Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2023 – 08:47 am GMT

PDB ID	:	4YA2
Title	:	Yeast 20S proteasome beta2-H116N 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 (1)) were used in the production of this report:

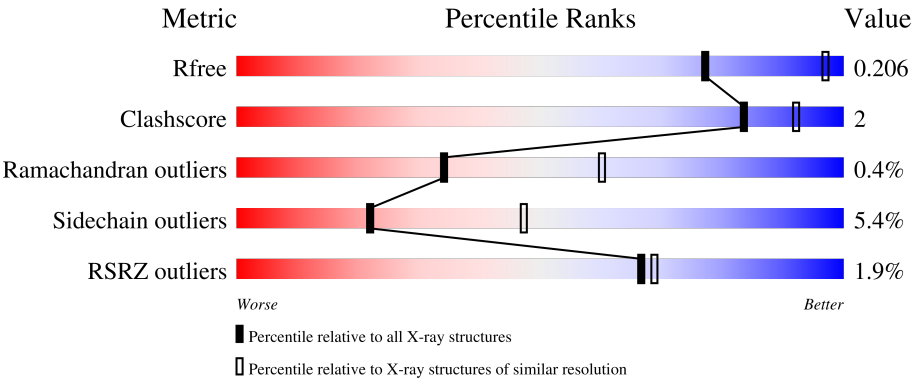
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2% 94% 6%
1	O	250	2% 94% 6%
2	B	258	3% 81% 13% • 5%
2	P	258	4% 83% 11% • 5%
3	C	254	5% 82% 9% • 6%

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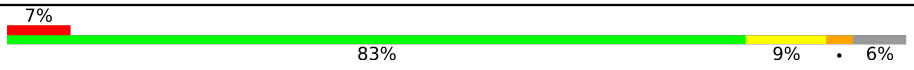
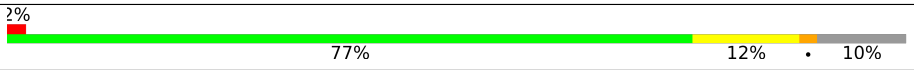
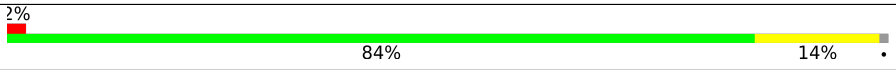
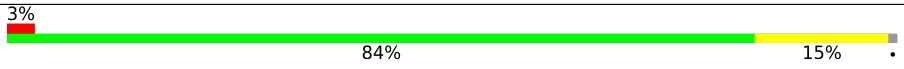
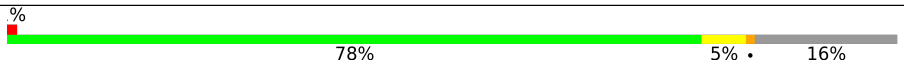
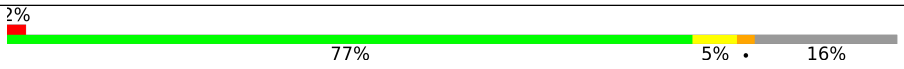
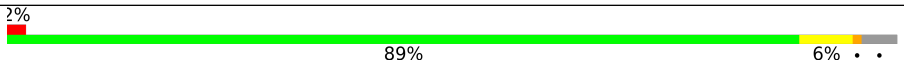
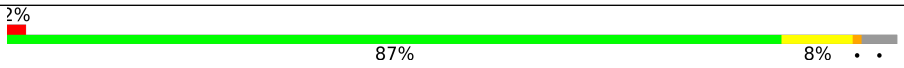
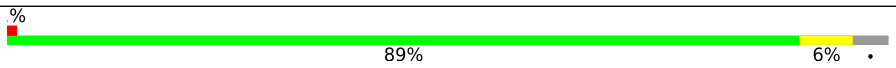
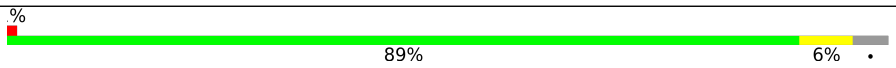
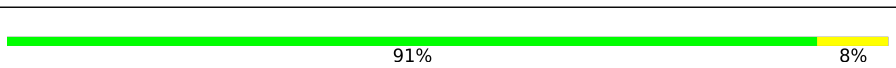
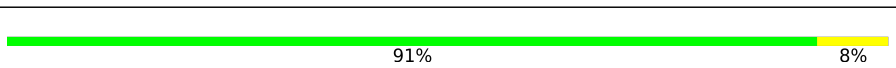
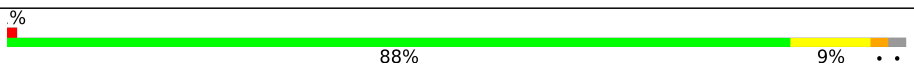
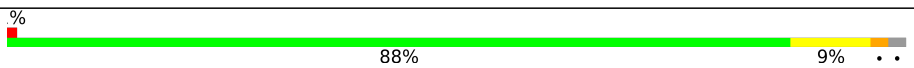
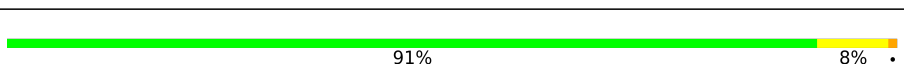
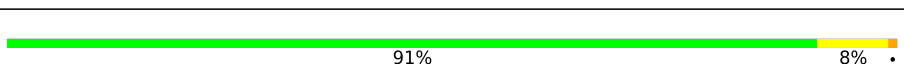
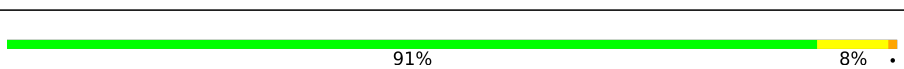
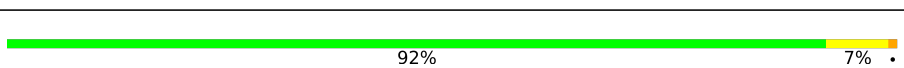
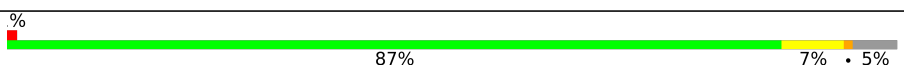
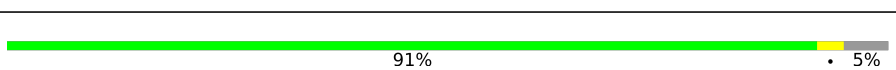
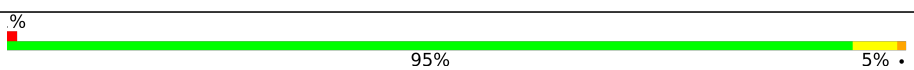
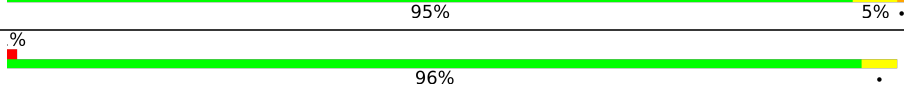
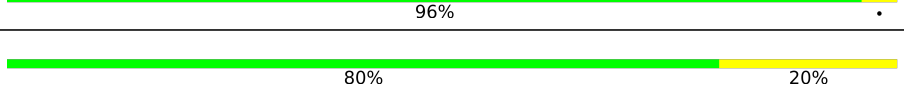
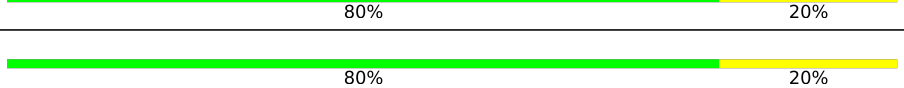
Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	c	5	
15	d	5	

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Mol	Chain	Length	Quality of chain
15	e	5	80% 20%
15	f	5	80% 20%
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 50225 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
			1682	1059	292	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1682	1059	292	324	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	116	ASN	HIS	engineered mutation	UNP P25043
V	116	ASN	HIS	engineered mutation	UNP P25043

- 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			
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	1	0
			1764	1120	305	335	4			
12	Z	222	Total	C	N	O	S	0	1	0
			1764	1120	305	335	4			

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

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

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

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

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

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

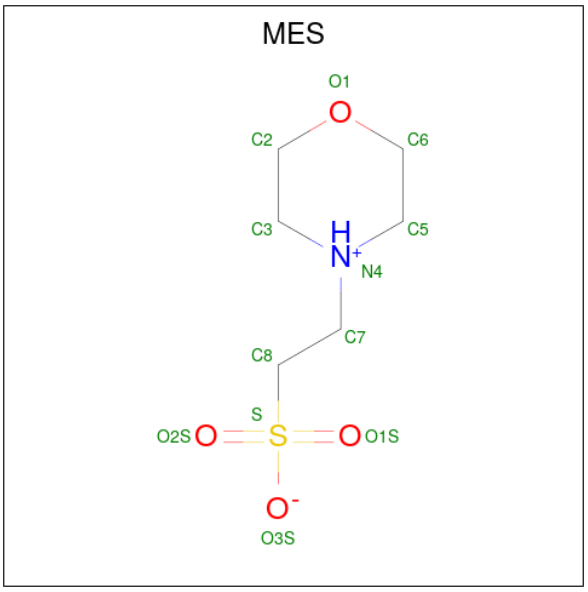
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	H	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

- 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	U	1	Total Cl 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	1	Total C N O S 12 6 1 4 1	0	0
18	V	1	Total C N O S 12 6 1 4 1	0	0
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	27	Total O 27 27	0	0
19	B	29	Total O 29 29	0	0
19	C	25	Total O 25 25	0	0
19	D	11	Total O 11 11	0	0
19	E	7	Total O 7 7	0	0
19	F	21	Total O 21 21	0	0
19	G	34	Total O 34 34	0	0
19	H	39	Total O 39 39	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	I	35	Total O 35 35	0	0
19	J	26	Total O 26 26	0	0
19	K	30	Total O 30 30	0	0
19	L	31	Total O 31 31	0	0
19	M	28	Total O 28 28	0	0
19	N	27	Total O 27 27	0	0
19	O	18	Total O 18 18	0	0
19	P	17	Total O 17 17	0	0
19	Q	9	Total O 9 9	0	0
19	R	9	Total O 9 9	0	0
19	S	7	Total O 7 7	0	0
19	T	18	Total O 18 18	0	0
19	U	25	Total O 25 25	0	0
19	V	33	Total O 33 33	0	0
19	W	24	Total O 24 24	0	0
19	X	31	Total O 31 31	0	0
19	Y	22	Total O 22 22	0	0
19	Z	23	Total O 23 23	0	0
19	a	41	Total O 41 41	0	0
19	b	32	Total O 32 32	0	0
19	c	1	Total O 1 1	0	0

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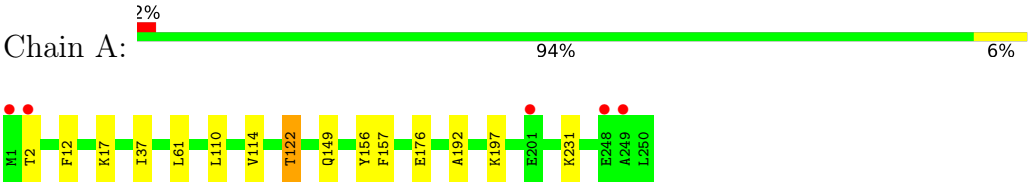
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	d	1	Total O 1 1	0	0
19	e	3	Total O 3 3	0	0
19	g	2	Total O 2 2	0	0
19	h	2	Total O 2 2	0	0

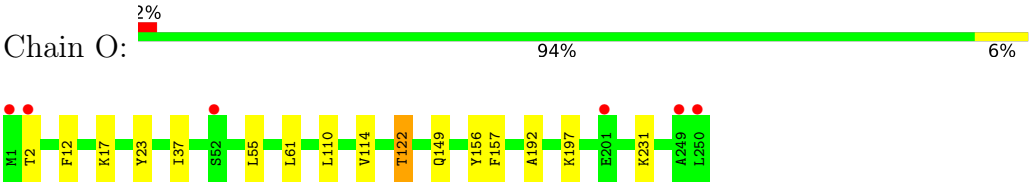
3 Residue-property plots (i)

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

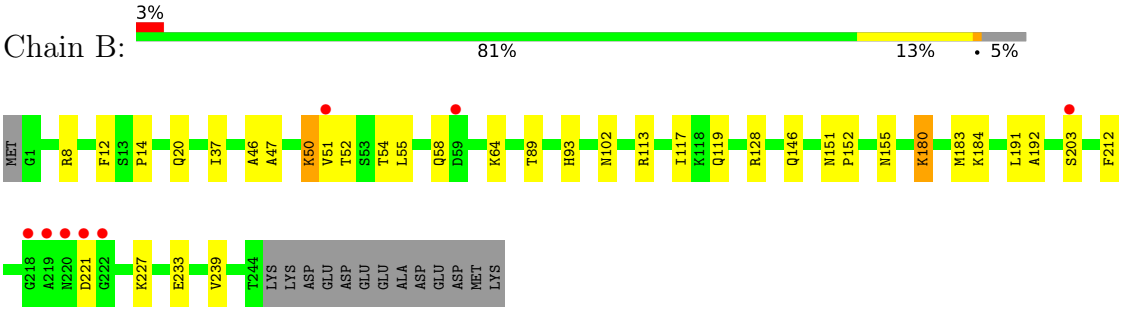
• Molecule 1: Proteasome subunit alpha type-2



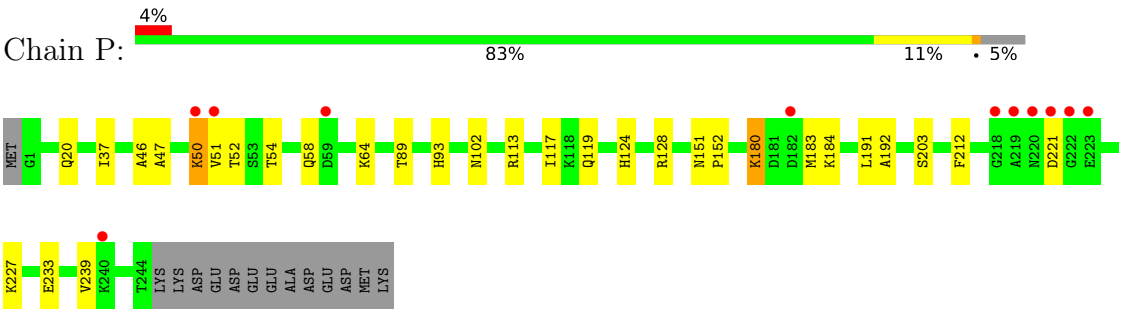
• Molecule 1: Proteasome subunit alpha type-2



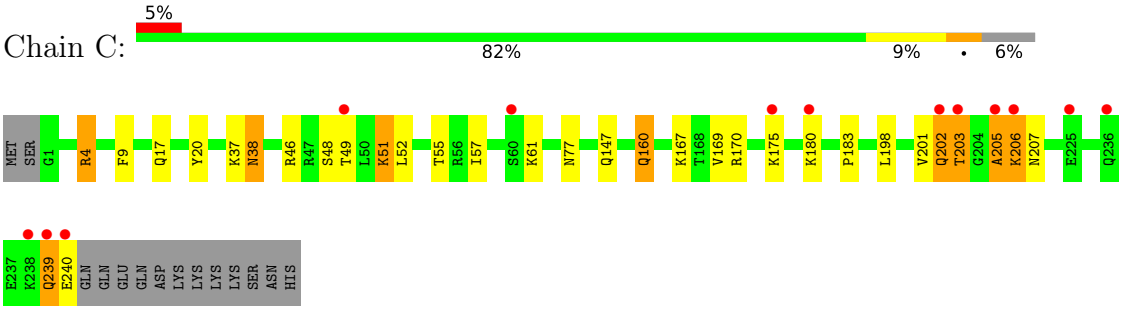
• Molecule 2: Proteasome subunit alpha type-3



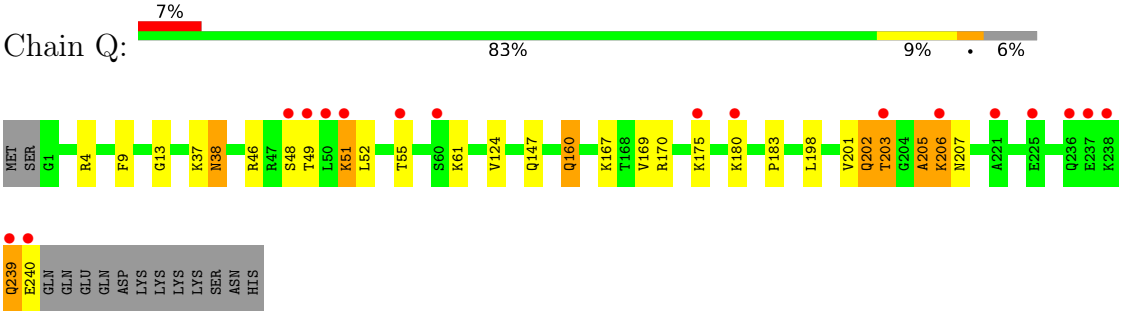
• Molecule 2: Proteasome subunit alpha type-3



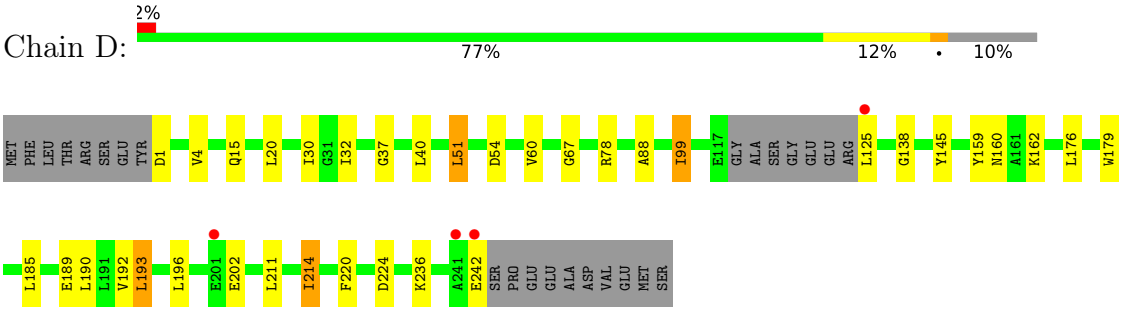
• Molecule 3: Proteasome subunit alpha type-4



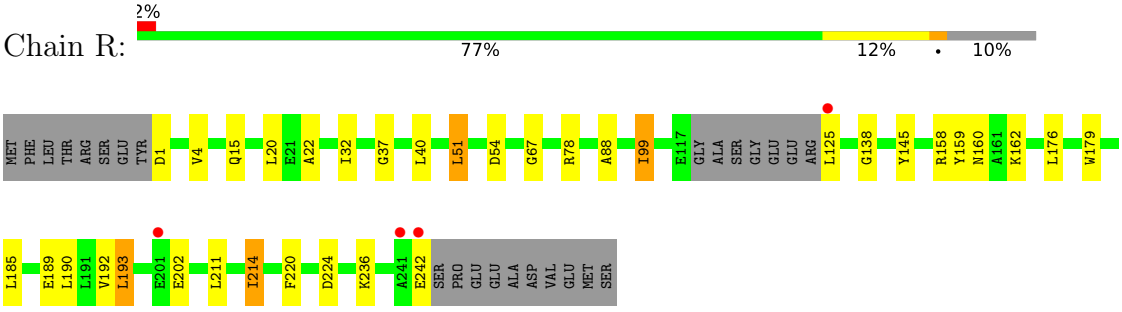
• Molecule 3: Proteasome subunit alpha type-4



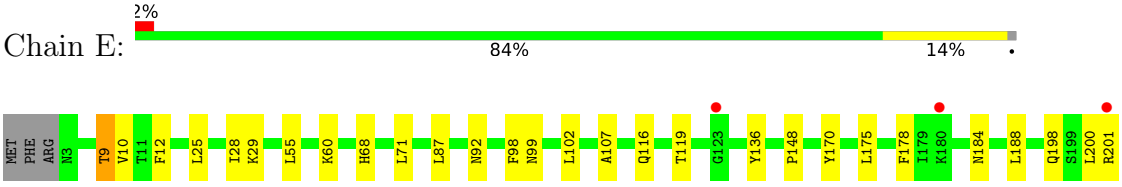
• Molecule 4: Proteasome subunit alpha type-5

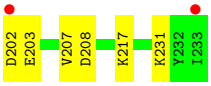


• Molecule 4: Proteasome subunit alpha type-5

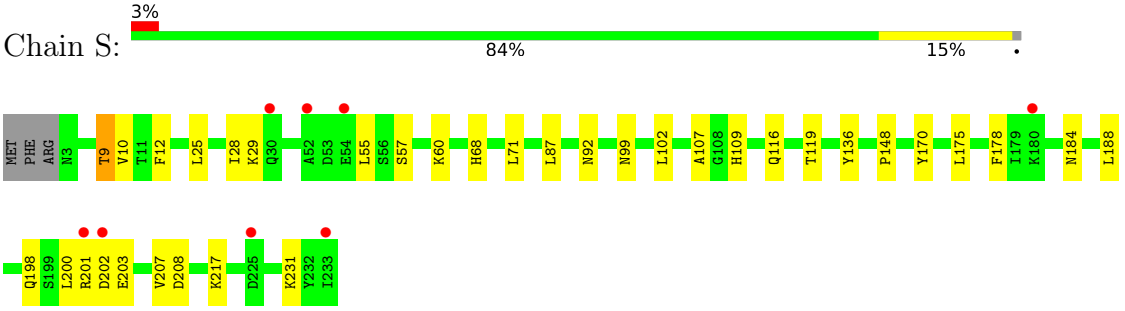


• Molecule 5: Proteasome subunit alpha type-6

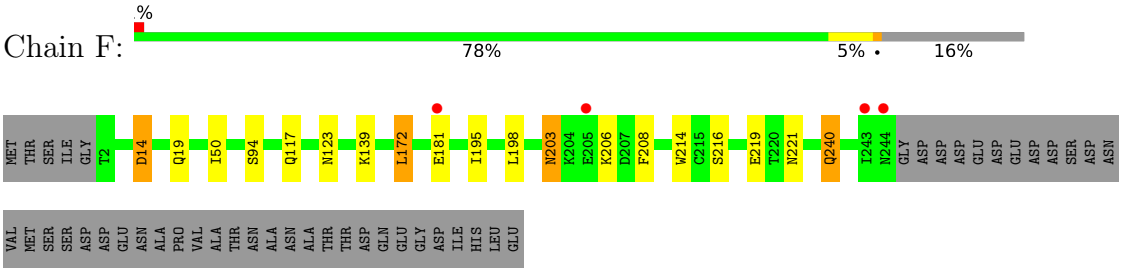




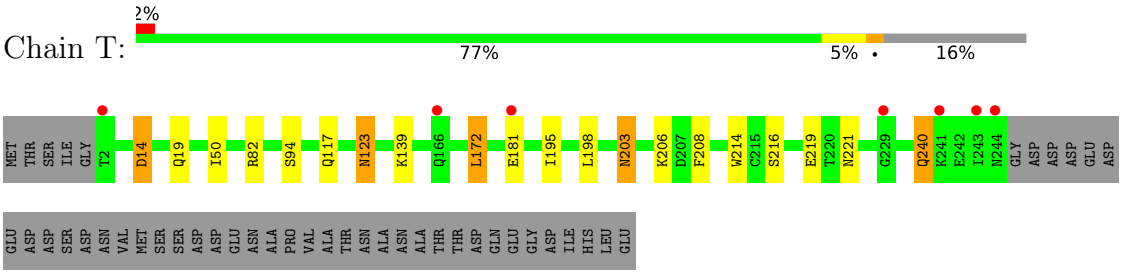
• Molecule 5: Proteasome subunit alpha type-6



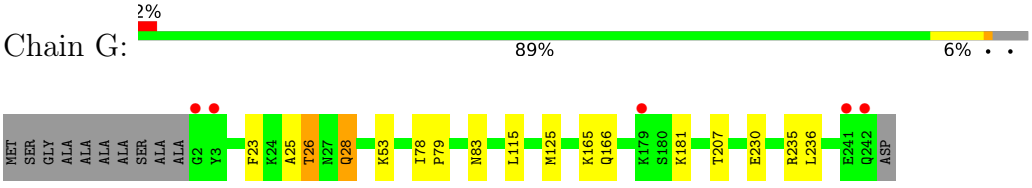
• Molecule 6: Probable proteasome subunit alpha type-7



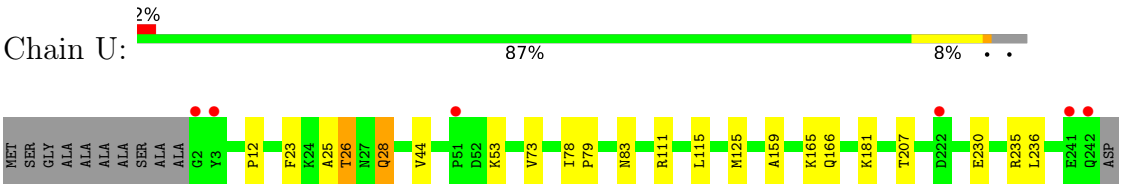
• Molecule 6: Probable proteasome subunit alpha type-7



• Molecule 7: Proteasome subunit alpha type-1

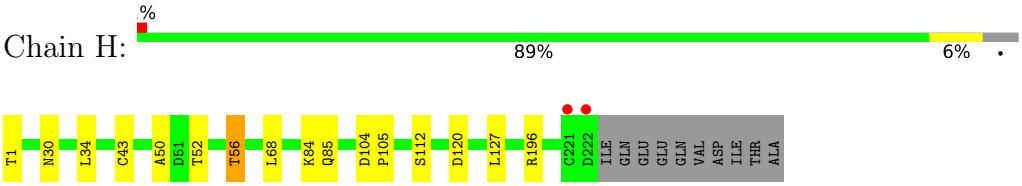


• Molecule 7: Proteasome subunit alpha type-1



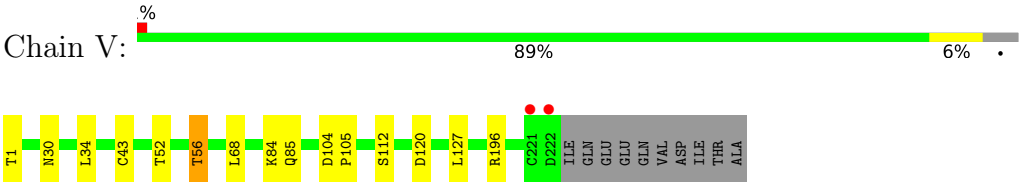
• Molecule 8: Proteasome subunit beta type-2

Chain H:



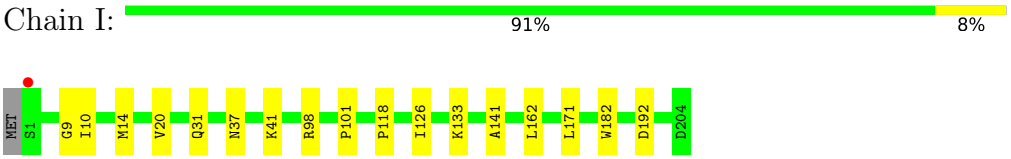
• Molecule 8: Proteasome subunit beta type-2

Chain V:



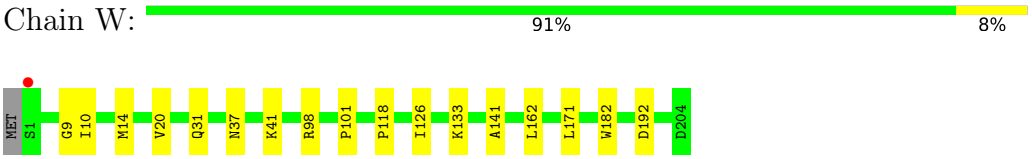
• Molecule 9: Proteasome subunit beta type-3

Chain I:



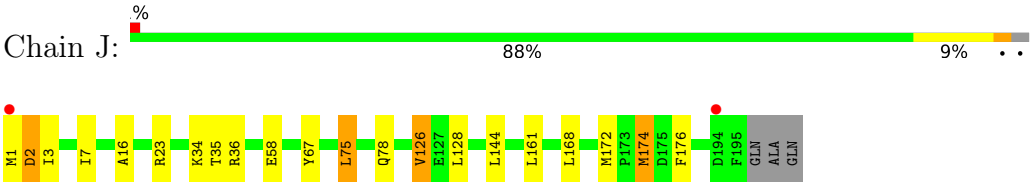
• Molecule 9: Proteasome subunit beta type-3

Chain W:



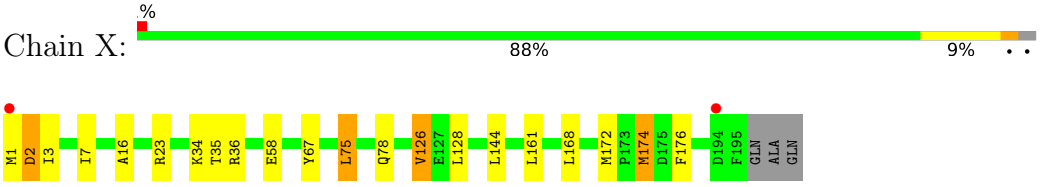
• Molecule 10: Proteasome subunit beta type-4

Chain J:



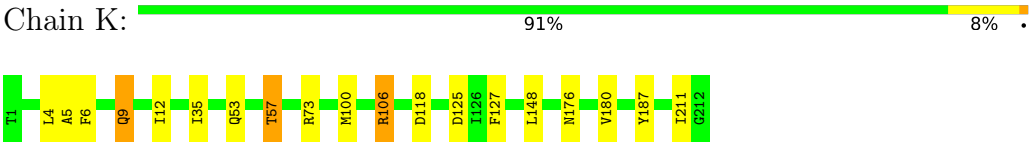
• Molecule 10: Proteasome subunit beta type-4

Chain X:



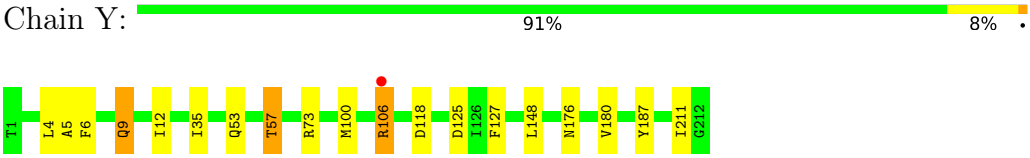
• Molecule 11: Proteasome subunit beta type-5

Chain K:



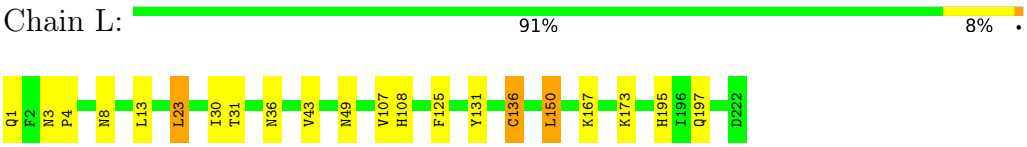
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



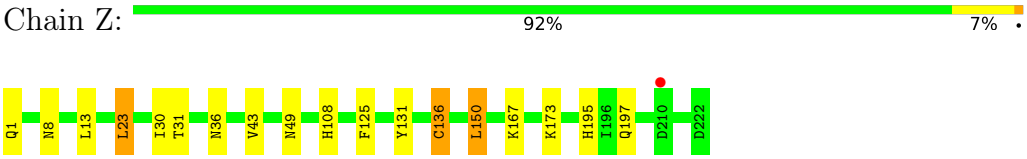
• Molecule 12: Proteasome subunit beta type-6

Chain L:



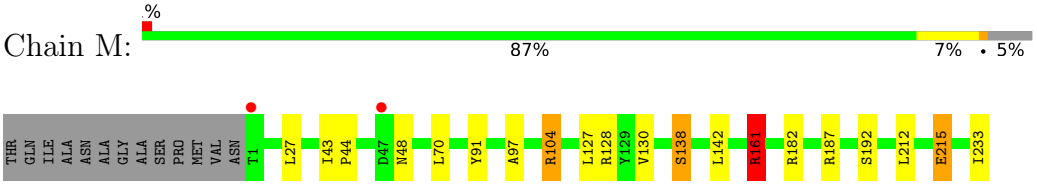
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



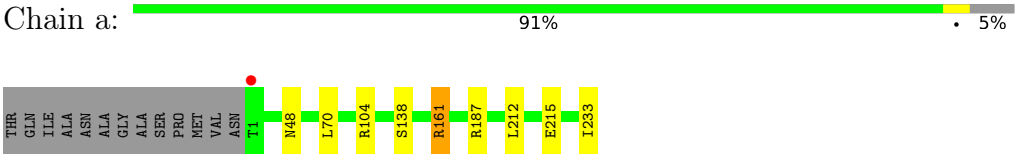
• Molecule 13: Proteasome subunit beta type-7

Chain M:



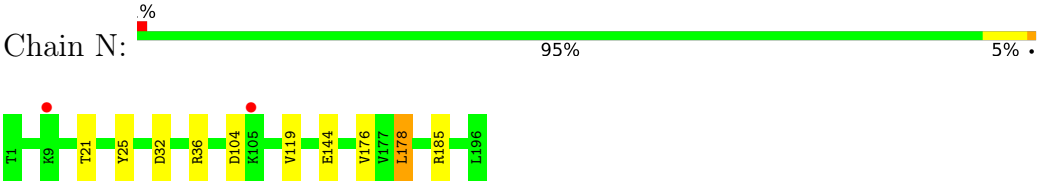
• Molecule 13: Proteasome subunit beta type-7

Chain a:



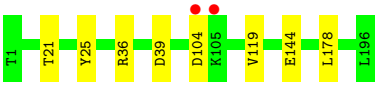
• Molecule 14: Proteasome subunit beta type-1

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	135.20Å 300.04Å 145.13Å 90.00° 113.14° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.6 (15.00-2.70) 95.6 (15.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.205 0.188 , 0.206	Depositor DCC
R_{free} test set	13782 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50225	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 2.56% 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: ACE, MES, CL, POL, MG, GAU

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	0.28	0/1952	0.51	0/2642
1	O	0.28	0/1952	0.51	0/2642
2	B	0.27	0/1934	0.55	0/2618
2	P	0.27	0/1934	0.55	0/2618
3	C	0.29	0/1910	0.56	0/2586
3	Q	0.28	0/1910	0.56	0/2586
4	D	0.28	0/1837	0.55	1/2475 (0.0%)
4	R	0.28	0/1837	0.55	1/2475 (0.0%)
5	E	0.28	0/1800	0.53	0/2433
5	S	0.27	0/1800	0.53	0/2433
6	F	0.28	0/1932	0.50	0/2609
6	T	0.28	0/1932	0.49	0/2609
7	G	0.28	0/1945	0.53	0/2634
7	U	0.28	0/1945	0.52	0/2634
8	H	0.29	0/1712	0.53	1/2322 (0.0%)
8	V	0.29	0/1712	0.52	1/2322 (0.0%)
9	I	0.27	0/1611	0.52	0/2174
9	W	0.27	0/1611	0.52	0/2174
10	J	0.27	0/1589	0.53	0/2142
10	X	0.27	0/1589	0.53	0/2142
11	K	0.27	0/1681	0.54	0/2274
11	Y	0.27	0/1681	0.55	0/2274
12	L	0.38	2/1806 (0.1%)	0.61	4/2435 (0.2%)
12	Z	0.32	0/1806	0.57	0/2435
13	M	0.28	0/1855	0.56	1/2514 (0.0%)
13	a	0.28	0/1855	0.56	1/2514 (0.0%)
14	N	0.78	4/1541 (0.3%)	0.57	3/2087 (0.1%)
14	b	0.77	4/1541 (0.3%)	0.57	3/2087 (0.1%)
15	c	0.53	0/13	1.20	0/17
15	d	0.48	0/13	1.12	0/17
15	e	0.31	0/13	1.10	0/17
15	f	0.54	0/13	1.19	0/17

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	g	0.49	0/13	1.13	0/17
15	h	0.32	0/13	1.12	0/17
All	All	0.34	10/50288 (0.0%)	0.54	16/67992 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	25	TYR	CE1-CZ	-16.72	1.16	1.38
14	b	25	TYR	CE1-CZ	-16.42	1.17	1.38
14	b	25	TYR	CG-CD2	-14.41	1.20	1.39
14	N	25	TYR	CG-CD2	-14.25	1.20	1.39
14	N	25	TYR	CG-CD1	-13.93	1.21	1.39
14	b	25	TYR	CG-CD1	-13.64	1.21	1.39
14	b	25	TYR	CE2-CZ	-12.38	1.22	1.38
14	N	25	TYR	CE2-CZ	-12.26	1.22	1.38
12	L	108[A]	HIS	CA-C	6.81	1.70	1.52
12	L	108[B]	HIS	CA-C	6.81	1.70	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	108[A]	HIS	CA-C-O	7.51	135.87	120.10
12	L	108[B]	HIS	CA-C-O	7.51	135.87	120.10
12	L	108[A]	HIS	CA-C-N	-5.83	104.38	117.20
12	L	108[B]	HIS	CA-C-N	-5.83	104.38	117.20
13	M	161	ARG	NE-CZ-NH1	5.80	123.20	120.30
13	a	161	ARG	NE-CZ-NH1	5.62	123.11	120.30
14	b	25	TYR	CB-CG-CD1	5.50	124.30	121.00
14	N	25	TYR	CD1-CE1-CZ	5.50	124.75	119.80
14	b	25	TYR	CD1-CE1-CZ	5.33	124.60	119.80
8	H	1	THR	N-CA-C	5.25	125.18	111.00
8	V	1	THR	N-CA-C	5.20	125.04	111.00
14	N	25	TYR	CD1-CG-CD2	-5.16	112.22	117.90
14	N	25	TYR	CB-CG-CD2	5.16	124.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	25	TYR	CD1-CG-CD2	-5.14	112.25	117.90
4	R	51	LEU	CA-CB-CG	5.03	126.88	115.30
4	D	51	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	107	VAL	Peptide

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	8	0
2	B	1904	0	1904	18	0
2	P	1904	0	1904	15	0
3	C	1881	0	1895	20	0
3	Q	1881	0	1895	15	0
4	D	1813	0	1797	11	0
4	R	1813	0	1797	12	0
5	E	1773	0	1775	12	0
5	S	1773	0	1775	13	0
6	F	1892	0	1883	7	0
6	T	1892	0	1883	9	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	7	0
8	H	1682	0	1684	5	0
8	V	1682	0	1684	4	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	10	0
11	K	1644	0	1592	9	0
11	Y	1644	0	1592	9	0
12	L	1764	0	1718	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1764	0	1718	8	0
13	M	1824	0	1832	9	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	2	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	1	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
18	c	12	0	13	0	0
19	A	27	0	0	0	0
19	B	29	0	0	0	0
19	C	25	0	0	0	0
19	D	11	0	0	0	0
19	E	7	0	0	0	0
19	F	21	0	0	0	0
19	G	34	0	0	0	0
19	H	39	0	0	0	0
19	I	35	0	0	0	0
19	J	26	0	0	0	0
19	K	30	0	0	0	0
19	L	31	0	0	0	0
19	M	28	0	0	0	0
19	N	27	0	0	0	0
19	O	18	0	0	0	0
19	P	17	0	0	0	0
19	Q	9	0	0	0	0
19	R	9	0	0	0	0
19	S	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	T	18	0	0	0	0
19	U	25	0	0	0	0
19	V	33	0	0	0	0
19	W	24	0	0	0	0
19	X	31	0	0	0	0
19	Y	22	0	0	0	0
19	Z	23	0	0	0	0
19	a	41	0	0	0	0
19	b	32	0	0	0	0
19	c	1	0	0	0	0
19	d	1	0	0	0	0
19	e	3	0	0	0	0
19	g	2	0	0	0	0
19	h	2	0	0	0	0
All	All	50225	0	49294	220	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 (220) 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:100:MET:HE3	11:K:127:PHE:HB2	1.60	0.82
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.62	0.81
11:K:53:GLN:O	11:K:57:THR:HG23	1.86	0.76
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.85	0.75
11:K:100:MET:CE	11:K:127:PHE:HB2	2.19	0.72
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.19	0.72
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.57	0.70
3:C:51:LYS:O	3:C:52:LEU:HB2	1.92	0.70
3:C:202:GLN:HG3	3:C:203:THR:H	1.57	0.68
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.92	0.68
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.59	0.67
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.59	0.67
11:Y:106:ARG:HH11	11:Y:106:ARG:HB3	1.63	0.63
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.81	0.63
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.81	0.62
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.81	0.62
11:K:106:ARG:HH11	11:K:106:ARG:HB3	1.64	0.61
7:G:23:PHE:O	7:G:26:THR:HB	2.01	0.61
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:23:PHE:O	7:U:26:THR:HB	2.00	0.60
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.84	0.60
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.83	0.60
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.83	0.59
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.66	0.59
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.67	0.58
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.85	0.58
2:P:50:LYS:HE3	2:P:50:LYS:HA	1.87	0.57
5:S:9:THR:HG21	5:S:119:THR:HA	1.86	0.57
2:B:50:LYS:HE3	2:B:50:LYS:HA	1.87	0.56
2:B:12:PHE:H	3:C:17:GLN:HE22	1.52	0.56
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.88	0.56
5:E:9:THR:HG21	5:E:119:THR:HA	1.86	0.55
5:S:12:PHE:H	6:T:19:GLN:HE22	1.54	0.55
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.88	0.55
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.88	0.55
4:R:185:LEU:O	4:R:189:GLU:HG3	2.06	0.55
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.55	0.55
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.06	0.54
3:C:201:VAL:O	3:C:202:GLN:HB2	2.07	0.54
4:D:185:LEU:O	4:D:189:GLU:HG3	2.07	0.54
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.73	0.54
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.38	0.54
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.38	0.54
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.91	0.53
5:E:12:PHE:H	6:F:19:GLN:HE22	1.57	0.53
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.91	0.53
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.89	0.52
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.72	0.52
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.23	0.51
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.92	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.51
12:L:8:ASN:HA	12:L:30:ILE:O	2.10	0.51
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.93	0.51
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.58	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
3:C:202:GLN:HG3	3:C:203:THR:N	2.23	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
7:G:25:ALA:O	7:G:28:GLN:HB2	2.11	0.50
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.42	0.50
7:U:25:ALA:O	7:U:28:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.42	0.50
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.11	0.50
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.47	0.50
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.47	0.50
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.93	0.50
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.42	0.49
1:A:37:ILE:HD12	1:A:192:ALA:HB2	1.94	0.49
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.58	0.49
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.94	0.49
8:H:52:THR:O	8:H:56:THR:HB	2.12	0.49
1:O:37:ILE:HD12	1:O:192:ALA:HB2	1.94	0.49
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.42	0.49
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.94	0.49
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.95	0.49
10:J:174:MET:HA	10:X:174:MET:HA	1.94	0.49
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.77	0.49
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.95	0.48
6:T:14:ASP:OD2	6:T:14:ASP:N	2.43	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.95	0.48
5:S:201:ARG:C	5:S:203:GLU:H	2.17	0.48
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.95	0.48
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.95	0.48
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.95	0.48
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.44	0.48
8:V:52:THR:O	8:V:56:THR:HB	2.14	0.48
5:E:170:TYR:HB2	5:E:198:GLN:HG3	1.95	0.48
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.29	0.48
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.96	0.47
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.96	0.47
2:B:227:LYS:NZ	2:B:233:GLU:OE2	2.48	0.47
5:E:201:ARG:C	5:E:203:GLU:H	2.17	0.47
5:S:170:TYR:HB2	5:S:198:GLN:HG3	1.95	0.47
6:F:14:ASP:OD2	6:F:14:ASP:N	2.43	0.47
2:P:227:LYS:NZ	2:P:233:GLU:OE2	2.48	0.47
8:V:84:LYS:HG3	8:V:85:GLN:N	2.28	0.47
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.48	0.47
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.48	0.47
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.97	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.50	0.46
8:H:84:LYS:HG3	8:H:85:GLN:N	2.28	0.46
4:R:158:ARG:HB3	5:S:57:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.51	0.46
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.98	0.46
2:B:37:ILE:HD12	2:B:192:ALA:HB2	1.98	0.46
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.98	0.46
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.98	0.46
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.46	0.46
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.96	0.46
1:O:55:LEU:HB3	7:U:159:ALA:O	2.14	0.46
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.46	0.46
3:C:201:VAL:HG13	3:C:202:GLN:N	2.32	0.45
2:P:37:ILE:HD12	2:P:192:ALA:HB2	1.99	0.45
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.50	0.45
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.82	0.45
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.51	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.51	0.45
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.32	0.45
2:B:155:ASN:ND2	3:C:77:ASN:HB2	2.32	0.45
3:C:9:PHE:H	4:D:15:GLN:HE22	1.64	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.45
14:N:32:ASP:OD2	14:N:185:ARG:NH2	2.50	0.45
9:W:14:MET:HB3	9:W:162:LEU:HD11	1.97	0.45
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.46	0.45
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.50	0.45
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.46	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
3:C:205:ALA:C	3:C:207:ASN:H	2.20	0.44
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.97	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.98	0.44
1:O:12:PHE:H	2:P:20:GLN:HE22	1.64	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.44
12:L:195:HIS:HD2	12:L:197:GLN:H	1.66	0.44
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.30	0.44
3:Q:205:ALA:C	3:Q:207:ASN:H	2.20	0.44
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.33	0.44
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.82	0.44
6:F:172:LEU:HD13	6:F:195:ILE:HD13	2.00	0.43
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.53	0.43
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.58	0.43
6:T:172:LEU:HD13	6:T:195:ILE:HD13	2.00	0.43
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:GLN:CG	3:C:203:THR:H	2.30	0.43
9:I:98:ARG:O	9:I:126:ILE:HD11	2.19	0.43
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.01	0.43
2:B:46:ALA:HB2	2:B:212:PHE:CE1	2.54	0.43
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.54	0.43
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.59	0.43
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.65	0.43
10:J:7:ILE:HD12	10:J:161:LEU:HD13	2.00	0.43
12:L:4:PRO:O	13:M:104:ARG:NH1	2.47	0.43
2:P:46:ALA:HB2	2:P:212:PHE:CE1	2.54	0.43
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.01	0.43
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.30	0.43
10:X:1:MET:HA	10:X:34:LYS:CE	2.49	0.43
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.53	0.42
11:K:5:ALA:HB3	11:K:100:MET:CE	2.49	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
4:R:159:TYR:CZ	4:R:162:LYS:HD3	2.54	0.42
10:X:7:ILE:HD12	10:X:161:LEU:HD13	2.00	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.42
4:D:159:TYR:CZ	4:D:162:LYS:HD3	2.55	0.42
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.42
10:J:168:LEU:O	10:J:172:MET:HB2	2.20	0.42
7:U:111:ARG:NH1	17:U:301:CL:CL	2.87	0.42
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.49	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.42
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.54	0.42
1:A:110:LEU:O	1:A:114:VAL:HG23	2.20	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.42
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.53	0.42
5:E:201:ARG:O	5:E:203:GLU:N	2.52	0.42
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.55	0.42
10:J:1:MET:HA	10:J:34:LYS:CE	2.49	0.42
3:Q:46:ARG:NH1	3:Q:206:LYS:O	2.53	0.42
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.94	0.42
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.42
2:B:180:LYS:O	2:B:183:MET:HB2	2.20	0.41
11:K:12:ILE:HB	11:K:180:VAL:HB	2.01	0.41
3:Q:13:GLY:O	4:R:22:ALA:HB2	2.19	0.41
5:E:68:HIS:HE1	5:E:102:LEU:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.01	0.41
10:X:168:LEU:O	10:X:172:MET:HB2	2.20	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
3:C:46:ARG:NH1	3:C:206:LYS:O	2.53	0.41
4:R:67:GLY:HA3	4:R:220:PHE:CD1	2.55	0.41
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.34	0.41
6:F:50:ILE:HG13	6:F:208:PHE:HA	2.02	0.41
8:H:112:SER:OG	8:H:120:ASP:HB2	2.20	0.41
3:C:38:ASN:N	3:C:38:ASN:HD22	2.19	0.41
13:M:182:ARG:NH2	13:M:215:GLU:O	2.50	0.41
5:S:200:LEU:O	5:S:201:ARG:HG2	2.21	0.41
7:U:44:VAL:HG21	7:U:73:VAL:HG11	2.03	0.41
2:P:180:LYS:O	2:P:183:MET:HB2	2.21	0.41
1:A:12:PHE:H	2:B:20:GLN:HE22	1.67	0.41
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.03	0.41
4:D:67:GLY:HA3	4:D:220:PHE:CD1	2.56	0.41
4:D:193:LEU:HD22	4:D:211:LEU:HD11	2.02	0.41
5:E:200:LEU:O	5:E:201:ARG:HG2	2.21	0.41
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.55	0.41
5:S:201:ARG:O	5:S:203:GLU:N	2.52	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.41
8:V:112:SER:OG	8:V:120:ASP:HB2	2.20	0.41
5:E:98:PHE:O	13:M:91:TYR:HA	2.21	0.40
11:K:6:PHE:HA	11:K:125:ASP:O	2.21	0.40
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.86	0.40
2:P:93:HIS:HB3	2:P:113:ARG:NH2	2.35	0.40
6:T:123:ASN:HD22	6:T:123:ASN:C	2.25	0.40
9:W:98:ARG:O	9:W:126:ILE:HD11	2.20	0.40
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.21	0.40
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.40
3:Q:38:ASN:HD22	3:Q:38:ASN:N	2.19	0.40
1:O:110:LEU:O	1:O:114:VAL:HG23	2.21	0.40
4:R:193:LEU:HD22	4:R:211:LEU:HD11	2.02	0.40
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.87	0.40
5:S:68:HIS:HE1	5:S:102:LEU:O	2.04	0.40
6:T:50:ILE:HG13	6:T:208:PHE:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	13	32
2	P	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	13	32
3	C	238/254 (94%)	229 (96%)	4 (2%)	5 (2%)	7	18
3	Q	238/254 (94%)	229 (96%)	4 (2%)	5 (2%)	7	18
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%)	216 (94%)	11 (5%)	2 (1%)	17	40
5	S	229/234 (98%)	216 (94%)	11 (5%)	2 (1%)	17	40
6	F	241/288 (84%)	234 (97%)	6 (2%)	1 (0%)	34	60
6	T	241/288 (84%)	234 (97%)	6 (2%)	1 (0%)	34	60
7	G	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
7	U	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (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%)	202 (96%)	6 (3%)	2 (1%)	15	37
11	Y	210/212 (99%)	202 (96%)	6 (3%)	2 (1%)	15	37
12	L	221/222 (100%)	215 (97%)	6 (3%)	0	100	100
12	Z	221/222 (100%)	215 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (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
15	h	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6290/6644 (95%)	6086 (97%)	176 (3%)	28 (0%)	34	60

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	52	THR
3	C	202	GLN
2	P	51	VAL
2	P	52	THR
3	Q	202	GLN
3	C	205	ALA
3	C	206	LYS
3	C	239	GLN
3	Q	205	ALA
3	Q	206	LYS
3	Q	239	GLN
2	B	221	ASP
5	E	231	LYS
10	J	2	ASP
11	K	9	GLN
2	P	221	ASP
5	S	231	LYS
10	X	2	ASP
11	Y	9	GLN
5	E	202	ASP
6	F	203	ASN
5	S	202	ASP
6	T	203	ASN
3	Q	183	PRO

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Mol	Chain	Res	Type
3	C	183	PRO
11	K	211	ILE
11	Y	211	ILE

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%)	202 (97%)	7 (3%)	38	67
1	O	209/209 (100%)	202 (97%)	7 (3%)	38	67
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	52
2	P	203/216 (94%)	193 (95%)	10 (5%)	25	52
3	C	212/226 (94%)	195 (92%)	17 (8%)	12	27
3	Q	212/226 (94%)	195 (92%)	17 (8%)	12	27
4	D	194/215 (90%)	176 (91%)	18 (9%)	9	21
4	R	194/215 (90%)	177 (91%)	17 (9%)	10	23
5	E	190/193 (98%)	176 (93%)	14 (7%)	13	32
5	S	190/193 (98%)	176 (93%)	14 (7%)	13	32
6	F	201/239 (84%)	188 (94%)	13 (6%)	17	38
6	T	201/239 (84%)	188 (94%)	13 (6%)	17	38
7	G	206/210 (98%)	193 (94%)	13 (6%)	18	40
7	U	206/210 (98%)	193 (94%)	13 (6%)	18	40
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%)	165 (95%)	8 (5%)	27	54
10	X	173/175 (99%)	165 (95%)	8 (5%)	27	54
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26 54
12	L	186/185 (100%)	179 (96%)	7 (4%)	33 62
12	Z	186/185 (100%)	177 (95%)	9 (5%)	25 53
13	M	199/208 (96%)	190 (96%)	9 (4%)	27 55
13	a	199/208 (96%)	190 (96%)	9 (4%)	27 55
14	N	162/162 (100%)	156 (96%)	6 (4%)	34 63
14	b	162/162 (100%)	155 (96%)	7 (4%)	29 57
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	5320/5546 (96%)	5032 (95%)	288 (5%)	22 47

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	197	LYS
1	A	231	LYS
2	B	50	LYS
2	B	54	THR
2	B	58	GLN
2	B	102	ASN
2	B	119	GLN
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	203	SER
2	B	239	VAL
3	C	4	ARG
3	C	37	LYS

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Mol	Chain	Res	Type
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	51	LYS
3	C	55	THR
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	203	THR
3	C	239	GLN
3	C	240	GLU
4	D	1	ASP
4	D	4	VAL
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	60	VAL
4	D	78	ARG
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	60	LYS
5	E	71	LEU
5	E	92	ASN
5	E	99	ASN

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Mol	Chain	Res	Type
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
6	F	14	ASP
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	198	LEU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	28	GLN
7	G	53	LYS
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	165	LYS
7	G	166	GLN
7	G	181	LYS
7	G	207	THR
7	G	230	GLU
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	31	GLN
9	I	37	ASN
9	I	133	LYS
9	I	171	LEU

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Mol	Chain	Res	Type
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	126	VAL
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	57	THR
11	K	73	ARG
11	K	106	ARG
11	K	118	ASP
11	K	148	LEU
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
12	L	173	LYS
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	212	LEU
13	M	215	GLU
13	M	233	ILE
14	N	21	THR
14	N	36	ARG
14	N	104	ASP
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	17	LYS

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Mol	Chain	Res	Type
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	197	LYS
1	O	231	LYS
2	P	50	LYS
2	P	54	THR
2	P	58	GLN
2	P	102	ASN
2	P	119	GLN
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	203	SER
2	P	239	VAL
3	Q	4	ARG
3	Q	37	LYS
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	51	LYS
3	Q	55	THR
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	167	LYS
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	203	THR
3	Q	239	GLN
3	Q	240	GLU
4	R	1	ASP
4	R	4	VAL
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	54	ASP
4	R	78	ARG
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU

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Mol	Chain	Res	Type
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
4	R	224	ASP
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	55	LEU
5	S	60	LYS
5	S	71	LEU
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
6	T	14	ASP
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	198	LEU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	28	GLN
7	U	53	LYS
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	165	LYS
7	U	166	GLN

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Mol	Chain	Res	Type
7	U	181	LYS
7	U	207	THR
7	U	230	GLU
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
8	V	127	LEU
8	V	196	ARG
9	W	31	GLN
9	W	37	ASN
9	W	133	LYS
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	126	VAL
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	73	ARG
11	Y	106	ARG
11	Y	118	ASP
11	Y	148	LEU
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	108[A]	HIS
12	Z	108[B]	HIS
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS

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Mol	Chain	Res	Type
12	Z	173	LYS
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	138	SER
13	a	161	ARG
13	a	187	ARG
13	a	212	LEU
13	a	215	GLU
13	a	233	ILE
14	b	21	THR
14	b	36	ARG
14	b	39	ASP
14	b	104	ASP
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	102	ASN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	100	ASN
4	D	225	ASN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN

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Mol	Chain	Res	Type
5	E	116	GLN
5	E	118	ASN
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	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	186	ASN
8	H	30	ASN
8	H	66	HIS
8	H	172	ASN
8	H	189	ASN
9	I	31	GLN
10	J	55	GLN
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	158	ASN
12	L	165	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
14	N	38	HIS
14	N	69	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN

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Mol	Chain	Res	Type
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	100	ASN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	186	ASN
8	V	30	ASN
8	V	66	HIS
8	V	172	ASN
8	V	189	ASN
9	W	31	GLN
10	X	55	GLN
10	X	86	GLN

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Mol	Chain	Res	Type
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	158	ASN
12	Z	165	ASN
12	Z	195	HIS
13	a	2	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
14	b	38	HIS
14	b	69	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	$\#\|Z\| > 2$
15	GAU	f	4	8,15	8,8,8	1.07	0	8,9,9	1.81	2 (25%)
15	GAU	e	4	14,15	8,8,8	1.05	0	8,9,9	1.80	1 (12%)
15	GAU	h	4	14,15	8,8,8	1.09	0	8,9,9	1.77	1 (12%)
15	GAU	c	4	8,15	8,8,8	1.10	0	8,9,9	1.82	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	GAU	g	4	11,15	8,8,8	1.13	1 (12%)	8,9,9	1.74	2 (25%)
15	GAU	d	4	11,15	8,8,8	1.11	1 (12%)	8,9,9	1.75	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	f	4	8,15	-	3/7/7/7	-
15	GAU	e	4	14,15	-	2/7/7/7	-
15	GAU	h	4	14,15	-	4/7/7/7	-
15	GAU	c	4	8,15	-	3/7/7/7	-
15	GAU	g	4	11,15	-	0/7/7/7	-
15	GAU	d	4	11,15	-	0/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	4	GAU	CG-CD	2.25	1.55	1.50
15	d	4	GAU	CG-CD	2.22	1.55	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	e	4	GAU	CG-CB-CA	-4.07	104.18	112.74
15	h	4	GAU	CG-CB-CA	-4.01	104.31	112.74
15	c	4	GAU	CG-CB-CA	-3.68	105.01	112.74
15	f	4	GAU	CG-CB-CA	-3.66	105.04	112.74
15	d	4	GAU	CG-CB-CA	-3.39	105.61	112.74
15	g	4	GAU	CG-CB-CA	-3.37	105.66	112.74
15	d	4	GAU	CB-CA-C	-2.40	108.97	112.25
15	g	4	GAU	CB-CA-C	-2.38	109.00	112.25
15	c	4	GAU	OE1-CD-CG	-2.13	116.23	123.08
15	f	4	GAU	OE1-CD-CG	-2.12	116.28	123.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	GAU	C-CA-CB-CG
15	f	4	GAU	C-CA-CB-CG
15	e	4	GAU	OE2-CD-CG-CB
15	h	4	GAU	OE2-CD-CG-CB
15	h	4	GAU	OE1-CD-CG-CB
15	e	4	GAU	OE1-CD-CG-CB
15	h	4	GAU	O-C-CA-CB
15	h	4	GAU	O-C-CA-N
15	c	4	GAU	OE1-CD-CG-CB
15	c	4	GAU	N-CA-CB-CG
15	f	4	GAU	N-CA-CB-CG
15	f	4	GAU	OE1-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	V	301	-	12,12,12	2.24	1 (8%)	14,16,16	1.22	3 (21%)
18	MES	c	101	-	12,12,12	2.18	1 (8%)	14,16,16	1.45	1 (7%)
18	MES	Y	301	-	12,12,12	2.23	1 (8%)	14,16,16	1.24	2 (14%)
18	MES	K	302	-	12,12,12	2.24	1 (8%)	14,16,16	1.37	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	V	301	-	-	5/6/14/14	0/1/1/1
18	MES	c	101	-	-	4/6/14/14	0/1/1/1
18	MES	Y	301	-	-	0/6/14/14	0/1/1/1
18	MES	K	302	-	-	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	-7.47	1.66	1.77
18	K	302	MES	C8-S	-7.46	1.66	1.77
18	Y	301	MES	C8-S	-7.44	1.66	1.77
18	c	101	MES	C8-S	-7.23	1.67	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	c	101	MES	O2S-S-C8	4.13	111.89	106.92
18	Y	301	MES	O2S-S-C8	2.65	110.10	106.92
18	K	302	MES	O3S-S-C8	2.48	109.78	105.77
18	Y	301	MES	O3S-S-C8	2.38	109.61	105.77
18	V	301	MES	O2S-S-C8	2.29	109.68	106.92
18	V	301	MES	O3S-S-C8	2.25	109.41	105.77
18	K	302	MES	O2S-S-C8	2.25	109.62	106.92
18	V	301	MES	O1S-S-C8	2.21	109.57	106.92

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	V	301	MES	C7-C8-S-O1S
18	c	101	MES	N4-C7-C8-S
18	V	301	MES	C7-C8-S-O3S
18	V	301	MES	C8-C7-N4-C5
18	c	101	MES	C7-C8-S-O3S
18	V	301	MES	C7-C8-S-O2S
18	c	101	MES	C7-C8-S-O1S
18	c	101	MES	C7-C8-S-O2S
18	V	301	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

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%)	-0.41	5 (2%)	65	67	37, 53, 85, 125	0
1	O	250/250 (100%)	-0.34	6 (2%)	59	60	36, 60, 100, 133	0
2	B	244/258 (94%)	-0.28	8 (3%)	46	46	37, 58, 109, 152	0
2	P	244/258 (94%)	-0.24	11 (4%)	33	31	39, 60, 108, 147	0
3	C	240/254 (94%)	-0.14	13 (5%)	25	24	40, 62, 117, 145	0
3	Q	240/254 (94%)	0.01	17 (7%)	16	14	44, 73, 145, 159	0
4	D	235/260 (90%)	-0.41	4 (1%)	70	72	40, 61, 96, 129	0
4	R	235/260 (90%)	-0.28	4 (1%)	70	72	46, 67, 100, 140	0
5	E	231/234 (98%)	-0.23	5 (2%)	62	63	44, 67, 99, 154	0
5	S	231/234 (98%)	-0.17	8 (3%)	44	44	44, 75, 115, 160	0
6	F	243/288 (84%)	-0.42	4 (1%)	72	74	38, 59, 106, 135	0
6	T	243/288 (84%)	-0.33	7 (2%)	51	52	39, 68, 118, 154	0
7	G	241/252 (95%)	-0.42	5 (2%)	63	65	35, 53, 89, 136	0
7	U	241/252 (95%)	-0.38	6 (2%)	57	59	37, 56, 88, 113	0
8	H	222/232 (95%)	-0.55	2 (0%)	84	85	35, 49, 77, 111	0
8	V	222/232 (95%)	-0.52	2 (0%)	84	85	34, 52, 76, 117	0
9	I	204/205 (99%)	-0.69	1 (0%)	91	92	35, 50, 77, 102	0
9	W	204/205 (99%)	-0.62	1 (0%)	91	92	31, 50, 79, 106	0
10	J	195/198 (98%)	-0.53	2 (1%)	82	83	35, 51, 78, 125	0
10	X	195/198 (98%)	-0.53	2 (1%)	82	83	38, 52, 78, 135	0
11	K	212/212 (100%)	-0.55	0	100	100	35, 50, 79, 107	0
11	Y	212/212 (100%)	-0.53	1 (0%)	91	92	39, 55, 84, 111	0
12	L	222/222 (100%)	-0.60	0	100	100	34, 53, 78, 92	0
12	Z	222/222 (100%)	-0.53	1 (0%)	91	92	34, 53, 84, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.58	2 (0%) 84 85	33, 51, 70, 83	0
13	a	233/246 (94%)	-0.58	1 (0%) 92 93	34, 50, 70, 79	0
14	N	196/196 (100%)	-0.63	2 (1%) 82 83	34, 46, 72, 101	0
14	b	196/196 (100%)	-0.61	2 (1%) 82 83	33, 48, 74, 95	0
15	c	2/5 (40%)	-1.19	0 100 100	43, 43, 43, 49	0
15	d	2/5 (40%)	-0.73	0 100 100	44, 44, 44, 45	0
15	e	2/5 (40%)	-0.69	0 100 100	43, 43, 43, 50	0
15	f	2/5 (40%)	-0.87	0 100 100	50, 50, 50, 51	0
15	g	2/5 (40%)	-0.43	0 100 100	54, 54, 54, 62	0
15	h	2/5 (40%)	-0.79	0 100 100	40, 40, 40, 51	0
All	All	6348/6644 (95%)	-0.42	122 (1%) 66 69	31, 56, 99, 160	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	206	LYS	7.0
3	Q	50	LEU	6.9
2	P	219	ALA	6.4
5	S	202	ASP	6.0
2	P	51	VAL	5.6
2	B	219	ALA	5.5
5	E	202	ASP	5.4
8	V	222	ASP	5.3
2	P	222	GLY	5.2
2	B	51	VAL	5.0
3	Q	49	THR	5.0
3	C	238	LYS	4.8
1	A	1	MET	4.8
2	B	220	ASN	4.6
1	O	249	ALA	4.6
2	P	218	GLY	4.6
3	Q	206	LYS	4.3
2	P	220	ASN	4.2
6	F	244	ASN	4.2
2	B	222	GLY	4.1
8	V	221	CYS	4.0
3	C	49	THR	4.0
7	G	242	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
2	P	59	ASP	3.8
10	X	194	ASP	3.8
3	Q	48	SER	3.8
6	T	244	ASN	3.6
8	H	221	CYS	3.6
6	F	205	GLU	3.6
7	G	2	GLY	3.5
3	Q	240	GLU	3.5
2	B	221	ASP	3.5
9	I	1	SER	3.4
13	a	1	THR	3.4
13	M	1	THR	3.3
4	R	241	ALA	3.2
2	P	221	ASP	3.2
3	Q	203	THR	3.2
3	Q	236	GLN	3.2
1	O	52	SER	3.1
2	B	203	SER	3.1
3	Q	238	LYS	3.1
4	D	242	GLU	3.1
3	Q	239	GLN	3.1
8	H	222	ASP	3.1
1	O	1	MET	3.0
4	R	242	GLU	3.0
6	T	243	ILE	2.9
1	A	2	THR	2.8
2	B	218	GLY	2.8
3	C	205	ALA	2.8
5	S	52	ALA	2.8
6	T	241	LYS	2.8
3	Q	225	GLU	2.8
5	S	54	GLU	2.7
7	U	242	GLN	2.7
7	G	241	GLU	2.7
10	J	194	ASP	2.7
3	C	203	THR	2.7
4	R	125	LEU	2.6
1	O	201	GLU	2.6
9	W	1	SER	2.6
2	P	182	ASP	2.6
3	Q	221	ALA	2.6
4	D	241	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
13	M	47	ASP	2.5
7	G	3	TYR	2.5
1	A	248	GLU	2.5
3	Q	175	LYS	2.5
4	R	201	GLU	2.5
10	J	1	MET	2.5
5	E	180	LYS	2.5
7	U	2	GLY	2.5
6	T	166	GLN	2.4
1	O	2	THR	2.4
3	C	175	LYS	2.4
6	T	181	GLU	2.4
5	E	233	ILE	2.4
11	Y	106	ARG	2.4
2	P	50	LYS	2.4
2	P	223	GLU	2.4
5	S	233	ILE	2.4
14	N	105	LYS	2.4
6	F	243	ILE	2.4
3	Q	237	GLU	2.4
2	B	59	ASP	2.4
6	T	229	GLY	2.4
1	A	201	GLU	2.3
3	C	240	GLU	2.3
7	G	179	LYS	2.3
3	C	225	GLU	2.3
7	U	241	GLU	2.3
14	N	9	LYS	2.3
3	Q	60	SER	2.3
6	T	2	THR	2.3
12	Z	210	ASP	2.3
5	E	123	GLY	2.3
1	A	249	ALA	2.3
3	C	236	GLN	2.2
6	F	181	GLU	2.2
5	S	225	ASP	2.2
5	E	201	ARG	2.2
7	U	222	ASP	2.2
5	S	201	ARG	2.2
7	U	3	TYR	2.2
14	b	105	LYS	2.1
3	C	202	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
5	S	30	GLN	2.1
3	C	60	SER	2.1
3	Q	55	THR	2.1
3	C	180	LYS	2.1
3	Q	51	LYS	2.1
10	X	1	MET	2.1
4	D	201	GLU	2.1
1	O	250	LEU	2.1
5	S	180	LYS	2.1
14	b	104	ASP	2.1
3	C	239	GLN	2.0
2	P	240	LYS	2.0
4	D	125	LEU	2.0
7	U	51	PRO	2.0
3	Q	180	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	GAU	h	4	9/9	0.92	0.16	41,45,50,57	0
15	GAU	g	4	9/9	0.93	0.14	40,60,64,64	0
15	GAU	e	4	9/9	0.93	0.16	43,44,52,53	0
15	GAU	c	4	9/9	0.94	0.14	41,54,58,58	0
15	GAU	d	4	9/9	0.95	0.11	37,46,49,49	0
15	GAU	f	4	9/9	0.98	0.08	49,53,57,63	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	H	301	1/1	0.60	0.30	74,74,74,74	0
18	MES	V	301	12/12	0.80	0.45	85,127,143,144	0
18	MES	Y	301	12/12	0.90	0.29	70,79,99,103	0
18	MES	c	101	12/12	0.90	0.35	84,108,115,117	0
18	MES	K	302	12/12	0.91	0.30	76,85,95,97	0
16	MG	G	301	1/1	0.91	0.18	53,53,53,53	0
16	MG	N	201	1/1	0.93	0.14	52,52,52,52	0
16	MG	I	301	1/1	0.94	0.30	74,74,74,74	0
16	MG	K	301	1/1	0.96	0.08	56,56,56,56	0
16	MG	L	301	1/1	0.99	0.04	62,62,62,62	0
16	MG	I	302	1/1	0.99	0.11	50,50,50,50	0
17	CL	G	302	1/1	0.99	0.12	47,47,47,47	0
17	CL	U	301	1/1	0.99	0.14	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.