Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2023 – 10:27 am GMT

PDB ID	:	4Y8L
Title	:	Yeast 20S proteasome in complex with Ac-APLL-ep
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-02-16
Resolution	:	2.40 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:

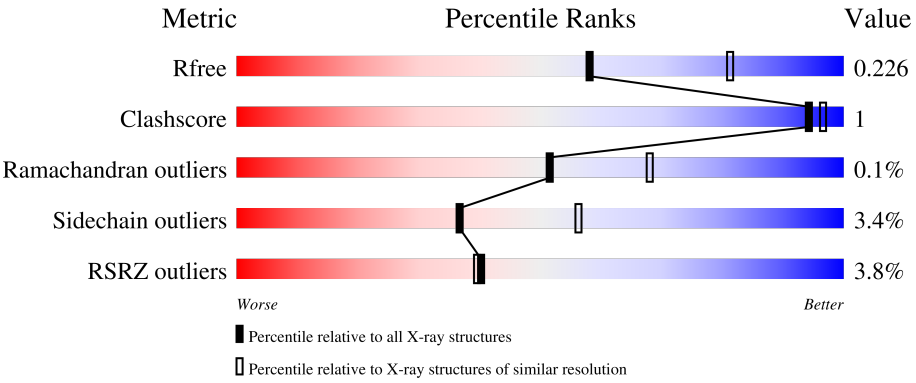
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	4% 97% .
1	O	250	5% 98% .
2	B	258	7% 90% 5% 5%
2	P	258	7% 90% . . 5%
3	C	254	8% 88% 5% . 6%

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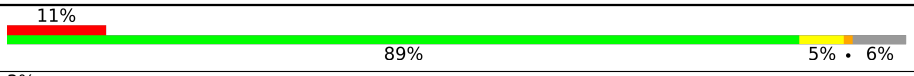
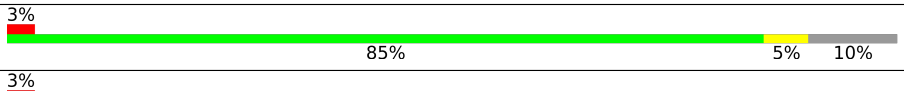
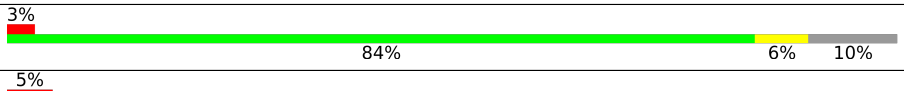
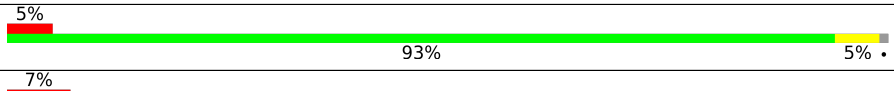
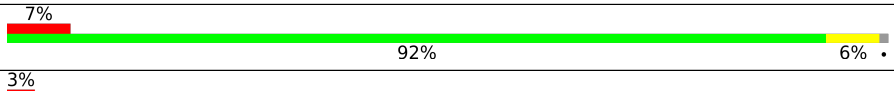
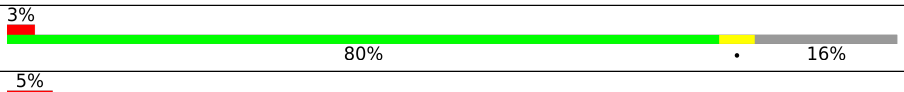
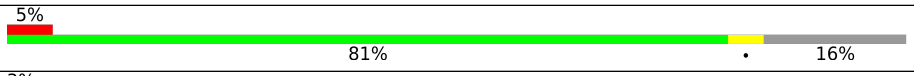
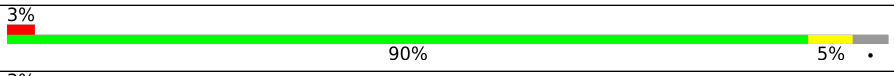
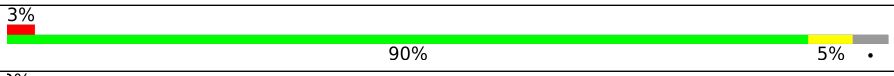
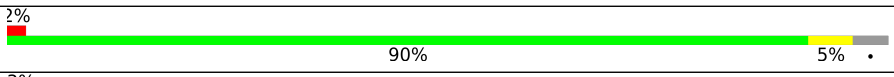
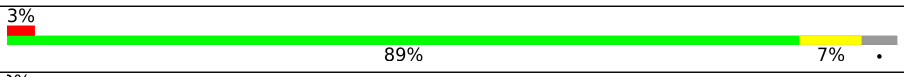
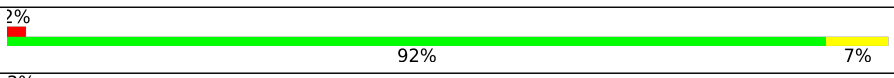
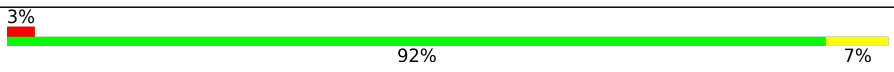
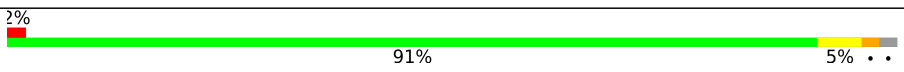
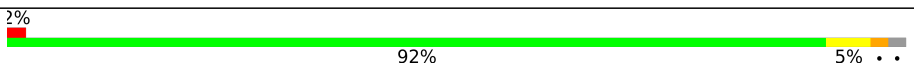
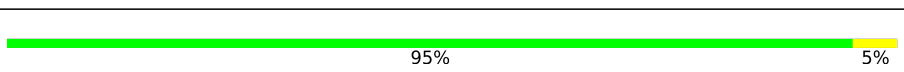
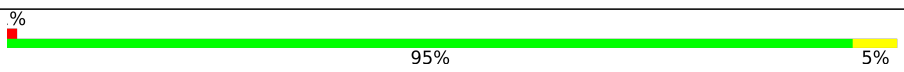
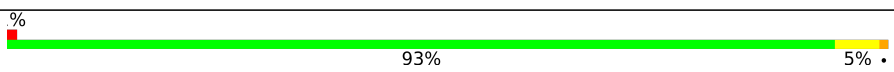
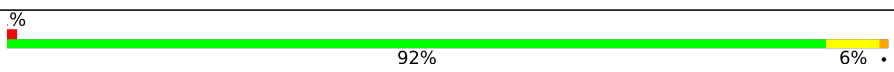
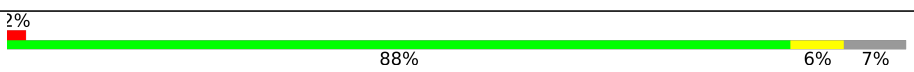
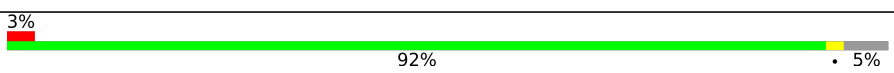
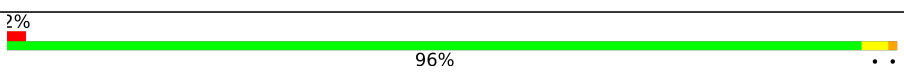
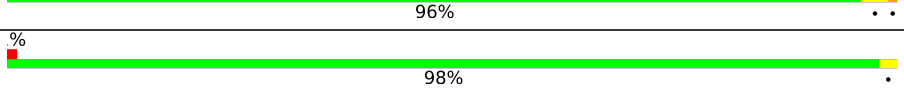
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	c	5	
15	d	5	

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Mol	Chain	Length	Quality of chain
15	e	5	80% 20%
15	f	5	80% 20%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 50603 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	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
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-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	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

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

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

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 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
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

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

- Molecule 12 is a protein called Proteasome subunit beta type-6.

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 type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	230	Total	C	N	O	S	0	0	0
			1797	1137	307	346	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 a protein called Ac-APLL-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			35	25	4	6			
15	d	5	Total	C	N	O	0	0	0
			35	25	4	6			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	e	5	Total C N O 35 25 4 6	0	0	0
15	f	5	Total C N O 35 25 4 6	0	0	0

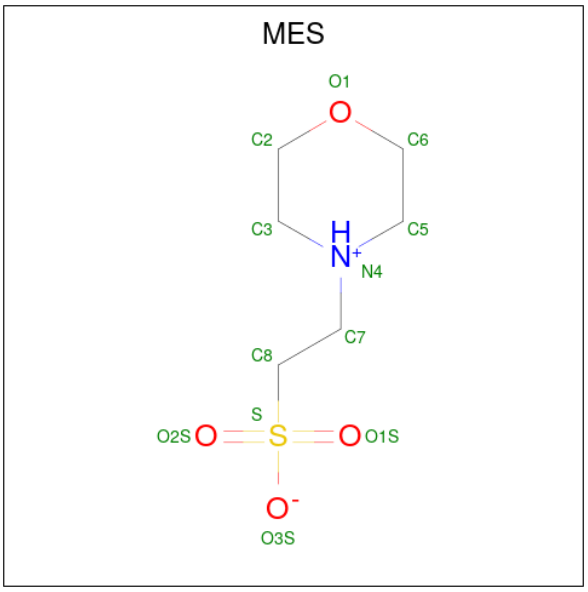
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	I	2	Total Mg 2 2	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	Z	1	Total Mg 1 1	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total Cl 1 1	0	0
17	N	1	Total Cl 1 1	0	0
17	U	1	Total Cl 1 1	0	0
17	b	1	Total Cl 1 1	0	0
17	d	1	Total Cl 1 1	0	0
17	f	1	Total Cl 1 1	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	1	Total C N O S 12 6 1 4 1	0	0
18	e	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	51	Total O 51 51	0	0
19	B	37	Total O 37 37	0	0
19	C	35	Total O 35 35	0	0
19	D	31	Total O 31 31	0	0
19	E	17	Total O 17 17	0	0
19	F	41	Total O 41 41	0	0
19	G	58	Total O 58 58	0	0
19	H	56	Total O 56 56	0	0
19	I	48	Total O 48 48	0	0
19	J	44	Total O 44 44	0	0

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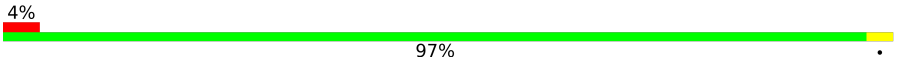
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	46	Total O 46 46	0	0
19	L	59	Total O 59 59	0	0
19	M	52	Total O 52 52	0	0
19	N	47	Total O 47 47	0	0
19	O	36	Total O 36 36	0	0
19	P	31	Total O 31 31	0	0
19	Q	23	Total O 23 23	0	0
19	R	18	Total O 18 18	0	0
19	S	17	Total O 17 17	0	0
19	T	32	Total O 32 32	0	0
19	U	57	Total O 57 57	0	0
19	V	32	Total O 32 32	0	0
19	W	39	Total O 39 39	0	0
19	X	46	Total O 46 46	0	0
19	Y	38	Total O 38 38	0	0
19	Z	58	Total O 58 58	0	0
19	a	59	Total O 59 59	0	0
19	b	43	Total O 43 43	0	0
19	d	2	Total O 2 2	0	0
19	e	1	Total O 1 1	0	0
19	f	3	Total O 3 3	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.

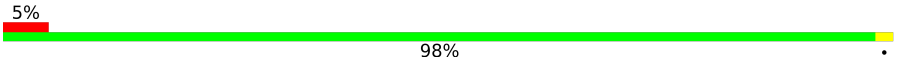
• Molecule 1: Proteasome subunit alpha type-2

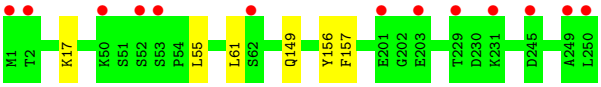
Chain A:



• Molecule 1: Proteasome subunit alpha type-2

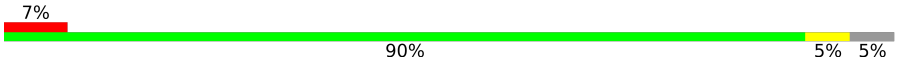
Chain O:

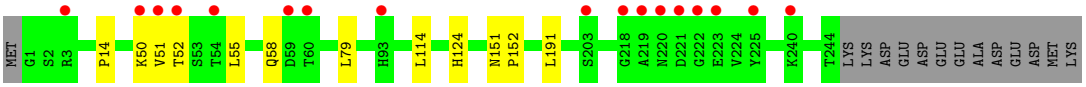




• Molecule 2: Proteasome subunit alpha type-3

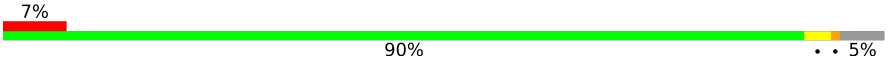
Chain B:

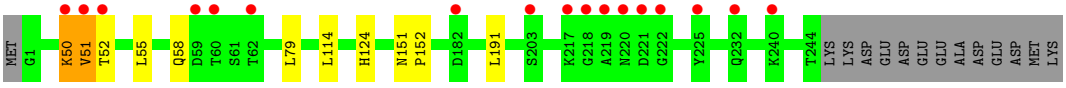




• Molecule 2: Proteasome subunit alpha type-3

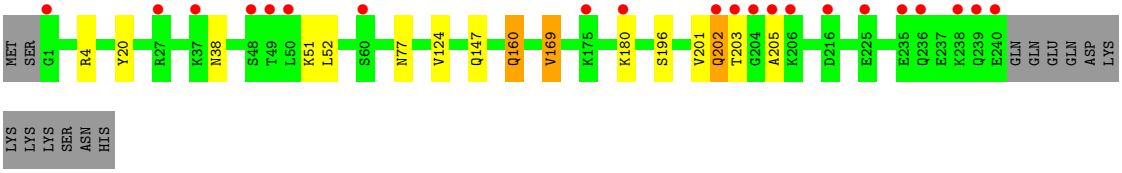
Chain P:





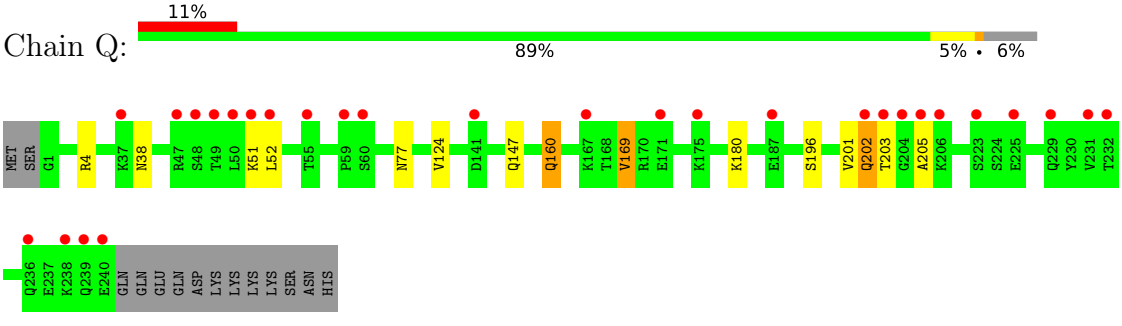
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



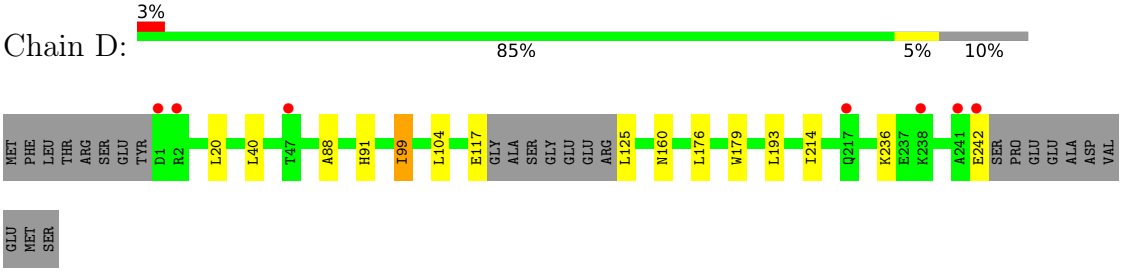
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



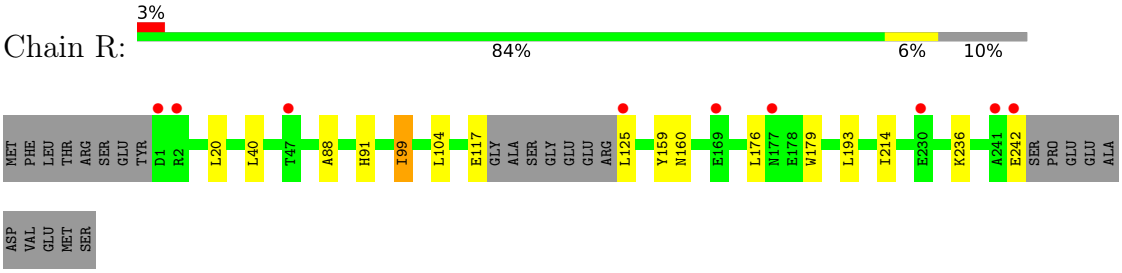
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



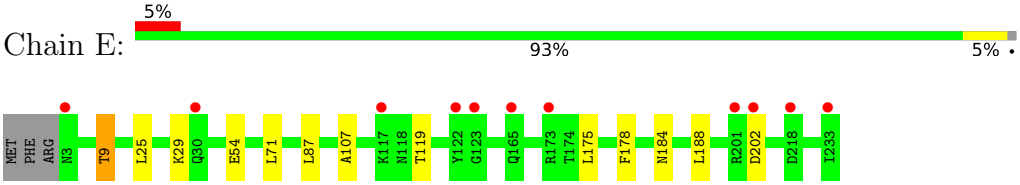
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



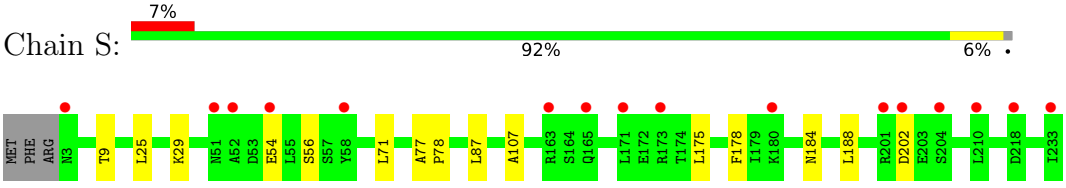
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



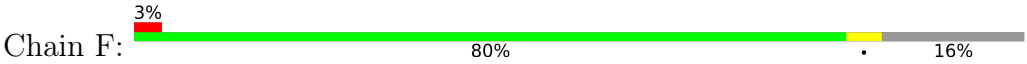
• Molecule 5: Proteasome subunit alpha type-6

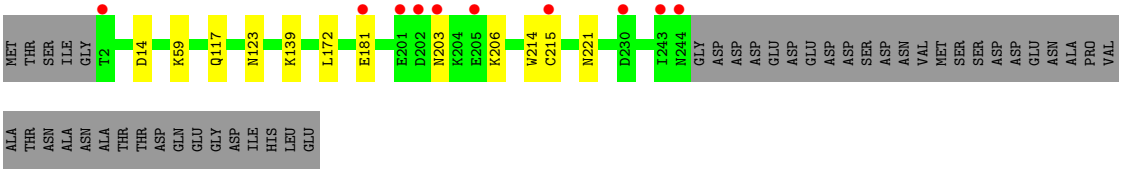
Chain S:



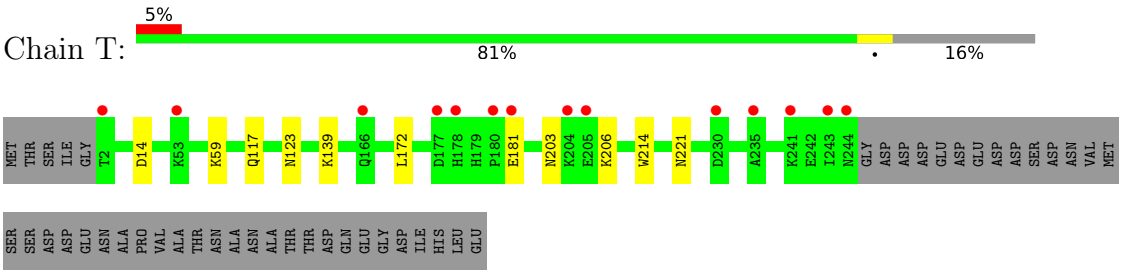
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:

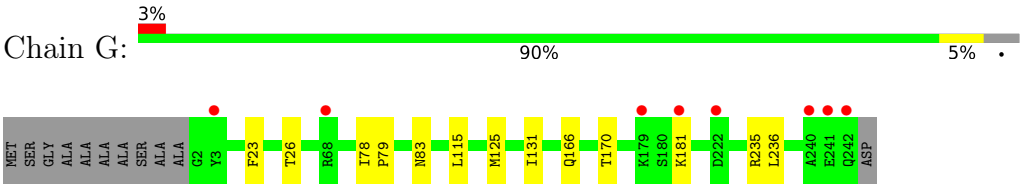




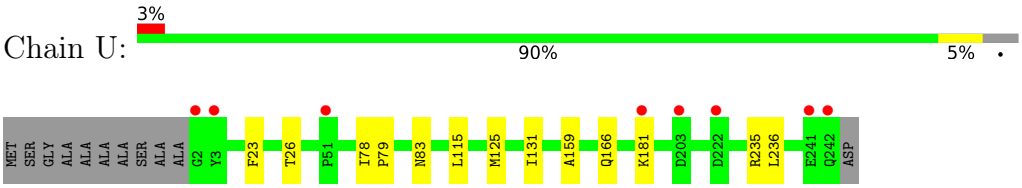
• Molecule 6: Probable proteasome subunit alpha type-7



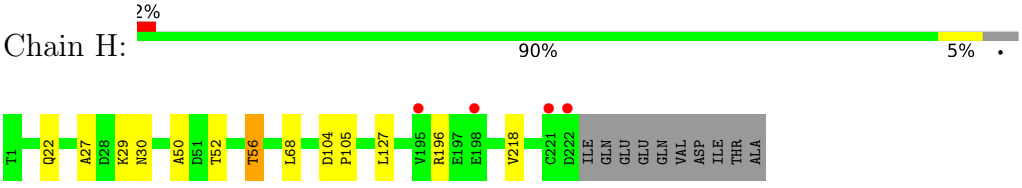
• Molecule 7: Proteasome subunit alpha type-1



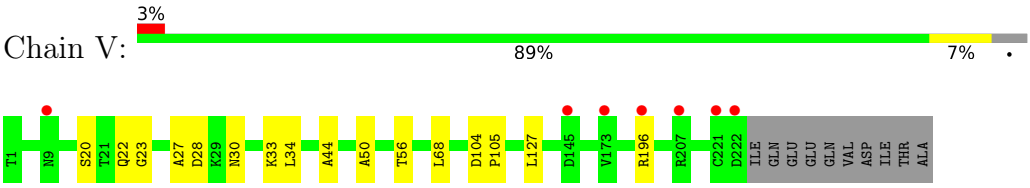
• Molecule 7: Proteasome subunit alpha type-1



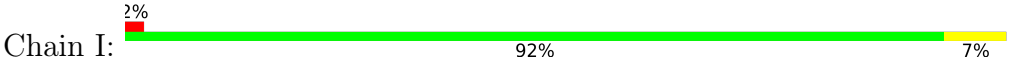
• Molecule 8: Proteasome subunit beta type-2

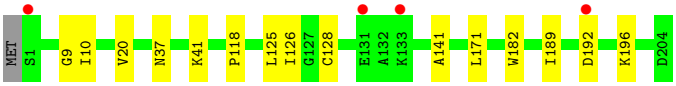


• Molecule 8: Proteasome subunit beta type-2



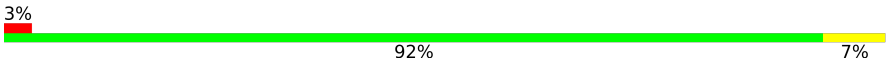
• Molecule 9: Proteasome subunit beta type-3

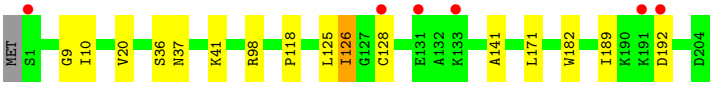




• Molecule 9: Proteasome subunit beta type-3

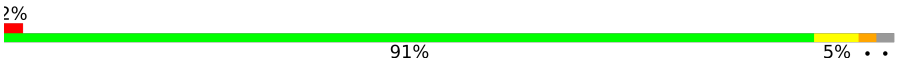
Chain W:





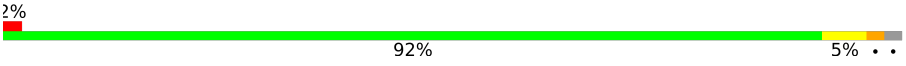
• Molecule 10: Proteasome subunit beta type-4

Chain J:



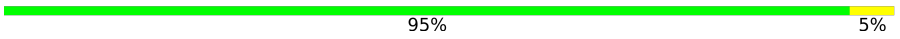
• Molecule 10: Proteasome subunit beta type-4

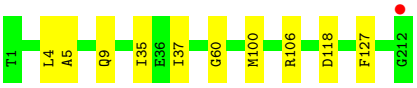
Chain X:



• Molecule 11: Proteasome subunit beta type-5

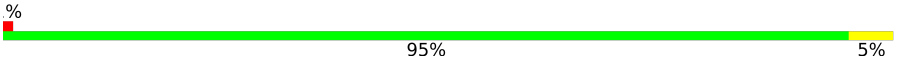
Chain K:

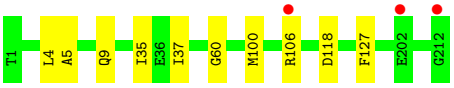




• Molecule 11: Proteasome subunit beta type-5

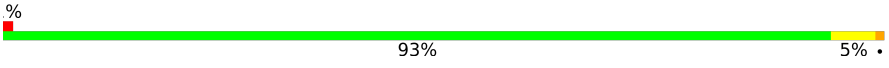
Chain Y:

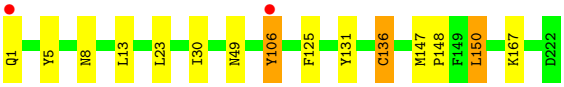




• Molecule 12: Proteasome subunit beta type-6

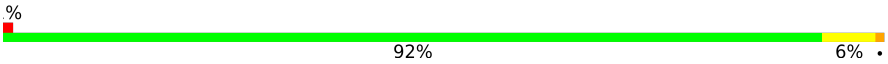
Chain L:





• Molecule 12: Proteasome subunit beta type-6

Chain Z:

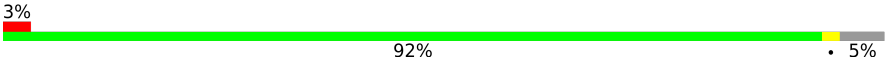


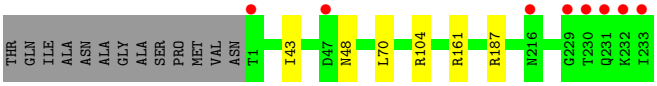
• Molecule 13: Proteasome subunit beta type-7

Chain M:

• Molecule 13: Proteasome subunit beta type-7

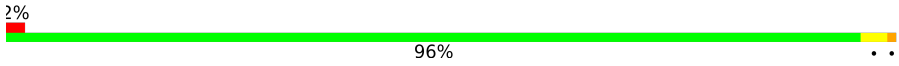
Chain a:

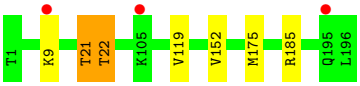




• Molecule 14: Proteasome subunit beta type-1

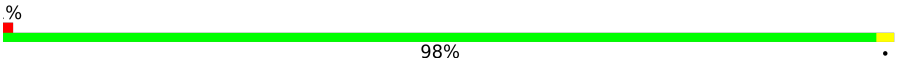
Chain N:

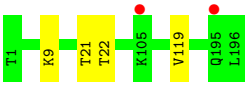




• Molecule 14: Proteasome subunit beta type-1

Chain b:





• Molecule 15: Ac-APLL-ep

Chain c:

• Molecule 15: Ac-APLL-ep

Chain d:

• Molecule 15: Ac-APLL-ep

Chain e:

• Molecule 15: Ac-APLL-ep

Chain f:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.61Å 299.76Å 144.95Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.40) 98.7 (15.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.208 , 0.224 0.211 , 0.226	Depositor DCC
R_{free} test set	20450 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.0	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	0.95	EDS
Total number of atoms	50603	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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: 05W, CL, ACE, MES, 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	0.27	0/1952	0.48	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.51	0/2586
4	D	0.26	0/1837	0.48	0/2475
4	R	0.26	0/1837	0.48	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.46	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.33	0/1715	0.49	0/2326
8	V	0.42	0/1715	0.50	1/2326 (0.0%)
9	I	0.29	0/1611	0.49	0/2174
9	W	0.27	0/1611	0.49	0/2174
10	J	0.26	0/1589	0.49	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.27	0/1681	0.49	0/2274
11	Y	0.27	0/1681	0.49	0/2274
12	L	0.27	0/1795	0.48	0/2420
12	Z	0.27	0/1795	0.47	0/2420
13	M	0.28	0/1828	0.51	0/2480
13	a	0.27	0/1855	0.51	0/2514
14	N	0.34	0/1541	0.51	0/2087
14	b	0.37	0/1541	0.51	0/2087
15	c	2.17	1/21 (4.8%)	1.20	0/29
15	d	2.15	1/21 (4.8%)	1.08	0/29
15	e	2.02	1/21 (4.8%)	1.10	0/29
15	f	2.02	1/21 (4.8%)	0.98	0/29

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.30	4/50251 (0.0%)	0.49	1/67950 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	3	PRO	CA-C	-8.22	1.36	1.52
15	e	3	PRO	CA-C	-7.75	1.37	1.52
15	d	3	PRO	CA-C	-7.27	1.38	1.52
15	f	3	PRO	CA-C	-6.82	1.39	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	23	GLY	C-N-CD	5.57	140.10	128.40

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	1915	0	1929	3	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	4	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	0	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1684	0	1688	6	0
8	V	1684	0	1688	6	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	10	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	7	0
11	K	1644	0	1592	5	0
11	Y	1644	0	1592	5	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	8	0
13	M	1797	0	1800	4	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	5	0
14	b	1512	0	1478	0	0
15	c	35	0	36	0	0
15	d	35	0	36	0	0
15	e	35	0	36	0	0
15	f	35	0	36	0	0
16	G	1	0	0	0	0
16	I	2	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	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
17	d	1	0	0	0	0
17	f	1	0	0	0	0
18	K	12	0	13	0	0
18	e	12	0	13	0	0
19	A	51	0	0	0	0
19	B	37	0	0	0	0
19	C	35	0	0	0	0
19	D	31	0	0	0	0
19	E	17	0	0	0	0
19	F	41	0	0	1	0
19	G	58	0	0	1	0
19	H	56	0	0	0	0
19	I	48	0	0	0	0
19	J	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	46	0	0	1	0
19	L	59	0	0	0	0
19	M	52	0	0	0	0
19	N	47	0	0	3	0
19	O	36	0	0	0	0
19	P	31	0	0	0	0
19	Q	23	0	0	0	0
19	R	18	0	0	0	0
19	S	17	0	0	0	0
19	T	32	0	0	0	0
19	U	57	0	0	0	0
19	V	32	0	0	0	0
19	W	39	0	0	0	0
19	X	46	0	0	0	0
19	Y	38	0	0	0	0
19	Z	58	0	0	0	0
19	a	59	0	0	0	0
19	b	43	0	0	0	0
19	d	2	0	0	0	0
19	e	1	0	0	0	0
19	f	3	0	0	0	0
All	All	50603	0	49194	118	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 1.

All (118) 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)
14:N:21:THR:HG23	19:N:329:HOH:O	1.48	1.13
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.46	0.94
14:N:21:THR:CG2	19:N:329:HOH:O	2.09	0.94
10:J:23:ARG:HD3	19:K:401:HOH:O	1.78	0.84
10:J:1:MET:O	10:J:2:ASP:HB2	1.87	0.73
10:X:1:MET:O	10:X:2:ASP:HB2	1.87	0.73
9:W:98:ARG:HD2	9:W:126:ILE:HD12	1.72	0.71
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.74	0.70
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.74	0.69
8:V:20:SER:OG	8:V:28:ASP:HB3	1.97	0.65
9:W:125:LEU:HG	9:W:126:ILE:HG22	1.80	0.64
9:W:98:ARG:CD	9:W:126:ILE:HD12	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:29:LYS:NZ	12:Z:193:GLU:OE2	2.24	0.60
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.83	0.60
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.83	0.59
8:H:52:THR:O	8:H:56:THR:HB	2.02	0.59
14:N:185:ARG:NH1	19:N:301:HOH:O	2.30	0.58
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.57
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.87	0.56
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.89	0.55
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.88	0.55
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.89	0.54
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.10	0.52
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.75	0.52
10:J:174:MET:HA	10:X:174:MET:HA	1.92	0.52
8:V:33:LYS:O	8:V:44:ALA:HA	2.10	0.52
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.75	0.50
8:V:34:LEU:HD12	8:V:44:ALA:HB2	1.92	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.50
9:W:126:ILE:O	9:W:126:ILE:HG13	2.12	0.50
3:C:201:VAL:O	3:C:202:GLN:CB	2.61	0.49
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.94	0.49
11:K:100:MET:CE	11:K:127:PHE:HB2	2.43	0.48
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.61	0.48
3:C:201:VAL:HG13	3:C:202:GLN:N	2.28	0.48
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.43	0.48
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.95	0.48
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.28	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.47
10:X:1:MET:O	10:X:2:ASP:CB	2.59	0.47
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.50	0.47
10:J:93:ARG:NH1	19:J:201:HOH:O	2.45	0.47
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.97	0.47
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.50	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.15	0.46
12:L:8:ASN:HA	12:L:30:ILE:O	2.15	0.46
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.45	0.46
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.15	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.46
6:F:215:CYS:HB3	19:F:308:HOH:O	2.16	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.45
3:C:201:VAL:O	3:C:202:GLN:HB2	2.15	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.45
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.17	0.45
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.45
1:O:55:LEU:HB3	7:U:159:ALA:O	2.17	0.45
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.99	0.44
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.98	0.44
14:N:22:THR:HG23	14:N:22:THR:O	2.17	0.44
3:C:51:LYS:O	3:C:52:LEU:HB2	2.16	0.44
10:J:1:MET:O	10:J:2:ASP:CB	2.60	0.44
8:H:27:ALA:O	12:Z:194:ARG:NH1	2.46	0.44
12:Z:5:TYR:CE1	12:Z:106:TYR:CD1	3.06	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.01	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.43
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.00	0.43
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.43
12:L:5:TYR:CE1	12:L:106:TYR:CD1	3.06	0.43
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.01	0.43
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.43
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.59	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.42
1:A:149:GLN:O	1:A:156:TYR:HA	2.20	0.42
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.01	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.59	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.41
11:K:5:ALA:HB3	11:K:100:MET:CE	2.50	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.53	0.41
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.02	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.01	0.41
9:I:125:LEU:HG	9:I:126:ILE:HG23	2.03	0.41
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.03	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.02	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.50	0.41
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.02	0.41
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.02	0.41
1:O:149:GLN:O	1:O:156:TYR:HA	2.20	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
5:E:9:THR:HG21	5:E:119:THR:HA	2.04	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	0.40
10:J:1:MET:HA	10:J:34:LYS:CE	2.51	0.40
1:A:57:MET:HE1	19:G:415:HOH:O	2.22	0.40
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.02	0.40
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.56	0.40
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	48
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	48
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	29
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	29
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
5	S	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
8	V	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	41
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	29	41
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	228/246 (93%)	221 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
15	c	3/5 (60%)	3 (100%)	0	0	100	100
15	d	3/5 (60%)	3 (100%)	0	0	100	100
15	e	3/5 (60%)	3 (100%)	0	0	100	100
15	f	3/5 (60%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6285/6634 (95%)	6131 (98%)	146 (2%)	8 (0%)	51 68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	206 (99%)	3 (1%)	67 82
1	O	209/209 (100%)	206 (99%)	3 (1%)	67 82
2	B	203/216 (94%)	196 (97%)	7 (3%)	37 56
2	P	203/216 (94%)	196 (97%)	7 (3%)	37 56
3	C	212/226 (94%)	204 (96%)	8 (4%)	33 51
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33 51
4	D	194/215 (90%)	184 (95%)	10 (5%)	23 38
4	R	194/215 (90%)	184 (95%)	10 (5%)	23 38
5	E	190/193 (98%)	182 (96%)	8 (4%)	30 47
5	S	190/193 (98%)	182 (96%)	8 (4%)	30 47
6	F	201/239 (84%)	190 (94%)	11 (6%)	21 35
6	T	201/239 (84%)	190 (94%)	11 (6%)	21 35
7	G	206/210 (98%)	199 (97%)	7 (3%)	37 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	56
8	H	181/190 (95%)	175 (97%)	6 (3%)	38	57
8	V	181/190 (95%)	176 (97%)	5 (3%)	43	63
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	70
9	W	172/173 (99%)	167 (97%)	5 (3%)	42	62
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	62
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	62
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	61
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	61
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	51
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	51
13	M	196/208 (94%)	190 (97%)	6 (3%)	40	60
13	a	199/208 (96%)	193 (97%)	6 (3%)	41	61
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	67
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	67
15	c	2/2 (100%)	2 (100%)	0	100	100
15	d	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	e	2/2 (100%)	2 (100%)	0	100	100
15	f	2/2 (100%)	2 (100%)	0	100	100
All	All	5317/5548 (96%)	5134 (97%)	183 (3%)	37	56

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	191	LEU
3	C	4	ARG

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Mol	Chain	Res	Type
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	40	LEU
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG

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Mol	Chain	Res	Type
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	21	THR
14	N	22	THR
14	N	119	VAL
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS

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Mol	Chain	Res	Type
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	40	LEU
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	59	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP

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Mol	Chain	Res	Type
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS

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Mol	Chain	Res	Type
14	b	21	THR
14	b	22	THR
14	b	119	VAL
15	d	3	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
8	H	57	GLN
9	I	37	ASN
10	J	55	GLN

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Mol	Chain	Res	Type
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	79	HIS
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
8	V	57	GLN

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Mol	Chain	Res	Type
8	V	66	HIS
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
13	a	2	GLN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 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	$\#\|Z\|>2$
18	MES	K	302	-	12,12,12	2.26	1 (8%)	14,16,16	1.24	2 (14%)
18	MES	e	101	-	12,12,12	2.21	1 (8%)	14,16,16	1.28	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	K	302	-	-	0/6/14/14	0/1/1/1
18	MES	e	101	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	302	MES	C8-S	-7.53	1.66	1.77
18	e	101	MES	C8-S	-7.38	1.67	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	e	101	MES	O2S-S-C8	2.74	110.22	106.92
18	K	302	MES	O3S-S-C8	2.57	109.92	105.77
18	e	101	MES	O3S-S-C8	2.45	109.73	105.77
18	K	302	MES	O2S-S-C8	2.19	109.55	106.92

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.14	10 (4%)	38	37	35, 50, 87, 128	0
1	O	250/250 (100%)	-0.05	13 (5%)	27	26	39, 56, 100, 132	0
2	B	244/258 (94%)	0.15	17 (6%)	16	15	36, 55, 105, 158	0
2	P	244/258 (94%)	0.14	17 (6%)	16	15	39, 59, 111, 161	0
3	C	240/254 (94%)	0.22	21 (8%)	10	9	36, 59, 124, 165	0
3	Q	240/254 (94%)	0.55	29 (12%)	4	3	46, 76, 160, 206	0
4	D	235/260 (90%)	-0.10	7 (2%)	50	49	40, 59, 94, 141	0
4	R	235/260 (90%)	0.00	9 (3%)	40	39	44, 65, 104, 157	0
5	E	231/234 (98%)	-0.00	11 (4%)	30	29	42, 61, 97, 140	0
5	S	231/234 (98%)	0.21	16 (6%)	16	15	42, 65, 109, 147	0
6	F	243/288 (84%)	-0.16	10 (4%)	37	36	37, 56, 107, 137	0
6	T	243/288 (84%)	0.06	14 (5%)	23	22	32, 61, 112, 154	0
7	G	241/252 (95%)	-0.12	8 (3%)	46	45	35, 52, 92, 151	0
7	U	241/252 (95%)	-0.16	8 (3%)	46	45	37, 51, 85, 132	0
8	H	222/232 (95%)	0.00	4 (1%)	68	66	37, 51, 81, 121	0
8	V	222/232 (95%)	0.18	7 (3%)	47	46	38, 53, 90, 131	0
9	I	204/205 (99%)	-0.33	4 (1%)	65	63	32, 46, 76, 97	0
9	W	204/205 (99%)	-0.28	6 (2%)	51	50	33, 48, 78, 101	0
10	J	195/198 (98%)	-0.32	3 (1%)	73	72	33, 47, 73, 119	0
10	X	195/198 (98%)	-0.38	3 (1%)	73	72	35, 48, 75, 127	0
11	K	212/212 (100%)	-0.30	1 (0%)	91	89	35, 48, 76, 94	0
11	Y	212/212 (100%)	-0.36	3 (1%)	75	73	36, 48, 78, 105	0
12	L	222/222 (100%)	-0.34	2 (0%)	84	82	33, 48, 74, 102	0
12	Z	222/222 (100%)	-0.33	2 (0%)	84	82	30, 48, 77, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	230/246 (93%)	-0.29	4 (1%) 70 68	29, 47, 73, 83	0
13	a	233/246 (94%)	-0.26	8 (3%) 45 44	31, 46, 70, 95	0
14	N	196/196 (100%)	-0.43	3 (1%) 73 72	31, 43, 72, 99	0
14	b	196/196 (100%)	-0.38	2 (1%) 82 80	32, 44, 74, 97	0
15	c	3/5 (60%)	-0.01	0 100 100	67, 67, 68, 72	0
15	d	3/5 (60%)	-0.32	0 100 100	53, 53, 58, 60	0
15	e	3/5 (60%)	-0.07	0 100 100	65, 65, 70, 74	0
15	f	3/5 (60%)	-0.45	0 100 100	56, 56, 60, 62	0
All	All	6345/6634 (95%)	-0.10	242 (3%) 40 39	29, 53, 98, 206	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	11.7
2	P	219	ALA	10.6
8	V	222	ASP	9.7
8	H	221	CYS	9.2
1	A	1	MET	8.9
1	O	1	MET	8.5
3	Q	206	LYS	8.2
2	P	51	VAL	8.2
8	H	222	ASP	8.0
3	Q	49	THR	7.8
3	Q	50	LEU	7.6
2	B	219	ALA	7.6
13	M	230	THR	7.4
8	V	221	CYS	7.1
3	Q	239	GLN	7.1
2	B	221	ASP	6.9
3	Q	48	SER	6.9
2	P	222	GLY	6.6
2	P	221	ASP	6.6
2	B	51	VAL	6.5
13	M	229	GLY	6.3
4	D	242	GLU	6.3
2	P	220	ASN	6.1
13	a	233	ILE	6.1
9	W	1	SER	6.1
3	C	206	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
3	C	49	THR	6.1
3	Q	238	LYS	5.9
2	P	218	GLY	5.7
5	E	202	ASP	5.7
3	Q	236	GLN	5.5
13	a	232	LYS	5.4
10	X	1	MET	5.3
2	B	218	GLY	5.2
11	Y	212	GLY	5.2
10	J	1	MET	5.1
5	S	202	ASP	5.1
13	a	1	THR	5.1
3	C	238	LYS	5.1
1	O	52	SER	5.0
1	O	249	ALA	4.8
2	P	59	ASP	4.6
6	T	241	LYS	4.6
10	X	194	ASP	4.6
10	J	194	ASP	4.6
9	I	1	SER	4.5
3	C	202	GLN	4.5
3	C	225	GLU	4.5
3	Q	51	LYS	4.3
9	I	133	LYS	4.3
3	Q	240	GLU	4.3
6	T	2	THR	4.2
3	Q	223	SER	4.2
3	C	205	ALA	4.2
6	F	244	ASN	4.2
6	T	181	GLU	4.1
13	a	231	GLN	4.1
7	U	222	ASP	4.0
7	G	242	GLN	4.0
6	F	202	ASP	4.0
6	F	243	ILE	4.0
5	E	233	ILE	3.9
3	Q	205	ALA	3.9
4	D	241	ALA	3.9
10	X	193	ASP	3.9
1	A	250	LEU	3.9
1	O	201	GLU	3.9
13	M	1	THR	3.8

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Mol	Chain	Res	Type	RSRZ
6	T	244	ASN	3.8
2	P	52	THR	3.7
3	C	48	SER	3.7
9	W	133	LYS	3.7
3	Q	202	GLN	3.7
2	B	222	GLY	3.7
11	K	212	GLY	3.6
4	D	1	ASP	3.6
5	S	180	LYS	3.6
5	E	123	GLY	3.6
3	C	236	GLN	3.5
6	T	243	ILE	3.4
5	S	173	ARG	3.4
3	C	37	LYS	3.4
3	Q	52	LEU	3.4
7	G	181	LYS	3.4
5	S	233	ILE	3.3
2	B	225	TYR	3.3
3	C	180	LYS	3.3
6	T	205	GLU	3.3
3	C	239	GLN	3.3
2	B	52	THR	3.3
7	G	241	GLU	3.2
5	S	54	GLU	3.2
3	Q	203	THR	3.2
7	U	242	GLN	3.2
13	a	230	THR	3.2
1	O	229	THR	3.2
2	B	240	LYS	3.1
6	F	2	THR	3.1
3	C	50	LEU	3.1
3	Q	232	THR	3.1
9	W	131	GLU	3.1
7	G	3	TYR	3.1
5	S	163	ARG	3.1
1	A	2	THR	3.1
1	O	250	LEU	3.1
6	F	205	GLU	3.0
2	B	50	LYS	3.0
6	T	180	PRO	3.0
3	Q	55	THR	3.0
5	E	201	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	Q	231	VAL	3.0
1	A	201	GLU	3.0
4	R	177	ASN	3.0
2	P	225	TYR	3.0
12	Z	1	GLN	3.0
9	W	191	LYS	3.0
1	O	2	THR	3.0
6	T	230	ASP	3.0
7	G	179	LYS	3.0
1	O	231	LYS	2.9
3	Q	47	ARG	2.9
3	C	240	GLU	2.9
5	S	3	ASN	2.9
6	F	215	CYS	2.9
10	J	193	ASP	2.9
9	I	131	GLU	2.9
6	F	181	GLU	2.8
11	Y	106	ARG	2.8
1	A	249	ALA	2.8
5	S	52	ALA	2.8
4	R	125	LEU	2.8
6	T	177	ASP	2.8
3	Q	229	GLN	2.8
14	b	195	GLN	2.8
1	O	50	LYS	2.8
7	G	222	ASP	2.8
14	N	195	GLN	2.7
7	U	3	TYR	2.7
5	S	171	LEU	2.7
3	Q	187	GLU	2.7
6	T	178	HIS	2.7
4	R	242	GLU	2.7
3	Q	204	GLY	2.7
3	Q	225	GLU	2.7
2	P	182	ASP	2.7
14	N	105	LYS	2.6
7	U	241	GLU	2.6
8	V	173	VAL	2.6
7	U	2	GLY	2.6
4	R	1	ASP	2.6
14	b	105	LYS	2.6
2	B	60	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	P	50	LYS	2.6
3	Q	60	SER	2.6
7	G	240	ALA	2.6
1	A	248	GLU	2.6
2	B	203	SER	2.5
3	Q	59	PRO	2.5
3	C	175	LYS	2.5
6	T	166	GLN	2.5
8	V	145	ASP	2.5
1	O	53	SER	2.5
2	P	232	GLN	2.5
3	Q	141	ASP	2.5
8	V	9	ASN	2.5
13	a	229	GLY	2.5
1	A	51	SER	2.5
1	A	229	THR	2.5
4	R	241	ALA	2.5
2	P	217	LYS	2.4
8	V	207	ARG	2.4
2	B	223	GLU	2.4
3	C	235	GLU	2.4
9	W	128	CYS	2.4
3	C	204	GLY	2.4
13	M	47	ASP	2.4
6	F	203	ASN	2.4
1	O	203	GLU	2.4
6	T	53	LYS	2.4
5	S	51	ASN	2.4
12	L	1	GLN	2.4
3	Q	171	GLU	2.4
4	R	2	ARG	2.3
3	C	203	THR	2.3
7	U	181	LYS	2.3
2	P	62	THR	2.3
7	U	203	ASP	2.3
8	V	196	ARG	2.3
1	A	182	GLU	2.3
3	C	1	GLY	2.3
4	D	47	THR	2.3
11	Y	202	GLU	2.3
4	D	217	GLN	2.3
9	W	192	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
12	Z	210	ASP	2.3
13	a	216	ASN	2.3
2	B	59	ASP	2.3
2	P	60	THR	2.3
5	S	165	GLN	2.3
5	S	218	ASP	2.3
5	S	210	LEU	2.3
2	B	54	THR	2.2
4	R	47	THR	2.2
4	D	238	LYS	2.2
5	E	117	LYS	2.2
4	R	169	GLU	2.2
5	E	122	TYR	2.2
2	P	203	SER	2.2
2	P	240	LYS	2.2
5	S	201	ARG	2.2
6	F	201	GLU	2.2
5	E	218	ASP	2.2
2	B	93	HIS	2.2
5	E	3	ASN	2.2
3	Q	175	LYS	2.1
3	C	27	ARG	2.1
3	Q	37	LYS	2.1
5	E	165	GLN	2.1
1	A	53	SER	2.1
7	G	68	ARG	2.1
6	T	235	ALA	2.1
6	F	230	ASP	2.1
5	E	173	ARG	2.1
6	T	204	LYS	2.1
5	S	204	SER	2.1
12	L	106	TYR	2.1
4	R	230	GLU	2.1
8	H	198	GLU	2.1
4	D	2	ARG	2.1
13	a	47	ASP	2.0
1	O	62	SER	2.0
2	B	3	ARG	2.0
1	O	245	ASP	2.0
3	C	216	ASP	2.0
7	U	51	PRO	2.0
3	C	60	SER	2.0

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Mol	Chain	Res	Type	RSRZ
5	S	58	TYR	2.0
9	I	192	ASP	2.0
3	Q	167	LYS	2.0
8	H	195	VAL	2.0
14	N	9	LYS	2.0
5	E	30	GLN	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
18	MES	e	101	12/12	0.86	0.26	62,81,84,86	0
18	MES	K	302	12/12	0.88	0.27	66,83,86,87	0
16	MG	I	301	1/1	0.94	0.18	49,49,49,49	0
16	MG	Z	301	1/1	0.95	0.18	57,57,57,57	0
16	MG	K	301	1/1	0.95	0.07	47,47,47,47	0
16	MG	N	201	1/1	0.95	0.08	39,39,39,39	0
17	CL	b	201	1/1	0.96	0.08	69,69,69,69	0
17	CL	f	101	1/1	0.96	0.18	30,30,30,30	0
16	MG	G	301	1/1	0.97	0.06	44,44,44,44	0
17	CL	d	101	1/1	0.98	0.11	30,30,30,30	0
16	MG	L	301	1/1	0.98	0.06	47,47,47,47	0
17	CL	G	302	1/1	0.99	0.14	30,30,30,30	0
17	CL	N	202	1/1	0.99	0.06	51,51,51,51	0
17	CL	U	301	1/1	0.99	0.16	30,30,30,30	0
16	MG	I	302	1/1	0.99	0.07	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.