Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 11:42 pm GMT

PDB ID	:	4Y8K
Title	:	Yeast 20S proteasome in complex with H-APLL-ep
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-02-16
Resolution	:	2.60 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:

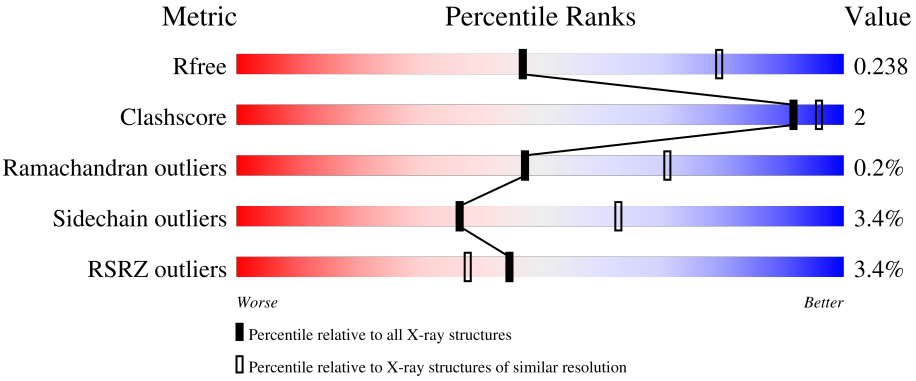
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	2% 99% ·
1	O	250	4% 98% ·
2	B	258	4% 90% · · 5%
2	P	258	5% 90% · · 5%
3	C	254	6% 89% 5% · 6%

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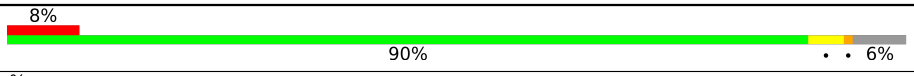
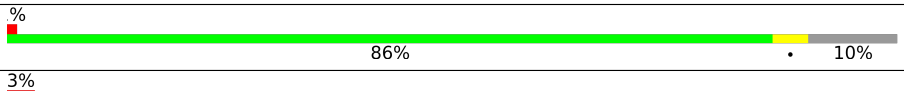
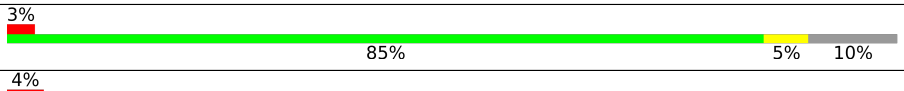
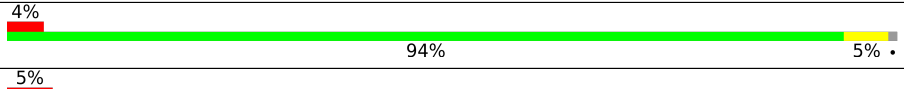
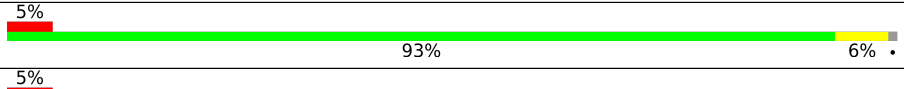
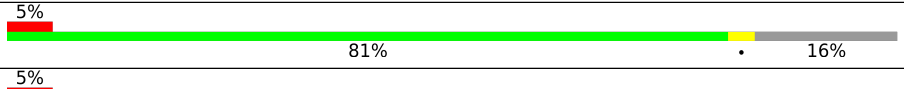
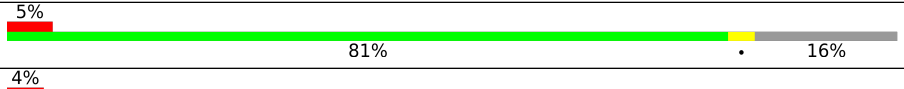
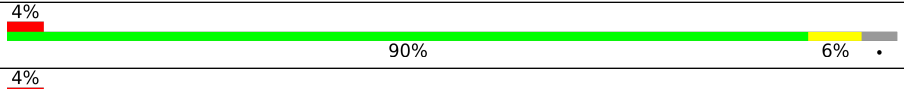
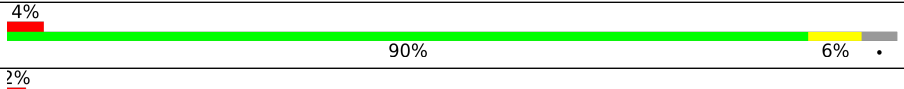
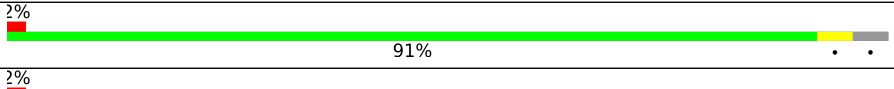
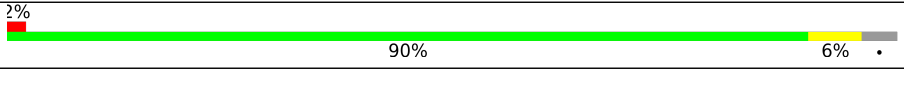
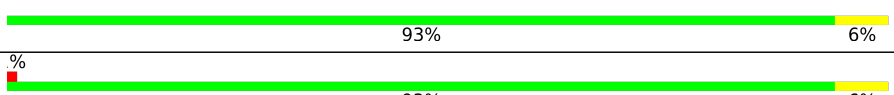
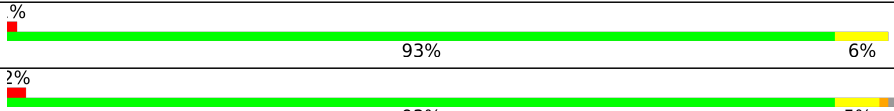
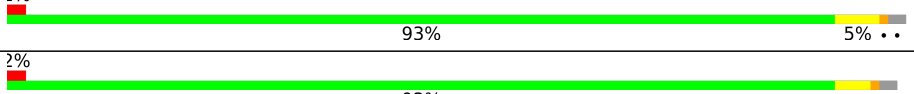
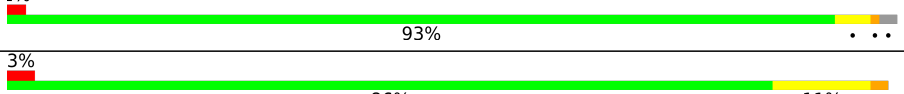
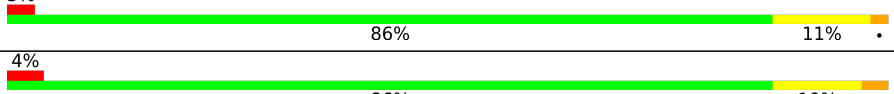
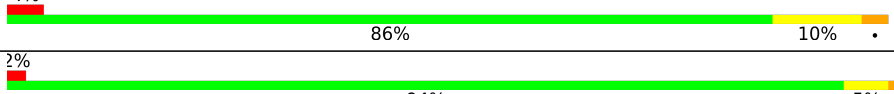
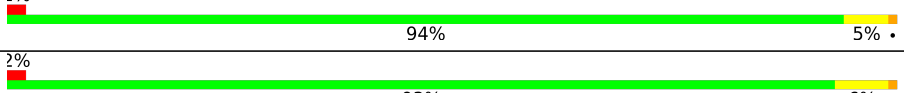
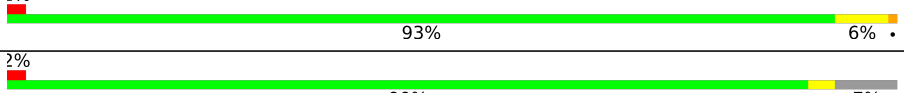
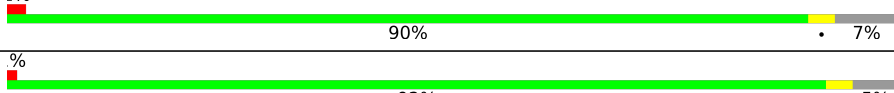
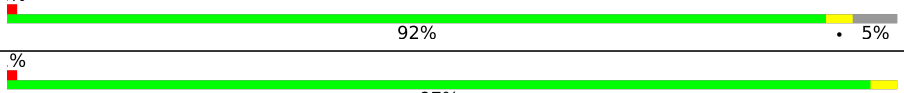
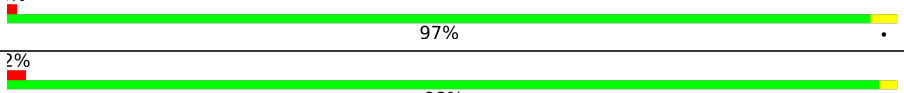
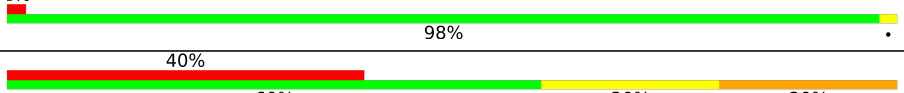
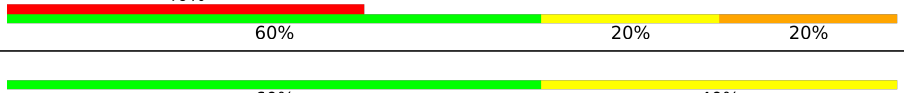
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	c	5	
15	d	5	

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Mol	Chain	Length	Quality of chain
15	e	5	
15	f	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	DCL	e	4	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49865 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 H-APLL-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			32	23	4	5			
15	d	5	Total	C	N	O	0	0	0
			32	23	4	5			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	e	5	Total C N O 32 23 4 5	0	0	0
15	f	5	Total C N O 32 23 4 5	0	0	0

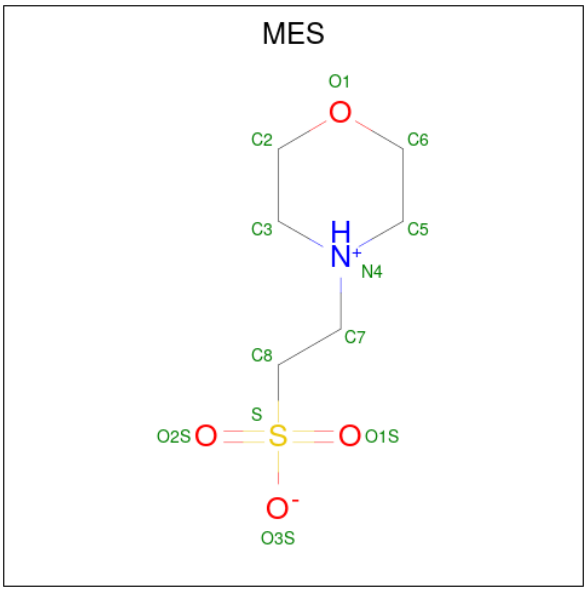
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- 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	Y	1	Total C N O S 12 6 1 4 1	0	0
18	c	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	17	Total O 17 17	0	0
19	B	20	Total O 20 20	0	0
19	C	15	Total O 15 15	0	0
19	D	3	Total O 3 3	0	0
19	E	5	Total O 5 5	0	0
19	F	17	Total O 17 17	0	0
19	G	27	Total O 27 27	0	0
19	H	16	Total O 16 16	0	0
19	I	18	Total O 18 18	0	0
19	J	17	Total O 17 17	0	0

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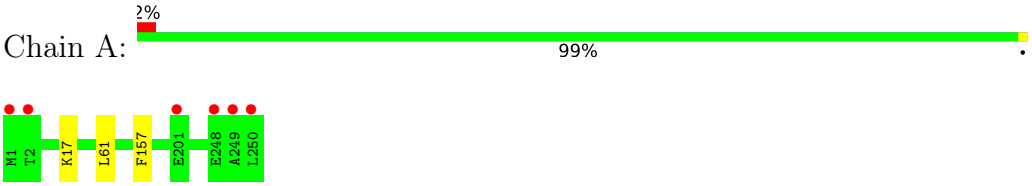
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	18	Total O 18 18	0	0
19	L	24	Total O 24 24	0	0
19	M	20	Total O 20 20	0	0
19	N	19	Total O 19 19	0	0
19	O	10	Total O 10 10	0	0
19	P	10	Total O 10 10	0	0
19	Q	9	Total O 9 9	0	0
19	R	8	Total O 8 8	0	0
19	S	5	Total O 5 5	0	0
19	T	11	Total O 11 11	0	0
19	U	18	Total O 18 18	0	0
19	V	19	Total O 19 19	0	0
19	W	12	Total O 12 12	0	0
19	X	16	Total O 16 16	0	0
19	Y	20	Total O 20 20	0	0
19	Z	15	Total O 15 15	0	0
19	a	24	Total O 24 24	0	0
19	b	15	Total O 15 15	0	0
19	d	2	Total O 2 2	0	0
19	f	3	Total O 3 3	0	0

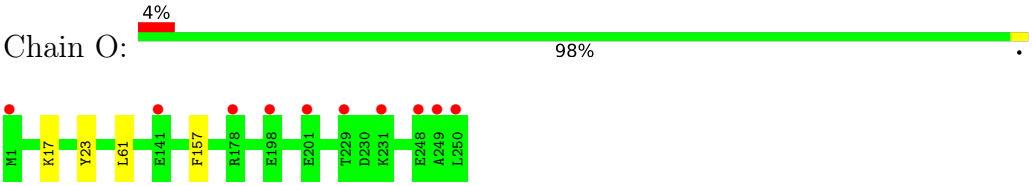
3 Residue-property plots (i)

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.

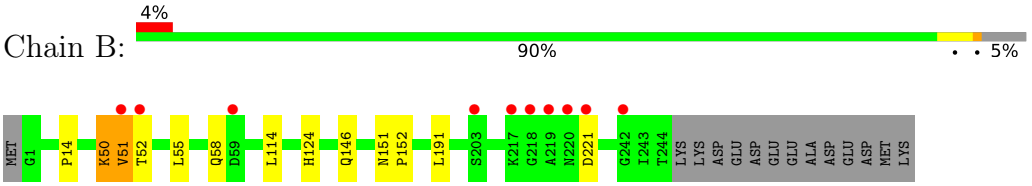
• Molecule 1: Proteasome subunit alpha type-2



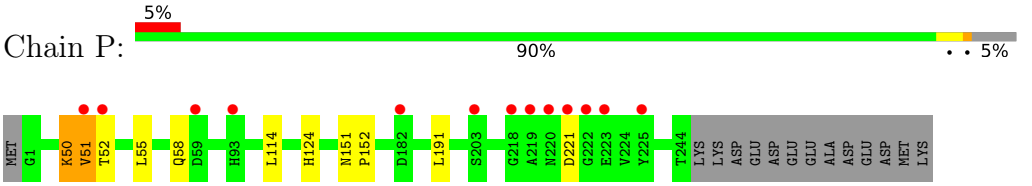
• Molecule 1: Proteasome subunit alpha type-2



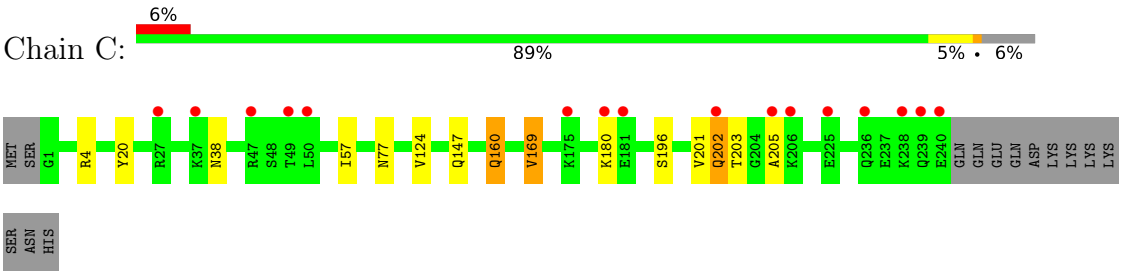
• Molecule 2: Proteasome subunit alpha type-3



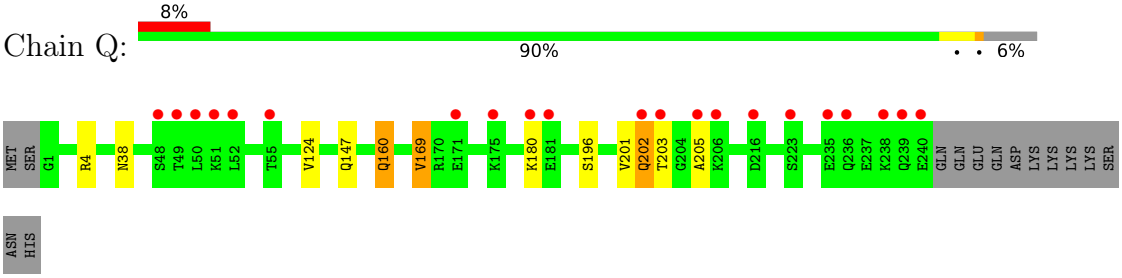
• Molecule 2: Proteasome subunit alpha type-3



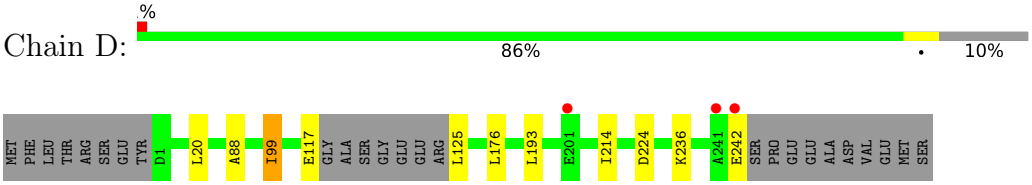
• Molecule 3: Proteasome subunit alpha type-4



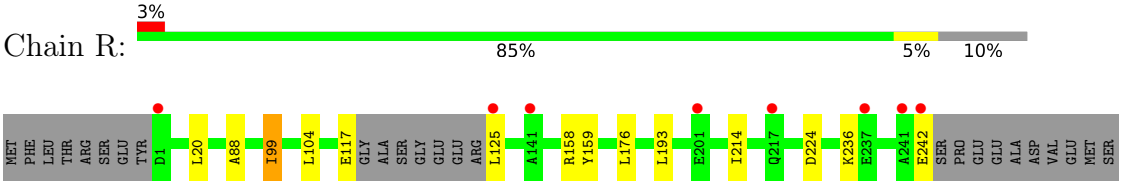
• Molecule 3: Proteasome subunit alpha type-4



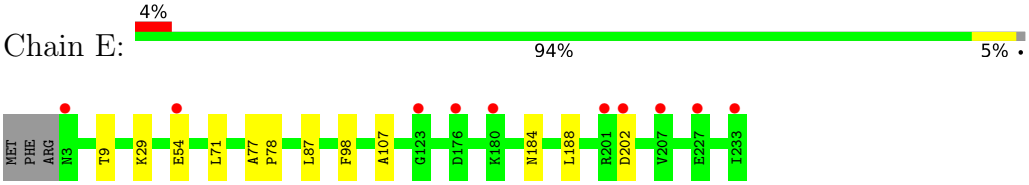
• Molecule 4: Proteasome subunit alpha type-5



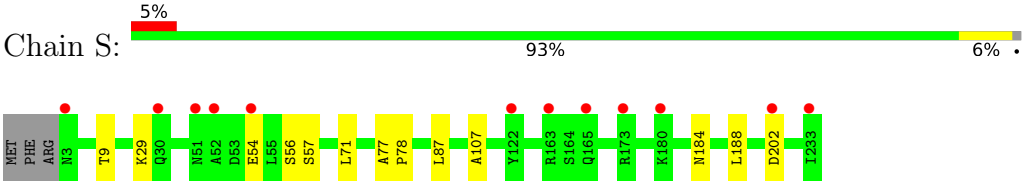
• Molecule 4: Proteasome subunit alpha type-5



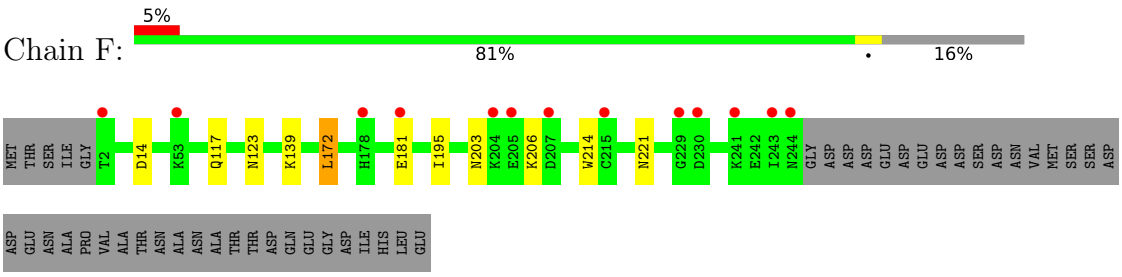
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 5: Proteasome subunit alpha type-6

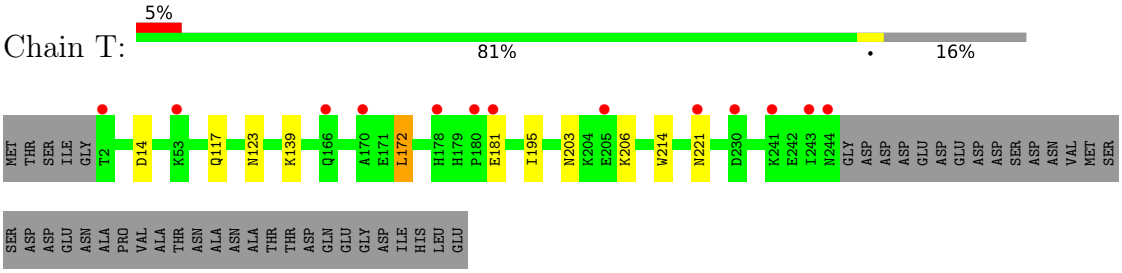


• Molecule 6: Probable proteasome subunit alpha type-7



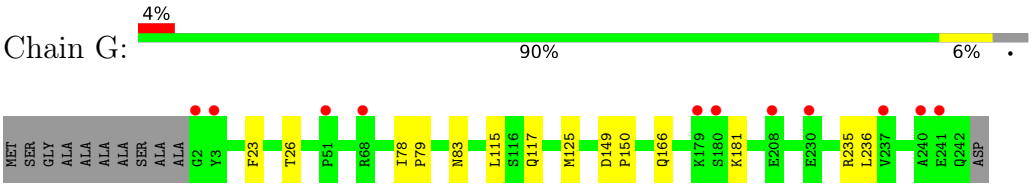
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



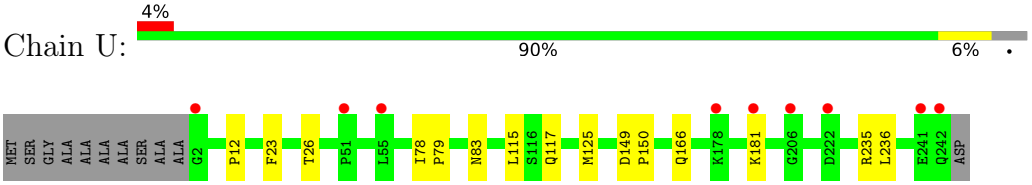
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



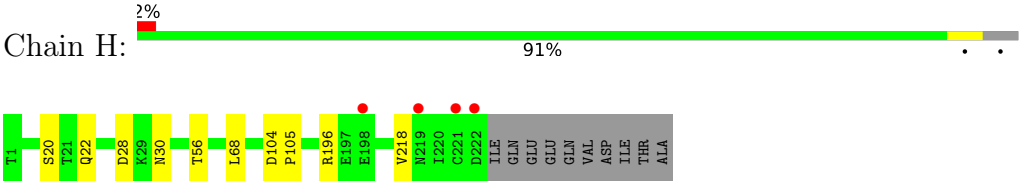
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



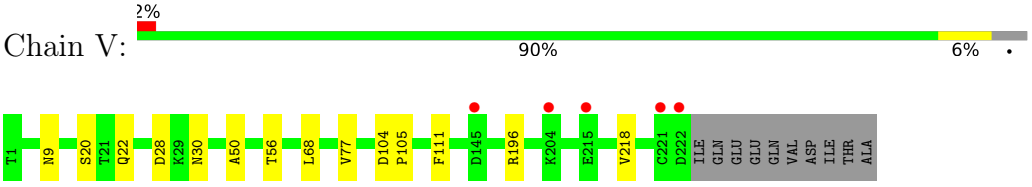
• Molecule 8: Proteasome subunit beta type-2

Chain H:



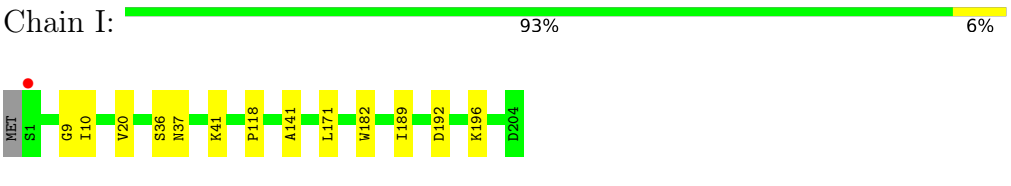
• Molecule 8: Proteasome subunit beta type-2

Chain V:



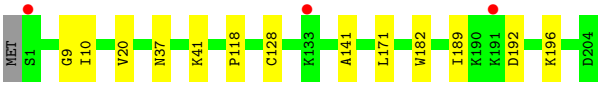
• Molecule 9: Proteasome subunit beta type-3

Chain I:



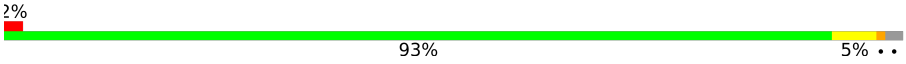
• Molecule 9: Proteasome subunit beta type-3

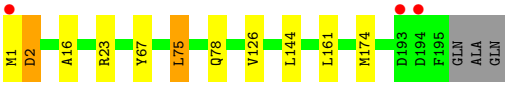
Chain W:



• Molecule 10: Proteasome subunit beta type-4

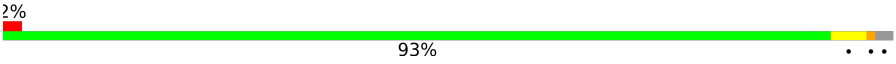
Chain J:

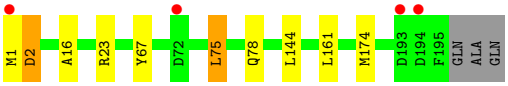




• Molecule 10: Proteasome subunit beta type-4

Chain X:



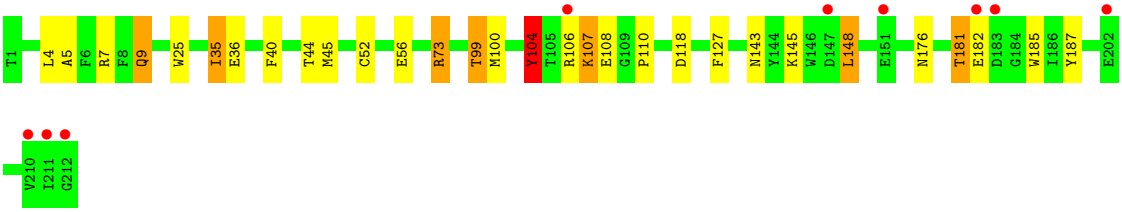


• Molecule 11: Proteasome subunit beta type-5

Chain K:

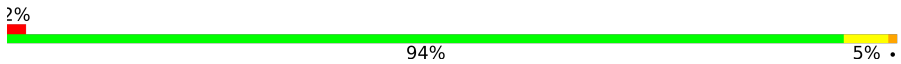
• Molecule 11: Proteasome subunit beta type-5

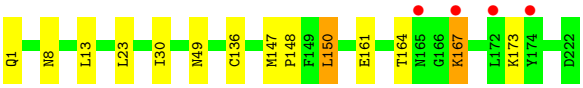
Chain Y:



• Molecule 12: Proteasome subunit beta type-6

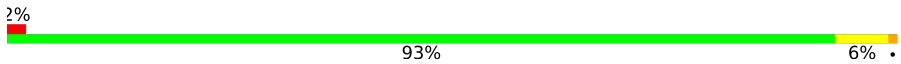
Chain L:

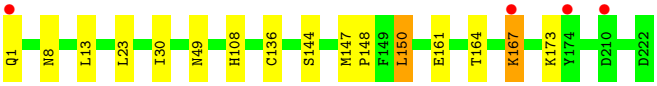




• Molecule 12: Proteasome subunit beta type-6

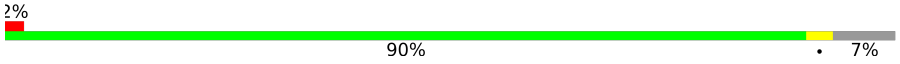
Chain Z:

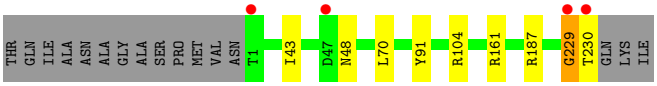




• Molecule 13: Proteasome subunit beta type-7

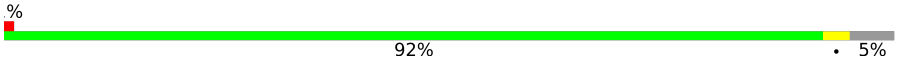
Chain M:

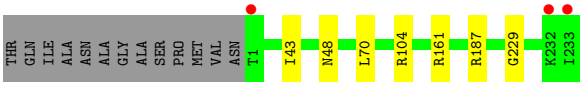




• Molecule 13: Proteasome subunit beta type-7

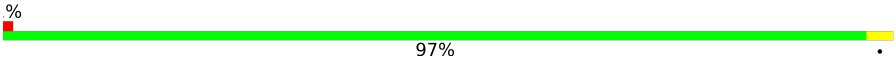
Chain a:

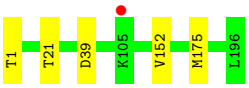




• Molecule 14: Proteasome subunit beta type-1

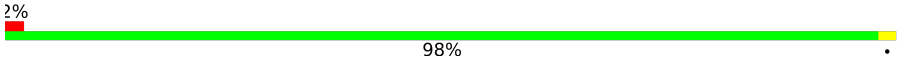
Chain N:





• Molecule 14: Proteasome subunit beta type-1

Chain b:



• Molecule 15: H-APLL-ep

Chain c:

• Molecule 15: H-APLL-ep

Chain d:

• Molecule 15: H-APLL-ep

Chain e:

• Molecule 15: H-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	136.56Å 300.72Å 145.43Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.60) 98.6 (15.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.209 , 0.236 0.214 , 0.238	Depositor DCC
R_{free} test set	16129 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.0	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	0.94	EDS
Total number of atoms	49865	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: POL, MES, CL, MG, DCL

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	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.28	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.28	0/1932	0.45	0/2609
6	T	0.28	0/1932	0.45	0/2609
7	G	0.28	0/1945	0.46	0/2634
7	U	0.28	0/1945	0.46	0/2634
8	H	0.26	0/1715	0.46	0/2326
8	V	0.26	0/1715	0.46	0/2326
9	I	0.28	0/1611	0.48	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.58	4/1681 (0.2%)	0.56	0/2274
11	Y	0.58	4/1681 (0.2%)	0.57	0/2274
12	L	0.28	0/1795	0.53	1/2420 (0.0%)
12	Z	0.28	0/1795	0.53	1/2420 (0.0%)
13	M	0.28	0/1828	0.51	0/2480
13	a	0.28	0/1855	0.51	0/2514
14	N	0.34	0/1541	0.51	1/2087 (0.0%)
14	b	0.33	0/1541	0.50	1/2087 (0.0%)
15	c	1.82	1/20 (5.0%)	1.39	0/27
15	d	1.58	1/20 (5.0%)	1.09	0/27
15	e	1.72	1/20 (5.0%)	1.38	0/27
15	f	1.60	1/20 (5.0%)	1.12	0/27

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.32	12/50247 (0.0%)	0.49	4/67942 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	104	TYR	CE1-CZ	-11.75	1.23	1.38
11	Y	104	TYR	CE1-CZ	-10.68	1.24	1.38
11	Y	104	TYR	CG-CD2	-9.77	1.26	1.39
11	K	104	TYR	CG-CD2	-9.32	1.27	1.39
11	Y	104	TYR	CG-CD1	-9.27	1.27	1.39
11	K	104	TYR	CG-CD1	-9.21	1.27	1.39
11	Y	104	TYR	CE2-CZ	-8.34	1.27	1.38
11	K	104	TYR	CE2-CZ	-8.13	1.27	1.38
15	e	2	PRO	CA-C	-7.33	1.38	1.52
15	c	2	PRO	CA-C	-7.31	1.38	1.52
15	f	2	PRO	CA-C	-6.45	1.40	1.52
15	d	2	PRO	CA-C	-6.33	1.40	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	173	LYS	CD-CE-NZ	8.49	131.24	111.70
12	L	173	LYS	CD-CE-NZ	8.01	130.12	111.70
14	N	1	THR	N-CA-C	5.18	124.98	111.00
14	b	1	THR	N-CA-C	5.14	124.89	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	0	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1904	0	1904	3	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	4	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	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1684	0	1688	3	0
8	V	1684	0	1688	6	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	3	0
11	K	1644	0	1592	29	0
11	Y	1644	0	1592	37	0
12	L	1757	0	1711	5	0
12	Z	1757	0	1711	7	0
13	M	1797	0	1800	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	1	0
14	b	1512	0	1478	0	0
15	c	32	0	41	0	0
15	d	32	0	41	0	0
15	e	32	0	41	0	0
15	f	32	0	41	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
18	Y	12	0	13	0	0
18	c	12	0	13	0	0
19	A	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	20	0	0	0	0
19	C	15	0	0	0	0
19	D	3	0	0	0	0
19	E	5	0	0	0	0
19	F	17	0	0	0	0
19	G	27	0	0	0	0
19	H	16	0	0	0	0
19	I	18	0	0	0	0
19	J	17	0	0	0	0
19	K	18	0	0	0	0
19	L	24	0	0	0	0
19	M	20	0	0	0	0
19	N	19	0	0	0	0
19	O	10	0	0	0	0
19	P	10	0	0	0	0
19	Q	9	0	0	0	0
19	R	8	0	0	0	0
19	S	5	0	0	0	0
19	T	11	0	0	0	0
19	U	18	0	0	0	0
19	V	19	0	0	0	0
19	W	12	0	0	0	0
19	X	16	0	0	0	0
19	Y	20	0	0	0	0
19	Z	15	0	0	1	0
19	a	24	0	0	0	0
19	b	15	0	0	0	0
19	d	2	0	0	0	0
19	f	3	0	0	0	0
All	All	49865	0	49214	141	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 2.

All (141) 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)
11:K:104:TYR:CE2	11:K:182:GLU:HG2	1.74	1.22
11:Y:40:PHE:CD1	11:Y:73:ARG:NH2	2.27	1.01
11:K:104:TYR:HE2	11:K:182:GLU:HG2	1.10	1.01
11:Y:104:TYR:CE1	11:Y:110:PRO:HD3	1.96	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:104:TYR:HE1	11:Y:110:PRO:HD3	1.29	0.92
11:K:104:TYR:CD2	11:K:182:GLU:HA	2.10	0.87
11:Y:40:PHE:HD1	11:Y:73:ARG:NH2	1.73	0.87
11:Y:44:THR:O	11:Y:99:THR:HG22	1.74	0.86
11:K:44:THR:O	11:K:99:THR:HG22	1.75	0.85
11:Y:104:TYR:HD2	11:Y:182:GLU:N	1.76	0.83
11:K:104:TYR:HD2	11:K:182:GLU:HA	1.43	0.81
11:Y:104:TYR:CD2	11:Y:182:GLU:N	2.52	0.77
11:K:35:ILE:HB	11:K:45:MET:HE3	1.68	0.74
11:K:35:ILE:HB	11:K:45:MET:CE	2.18	0.74
11:K:104:TYR:CE1	11:K:110:PRO:HD3	2.23	0.74
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.18	0.73
10:X:1:MET:O	10:X:2:ASP:HB2	1.89	0.72
11:Y:104:TYR:CE1	11:Y:110:PRO:CD	2.74	0.71
10:J:1:MET:O	10:J:2:ASP:HB2	1.89	0.71
11:Y:104:TYR:HD2	11:Y:181:THR:C	1.94	0.71
11:Y:40:PHE:HD1	11:Y:73:ARG:HH21	1.33	0.70
11:Y:40:PHE:CD1	11:Y:73:ARG:CZ	2.74	0.70
12:L:164:THR:O	12:L:167:LYS:HB2	1.96	0.65
11:Y:104:TYR:CE2	11:Y:182:GLU:HG3	2.32	0.65
11:Y:35:ILE:HB	11:Y:45:MET:HE2	1.79	0.64
12:Z:164:THR:O	12:Z:167:LYS:HB2	1.98	0.64
12:Z:108:HIS:HB2	19:Z:410:HOH:O	1.97	0.63
11:K:104:TYR:CD2	11:K:182:GLU:CA	2.81	0.63
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.82	0.62
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.32	0.62
11:Y:7:ARG:NH1	11:Y:110:PRO:O	2.31	0.62
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.82	0.62
11:K:7:ARG:NH1	11:K:110:PRO:O	2.34	0.61
11:Y:104:TYR:HE1	11:Y:110:PRO:CD	2.09	0.61
11:Y:35:ILE:HB	11:Y:45:MET:HE3	1.85	0.58
11:Y:104:TYR:CD2	11:Y:182:GLU:HA	2.38	0.58
11:Y:104:TYR:CD2	11:Y:182:GLU:CA	2.88	0.56
11:K:104:TYR:CE1	11:K:110:PRO:CD	2.88	0.56
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.88	0.54
11:Y:56:GLU:OE2	11:Y:99:THR:HG21	2.07	0.54
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.89	0.54
11:Y:104:TYR:CE2	11:Y:182:GLU:CG	2.90	0.54
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.90	0.54
8:V:20:SER:OG	8:V:28:ASP:HB3	2.08	0.54
11:K:56:GLU:OE2	11:K:99:THR:HG21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:SER:OG	8:H:28:ASP:HB3	2.09	0.53
14:N:152:VAL:HA	14:N:175:MET:HE1	1.91	0.53
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.90	0.53
11:Y:56:GLU:OE2	11:Y:99:THR:CG2	2.57	0.52
11:K:56:GLU:OE2	11:K:99:THR:CG2	2.57	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.51
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.46	0.51
11:K:104:TYR:HE2	11:K:182:GLU:CG	2.02	0.51
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.46	0.51
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.92	0.50
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.93	0.50
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.44	0.49
11:K:36:GLU:OE1	11:K:185:TRP:CH2	2.65	0.49
13:M:229:GLY:HA2	8:V:111:PHE:CE1	2.47	0.49
11:Y:36:GLU:OE1	11:Y:185:TRP:CH2	2.65	0.49
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.94	0.49
3:C:201:VAL:O	3:C:202:GLN:CB	2.60	0.49
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.60	0.49
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.78	0.48
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.96	0.48
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.96	0.48
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.96	0.48
13:M:230:THR:HG22	8:V:77:VAL:HB	1.96	0.48
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.96	0.47
11:K:35:ILE:HB	11:K:45:MET:HE2	1.96	0.47
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.96	0.47
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	1.97	0.46
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.47	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.79	0.46
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.46
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.46	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
11:K:35:ILE:HG21	11:K:56:GLU:HB3	1.97	0.46
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.98	0.46
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.50	0.46
11:K:100:MET:CE	11:K:127:PHE:HB2	2.46	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.98	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
3:C:201:VAL:HG13	3:C:202:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:8:ASN:HA	12:L:30:ILE:O	2.16	0.45
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.52	0.45
11:K:5:ALA:HB3	11:K:100:MET:CE	2.46	0.45
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.45
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.32	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.98	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.16	0.44
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.00	0.44
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.99	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.44
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.44
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.00	0.44
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.53	0.44
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.46	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.44
5:E:98:PHE:O	13:M:91:TYR:HA	2.18	0.43
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.99	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.43
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.48	0.43
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.53	0.43
11:K:1:THR:HG22	11:K:2:THR:N	2.34	0.43
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.49	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.49	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.42
11:K:104:TYR:CD2	11:K:182:GLU:HG2	2.42	0.42
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.19	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.42
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.01	0.42
11:Y:9:GLN:NE2	11:Y:148:LEU:O	2.52	0.42
11:Y:40:PHE:CE1	11:Y:73:ARG:CZ	3.03	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.01	0.41
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.35	0.41
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.50	0.41
4:R:158:ARG:HB3	5:S:57:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
11:K:104:TYR:CZ	11:K:110:PRO:HD3	2.55	0.41
12:Z:161:GLU:HB3	12:Z:164:THR:HG21	2.01	0.41
3:C:201:VAL:O	3:C:202:GLN:HB2	2.20	0.41
10:J:1:MET:O	10:J:2:ASP:CB	2.66	0.41
11:K:9:GLN:NE2	11:K:148:LEU:O	2.54	0.41
12:L:161:GLU:HB3	12:L:164:THR:HG21	2.01	0.41
4:R:99:ILE:HD11	4:R:104:LEU:HB2	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.40
11:Y:40:PHE:CD1	11:Y:73:ARG:NE	2.89	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	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%)	241 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	39
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	39
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	19	39
3	Q	238/254 (94%)	229 (96%)	7 (3%)	2 (1%)	19	39
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	234 (98%)	5 (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%)	4 (2%)	1 (0%)	29	52
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%)	189 (98%)	3 (2%)	1 (0%)	29	52
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	228/246 (93%)	222 (97%)	5 (2%)	1 (0%)	34	57
13	a	231/246 (94%)	225 (97%)	5 (2%)	1 (0%)	34	57
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	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
15	d	2/5 (40%)	2 (100%)	0	0	100	100
15	e	2/5 (40%)	2 (100%)	0	0	100	100
15	f	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6281/6634 (95%)	6109 (97%)	159 (2%)	13 (0%)	47	71

All (13) 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

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Mol	Chain	Res	Type
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP
8	V	9	ASN
13	M	229	GLY
13	a	229	GLY

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	85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	85
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	67
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	67
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	59
3	Q	212/226 (94%)	205 (97%)	7 (3%)	38	64
4	D	194/215 (90%)	184 (95%)	10 (5%)	23	46
4	R	194/215 (90%)	184 (95%)	10 (5%)	23	46
5	E	190/193 (98%)	183 (96%)	7 (4%)	34	60
5	S	190/193 (98%)	183 (96%)	7 (4%)	34	60
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	47
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	47
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	58
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	58
8	H	181/190 (95%)	176 (97%)	5 (3%)	43	69
8	V	181/190 (95%)	176 (97%)	5 (3%)	43	69
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	75
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	173/175 (99%)	168 (97%)	5 (3%)	42 68
10	X	173/175 (99%)	168 (97%)	5 (3%)	42 68
11	K	169/169 (100%)	160 (95%)	9 (5%)	22 45
11	Y	169/169 (100%)	157 (93%)	12 (7%)	14 29
12	L	185/185 (100%)	179 (97%)	6 (3%)	39 65
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39 65
13	M	196/208 (94%)	190 (97%)	6 (3%)	40 66
13	a	199/208 (96%)	193 (97%)	6 (3%)	41 67
14	N	162/162 (100%)	160 (99%)	2 (1%)	71 87
14	b	162/162 (100%)	160 (99%)	2 (1%)	71 87
15	c	2/2 (100%)	1 (50%)	1 (50%)	0 0
15	d	2/2 (100%)	2 (100%)	0	100 100
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%)	5136 (97%)	181 (3%)	37 63

All (181) 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	114	LEU
2	B	191	LEU
3	C	4	ARG
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

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Mol	Chain	Res	Type
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	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
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	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	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP

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Mol	Chain	Res	Type
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	107	LYS
11	K	118	ASP
11	K	143	ASN
11	K	148	LEU
11	K	181	THR
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
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	21	THR
14	N	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN

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Mol	Chain	Res	Type
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	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	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
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	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
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	56	THR
8	V	68	LEU

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Mol	Chain	Res	Type
8	V	196	ARG
9	W	37	ASN
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	73	ARG
11	Y	99	THR
11	Y	104	TYR
11	Y	106	ARG
11	Y	107	LYS
11	Y	118	ASP
11	Y	143	ASN
11	Y	148	LEU
11	Y	181	THR
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
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	21	THR
14	b	39	ASP
15	c	2	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS

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Mol	Chain	Res	Type
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
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	86	ASN
6	F	117	GLN
6	F	123	ASN
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
11	K	9	GLN
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	48	ASN
13	M	102	GLN
1	O	94	HIS
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN

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Mol	Chain	Res	Type
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
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	86	ASN
6	T	117	GLN
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
9	W	37	ASN
10	X	55	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	DCL	c	4	11,15	7,7,7	0.65	0	6,8,8	1.00	1 (16%)
15	DCL	e	4	11,15	7,7,7	0.48	0	6,8,8	0.90	0
15	DCL	d	4	14,15	7,7,7	0.64	0	6,8,8	1.30	1 (16%)
15	DCL	f	4	14,15	7,7,7	0.69	0	6,8,8	1.28	1 (16%)

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
15	DCL	c	4	11,15	-	3/6/6/6	-
15	DCL	e	4	11,15	-	2/6/6/6	-
15	DCL	d	4	14,15	-	3/6/6/6	-
15	DCL	f	4	14,15	-	3/6/6/6	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	d	4	DCL	CB-CA-C	-2.55	107.60	111.79
15	f	4	DCL	CB-CA-C	-2.48	107.73	111.79
15	c	4	DCL	O-C-CA	-2.09	103.27	111.52

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	DCL	N-CA-CB-CG
15	c	4	DCL	C-CA-CB-CG
15	d	4	DCL	N-CA-CB-CG
15	d	4	DCL	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
15	e	4	DCL	N-CA-CB-CG
15	e	4	DCL	C-CA-CB-CG
15	f	4	DCL	N-CA-CB-CG
15	f	4	DCL	C-CA-CB-CG
15	f	4	DCL	CA-CB-CG-CD2
15	d	4	DCL	CA-CB-CG-CD2
15	c	4	DCL	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 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	c	101	-	12,12,12	2.22	1 (8%)	14,16,16	1.22	2 (14%)
18	MES	Y	301	-	12,12,12	2.21	1 (8%)	14,16,16	1.24	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	c	101	-	-	0/6/14/14	0/1/1/1
18	MES	Y	301	-	-	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	c	101	MES	C8-S	-7.38	1.67	1.77
18	Y	301	MES	C8-S	-7.33	1.67	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Y	301	MES	O2S-S-C8	2.81	110.30	106.92
18	c	101	MES	O2S-S-C8	2.53	109.96	106.92
18	c	101	MES	O3S-S-C8	2.33	109.53	105.77
18	Y	301	MES	O3S-S-C8	2.32	109.53	105.77

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	6 (2%)	59	53	36, 50, 88, 129	0
1	O	250/250 (100%)	0.01	10 (4%)	38	31	42, 59, 105, 136	0
2	B	244/258 (94%)	-0.07	10 (4%)	37	30	36, 55, 103, 159	0
2	P	244/258 (94%)	0.02	13 (5%)	26	20	41, 60, 109, 159	0
3	C	240/254 (94%)	0.02	16 (6%)	17	13	37, 58, 122, 161	0
3	Q	240/254 (94%)	0.24	21 (8%)	10	7	42, 72, 153, 193	0
4	D	235/260 (90%)	-0.25	3 (1%)	77	73	41, 61, 94, 142	0
4	R	235/260 (90%)	-0.17	8 (3%)	45	38	41, 62, 102, 156	0
5	E	231/234 (98%)	0.06	10 (4%)	35	28	43, 63, 99, 141	0
5	S	231/234 (98%)	0.08	12 (5%)	27	21	48, 73, 115, 155	0
6	F	243/288 (84%)	0.10	13 (5%)	26	20	37, 58, 111, 138	0
6	T	243/288 (84%)	0.15	13 (5%)	26	20	36, 68, 126, 161	0
7	G	241/252 (95%)	0.06	11 (4%)	32	26	37, 54, 96, 150	0
7	U	241/252 (95%)	0.07	9 (3%)	41	34	41, 56, 93, 138	0
8	H	222/232 (95%)	-0.20	4 (1%)	68	64	35, 48, 81, 118	0
8	V	222/232 (95%)	0.08	5 (2%)	60	54	38, 54, 90, 130	0
9	I	204/205 (99%)	-0.55	1 (0%)	91	89	30, 47, 76, 96	0
9	W	204/205 (99%)	-0.46	3 (1%)	73	70	32, 50, 82, 103	0
10	J	195/198 (98%)	-0.38	3 (1%)	73	70	32, 49, 75, 114	0
10	X	195/198 (98%)	-0.38	4 (2%)	63	58	36, 51, 77, 129	0
11	K	212/212 (100%)	-0.17	7 (3%)	46	39	38, 54, 89, 108	0
11	Y	212/212 (100%)	-0.10	9 (4%)	36	29	40, 54, 90, 116	0
12	L	222/222 (100%)	-0.34	4 (1%)	68	64	35, 51, 89, 122	0
12	Z	222/222 (100%)	-0.32	4 (1%)	68	64	33, 52, 89, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	230/246 (93%)	-0.26	4 (1%) 70 66	31, 49, 77, 88	0
13	a	233/246 (94%)	-0.27	3 (1%) 77 73	33, 50, 74, 101	0
14	N	196/196 (100%)	-0.20	1 (0%) 91 89	32, 45, 75, 104	0
14	b	196/196 (100%)	-0.22	4 (2%) 65 60	32, 46, 77, 101	0
15	c	3/5 (60%)	3.56	2 (66%) 0 0	78, 78, 84, 84	0
15	d	3/5 (60%)	-0.12	0 100 100	49, 49, 53, 56	0
15	e	3/5 (60%)	4.08	3 (100%) 0 0	80, 80, 88, 90	0
15	f	3/5 (60%)	-0.15	0 100 100	52, 52, 56, 56	0
All	All	6345/6634 (95%)	-0.11	216 (3%) 45 38	30, 55, 102, 193	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	8.3
3	Q	49	THR	7.8
1	O	1	MET	7.3
3	C	206	LYS	7.1
8	V	222	ASP	6.9
2	P	218	GLY	6.8
2	B	220	ASN	6.7
15	c	1	ALA	6.4
2	P	219	ALA	6.4
2	P	221	ASP	6.3
2	B	218	GLY	6.2
2	P	222	GLY	6.1
5	S	202	ASP	5.9
10	X	1	MET	5.8
2	B	51	VAL	5.8
2	P	51	VAL	5.8
3	Q	206	LYS	5.8
8	V	221	CYS	5.7
3	Q	50	LEU	5.6
13	M	230	THR	5.5
10	X	194	ASP	5.5
1	A	1	MET	5.2
6	F	241	LYS	5.0
9	W	1	SER	4.9
5	E	202	ASP	4.9
3	Q	240	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
2	P	220	ASN	4.8
15	e	2	PRO	4.6
2	B	221	ASP	4.6
10	J	1	MET	4.6
2	P	203	SER	4.5
3	Q	51	LYS	4.5
3	C	49	THR	4.5
1	O	249	ALA	4.4
8	H	221	CYS	4.4
9	I	1	SER	4.4
6	T	243	ILE	4.4
3	Q	236	GLN	4.4
1	O	201	GLU	4.2
3	Q	238	LYS	4.2
3	C	202	GLN	4.2
10	X	193	ASP	4.2
6	T	180	PRO	4.2
3	C	239	GLN	4.1
15	e	3	LEU	4.1
3	C	238	LYS	4.1
7	G	240	ALA	4.1
5	S	233	ILE	4.1
3	C	236	GLN	4.0
3	Q	48	SER	4.0
13	a	1	THR	4.0
2	P	52	THR	4.0
11	Y	147	ASP	3.9
4	R	242	GLU	3.9
4	D	242	GLU	3.9
7	U	206	GLY	3.9
5	E	233	ILE	3.8
3	Q	239	GLN	3.8
2	P	59	ASP	3.7
7	U	242	GLN	3.6
10	J	193	ASP	3.6
4	R	241	ALA	3.6
15	e	1	ALA	3.5
6	T	241	LYS	3.5
7	G	179	LYS	3.5
8	H	222	ASP	3.5
7	G	3	TYR	3.4
6	T	178	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
6	F	244	ASN	3.4
3	Q	205	ALA	3.3
3	Q	55	THR	3.3
15	c	2	PRO	3.3
6	F	215	CYS	3.3
12	L	172	LEU	3.3
10	J	194	ASP	3.2
12	Z	174	TYR	3.2
3	C	205	ALA	3.2
7	U	222	ASP	3.2
2	B	217	LYS	3.2
9	W	133	LYS	3.2
12	L	165	ASN	3.2
3	C	225	GLU	3.2
1	A	250	LEU	3.2
5	S	52	ALA	3.2
6	F	243	ILE	3.1
13	M	229	GLY	3.1
3	C	50	LEU	3.1
5	E	201	ARG	3.1
11	Y	106	ARG	3.1
6	F	229	GLY	3.1
11	K	147	ASP	3.1
8	H	198	GLU	3.0
2	B	242	GLY	3.0
11	K	182	GLU	3.0
3	Q	171	GLU	2.9
2	P	225	TYR	2.9
7	G	237	VAL	2.9
11	Y	210	VAL	2.9
3	Q	223	SER	2.9
13	a	233	ILE	2.9
1	A	248	GLU	2.9
6	F	178	HIS	2.8
2	B	203	SER	2.8
11	Y	212	GLY	2.8
4	D	241	ALA	2.8
5	E	54	GLU	2.8
13	M	47	ASP	2.7
5	S	122	TYR	2.7
1	O	231	LYS	2.7
1	O	250	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	207	ASP	2.7
6	F	205	GLU	2.7
14	b	104	ASP	2.7
1	O	229	THR	2.6
5	S	3	ASN	2.6
6	T	181	GLU	2.6
6	T	2	THR	2.6
2	P	182	ASP	2.6
5	E	180	LYS	2.6
7	G	2	GLY	2.6
13	M	1	THR	2.6
6	F	53	LYS	2.6
6	T	53	LYS	2.6
1	O	178	ARG	2.6
6	F	181	GLU	2.6
8	V	215	GLU	2.6
7	G	180	SER	2.6
3	C	175	LYS	2.5
3	Q	235	GLU	2.5
8	V	145	ASP	2.5
7	U	181	LYS	2.5
1	A	249	ALA	2.5
5	S	54	GLU	2.5
12	L	174	TYR	2.5
7	G	51	PRO	2.5
11	Y	182	GLU	2.5
12	Z	167	LYS	2.5
6	T	244	ASN	2.5
7	G	208	GLU	2.4
6	F	2	THR	2.4
11	Y	211	ILE	2.4
3	Q	202	GLN	2.4
11	K	211	ILE	2.4
3	C	181	GLU	2.4
7	G	230	GLU	2.4
7	G	241	GLU	2.4
3	Q	180	LYS	2.4
9	W	191	LYS	2.4
11	K	210	VAL	2.4
3	C	37	LYS	2.4
11	Y	202	GLU	2.4
6	T	166	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
11	K	212	GLY	2.4
1	O	248	GLU	2.4
11	Y	183	ASP	2.4
5	E	176	ASP	2.4
5	S	51	ASN	2.4
13	a	232	LYS	2.4
11	K	23	GLY	2.4
14	N	105	LYS	2.4
3	C	47	ARG	2.4
1	A	2	THR	2.3
12	Z	210	ASP	2.3
7	U	51	PRO	2.3
3	Q	216	ASP	2.3
1	O	141	GLU	2.3
11	K	183	ASP	2.3
4	R	201	GLU	2.3
6	T	205	GLU	2.3
5	S	180	LYS	2.3
3	Q	52	LEU	2.3
5	S	30	GLN	2.3
3	C	240	GLU	2.3
7	U	55	LEU	2.3
12	L	167	LYS	2.3
3	Q	181	GLU	2.3
7	G	68	ARG	2.3
2	P	223	GLU	2.3
3	Q	203	THR	2.3
7	U	241	GLU	2.3
2	B	59	ASP	2.3
12	Z	1	GLN	2.2
1	A	201	GLU	2.2
5	S	165	GLN	2.2
7	U	178	LYS	2.2
4	D	201	GLU	2.2
6	F	204	LYS	2.2
10	X	72	ASP	2.2
14	b	105	LYS	2.1
4	R	125	LEU	2.1
14	b	195	GLN	2.1
6	T	230	ASP	2.1
4	R	141	ALA	2.1
4	R	1	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	S	163	ARG	2.1
6	T	170	ALA	2.1
2	B	52	THR	2.1
5	S	173	ARG	2.1
2	P	93	HIS	2.1
5	E	227	GLU	2.1
3	Q	175	LYS	2.1
8	H	219	ASN	2.1
5	E	123	GLY	2.1
4	R	217	GLN	2.1
11	Y	151	GLU	2.1
14	b	71	GLY	2.1
5	E	207	VAL	2.0
3	C	27	ARG	2.0
1	O	198	GLU	2.0
4	R	237	GLU	2.0
6	T	221	ASN	2.0
3	C	180	LYS	2.0
6	F	230	ASP	2.0
7	U	2	GLY	2.0
5	E	3	ASN	2.0
8	V	204	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	DCL	e	4	8/8	0.62	0.43	77,81,82,83	0
15	DCL	c	4	8/8	0.81	0.28	70,78,79,79	0
15	DCL	d	4	8/8	0.86	0.23	51,56,58,58	0
15	DCL	f	4	8/8	0.93	0.21	50,57,62,62	0

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
16	MG	Z	301	1/1	0.71	0.18	67,67,67,67	0
18	MES	Y	301	12/12	0.79	0.39	76,84,97,106	0
18	MES	c	101	12/12	0.86	0.37	79,86,100,102	0
16	MG	I	302	1/1	0.93	0.07	54,54,54,54	0
16	MG	N	201	1/1	0.96	0.14	46,46,46,46	0
16	MG	I	301	1/1	0.96	0.37	63,63,63,63	0
16	MG	G	301	1/1	0.96	0.07	41,41,41,41	0
16	MG	K	301	1/1	0.96	0.09	56,56,56,56	0
16	MG	L	301	1/1	0.97	0.04	54,54,54,54	0
17	CL	b	201	1/1	0.97	0.23	63,63,63,63	0
17	CL	G	302	1/1	0.99	0.18	30,30,30,30	0
17	CL	N	202	1/1	0.99	0.06	43,43,43,43	0
17	CL	U	301	1/1	0.99	0.23	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.