Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 08:29 am GMT

PDB ID	:	4YA7
Title	:	Yeast 20S proteasome beta2-H114D mutant in complex with Ac-LAE-ep
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-02-17
Resolution	:	2.70 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 (i)) were used in the production of this report:

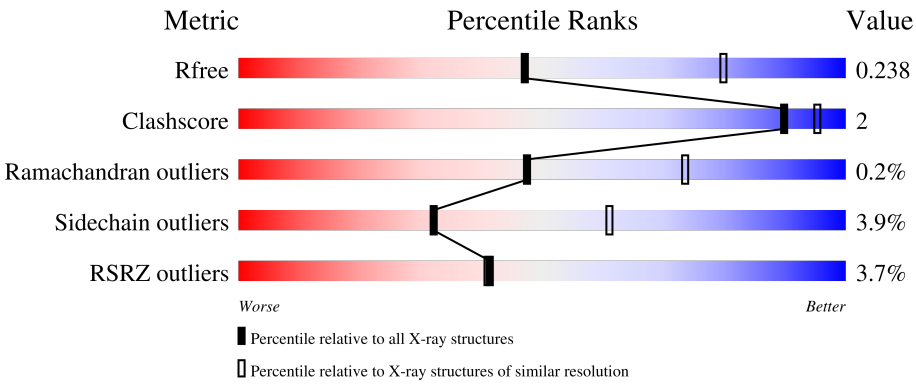
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	3% 95% 5%
1	O	250	5% 95% 5%
2	B	258	6% 86% 8% 5%
2	P	258	6% 86% 8% 5%
3	C	254	9% 87% 7% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	13% 87% 6% 6%
4	D	260	2% 84% 6% 10%
4	R	260	3% 82% 8% 10%
5	E	234	5% 89% 9%
5	S	234	5% 87% 11%
6	F	288	3% 79% 5% 16%
6	T	288	6% 79% 5% 16%
7	G	252	4% 90% 6%
7	U	252	3% 89% 6%
8	H	232	% 89% 6%
8	V	232	2% 91% 5%
9	I	205	% 92% 7%
9	W	205	% 93% 5%
10	J	198	2% 90% 7%
10	X	198	2% 90% 7%
11	K	212	% 89% 10%
11	Y	212	2% 92% 8%
12	L	222	% 92% 8%
12	Z	222	% 92% 7%
13	M	246	% 89% 6% 5%
13	a	246	2% 91% 5%
14	N	196	2% 96%
14	b	196	% 97%
15	c	5	80% 20%
15	d	5	80% 20%

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

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 50429 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
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	235	1813	1136	304	366	7	0	0	0
4	R	235	1813	1136	304	366	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	231	1773	1114	307	348	4	0	0	0
5	S	231	1773	1114	307	348	4	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	222	1682	1059	291	325	7	0	0	0
8	V	222	1682	1059	291	325	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	114	ASP	HIS	engineered mutation	UNP P25043
V	114	ASP	HIS	engineered mutation	UNP P25043

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1581	1010	258	305	8	0	0	0
9	W	204	1581	1010	258	305	8	0	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1757	1115	303	335	4	0	0	0
12	Z	222	1764	1120	305	335	4	0	1	0

- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

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

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

- Molecule 15 is a protein called Ac-LAE-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	c	5	29	19	3	7	0	0	0
15	d	5	29	19	3	7	0	0	0
15	e	5	29	19	3	7	0	0	0
15	f	5	29	19	3	7	0	0	0
15	g	5	29	19	3	7	0	0	0
15	h	5	29	19	3	7	0	0	0

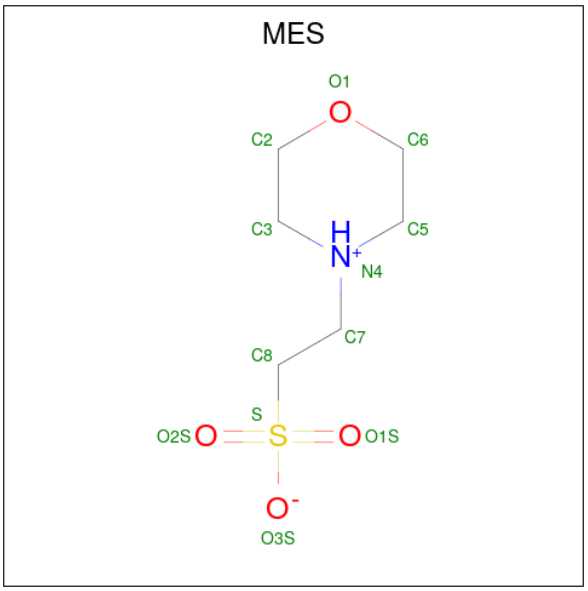
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
16	G	1	1	1	0	0
16	H	1	1	1	0	0
16	I	2	2	2	0	0
16	K	1	1	1	0	0
16	L	1	1	1	0	0
16	N	1	1	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
17	G	1	1	1	0	0
17	U	1	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
			Total	C	N	O	S		
18	H	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
18	K	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
18	V	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
18	Y	1	12	6	1	4	1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	A	44	44	44	0	0
			Total	O		
19	B	34	34	34	0	0
			Total	O		
19	C	22	22	22	0	0
			Total	O		
19	D	19	19	19	0	0
			Total	O		
19	E	21	21	21	0	0
			Total	O		
19	F	26	26	26	0	0
			Total	O		
19	G	36	36	36	0	0
			Total	O		
19	H	50	50	50	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	I	40	Total O 40 40	0	0
19	J	43	Total O 43 43	0	0
19	K	27	Total O 27 27	0	0
19	L	52	Total O 52 52	0	0
19	M	42	Total O 42 42	0	0
19	N	26	Total O 26 26	0	0
19	O	30	Total O 30 30	0	0
19	P	23	Total O 23 23	0	0
19	Q	18	Total O 18 18	0	0
19	R	18	Total O 18 18	0	0
19	S	11	Total O 11 11	0	0
19	T	27	Total O 27 27	0	0
19	U	31	Total O 31 31	0	0
19	V	43	Total O 43 43	0	0
19	W	35	Total O 35 35	0	0
19	X	29	Total O 29 29	0	0
19	Y	28	Total O 28 28	0	0
19	Z	52	Total O 52 52	0	0
19	a	36	Total O 36 36	0	0
19	b	30	Total O 30 30	0	0
19	d	1	Total O 1 1	0	0

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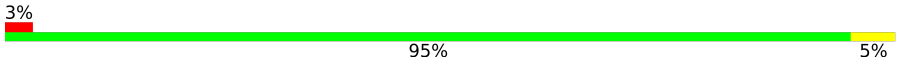
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	e	1	1	1	0	0
			Total	O		
19	f	1	1	1	0	0
			Total	O		
19	g	3	3	3	0	0

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.

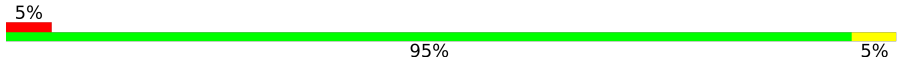
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



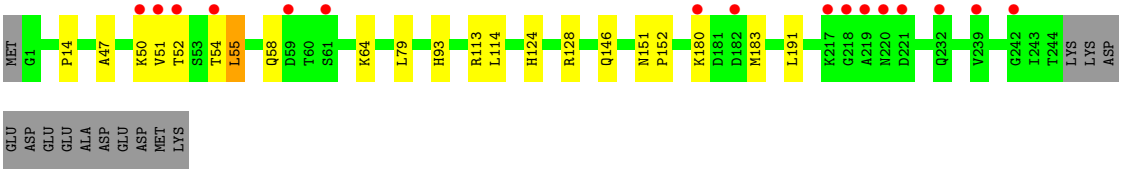
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



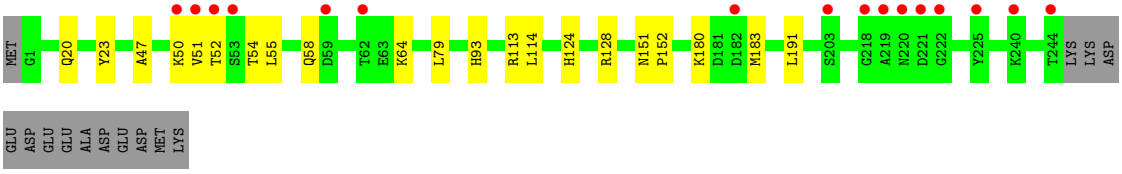
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



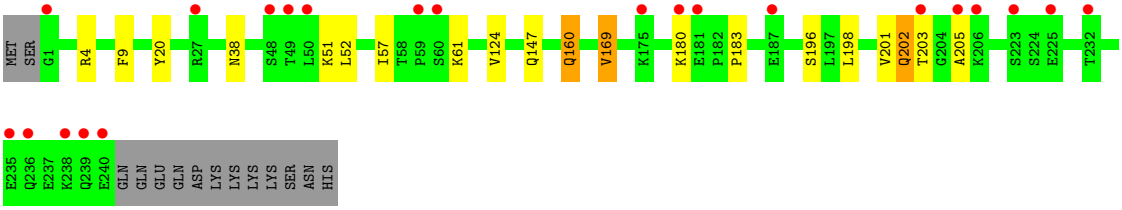
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



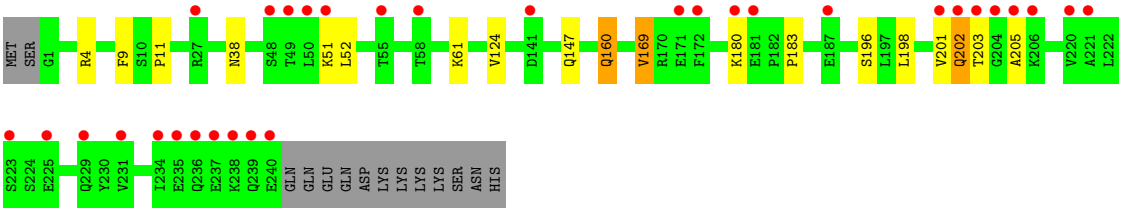
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



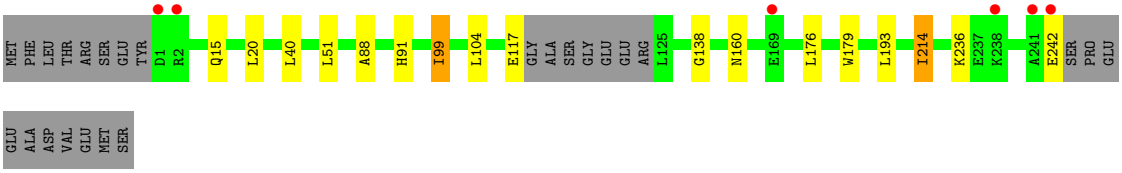
- Molecule 3: Proteasome subunit alpha type-4

Chain Q:



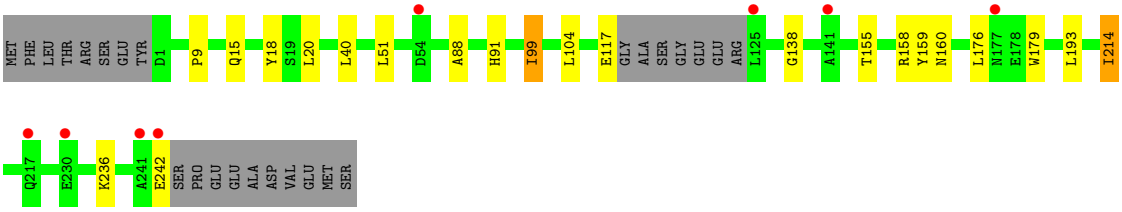
- Molecule 4: Proteasome subunit alpha type-5

Chain D:



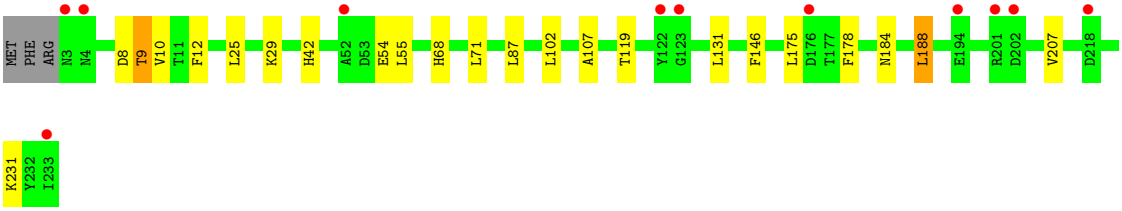
- Molecule 4: Proteasome subunit alpha type-5

Chain R:



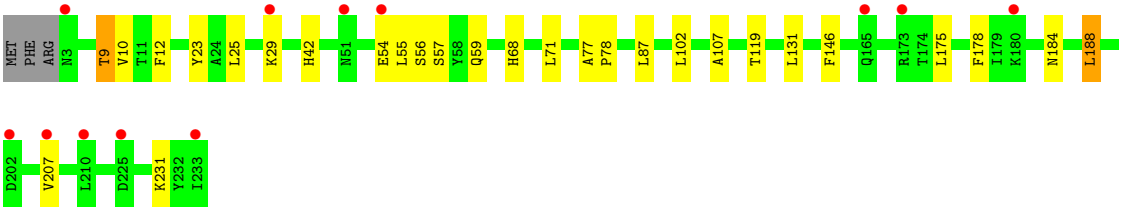
- Molecule 5: Proteasome subunit alpha type-6

Chain E:



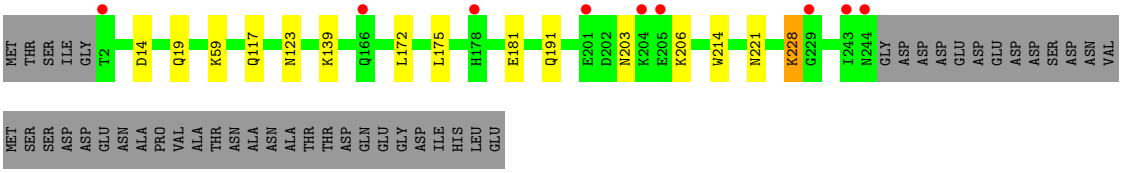
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



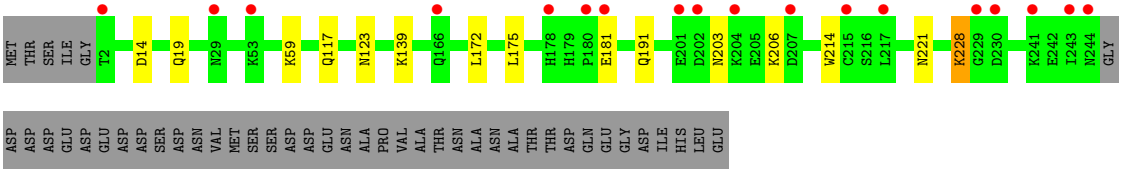
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



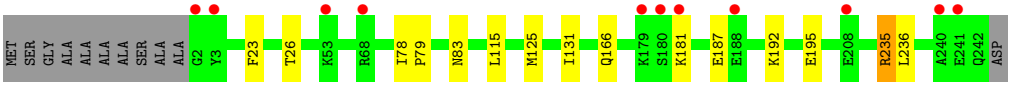
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



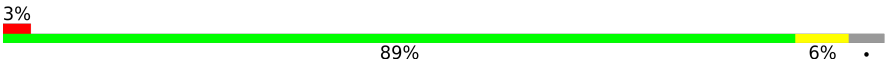
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



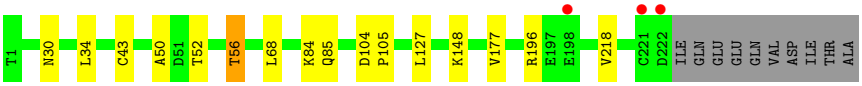
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



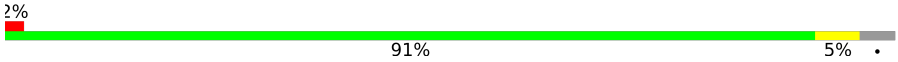
• Molecule 8: Proteasome subunit beta type-2

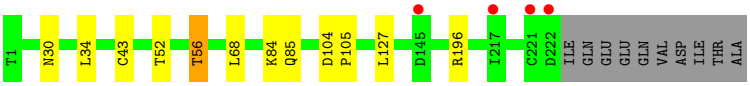
Chain H:



• Molecule 8: Proteasome subunit beta type-2

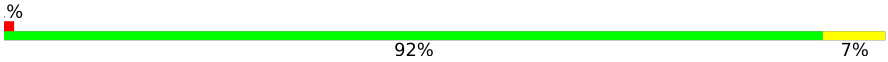
Chain V:





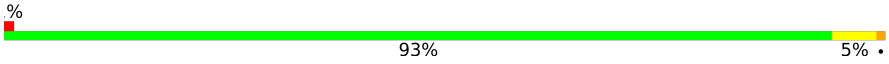
• Molecule 9: Proteasome subunit beta type-3

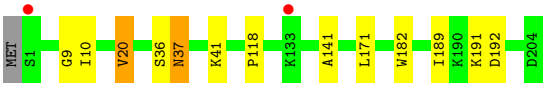
Chain I:



• Molecule 9: Proteasome subunit beta type-3

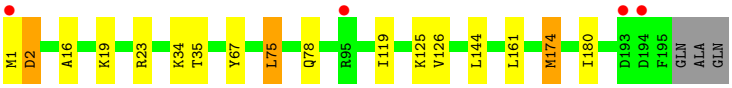
Chain W:





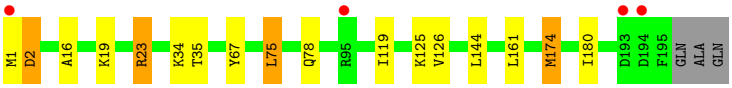
• Molecule 10: Proteasome subunit beta type-4

Chain J:



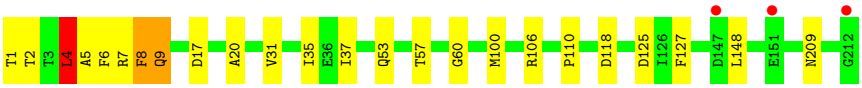
• Molecule 10: Proteasome subunit beta type-4

Chain X:



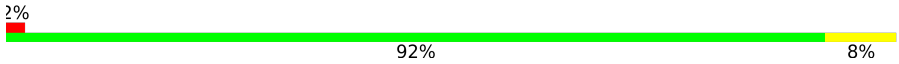
• Molecule 11: Proteasome subunit beta type-5

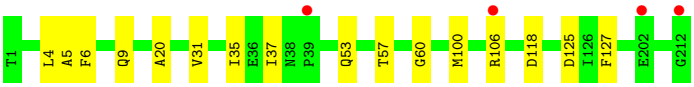
Chain K:



• Molecule 11: Proteasome subunit beta type-5

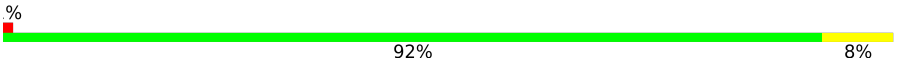
Chain Y:





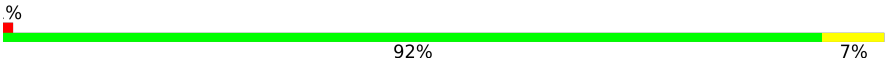
• Molecule 12: Proteasome subunit beta type-6

Chain L:



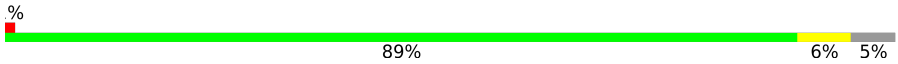
• Molecule 12: Proteasome subunit beta type-6

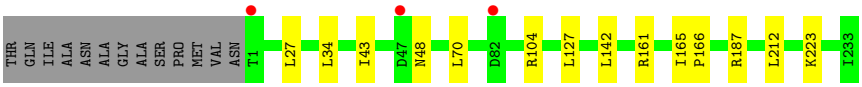
Chain Z:



• Molecule 13: Proteasome subunit beta type-7

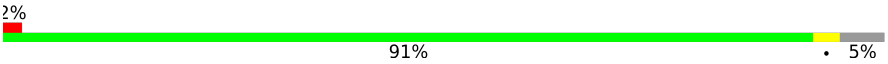
Chain M:

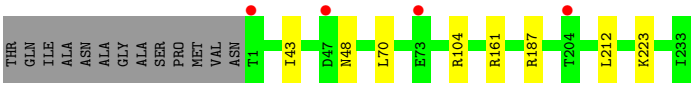




• Molecule 13: Proteasome subunit beta type-7

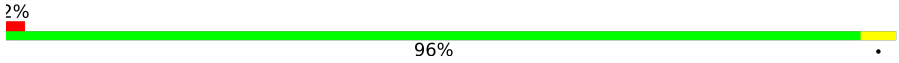
Chain a:

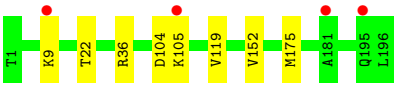




• Molecule 14: Proteasome subunit beta type-1

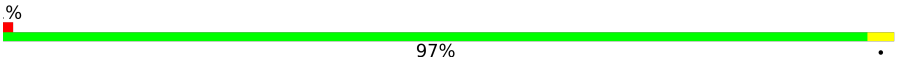
Chain N:

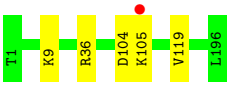




• Molecule 14: Proteasome subunit beta type-1

Chain b:





- Molecule 15: Ac-LAE-ep

Chain c:

- Molecule 15: Ac-LAE-ep

Chain d:

- Molecule 15: Ac-LAE-ep

Chain e:

- Molecule 15: Ac-LAE-ep

Chain f:

- Molecule 15: Ac-LAE-ep

Chain g:

- Molecule 15: Ac-LAE-ep

Chain h:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.02Å 299.94Å 144.88Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-2.70) 96.0 (15.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.215 , 0.237 0.217 , 0.238	Depositor DCC
R_{free} test set	13803 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	50429	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, MG, CL, POL, GAU, MES

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	0.48	0/2642
2	B	0.27	0/1934	0.51	0/2618
2	P	0.27	0/1934	0.51	0/2618
3	C	0.27	0/1910	0.52	0/2586
3	Q	0.27	0/1910	0.51	0/2586
4	D	0.26	0/1837	0.49	0/2475
4	R	0.26	0/1837	0.49	0/2475
5	E	0.27	0/1800	0.48	0/2433
5	S	0.27	0/1800	0.49	0/2433
6	F	0.27	0/1932	0.47	0/2609
6	T	0.27	0/1932	0.47	0/2609
7	G	0.27	0/1945	0.49	0/2634
7	U	0.27	0/1945	0.48	0/2634
8	H	0.25	0/1712	0.50	0/2322
8	V	0.26	0/1712	0.49	0/2322
9	I	0.28	0/1611	0.50	0/2174
9	W	0.28	0/1611	0.50	0/2174
10	J	0.26	0/1589	0.49	0/2142
10	X	0.26	0/1589	0.49	0/2142
11	K	0.41	0/1681	0.52	1/2274 (0.0%)
11	Y	0.26	0/1681	0.50	0/2274
12	L	0.27	0/1795	0.49	0/2420
12	Z	0.29	0/1806	0.49	0/2435
13	M	0.27	0/1855	0.52	0/2514
13	a	0.27	0/1855	0.52	0/2514
14	N	0.29	0/1541	0.49	0/2087
14	b	0.29	0/1541	0.49	0/2087
15	c	0.34	0/13	1.26	0/17
15	d	1.16	0/13	1.61	0/17
15	e	0.34	0/13	1.20	0/17
15	f	1.09	0/13	1.46	0/17

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	g	0.99	0/13	1.26	0/17
15	h	1.02	0/13	1.10	0/17
All	All	0.28	0/50277	0.50	1/67977 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	4	LEU	CA-CB-CG	5.30	127.50	115.30

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	6	0
1	O	1915	0	1929	7	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	10	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	11	0
5	E	1773	0	1775	7	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	7	0
8	H	1682	0	1682	6	0
8	V	1682	0	1682	3	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1561	0	1569	11	0
11	K	1644	0	1592	14	0
11	Y	1644	0	1592	8	0
12	L	1757	0	1711	6	0
12	Z	1764	0	1718	6	0
13	M	1824	0	1832	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	29	0	30	0	0
15	d	29	0	30	0	0
15	e	29	0	30	0	0
15	f	29	0	30	0	0
15	g	29	0	30	0	0
15	h	29	0	30	0	0
16	G	1	0	0	0	0
16	H	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
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	H	12	0	13	0	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	44	0	0	1	0
19	B	34	0	0	0	0
19	C	22	0	0	0	0
19	D	19	0	0	0	0
19	E	21	0	0	0	0
19	F	26	0	0	0	0
19	G	36	0	0	0	0
19	H	50	0	0	0	0
19	I	40	0	0	0	0
19	J	43	0	0	0	0
19	K	27	0	0	0	0
19	L	52	0	0	0	0
19	M	42	0	0	0	0
19	N	26	0	0	0	0
19	O	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	23	0	0	0	0
19	Q	18	0	0	0	0
19	R	18	0	0	0	0
19	S	11	0	0	0	0
19	T	27	0	0	0	0
19	U	31	0	0	0	0
19	V	43	0	0	0	0
19	W	35	0	0	0	0
19	X	29	0	0	0	0
19	Y	28	0	0	1	0
19	Z	52	0	0	0	0
19	a	36	0	0	0	0
19	b	30	0	0	0	0
19	d	1	0	0	0	0
19	e	1	0	0	0	0
19	f	1	0	0	0	0
19	g	3	0	0	0	0
All	All	50429	0	49283	162	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 (162) 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)
10:J:1:MET:O	10:J:2:ASP:HB2	1.84	0.77
10:X:1:MET:O	10:X:2:ASP:HB2	1.84	0.75
11:K:9:GLN:NE2	11:K:148:LEU:O	2.20	0.75
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.70	0.73
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.71	0.73
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.70	0.72
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.70	0.71
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.72	0.70
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.77	0.67
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.75	0.67
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.80	0.64
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.01	0.61
3:C:51:LYS:O	3:C:52:LEU:HB2	2.01	0.61
11:K:100:MET:CE	11:K:127:PHE:HB2	2.32	0.59
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.68	0.58
5:S:12:PHE:H	6:T:19:GLN:HE22	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:5:ALA:HB3	11:K:100:MET:CE	2.34	0.57
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.32	0.57
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.57
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.69	0.57
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.70	0.56
7:G:23:PHE:O	7:G:26:THR:HB	2.05	0.56
14:N:152:VAL:HA	14:N:175:MET:HE1	1.87	0.56
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.86	0.56
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.40	0.56
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.55
8:H:52:THR:O	8:H:56:THR:HB	2.07	0.55
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.54
8:V:52:THR:O	8:V:56:THR:HB	2.07	0.54
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.73	0.54
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.91	0.53
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.91	0.53
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.91	0.53
5:E:12:PHE:H	6:F:19:GLN:HE22	1.55	0.52
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.74	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.51
5:E:9:THR:HG21	5:E:119:THR:HA	1.93	0.51
5:S:9:THR:HG21	5:S:119:THR:HA	1.92	0.51
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.92	0.51
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.74	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
11:K:6:PHE:HA	11:K:125:ASP:O	2.11	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.93	0.51
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.51
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.93	0.51
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.92	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.94	0.50
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.93	0.50
10:J:1:MET:O	10:J:2:ASP:CB	2.59	0.50
12:L:8:ASN:HA	12:L:30:ILE:O	2.13	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.93	0.49
3:C:201:VAL:HG13	3:C:202:GLN:N	2.28	0.49
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.94	0.49
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.12	0.49
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.59	0.49
8:H:50:ALA:HB3	9:I:126:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.28	0.48
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.94	0.48
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.13	0.48
3:C:201:VAL:O	3:C:202:GLN:HB2	2.13	0.48
10:J:174:MET:HA	10:X:174:MET:HA	1.95	0.48
11:K:53:GLN:O	11:K:57:THR:HG23	2.14	0.47
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.80	0.47
7:U:26:THR:HG21	7:U:131:ILE:HD12	1.97	0.47
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.95	0.47
10:J:1:MET:HA	10:J:34:LYS:HE3	1.96	0.47
10:X:1:MET:O	10:X:2:ASP:CB	2.58	0.47
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.13	0.47
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.79	0.47
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.98	0.47
7:G:26:THR:HG21	7:G:131:ILE:HD12	1.96	0.46
10:X:1:MET:HA	10:X:34:LYS:HE3	1.96	0.46
1:O:149:GLN:O	1:O:156:TYR:HA	2.16	0.46
4:R:158:ARG:HB3	5:S:57:SER:HB3	1.97	0.46
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.51	0.46
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.97	0.46
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.98	0.46
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.97	0.46
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.98	0.46
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.51	0.46
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.98	0.45
6:T:228:LYS:HB2	6:T:228:LYS:HE3	1.72	0.45
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.31	0.45
4:R:155:THR:HG23	5:S:59:GLN:HE22	1.82	0.45
1:A:149:GLN:O	1:A:156:TYR:HA	2.15	0.45
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.97	0.45
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.97	0.45
11:K:7:ARG:NH1	11:K:110:PRO:O	2.47	0.45
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.99	0.45
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.99	0.45
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.98	0.45
11:K:4:LEU:CD2	11:K:4:LEU:C	2.85	0.45
12:L:147:MET:N	12:L:148:PRO:HD2	2.31	0.45
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.52	0.45
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.98	0.45
5:S:68:HIS:HE1	5:S:102:LEU:O	2.00	0.45
5:S:131:LEU:HB2	5:S:146:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:180:LYS:O	2:P:183:MET:HB2	2.17	0.45
1:A:236:ARG:NH2	19:A:301:HOH:O	2.49	0.44
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.53	0.44
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.99	0.44
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.45	0.44
10:J:1:MET:HA	10:J:34:LYS:CE	2.47	0.44
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.98	0.44
2:B:180:LYS:O	2:B:183:MET:HB2	2.17	0.44
5:E:68:HIS:HE1	5:E:102:LEU:O	2.00	0.44
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.99	0.44
10:X:1:MET:HA	10:X:34:LYS:CE	2.47	0.44
8:H:84:LYS:HG3	8:H:85:GLN:N	2.33	0.44
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.99	0.44
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.44
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.53	0.44
3:C:9:PHE:H	4:D:15:GLN:HE22	1.65	0.44
5:E:131:LEU:HB2	5:E:146:PHE:HB3	1.99	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.66	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.18	0.43
11:K:1:THR:HG22	11:K:2:THR:N	2.33	0.43
12:L:195:HIS:HD2	12:L:197:GLN:H	1.66	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.00	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.00	0.43
8:V:84:LYS:HG3	8:V:85:GLN:N	2.33	0.43
1:O:12:PHE:H	2:P:20:GLN:HE22	1.67	0.43
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.54	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.00	0.42
1:O:119:GLN:O	1:O:122:THR:HB	2.19	0.42
4:R:138:GLY:HA2	4:R:214:ILE:HG12	2.01	0.42
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.00	0.42
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.54	0.42
4:D:138:GLY:HA2	4:D:214:ILE:HG12	2.00	0.42
10:X:19:LYS:HD3	10:X:180:ILE:HG13	2.01	0.42
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:HIS:HB2	5:E:188:LEU:HD12	2.02	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.42
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.50	0.42
11:K:209:ASN:O	9:W:37:ASN:ND2	2.52	0.42
10:X:23:ARG:HG2	19:Y:420:HOH:O	2.20	0.42
1:A:119:GLN:O	1:A:122:THR:HB	2.20	0.42
1:A:176:GLU:HG2	2:B:55:LEU:HD13	2.02	0.42
10:J:19:LYS:HD3	10:J:180:ILE:HG13	2.00	0.42
5:S:42:HIS:HB2	5:S:188:LEU:HD12	2.02	0.41
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.55	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.01	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.41
11:K:8:PHE:CD1	11:K:8:PHE:N	2.88	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
1:A:110:LEU:O	1:A:114:VAL:HG23	2.20	0.41
6:F:228:LYS:HB2	6:F:228:LYS:HE3	1.72	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.41
6:T:175:LEU:HD21	6:T:191:GLN:NE2	2.36	0.41
6:F:175:LEU:HD21	6:F:191:GLN:NE2	2.35	0.40
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.40
8:H:148:LYS:HE3	8:H:177:VAL:HG11	2.03	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	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%)	5 (2%)	1 (0%)	34 60
1	O	248/250 (99%)	242 (98%)	5 (2%)	1 (0%)	34 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	60
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	60
3	C	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	12	30
3	Q	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	12	30
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
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%)	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%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	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%)	189 (98%)	3 (2%)	1 (0%)	29	54
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	54
11	K	210/212 (99%)	205 (98%)	5 (2%)	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	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	225 (97%)	6 (3%)	0	100	100
13	a	231/246 (94%)	225 (97%)	6 (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	2/5 (40%)	2 (100%)	0	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
15	g	2/5 (40%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	h	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6289/6644 (95%)	6123 (97%)	154 (2%)	12 (0%)	47	73

All (12) 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
1	A	3	ASP
1	O	3	ASP
3	C	183	PRO
3	Q	183	PRO

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	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	61
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	61
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	62
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	62
4	D	194/215 (90%)	184 (95%)	10 (5%)	23	49
4	R	194/215 (90%)	184 (95%)	10 (5%)	23	49
5	E	190/193 (98%)	178 (94%)	12 (6%)	18	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	190/193 (98%)	179 (94%)	11 (6%)	20	43
6	F	201/239 (84%)	189 (94%)	12 (6%)	19	42
6	T	201/239 (84%)	189 (94%)	12 (6%)	19	42
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	66
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	66
8	H	181/190 (95%)	174 (96%)	7 (4%)	32	61
8	V	181/190 (95%)	174 (96%)	7 (4%)	32	61
9	I	172/173 (99%)	166 (96%)	6 (4%)	36	65
9	W	172/173 (99%)	166 (96%)	6 (4%)	36	65
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	65
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	65
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	59
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	70
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	62
12	Z	186/185 (100%)	180 (97%)	6 (3%)	39	68
13	M	199/208 (96%)	191 (96%)	8 (4%)	31	60
13	a	199/208 (96%)	191 (96%)	8 (4%)	31	60
14	N	162/162 (100%)	156 (96%)	6 (4%)	34	63
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	69
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
All	All	5319/5546 (96%)	5110 (96%)	209 (4%)	32	61

All (209) 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

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Mol	Chain	Res	Type
2	B	50	LYS
2	B	52	THR
2	B	54	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
3	C	38	ASN
3	C	61	LYS
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	51	LEU
4	D	99	ILE
4	D	117	GLU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	231	LYS
6	F	14	ASP
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN

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Mol	Chain	Res	Type
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
6	F	228	LYS
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	20	VAL
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	191	LYS
9	I	192	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	8	PHE
11	K	9	GLN
11	K	17	ASP
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN

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Mol	Chain	Res	Type
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
13	M	212	LEU
13	M	223	LYS
14	N	9	LYS
14	N	22	THR
14	N	36	ARG
14	N	104	ASP
14	N	105	LYS
14	N	119	VAL
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	54	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	61	LYS
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	51	LEU

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Mol	Chain	Res	Type
4	R	99	ILE
4	R	117	GLU
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	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	231	LYS
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
6	T	221	ASN
6	T	228	LYS
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	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU

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Mol	Chain	Res	Type
8	V	127	LEU
8	V	196	ARG
9	W	20	VAL
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
9	W	191	LYS
9	W	192	ASP
10	X	23	ARG
10	X	35	THR
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	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
13	a	212	LEU
13	a	223	LYS
14	b	9	LYS
14	b	36	ARG
14	b	104	ASP
14	b	105	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) 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	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
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	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
8	H	57	GLN
8	H	66	HIS
9	I	37	ASN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN

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Mol	Chain	Res	Type
12	L	95	HIS
12	L	158	ASN
12	L	165	ASN
13	M	2	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	146	GLN
4	R	198	GLN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
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	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN

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Mol	Chain	Res	Type
7	U	175	ASN
8	V	57	GLN
8	V	66	HIS
8	V	165	ASN
10	X	37	GLN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
12	Z	165	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	$\#\|Z\| > 2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	GAU	g	4	14,15	8,8,8	1.74	2 (25%)	8,9,9	1.90	3 (37%)
15	GAU	e	4	11,15	8,8,8	1.15	1 (12%)	8,9,9	1.61	2 (25%)
15	GAU	f	4	14,15	8,8,8	1.44	1 (12%)	8,9,9	1.67	2 (25%)
15	GAU	c	4	8,15	8,8,8	1.07	0	8,9,9	1.82	3 (37%)
15	GAU	d	4	11,15	8,8,8	1.49	1 (12%)	8,9,9	1.37	0
15	GAU	h	4	8,15	8,8,8	1.29	2 (25%)	8,9,9	1.52	2 (25%)

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	GAU	g	4	14,15	-	1/7/7/7	-
15	GAU	e	4	11,15	-	0/7/7/7	-
15	GAU	f	4	14,15	-	2/7/7/7	-
15	GAU	c	4	8,15	-	0/7/7/7	-
15	GAU	d	4	11,15	-	0/7/7/7	-
15	GAU	h	4	8,15	-	2/7/7/7	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	4	GAU	CB-CA	-3.49	1.48	1.53
15	h	4	GAU	O-C	-2.71	1.31	1.42
15	f	4	GAU	OE2-CD	-2.51	1.22	1.30
15	g	4	GAU	OE2-CD	-2.47	1.22	1.30
15	e	4	GAU	CG-CD	2.18	1.55	1.50
15	d	4	GAU	OE2-CD	-2.06	1.23	1.30
15	h	4	GAU	OE2-CD	-2.00	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c	4	GAU	CG-CB-CA	-3.56	105.27	112.74
15	f	4	GAU	CG-CB-CA	-3.16	106.10	112.74
15	g	4	GAU	CB-CA-N	-3.14	99.91	109.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	g	4	GAU	CG-CB-CA	-3.07	106.28	112.74
15	e	4	GAU	CG-CB-CA	-3.03	106.37	112.74
15	h	4	GAU	CB-CA-N	-2.42	102.01	109.03
15	f	4	GAU	CB-CA-N	-2.21	102.62	109.03
15	e	4	GAU	CB-CA-C	-2.19	109.26	112.25
15	c	4	GAU	OE1-CD-CG	-2.14	116.21	123.08
15	h	4	GAU	OE1-CD-CG	-2.09	116.36	123.08
15	g	4	GAU	OE1-CD-CG	-2.07	116.43	123.08
15	c	4	GAU	CB-CA-C	-2.04	109.46	112.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	h	4	GAU	C-CA-CB-CG
15	f	4	GAU	O-C-CA-CB
15	f	4	GAU	O-C-CA-N
15	h	4	GAU	N-CA-CB-CG
15	g	4	GAU	OE2-CD-CG-CB

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, 9 are monoatomic - leaving 4 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	2.21	1 (8%)	14,16,16	1.34	2 (14%)
18	MES	Y	301	-	12,12,12	2.25	1 (8%)	14,16,16	1.35	2 (14%)
18	MES	H	302	-	12,12,12	2.25	1 (8%)	14,16,16	1.35	2 (14%)
18	MES	V	301	-	12,12,12	2.30	1 (8%)	14,16,16	1.26	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	Y	301	-	-	0/6/14/14	0/1/1/1
18	MES	H	302	-	-	5/6/14/14	0/1/1/1
18	MES	V	301	-	-	0/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	301	MES	C8-S	-7.69	1.66	1.77
18	H	302	MES	C8-S	-7.51	1.66	1.77
18	Y	301	MES	C8-S	-7.50	1.66	1.77
18	K	302	MES	C8-S	-7.36	1.67	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	302	MES	O2S-S-C8	3.10	110.65	106.92
18	K	302	MES	O3S-S-C8	2.98	110.58	105.77
18	V	301	MES	O2S-S-C8	2.72	110.20	106.92
18	Y	301	MES	O2S-S-C8	2.72	110.19	106.92
18	Y	301	MES	O3S-S-C8	2.60	109.97	105.77
18	V	301	MES	O3S-S-C8	2.43	109.69	105.77
18	H	302	MES	O3S-S-C8	2.29	109.48	105.77
18	K	302	MES	O2S-S-C8	2.14	109.49	106.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	H	302	MES	C7-C8-S-O2S
18	H	302	MES	C7-C8-S-O3S
18	H	302	MES	C8-C7-N4-C5
18	H	302	MES	C7-C8-S-O1S
18	H	302	MES	C8-C7-N4-C3

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.10	8 (3%)	47	48	32, 45, 81, 121	0
1	O	250/250 (100%)	0.02	13 (5%)	27	25	37, 53, 97, 126	0
2	B	244/258 (94%)	0.08	16 (6%)	18	16	33, 50, 100, 154	0
2	P	244/258 (94%)	0.15	16 (6%)	18	16	37, 54, 106, 155	0
3	C	240/254 (94%)	0.20	22 (9%)	9	7	32, 54, 117, 155	0
3	Q	240/254 (94%)	0.48	32 (13%)	3	2	43, 70, 151, 195	0
4	D	235/260 (90%)	-0.05	6 (2%)	56	57	38, 57, 89, 136	0
4	R	235/260 (90%)	0.10	8 (3%)	45	45	43, 61, 99, 145	0
5	E	231/234 (98%)	0.11	11 (4%)	30	28	40, 60, 95, 137	0
5	S	231/234 (98%)	0.33	12 (5%)	27	25	42, 69, 113, 152	0
6	F	243/288 (84%)	-0.05	9 (3%)	41	41	38, 56, 104, 138	0
6	T	243/288 (84%)	0.15	18 (7%)	14	12	38, 63, 114, 152	0
7	G	241/252 (95%)	-0.11	11 (4%)	32	31	32, 47, 88, 139	0
7	U	241/252 (95%)	-0.12	7 (2%)	51	52	35, 49, 84, 128	0
8	H	222/232 (95%)	-0.27	3 (1%)	75	77	30, 41, 69, 107	0
8	V	222/232 (95%)	-0.24	4 (1%)	68	70	31, 45, 69, 112	0
9	I	204/205 (99%)	-0.45	3 (1%)	73	76	28, 42, 68, 93	0
9	W	204/205 (99%)	-0.43	2 (0%)	82	83	29, 42, 72, 99	0
10	J	195/198 (98%)	-0.34	4 (2%)	63	65	29, 42, 68, 118	0
10	X	195/198 (98%)	-0.26	4 (2%)	63	65	33, 45, 69, 122	0
11	K	212/212 (100%)	-0.27	3 (1%)	75	77	33, 46, 72, 87	0
11	Y	212/212 (100%)	-0.17	4 (1%)	66	69	35, 48, 79, 105	0
12	L	222/222 (100%)	-0.36	2 (0%)	84	85	29, 45, 72, 98	0
12	Z	222/222 (100%)	-0.30	2 (0%)	84	85	31, 45, 74, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.35	3 (1%)	77	78	27, 43, 63, 75	0
13	a	233/246 (94%)	-0.34	4 (1%)	70	72	30, 41, 63, 73	0
14	N	196/196 (100%)	-0.37	4 (2%)	65	67	28, 39, 65, 92	0
14	b	196/196 (100%)	-0.38	1 (0%)	91	92	30, 40, 68, 90	0
15	c	2/5 (40%)	-0.46	0	100	100	45, 45, 45, 48	0
15	d	2/5 (40%)	-0.55	0	100	100	63, 63, 63, 67	0
15	e	2/5 (40%)	-0.38	0	100	100	67, 67, 67, 73	0
15	f	2/5 (40%)	-0.60	0	100	100	48, 48, 48, 57	0
15	g	2/5 (40%)	-0.43	0	100	100	44, 44, 44, 51	0
15	h	2/5 (40%)	-0.74	0	100	100	47, 47, 47, 54	0
All	All	6348/6644 (95%)	-0.11	232 (3%)	41	41	27, 49, 95, 195	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	9.4
2	P	222	GLY	8.7
2	B	218	GLY	8.3
3	Q	50	LEU	7.8
5	S	202	ASP	7.8
2	B	219	ALA	7.5
2	P	219	ALA	7.0
2	P	51	VAL	6.0
4	R	241	ALA	5.6
3	C	205	ALA	5.4
3	Q	49	THR	5.4
3	Q	206	LYS	5.3
3	Q	239	GLN	5.3
6	F	244	ASN	5.3
3	C	206	LYS	5.2
6	T	243	ILE	5.1
2	B	51	VAL	5.0
1	O	1	MET	5.0
7	U	2	GLY	5.0
3	C	240	GLU	4.9
9	W	1	SER	4.9
2	B	221	ASP	4.9
10	X	1	MET	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	242	GLY	4.8
2	B	220	ASN	4.7
2	P	221	ASP	4.7
1	O	201	GLU	4.5
13	M	47	ASP	4.5
3	Q	236	GLN	4.5
5	E	201	ARG	4.5
7	G	240	ALA	4.5
6	T	244	ASN	4.3
14	N	105	LYS	4.3
3	C	49	THR	4.3
3	Q	240	GLU	4.3
10	X	194	ASP	4.3
3	Q	229	GLN	4.2
7	U	242	GLN	4.2
1	O	249	ALA	4.1
5	S	180	LYS	4.0
3	Q	203	THR	4.0
4	D	1	ASP	3.9
8	V	221	CYS	3.9
2	P	52	THR	3.9
5	S	233	ILE	3.9
6	T	178	HIS	3.8
7	U	241	GLU	3.8
3	C	238	LYS	3.8
8	H	222	ASP	3.8
2	B	59	ASP	3.8
10	J	194	ASP	3.7
3	Q	48	SER	3.7
6	T	201	GLU	3.6
5	E	202	ASP	3.6
2	B	217	LYS	3.6
2	P	220	ASN	3.6
3	C	180	LYS	3.5
3	C	203	THR	3.5
9	I	1	SER	3.5
6	T	241	LYS	3.5
5	S	3	ASN	3.5
3	Q	180	LYS	3.5
6	T	181	GLU	3.5
6	T	180	PRO	3.5
2	P	59	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
3	Q	55	THR	3.4
3	Q	205	ALA	3.4
7	G	188	GLU	3.4
8	V	222	ASP	3.4
5	S	54	GLU	3.4
1	O	248	GLU	3.4
3	Q	204	GLY	3.4
6	F	205	GLU	3.4
3	C	1	GLY	3.3
6	F	178	HIS	3.3
4	R	242	GLU	3.3
2	P	218	GLY	3.3
7	G	3	TYR	3.3
4	R	177	ASN	3.3
3	Q	220	VAL	3.3
1	O	203	GLU	3.3
2	P	203	SER	3.2
10	J	193	ASP	3.2
5	S	173	ARG	3.2
8	H	221	CYS	3.2
3	C	225	GLU	3.1
6	T	29	ASN	3.1
5	E	233	ILE	3.1
1	O	2	THR	3.1
6	F	201	GLU	3.1
10	X	193	ASP	3.1
4	D	242	GLU	3.1
5	S	51	ASN	3.1
7	G	179	LYS	3.1
3	Q	225	GLU	3.1
2	P	240	LYS	3.1
3	Q	202	GLN	3.1
2	B	180	LYS	3.0
11	K	151	GLU	3.0
13	M	1	THR	3.0
9	I	192	ASP	3.0
13	a	1	THR	3.0
4	R	125	LEU	3.0
7	G	241	GLU	3.0
2	P	50	LYS	3.0
9	W	133	LYS	3.0
11	K	147	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
6	T	2	THR	2.9
5	S	207	VAL	2.9
3	C	236	GLN	2.9
4	R	230	GLU	2.9
6	F	243	ILE	2.9
6	F	229	GLY	2.9
1	A	54	PRO	2.9
1	A	201	GLU	2.8
3	C	239	GLN	2.8
5	E	122	TYR	2.8
1	O	250	LEU	2.8
1	O	169	VAL	2.8
12	Z	172	LEU	2.8
3	Q	171	GLU	2.7
11	Y	212	GLY	2.7
1	A	2	THR	2.7
3	Q	201	VAL	2.7
3	C	223	SER	2.7
3	Q	58	THR	2.7
7	U	222	ASP	2.7
4	D	241	ALA	2.7
4	R	141	ALA	2.7
3	C	181	GLU	2.7
6	T	207	ASP	2.7
5	E	4	ASN	2.6
6	T	230	ASP	2.6
1	O	52	SER	2.6
7	U	3	TYR	2.6
12	Z	210	ASP	2.6
1	A	51	SER	2.6
2	B	182	ASP	2.6
14	N	195	GLN	2.6
6	T	229	GLY	2.6
6	F	2	THR	2.6
6	T	215	CYS	2.6
5	E	176	ASP	2.6
1	O	141	GLU	2.6
11	Y	106	ARG	2.6
10	J	1	MET	2.6
1	O	231	LYS	2.6
3	Q	223	SER	2.6
3	C	59	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	238	LYS	2.5
1	A	229	THR	2.5
11	Y	202	GLU	2.5
6	T	202	ASP	2.5
7	G	208	GLU	2.5
3	Q	172	PHE	2.5
12	L	165	ASN	2.5
13	M	82	ASP	2.5
6	T	204	LYS	2.4
4	R	54	ASP	2.4
2	B	232	GLN	2.4
7	G	2	GLY	2.4
2	P	182	ASP	2.4
11	K	212	GLY	2.4
1	A	249	ALA	2.4
5	E	52	ALA	2.4
3	Q	141	ASP	2.4
3	Q	234	ILE	2.4
3	Q	181	GLU	2.4
5	E	3	ASN	2.4
3	C	187	GLU	2.4
6	T	166	GLN	2.4
5	E	218	ASP	2.3
5	S	29	LYS	2.3
6	T	53	LYS	2.3
7	G	180	SER	2.3
12	L	167	LYS	2.3
2	P	244	THR	2.3
3	Q	51	LYS	2.3
7	G	53	LYS	2.3
2	P	53	SER	2.3
4	D	169	GLU	2.3
1	O	61	LEU	2.3
3	C	60	SER	2.3
5	E	123	GLY	2.3
3	Q	221	ALA	2.3
14	b	105	LYS	2.3
3	Q	237	GLU	2.3
2	B	239	VAL	2.3
3	Q	187	GLU	2.3
3	C	50	LEU	2.3
6	F	204	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	61	SER	2.3
6	F	166	GLN	2.3
3	C	27	ARG	2.3
8	V	217	ILE	2.3
3	C	175	LYS	2.2
3	Q	238	LYS	2.2
3	Q	235	GLU	2.2
2	B	52	THR	2.2
7	U	203	ASP	2.2
1	O	62	SER	2.2
3	Q	27	ARG	2.2
3	C	232	THR	2.2
3	Q	231	VAL	2.2
4	R	217	GLN	2.2
5	E	194	GLU	2.2
9	I	133	LYS	2.2
13	a	73	GLU	2.2
2	P	62	THR	2.2
5	S	225	ASP	2.2
7	G	68	ARG	2.2
2	B	54	THR	2.1
13	a	204	THR	2.1
5	S	165	GLN	2.1
14	N	181	ALA	2.1
3	C	48	SER	2.1
7	U	181	LYS	2.1
7	G	181	LYS	2.1
13	a	47	ASP	2.1
1	A	248	GLU	2.1
8	V	145	ASP	2.1
10	J	95	ARG	2.1
5	S	210	LEU	2.1
10	X	95	ARG	2.1
2	P	225	TYR	2.1
3	C	235	GLU	2.1
8	H	198	GLU	2.1
2	B	50	LYS	2.1
4	D	2	ARG	2.1
11	Y	39	PRO	2.0
14	N	9	LYS	2.0
6	T	217	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	GAU	e	4	9/9	0.88	0.20	66,71,76,78	0
15	GAU	g	4	9/9	0.93	0.16	46,49,51,51	0
15	GAU	d	4	9/9	0.94	0.15	53,63,70,70	0
15	GAU	c	4	9/9	0.95	0.16	50,53,60,60	0
15	GAU	h	4	9/9	0.95	0.13	47,54,63,64	0
15	GAU	f	4	9/9	0.96	0.14	49,54,55,57	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	H	301	1/1	0.45	0.24	62,62,62,62	0
18	MES	V	301	12/12	0.88	0.30	72,109,123,125	0
18	MES	H	302	12/12	0.89	0.33	62,98,113,113	0
18	MES	K	302	12/12	0.90	0.29	66,83,84,85	0
18	MES	Y	301	12/12	0.90	0.30	71,81,85,86	0
16	MG	K	301	1/1	0.94	0.10	51,51,51,51	0
17	CL	U	301	1/1	0.95	0.12	33,33,33,33	0
16	MG	I	302	1/1	0.96	0.17	56,56,56,56	0
16	MG	G	301	1/1	0.97	0.10	42,42,42,42	0
16	MG	N	201	1/1	0.98	0.08	42,42,42,42	0
16	MG	L	301	1/1	0.98	0.05	42,42,42,42	0
17	CL	G	302	1/1	0.99	0.04	39,39,39,39	0
16	MG	I	301	1/1	0.99	0.08	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.