



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:30 PM UTC

PDB ID : 9AW3 / pdb_00009aw3
Title : Yeast 20S proteasome soaked with MA9 crude extract
Authors : Meneghello, R.; Rustiguel, J.K.; Fernandes, A.Z.N.; Trivella, D.B.B.
Deposited on : 2024-03-05
Resolution : 3.42 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

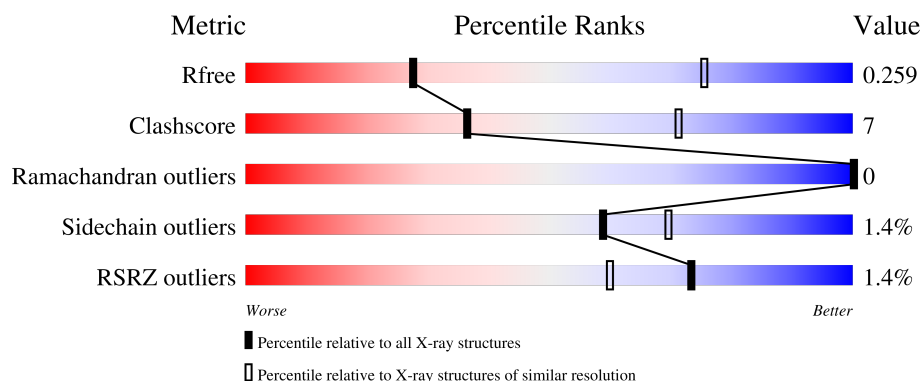
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	250	0% 78% 21% .
1	O	250	0% 81% 18%
2	B	258	3% 76% 18% 6%
2	P	258	3% 74% 20% 5%
3	C	254	2% 76% 18% .

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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

There are 17 unique types of molecules in this entry. The entry contains 49260 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1897	1207	313	374	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1893	1198	315	377	3			
2	P	244	Total	C	N	O	S	0	0	0
			1909	1206	322	378	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	243	Total	C	N	O	S	0	0	0
			1910	1193	333	380	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1853	1157	325	367	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	237	Total	C	N	O	S	0	0	0
			1833	1147	309	370	7			
4	R	236	Total	C	N	O	S	0	0	0
			1718	1075	290	346	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1745	1095	301	345	4			
5	S	232	Total	C	N	O	S	0	0	0
			1774	1114	307	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	245	Total	C	N	O	S	0	0	0
			1884	1198	328	354	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	242	Total	C	N	O	S	0	0	0
			1904	1211	320	365	8			
7	U	242	Total	C	N	O	S	0	0	0
			1910	1215	318	369	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	221	Total	C	N	O	S	0	0	0
			1656	1045	284	320	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1569	1003	257	301	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 type-4.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1547	984	262	295	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
			1749	1110	302	333	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
			1809	1142	310	350	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
			1508	952	249	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1495	945	245	298	7			

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

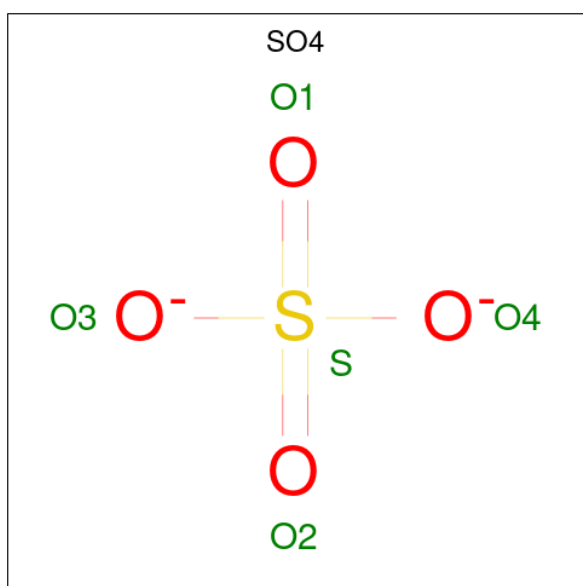
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	M	1	Total	O	S	0	0
			5	4	1		
16	a	1	Total	O	S	0	0
			5	4	1		
16	a	1	Total	O	S	0	0
			5	4	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	12	Total O 12 12	0	0
17	C	5	Total O 5 5	0	0
17	D	5	Total O 5 5	0	0
17	E	4	Total O 4 4	0	0
17	F	8	Total O 8 8	0	0
17	G	2	Total O 2 2	0	0
17	O	5	Total O 5 5	0	0
17	P	8	Total O 8 8	0	0
17	Q	11	Total O 11 11	0	0
17	R	1	Total O 1 1	0	0
17	S	4	Total O 4 4	0	0
17	T	3	Total O 3 3	0	0
17	U	5	Total O 5 5	0	0
17	H	12	Total O 12 12	0	0
17	I	3	Total O 3 3	0	0
17	J	6	Total O 6 6	0	0
17	K	2	Total O 2 2	0	0
17	L	5	Total O 5 5	0	0
17	M	12	Total O 12 12	0	0
17	N	6	Total O 6 6	0	0
17	V	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	2	Total 2	O 2	0	0
17	X	10	Total 10	O 10	0	0
17	Y	7	Total 7	O 7	0	0
17	Z	6	Total 6	O 6	0	0
17	a	14	Total 14	O 14	0	0
17	b	2	Total 2	O 2	0	0

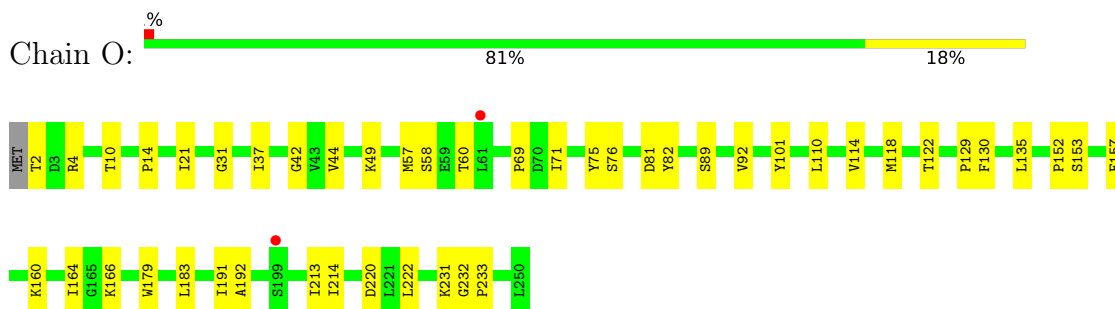
3 Residue-property plots [i](#)

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

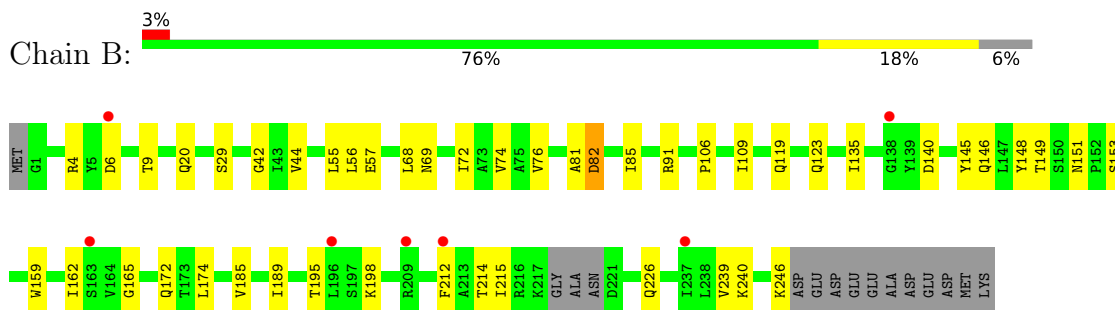
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2

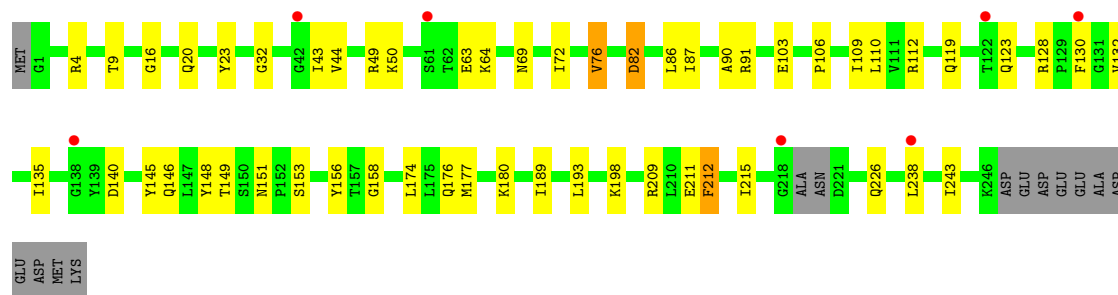


- Molecule 2: Proteasome subunit alpha type-3

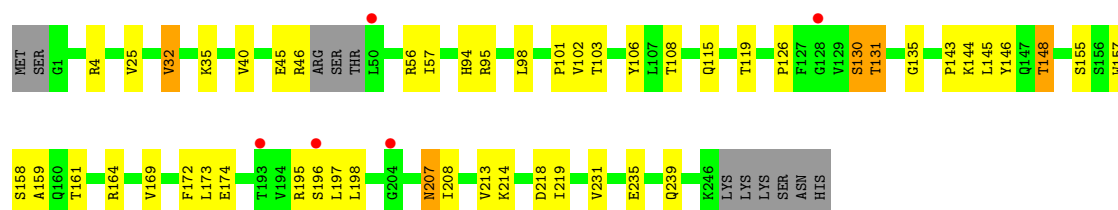
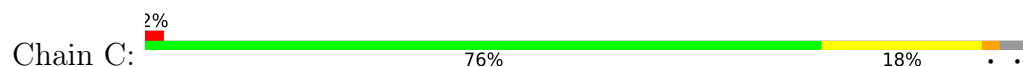


- Molecule 2: Proteasome subunit alpha type-3

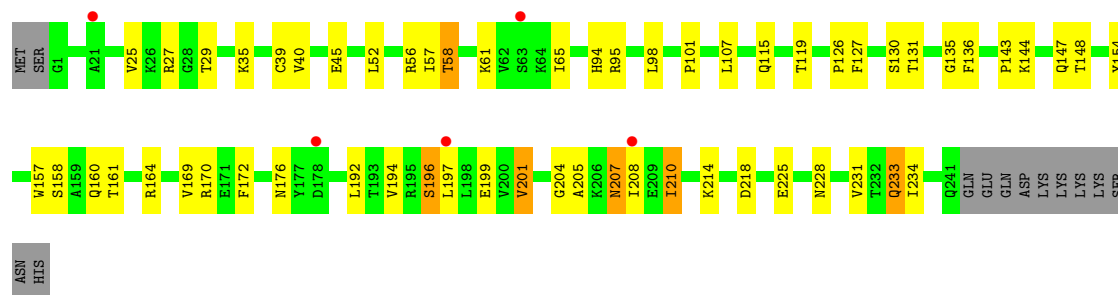
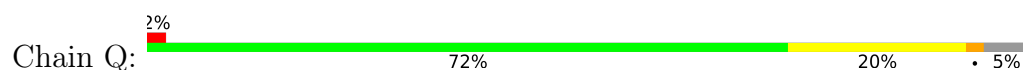




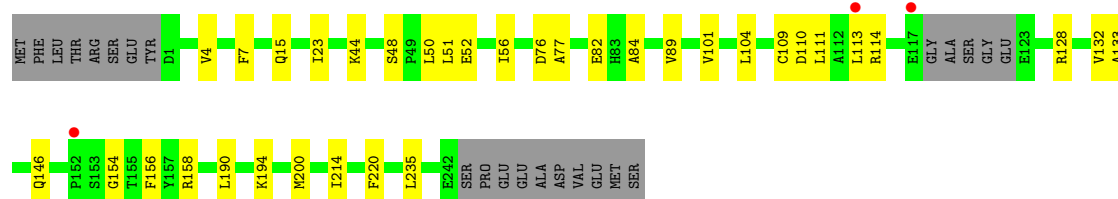
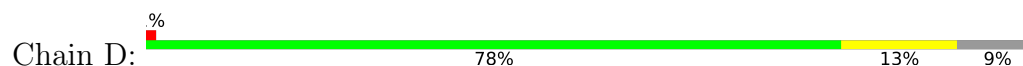
• Molecule 3: Proteasome subunit alpha type-4



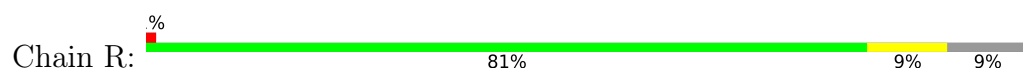
• Molecule 3: Proteasome subunit alpha type-4

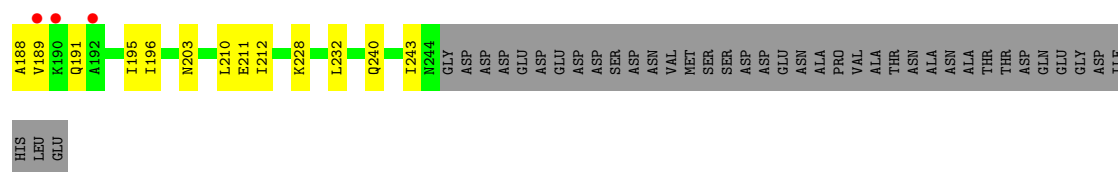


• Molecule 4: Proteasome subunit alpha type-5

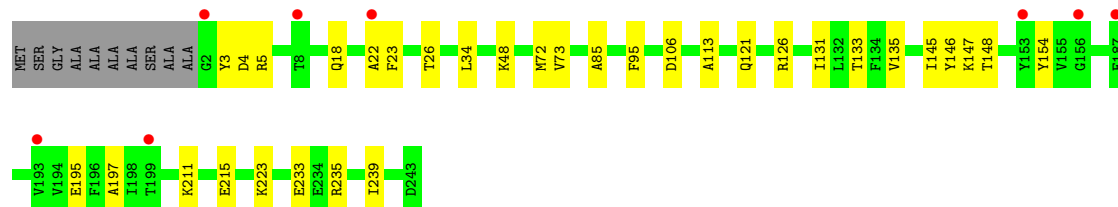
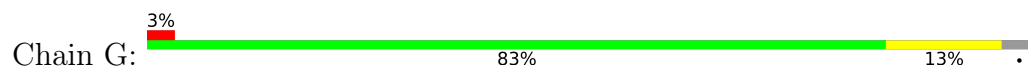


• Molecule 4: Proteasome subunit alpha type-5

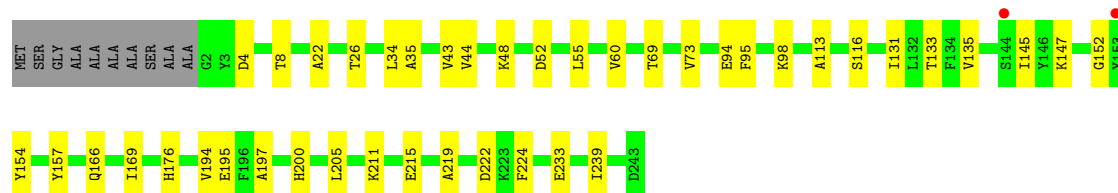
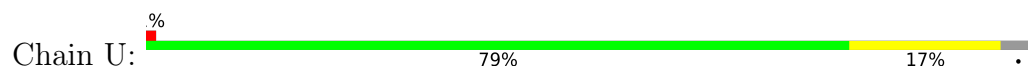




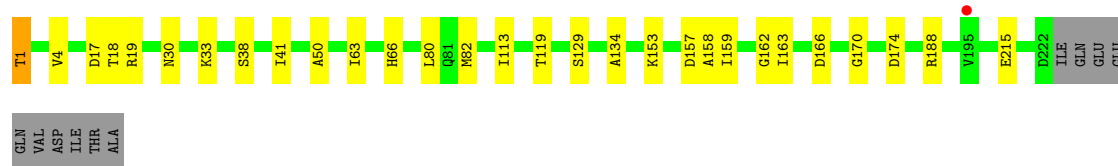
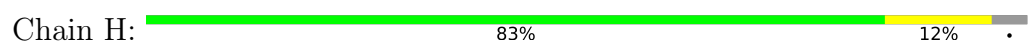
- Molecule 7: Proteasome subunit alpha type-1



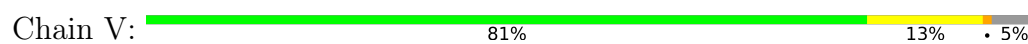
- Molecule 7: Proteasome subunit alpha type-1



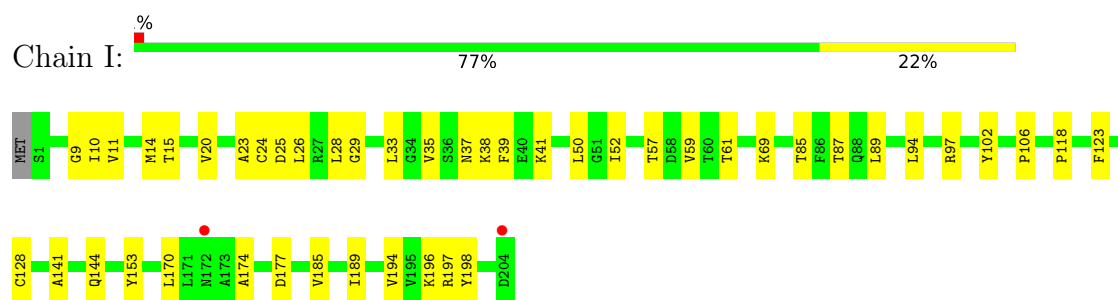
- Molecule 8: proteasome endopeptidase complex



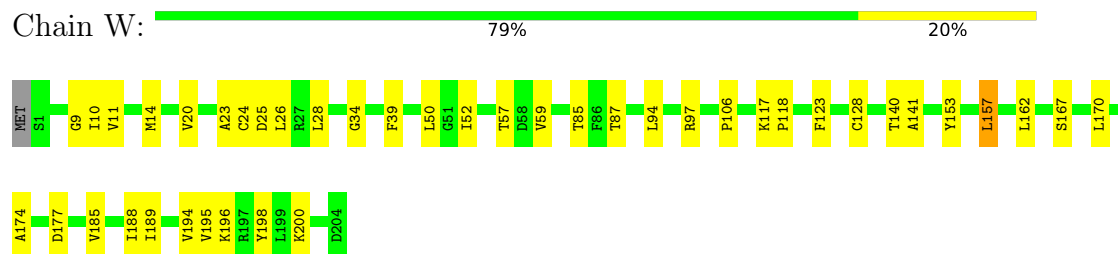
- Molecule 8: proteasome endopeptidase complex



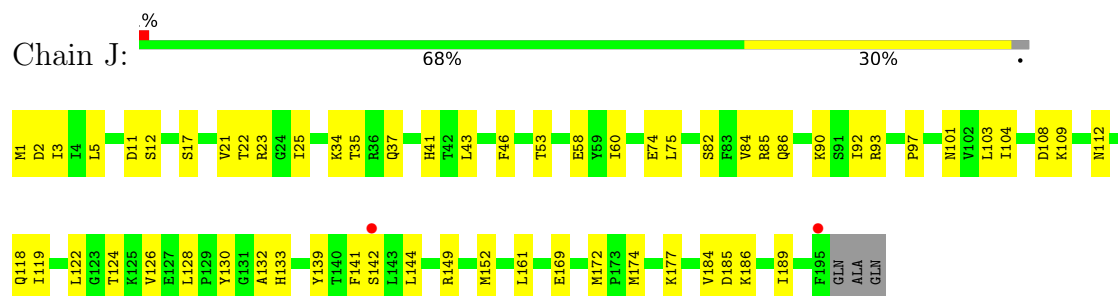
- Molecule 9: Proteasome subunit beta type-3



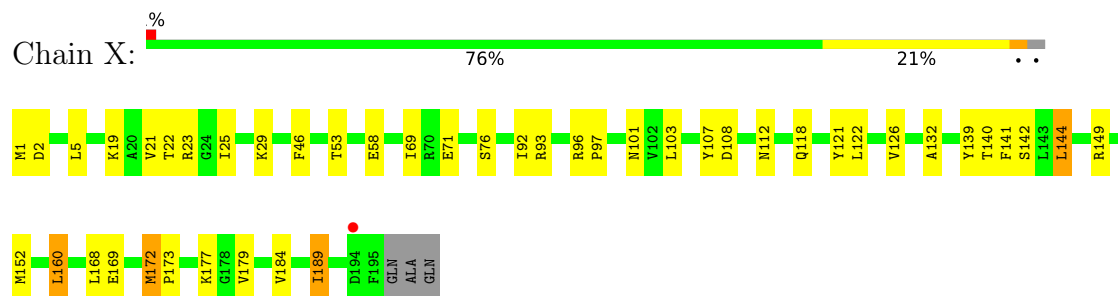
- Molecule 9: Proteasome subunit beta type-3



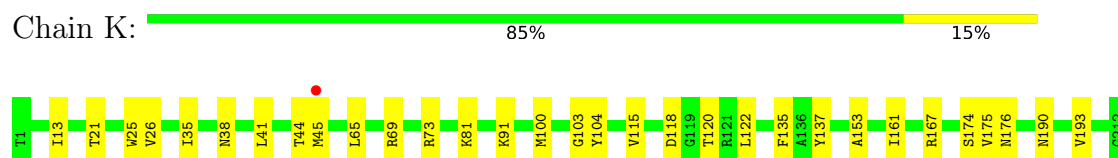
- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4

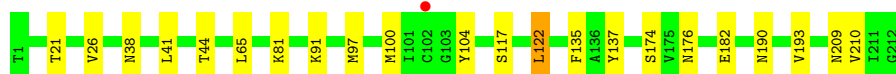


- Molecule 11: proteasome endopeptidase complex



- Molecule 11: proteasome endopeptidase complex

Chain Y:  90% 10%



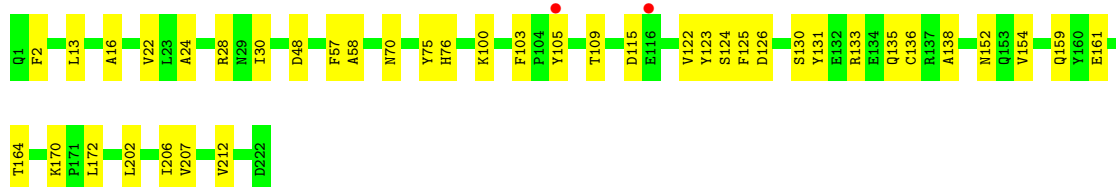
- Molecule 12: PRE7 isoform 1

Chain L:  83% 17%



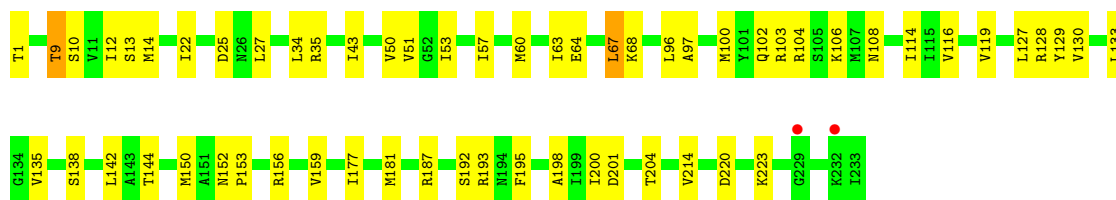
- Molecule 12: PRE7 isoform 1

Chain Z:  82% 18%



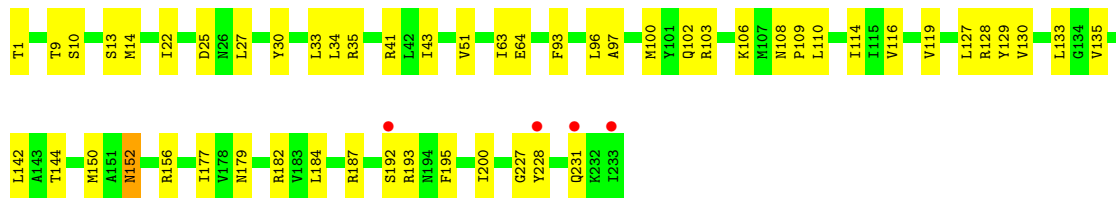
- Molecule 13: Proteasome subunit beta

Chain M:  75% 24%



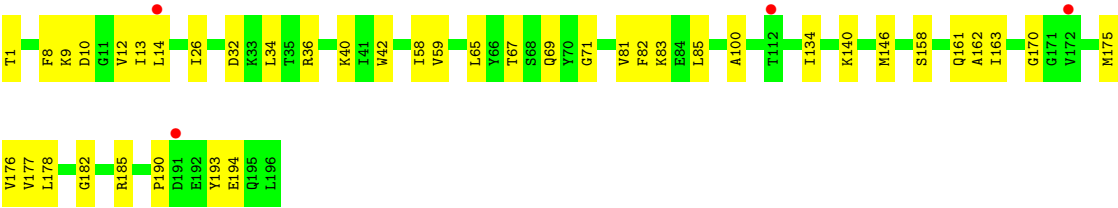
- Molecule 13: Proteasome subunit beta

Chain a:  77% 22%

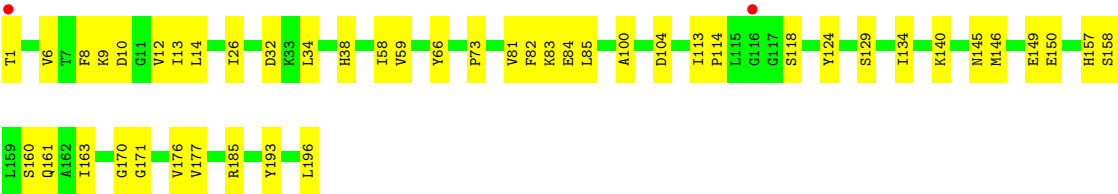
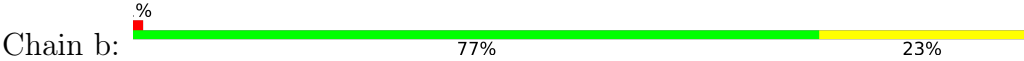


- Molecule 14: Proteasome subunit beta type-1

Chain N:  79% 21%



● Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.96Å 301.46Å 142.65Å 90.00° 111.98° 90.00°	Depositor
Resolution (Å)	29.84 – 3.42 29.84 – 3.42	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.84-3.42) 84.3 (29.84-3.42)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.21-5207	Depositor
R, R_{free}	0.215 , 0.259 0.215 , 0.259	Depositor DCC
R_{free} test set	6917 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	1.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49260	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/1934	0.28	0/2618
1	O	0.09	0/1944	0.27	0/2632
2	B	0.09	0/1922	0.26	0/2600
2	P	0.09	0/1938	0.27	0/2619
3	C	0.11	0/1938	0.30	0/2621
3	Q	0.11	0/1881	0.31	0/2551
4	D	0.09	0/1857	0.26	0/2501
4	R	0.08	0/1742	0.24	0/2365
5	E	0.11	0/1771	0.30	0/2399
5	S	0.10	0/1801	0.29	0/2436
6	F	0.10	0/1936	0.28	0/2614
6	T	0.10	0/1924	0.28	0/2603
7	G	0.09	0/1942	0.26	0/2631
7	U	0.09	0/1948	0.27	0/2638
8	H	0.08	0/1715	0.26	0/2326
8	V	0.08	0/1687	0.26	0/2293
9	I	0.09	0/1599	0.28	0/2160
9	W	0.09	0/1611	0.29	0/2174
10	J	0.09	0/1589	0.26	0/2142
10	X	0.10	0/1575	0.28	0/2126
11	K	0.09	0/1681	0.26	0/2274
11	Y	0.09	0/1681	0.26	0/2274
12	L	0.09	0/1795	0.27	0/2420
12	Z	0.09	0/1787	0.27	0/2411
13	M	0.10	0/1855	0.30	0/2514
13	a	0.10	0/1840	0.29	0/2498
14	N	0.09	0/1537	0.26	0/2083
14	b	0.11	0/1524	0.29	0/2068
All	All	0.09	0/49954	0.28	0/67591

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1897	0	1901	33	0
1	O	1907	0	1917	26	0
2	B	1893	0	1893	31	0
2	P	1909	0	1918	35	0
3	C	1910	0	1916	34	0
3	Q	1853	0	1837	38	0
4	D	1833	0	1816	25	0
4	R	1718	0	1594	17	0
5	E	1745	0	1722	33	0
5	S	1774	0	1766	35	0
6	F	1896	0	1889	23	0
6	T	1884	0	1859	28	0
7	G	1904	0	1886	23	0
7	U	1910	0	1894	22	0
8	H	1684	0	1688	18	0
8	V	1656	0	1640	20	0
9	I	1569	0	1555	32	0
9	W	1581	0	1574	30	0
10	J	1561	0	1569	40	0
10	X	1547	0	1543	33	0
11	K	1644	0	1595	22	0
11	Y	1644	0	1595	16	0
12	L	1757	0	1711	21	0
12	Z	1749	0	1696	25	0
13	M	1824	0	1832	41	0
13	a	1809	0	1792	32	0
14	N	1508	0	1470	25	0
14	b	1495	0	1446	28	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	M	5	0	0	0	0
16	a	10	0	0	0	0
17	A	5	0	0	0	0
17	B	12	0	0	0	0
17	C	5	0	0	0	0
17	D	5	0	0	0	0
17	E	4	0	0	0	0
17	F	8	0	0	0	0
17	G	2	0	0	0	0
17	H	12	0	0	0	0
17	I	3	0	0	0	0
17	J	6	0	0	0	0
17	K	2	0	0	0	0
17	L	5	0	0	0	0
17	M	12	0	0	1	0
17	N	6	0	0	0	0
17	O	5	0	0	0	0
17	P	8	0	0	0	0
17	Q	11	0	0	0	0
17	R	1	0	0	0	0
17	S	4	0	0	0	0
17	T	3	0	0	0	0
17	U	5	0	0	0	0
17	V	12	0	0	1	0
17	W	2	0	0	0	0
17	X	10	0	0	0	0
17	Y	7	0	0	1	0
17	Z	6	0	0	0	0
17	a	14	0	0	1	0
17	b	2	0	0	0	0
All	All	49260	0	48514	706	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 7.

All (706) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:GLY:O	3:C:144:LYS:HB2	1.73	0.87
1:A:38:LYS:NZ	2:B:57:GLU:OE1	2.16	0.77
2:P:63:GLU:HG3	2:P:64:LYS:HG2	1.69	0.74
10:X:92:ILE:HA	10:X:97:PRO:HB3	1.70	0.73
5:S:80:ALA:HB2	5:S:129:VAL:HG21	1.72	0.72
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.72	0.72
13:M:201:ASP:HB3	13:M:204:THR:HG22	1.70	0.72
3:Q:135:GLY:O	3:Q:144:LYS:HB2	1.91	0.71
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.72	0.71
13:M:103:ARG:NH1	13:M:108:ASN:O	2.24	0.70
2:B:44:VAL:HG12	2:B:214:THR:HG22	1.74	0.69
13:M:9:THR:OG1	13:M:10:SER:N	2.25	0.69
3:C:45:GLU:OE2	3:C:164:ARG:NH2	2.25	0.69
2:B:215:ILE:HG12	2:B:226:GLN:HG2	1.75	0.68
2:P:140:ASP:OD2	2:P:146:GLN:NE2	2.26	0.68
9:I:189:ILE:HG23	9:I:194:VAL:HG22	1.74	0.68
10:X:58:GLU:OE1	11:Y:81:LYS:NZ	2.26	0.68
5:E:163:ARG:NH1	5:E:200:LEU:O	2.26	0.68
6:T:39:ASN:ND2	6:T:183:LEU:O	2.27	0.67
2:B:135:ILE:HG12	2:B:149:THR:HG22	1.77	0.67
10:X:92:ILE:HG21	10:X:122:LEU:HA	1.74	0.67
11:Y:44:THR:HG21	11:Y:100:MET:HE2	1.77	0.67
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.76	0.66
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.77	0.66
10:J:92:ILE:HG21	10:J:122:LEU:HA	1.78	0.65
3:Q:95:ARG:HE	3:Q:101:PRO:HG3	1.62	0.65
5:S:49:LYS:HB2	5:S:58:TYR:HB3	1.77	0.65
14:b:9:LYS:HG3	14:b:145:ASN:HB3	1.79	0.65
5:S:116:GLN:NE2	5:S:120:GLN:OE1	2.29	0.64
1:A:222:LEU:HG	1:A:232:GLY:HA2	1.79	0.64
12:L:124:SER:O	12:L:131:TYR:HA	1.98	0.64
8:H:17:ASP:OD1	8:H:33:LYS:NZ	2.28	0.64
13:M:63:ILE:HD13	13:M:114:ILE:HD11	1.80	0.64
2:P:193:LEU:HG	2:P:243:ILE:HD12	1.79	0.64
8:H:215:GLU:HG3	9:I:197:ARG:HG2	1.79	0.64
3:Q:172:PHE:O	3:Q:176:ASN:ND2	2.31	0.64
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	1.80	0.63
12:Z:152:ASN:O	12:Z:159:GLN:NE2	2.29	0.63
1:O:49:LYS:HE3	1:O:58:SER:HB2	1.81	0.63
4:R:4:VAL:HG23	4:R:15:GLN:HG3	1.80	0.63
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.79	0.63
2:P:16:GLY:O	3:Q:27:ARG:NH2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:82:ASP:HB3	2:P:130:PHE:HD1	1.63	0.63
4:D:44:LYS:HD3	4:D:56:ILE:HB	1.80	0.63
3:Q:197:LEU:HD13	3:Q:208:ILE:HD12	1.80	0.62
7:U:48:LYS:HB2	7:U:215:GLU:HG3	1.79	0.62
9:W:97:ARG:HH22	10:X:93:ARG:HD3	1.64	0.62
2:P:119:GLN:NE2	2:P:123:GLN:OE1	2.30	0.62
4:R:113:LEU:HD12	5:S:78:PRO:HB2	1.82	0.62
11:K:21:THR:HG22	11:K:26:VAL:HA	1.82	0.62
10:J:92:ILE:HA	10:J:97:PRO:HB3	1.80	0.62
8:H:174:ASP:OD2	8:H:188:ARG:NH1	2.33	0.62
9:W:189:ILE:HG23	9:W:194:VAL:HG22	1.81	0.62
13:a:27:LEU:HD11	13:a:34:LEU:HB3	1.82	0.62
13:a:63:ILE:HD13	13:a:114:ILE:HD11	1.80	0.62
11:K:44:THR:HG21	11:K:100:MET:HE2	1.83	0.61
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.82	0.61
12:Z:109:THR:HB	12:Z:125:PHE:HB2	1.82	0.61
14:b:146:MET:HB3	14:b:150:GLU:HG3	1.82	0.61
6:T:189:VAL:HG13	6:T:212:ILE:HG21	1.81	0.61
11:Y:21:THR:HG22	11:Y:26:VAL:HA	1.83	0.61
7:G:148:THR:HG22	7:G:154:TYR:HB2	1.83	0.60
4:R:140:ASP:OD2	4:R:146:GLN:NE2	2.34	0.60
3:C:155:SER:HB3	4:D:51:LEU:HD11	1.83	0.60
3:Q:39:CYS:HA	3:Q:136:PHE:HZ	1.65	0.60
9:I:97:ARG:HD3	9:I:102:TYR:HE1	1.66	0.60
10:J:108:ASP:O	10:J:112:ASN:N	2.35	0.60
11:K:35:ILE:HD11	11:K:45:MET:HE3	1.82	0.60
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.82	0.60
14:b:160:SER:HB3	14:b:193:TYR:HB2	1.83	0.60
4:R:19:SER:OG	4:R:130:PHE:O	2.20	0.59
13:a:35:ARG:NH2	17:a:401:HOH:O	2.34	0.59
9:I:23:ALA:HB1	9:I:170:LEU:HD22	1.84	0.59
13:M:13:SER:HB3	13:M:22:ILE:HG13	1.84	0.59
2:P:90:ALA:HB1	2:P:110:LEU:HD21	1.84	0.59
13:a:10:SER:O	13:a:41:ARG:NH2	2.30	0.59
10:J:130:TYR:HB2	10:J:144:LEU:HD13	1.84	0.59
12:L:109:THR:HB	12:L:125:PHE:HB2	1.84	0.59
5:E:69:MET:HE3	5:E:87:LEU:HD21	1.85	0.58
3:Q:35:LYS:HE3	3:Q:143:PRO:HB2	1.85	0.58
6:T:12:SER:OG	6:T:14:ASP:OD1	2.21	0.58
13:a:13:SER:HB3	13:a:22:ILE:HG13	1.84	0.58
12:L:207:VAL:HG22	12:L:212:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:23:ALA:HB1	9:W:170:LEU:HD22	1.86	0.58
2:P:193:LEU:HD21	2:P:238:LEU:HD23	1.85	0.58
8:H:38:SER:HB3	8:H:41:ILE:HB	1.86	0.58
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.86	0.58
2:B:140:ASP:OD2	2:B:146:GLN:NE2	2.35	0.58
3:C:198:LEU:HD11	3:C:231:VAL:HG13	1.86	0.58
3:C:46:ARG:HB3	3:C:207:ASN:HA	1.84	0.58
7:U:52:ASP:HB3	7:U:55:LEU:HD23	1.84	0.58
9:I:15:THR:HG22	9:I:20:VAL:HG12	1.86	0.58
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.86	0.58
3:C:169:VAL:HG13	3:C:196:SER:HB2	1.86	0.57
10:X:152:MET:HE1	10:X:160:LEU:HD22	1.86	0.57
4:D:23:ILE:HD13	4:D:133:ALA:HB2	1.86	0.57
6:F:131:SER:HB2	6:F:161:THR:HG21	1.86	0.57
5:E:170:TYR:O	5:E:174:THR:OG1	2.22	0.57
3:Q:65:ILE:HG21	3:Q:107:LEU:HD21	1.85	0.57
9:I:14:MET:HE3	9:I:153:TYR:HD1	1.69	0.57
12:L:126:ASP:OD1	12:L:130:SER:N	2.37	0.57
13:M:35:ARG:NH2	17:M:401:HOH:O	2.38	0.57
3:C:56:ARG:HG3	3:C:57:ILE:HG23	1.84	0.57
3:Q:56:ARG:HG3	3:Q:57:ILE:HG23	1.85	0.57
4:R:161:ALA:HB3	5:S:55:LEU:HD13	1.86	0.57
6:F:189:VAL:HG13	6:F:212:ILE:HG21	1.87	0.57
10:X:22:THR:O	10:X:23:ARG:NH1	2.38	0.57
13:a:96:LEU:O	13:a:100:MET:HG2	2.05	0.57
1:A:119:GLN:NE2	1:A:123:GLN:OE1	2.37	0.57
12:Z:207:VAL:HG22	12:Z:212:VAL:HG22	1.86	0.57
7:G:23:PHE:O	7:G:26:THR:OG1	2.20	0.56
5:S:105:GLU:HG2	5:S:109:HIS:CE1	2.39	0.56
3:C:172:PHE:HZ	3:C:195:ARG:HE	1.52	0.56
2:B:119:GLN:NE2	2:B:123:GLN:OE1	2.35	0.56
3:Q:225:GLU:N	3:Q:225:GLU:OE1	2.36	0.56
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.87	0.56
7:U:69:THR:HG22	7:U:222:ASP:HA	1.88	0.56
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.87	0.56
14:b:134:ILE:HD12	14:b:158:SER:HB3	1.86	0.56
10:J:139:TYR:OH	10:X:25:ILE:O	2.23	0.56
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.87	0.56
4:R:83:HIS:CG	4:R:111:LEU:HD11	2.41	0.56
5:S:114:LYS:HD2	5:S:117:LYS:HD3	1.87	0.56
8:H:1:THR:HG23	8:H:33:LYS:HZ3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:153:LYS:NZ	8:H:157:ASP:OD2	2.31	0.56
11:K:135:PHE:HB3	10:X:142:SER:HB3	1.88	0.56
12:L:4:PRO:O	13:M:104:ARG:NH1	2.38	0.56
14:b:171:GLY:O	14:b:193:TYR:OH	2.23	0.56
5:E:116:GLN:NE2	5:E:120:GLN:OE1	2.39	0.56
3:Q:194:VAL:HG13	3:Q:234:ILE:HD11	1.87	0.56
9:W:52:ILE:HG22	9:W:59:VAL:HG22	1.87	0.56
10:J:172:MET:HE3	10:J:174:MET:HB2	1.87	0.55
4:D:4:VAL:HG13	4:D:15:GLN:HG3	1.88	0.55
12:Z:126:ASP:OD1	12:Z:130:SER:N	2.38	0.55
2:P:103:GLU:OE2	10:X:76:SER:OG	2.23	0.55
6:T:210:LEU:HD21	6:T:212:ILE:HD11	1.88	0.55
3:Q:197:LEU:O	3:Q:201:VAL:HG13	2.06	0.55
6:F:186:ARG:NH1	6:F:234:GLU:OE2	2.40	0.55
2:P:193:LEU:HD13	2:P:212:PHE:HE2	1.69	0.55
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.88	0.55
5:E:28:ILE:HD11	5:E:148:PRO:HD3	1.89	0.55
3:Q:45:GLU:OE2	3:Q:164:ARG:NH2	2.33	0.55
12:L:64:LEU:HD21	12:L:97:LEU:HD21	1.89	0.55
12:Z:124:SER:O	12:Z:131:TYR:HA	2.07	0.55
13:M:25:ASP:HA	13:M:195:PHE:HA	1.87	0.55
3:C:174:GLU:HG2	4:D:50:LEU:HD13	1.89	0.55
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.89	0.55
1:O:69:PRO:HB3	1:O:233:PRO:HB3	1.89	0.55
9:W:188:ILE:HB	9:W:195:VAL:HG12	1.89	0.55
9:I:52:ILE:HG22	9:I:59:VAL:HG22	1.88	0.54
4:D:111:LEU:HD12	4:D:114:ARG:HD2	1.88	0.54
3:Q:201:VAL:HG11	3:Q:208:ILE:HD11	1.89	0.54
11:Y:97:MET:N	11:Y:117:SER:OG	2.36	0.54
3:C:35:LYS:HD2	3:C:158:SER:HA	1.89	0.54
4:D:76:ASP:OD2	4:D:128:ARG:NH1	2.34	0.54
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.89	0.54
4:D:109:CYS:SG	4:D:156:PHE:HB3	2.48	0.54
7:G:135:VAL:HG12	7:G:145:ILE:HG12	1.89	0.54
13:M:129:TYR:HE2	13:M:144:THR:HG22	1.73	0.54
14:b:114:PRO:HD2	14:b:118:SER:O	2.07	0.54
6:T:23:ALA:O	6:T:27:VAL:HG13	2.07	0.54
6:T:228:LYS:HA	6:T:232:LEU:HD12	1.90	0.54
9:W:189:ILE:HD13	9:W:194:VAL:HG13	1.90	0.54
10:J:177:LYS:NZ	10:X:169:GLU:O	2.40	0.54
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:38:SER:HB3	8:V:41:ILE:HB	1.90	0.54
2:B:189:ILE:HG12	2:B:212:PHE:HZ	1.73	0.53
3:C:235:GLU:O	3:C:239:GLN:HG2	2.07	0.53
10:J:12:SER:HB3	10:J:185:ASP:HB3	1.91	0.53
12:L:24:ALA:HB1	12:L:202:LEU:HD11	1.89	0.53
13:a:227:GLY:HA3	13:a:231:GLN:HB2	1.89	0.53
2:B:149:THR:HG21	2:B:162:ILE:HG12	1.89	0.53
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.91	0.53
10:J:46:PHE:HD2	10:J:53:THR:HB	1.74	0.53
8:V:13:VAL:HG12	8:V:177:VAL:HG13	1.89	0.53
13:a:51:VAL:HG13	13:a:114:ILE:HG23	1.90	0.53
5:E:210:LEU:HB3	5:E:229:VAL:HG21	1.89	0.53
1:O:222:LEU:HG	1:O:232:GLY:HA2	1.89	0.53
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.91	0.53
1:A:49:LYS:NZ	1:A:61:LEU:O	2.29	0.53
3:C:95:ARG:HE	3:C:101:PRO:HG3	1.74	0.53
14:N:58:ILE:HG22	14:N:85:LEU:HD11	1.91	0.53
1:A:116:LYS:NZ	1:A:120:GLU:OE2	2.35	0.53
3:Q:233:GLN:NE2	3:Q:233:GLN:O	2.42	0.53
6:T:118:ALA:HA	6:T:121:LEU:HD12	1.90	0.53
8:H:134:ALA:HB1	8:H:158:ALA:HB1	1.91	0.53
10:J:60:ILE:HD12	10:J:84:VAL:HG12	1.91	0.53
9:W:10:ILE:HD11	9:W:174:ALA:HB2	1.91	0.53
9:W:26:LEU:HD21	9:W:185:VAL:HG13	1.89	0.53
3:C:40:VAL:HG22	3:C:143:PRO:HB3	1.91	0.53
13:M:96:LEU:O	13:M:100:MET:HG2	2.09	0.53
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.91	0.53
10:J:25:ILE:O	10:X:139:TYR:OH	2.27	0.52
3:C:197:LEU:HD23	3:C:208:ILE:HD12	1.90	0.52
4:R:23:ILE:HD13	4:R:133:ALA:HB2	1.90	0.52
6:F:186:ARG:HG3	6:F:231:LEU:HD11	1.91	0.52
9:I:10:ILE:HD11	9:I:174:ALA:HB2	1.91	0.52
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.90	0.52
13:a:103:ARG:HD3	13:a:110:LEU:HG	1.92	0.52
4:D:101:VAL:HB	4:D:146:GLN:HE21	1.75	0.52
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.90	0.52
6:F:9:SER:HB2	7:G:126:ARG:HG2	1.92	0.52
5:S:70:GLY:HA3	5:S:221:PHE:CZ	2.45	0.52
5:S:174:THR:HG22	5:S:177:THR:HB	1.91	0.52
11:K:176:ASN:OD1	11:K:190:ASN:ND2	2.35	0.52
6:T:24:VAL:O	6:T:27:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:THR:HG22	3:C:126:PRO:HB3	1.92	0.52
4:D:194:LYS:HB2	4:D:235:LEU:HD11	1.92	0.52
1:O:42:GLY:HA2	1:O:214:ILE:O	2.10	0.52
10:J:5:LEU:HD23	10:J:132:ALA:HB2	1.91	0.52
1:A:44:VAL:HG22	1:A:213:ILE:HG22	1.92	0.52
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.92	0.52
4:D:113:LEU:HD22	5:E:78:PRO:HB2	1.91	0.51
3:Q:29:THR:OG1	3:Q:61:LYS:NZ	2.32	0.51
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.92	0.51
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.92	0.51
9:W:157:LEU:HD13	9:W:162:LEU:HB2	1.92	0.51
3:C:35:LYS:NZ	4:D:52:GLU:OE2	2.39	0.51
7:U:135:VAL:HG12	7:U:145:ILE:HG12	1.90	0.51
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.92	0.51
14:N:176:VAL:HG22	14:N:185:ARG:HD2	1.92	0.51
11:Y:44:THR:OG1	11:Y:100:MET:N	2.34	0.51
13:a:227:GLY:HA2	13:a:231:GLN:HE21	1.75	0.51
8:H:19:ARG:O	8:H:33:LYS:NZ	2.38	0.51
13:a:179:ASN:OD1	13:a:182:ARG:NH2	2.44	0.51
3:C:102:VAL:HG13	3:C:106:TYR:HD2	1.76	0.51
10:J:149:ARG:HB2	10:J:152:MET:HG3	1.93	0.51
13:M:193:ARG:HG3	13:M:214:VAL:HB	1.93	0.51
6:F:175:LEU:HD11	6:F:191:GLN:HG2	1.93	0.51
9:I:29:GLY:HA2	9:I:35:VAL:HG23	1.92	0.51
8:V:120:ASP:OD1	8:V:120:ASP:N	2.42	0.51
9:W:14:MET:HE3	9:W:153:TYR:HD1	1.76	0.51
1:A:122:THR:HG22	1:A:129:PRO:HB3	1.92	0.51
2:P:106:PRO:HD2	2:P:109:ILE:HD12	1.92	0.51
3:Q:25:VAL:HG11	3:Q:130:SER:HB2	1.92	0.51
14:N:40:LYS:HE2	14:N:182:GLY:HA2	1.92	0.51
7:G:48:LYS:HB2	7:G:215:GLU:HG3	1.92	0.51
13:M:150:MET:HE1	13:M:187:ARG:HG3	1.93	0.51
2:P:82:ASP:HB3	2:P:130:PHE:CD1	2.44	0.50
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.93	0.50
11:Y:209:ASN:ND2	17:Y:401:HOH:O	2.43	0.50
13:a:129:TYR:HE2	13:a:144:THR:HG22	1.75	0.50
3:Q:131:THR:HB	3:Q:148:THR:HB	1.94	0.50
3:Q:201:VAL:CG1	3:Q:208:ILE:HD11	2.41	0.50
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.94	0.50
13:M:27:LEU:HD11	13:M:34:LEU:HB3	1.93	0.50
13:M:43:ILE:HG13	13:M:64:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.92	0.50
13:M:152:ASN:O	13:M:156:ARG:HG3	2.11	0.50
14:N:161:GLN:HE21	14:b:140:LYS:HE2	1.75	0.50
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.46	0.50
1:O:81:ASP:HB3	1:O:130:PHE:HD2	1.77	0.50
5:S:105:GLU:HG2	5:S:109:HIS:HE1	1.77	0.50
6:T:146:MET:HB3	6:T:156:TYR:CE1	2.47	0.50
5:S:28:ILE:HD11	5:S:148:PRO:HD3	1.94	0.50
5:S:209:ASN:N	5:S:209:ASN:OD1	2.45	0.50
6:T:184:SER:O	6:T:188:ALA:N	2.40	0.50
13:M:12:ILE:HG12	13:M:181:MET:HE2	1.94	0.50
14:N:134:ILE:HD12	14:N:158:SER:HB3	1.94	0.50
2:B:106:PRO:HD2	2:B:109:ILE:HD12	1.94	0.49
10:J:86:GLN:HG2	10:J:90:LYS:HE3	1.93	0.49
13:M:51:VAL:HG22	13:M:116:VAL:HG22	1.94	0.49
1:O:220:ASP:OD1	1:O:220:ASP:N	2.45	0.49
5:S:175:LEU:HA	5:S:178:PHE:CE1	2.47	0.49
13:M:50:VAL:HG23	13:M:200:ILE:HD11	1.94	0.49
8:V:112:SER:OG	8:V:120:ASP:OD1	2.25	0.49
2:B:239:VAL:HG11	2:B:246:LYS:HB3	1.94	0.49
2:P:112:ARG:NH2	10:X:71:GLU:OE2	2.45	0.49
6:F:147:LEU:HD13	6:F:153:TYR:HB3	1.93	0.49
14:N:26:ILE:HB	13:a:187:ARG:HA	1.95	0.49
8:V:213:LEU:HG	9:W:200:LYS:HB2	1.94	0.49
1:A:69:PRO:HB3	1:A:233:PRO:HB3	1.94	0.49
2:B:151:ASN:OD1	2:B:153:SER:OG	2.25	0.49
2:P:4:ARG:HH12	6:T:7:SER:HB2	1.77	0.49
3:Q:228:ASN:HA	3:Q:231:VAL:HG22	1.92	0.49
11:K:44:THR:OG1	11:K:100:MET:N	2.38	0.49
14:b:12:VAL:HG21	14:b:100:ALA:HB1	1.95	0.49
14:b:59:VAL:HG11	14:b:82:PHE:CE2	2.47	0.49
2:P:32:GLY:N	2:P:50:LYS:HD2	2.27	0.49
7:U:169:ILE:HD11	7:U:205:LEU:HD21	1.95	0.49
14:N:140:LYS:HE3	14:b:161:GLN:HE21	1.78	0.49
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.95	0.49
14:b:1:THR:O	14:b:129:SER:N	2.46	0.49
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.95	0.49
7:G:4:ASP:N	7:G:4:ASP:OD1	2.46	0.49
7:G:48:LYS:HE3	7:G:215:GLU:HG2	1.94	0.49
1:O:31:GLY:O	1:O:166:LYS:HG3	2.12	0.49
9:I:61:THR:HG23	10:J:85:ARG:HH22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:30:TYR:N	13:a:33:LEU:O	2.43	0.49
4:D:77:ALA:HB2	4:D:132:VAL:HG11	1.94	0.48
5:E:44:VAL:HG23	5:E:188:LEU:HD23	1.93	0.48
5:E:103:ALA:HB3	5:E:106:ARG:HG3	1.94	0.48
5:E:70:GLY:HA3	5:E:221:PHE:CZ	2.49	0.48
2:P:43:ILE:HD11	2:P:145:TYR:HB3	1.95	0.48
8:V:19:ARG:NH2	8:V:167:LEU:O	2.46	0.48
10:X:19:LYS:NZ	10:X:179:VAL:O	2.46	0.48
5:S:163:ARG:O	5:S:199:SER:OG	2.25	0.48
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.94	0.48
10:X:1:MET:HG2	10:X:2:ASP:H	1.78	0.48
14:b:59:VAL:HG22	14:b:81:VAL:HG12	1.94	0.48
3:Q:115:GLN:HG2	3:Q:127:PHE:CD2	2.49	0.48
3:Q:161:THR:HG21	3:Q:169:VAL:HB	1.95	0.48
1:A:245:ASP:O	1:A:248:GLU:HG2	2.13	0.48
13:M:102:GLN:O	13:M:106:LYS:HG2	2.14	0.48
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.79	0.48
1:A:149:GLN:O	1:A:156:TYR:HA	2.13	0.48
7:U:113:ALA:HB2	7:U:154:TYR:HB3	1.96	0.48
2:B:159:TRP:CD2	2:B:162:ILE:HD13	2.49	0.48
3:C:207:ASN:OD1	3:C:207:ASN:N	2.47	0.48
6:F:240:GLN:O	6:F:243:ILE:HG22	2.14	0.48
2:P:69:ASN:OD1	2:P:72:ILE:N	2.47	0.48
9:I:26:LEU:HD11	9:I:185:VAL:HG13	1.96	0.48
2:B:174:LEU:HD13	2:B:195:THR:HA	1.95	0.48
2:P:82:ASP:OD1	2:P:82:ASP:N	2.46	0.48
6:T:147:LEU:HD13	6:T:153:TYR:HB3	1.96	0.47
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.96	0.47
9:W:140:THR:OG1	9:W:177:ASP:OD2	2.32	0.47
10:X:101:ASN:OD1	10:X:121:TYR:N	2.43	0.47
3:C:25:VAL:HG11	3:C:130:SER:HB2	1.97	0.47
8:H:1:THR:O	8:H:129:SER:N	2.47	0.47
12:L:134:GLU:OE2	12:L:137:ARG:NH1	2.48	0.47
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.96	0.47
1:A:114:VAL:O	1:A:118:MET:HG3	2.14	0.47
5:S:49:LYS:HB3	5:S:59:GLN:O	2.13	0.47
10:J:58:GLU:OE1	11:K:81:LYS:NZ	2.35	0.47
4:D:84:ALA:HB1	4:D:104:LEU:HD11	1.96	0.47
4:D:158:ARG:HB3	5:E:57:SER:HB3	1.97	0.47
1:O:4:ARG:NH2	4:R:117:GLU:OE1	2.48	0.47
10:J:119:ILE:HA	10:J:124:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:184:VAL:HG12	10:X:189:ILE:HG22	1.96	0.47
14:b:58:ILE:HG22	14:b:85:LEU:HD21	1.96	0.47
7:G:195:GLU:HG3	7:G:235:ARG:HD3	1.97	0.47
7:U:22:ALA:O	7:U:26:THR:HG23	2.15	0.47
7:U:26:THR:HG21	7:U:131:ILE:HG13	1.96	0.47
2:B:68:LEU:O	2:B:91:ARG:HG2	2.15	0.47
1:O:114:VAL:O	1:O:118:MET:HG3	2.15	0.47
2:P:176:GLN:HB2	3:Q:52:LEU:HD21	1.97	0.47
5:S:35:VAL:HG13	5:S:46:VAL:HG23	1.97	0.47
5:S:196:ILE:O	5:S:200:LEU:HG	2.15	0.47
9:I:50:LEU:HD11	9:I:106:PRO:HB3	1.97	0.47
10:J:1:MET:HG2	10:J:2:ASP:H	1.80	0.47
10:J:46:PHE:CD2	10:J:53:THR:HB	2.50	0.47
6:F:118:ALA:HA	6:F:121:LEU:HD13	1.97	0.47
10:J:3:ILE:HD11	10:J:172:MET:HE1	1.96	0.47
14:N:194:GLU:OE1	13:a:193:ARG:NH1	2.48	0.47
3:Q:161:THR:O	3:Q:170:ARG:NH2	2.48	0.47
14:N:59:VAL:HG22	14:N:81:VAL:HG12	1.97	0.47
1:A:220:ASP:OD1	1:A:220:ASP:N	2.45	0.47
3:Q:157:TRP:CZ3	4:R:48:SER:HB3	2.50	0.47
13:M:51:VAL:HG13	13:M:114:ILE:HG23	1.97	0.47
12:Z:172:LEU:HD23	12:Z:172:LEU:H	1.80	0.47
2:P:215:ILE:HG12	2:P:226:GLN:HG2	1.96	0.46
5:S:35:VAL:HB	5:S:159:ALA:HB2	1.97	0.46
5:S:92:ASN:ND2	12:Z:70:ASN:OD1	2.41	0.46
7:U:4:ASP:OD1	7:U:4:ASP:N	2.45	0.46
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.42	0.46
11:K:38:ASN:HD21	11:K:41:LEU:HD12	1.80	0.46
1:O:122:THR:HG22	1:O:129:PRO:HB3	1.97	0.46
1:A:101:TYR:HB3	9:I:85:THR:HG23	1.98	0.46
6:F:91:GLU:HB3	6:F:111:ARG:HH11	1.80	0.46
3:Q:35:LYS:HD3	3:Q:158:SER:HA	1.97	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.46
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.98	0.46
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.97	0.46
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.79	0.46
12:Z:57:PHE:HZ	13:a:133:LEU:HB3	1.81	0.46
5:E:32:SER:HB2	5:E:48:LEU:HD23	1.97	0.46
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.51	0.46
1:O:118:MET:HE2	1:O:152:PRO:HA	1.97	0.46
9:I:33:LEU:HD11	10:J:141:PHE:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:MET:HE2	1:A:152:PRO:HA	1.97	0.46
1:A:127:VAL:HG23	7:G:121:GLN:HG2	1.98	0.46
1:A:137:ALA:HB3	1:A:214:ILE:HD13	1.98	0.46
7:U:116:SER:HB2	7:U:152:GLY:HA2	1.98	0.46
12:L:13:LEU:HD13	12:L:138:ALA:HB2	1.97	0.46
14:N:59:VAL:HG11	14:N:82:PHE:CE2	2.51	0.46
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.97	0.46
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.46
10:J:101:ASN:HB3	10:J:133:HIS:CE1	2.50	0.46
1:A:111:VAL:HG22	1:A:136:ILE:HD12	1.98	0.46
7:G:34:LEU:HD11	7:G:197:ALA:HB1	1.98	0.46
7:U:94:GLU:HG2	7:U:98:LYS:HE2	1.98	0.46
8:H:18:THR:HB	8:H:30:ASN:HA	1.97	0.46
13:M:187:ARG:HA	14:b:26:ILE:HB	1.97	0.46
13:a:150:MET:HE3	13:a:184:LEU:HD23	1.98	0.46
3:Q:147:GLN:O	3:Q:154:TYR:HA	2.16	0.46
1:A:118:MET:HE3	1:A:130:PHE:HB2	1.98	0.46
2:B:146:GLN:HB3	2:B:148:TYR:CE1	2.51	0.46
6:T:97:LYS:NZ	14:b:84:GLU:OE2	2.40	0.46
10:J:22:THR:HG21	10:X:173:PRO:HG3	1.98	0.46
2:B:69:ASN:OD1	2:B:72:ILE:N	2.49	0.45
4:D:89:VAL:HG21	11:K:65:LEU:HG	1.98	0.45
1:O:37:ILE:HD13	1:O:192:ALA:HB2	1.97	0.45
7:U:195:GLU:HA	7:U:239:ILE:HD11	1.97	0.45
10:J:82:SER:HA	10:J:85:ARG:HG2	1.98	0.45
10:X:107:TYR:HE1	10:X:112:ASN:C	2.24	0.45
5:E:196:ILE:O	5:E:200:LEU:HG	2.16	0.45
1:O:71:ILE:HG21	1:O:110:LEU:HD23	1.98	0.45
5:S:210:LEU:HB3	5:S:229:VAL:HG21	1.97	0.45
14:N:8:PHE:HB2	14:N:146:MET:O	2.15	0.45
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.98	0.45
1:A:176:GLU:HG2	2:B:55:LEU:HG	1.99	0.45
7:G:113:ALA:HB2	7:G:154:TYR:HB3	1.97	0.45
5:S:200:LEU:HB3	5:S:203:GLU:HG3	1.97	0.45
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.45
1:A:197:LYS:HB2	1:A:204:PHE:CE2	2.51	0.45
3:Q:94:HIS:O	3:Q:98:LEU:HB2	2.17	0.45
6:T:46:VAL:HG11	6:T:62:LYS:HB2	1.98	0.45
8:V:134:ALA:HB1	8:V:158:ALA:HB1	1.99	0.45
7:G:22:ALA:O	7:G:26:THR:HG23	2.17	0.45
2:P:174:LEU:HA	2:P:177:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:109:CYS:SG	4:R:156:PHE:HB3	2.57	0.45
6:F:82:ARG:HA	6:F:85:VAL:HG22	1.99	0.45
7:U:34:LEU:HD11	7:U:197:ALA:HB1	1.99	0.45
8:V:217:ILE:HD12	9:W:194:VAL:O	2.17	0.45
10:X:46:PHE:HD2	10:X:53:THR:HB	1.81	0.45
14:b:6:VAL:HG22	14:b:124:TYR:HB2	1.98	0.45
14:b:104:ASP:OD1	14:b:104:ASP:N	2.49	0.45
6:F:189:VAL:HG11	6:F:227:VAL:HG11	1.98	0.45
1:O:101:TYR:HB3	9:W:85:THR:HG23	1.98	0.45
3:Q:157:TRP:HZ3	4:R:48:SER:HB3	1.82	0.45
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.99	0.45
10:J:41:HIS:N	10:J:74:GLU:OE2	2.49	0.45
11:K:120:THR:HG23	11:K:122:LEU:HD13	1.99	0.45
11:Y:176:ASN:OD1	11:Y:190:ASN:ND2	2.39	0.45
7:G:147:LYS:O	7:G:154:TYR:HA	2.16	0.45
11:K:167:ARG:NE	10:X:141:PHE:HB3	2.31	0.45
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.45
13:a:14:MET:HG2	13:a:177:ILE:HD11	1.98	0.45
13:a:25:ASP:HA	13:a:195:PHE:HA	1.99	0.45
5:E:49:LYS:N	5:E:209:ASN:O	2.40	0.45
5:E:105:GLU:O	5:E:109:HIS:ND1	2.50	0.45
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.99	0.45
2:P:9:THR:HB	2:P:20:GLN:HG3	1.98	0.45
6:T:52:SER:H	6:T:55:LEU:HD13	1.82	0.45
12:L:10:GLY:HA3	12:L:42:LYS:HE3	1.99	0.45
12:Z:48:ASP:OD2	12:Z:76:HIS:NE2	2.48	0.45
2:B:29:SER:HA	2:B:165:GLY:O	2.17	0.44
4:D:109:CYS:HB3	4:D:154:GLY:O	2.17	0.44
5:E:175:LEU:HA	5:E:178:PHE:CE1	2.52	0.44
6:F:236:ILE:O	6:F:240:GLN:HG2	2.17	0.44
3:Q:119:THR:HG22	3:Q:126:PRO:HB3	1.98	0.44
5:S:2:ARG:HB2	5:S:19:PHE:CZ	2.52	0.44
9:I:11:VAL:HG22	9:I:24:CYS:HB2	1.99	0.44
1:A:106:PRO:HD2	1:A:109:LEU:HD12	1.99	0.44
3:Q:40:VAL:HG22	3:Q:143:PRO:HB3	1.99	0.44
13:a:119:VAL:HG23	13:a:200:ILE:HG22	1.99	0.44
5:E:134:ILE:HD11	5:E:221:PHE:HE1	1.82	0.44
7:G:5:ARG:O	7:G:18:GLN:NE2	2.50	0.44
9:W:196:LYS:HE3	9:W:198:TYR:CE1	2.53	0.44
1:A:211:LEU:HD22	1:A:238:LEU:HD22	2.00	0.44
3:C:32:VAL:HG11	3:C:169:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:VAL:HG22	1:O:213:ILE:HG22	1.98	0.44
2:B:174:LEU:HD11	2:B:198:LYS:HD3	2.00	0.44
7:U:73:VAL:HG13	7:U:133:THR:HB	2.00	0.44
10:J:11:ASP:OD1	10:J:11:ASP:N	2.50	0.44
6:T:154:TRP:HB2	6:T:156:TYR:CE1	2.53	0.44
7:U:219:ALA:HB2	7:U:224:PHE:HD1	1.83	0.44
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.86	0.44
4:D:110:ASP:OD2	5:E:81:ARG:NE	2.51	0.44
1:O:231:LYS:HE2	1:O:231:LYS:HB2	1.88	0.44
2:P:158:GLY:H	3:Q:58:THR:HG22	1.83	0.44
3:Q:160:GLN:NE2	3:Q:170:ARG:HH21	2.16	0.44
10:J:35:THR:HB	10:J:43:LEU:HD11	1.99	0.44
9:W:141:ALA:HB2	9:W:177:ASP:HB2	1.99	0.44
13:a:1:THR:N	13:a:108:ASN:OD1	2.51	0.44
5:E:174:THR:HG22	5:E:177:THR:OG1	2.18	0.44
10:J:109:LYS:HE3	10:J:186:LYS:HB2	1.99	0.44
8:V:18:THR:HB	8:V:30:ASN:HA	1.99	0.44
9:W:117:LYS:HB3	9:W:117:LYS:HE2	1.79	0.44
3:C:94:HIS:O	3:C:98:LEU:HB2	2.18	0.44
5:E:25:LEU:HD23	5:E:28:ILE:HD12	2.00	0.44
14:N:8:PHE:CE2	14:N:10:ASP:HB2	2.53	0.44
7:G:195:GLU:HA	7:G:239:ILE:HD11	1.99	0.43
11:K:91:LYS:NZ	11:K:118:ASP:O	2.45	0.43
10:X:5:LEU:HD23	10:X:132:ALA:HB2	2.00	0.43
10:X:103:LEU:HD23	10:X:118:GLN:HA	1.99	0.43
12:Z:136:CYS:SG	12:Z:154:VAL:HG11	2.58	0.43
13:a:43:ILE:HG13	13:a:64:GLU:HG2	1.99	0.43
14:b:14:LEU:HD13	14:b:176:VAL:HG13	1.99	0.43
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.53	0.43
11:K:73:ARG:NH2	11:K:104:TYR:O	2.38	0.43
8:V:22:GLN:NE2	17:V:401:HOH:O	2.38	0.43
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.53	0.43
2:P:49:ARG:N	2:P:209:ARG:O	2.46	0.43
2:P:76:VAL:HG23	2:P:132:VAL:HG13	1.99	0.43
4:R:97:GLU:OE2	12:Z:75:TYR:OH	2.25	0.43
5:S:44:VAL:HG23	5:S:188:LEU:HD23	2.00	0.43
12:Z:161:GLU:O	12:Z:164:THR:HG22	2.18	0.43
2:B:42:GLY:HA2	2:B:145:TYR:CE1	2.54	0.43
2:B:82:ASP:OD1	2:B:82:ASP:N	2.48	0.43
6:F:29:ASN:HA	6:F:163:LYS:NZ	2.34	0.43
6:F:169:LYS:HB2	6:F:169:LYS:HE3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:41:LEU:HD23	11:K:103:GLY:HA3	1.99	0.43
11:Y:104:TYR:HB3	11:Y:182:GLU:HA	2.00	0.43
14:b:13:ILE:HG12	14:b:177:VAL:HG13	2.00	0.43
14:b:157:HIS:ND1	14:b:196:LEU:HD13	2.33	0.43
1:O:21:ILE:HG21	1:O:153:SER:HB3	2.01	0.43
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.99	0.43
7:U:147:LYS:HB3	7:U:157:TYR:HE2	1.84	0.43
13:M:22:ILE:HG22	13:M:198:ALA:HB3	2.00	0.43
14:b:8:PHE:CE2	14:b:10:ASP:HB2	2.53	0.43
3:C:157:TRP:CE2	4:D:51:LEU:HD13	2.53	0.43
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.54	0.43
5:S:179:ILE:HG23	5:S:180:LYS:HG3	1.99	0.43
9:I:144:GLN:OE1	9:I:144:GLN:N	2.43	0.43
14:N:32:ASP:OD2	14:N:185:ARG:NH2	2.52	0.43
14:N:83:LYS:HE3	14:N:83:LYS:HB3	1.80	0.43
9:W:11:VAL:HG22	9:W:24:CYS:HB2	2.00	0.43
9:W:50:LEU:HD11	9:W:106:PRO:HB3	2.01	0.43
10:X:140:THR:O	10:X:144:LEU:HD22	2.18	0.43
12:Z:115:ASP:OD2	12:Z:133:ARG:NH2	2.51	0.43
3:C:102:VAL:HG12	3:C:103:THR:O	2.19	0.43
10:J:92:ILE:HD12	10:J:93:ARG:HG3	2.01	0.43
1:A:49:LYS:HD2	1:A:210:GLU:HB2	2.01	0.43
2:P:86:LEU:HD21	2:P:130:PHE:CE2	2.54	0.43
5:S:226:GLY:O	5:S:229:VAL:HG22	2.19	0.43
6:T:196:ILE:HG21	6:T:210:LEU:HD13	2.01	0.43
8:H:162:GLY:O	8:H:166:ASP:HB3	2.18	0.43
11:K:25:TRP:HH2	12:L:147:MET:HB2	1.83	0.43
10:X:168:LEU:O	10:X:172:MET:HB2	2.19	0.43
14:b:163:ILE:HG23	14:b:170:GLY:HA2	2.00	0.43
2:B:6:ASP:HB3	3:C:4:ARG:HH12	1.84	0.43
2:B:81:ALA:O	2:B:85:ILE:HG12	2.19	0.43
2:B:189:ILE:HG12	2:B:212:PHE:CZ	2.51	0.43
6:T:91:GLU:OE1	6:T:111:ARG:NH1	2.51	0.43
14:b:83:LYS:HE3	14:b:83:LYS:HB3	1.76	0.43
1:A:180:ASN:HD22	1:A:182:GLU:H	1.67	0.43
13:M:68:LYS:HB3	13:M:68:LYS:HE2	1.86	0.43
13:a:102:GLN:O	13:a:106:LYS:HG2	2.18	0.43
3:C:213:VAL:HG13	3:C:219:ILE:HG13	2.00	0.42
5:E:79:ASP:O	5:E:82:VAL:HG12	2.19	0.42
7:G:73:VAL:HG13	7:G:133:THR:HB	2.00	0.42
2:P:149:THR:O	2:P:156:TYR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:32:SER:OG	5:S:48:LEU:O	2.23	0.42
9:I:9:GLY:HA2	9:I:25:ASP:OD2	2.18	0.42
13:M:12:ILE:HD11	13:M:177:ILE:HG23	2.01	0.42
8:V:7:LYS:HD2	8:V:110:LEU:HB3	2.01	0.42
5:S:181:ILE:HB	5:S:188:LEU:HD13	2.01	0.42
6:T:46:VAL:HG12	6:T:211:GLU:HB3	2.01	0.42
6:T:171:GLU:HG2	6:T:195:ILE:HG12	2.01	0.42
6:T:240:GLN:O	6:T:243:ILE:HG22	2.20	0.42
10:X:172:MET:HE3	10:X:172:MET:HB3	1.85	0.42
6:F:154:TRP:HB2	6:F:156:TYR:CE1	2.54	0.42
1:O:135:LEU:HD23	1:O:135:LEU:HA	1.90	0.42
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.34	0.42
10:X:46:PHE:CD2	10:X:53:THR:HB	2.55	0.42
10:X:96:ARG:HH11	11:Y:91:LYS:HB3	1.83	0.42
11:Y:174:SER:HA	11:Y:193:VAL:HG23	2.02	0.42
13:a:152:ASN:O	13:a:156:ARG:HG3	2.19	0.42
14:b:66:TYR:CD1	14:b:73:PRO:HB3	2.53	0.42
7:G:26:THR:HG21	7:G:131:ILE:HG13	2.02	0.42
11:K:174:SER:HA	11:K:193:VAL:HG23	2.00	0.42
13:M:220:ASP:OD2	13:M:223:LYS:NZ	2.49	0.42
8:V:48:THR:HB	8:V:51:ASP:HB2	2.01	0.42
1:A:179:TRP:CE3	1:A:183:LEU:HD12	2.55	0.42
2:B:146:GLN:HB3	2:B:148:TYR:HE1	1.83	0.42
3:C:131:THR:HB	3:C:148:THR:HG22	2.01	0.42
7:G:223:LYS:HD2	7:G:223:LYS:HA	1.81	0.42
1:O:183:LEU:HD21	1:O:191:ILE:HD12	2.02	0.42
2:P:146:GLN:HB3	2:P:148:TYR:CE2	2.55	0.42
2:P:174:LEU:HD21	2:P:198:LYS:HE2	2.01	0.42
8:H:4:VAL:HG22	8:H:159:ILE:HD11	2.02	0.42
12:L:214:LYS:HB2	12:L:214:LYS:HE3	1.79	0.42
13:M:67:LEU:HD11	13:M:96:LEU:HD21	2.01	0.42
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.01	0.42
12:Z:123:TYR:CE2	12:Z:133:ARG:HB2	2.54	0.42
12:Z:170:LYS:HE3	12:Z:170:LYS:HB2	1.81	0.42
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.01	0.42
5:E:146:PHE:HD1	5:E:152:VAL:HG22	1.83	0.42
13:M:1:THR:N	13:M:108:ASN:OD1	2.43	0.42
12:Z:58:ALA:HB3	13:a:135:VAL:HG13	2.01	0.42
12:Z:100:LYS:HE2	12:Z:103:PHE:O	2.20	0.42
2:B:240:LYS:HE3	2:B:240:LYS:HB3	1.94	0.42
5:E:156:TYR:OH	6:F:57:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:175:LEU:HD21	6:F:191:GLN:HG2	2.02	0.42
7:U:176:HIS:HB2	7:U:200:HIS:HE1	1.84	0.42
10:J:37:GLN:HG3	10:J:189:ILE:HD13	2.00	0.42
6:T:82:ARG:HA	6:T:85:VAL:HG22	2.02	0.42
9:I:37:ASN:HD21	11:Y:210:VAL:HA	1.85	0.42
6:F:184:SER:O	6:F:188:ALA:N	2.40	0.42
1:O:89:SER:HA	1:O:92:VAL:HG12	2.02	0.42
10:J:103:LEU:HD23	10:J:118:GLN:HA	2.01	0.42
13:M:63:ILE:O	13:M:67:LEU:HD13	2.19	0.42
6:T:191:GLN:O	6:T:195:ILE:HG13	2.20	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.00	0.42
10:J:142:SER:HB3	11:Y:135:PHE:HB3	2.02	0.42
11:K:115:VAL:HA	11:K:120:THR:O	2.20	0.42
14:N:9:LYS:HG2	14:N:146:MET:O	2.20	0.42
14:b:113:ILE:HA	14:b:118:SER:O	2.19	0.42
3:C:115:GLN:O	3:C:119:THR:HG23	2.20	0.41
2:P:151:ASN:OD1	2:P:153:SER:OG	2.24	0.41
3:Q:205:ALA:HB2	3:Q:231:VAL:HG21	2.02	0.41
12:L:164:THR:O	12:L:167:LYS:HD3	2.20	0.41
11:Y:38:ASN:HD21	11:Y:41:LEU:HD12	1.85	0.41
12:Z:13:LEU:HD13	12:Z:138:ALA:HB2	2.02	0.41
5:E:139:SER:HB2	5:E:142:HIS:NE2	2.35	0.41
3:Q:204:GLY:H	3:Q:207:ASN:HD21	1.67	0.41
12:L:204:ILE:HG12	12:L:215:GLU:HB2	2.02	0.41
5:E:226:GLY:O	5:E:229:VAL:HG22	2.20	0.41
1:O:160:LYS:HD3	1:O:179:TRP:CH2	2.56	0.41
10:X:5:LEU:HD21	10:X:140:THR:HG21	2.02	0.41
13:a:27:LEU:HB2	13:a:192:SER:HB2	2.02	0.41
14:b:38:HIS:CD2	14:b:73:PRO:HD2	2.55	0.41
5:S:170:TYR:O	5:S:174:THR:OG1	2.34	0.41
9:I:69:LYS:HD3	9:I:89:LEU:HD11	2.02	0.41
9:I:196:LYS:HE2	9:I:198:TYR:CE1	2.56	0.41
12:L:175:LEU:HD12	12:L:179:GLU:HB3	2.02	0.41
12:L:204:ILE:CG1	12:L:215:GLU:HB2	2.51	0.41
12:Z:2:PHE:CE1	13:a:109:PRO:HG3	2.55	0.41
12:Z:22:VAL:HG12	12:Z:206:ILE:HG12	2.02	0.41
13:a:51:VAL:HG22	13:a:116:VAL:HG22	2.02	0.41
1:A:190:HIS:O	1:A:194:LEU:HG	2.20	0.41
4:D:200:MET:HE2	4:D:200:MET:HB3	1.94	0.41
6:F:110:ASP:OD1	6:F:153:TYR:OH	2.27	0.41
7:U:43:VAL:HG11	7:U:194:VAL:HA	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:VAL:HG11	11:K:122:LEU:HD21	2.02	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.56	0.41
4:D:214:ILE:HG13	4:D:220:PHE:HD1	1.86	0.41
1:O:76:SER:HB2	1:O:164:ILE:HG23	2.02	0.41
4:R:113:LEU:HD23	4:R:113:LEU:HA	1.92	0.41
7:U:95:PHE:CE2	8:V:66:HIS:HE1	2.38	0.41
14:N:134:ILE:HD13	14:N:162:ALA:HB2	2.02	0.41
9:W:87:THR:HG23	9:W:123:PHE:CZ	2.56	0.41
14:b:32:ASP:OD2	14:b:185:ARG:NH2	2.53	0.41
1:A:172:LYS:O	1:A:176:GLU:HG3	2.20	0.41
7:G:95:PHE:CE2	8:H:66:HIS:HE1	2.39	0.41
1:O:10:THR:O	2:P:128:ARG:HD3	2.21	0.41
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.56	0.41
7:U:211:LYS:HD3	7:U:233:GLU:HB2	2.03	0.41
9:I:35:VAL:HG12	10:J:128:LEU:HD11	2.03	0.41
12:L:160:TYR:CG	12:L:166:GLY:HA2	2.56	0.41
4:D:7:PHE:CE1	5:E:125:ARG:HD2	2.55	0.41
1:O:57:MET:HE3	1:O:60:THR:HG21	2.02	0.41
5:S:215:VAL:HB	5:S:221:PHE:HD1	1.85	0.41
9:I:87:THR:HG23	9:I:123:PHE:CZ	2.56	0.41
13:M:150:MET:C	13:M:153:PRO:HD2	2.46	0.41
14:N:67:THR:HA	14:N:71:GLY:O	2.20	0.41
1:A:18:LEU:HD13	1:A:21:ILE:HD12	2.02	0.41
2:B:4:ARG:HH12	7:G:3:TYR:HE1	1.69	0.41
3:C:157:TRP:HZ3	4:D:48:SER:HB3	1.84	0.41
3:C:159:ALA:HB1	3:C:173:LEU:HD13	2.02	0.41
4:D:82:GLU:OE1	11:K:69:ARG:HD3	2.20	0.41
5:E:111:LEU:HD23	5:E:111:LEU:HA	1.97	0.41
7:G:211:LYS:HD3	7:G:233:GLU:HB2	2.03	0.41
2:P:87:ILE:O	2:P:91:ARG:HG3	2.21	0.41
9:I:28:LEU:HD22	9:I:39:PHE:CD2	2.56	0.41
10:J:23:ARG:HA	10:J:23:ARG:HD3	1.77	0.41
10:J:84:VAL:HG21	10:J:104:ILE:HD11	2.03	0.41
11:K:13:ILE:HG13	11:K:153:ALA:HB1	2.03	0.41
11:K:161:ILE:HG21	11:K:175:VAL:HG13	2.02	0.41
12:L:20:PHE:HE2	12:L:180:VAL:HG11	1.86	0.41
12:L:28:ARG:HG2	12:L:30:ILE:HG23	2.02	0.41
14:N:14:LEU:O	14:N:175:MET:HA	2.20	0.41
9:W:28:LEU:HD22	9:W:39:PHE:CD2	2.56	0.41
10:X:29:LYS:HD2	11:Y:122:LEU:HD12	2.03	0.41
12:Z:16:ALA:HB3	12:Z:135:GLN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:28:ARG:HG2	12:Z:30:ILE:HG23	2.03	0.41
3:C:161:THR:HG21	3:C:169:VAL:HB	2.03	0.41
5:E:145:GLU:OE2	5:E:147:GLN:NE2	2.53	0.41
3:Q:210:ILE:O	3:Q:210:ILE:HG13	2.21	0.41
6:T:48:LYS:NZ	6:T:59:LYS:O	2.39	0.41
13:M:53:ILE:HB	13:M:60:MET:HG3	2.01	0.41
8:V:162:GLY:O	8:V:166:ASP:HB3	2.21	0.41
11:Y:97:MET:H	11:Y:117:SER:HG	1.65	0.41
1:A:247:LEU:HA	1:A:250:LEU:HG	2.01	0.40
3:C:102:VAL:HG13	3:C:106:TYR:CD2	2.55	0.40
5:E:155:LEU:HD23	6:F:55:LEU:HA	2.02	0.40
4:R:62:ILE:HB	4:R:66:ILE:HG22	2.03	0.40
10:J:184:VAL:HG13	10:J:189:ILE:HG13	2.03	0.40
1:A:176:GLU:HA	2:B:55:LEU:HD21	2.03	0.40
2:B:162:ILE:HD12	2:B:172:GLN:OE1	2.21	0.40
3:C:35:LYS:HE3	3:C:145:LEU:HB3	2.01	0.40
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.57	0.40
8:H:63:ILE:HG12	8:H:82:MET:HE1	2.04	0.40
13:M:57:ILE:HG23	13:M:60:MET:HE2	2.02	0.40
9:W:9:GLY:HA2	9:W:25:ASP:OD2	2.20	0.40
10:X:92:ILE:HD12	10:X:93:ARG:HG3	2.02	0.40
10:X:108:ASP:O	10:X:112:ASN:N	2.54	0.40
13:a:93:PHE:CZ	13:a:128:ARG:HG2	2.57	0.40
1:A:200:VAL:HG21	1:A:204:PHE:CD1	2.57	0.40
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.04	0.40
4:D:190:LEU:HD22	4:D:235:LEU:HB2	2.03	0.40
2:P:180:LYS:HB3	2:P:180:LYS:HE2	1.92	0.40
5:S:155:LEU:HD23	6:T:55:LEU:HA	2.03	0.40
7:U:35:ALA:HB2	7:U:44:VAL:HG12	2.03	0.40
10:J:17:SER:HB3	10:J:34:LYS:HB2	2.03	0.40
11:K:167:ARG:NH1	9:W:34:GLY:O	2.54	0.40
13:M:14:MET:HG2	13:M:177:ILE:HD11	2.02	0.40
8:V:210:THR:HG21	9:W:167:SER:HB3	2.03	0.40
14:b:149:GLU:OE1	14:b:149:GLU:N	2.55	0.40
1:A:94:HIS:HA	1:A:98:LYS:HB3	2.03	0.40
2:B:9:THR:HB	2:B:20:GLN:HG3	2.03	0.40
2:B:185:VAL:O	2:B:189:ILE:HG13	2.21	0.40
7:G:72:MET:HE1	7:G:85:ALA:HA	2.02	0.40
3:Q:192:LEU:O	3:Q:196:SER:OG	2.32	0.40
10:J:75:LEU:HD23	10:J:75:LEU:HA	1.96	0.40
10:J:169:GLU:O	10:X:177:LYS:NZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:130:VAL:HA	13:M:135:VAL:O	2.22	0.40
14:N:190:PRO:HA	14:N:193:TYR:CE2	2.57	0.40
6:F:128:PHE:O	6:F:149:PRO:HB3	2.22	0.40
2:P:44:VAL:HG21	2:P:189:ILE:HG12	2.03	0.40
12:L:114:LEU:HD23	12:L:120:GLY:HA2	2.03	0.40
13:M:104:ARG:HD3	13:M:133:LEU:O	2.21	0.40
13:M:150:MET:O	13:M:153:PRO:HD2	2.21	0.40
14:N:12:VAL:HG21	14:N:100:ALA:HB1	2.02	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	246/250 (98%)	241 (98%)	5 (2%)	0	100	100
1	O	247/250 (99%)	242 (98%)	5 (2%)	0	100	100
2	B	239/258 (93%)	233 (98%)	6 (2%)	0	100	100
2	P	240/258 (93%)	234 (98%)	6 (2%)	0	100	100
3	C	239/254 (94%)	233 (98%)	6 (2%)	0	100	100
3	Q	239/254 (94%)	233 (98%)	6 (2%)	0	100	100
4	D	233/260 (90%)	227 (97%)	6 (3%)	0	100	100
4	R	232/260 (89%)	228 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	225 (98%)	4 (2%)	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	243/287 (85%)	236 (97%)	7 (3%)	0	100	100
7	G	240/252 (95%)	230 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	U	240/252 (95%)	229 (95%)	11 (5%)	0	100	100
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	219/232 (94%)	213 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
9	W	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	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%)	220 (95%)	11 (5%)	0	100	100
13	a	231/233 (99%)	219 (95%)	12 (5%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6278/6586 (95%)	6083 (97%)	195 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/209 (99%)	206 (100%)	0	100	100
1	O	208/209 (100%)	206 (99%)	2 (1%)	68	74
2	B	202/216 (94%)	198 (98%)	4 (2%)	48	65
2	P	204/216 (94%)	199 (98%)	5 (2%)	42	61
3	C	215/226 (95%)	210 (98%)	5 (2%)	44	62
3	Q	204/226 (90%)	197 (97%)	7 (3%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	196/215 (91%)	196 (100%)	0	100	100
4	R	167/215 (78%)	165 (99%)	2 (1%)	63	72
5	E	184/193 (95%)	179 (97%)	5 (3%)	39	60
5	S	189/193 (98%)	183 (97%)	6 (3%)	34	57
6	F	201/238 (84%)	199 (99%)	2 (1%)	68	74
6	T	197/238 (83%)	194 (98%)	3 (2%)	57	69
7	G	204/210 (97%)	204 (100%)	0	100	100
7	U	206/210 (98%)	204 (99%)	2 (1%)	68	74
8	H	181/190 (95%)	180 (99%)	1 (1%)	78	80
8	V	176/190 (93%)	173 (98%)	3 (2%)	53	67
9	I	169/173 (98%)	168 (99%)	1 (1%)	78	80
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	72
10	J	173/175 (99%)	171 (99%)	2 (1%)	63	72
10	X	169/175 (97%)	162 (96%)	7 (4%)	27	52
11	K	169/169 (100%)	168 (99%)	1 (1%)	78	80
11	Y	169/169 (100%)	166 (98%)	3 (2%)	51	66
12	L	185/185 (100%)	185 (100%)	0	100	100
12	Z	183/185 (99%)	183 (100%)	0	100	100
13	M	199/199 (100%)	196 (98%)	3 (2%)	57	69
13	a	195/199 (98%)	192 (98%)	3 (2%)	57	69
14	N	161/162 (99%)	159 (99%)	2 (1%)	63	72
14	b	158/162 (98%)	157 (99%)	1 (1%)	78	80
All	All	5242/5520 (95%)	5170 (99%)	72 (1%)	59	69

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	56	LEU
2	B	74	VAL
2	B	76	VAL
2	B	82	ASP
3	C	32	VAL
3	C	130	SER
3	C	131	THR

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Mol	Chain	Res	Type
3	C	148	THR
3	C	207	ASN
5	E	15	THR
5	E	48	LEU
5	E	53	ASP
5	E	87	LEU
5	E	174	THR
6	F	130	VAL
6	F	242	GLU
1	O	2	THR
1	O	157	PHE
2	P	76	VAL
2	P	82	ASP
2	P	135	ILE
2	P	211	GLU
2	P	212	PHE
3	Q	58	THR
3	Q	196	SER
3	Q	199	GLU
3	Q	201	VAL
3	Q	207	ASN
3	Q	210	ILE
3	Q	233	GLN
4	R	4	VAL
4	R	47	THR
5	S	9	THR
5	S	35	VAL
5	S	49	LYS
5	S	174	THR
5	S	206	THR
5	S	209	ASN
6	T	27	VAL
6	T	130	VAL
6	T	203	ASN
7	U	8	THR
7	U	166	GLN
8	H	1	THR
9	I	57	THR
10	J	126	VAL
10	J	161	LEU
11	K	137	TYR
13	M	9	THR

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Mol	Chain	Res	Type
13	M	67	LEU
13	M	159	VAL
14	N	1	THR
14	N	178	LEU
8	V	63	ILE
8	V	120	ASP
8	V	217	ILE
9	W	57	THR
9	W	157	LEU
10	X	21	VAL
10	X	69	ILE
10	X	126	VAL
10	X	144	LEU
10	X	160	LEU
10	X	172	MET
10	X	189	ILE
11	Y	65	LEU
11	Y	122	LEU
11	Y	137	TYR
13	a	9	THR
13	a	152	ASN
13	a	228	TYR
14	b	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	242	GLN
4	D	210	GLN
5	E	90	GLN
6	F	58	GLN
2	P	88	ASN
3	Q	53	GLN
3	Q	92	GLN
3	Q	165	ASN
3	Q	239	GLN
4	R	210	GLN
7	U	166	GLN
7	U	184	HIS
8	H	22	GLN
8	H	30	ASN
8	H	85	GLN

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Mol	Chain	Res	Type
8	H	189	ASN
8	H	194	ASN
8	H	219	ASN
9	I	168	GLN
9	I	172	ASN
11	K	29	GLN
11	K	188	HIS
13	M	203	ASN
14	N	141	ASN
14	N	161	GLN
8	V	30	ASN
8	V	160	GLN
8	V	189	ASN
10	X	37	GLN
10	X	86	GLN
11	Y	29	GLN
11	Y	188	HIS
12	Z	95	HIS
12	Z	158	ASN
13	a	26	ASN
13	a	74	ASN
13	a	203	ASN
14	b	106	ASN

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 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	$\# Z > 2$
16	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.08	0
16	SO4	a	301	-	4,4,4	0.67	0	6,6,6	0.07	0
16	SO4	M	301	-	4,4,4	0.67	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	248/250 (99%)	0.33	3 (1%) 76 64	65, 98, 134, 168	0
1	O	249/250 (99%)	0.29	2 (0%) 82 71	63, 100, 137, 166	0
2	B	243/258 (94%)	0.43	7 (2%) 53 39	70, 108, 146, 165	0
2	P	244/258 (94%)	0.52	7 (2%) 53 39	64, 100, 135, 158	0
3	C	243/254 (95%)	0.43	5 (2%) 63 48	66, 104, 155, 179	0
3	Q	241/254 (94%)	0.55	5 (2%) 63 48	65, 112, 152, 184	0
4	D	237/260 (91%)	0.36	3 (1%) 75 61	66, 101, 131, 155	0
4	R	236/260 (90%)	0.49	2 (0%) 82 71	72, 114, 142, 170	0
5	E	231/234 (98%)	0.53	4 (1%) 69 54	72, 116, 155, 175	0
5	S	232/234 (99%)	0.58	7 (3%) 52 38	68, 114, 164, 182	0
6	F	244/287 (85%)	0.52	6 (2%) 58 43	60, 106, 144, 161	0
6	T	245/287 (85%)	0.41	4 (1%) 70 57	61, 98, 135, 156	0
7	G	242/252 (96%)	0.45	8 (3%) 49 36	58, 96, 126, 183	0
7	U	242/252 (96%)	0.38	2 (0%) 82 71	62, 94, 131, 164	0
8	H	222/232 (95%)	0.32	1 (0%) 87 78	52, 96, 125, 184	0
8	V	221/232 (95%)	0.31	1 (0%) 87 78	64, 95, 119, 157	0
9	I	204/205 (99%)	0.37	2 (0%) 79 67	63, 94, 123, 139	0
9	W	204/205 (99%)	0.29	0 100 100	60, 85, 116, 140	0
10	J	195/198 (98%)	0.30	2 (1%) 79 67	63, 90, 117, 154	0
10	X	195/198 (98%)	0.31	1 (0%) 87 78	57, 84, 110, 132	0
11	K	212/212 (100%)	0.29	1 (0%) 87 78	59, 87, 115, 132	0
11	Y	212/212 (100%)	0.43	1 (0%) 87 78	67, 99, 127, 143	0
12	L	222/222 (100%)	0.29	0 100 100	64, 92, 121, 160	0
12	Z	222/222 (100%)	0.47	2 (0%) 81 69	69, 99, 135, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	0.38	2 (0%) 81 69	64, 94, 136, 160	0
13	a	233/233 (100%)	0.38	4 (1%) 69 54	58, 86, 128, 164	0
14	N	196/196 (100%)	0.35	4 (2%) 65 50	62, 86, 117, 135	0
14	b	196/196 (100%)	0.36	2 (1%) 79 67	59, 86, 114, 135	0
All	All	6344/6586 (96%)	0.40	88 (1%) 73 60	52, 97, 140, 184	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	a	233	ILE	3.8
14	N	172	VAL	3.7
3	C	193	THR	3.2
2	P	218	GLY	3.1
7	G	187	GLU	3.0
3	Q	21	ALA	2.9
13	M	229	GLY	2.9
3	Q	178	ASP	2.8
7	U	153	TYR	2.8
6	F	215	CYS	2.8
9	I	204	ASP	2.8
2	P	138	GLY	2.8
7	G	8	THR	2.8
3	C	204	GLY	2.7
4	R	243	SER	2.7
11	K	45	MET	2.7
2	B	6	ASP	2.7
6	F	33	SER	2.6
2	P	42	GLY	2.6
8	H	195	VAL	2.6
4	D	152	PRO	2.6
6	T	192	ALA	2.6
3	Q	208	ILE	2.5
7	G	199	THR	2.5
5	S	178	PHE	2.5
12	Z	105	TYR	2.5
2	B	209	ARG	2.5
2	B	163	SER	2.4
2	B	138	GLY	2.4
2	B	237	ILE	2.4
5	S	65	CYS	2.4
10	J	142	SER	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	122	TYR	2.4
5	E	120	GLN	2.4
6	F	32	THR	2.3
7	G	156	GLY	2.3
14	N	14	LEU	2.3
1	A	204	PHE	2.3
14	b	1	THR	2.3
3	Q	197	LEU	2.3
13	a	228	TYR	2.3
5	S	8	ASP	2.3
13	a	231	GLN	2.3
14	b	116	GLY	2.3
3	C	128	GLY	2.2
5	S	128	GLY	2.2
2	P	122	THR	2.2
1	O	61	LEU	2.2
5	S	157	GLY	2.2
3	Q	63	SER	2.2
7	G	193	VAL	2.2
6	F	222	GLY	2.2
9	I	172	ASN	2.2
4	D	113	LEU	2.2
6	F	172	LEU	2.2
2	P	130	PHE	2.2
7	G	153	TYR	2.2
2	P	238	LEU	2.2
10	J	195	PHE	2.2
14	N	112	THR	2.1
7	U	144	SER	2.1
14	N	191	ASP	2.1
6	T	190	LYS	2.1
13	M	232	LYS	2.1
8	V	196	ARG	2.1
3	C	196	SER	2.1
13	a	192	SER	2.1
6	F	31	THR	2.1
5	S	52	ALA	2.1
2	B	212	PHE	2.1
1	A	6	SER	2.1
1	O	199	SER	2.1
2	P	61	SER	2.1
1	A	183	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	2	GLY	2.1
4	D	117	GLU	2.1
6	T	189	VAL	2.0
2	B	196	LEU	2.0
3	C	50	LEU	2.0
10	X	194	ASP	2.0
4	R	48	SER	2.0
5	S	56	SER	2.0
5	E	69	MET	2.0
5	E	11	THR	2.0
7	G	22	ALA	2.0
11	Y	102	CYS	2.0
12	Z	116	GLU	2.0
6	T	0	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	W	301	1/1	0.63	0.14	72,72,72,72	0
16	SO4	a	301	5/5	0.81	0.17	70,89,104,113	5
16	SO4	a	302	5/5	0.82	0.25	100,106,147,171	0
15	MG	Z	301	1/1	0.84	0.09	68,68,68,68	0
15	MG	L	301	1/1	0.86	0.16	62,62,62,62	0
15	MG	Y	301	1/1	0.87	0.08	114,114,114,114	0
15	MG	V	301	1/1	0.89	0.13	100,100,100,100	0
16	SO4	M	301	5/5	0.89	0.26	108,113,168,170	0
15	MG	I	301	1/1	0.90	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	H	301	1/1	0.95	0.09	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.