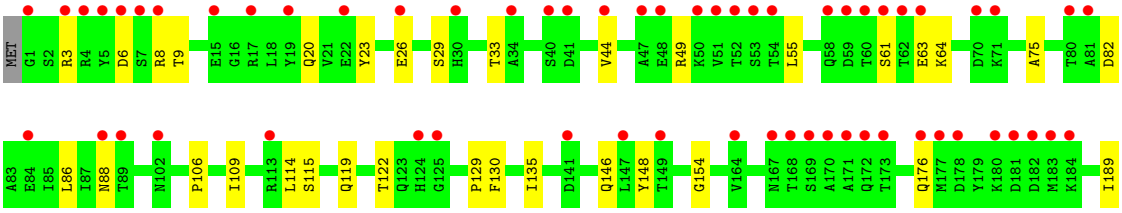


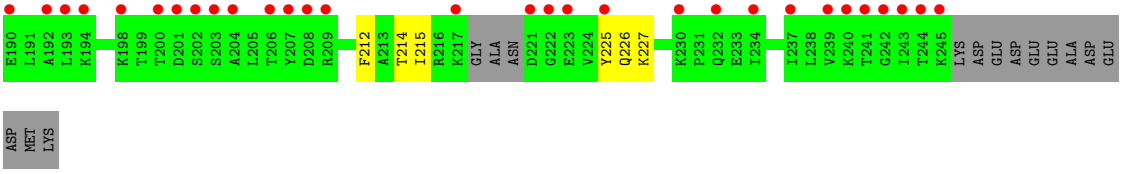


• Molecule 2: PRE9 isoform 1

Chain B:

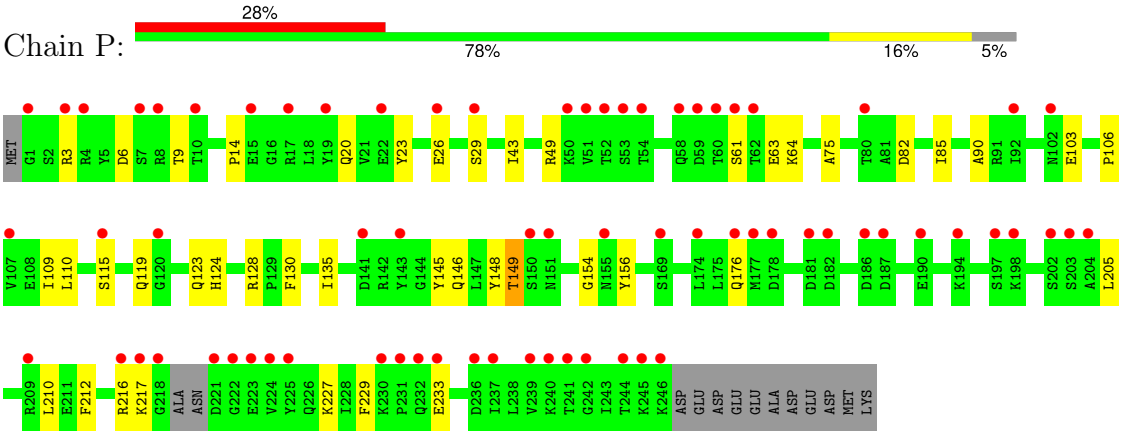






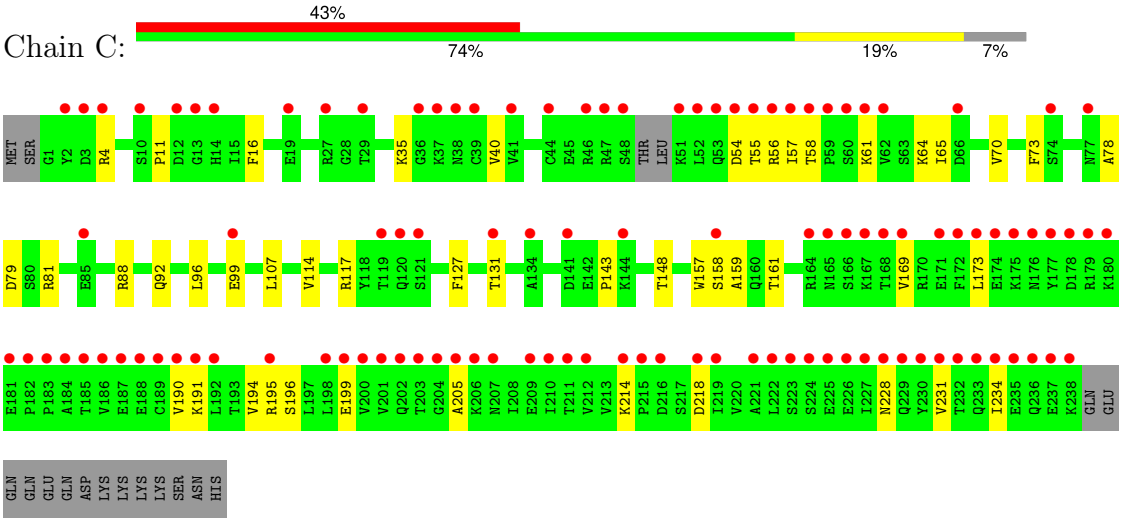
• Molecule 2: PRE9 isoform 1

Chain P:



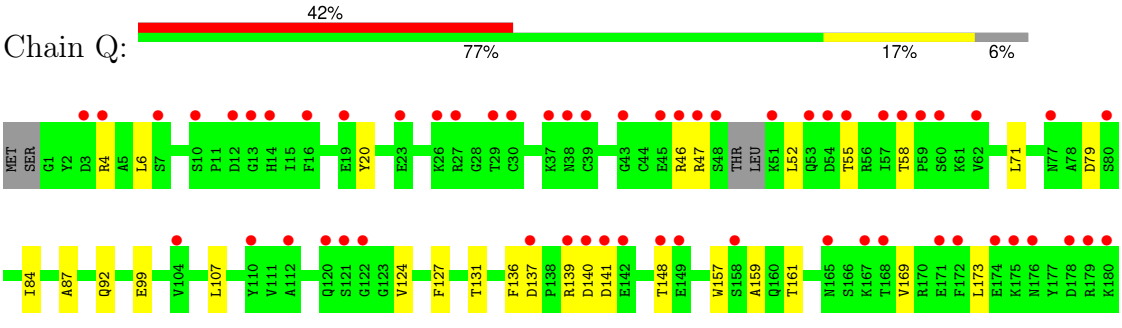
• Molecule 3: PRE6 isoform 1

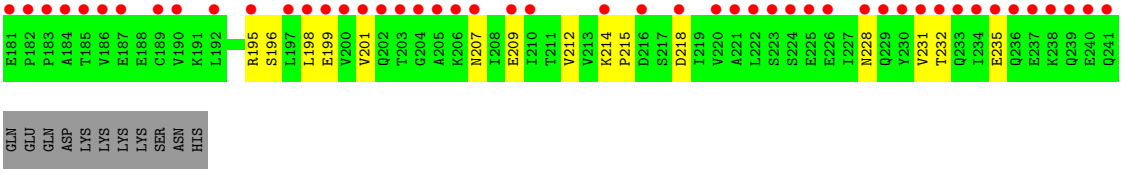
Chain C:



• Molecule 3: PRE6 isoform 1

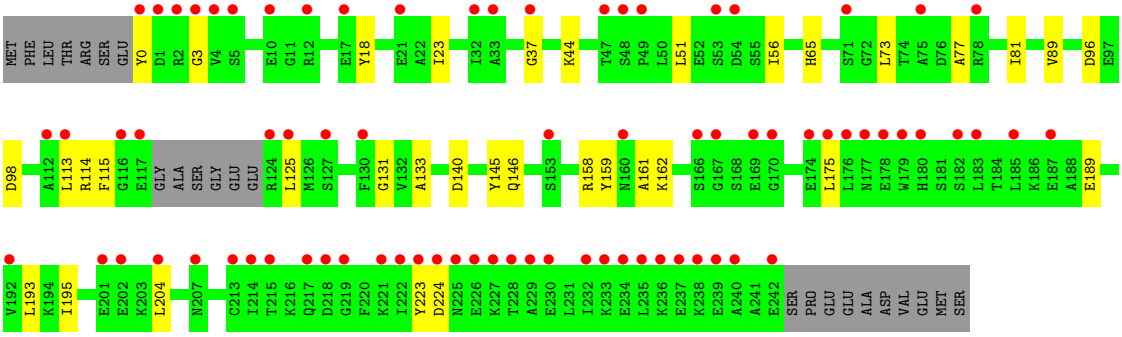
Chain Q:





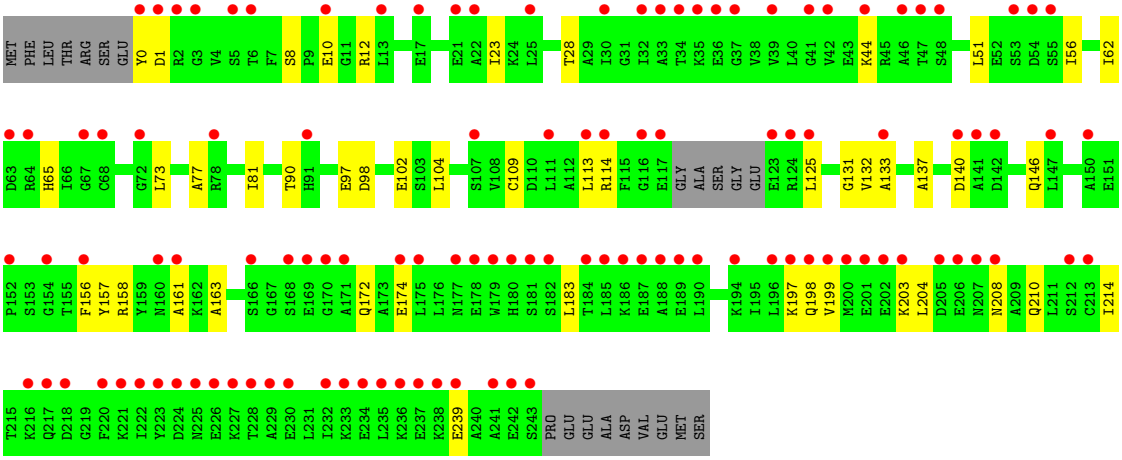
• Molecule 4: PUP2 isoform 1

Chain D:



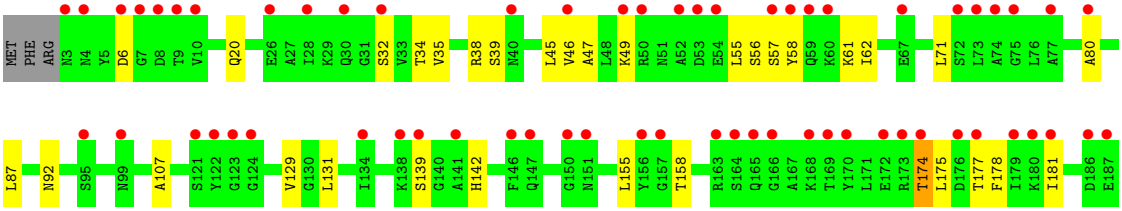
• Molecule 4: PUP2 isoform 1

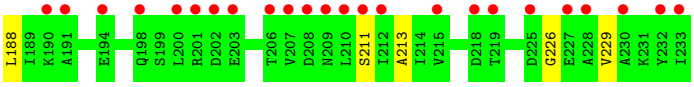
Chain R:



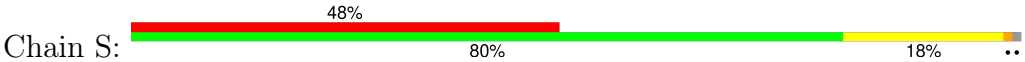
• Molecule 5: PRE5 isoform 1

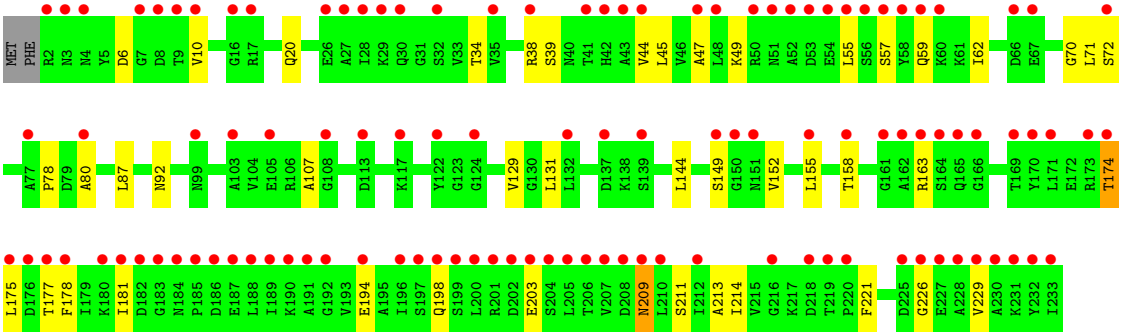
Chain E:



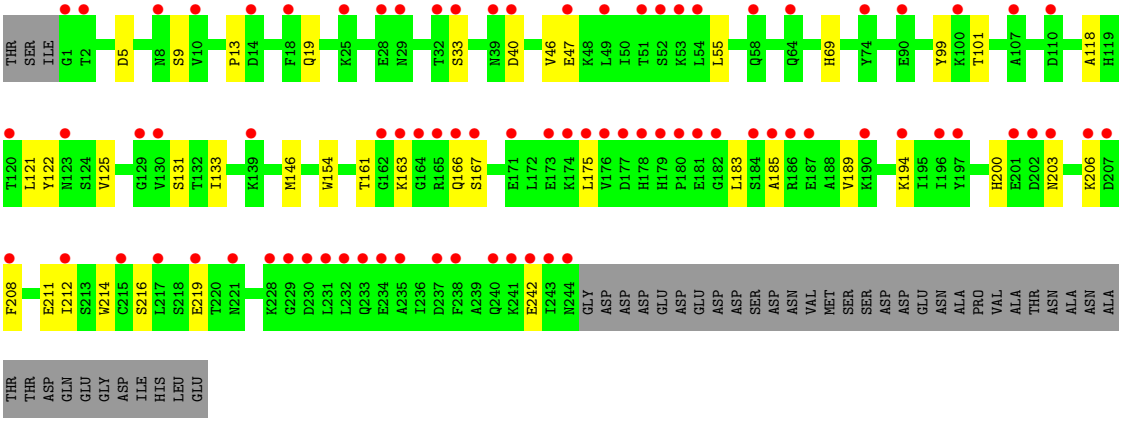


• Molecule 5: PRE5 isoform 1

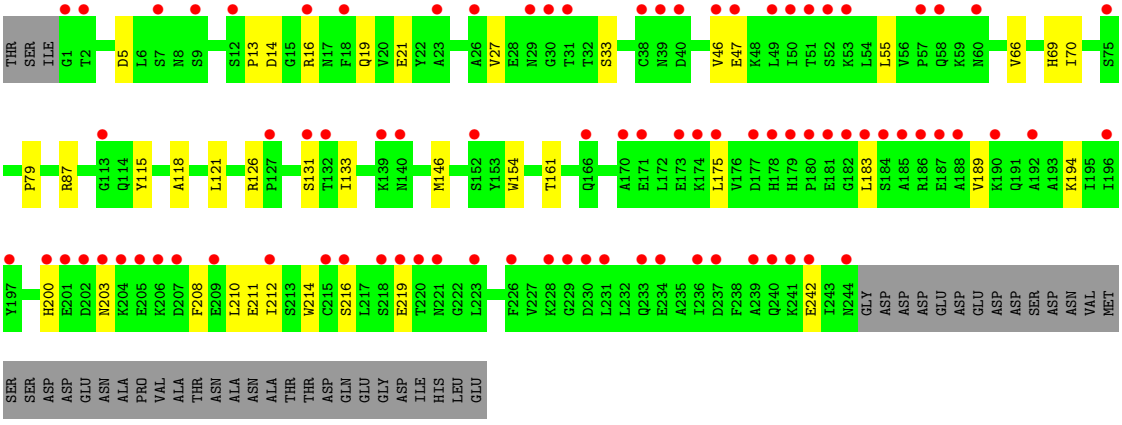




• Molecule 6: PRE10 isoform 1

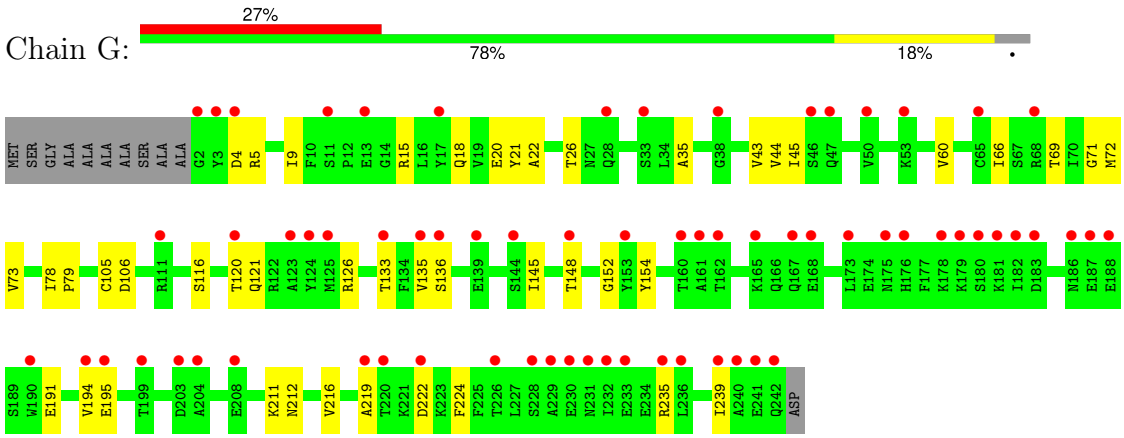


• Molecule 6: PRE10 isoform 1



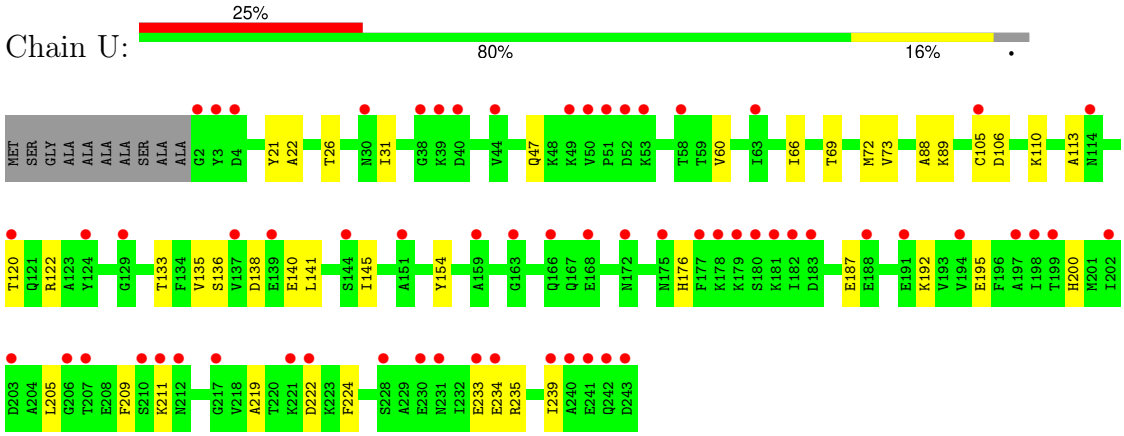
• Molecule 7: SCL1 isoform 1

Chain G:



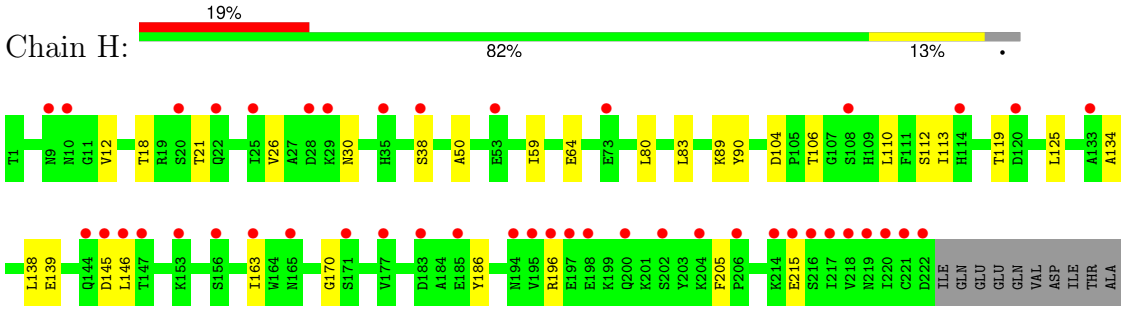
• Molecule 7: SCL1 isoform 1

Chain U:



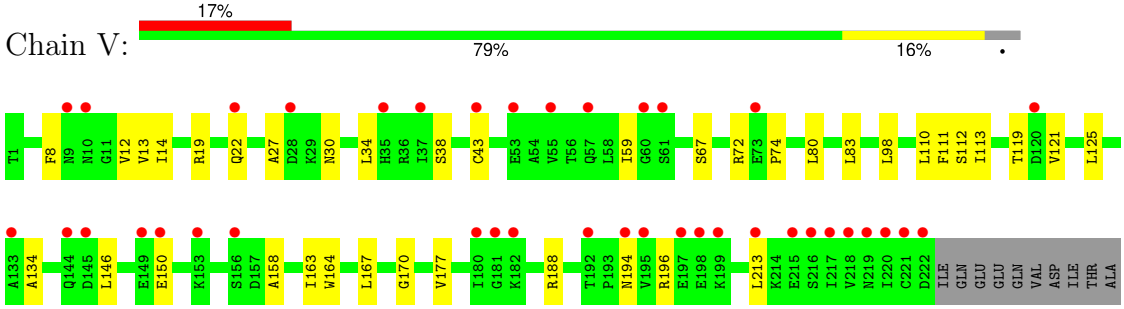
• Molecule 8: proteasome endopeptidase complex

Chain H:



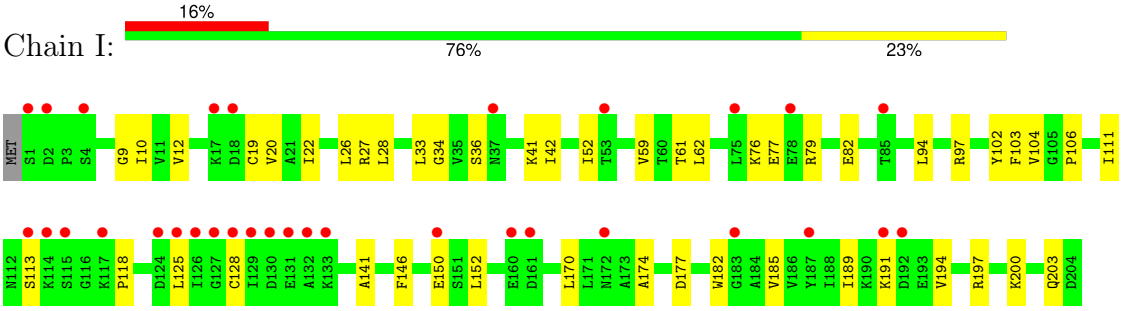
• Molecule 8: proteasome endopeptidase complex

Chain V:



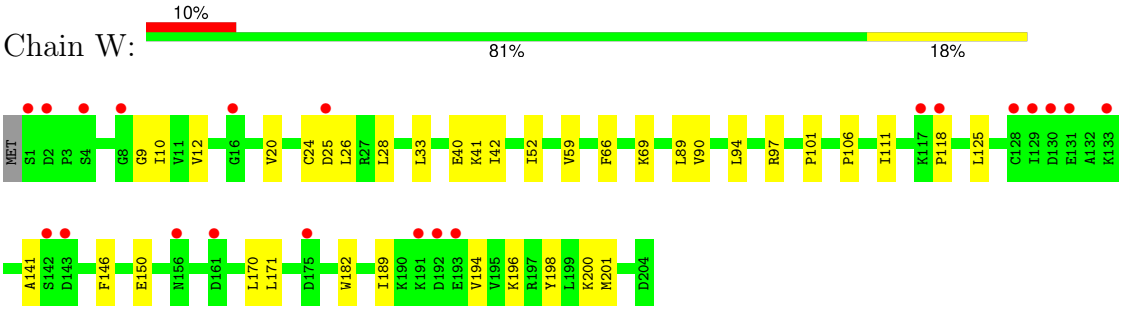
• Molecule 9: PUP3 isoform 1

Chain I:



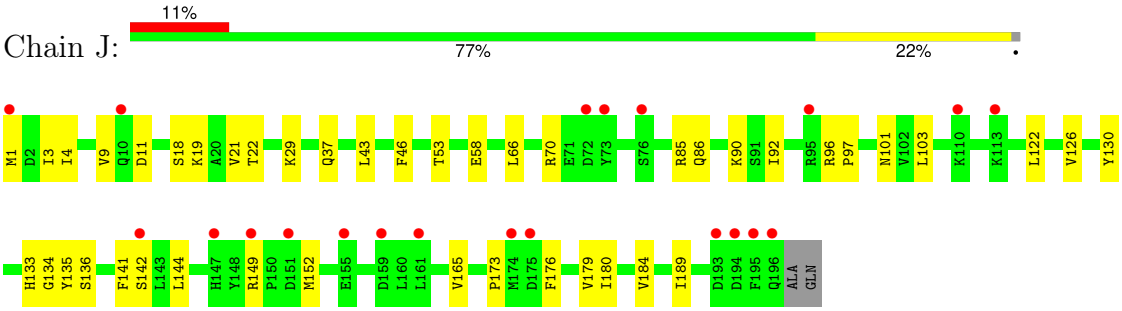
• Molecule 9: PUP3 isoform 1

Chain W:



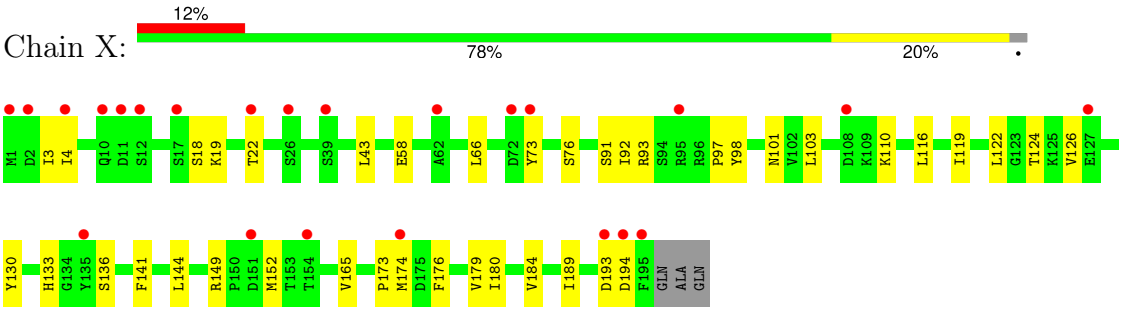
• Molecule 10: Proteasome subunit beta

Chain J:



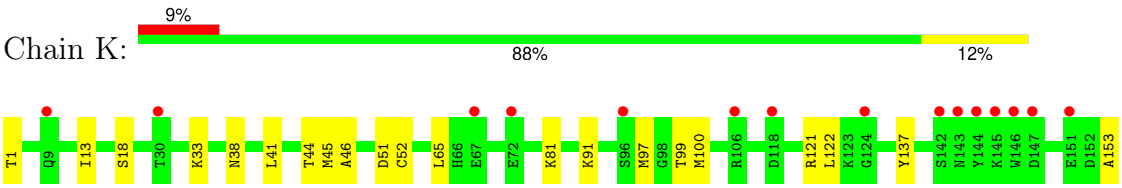
• Molecule 10: Proteasome subunit beta

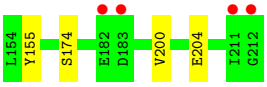
Chain X:



• Molecule 11: proteasome endopeptidase complex

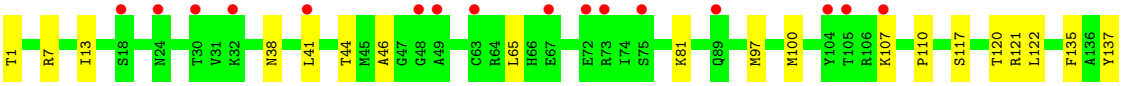
Chain K:





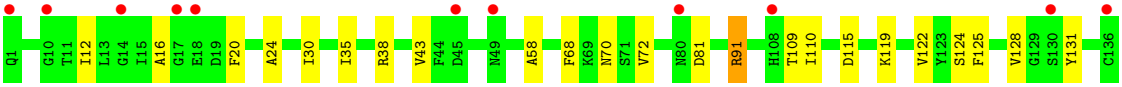
• Molecule 11: proteasome endopeptidase complex

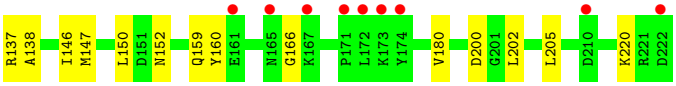
Chain Y:



• Molecule 12: PRE7 isoform 1

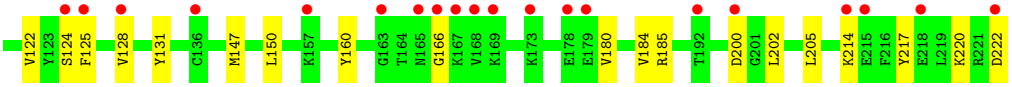
Chain L:





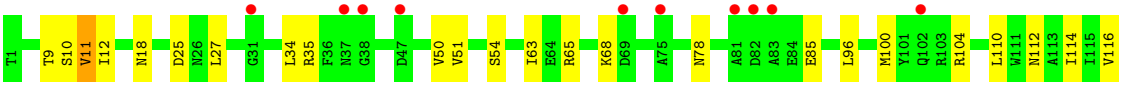
• Molecule 12: PRE7 isoform 1

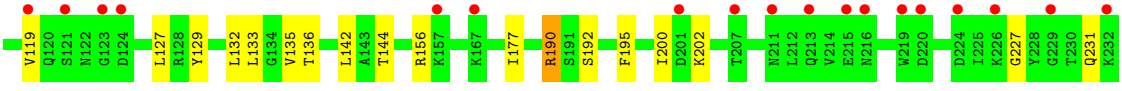
Chain Z:



• Molecule 13: Proteasome subunit beta

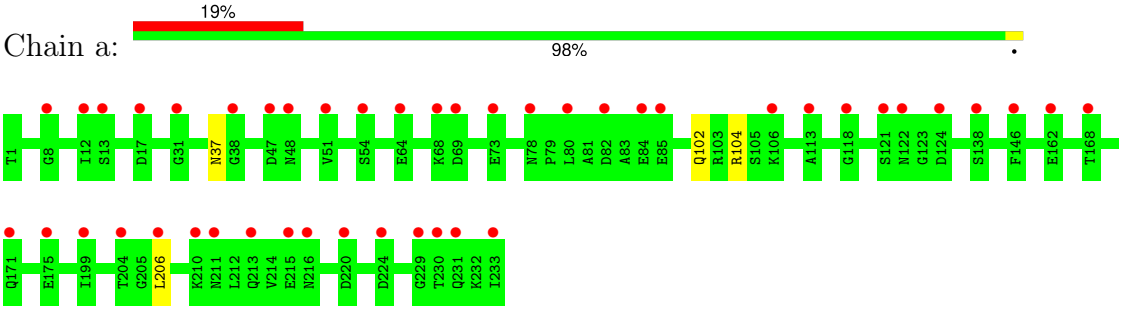
Chain M:





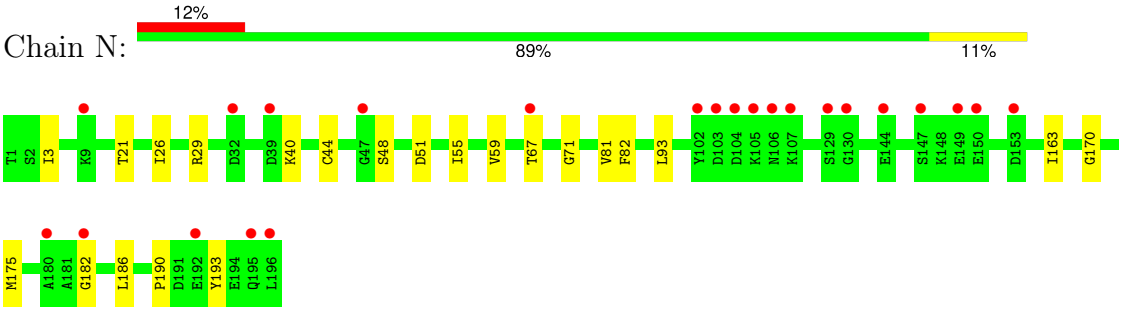
• Molecule 13: Proteasome subunit beta

Chain a:



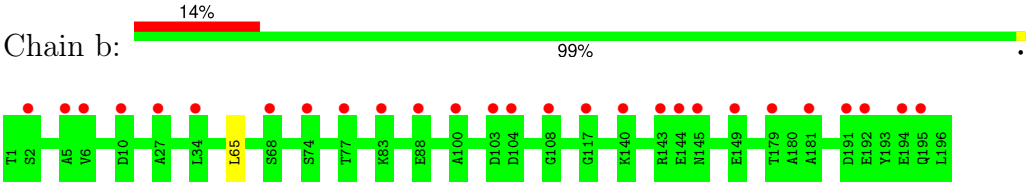
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	6918 reflections (5.05%)	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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.25	0/1944	0.47	0/2632
1	O	0.25	0/1944	0.47	0/2632
2	B	0.24	0/1923	0.48	0/2600
2	P	0.24	0/1938	0.49	0/2619
3	C	0.24	0/1876	0.49	0/2538
3	Q	0.24	0/1903	0.49	0/2574
4	D	0.24	0/1861	0.48	0/2507
4	R	0.24	0/1875	0.46	0/2526
5	E	0.24	0/1797	0.48	0/2429
5	S	0.24	0/1811	0.49	0/2447
6	F	0.25	0/1936	0.46	0/2614
6	T	0.25	0/1934	0.46	0/2611
7	G	0.25	0/1945	0.46	0/2634
7	U	0.26	0/1951	0.46	0/2641
8	H	0.24	0/1715	0.46	0/2326
8	V	0.25	0/1711	0.46	0/2321
9	I	0.25	0/1611	0.49	0/2174
9	W	0.25	0/1611	0.49	0/2174
10	J	0.25	0/1598	0.48	0/2154
10	X	0.25	0/1589	0.48	0/2142
11	K	0.25	0/1681	0.48	0/2274
11	Y	0.25	0/1681	0.47	0/2274
12	L	0.26	0/1795	0.49	0/2420
12	Z	0.25	0/1795	0.48	0/2420
13	M	0.25	0/1855	0.51	0/2514
13	a	0.25	0/1855	0.49	0/2514
14	N	0.24	0/1541	0.46	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.25	0/50217	0.48	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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1917	23	0
1	O	1907	0	1917	30	0
2	B	1894	0	1897	26	0
2	P	1909	0	1918	27	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	29	0
6	F	1896	0	1889	23	0
6	T	1894	0	1884	23	0
7	G	1907	0	1901	27	0
7	U	1913	0	1903	29	0
8	H	1684	0	1688	19	0
8	V	1680	0	1683	27	0
9	I	1581	0	1574	34	0
9	W	1581	0	1574	24	0
10	J	1570	0	1577	34	0
10	X	1561	0	1569	27	0
11	K	1644	0	1595	17	0
11	Y	1644	0	1595	20	0
12	L	1757	0	1711	23	0
12	Z	1757	0	1710	22	0
13	M	1824	0	1832	27	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	12	0
14	b	1512	0	1481	0	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	573	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 (573) 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
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
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
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	1.80	0.64
12:L:38:ARG:NH1	12:L:200:ASP:OD1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:66:ILE:HD11	7:G:72:MET:HE2	1.81	0.61
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
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
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
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
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
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
2:B:82:ASP:HB3	2:B:130:PHE:HD1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
10:J:1:MET:HE1	10:J:134:GLY:HA3	1.86	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
7:U:66:ILE:HD11	7:U:72:MET:HE2	1.88	0.55
8:H:104:ASP:OD1	8:H:106:THR:OG1	2.18	0.55
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
5:E:174:THR:HG22	5:E:177:THR:HB	1.88	0.55
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
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:159:ARG:HH12	11:Y:163:ALA:HB2	1.73	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
4:D:89:VAL:HG21	11:K:65:LEU:HG	1.91	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:125:LEU:H	9:W:125:LEU:HD23	1.78	0.48
6:T:194:LYS:HD2	6:T:242:GLU:HG3	1.94	0.48
11:K:155:TYR:OH	11:K:204:GLU:OE2	2.26	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:ILE:HG21	3:C:107:LEU:HD21	1.96	0.47
10:J:1:MET:HE1	10:J:135:TYR:H	1.79	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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:21:ILE:HD12	1:A:153:SER:HA	1.98	0.46
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
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
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
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
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
1:A:108:LYS:NZ	17:A:301:HOH:O	2.47	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:X:58:GLU:OE1	11:Y:81:LYS:NZ	2.35	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
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
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
1:A:104:TYR:HH	8:H:64:GLU:CD	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:T:14:ASP:CG	6:T:16:ARG:HD3	2.38	0.44
11:Y:44:THR:HG21	11:Y:100:MET:HE3	2.00	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
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
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:R:77:ALA:HB2	4:R:132:VAL:HG21	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
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
11:K:44:THR:HG21	11:K:100:MET:HE3	2.01	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
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: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
11:K:1:THR:HG23	11:K:33:LYS:HZ3	1.85	0.42
11:K:45:MET:HE3	11:K:52:CYS:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:120:THR:HG22	11:Y:122:LEU:HG	2.01	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
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
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
10:J:92:ILE:HG21	10:J:122:LEU:HD23	2.03	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
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
4:D:189:GLU:OE2	4:D:223:TYR:OH	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:26:GLU:O	2:B:29:SER:OG	2.26	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
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
1:A:14:PRO:HA	2:B:23:TYR:CD1	2.56	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:100:MET:HE3	13:M:132:LEU:HA	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:62:LEU:HD23	9:I:62:LEU:HA	1.88	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
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
2:P:227:LYS:NZ	2:P:233:GLU:OE2	2.51	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
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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
8	H	220/232 (95%)	209 (95%)	9 (4%)	2 (1%)	14	44
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	208/209 (100%)	206 (99%)	2 (1%)	73 84
1	O	208/209 (100%)	206 (99%)	2 (1%)	73 84
2	B	202/216 (94%)	201 (100%)	1 (0%)	86 91
2	P	204/216 (94%)	203 (100%)	1 (0%)	86 91
3	C	208/226 (92%)	208 (100%)	0	100 100
3	Q	211/226 (93%)	208 (99%)	3 (1%)	62 78
4	D	196/215 (91%)	196 (100%)	0	100 100
4	R	197/215 (92%)	196 (100%)	1 (0%)	86 91
5	E	189/193 (98%)	187 (99%)	2 (1%)	70 82
5	S	191/193 (99%)	188 (98%)	3 (2%)	58 75
6	F	201/238 (84%)	199 (99%)	2 (1%)	73 84
6	T	200/238 (84%)	197 (98%)	3 (2%)	60 77
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%)	180 (99%)	1 (1%)	84 90
8	V	179/190 (94%)	178 (99%)	1 (1%)	84 90
9	I	172/173 (99%)	171 (99%)	1 (1%)	84 90
9	W	172/173 (99%)	170 (99%)	2 (1%)	67 80
10	J	174/175 (99%)	173 (99%)	1 (1%)	84 90
10	X	173/175 (99%)	172 (99%)	1 (1%)	84 90
11	K	169/169 (100%)	168 (99%)	1 (1%)	84 90
11	Y	169/169 (100%)	167 (99%)	2 (1%)	67 80
12	L	185/185 (100%)	182 (98%)	3 (2%)	58 75
12	Z	185/185 (100%)	184 (100%)	1 (0%)	86 91
13	M	199/199 (100%)	196 (98%)	3 (2%)	60 77
13	a	199/199 (100%)	195 (98%)	4 (2%)	50 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	162/162 (100%)	162 (100%)	0	100 100
14	b	162/162 (100%)	161 (99%)	1 (1%)	84 90
All	All	5308/5520 (96%)	5266 (99%)	42 (1%)	79 87

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	PHE
1	A	174	PHE
2	B	33	THR
5	E	34	THR
5	E	174	THR
6	F	69	HIS
6	F	214	TRP
1	O	157	PHE
1	O	169	VAL
2	P	149	THR
3	Q	131	THR
3	Q	148	THR
3	Q	212	VAL
4	R	183	LEU
5	S	34	THR
5	S	174	THR
5	S	209	ASN
6	T	69	HIS
6	T	203	ASN
6	T	214	TRP
8	H	38	SER
9	I	146	PHE
10	J	136	SER
11	K	137	TYR
12	L	81	ASP
12	L	91	ARG
12	L	128	VAL
13	M	11	VAL
13	M	127	LEU
13	M	190	ARG
8	V	38	SER
9	W	146	PHE
9	W	182	TRP
10	X	174	MET

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Mol	Chain	Res	Type
11	Y	65	LEU
11	Y	137	TYR
12	Z	128	VAL
13	a	37	ASN
13	a	102	GLN
13	a	104	ARG
13	a	206	LEU
14	b	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	L	303	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	E	304	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	304	-	4,4,4	0.68	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SO4	H	302	-	4,4,4	0.68	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	K	303	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	N	201	-	4,4,4	0.66	0	6,6,6	0.09	0
15	SO4	a	303	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	B	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	Z	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	M	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	304	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	Z	303	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	M	303	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	S	301	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	D	301	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	b	201	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	K	304	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	F	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	J	201	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	301	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	I	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	J	202	-	4,4,4	0.67	0	6,6,6	0.10	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	E	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	E	301	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	F	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	R	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	U	301	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	P	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	L	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	V	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	G	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	H	303	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	E	303	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	T	301	-	4,4,4	0.67	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	N	203	-	4,4,4	0.68	0	6,6,6	0.10	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	N	201	SO4	1	0
15	R	301	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	249/250 (99%)	1.60	76 (30%)	1	1	18, 38, 73, 97	0
1	O	249/250 (99%)	1.46	64 (25%)	2	2	11, 34, 71, 96	0
2	B	242/258 (93%)	1.94	90 (37%)	1	1	19, 45, 77, 104	0
2	P	244/258 (94%)	1.60	71 (29%)	1	2	15, 35, 73, 97	0
3	C	236/254 (92%)	2.10	110 (46%)	0	1	17, 50, 94, 112	0
3	Q	239/254 (94%)	2.02	106 (44%)	1	1	19, 48, 90, 116	0
4	D	237/260 (91%)	1.74	77 (32%)	1	1	14, 40, 65, 105	0
4	R	239/260 (91%)	2.16	116 (48%)	0	1	20, 52, 79, 103	0
5	E	231/234 (98%)	1.87	86 (37%)	1	1	21, 41, 70, 89	0
5	S	232/234 (99%)	2.25	113 (48%)	0	0	24, 46, 80, 93	0
6	F	244/287 (85%)	1.74	82 (33%)	1	1	18, 39, 75, 83	0
6	T	244/287 (85%)	1.91	86 (35%)	1	1	18, 40, 78, 107	0
7	G	241/252 (95%)	1.48	68 (28%)	1	2	15, 35, 60, 93	0
7	U	242/252 (96%)	1.49	63 (26%)	2	2	15, 35, 62, 92	0
8	H	222/232 (95%)	1.30	45 (20%)	3	4	12, 31, 55, 95	0
8	V	222/232 (95%)	1.16	39 (17%)	4	5	16, 28, 53, 87	0
9	I	204/205 (99%)	1.14	32 (15%)	6	6	14, 29, 55, 80	0
9	W	204/205 (99%)	0.98	21 (10%)	13	13	12, 23, 48, 76	0
10	J	196/198 (98%)	1.03	21 (10%)	12	12	15, 30, 50, 102	0
10	X	195/198 (98%)	1.00	23 (11%)	10	11	12, 27, 52, 106	0
11	K	212/212 (100%)	1.03	19 (8%)	17	15	12, 25, 45, 83	0
11	Y	212/212 (100%)	1.17	35 (16%)	5	6	15, 31, 51, 69	0
12	L	222/222 (100%)	0.91	20 (9%)	17	15	11, 23, 42, 60	0
12	Z	222/222 (100%)	1.27	39 (17%)	4	5	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%)	0.97	29 (12%) 9 10	12, 26, 47, 66	0
13	a	233/233 (100%)	1.28	45 (19%) 4 4	15, 30, 52, 74	0
14	N	196/196 (100%)	0.97	23 (11%) 10 11	16, 28, 54, 83	0
14	b	196/196 (100%)	1.01	27 (13%) 8 8	13, 27, 54, 69	0
All	All	6338/6586 (96%)	1.47	1626 (25%) 2 2	11, 34, 72, 116	0

All (1626) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	40	ASP	7.3
3	Q	241	GLN	7.2
2	P	218	GLY	7.2
5	S	187	GLU	7.2
6	F	244	ASN	7.0
3	C	236	GLN	7.0
4	D	117	GLU	6.8
2	B	54	THR	6.8
9	W	131	GLU	6.8
2	B	59	ASP	6.7
4	D	0	TYR	6.7
5	S	54	GLU	6.7
2	P	222	GLY	6.6
6	T	51	THR	6.6
2	B	244	THR	6.4
10	X	193	ASP	6.4
6	T	181	GLU	6.3
7	G	188	GLU	6.1
3	C	168	THR	6.1
9	I	192	ASP	6.1
2	P	54	THR	6.0
2	B	7	SER	5.9
2	B	223	GLU	5.8
3	C	58	THR	5.8
3	Q	237	GLU	5.8
3	C	171	GLU	5.8
3	Q	234	ILE	5.7
4	R	0	TYR	5.7
3	C	228	ASN	5.7
5	E	203	GLU	5.7
3	Q	58	THR	5.6
5	E	123	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
6	T	207	ASP	5.5
1	O	249	ALA	5.5
4	R	1	ASP	5.5
4	R	201	GLU	5.4
3	C	204	GLY	5.4
5	S	200	LEU	5.4
9	I	131	GLU	5.4
1	A	52	SER	5.4
7	U	222	ASP	5.4
6	F	242	GLU	5.4
5	S	51	ASN	5.4
4	D	224	ASP	5.4
8	H	221	CYS	5.4
2	B	40	SER	5.4
10	J	194	ASP	5.3
3	C	38	ASN	5.3
5	E	3	ASN	5.3
3	C	237	GLU	5.3
3	Q	225	GLU	5.3
5	E	227	GLU	5.3
5	S	203	GLU	5.3
3	Q	48	SER	5.3
4	D	1	ASP	5.3
2	P	1	GLY	5.3
3	C	175	LYS	5.2
7	G	2	GLY	5.2
5	S	233	ILE	5.2
5	E	177	THR	5.2
10	J	196	GLN	5.2
8	V	222	ASP	5.2
4	R	243	SER	5.2
1	A	248	GLU	5.1
5	S	124	GLY	5.1
3	Q	240	GLU	5.1
8	H	108	SER	5.1
5	S	186	ASP	5.1
5	S	229	VAL	5.1
10	X	194	ASP	5.1
5	S	226	GLY	5.0
7	G	180	SER	5.0
4	D	2	ARG	5.0
2	P	61	SER	5.0

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Mol	Chain	Res	Type	RSRZ
3	Q	229	GLN	5.0
5	S	173	ARG	5.0
3	Q	239	GLN	5.0
3	C	184	ALA	5.0
5	S	207	VAL	4.9
3	Q	167	LYS	4.9
6	T	204	LYS	4.9
5	S	32	SER	4.9
2	P	221	ASP	4.9
4	R	202	GLU	4.9
3	Q	55	THR	4.9
6	T	2	THR	4.9
2	B	62	THR	4.9
5	S	56	SER	4.9
6	T	241	LYS	4.9
6	F	182	GLY	4.9
1	O	62	SER	4.9
6	F	184	SER	4.9
4	D	54	ASP	4.8
7	G	179	LYS	4.8
4	D	177	ASN	4.8
4	R	242	GLU	4.8
5	S	205	LEU	4.8
7	U	243	ASP	4.8
13	a	85	GLU	4.8
5	E	174	THR	4.8
6	T	178	HIS	4.8
7	G	3	TYR	4.8
3	C	48	SER	4.8
4	D	226	GLU	4.8
2	P	245	LYS	4.8
7	G	242	GLN	4.8
6	T	205	GLU	4.8
1	A	2	THR	4.8
3	Q	236	GLN	4.7
7	G	124	TYR	4.7
4	R	234	GLU	4.7
1	A	250	LEU	4.7
1	O	167	GLY	4.7
4	D	242	GLU	4.7
6	T	39	ASN	4.7
3	C	37	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
3	C	223	SER	4.7
6	T	206	LYS	4.7
6	T	166	GLN	4.7
5	S	202	ASP	4.6
6	F	237	ASP	4.6
4	R	123	GLU	4.6
9	W	133	LYS	4.6
8	H	218	VAL	4.6
6	T	237	ASP	4.6
3	Q	238	LYS	4.6
8	V	198	GLU	4.6
5	S	52	ALA	4.6
7	U	242	GLN	4.6
13	a	211	ASN	4.6
6	T	180	PRO	4.6
2	B	202	SER	4.6
3	C	60	SER	4.6
3	Q	202	GLN	4.6
9	I	133	LYS	4.6
1	O	250	LEU	4.6
6	T	187	GLU	4.6
2	P	203	SER	4.5
4	R	169	GLU	4.5
2	B	168	THR	4.5
5	E	190	LYS	4.5
5	S	58	TYR	4.5
3	Q	232	THR	4.5
6	T	184	SER	4.5
1	O	244	ASN	4.5
6	F	230	ASP	4.5
6	T	230	ASP	4.5
2	P	242	GLY	4.5
5	E	121	SER	4.5
6	F	181	GLU	4.4
2	P	59	ASP	4.4
1	A	202	GLY	4.4
2	B	51	VAL	4.4
6	T	173	GLU	4.4
1	A	4	ARG	4.4
4	R	3	GLY	4.4
13	a	82	ASP	4.4
1	A	200	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	203	THR	4.4
2	B	171	ALA	4.4
1	O	52	SER	4.4
4	R	226	GLU	4.4
8	V	120	ASP	4.4
1	A	198	GLU	4.4
4	D	180	HIS	4.3
6	T	218	SER	4.3
2	B	3	ARG	4.3
3	Q	230	TYR	4.3
14	b	191	ASP	4.3
6	F	1	GLY	4.3
1	O	141	GLU	4.3
3	Q	59	PRO	4.3
5	E	77	ALA	4.3
7	U	203	ASP	4.3
3	C	235	GLU	4.3
4	R	178	GLU	4.3
5	S	204	SER	4.3
5	S	169	THR	4.3
2	B	245	LYS	4.3
7	G	181	LYS	4.3
11	K	212	GLY	4.3
3	C	185	THR	4.3
3	C	232	THR	4.3
5	S	209	ASN	4.3
3	Q	235	GLU	4.2
12	Z	169	LYS	4.2
3	Q	207	ASN	4.2
5	E	209	ASN	4.2
13	a	216	ASN	4.2
4	R	217	GLN	4.2
2	B	201	ASP	4.2
3	Q	218	ASP	4.2
4	R	224	ASP	4.2
5	E	95	SER	4.2
4	R	177	ASN	4.2
3	C	180	LYS	4.2
13	a	215	GLU	4.2
2	B	173	THR	4.2
5	S	231	LYS	4.2
3	C	221	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	P	182	ASP	4.2
6	F	40	ASP	4.2
14	b	104	ASP	4.2
5	S	181	ILE	4.2
3	Q	185	THR	4.2
3	C	238	LYS	4.2
3	Q	180	LYS	4.2
5	S	117	LYS	4.2
7	G	228	SER	4.2
3	C	186	VAL	4.2
5	S	227	GLU	4.2
8	H	28	ASP	4.2
5	S	198	GLN	4.1
7	U	124	TYR	4.1
4	R	216	LYS	4.1
5	E	202	ASP	4.1
3	C	167	LYS	4.1
3	Q	199	GLU	4.1
5	S	206	THR	4.1
1	A	177	LYS	4.1
2	P	236	ASP	4.1
1	O	203	GLU	4.1
3	C	209	GLU	4.1
4	R	239	GLU	4.1
2	B	221	ASP	4.1
1	A	249	ALA	4.1
8	V	182	LYS	4.1
3	Q	10	SER	4.1
3	C	199	GLU	4.0
2	B	232	GLN	4.0
6	T	240	GLN	4.0
3	Q	38	ASN	4.0
2	B	222	GLY	4.0
2	B	204	ALA	4.0
5	S	57	SER	4.0
2	B	208	ASP	4.0
4	R	2	ARG	4.0
6	F	234	GLU	4.0
1	A	54	PRO	4.0
6	F	202	ASP	4.0
6	T	200	HIS	4.0
3	C	201	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
7	G	178	LYS	4.0
3	Q	204	GLY	4.0
4	D	214	ILE	4.0
4	R	46	ALA	4.0
5	S	230	ALA	4.0
2	B	225	TYR	3.9
2	B	176	GLN	3.9
3	Q	233	GLN	3.9
2	B	217	LYS	3.9
3	C	225	GLU	3.9
4	D	169	GLU	3.9
3	Q	203	THR	3.9
10	X	1	MET	3.9
1	O	245	ASP	3.9
3	C	234	ILE	3.9
2	B	34	ALA	3.9
6	T	242	GLU	3.9
2	B	88	ASN	3.9
7	U	181	LYS	3.9
3	Q	53	GLN	3.9
3	Q	137	ASP	3.9
6	T	202	ASP	3.9
11	Y	72	GLU	3.9
1	A	231	LYS	3.9
10	J	195	PHE	3.9
1	A	220	ASP	3.9
4	D	4	VAL	3.9
6	F	178	HIS	3.9
5	S	196	ILE	3.9
3	Q	51	LYS	3.9
3	C	187	GLU	3.8
2	P	239	VAL	3.8
6	T	244	ASN	3.8
2	B	242	GLY	3.8
4	R	221	LYS	3.8
2	B	113	ARG	3.8
2	B	182	ASP	3.8
2	P	178	ASP	3.8
5	E	8	ASP	3.8
5	E	225	ASP	3.8
3	C	174	GLU	3.8
5	S	59	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
7	U	240	ALA	3.8
5	S	197	SER	3.8
5	S	77	ALA	3.8
5	S	201	ARG	3.8
8	V	219	ASN	3.8
1	A	3	ASP	3.8
6	T	177	ASP	3.8
2	B	52	THR	3.8
3	C	46	ARG	3.8
2	B	53	SER	3.8
1	O	181	ASP	3.8
4	R	236	LYS	3.8
6	F	207	ASP	3.8
4	R	124	ARG	3.8
6	F	179	HIS	3.8
3	Q	165	ASN	3.7
6	F	29	ASN	3.7
10	X	10	GLN	3.7
6	T	53	LYS	3.7
5	S	2	ARG	3.7
14	N	149	GLU	3.7
1	O	207	ASP	3.7
5	S	218	ASP	3.7
8	H	222	ASP	3.7
3	C	55	THR	3.7
1	A	240	SER	3.7
1	O	200	VAL	3.7
7	U	178	LYS	3.7
4	R	187	GLU	3.7
6	T	171	GLU	3.7
2	B	178	ASP	3.7
5	S	225	ASP	3.7
5	E	59	GLN	3.7
7	U	53	LYS	3.7
6	F	180	PRO	3.7
5	E	233	ILE	3.7
13	M	38	GLY	3.7
5	S	53	ASP	3.7
9	W	192	ASP	3.7
10	X	11	ASP	3.7
8	V	43	CYS	3.7
4	D	116	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	O	61	LEU	3.7
3	C	216	ASP	3.7
5	E	218	ASP	3.7
4	R	114	ARG	3.7
5	S	165	GLN	3.7
4	R	225	ASN	3.7
5	E	187	GLU	3.6
4	R	194	LYS	3.6
5	S	190	LYS	3.6
5	E	122	TYR	3.6
9	I	130	ASP	3.6
3	C	10	SER	3.6
4	D	229	ALA	3.6
3	C	13	GLY	3.6
1	O	201	GLU	3.6
2	B	60	THR	3.6
11	Y	147	ASP	3.6
4	R	179	TRP	3.6
4	D	182	SER	3.6
5	E	191	ALA	3.6
8	V	195	VAL	3.6
2	B	207	TYR	3.6
3	C	227	ILE	3.6
3	C	233	GLN	3.6
7	G	222	ASP	3.6
9	I	18	ASP	3.6
1	O	53	SER	3.6
8	V	10	ASN	3.6
3	C	230	TYR	3.6
1	O	2	THR	3.6
4	R	203	LYS	3.6
6	F	177	ASP	3.6
8	V	221	CYS	3.6
6	T	221	ASN	3.6
3	C	56	ARG	3.5
3	C	141	ASP	3.5
4	R	218	ASP	3.5
8	H	145	ASP	3.5
2	B	237	ILE	3.5
4	D	221	LYS	3.5
5	S	232	TYR	3.5
3	C	53	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
6	T	175	LEU	3.5
4	R	205	ASP	3.5
11	Y	210	VAL	3.5
3	Q	171	GLU	3.5
7	U	233	GLU	3.5
8	H	217	ILE	3.5
9	W	1	SER	3.5
10	X	135	TYR	3.5
5	E	219	THR	3.5
6	F	2	THR	3.5
9	W	130	ASP	3.5
12	Z	214	LYS	3.5
2	P	202	SER	3.5
3	C	39	CYS	3.5
7	G	241	GLU	3.5
2	B	167	ASN	3.5
5	E	169	THR	3.5
4	R	33	ALA	3.5
5	E	207	VAL	3.5
5	S	192	GLY	3.5
3	C	12	ASP	3.5
7	U	52	ASP	3.5
9	I	2	ASP	3.5
3	C	226	GLU	3.4
14	b	192	GLU	3.4
5	S	151	ASN	3.4
8	H	9	ASN	3.4
13	a	78	ASN	3.4
6	F	162	GLY	3.4
6	T	1	GLY	3.4
2	B	4	ARG	3.4
3	Q	47	ARG	3.4
11	K	106	ARG	3.4
5	S	132	LEU	3.4
5	S	176	ASP	3.4
9	W	143	ASP	3.4
2	B	15	GLU	3.4
7	U	241	GLU	3.4
1	O	51	SER	3.4
3	Q	60	SER	3.4
4	D	48	SER	3.4
1	O	197	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
3	Q	37	LYS	3.4
6	F	163	LYS	3.4
6	F	241	LYS	3.4
5	S	30	GLN	3.4
6	F	58	GLN	3.4
4	R	21	GLU	3.4
6	T	174	LYS	3.4
1	A	206	GLY	3.4
2	B	125	GLY	3.4
4	R	47	THR	3.4
7	U	2	GLY	3.4
8	H	216	SER	3.4
2	P	151	ASN	3.4
4	R	207	ASN	3.4
2	B	8	ARG	3.4
4	D	113	LEU	3.4
3	Q	220	VAL	3.4
8	V	218	VAL	3.4
11	Y	157	GLY	3.4
2	P	237	ILE	3.4
7	U	212	ASN	3.4
1	O	247	LEU	3.4
6	F	231	LEU	3.4
14	N	196	LEU	3.4
4	R	35	LYS	3.4
4	D	112	ALA	3.4
4	D	201	GLU	3.4
14	b	194	GLU	3.4
5	E	201	ARG	3.4
5	S	66	ASP	3.4
7	U	183	ASP	3.4
5	S	9	THR	3.4
2	P	197	SER	3.4
3	C	44	CYS	3.3
3	C	52	LEU	3.3
8	V	22	GLN	3.3
8	V	144	GLN	3.3
10	J	10	GLN	3.3
1	A	203	GLU	3.3
3	C	181	GLU	3.3
5	E	186	ASP	3.3
13	M	47	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
5	E	73	LEU	3.3
6	T	52	SER	3.3
2	P	246	LYS	3.3
3	C	144	LYS	3.3
3	C	176	ASN	3.3
3	C	202	GLN	3.3
6	F	221	ASN	3.3
8	H	10	ASN	3.3
5	S	185	PRO	3.3
1	O	190	HIS	3.3
3	Q	43	GLY	3.3
5	S	161	GLY	3.3
6	F	243	ILE	3.3
3	Q	158	SER	3.3
2	B	193	LEU	3.3
3	Q	206	LYS	3.3
5	S	177	THR	3.3
7	G	183	ASP	3.3
13	a	69	ASP	3.3
8	H	202	SER	3.3
11	Y	75	SER	3.3
3	C	200	VAL	3.3
6	T	203	ASN	3.3
7	G	194	VAL	3.3
7	G	240	ALA	3.3
7	U	182	ILE	3.3
7	G	230	GLU	3.3
7	U	168	GLU	3.3
13	M	215	GLU	3.3
1	A	50	LYS	3.3
2	B	184	LYS	3.3
3	C	51	LYS	3.3
3	Q	26	LYS	3.3
4	R	238	LYS	3.3
6	F	139	LYS	3.3
5	S	178	PHE	3.3
7	G	229	ALA	3.3
14	b	68	SER	3.3
6	T	57	PRO	3.3
11	K	124	GLY	3.3
1	O	231	LYS	3.2
6	F	206	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
12	L	172	LEU	3.3
1	A	208	THR	3.2
1	O	204	PHE	3.2
10	X	195	PHE	3.2
13	M	69	ASP	3.2
8	H	38	SER	3.2
7	U	231	ASN	3.2
7	U	105	CYS	3.2
1	A	120	GLU	3.2
2	P	223	GLU	3.2
5	S	122	TYR	3.2
6	F	201	GLU	3.2
8	H	197	GLU	3.2
2	P	10	THR	3.2
4	R	171	ALA	3.2
2	P	232	GLN	3.2
10	J	193	ASP	3.2
11	Y	152	ASP	3.2
14	N	103	ASP	3.2
1	O	240	SER	3.2
3	Q	7	SER	3.2
5	E	57	SER	3.2
4	D	225	ASN	3.2
1	A	242	GLU	3.2
1	O	242	GLU	3.2
2	B	63	GLU	3.2
5	S	194	GLU	3.2
4	R	42	VAL	3.2
2	P	241	THR	3.2
7	U	207	THR	3.2
11	Y	30	THR	3.2
1	A	241	GLN	3.2
4	R	111	LEU	3.2
1	A	245	ASP	3.2
4	D	219	GLY	3.2
3	C	121	SER	3.2
3	C	166	SER	3.2
3	Q	223	SER	3.2
6	F	187	GLU	3.2
7	G	139	GLU	3.2
8	H	215	GLU	3.2
3	Q	189	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
4	R	241	ALA	3.2
6	T	226	PHE	3.2
2	P	8	ARG	3.2
3	Q	140	ASP	3.2
4	D	5	SER	3.2
4	D	127	SER	3.2
4	R	180	HIS	3.2
2	B	102	ASN	3.2
1	A	201	GLU	3.2
2	P	204	ALA	3.2
6	F	217	LEU	3.2
3	Q	183	PRO	3.1
3	C	179	ARG	3.1
3	C	229	GLN	3.1
5	E	165	GLN	3.1
3	C	218	ASP	3.1
8	V	35	HIS	3.1
4	D	153	SER	3.1
10	J	1	MET	3.1
3	Q	187	GLU	3.1
4	R	233	LYS	3.1
6	T	231	LEU	3.1
8	V	220	ILE	3.1
9	I	128	CYS	3.1
2	B	1	GLY	3.1
6	T	182	GLY	3.1
3	Q	3	ASP	3.1
4	R	140	ASP	3.1
7	G	4	ASP	3.1
2	B	240	LYS	3.1
5	S	180	LYS	3.1
11	Y	199	LYS	3.1
2	B	203	SER	3.1
1	O	248	GLU	3.1
4	R	36	GLU	3.1
10	J	155	GLU	3.1
13	a	84	GLU	3.1
6	T	50	ILE	3.1
13	a	229	GLY	3.1
5	E	30	GLN	3.1
4	R	186	LYS	3.1
6	T	190	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
9	W	191	LYS	3.1
7	U	50	VAL	3.1
5	E	176	ASP	3.1
1	A	199	SER	3.1
6	T	216	SER	3.1
12	L	174	TYR	3.1
11	Y	203	GLU	3.1
4	R	228	THR	3.1
7	U	206	GLY	3.1
1	O	17	LYS	3.1
5	E	179	ILE	3.1
5	S	208	ASP	3.1
13	M	233	ILE	3.1
13	a	47	ASP	3.1
1	A	8	SER	3.1
4	R	237	GLU	3.1
1	O	206	GLY	3.1
3	C	59	PRO	3.1
6	F	129	GLY	3.1
2	P	194	LYS	3.1
5	E	49	LYS	3.1
3	Q	4	ARG	3.1
5	E	52	ALA	3.1
1	A	209	ILE	3.1
3	C	3	ASP	3.0
3	Q	141	ASP	3.0
7	G	186	ASN	3.0
5	E	198	GLN	3.0
6	F	166	GLN	3.0
4	D	179	TRP	3.0
4	R	230	GLU	3.0
14	N	153	ASP	3.0
2	B	180	LYS	3.0
3	C	206	LYS	3.0
6	T	228	LYS	3.0
3	C	215	PRO	3.0
4	R	182	SER	3.0
5	S	139	SER	3.0
3	C	207	ASN	3.0
4	R	208	ASN	3.0
3	C	47	ARG	3.0
4	R	25	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
6	F	233	GLN	3.0
1	O	243	ILE	3.0
5	S	228	ALA	3.0
4	R	227	LYS	3.0
5	E	232	TYR	3.0
4	D	174	GLU	3.0
4	D	239	GLU	3.0
4	R	174	GLU	3.0
7	G	233	GLU	3.0
8	V	197	GLU	3.0
11	Y	151	GLU	3.0
5	S	166	GLY	3.0
11	K	96	SER	3.0
13	a	121	SER	3.0
5	S	219	THR	3.0
6	F	203	ASN	3.0
2	B	172	GLN	3.0
3	Q	172	PHE	3.0
2	B	47	ALA	3.0
5	E	170	TYR	3.0
3	Q	19	GLU	3.0
4	R	37	GLY	3.0
1	A	181	ASP	3.0
1	A	6	SER	3.0
1	A	61	LEU	3.0
1	A	178	ARG	3.0
2	B	239	VAL	3.0
2	P	62	THR	3.0
4	D	47	THR	3.0
4	R	190	LEU	3.0
5	S	55	LEU	3.0
10	J	142	SER	3.0
7	U	120	THR	3.0
8	H	22	GLN	3.0
8	H	133	ALA	3.0
13	a	233	ILE	3.0
10	J	113	LYS	3.0
1	A	48	GLU	3.0
4	D	37	GLY	3.0
4	D	187	GLU	3.0
7	U	217	GLY	3.0
12	Z	215	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	Q	197	LEU	3.0
1	A	230	ASP	3.0
9	I	124	ASP	3.0
14	N	104	ASP	3.0
1	A	51	SER	3.0
3	Q	121	SER	3.0
4	D	53	SER	3.0
4	R	5	SER	3.0
5	S	41	THR	3.0
12	Z	124	SER	3.0
4	R	188	ALA	3.0
12	Z	80	ASN	3.0
13	M	216	ASN	3.0
6	T	58	GLN	2.9
4	D	213	CYS	2.9
5	S	170	TYR	2.9
4	D	21	GLU	2.9
10	J	161	LEU	2.9
3	C	210	ILE	2.9
5	E	141	ALA	2.9
5	S	164	SER	2.9
6	T	185	ALA	2.9
8	V	156	SER	2.9
7	G	167	GLN	2.9
2	B	17	ARG	2.9
5	E	58	TYR	2.9
1	A	247	LEU	2.9
5	E	26	GLU	2.9
7	U	188	GLU	2.9
2	B	198	LYS	2.9
3	C	211	THR	2.9
6	T	31	THR	2.9
8	H	147	THR	2.9
9	I	115	SER	2.9
5	E	99	ASN	2.9
3	Q	27	ARG	2.9
3	C	190	VAL	2.9
3	C	222	LEU	2.9
1	A	228	PRO	2.9
3	C	214	LYS	2.9
8	V	217	ILE	2.9
3	Q	168	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	22	ASP	2.9
2	B	181	ASP	2.9
3	Q	54	ASP	2.9
2	B	61	SER	2.9
3	C	27	ARG	2.9
4	R	48	SER	2.9
5	S	50	ARG	2.9
6	F	64	GLN	2.9
6	T	179	HIS	2.9
4	D	175	LEU	2.9
4	R	235	LEU	2.9
3	Q	122	GLY	2.9
12	Z	166	GLY	2.9
5	E	60	LYS	2.9
11	Y	155	TYR	2.9
12	L	173	LYS	2.9
1	O	198	GLU	2.9
2	P	233	GLU	2.9
4	D	178	GLU	2.9
4	D	237	GLU	2.9
4	R	117	GLU	2.9
12	L	18	GLU	2.9
13	a	162	GLU	2.9
6	F	32	THR	2.9
7	G	133	THR	2.9
6	F	186	ARG	2.9
4	R	200	MET	2.9
1	O	202	GLY	2.9
5	S	4	ASN	2.9
2	B	230	LYS	2.9
6	F	197	TYR	2.9
9	I	132	ALA	2.8
5	S	48	LEU	2.8
1	O	199	SER	2.8
1	O	237	LYS	2.8
5	E	180	LYS	2.8
6	F	14	ASP	2.8
8	V	145	ASP	2.8
11	K	118	ASP	2.8
4	R	154	GLY	2.8
3	Q	182	PRO	2.8
2	B	243	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	232	ILE	2.8
13	M	219	TRP	2.8
1	O	46	ALA	2.8
6	T	201	GLU	2.8
11	K	182	GLU	2.8
7	U	58	THR	2.8
2	P	224	VAL	2.8
1	O	3	ASP	2.8
2	B	6	ASP	2.8
9	W	25	ASP	2.8
10	J	175	ASP	2.8
12	Z	10	GLY	2.8
5	S	199	SER	2.8
7	U	180	SER	2.8
2	P	155	ASN	2.8
5	S	163	ARG	2.8
14	b	100	ALA	2.8
11	Y	107	LYS	2.8
4	D	228	THR	2.8
5	S	44	VAL	2.8
7	G	65	CYS	2.8
5	S	189	ILE	2.8
9	I	113	SER	2.8
10	J	76	SER	2.8
13	a	54	SER	2.8
3	Q	195	ARG	2.8
12	L	165	ASN	2.8
6	F	49	LEU	2.8
1	A	60	THR	2.8
12	Z	163	GLY	2.8
5	E	212	ILE	2.8
3	C	178	ASP	2.8
3	C	2	TYR	2.8
4	R	22	ALA	2.8
5	S	3	ASN	2.8
8	H	194	ASN	2.8
5	E	200	LEU	2.8
11	K	67	GLU	2.8
11	Y	202	GLU	2.8
5	E	10	VAL	2.8
2	B	149	THR	2.8
5	E	9	THR	2.8

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Mol	Chain	Res	Type	RSRZ
6	F	164	GLY	2.8
5	E	181	ILE	2.8
13	M	102	GLN	2.7
13	a	171	GLN	2.7
6	F	215	CYS	2.7
6	F	235	ALA	2.7
1	A	29	LYS	2.7
4	D	223	TYR	2.7
5	E	208	ASP	2.7
5	S	60	LYS	2.7
6	T	75	SER	2.7
1	A	176	GLU	2.7
5	E	54	GLU	2.7
6	T	47	GLU	2.7
1	A	64	VAL	2.7
3	Q	201	VAL	2.7
1	A	229	THR	2.7
4	R	41	GLY	2.7
6	T	229	GLY	2.7
7	G	160	THR	2.7
13	M	123	GLY	2.7
1	O	241	GLN	2.7
2	P	176	GLN	2.7
3	Q	221	ALA	2.7
4	R	44	LYS	2.7
4	R	212	SER	2.7
11	K	142	SER	2.7
2	B	48	GLU	2.7
3	Q	23	GLU	2.7
8	H	219	ASN	2.7
12	L	171	PRO	2.7
6	F	240	GLN	2.7
7	G	28	GLN	2.7
8	V	153	LYS	2.7
4	D	176	LEU	2.7
4	D	235	LEU	2.7
4	R	113	LEU	2.7
6	F	54	LEU	2.7
11	Y	144	TYR	2.7
1	A	58	SER	2.7
2	P	150	SER	2.7
12	Z	32	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
13	M	121	SER	2.7
14	b	2	SER	2.7
5	S	99	ASN	2.7
9	I	150	GLU	2.7
11	Y	67	GLU	2.7
9	W	8	GLY	2.7
11	Y	211	ILE	2.7
6	T	18	PHE	2.7
12	L	17	GLY	2.7
2	P	60	THR	2.7
8	H	206	PRO	2.7
3	C	14	HIS	2.7
4	D	33	ALA	2.7
7	G	161	ALA	2.7
11	Y	49	ALA	2.7
13	M	213	GLN	2.7
2	B	183	MET	2.7
8	H	196	ARG	2.7
3	Q	12	ASP	2.7
5	E	32	SER	2.7
5	E	53	ASP	2.7
6	T	12	SER	2.7
6	T	219	GLU	2.7
6	T	234	GLU	2.7
3	Q	176	ASN	2.7
14	N	106	ASN	2.7
4	D	170	GLY	2.7
12	Z	167	LYS	2.7
2	B	206	THR	2.7
4	R	6	THR	2.7
2	B	147	LEU	2.7
4	R	229	ALA	2.7
7	U	151	ALA	2.7
13	a	113	ALA	2.7
8	V	57	GLN	2.7
12	L	1	GLN	2.7
10	X	174	MET	2.7
3	C	231	VAL	2.7
4	R	223	TYR	2.7
4	R	64	ARG	2.7
6	T	212	ILE	2.6
8	H	73	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
11	K	151	GLU	2.6
11	Y	182	GLU	2.6
1	A	216	ASP	2.6
2	B	141	ASP	2.6
10	X	151	ASP	2.6
13	M	211	ASN	2.6
1	O	196	LEU	2.6
1	O	229	THR	2.6
2	P	52	THR	2.6
3	Q	29	THR	2.6
4	D	75	ALA	2.6
4	R	161	ALA	2.6
5	S	43	ALA	2.6
5	S	220	PRO	2.6
6	T	132	THR	2.6
7	G	204	ALA	2.6
13	M	75	ALA	2.6
4	R	199	VAL	2.6
1	A	17	LYS	2.6
6	T	236	ILE	2.6
7	G	182	ILE	2.6
1	A	184	GLU	2.6
2	B	84	GLU	2.6
3	Q	209	GLU	2.6
6	F	173	GLU	2.6
8	H	185	GLU	2.6
9	W	128	CYS	2.6
2	B	70	ASP	2.6
4	D	166	SER	2.6
7	G	46	SER	2.6
2	B	192	ALA	2.6
6	T	192	ALA	2.6
2	B	241	THR	2.6
2	P	244	THR	2.6
12	Z	27	THR	2.6
2	P	177	MET	2.6
3	C	4	ARG	2.6
10	J	95	ARG	2.6
4	D	233	LYS	2.6
5	E	168	LYS	2.6
6	T	197	TYR	2.6
11	Y	145	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	Q	181	GLU	2.6
6	F	219	GLU	2.6
9	I	78	GLU	2.6
3	C	189	CYS	2.6
6	F	175	LEU	2.6
1	O	230	ASP	2.6
3	C	205	ALA	2.6
4	R	63	ASP	2.6
5	E	6	ASP	2.6
7	G	33	SER	2.6
14	N	180	ALA	2.6
6	T	60	ASN	2.6
2	B	30	HIS	2.6
2	P	4	ARG	2.6
3	Q	46	ARG	2.6
6	T	16	ARG	2.6
3	C	169	VAL	2.6
2	B	58	GLN	2.6
1	A	37	ILE	2.6
7	U	3	TYR	2.6
9	I	126	ILE	2.6
9	I	129	ILE	2.6
4	D	185	LEU	2.6
3	C	188	GLU	2.6
8	H	198	GLU	2.6
12	Z	179	GLU	2.6
1	A	76	SER	2.6
2	P	169	SER	2.6
4	R	107	SER	2.6
5	E	173	ARG	2.6
5	S	72	SER	2.6
5	S	113	ASP	2.6
7	G	136	SER	2.6
13	a	224	ASP	2.6
1	A	33	THR	2.6
3	Q	186	VAL	2.6
4	R	34	THR	2.6
5	E	40	ASN	2.6
4	D	238	LYS	2.6
4	R	197	LYS	2.6
7	G	232	ILE	2.6
7	U	63	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
12	Z	86	ILE	2.6
6	F	74	TYR	2.6
14	N	102	TYR	2.6
1	A	42	GLY	2.6
1	A	238	LEU	2.6
14	N	182	GLY	2.6
2	B	26	GLU	2.6
3	Q	174	GLU	2.6
4	D	202	GLU	2.6
4	R	189	GLU	2.6
8	V	73	GLU	2.6
2	B	50	LYS	2.6
2	B	169	SER	2.6
4	R	213	CYS	2.6
3	Q	178	ASP	2.6
10	J	110	LYS	2.6
14	b	179	THR	2.6
8	H	220	ILE	2.5
5	S	155	LEU	2.5
5	S	7	GLY	2.5
1	O	105	PRO	2.5
3	C	85	GLU	2.5
1	A	166	LYS	2.5
2	B	164	VAL	2.5
3	Q	175	LYS	2.5
5	E	46	VAL	2.5
7	U	137	VAL	2.5
1	O	40	THR	2.5
1	O	60	THR	2.5
3	Q	39	CYS	2.5
13	a	138	SER	2.5
6	F	212	ILE	2.5
7	U	172	ASN	2.5
7	G	190	TRP	2.5
7	U	166	GLN	2.5
11	Y	146	TRP	2.5
6	F	232	LEU	2.5
6	T	49	LEU	2.5
2	B	19	TYR	2.5
5	E	7	GLY	2.5
5	E	166	GLY	2.5
6	T	113	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
11	Y	48	GLY	2.5
4	R	133	ALA	2.5
5	S	191	ALA	2.5
14	b	181	ALA	2.5
2	P	15	GLU	2.5
4	R	152	PRO	2.5
7	G	168	GLU	2.5
14	N	192	GLU	2.5
11	Y	200	VAL	2.5
1	O	146	SER	2.5
2	B	89	THR	2.5
2	P	80	THR	2.5
3	C	29	THR	2.5
12	Z	108	HIS	2.5
9	W	4	SER	2.5
5	S	8	ASP	2.5
7	U	40	ASP	2.5
4	D	204	LEU	2.5
7	U	114	ASN	2.5
7	U	175	ASN	2.5
1	O	246	ARG	2.5
4	D	12	ARG	2.5
6	T	30	GLY	2.5
10	J	73	TYR	2.5
6	F	228	LYS	2.5
6	T	170	ALA	2.5
8	H	153	LYS	2.5
14	b	27	ALA	2.5
1	O	184	GLU	2.5
3	C	19	GLU	2.5
3	Q	231	VAL	2.5
7	G	208	GLU	2.5
4	R	185	LEU	2.5
1	A	246	ARG	2.5
2	P	53	SER	2.5
4	R	78	ARG	2.5
5	S	149	SER	2.5
6	T	152	SER	2.5
10	X	26	SER	2.5
4	R	142	ASP	2.5
10	X	72	ASP	2.5
12	Z	1	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
14	b	195	GLN	2.5
7	U	38	GLY	2.5
2	B	170	ALA	2.5
2	B	194	LYS	2.5
2	P	217	LYS	2.5
4	D	236	LYS	2.5
6	T	139	LYS	2.5
7	G	165	LYS	2.5
7	U	49	LYS	2.5
3	C	62	VAL	2.5
8	H	195	VAL	2.5
1	O	176	GLU	2.5
4	R	10	GLU	2.5
12	Z	218	GLU	2.5
4	R	222	ILE	2.5
5	S	212	ILE	2.5
14	b	34	LEU	2.5
3	Q	16	PHE	2.5
4	D	215	THR	2.5
5	E	50	ARG	2.5
6	T	220	THR	2.5
8	V	61	SER	2.5
10	X	108	ASP	2.5
11	K	147	ASP	2.5
12	Z	26	ASP	2.5
13	M	124	ASP	2.5
13	a	38	GLY	2.5
6	T	38	CYS	2.5
2	P	51	VAL	2.5
2	P	26	GLU	2.5
6	F	28	GLU	2.5
7	U	191	GLU	2.5
6	T	186	ARG	2.4
14	b	143	ARG	2.4
2	B	124	HIS	2.4
7	U	199	THR	2.4
2	P	120	GLY	2.4
5	S	16	GLY	2.4
6	F	229	GLY	2.4
9	I	127	GLY	2.4
1	A	161	ALA	2.4
3	C	158	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	244	ASN	2.4
2	B	5	TYR	2.4
5	E	230	ALA	2.4
7	G	144	SER	2.4
9	I	4	SER	2.4
10	X	17	SER	2.4
2	P	141	ASP	2.4
4	R	54	ASP	2.4
6	F	39	ASN	2.4
8	V	194	ASN	2.4
9	W	156	ASN	2.4
10	J	72	ASP	2.4
12	L	210	ASP	2.4
12	Z	117	ASP	2.4
12	Z	136	CYS	2.4
2	B	190	GLU	2.4
11	K	211	ILE	2.4
3	Q	139	ARG	2.4
13	a	73	GLU	2.4
13	a	175	GLU	2.4
6	F	25	LYS	2.4
13	a	210	LYS	2.4
14	N	105	LYS	2.4
7	G	226	THR	2.4
12	Z	192	THR	2.4
1	O	16	GLY	2.4
12	L	10	GLY	2.4
2	P	58	GLN	2.4
3	Q	120	GLN	2.4
1	A	133	SER	2.4
2	P	7	SER	2.4
3	C	74	SER	2.4
9	W	142	SER	2.4
1	A	180	ASN	2.4
1	O	187	ASP	2.4
2	P	187	ASP	2.4
3	Q	77	ASN	2.4
9	I	172	ASN	2.4
13	a	48	ASN	2.4
14	b	103	ASP	2.4
6	T	183	LEU	2.4
7	G	239	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	22	GLU	2.4
5	E	194	GLU	2.4
8	V	53	GLU	2.4
13	a	64	GLU	2.4
1	O	166	LYS	2.4
4	R	170	GLY	2.4
7	G	199	THR	2.4
13	M	207	THR	2.4
5	S	162	ALA	2.4
3	Q	190	VAL	2.4
7	U	194	VAL	2.4
1	A	62	SER	2.4
1	O	219	PRO	2.4
4	D	71	SER	2.4
4	R	53	SER	2.4
7	G	11	SER	2.4
1	A	70	ASP	2.4
1	O	205	ASN	2.4
3	C	66	ASP	2.4
3	C	198	LEU	2.4
5	E	163	ARG	2.4
7	U	198	ILE	2.4
11	K	143	ASN	2.4
12	Z	165	ASN	2.4
3	Q	30	CYS	2.4
8	H	204	LYS	2.4
14	N	107	LYS	2.4
4	D	230	GLU	2.4
4	R	220	PHE	2.4
6	F	47	GLU	2.4
9	I	160	GLU	2.4
14	b	149	GLU	2.4
3	Q	184	ALA	2.4
2	B	44	VAL	2.4
6	F	176	VAL	2.4
7	G	135	VAL	2.4
14	N	195	GLN	2.4
3	C	177	TYR	2.4
5	S	17	ARG	2.4
2	P	29	SER	2.4
3	Q	224	SER	2.4
4	R	30	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
7	U	210	SER	2.4
8	H	156	SER	2.4
13	a	13	SER	2.4
3	C	54	ASP	2.4
3	C	61	LYS	2.4
1	A	143	ASN	2.4
4	D	218	ASP	2.4
6	F	53	LYS	2.4
13	M	226	LYS	2.4
5	S	150	GLY	2.4
2	B	81	ALA	2.4
2	B	200	THR	2.4
4	D	192	VAL	2.4
6	F	130	VAL	2.4
11	K	30	THR	2.4
8	H	144	GLN	2.4
9	I	125	LEU	2.3
8	H	214	LYS	2.3
9	I	117	LYS	2.3
13	a	199	ILE	2.3
5	E	139	SER	2.3
6	F	33	SER	2.3
10	X	12	SER	2.3
3	C	165	ASN	2.3
4	R	160	ASN	2.3
6	T	29	ASN	2.3
10	J	159	ASP	2.3
12	L	80	ASN	2.3
12	Z	36	ASN	2.3
7	U	139	GLU	2.3
1	A	188	ALA	2.3
4	D	3	GLY	2.3
5	S	42	HIS	2.3
13	M	81	ALA	2.3
2	P	17	ARG	2.3
6	F	51	THR	2.3
7	G	111	ARG	2.3
8	V	192	THR	2.3
13	a	168	THR	2.3
3	C	191	LYS	2.3
3	Q	222	LEU	2.3
10	X	4	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
6	F	208	PHE	2.3
4	R	181	SER	2.3
14	N	129	SER	2.3
14	N	147	SER	2.3
4	D	207	ASN	2.3
5	E	4	ASN	2.3
5	S	105	GLU	2.3
7	G	13	GLU	2.3
8	V	215	GLU	2.3
14	N	144	GLU	2.3
4	R	68	CYS	2.3
4	R	116	GLY	2.3
11	Y	63	CYS	2.3
8	H	114	HIS	2.3
13	a	118	GLY	2.3
3	C	164	ARG	2.3
6	F	174	LYS	2.3
7	G	173	LEU	2.3
7	U	221	LYS	2.3
3	C	131	THR	2.3
4	D	32	ILE	2.3
1	O	5	TYR	2.3
3	C	224	SER	2.3
2	B	177	MET	2.3
2	P	190	GLU	2.3
3	C	77	ASN	2.3
8	H	53	GLU	2.3
10	J	151	ASP	2.3
12	Z	116	GLU	2.3
12	Z	200	ASP	2.3
13	M	37	ASN	2.3
1	A	170	ALA	2.3
1	O	165	GLY	2.3
3	C	212	VAL	2.3
14	N	130	GLY	2.3
11	Y	32	LYS	2.3
13	a	206	LEU	2.3
6	F	120	THR	2.3
4	D	217	GLN	2.3
12	Z	33	TYR	2.3
3	C	99	GLU	2.3
3	C	134	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
5	S	103	ALA	2.3
6	F	185	ALA	2.3
12	Z	37	SER	2.3
3	Q	45	GLU	2.3
4	R	17	GLU	2.3
6	T	209	GLU	2.3
7	G	38	GLY	2.3
5	S	184	ASN	2.3
6	F	190	LYS	2.3
8	V	150	GLU	2.3
3	Q	192	LEU	2.3
3	Q	198	LEU	2.3
3	Q	216	ASP	2.3
12	L	222	ASP	2.3
13	a	220	ASP	2.3
12	L	108	HIS	2.3
7	G	120	THR	2.3
14	N	67	THR	2.3
4	R	198	GLN	2.3
11	Y	89	GLN	2.3
13	a	231	GLN	2.3
5	S	38	ARG	2.3
2	P	50	LYS	2.3
2	P	240	LYS	2.3
7	U	179	LYS	2.3
9	I	17	LYS	2.3
9	W	117	LYS	2.3
12	L	167	LYS	2.3
3	Q	112	ALA	2.3
6	T	239	ALA	2.3
13	a	31	GLY	2.3
1	A	210	GLU	2.3
3	C	192	LEU	2.3
5	E	72	SER	2.3
5	S	26	GLU	2.3
11	Y	18	SER	2.3
11	Y	41	LEU	2.3
1	O	139	HIS	2.2
2	B	41	ASP	2.2
7	G	175	ASN	2.2
7	U	30	ASN	2.2
8	H	120	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
8	V	9	ASN	2.2
9	I	37	ASN	2.2
13	a	17	ASP	2.2
14	N	39	ASP	2.2
1	A	162	THR	2.2
4	R	156	PHE	2.2
9	W	118	PRO	2.2
5	E	147	GLN	2.2
3	C	195	ARG	2.2
6	F	100	LYS	2.2
3	Q	62	VAL	2.2
4	R	39	VAL	2.2
5	S	10	VAL	2.2
1	A	232	GLY	2.2
4	D	183	LEU	2.2
4	R	150	ALA	2.2
5	E	210	LEU	2.2
5	S	216	GLY	2.2
8	V	133	ALA	2.2
9	W	16	GLY	2.2
13	M	31	GLY	2.2
6	F	171	GLU	2.2
7	G	195	GLU	2.2
11	K	72	GLU	2.2
4	R	91	HIS	2.2
4	R	168	SER	2.2
5	E	211	SER	2.2
5	S	28	ILE	2.2
8	V	37	ILE	2.2
9	W	129	ILE	2.2
10	X	39	SER	2.2
1	O	41	ASN	2.2
2	P	181	ASP	2.2
5	E	146	PHE	2.2
7	G	148	THR	2.2
10	X	95	ARG	2.2
7	G	153	TYR	2.2
13	M	232	LYS	2.2
12	Z	128	VAL	2.2
2	P	174	LEU	2.2
3	Q	205	ALA	2.2
5	S	210	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
10	X	62	ALA	2.2
3	Q	13	GLY	2.2
1	A	227	ILE	2.2
1	O	209	ILE	2.2
2	B	234	ILE	2.2
4	D	222	ILE	2.2
1	O	59	GLU	2.2
12	Z	178	GLU	2.2
1	A	53	SER	2.2
4	R	55	SER	2.2
3	C	172	PHE	2.2
7	G	231	ASN	2.2
9	W	2	ASP	2.2
9	W	175	ASP	2.2
12	L	49	ASN	2.2
13	M	220	ASP	2.2
5	E	206	THR	2.2
14	N	9	LYS	2.2
1	O	30	GLN	2.2
3	C	120	GLN	2.2
6	T	215	CYS	2.2
8	H	200	GLN	2.2
6	F	10	VAL	2.2
6	T	46	VAL	2.2
4	R	196	LEU	2.2
5	E	80	ALA	2.2
6	T	188	ALA	2.2
5	S	183	GLY	2.2
3	Q	57	ILE	2.2
1	O	182	GLU	2.2
7	G	187	GLU	2.2
9	W	193	GLU	2.2
11	Y	195	GLU	2.2
2	P	209	ARG	2.2
6	T	131	SER	2.2
7	U	51	PRO	2.2
11	K	146	TRP	2.2
2	P	198	LYS	2.2
11	Y	143	ASN	2.2
11	Y	208	ASN	2.2
13	a	106	LYS	2.2
13	a	124	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
9	I	53	THR	2.2
1	A	194	LEU	2.2
2	P	19	TYR	2.2
3	C	41	VAL	2.2
4	R	13	LEU	2.2
7	G	17	TYR	2.2
7	G	50	VAL	2.2
7	G	236	LEU	2.2
4	D	240	ALA	2.2
7	G	219	ALA	2.2
3	C	36	GLY	2.2
4	D	167	GLY	2.2
3	C	57	ILE	2.2
1	A	190	HIS	2.2
2	B	209	ARG	2.2
2	P	3	ARG	2.2
6	F	238	PHE	2.2
11	Y	73	ARG	2.2
1	O	50	LYS	2.2
12	Z	173	LYS	2.2
5	E	164	SER	2.2
6	F	167	SER	2.2
7	U	228	SER	2.2
5	E	151	ASN	2.2
6	F	123	ASN	2.2
3	C	119	THR	2.2
4	R	147	LEU	2.2
5	S	35	VAL	2.2
6	F	110	ASP	2.2
6	T	223	LEU	2.2
9	I	75	LEU	2.2
12	Z	168	VAL	2.2
13	a	230	THR	2.2
14	N	32	ASP	2.2
3	Q	110	TYR	2.2
5	S	108	GLY	2.1
7	U	163	GLY	2.1
8	V	60	GLY	2.1
13	M	229	GLY	2.1
5	E	28	ILE	2.1
6	T	196	ILE	2.1
8	V	180	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	235	ARG	2.1
2	P	230	LYS	2.1
5	E	138	LYS	2.1
5	S	29	LYS	2.1
3	Q	142	GLU	2.1
4	D	130	PHE	2.1
8	H	29	LYS	2.1
10	J	147	HIS	2.1
12	Z	18	GLU	2.1
13	a	146	PHE	2.1
10	J	174	MET	2.1
1	A	34	SER	2.1
2	P	115	SER	2.1
12	L	130	SER	2.1
13	a	80	LEU	2.1
2	P	102	ASN	2.1
4	D	160	ASN	2.1
5	S	174	THR	2.1
14	b	145	ASN	2.1
1	A	151	ASP	2.1
5	S	137	ASP	2.1
6	T	23	ALA	2.1
6	T	26	ALA	2.1
7	G	123	ALA	2.1
8	H	183	ASP	2.1
13	M	82	ASP	2.1
2	P	92	ILE	2.1
3	C	219	ILE	2.1
7	U	202	ILE	2.1
7	G	53	LYS	2.1
7	U	39	LYS	2.1
8	V	199	LYS	2.1
12	L	136	CYS	2.1
7	U	230	GLU	2.1
7	U	234	GLU	2.1
2	P	231	PRO	2.1
4	D	49	PRO	2.1
4	D	125	LEU	2.1
5	S	188	LEU	2.1
7	U	44	VAL	2.1
4	R	166	SER	2.1
6	T	7	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	148	THR	2.1
4	R	141	ALA	2.1
5	S	47	ALA	2.1
5	S	80	ALA	2.1
5	S	158	THR	2.1
7	G	162	THR	2.1
7	G	220	THR	2.1
14	b	5	ALA	2.1
14	b	77	THR	2.1
6	F	8	ASN	2.1
12	Z	29	ASN	2.1
1	A	138	GLY	2.1
1	O	149	GLN	2.1
2	P	186	ASP	2.1
5	E	75	GLY	2.1
5	E	157	GLY	2.1
7	G	203	ASP	2.1
7	U	239	ILE	2.1
11	K	9	GLN	2.1
12	L	45	ASP	2.1
12	Z	81	ASP	2.1
4	D	124	ARG	2.1
4	D	227	LYS	2.1
6	F	165	ARG	2.1
6	F	194	LYS	2.1
7	G	68	ARG	2.1
7	U	211	LYS	2.1
12	Z	157	LYS	2.1
14	b	140	LYS	2.1
3	C	173	LEU	2.1
3	C	182	PRO	2.1
5	S	67	GLU	2.1
4	R	125	LEU	2.1
5	S	171	LEU	2.1
5	S	175	LEU	2.1
3	Q	104	VAL	2.1
5	E	228	ALA	2.1
1	O	34	SER	2.1
2	B	80	THR	2.1
3	Q	80	SER	2.1
1	A	205	ASN	2.1
1	O	180	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	71	LYS	2.1
2	P	216	ARG	2.1
2	P	225	TYR	2.1
5	E	134	ILE	2.1
8	H	25	ILE	2.1
10	X	22	THR	2.1
14	b	74	SER	2.1
4	R	67	GLY	2.1
4	R	72	GLY	2.1
5	E	150	GLY	2.1
8	H	165	ASN	2.1
9	I	191	LYS	2.1
12	Z	106	TYR	2.1
3	Q	228	ASN	2.1
6	T	233	GLN	2.1
13	M	157	LYS	2.1
1	A	207	ASP	2.1
9	I	161	ASP	2.1
9	W	161	ASP	2.1
10	X	2	ASP	2.1
14	b	10	ASP	2.1
1	O	54	PRO	2.1
3	Q	14	HIS	2.1
7	G	125	MET	2.1
6	F	90	GLU	2.1
6	T	127	PRO	2.1
8	H	35	HIS	2.1
8	V	213	LEU	2.1
3	Q	200	VAL	2.1
4	D	10	GLU	2.1
5	E	172	GLU	2.1
5	E	215	VAL	2.1
8	V	55	VAL	2.1
13	M	119	VAL	2.1
5	E	74	ALA	2.1
13	M	83	ALA	2.1
1	A	197	LYS	2.1
3	Q	179	ARG	2.1
4	D	78	ARG	2.1
6	F	196	ILE	2.1
10	J	149	ARG	2.1
13	M	167	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
14	b	83	LYS	2.1
8	V	181	GLY	2.1
9	I	85	THR	2.1
8	V	216	SER	2.1
9	I	1	SER	2.1
9	I	187	TYR	2.1
10	X	73	TYR	2.1
11	Y	104	TYR	2.1
11	Y	105	THR	2.1
14	b	117	GLY	2.1
6	T	9	SER	2.1
13	a	213	GLN	2.1
12	Z	87	ASN	2.1
5	S	182	ASP	2.1
7	U	4	ASP	2.1
13	M	201	ASP	2.1
4	R	175	LEU	2.1
8	H	177	VAL	2.1
13	a	51	VAL	2.1
8	V	149	GLU	2.1
10	X	127	GLU	2.1
14	N	150	GLU	2.1
14	b	144	GLU	2.1
1	A	172	LYS	2.0
7	U	129	GLY	2.0
9	I	183	GLY	2.0
4	R	184	THR	2.0
5	E	156	TYR	2.0
11	K	144	TYR	2.0
13	a	204	THR	2.0
6	F	52	SER	2.0
7	G	47	GLN	2.0
7	U	144	SER	2.0
8	H	20	SER	2.0
7	U	177	PHE	2.0
12	Z	125	PHE	2.0
13	a	122	ASN	2.0
8	H	146	LEU	2.0
8	V	28	ASP	2.0
13	M	224	ASP	2.0
2	P	107	VAL	2.0
14	b	6	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
7	G	176	HIS	2.0
1	O	178	ARG	2.0
3	Q	149	GLU	2.0
4	D	17	GLU	2.0
4	D	234	GLU	2.0
5	E	67	GLU	2.0
13	a	68	LYS	2.0
3	Q	210	ILE	2.0
4	R	232	ILE	2.0
5	S	27	ALA	2.0
6	F	107	ALA	2.0
7	U	197	ALA	2.0
13	a	12	ILE	2.0
11	Y	212	GLY	2.0
13	a	8	GLY	2.0
2	P	143	TYR	2.0
10	X	154	THR	2.0
6	F	18	PHE	2.0
8	H	171	SER	2.0
6	T	140	ASN	2.0
11	Y	24	ASN	2.0
11	K	183	ASP	2.0
12	Z	222	ASP	2.0
3	C	183	PRO	2.0
3	Q	214	LYS	2.0
9	I	114	LYS	2.0
11	K	145	LYS	2.0
2	P	22	GLU	2.0
3	Q	226	GLU	2.0
4	R	32	ILE	2.0
4	R	206	GLU	2.0
7	U	159	ALA	2.0
8	H	163	ILE	2.0
12	L	161	GLU	2.0
12	Z	40	GLU	2.0
14	b	88	GLU	2.0
5	E	124	GLY	2.0
12	L	14	GLY	2.0
14	N	47	GLY	2.0
14	b	108	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.