



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:53 PM UTC

PDB ID : 4Y8H / pdb_00004y8h
Title : Yeast 20S proteasome in complex with N3-APAL-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

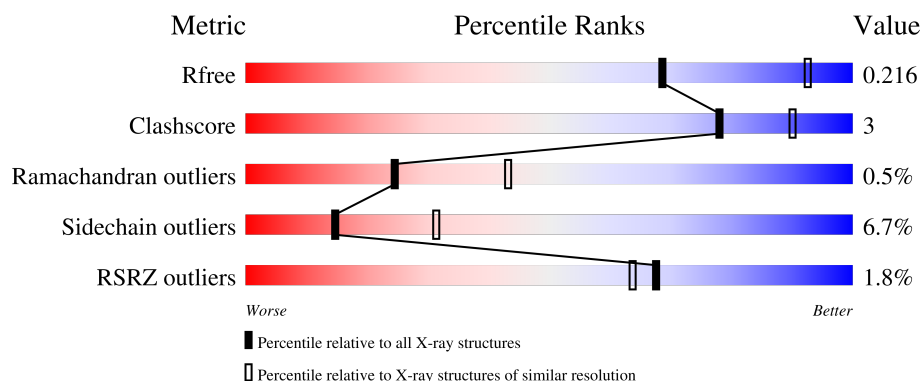
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	250	2% 92% 7% .
1	O	250	2% 92% 7% .
2	B	258	5% 79% 14% 5%
2	P	258	4% 79% 14% 5%
3	C	254	3% 82% 10% 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	6	
15	d	6	

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Mol	Chain	Length	Quality of chain
15	e	6	67% 17% 17%
15	f	6	17% 67% 33%
15	g	6	50% 50%
15	h	6	83% 17%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50485 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	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 N3-APAL-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	6	Total	C	N	O	0	0	0
			35	22	7	6			
15	d	6	Total	C	N	O	0	0	0
			35	22	7	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	6	Total	C	N	O	0	0	0
			35	22	7	6			
15	f	6	Total	C	N	O	0	0	0
			35	22	7	6			
15	g	6	Total	C	N	O	0	0	0
			35	22	7	6			
15	h	6	Total	C	N	O	0	0	0
			35	22	7	6			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	44	Total	O	0	0
			44	44		
19	B	37	Total	O	0	0
			37	37		
19	C	22	Total	O	0	0
			22	22		
19	D	19	Total	O	0	0
			19	19		
19	E	19	Total	O	0	0
			19	19		
19	F	29	Total	O	0	0
			29	29		
19	G	46	Total	O	0	0
			46	46		
19	H	55	Total	O	0	0
			55	55		
19	I	42	Total	O	0	0
			42	42		
19	J	34	Total	O	0	0
			34	34		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	43	Total O 43 43	0	0
19	L	48	Total O 48 48	0	0
19	M	43	Total O 43 43	0	0
19	N	37	Total O 37 37	0	0
19	O	21	Total O 21 21	0	0
19	P	21	Total O 21 21	0	0
19	Q	20	Total O 20 20	0	0
19	R	16	Total O 16 16	0	0
19	S	13	Total O 13 13	0	0
19	T	23	Total O 23 23	0	0
19	U	30	Total O 30 30	0	0
19	V	38	Total O 38 38	0	0
19	W	34	Total O 34 34	0	0
19	X	31	Total O 31 31	0	0
19	Y	34	Total O 34 34	0	0
19	Z	41	Total O 41 41	0	0
19	a	55	Total O 55 55	0	0
19	b	35	Total O 35 35	0	0
19	c	3	Total O 3 3	0	0
19	d	2	Total O 2 2	0	0
19	e	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	f	2	Total	O	0	0
			2	2		
19	g	2	Total	O	0	0
			2	2		
19	h	2	Total	O	0	0
			2	2		

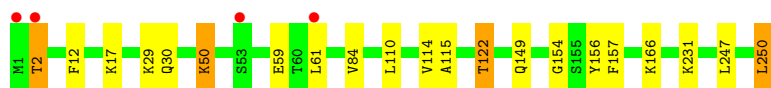
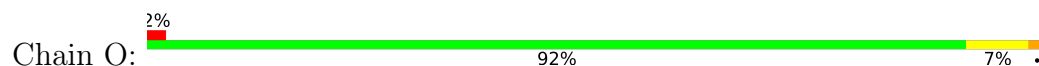
3 Residue-property plots [i](#)

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.

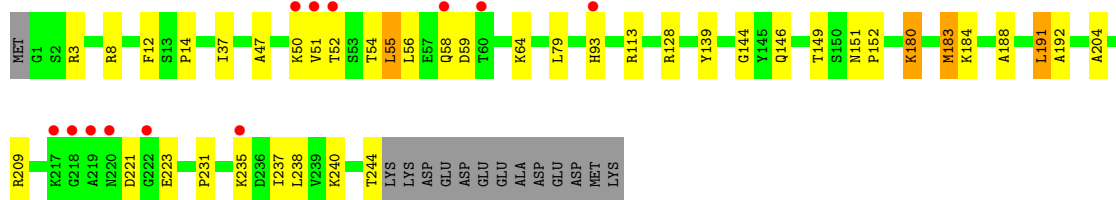
- Molecule 1: Proteasome subunit alpha type-2



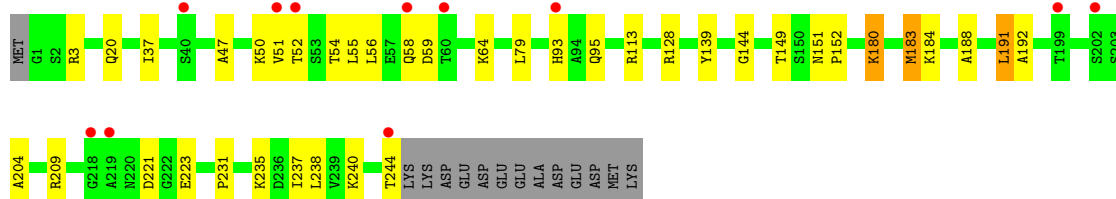
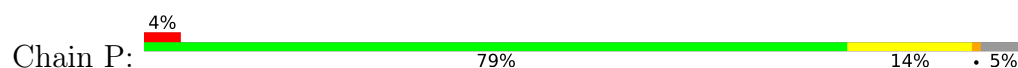
- Molecule 1: Proteasome subunit alpha type-2



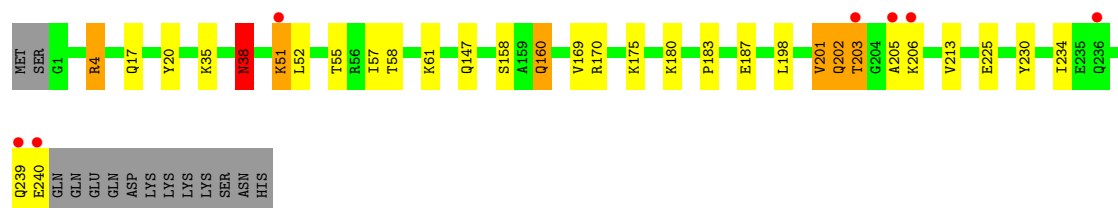
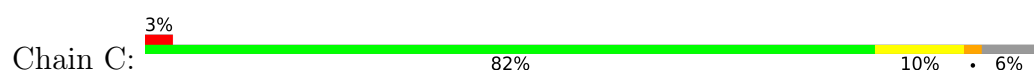
- Molecule 2: Proteasome subunit alpha type-3



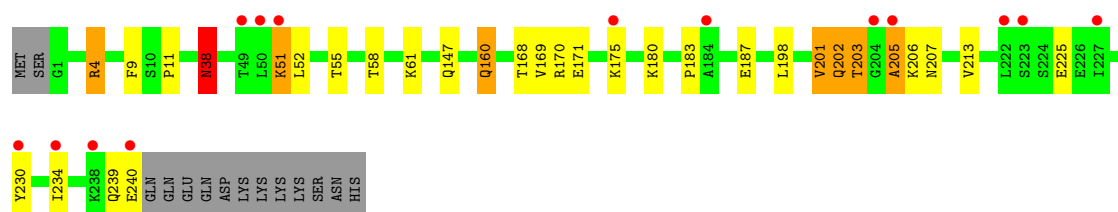
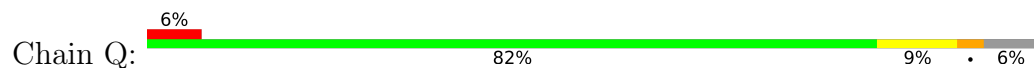
- Molecule 2: Proteasome subunit alpha type-3



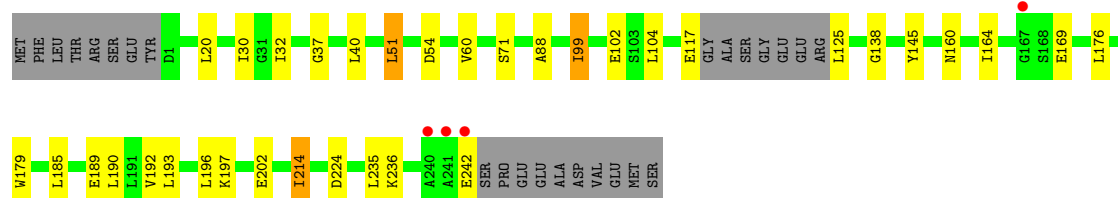
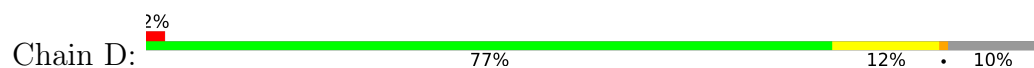
- Molecule 3: Proteasome subunit alpha type-4



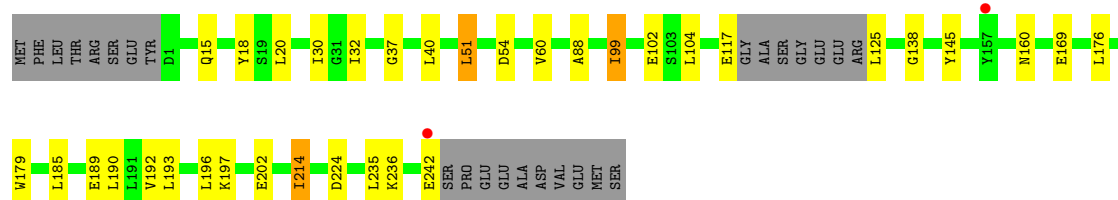
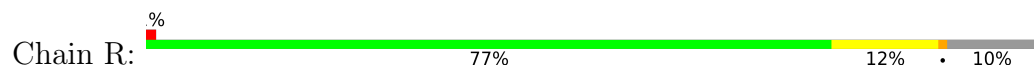
- Molecule 3: Proteasome subunit alpha type-4



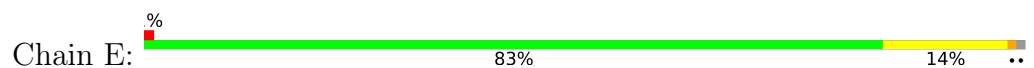
- Molecule 4: Proteasome subunit alpha type-5

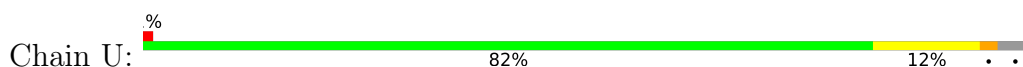


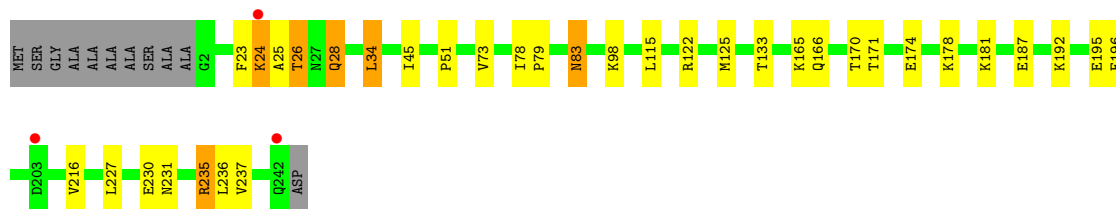
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 5: Proteasome subunit alpha type-6







• Molecule 8: Proteasome subunit beta type-2

Chain H: 88% 8% .



• Molecule 8: Proteasome subunit beta type-2

Chain V: 87% 8% .



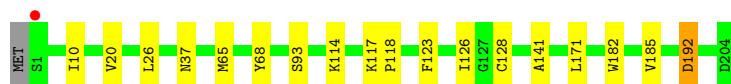
• Molecule 9: Proteasome subunit beta type-3

Chain I: 90% 9% .



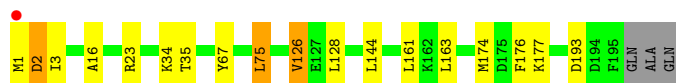
• Molecule 9: Proteasome subunit beta type-3

Chain W: 91% 8%



• Molecule 10: Proteasome subunit beta type-4

Chain J: 89% 8% ..



• Molecule 10: Proteasome subunit beta type-4

Chain X: 90% 7% ..



- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain K: 93% 6%



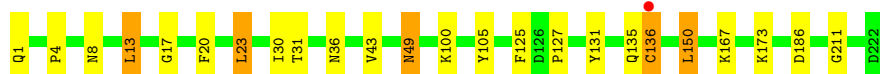
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain Y: 91% 8%



- Molecule 12: Proteasome subunit beta type-6

Chain L: 89% 9%



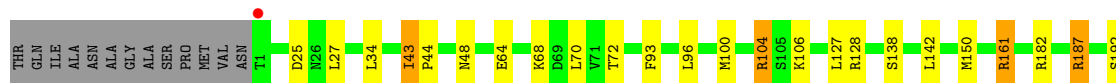
- Molecule 12: Proteasome subunit beta type-6

Chain Z: 90% 8%



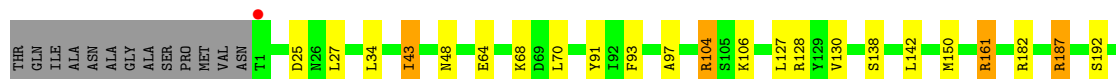
- Molecule 13: Proteasome subunit beta type-7

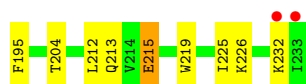
Chain M: 81% 11% 5%



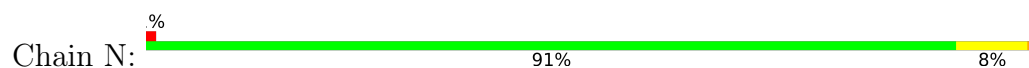
- Molecule 13: Proteasome subunit beta type-7

Chain a: 82% 11% 5%

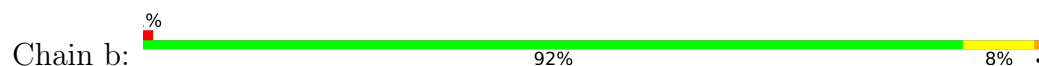




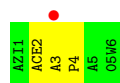
- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



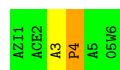
- Molecule 15: N3-APAL-ep



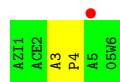
- Molecule 15: N3-APAL-ep



- Molecule 15: N3-APAL-ep



- Molecule 15: N3-APAL-ep



- Molecule 15: N3-APAL-ep





- Molecule 15: N3-APAL-ep

Chain h: 83% 17%

A horizontal bar chart for Chain h. The bar is divided into two segments: a long green segment on the left representing 83% and a shorter yellow segment on the right representing 17%.



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.32Å 300.79Å 145.46Å 90.00° 113.64° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.50) 98.7 (15.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.201 , 0.214 0.203 , 0.216	Depositor DCC
R_{free} test set	18194 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50485	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 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, AZI, MES, ACE, MG, 05W

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	0.40	0/1952	0.74	0/2642
1	O	0.40	0/1952	0.74	0/2642
2	B	0.39	0/1934	0.75	0/2618
2	P	0.39	0/1934	0.75	0/2618
3	C	0.40	0/1910	0.79	1/2586 (0.0%)
3	Q	0.40	0/1910	0.79	1/2586 (0.0%)
4	D	0.39	0/1837	0.70	0/2475
4	R	0.39	0/1837	0.71	0/2475
5	E	0.38	0/1800	0.73	0/2433
5	S	0.38	0/1800	0.73	0/2433
6	F	0.39	0/1932	0.72	0/2609
6	T	0.39	0/1932	0.72	0/2609
7	G	0.39	0/1945	0.72	0/2634
7	U	0.39	0/1945	0.72	0/2634
8	H	0.38	0/1715	0.68	0/2326
8	V	0.43	1/1715 (0.1%)	0.69	0/2326
9	I	0.37	0/1611	0.72	0/2174
9	W	0.38	0/1611	0.73	0/2174
10	J	0.38	0/1589	0.69	0/2142
10	X	0.37	0/1589	0.70	0/2142
11	K	0.40	1/1681 (0.1%)	0.69	0/2274
11	Y	0.42	2/1681 (0.1%)	0.70	0/2274
12	L	0.39	0/1795	0.68	0/2420
12	Z	0.37	0/1795	0.68	0/2420
13	M	0.39	0/1855	0.70	0/2514
13	a	0.39	0/1855	0.70	0/2514
14	N	0.49	1/1541 (0.1%)	0.76	1/2087 (0.0%)
14	b	0.44	0/1541	0.75	1/2087 (0.0%)
15	c	2.62	1/18 (5.6%)	2.98	2/25 (8.0%)
15	d	3.23	1/18 (5.6%)	2.02	0/25
15	e	3.33	2/18 (11.1%)	2.12	2/25 (8.0%)
15	f	2.75	1/18 (5.6%)	2.54	2/25 (8.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	3.12	1/18 (5.6%)	2.25	2/25 (8.0%)
15	h	1.94	1/18 (5.6%)	1.29	0/25
All	All	0.42	12/50302 (0.0%)	0.73	12/68018 (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
9	I	0	1
9	W	0	1
12	L	0	1
12	Z	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	4	PRO	CA-C	-10.93	1.39	1.52
15	d	4	PRO	CA-C	-10.75	1.39	1.52
15	e	4	PRO	CA-C	-10.47	1.37	1.52
15	f	4	PRO	CA-C	-10.10	1.40	1.52
15	c	4	PRO	CA-C	-9.58	1.41	1.52
15	h	4	PRO	CA-C	-7.45	1.41	1.52
15	e	4	PRO	CA-CB	-6.57	1.44	1.53
11	K	1	THR	CB-OG1	-6.40	1.33	1.43
11	Y	1	THR	CB-OG1	-6.35	1.33	1.43
8	V	1	THR	CB-OG1	-5.92	1.34	1.43
14	N	1	THR	CB-OG1	-5.53	1.34	1.43
11	Y	2	THR	C-O	-5.00	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	3	ALA	CA-C-N	9.67	129.75	119.89
15	c	3	ALA	C-N-CA	9.67	129.75	119.89
15	f	3	ALA	CA-C-N	7.02	127.01	119.78
15	f	3	ALA	C-N-CA	7.02	127.01	119.78
3	Q	201	VAL	N-CA-C	6.29	116.92	110.82
3	C	201	VAL	N-CA-C	6.17	116.80	110.82
14	b	22	THR	CB-CA-C	5.84	120.44	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	22	THR	CB-CA-C	5.45	119.85	111.85
15	e	3	ALA	CA-C-N	5.45	126.65	119.84
15	e	3	ALA	C-N-CA	5.45	126.65	119.84
15	g	3	ALA	CA-C-N	5.24	125.17	119.78
15	g	3	ALA	C-N-CA	5.24	125.17	119.78

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	192	ASP	Peptide
12	L	135	GLN	Peptide
9	W	192	ASP	Peptide
12	Z	135	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	7	0
1	O	1915	0	1929	8	0
2	B	1904	0	1904	20	0
2	P	1904	0	1904	18	0
3	C	1881	0	1895	16	0
3	Q	1881	0	1895	16	0
4	D	1813	0	1797	12	0
4	R	1813	0	1797	12	0
5	E	1773	0	1775	12	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	10	0
6	T	1892	0	1883	11	0
7	G	1907	0	1901	13	0
7	U	1907	0	1901	13	0
8	H	1684	0	1685	6	0
8	V	1684	0	1685	6	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1561	0	1569	9	0
10	X	1561	0	1569	8	0
11	K	1644	0	1592	8	0
11	Y	1644	0	1592	10	0
12	L	1757	0	1711	14	0
12	Z	1757	0	1711	12	0
13	M	1824	0	1832	15	0
13	a	1824	0	1832	13	0
14	N	1512	0	1478	8	0
14	b	1512	0	1479	7	0
15	c	35	0	30	1	0
15	d	35	0	30	1	0
15	e	35	0	30	0	0
15	f	35	0	30	0	0
15	g	35	0	30	1	0
15	h	35	0	30	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	2	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	K	12	0	13	0	0
18	g	12	0	13	0	0
19	A	44	0	0	0	0
19	B	37	0	0	0	0
19	C	22	0	0	0	0
19	D	19	0	0	1	0
19	E	19	0	0	0	0
19	F	29	0	0	0	0
19	G	46	0	0	0	0
19	H	55	0	0	0	0
19	I	42	0	0	0	0
19	J	34	0	0	0	0
19	K	43	0	0	0	0
19	L	48	0	0	0	0
19	M	43	0	0	0	0
19	N	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	21	0	0	0	0
19	P	21	0	0	0	0
19	Q	20	0	0	0	0
19	R	16	0	0	0	0
19	S	13	0	0	0	0
19	T	23	0	0	0	0
19	U	30	0	0	0	0
19	V	38	0	0	0	0
19	W	34	0	0	0	0
19	X	31	0	0	0	0
19	Y	34	0	0	0	0
19	Z	41	0	0	0	0
19	a	55	0	0	0	0
19	b	35	0	0	0	0
19	c	3	0	0	0	0
19	d	2	0	0	0	0
19	e	2	0	0	0	0
19	f	2	0	0	0	0
19	g	2	0	0	0	0
19	h	2	0	0	0	0
All	All	50485	0	49257	279	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 3.

All (279) 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	1.58	0.86
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.58	0.85
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.88	0.73
11:K:53:GLN:O	11:K:57:THR:HG23	1.88	0.72
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.73	0.71
3:C:201:VAL:O	3:C:202:GLN:HB2	1.92	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.73	0.69
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.92	0.69
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.58	0.69
3:C:51:LYS:O	3:C:52:LEU:HB2	1.92	0.68
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.59	0.68
3:Q:201:VAL:O	3:Q:202:GLN:HB2	1.92	0.68
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:GLN:HG3	3:C:203:THR:H	1.58	0.67
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.77	0.66
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.26	0.66
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.77	0.66
7:G:23:PHE:O	7:G:26:THR:HB	1.96	0.66
11:K:100:MET:CE	11:K:127:PHE:HB2	2.26	0.65
7:U:23:PHE:O	7:U:26:THR:HB	1.97	0.64
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.81	0.63
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.80	0.62
14:N:152:VAL:HA	14:N:175:MET:HE1	1.83	0.60
14:b:152:VAL:HA	14:b:175:MET:HE1	1.83	0.59
5:S:12:PHE:H	6:T:19:GLN:HE22	1.51	0.58
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.51	0.58
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.85	0.58
3:C:201:VAL:O	3:C:202:GLN:CB	2.52	0.57
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.86	0.57
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.85	0.57
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.70	0.56
8:H:52:THR:O	8:H:56:THR:HB	2.06	0.56
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.69	0.56
11:Y:49:ALA:HA	15:g:6:05W:H17	1.86	0.56
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.71	0.56
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.32	0.56
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.71	0.56
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.88	0.56
11:K:100:MET:HE3	11:K:127:PHE:CB	2.32	0.56
6:F:123:ASN:C	6:F:123:ASN:HD22	2.14	0.56
8:V:52:THR:O	8:V:56:THR:HB	2.06	0.56
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.88	0.55
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.21	0.55
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.88	0.55
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.88	0.55
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.88	0.55
6:T:123:ASN:C	6:T:123:ASN:HD22	2.14	0.55
2:B:183:MET:HE1	2:B:191:LEU:HD12	1.90	0.54
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.43	0.54
6:T:31:THR:HB	6:T:47:GLU:HG2	1.90	0.54
2:P:183:MET:HE1	2:P:191:LEU:HD12	1.90	0.54
7:G:34:LEU:C	7:G:34:LEU:HD23	2.33	0.54
5:E:12:PHE:H	6:F:19:GLN:HE22	1.56	0.54
6:F:31:THR:HB	6:F:47:GLU:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.91	0.53
14:N:185:ARG:NH1	19:N:301:HOH:O	2.40	0.53
10:X:1:MET:HA	10:X:34:LYS:CE	2.39	0.53
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.09	0.53
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.92	0.52
12:L:8:ASN:HA	12:L:30:ILE:O	2.09	0.52
11:Y:106:ARG:HH11	11:Y:106:ARG:HB3	1.74	0.52
11:K:106:ARG:HH11	11:K:106:ARG:HB3	1.74	0.52
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.91	0.52
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.91	0.52
10:J:1:MET:HA	10:J:34:LYS:HE3	1.91	0.52
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.58	0.52
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.75	0.52
7:U:34:LEU:C	7:U:34:LEU:HD23	2.34	0.52
10:J:1:MET:HA	10:J:34:LYS:CE	2.39	0.52
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.75	0.52
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.75	0.52
3:C:230:TYR:O	3:C:234:ILE:HG13	2.09	0.51
3:Q:230:TYR:O	3:Q:234:ILE:HG13	2.09	0.51
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.91	0.51
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.58	0.51
10:X:1:MET:HA	10:X:34:LYS:HE3	1.90	0.51
2:B:204:ALA:O	2:B:209:ARG:NH2	2.44	0.51
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.46	0.51
9:I:101:PRO:HB3	9:I:126:ILE:CD1	2.41	0.51
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.58	0.51
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.93	0.51
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.46	0.51
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.46	0.51
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.92	0.51
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.93	0.51
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.93	0.50
2:P:204:ALA:O	2:P:209:ARG:NH2	2.44	0.50
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.93	0.50
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.93	0.50
13:M:150:MET:HE1	13:M:187:ARG:HG2	1.93	0.50
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.94	0.50
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.93	0.50
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.93	0.49
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.93	0.49
4:D:99:ILE:HG22	19:D:307:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.48	0.49
4:R:51:LEU:C	4:R:51:LEU:HD12	2.37	0.49
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.93	0.49
8:V:84:LYS:HG3	8:V:85:GLN:N	2.27	0.49
5:E:68:HIS:HE1	5:E:102:LEU:O	1.96	0.49
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.94	0.48
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.78	0.48
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.95	0.48
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.78	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.48
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.48	0.48
4:D:99:ILE:HD13	4:D:104:LEU:HB2	1.96	0.48
6:F:194:LYS:HD3	6:F:242:GLU:HG3	1.96	0.48
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.41	0.48
3:Q:202:GLN:CG	3:Q:203:THR:H	2.26	0.48
5:S:68:HIS:HE1	5:S:102:LEU:O	1.96	0.48
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.95	0.48
6:T:194:LYS:HD3	6:T:242:GLU:HG3	1.96	0.48
8:V:50:ALA:HB3	9:W:126:ILE:HD12	1.94	0.48
5:E:9:THR:HG21	5:E:119:THR:HA	1.96	0.48
9:I:65:MET:HE1	9:I:93:SER:HB3	1.96	0.48
7:U:73:VAL:HG12	7:U:133:THR:HB	1.95	0.48
7:G:73:VAL:HG12	7:G:133:THR:HB	1.96	0.47
4:R:99:ILE:HD13	4:R:104:LEU:HB2	1.96	0.47
4:D:51:LEU:HD12	4:D:51:LEU:C	2.38	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.47
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.41	0.47
3:C:51:LYS:HD2	3:C:51:LYS:HA	1.73	0.47
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.97	0.47
2:P:59:ASP:HB3	2:P:231:PRO:HG2	1.96	0.47
2:P:183:MET:HE2	2:P:188:ALA:HA	1.96	0.47
5:S:9:THR:HG21	5:S:119:THR:HA	1.96	0.47
8:H:84:LYS:HG3	8:H:85:GLN:N	2.28	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.47
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.47
2:B:3:ARG:NH1	5:E:122:TYR:OH	2.47	0.47
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.97	0.47
4:R:185:LEU:O	4:R:189:GLU:HG3	2.15	0.47
2:B:237:ILE:HD12	2:B:240:LYS:HE3	1.97	0.47
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.47
1:A:149:GLN:O	1:A:156:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ASP:HB3	2:B:231:PRO:HG2	1.97	0.46
9:W:65:MET:HE1	9:W:93:SER:HB3	1.96	0.46
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.97	0.46
2:P:180:LYS:O	2:P:183:MET:HB2	2.16	0.46
13:M:43:ILE:HG21	13:M:64:GLU:HG2	1.97	0.46
4:D:185:LEU:O	4:D:189:GLU:HG3	2.16	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.46
2:B:183:MET:HE2	2:B:188:ALA:HA	1.96	0.46
13:M:182:ARG:NH2	13:M:215:GLU:O	2.49	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.46	0.46
8:H:22:GLN:HE22	15:c:2:ACE:C	2.24	0.46
7:U:45:ILE:HG22	7:U:216:VAL:HG13	1.98	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.45
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.42	0.45
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.80	0.45
13:a:43:ILE:HG21	13:a:64:GLU:HG2	1.97	0.45
7:G:45:ILE:HG22	7:G:216:VAL:HG13	1.98	0.45
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.98	0.45
2:P:237:ILE:HD12	2:P:240:LYS:HE3	1.96	0.45
3:C:38:ASN:N	3:C:38:ASN:HD22	2.15	0.45
11:K:86:LEU:C	11:K:86:LEU:HD13	2.42	0.45
6:T:146:MET:HE3	6:T:161:THR:HB	1.98	0.45
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.97	0.45
13:a:182:ARG:NH2	13:a:215:GLU:O	2.49	0.45
2:B:180:LYS:O	2:B:183:MET:HB2	2.16	0.45
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.98	0.45
1:A:50:LYS:O	1:A:50:LYS:HG3	2.17	0.45
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.98	0.45
6:F:146:MET:HE3	6:F:161:THR:HB	1.98	0.45
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.15	0.45
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.45	0.45
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.99	0.45
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.99	0.44
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.44
5:E:155:LEU:HD13	5:E:158:THR:HB	2.00	0.44
5:E:226:GLY:O	5:E:229:VAL:HG22	2.18	0.44
14:N:137:TYR:CE1	14:b:140:LYS:HG3	2.53	0.44
5:S:155:LEU:HD13	5:S:158:THR:HB	2.00	0.44
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.52	0.44
1:A:247:LEU:O	1:A:250:LEU:HB2	2.18	0.44
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.53	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.44
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.52	0.44
7:G:196:PHE:CD1	7:G:196:PHE:C	2.96	0.44
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.99	0.43
3:Q:51:LYS:HD2	3:Q:51:LYS:HA	1.74	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.53	0.43
5:S:226:GLY:O	5:S:229:VAL:HG22	2.17	0.43
1:O:12:PHE:H	2:P:20:GLN:HE22	1.66	0.43
7:U:196:PHE:CD1	7:U:196:PHE:C	2.96	0.43
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.53	0.43
12:L:127:PRO:HG2	15:d:2:ACE:H2	2.00	0.43
13:M:187:ARG:HG3	14:b:25:TYR:CE1	2.53	0.43
1:O:50:LYS:O	1:O:50:LYS:HG3	2.18	0.43
13:a:25:ASP:HA	13:a:195:PHE:CB	2.49	0.43
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.54	0.43
1:O:247:LEU:O	1:O:250:LEU:HB2	2.18	0.43
2:P:37:ILE:HD12	2:P:192:ALA:HB2	2.01	0.43
2:B:37:ILE:HD12	2:B:192:ALA:HB2	2.00	0.43
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.58	0.43
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.54	0.43
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.31	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.42
13:a:93:PHE:CE2	13:a:128:ARG:HD3	2.54	0.42
11:K:6:PHE:HA	11:K:125:ASP:O	2.19	0.42
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.83	0.42
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.02	0.42
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.49	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.42
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.54	0.42
5:S:71:LEU:C	5:S:71:LEU:HD23	2.44	0.42
2:B:93:HIS:CG	2:B:113:ARG:HE	2.37	0.42
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.55	0.42
6:T:34:ILE:HG22	6:T:160:ALA:HB2	2.02	0.42
6:T:238:PHE:O	6:T:242:GLU:HG2	2.20	0.42
13:M:25:ASP:HA	13:M:195:PHE:CB	2.49	0.42
2:P:93:HIS:CG	2:P:113:ARG:HE	2.37	0.42
3:C:202:GLN:CG	3:C:203:THR:H	2.26	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.42
5:E:71:LEU:C	5:E:71:LEU:HD23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:193:ASP:OD1	10:J:193:ASP:N	2.52	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.20	0.42
6:F:238:PHE:O	6:F:242:GLU:HG2	2.19	0.42
13:M:93:PHE:CE2	13:M:128:ARG:HD3	2.54	0.42
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.50	0.42
7:U:83:ASN:ND2	7:U:83:ASN:C	2.78	0.42
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.55	0.41
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.60	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.54	0.41
10:J:177:LYS:NZ	10:X:169:GLU:O	2.53	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.55	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.55	0.41
13:a:27:LEU:HB2	13:a:192:SER:HB3	2.02	0.41
1:A:110:LEU:O	1:A:114:VAL:HG23	2.20	0.41
7:G:170:THR:O	7:G:174:GLU:HG3	2.20	0.41
10:J:174:MET:HA	10:X:174:MET:HA	2.02	0.41
1:O:115:ALA:HB1	1:O:154:GLY:O	2.20	0.41
7:G:83:ASN:C	7:G:83:ASN:ND2	2.78	0.41
9:I:7:ASN:HA	9:I:29:GLY:O	2.21	0.41
12:L:186:ASP:OD2	8:V:203:TYR:OH	2.36	0.41
6:T:13:PRO:O	7:U:24:LYS:HD2	2.21	0.41
12:L:4:PRO:O	13:M:104:ARG:NH1	2.49	0.41
6:T:165:ARG:HG2	6:T:166:GLN:N	2.36	0.41
6:F:34:ILE:HG22	6:F:160:ALA:HB2	2.02	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.41
2:B:12:PHE:H	3:C:17:GLN:HE22	1.68	0.41
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.50	0.41
9:I:123:PHE:HA	9:I:128:CYS:O	2.20	0.41
7:U:25:ALA:O	7:U:28:GLN:HB2	2.21	0.41
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.03	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.55	0.41
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.56	0.41
4:D:71:SER:HB3	4:D:164:ILE:HD12	2.03	0.41
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.50	0.41
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.56	0.41
3:Q:205:ALA:C	3:Q:207:ASN:H	2.29	0.41
9:W:123:PHE:HA	9:W:128:CYS:O	2.21	0.41
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.54	0.41
7:G:25:ALA:O	7:G:28:GLN:HB2	2.21	0.40
7:G:101:TYR:OH	8:H:66:HIS:HE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.03	0.40
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.50	0.40
7:U:170:THR:O	7:U:174:GLU:HG3	2.21	0.40
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.03	0.40
3:C:35:LYS:HG2	3:C:158:SER:O	2.21	0.40
6:F:165:ARG:HG2	6:F:166:GLN:N	2.36	0.40
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.57	0.40
5:S:98:PHE:O	13:a:91:TYR:HA	2.20	0.40
13:a:97:ALA:HA	13:a:130:VAL:HG21	2.04	0.40
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.03	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	0.40
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.21	0.40
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.35	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	0.40
5:E:61:LYS:O	5:E:72:SER:HA	2.22	0.40
14:N:13:ILE:HG21	14:N:175:MET:CE	2.52	0.40
1:O:110:LEU:O	1:O:114:VAL:HG23	2.22	0.40
2:P:3:ARG:HG3	3:Q:4:ARG:CZ	2.51	0.40
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.57	0.40
6:T:78:ILE:HB	6:T:79:PRO:HD3	2.04	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%)	239 (96%)	7 (3%)	2 (1%)	16	31
1	O	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	16	31
2	B	242/258 (94%)	230 (95%)	9 (4%)	3 (1%)	10	20
2	P	242/258 (94%)	230 (95%)	9 (4%)	3 (1%)	10	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	227 (95%)	6 (2%)	5 (2%)	5	9
3	Q	238/254 (94%)	227 (95%)	6 (2%)	5 (2%)	5	9
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	217 (95%)	12 (5%)	0	100	100
5	S	229/234 (98%)	217 (95%)	12 (5%)	0	100	100
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	236 (99%)	2 (1%)	1 (0%)	30	49
7	U	239/252 (95%)	235 (98%)	3 (1%)	1 (0%)	30	49
8	H	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	24	43
8	V	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	24	43
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%)	24	43
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	43
11	K	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	24	43
11	Y	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	24	43
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
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	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
15	d	3/6 (50%)	2 (67%)	0	1 (33%)	0	0
15	e	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
15	f	3/6 (50%)	3 (100%)	0	0	100	100
15	g	3/6 (50%)	3 (100%)	0	0	100	100
15	h	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	6294/6650 (95%)	6090 (97%)	175 (3%)	29 (0%)	24	43

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	52	THR
3	C	202	GLN
3	C	205	ALA
1	O	2	THR
2	P	52	THR
3	Q	202	GLN
3	Q	205	ALA
2	B	51	VAL
3	C	38	ASN
8	H	9	ASN
10	J	2	ASP
2	P	51	VAL
3	Q	38	ASN
8	V	9	ASN
10	X	2	ASP
11	K	9	GLN
11	Y	9	GLN
2	B	221	ASP
3	C	183	PRO
2	P	221	ASP
3	Q	183	PRO
15	d	3	ALA
3	C	206	LYS
3	Q	206	LYS
1	A	166	LYS
1	O	166	LYS
7	G	51	PRO
7	U	51	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	197 (94%)	12 (6%)	18	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	209/209 (100%)	197 (94%)	12 (6%)	18	39
2	B	203/216 (94%)	188 (93%)	15 (7%)	13	27
2	P	203/216 (94%)	188 (93%)	15 (7%)	13	27
3	C	212/226 (94%)	195 (92%)	17 (8%)	11	24
3	Q	212/226 (94%)	195 (92%)	17 (8%)	11	24
4	D	194/215 (90%)	174 (90%)	20 (10%)	7	14
4	R	194/215 (90%)	174 (90%)	20 (10%)	7	14
5	E	190/193 (98%)	172 (90%)	18 (10%)	8	17
5	S	190/193 (98%)	172 (90%)	18 (10%)	8	17
6	F	201/239 (84%)	183 (91%)	18 (9%)	9	19
6	T	201/239 (84%)	183 (91%)	18 (9%)	9	19
7	G	206/210 (98%)	188 (91%)	18 (9%)	9	21
7	U	206/210 (98%)	188 (91%)	18 (9%)	9	21
8	H	181/190 (95%)	172 (95%)	9 (5%)	22	44
8	V	181/190 (95%)	172 (95%)	9 (5%)	22	44
9	I	172/173 (99%)	165 (96%)	7 (4%)	27	53
9	W	172/173 (99%)	166 (96%)	6 (4%)	32	58
10	J	173/175 (99%)	166 (96%)	7 (4%)	28	54
10	X	173/175 (99%)	166 (96%)	7 (4%)	28	54
11	K	169/169 (100%)	163 (96%)	6 (4%)	31	58
11	Y	169/169 (100%)	163 (96%)	6 (4%)	31	58
12	L	185/185 (100%)	177 (96%)	8 (4%)	26	51
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	51
13	M	199/208 (96%)	183 (92%)	16 (8%)	11	24
13	a	199/208 (96%)	183 (92%)	16 (8%)	11	24
14	N	162/162 (100%)	154 (95%)	8 (5%)	22	45
14	b	162/162 (100%)	154 (95%)	8 (5%)	22	45
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%)	0	1 (100%)	0	0
15	f	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
All	All	5318/5546 (96%)	4960 (93%)	358 (7%)	15	31

All (358) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	29	LYS
1	A	30	GLN
1	A	50	LYS
1	A	59	GLU
1	A	61	LEU
1	A	84	VAL
1	A	122	THR
1	A	157	PHE
1	A	231	LYS
1	A	250	LEU
2	B	50	LYS
2	B	54	THR
2	B	55	LEU
2	B	56	LEU
2	B	58	GLN
2	B	79	LEU
2	B	149	THR
2	B	180	LYS
2	B	183	MET
2	B	184	LYS
2	B	191	LEU
2	B	223	GLU
2	B	235	LYS
2	B	238	LEU
2	B	244	THR
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	55	THR
3	C	58	THR
3	C	61	LYS
3	C	147	GLN

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Mol	Chain	Res	Type
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	213	VAL
3	C	225	GLU
3	C	239	GLN
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	60	VAL
4	D	99	ILE
4	D	102	GLU
4	D	117	GLU
4	D	125	LEU
4	D	169	GLU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	197	LYS
4	D	202	GLU
4	D	214	ILE
4	D	224	ASP
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	4	ASN
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	61	LYS
5	E	71	LEU
5	E	92	ASN
5	E	144	LEU

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Mol	Chain	Res	Type
5	E	179	ILE
5	E	180	LYS
5	E	188	LEU
5	E	207	VAL
5	E	219	THR
5	E	231	LYS
6	F	14	ASP
6	F	47	GLU
6	F	58	GLN
6	F	59	LYS
6	F	68	ARG
6	F	96	LYS
6	F	123	ASN
6	F	139	LYS
6	F	148	GLU
6	F	165	ARG
6	F	172	LEU
6	F	174	LYS
6	F	181	GLU
6	F	187	GLU
6	F	203	ASN
6	F	221	ASN
6	F	228	LYS
6	F	241	LYS
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	34	LEU
7	G	83	ASN
7	G	98	LYS
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	165	LYS
7	G	166	GLN
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
7	G	237	VAL

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Mol	Chain	Res	Type
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	153	LYS
8	H	196	ARG
8	H	198	GLU
9	I	37	ASN
9	I	114	LYS
9	I	117	LYS
9	I	126	ILE
9	I	171	LEU
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	126	VAL
10	J	144	LEU
10	J	163	LEU
11	K	4	LEU
11	K	35	ILE
11	K	57	THR
11	K	73	ARG
11	K	106	ARG
11	K	148	LEU
12	L	1	GLN
12	L	13	LEU
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	43	ILE
13	M	48	ASN
13	M	68	LYS
13	M	70	LEU
13	M	104	ARG

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Mol	Chain	Res	Type
13	M	106	LYS
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	204	THR
13	M	212	LEU
13	M	213	GLN
13	M	215	GLU
13	M	225	ILE
13	M	226	LYS
13	M	232	LYS
14	N	9	LYS
14	N	21	THR
14	N	22	THR
14	N	36	ARG
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	17	LYS
1	O	29	LYS
1	O	30	GLN
1	O	50	LYS
1	O	59	GLU
1	O	61	LEU
1	O	84	VAL
1	O	122	THR
1	O	157	PHE
1	O	231	LYS
1	O	250	LEU
2	P	50	LYS
2	P	54	THR
2	P	55	LEU
2	P	56	LEU
2	P	58	GLN
2	P	79	LEU
2	P	149	THR
2	P	180	LYS
2	P	183	MET
2	P	184	LYS
2	P	191	LEU

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Mol	Chain	Res	Type
2	P	223	GLU
2	P	235	LYS
2	P	238	LEU
2	P	244	THR
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	55	THR
3	Q	58	THR
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	203	THR
3	Q	213	VAL
3	Q	225	GLU
3	Q	239	GLN
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	54	ASP
4	R	60	VAL
4	R	99	ILE
4	R	102	GLU
4	R	117	GLU
4	R	125	LEU
4	R	169	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	197	LYS
4	R	202	GLU
4	R	214	ILE
4	R	224	ASP
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN

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Mol	Chain	Res	Type
5	S	4	ASN
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	61	LYS
5	S	71	LEU
5	S	92	ASN
5	S	144	LEU
5	S	179	ILE
5	S	180	LYS
5	S	188	LEU
5	S	207	VAL
5	S	219	THR
5	S	231	LYS
6	T	14	ASP
6	T	47	GLU
6	T	58	GLN
6	T	59	LYS
6	T	68	ARG
6	T	96	LYS
6	T	123	ASN
6	T	139	LYS
6	T	148	GLU
6	T	165	ARG
6	T	172	LEU
6	T	174	LYS
6	T	181	GLU
6	T	187	GLU
6	T	203	ASN
6	T	221	ASN
6	T	228	LYS
6	T	241	LYS
7	U	24	LYS
7	U	26	THR
7	U	28	GLN
7	U	34	LEU
7	U	83	ASN
7	U	98	LYS
7	U	115	LEU

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Mol	Chain	Res	Type
7	U	122	ARG
7	U	125	MET
7	U	165	LYS
7	U	166	GLN
7	U	171	THR
7	U	178	LYS
7	U	181	LYS
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
7	U	237	VAL
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	153	LYS
8	V	196	ARG
8	V	198	GLU
9	W	37	ASN
9	W	114	LYS
9	W	117	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	126	VAL
10	X	144	LEU
10	X	163	LEU
11	Y	4	LEU
11	Y	35	ILE
11	Y	57	THR
11	Y	73	ARG
11	Y	106	ARG
11	Y	148	LEU
12	Z	1	GLN
12	Z	13	LEU
12	Z	23	LEU

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Mol	Chain	Res	Type
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	173	LYS
13	a	43	ILE
13	a	48	ASN
13	a	68	LYS
13	a	70	LEU
13	a	104	ARG
13	a	106	LYS
13	a	138	SER
13	a	161	ARG
13	a	187	ARG
13	a	204	THR
13	a	212	LEU
13	a	213	GLN
13	a	215	GLU
13	a	225	ILE
13	a	226	LYS
13	a	232	LYS
14	b	9	LYS
14	b	21	THR
14	b	22	THR
14	b	36	ARG
14	b	115	LEU
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU
15	e	4	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	149	GLN
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN

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Mol	Chain	Res	Type
2	B	124	HIS
2	B	146	GLN
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	38	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
4	D	15	GLN
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
7	G	186	ASN
8	H	22	GLN
8	H	30	ASN
8	H	57	GLN

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Mol	Chain	Res	Type
8	H	66	HIS
8	H	86	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	63	ASN
9	I	88	GLN
10	J	10	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	188	HIS
11	K	208	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
1	O	149	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN

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Mol	Chain	Res	Type
2	P	123	GLN
2	P	124	HIS
2	P	146	GLN
2	P	176	GLN
2	P	232	GLN
3	Q	38	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	165	ASN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	57	GLN
8	V	86	HIS
8	V	91	GLN
8	V	141	HIS

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Mol	Chain	Res	Type
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	63	ASN
10	X	10	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	133	HIS
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	188	HIS
11	Y	208	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	94	GLN
12	Z	153	GLN
12	Z	159	GLN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
14	b	38	HIS
14	b	69	GLN
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	MES	K	302	-	12,12,12	2.25	1 (8%)	15,16,16	1.17	1 (6%)
18	MES	g	101	-	12,12,12	2.30	1 (8%)	15,16,16	1.11	1 (6%)

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	g	101	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	g	101	MES	C8-S	-7.69	1.66	1.77
18	K	302	MES	C8-S	-7.49	1.67	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	302	MES	O3S-S-C8	2.35	110.60	106.00
18	g	101	MES	O2S-S-C8	2.21	110.07	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.22	5 (2%) 65 61	30, 48, 79, 122	0
1	O	250/250 (100%)	-0.12	4 (1%) 70 67	34, 55, 94, 128	0
2	B	244/258 (94%)	0.01	12 (4%) 35 31	32, 52, 101, 146	0
2	P	244/258 (94%)	0.17	11 (4%) 38 33	37, 56, 104, 151	0
3	C	240/254 (94%)	0.08	7 (2%) 53 49	32, 55, 119, 144	0
3	Q	240/254 (94%)	0.31	14 (5%) 29 25	36, 68, 144, 165	0
4	D	235/260 (90%)	-0.06	4 (1%) 69 65	34, 57, 90, 141	0
4	R	235/260 (90%)	-0.03	2 (0%) 81 78	37, 59, 98, 144	0
5	E	231/234 (98%)	-0.01	3 (1%) 75 71	38, 60, 92, 132	0
5	S	231/234 (98%)	0.13	4 (1%) 69 65	39, 63, 104, 141	0
6	F	243/288 (84%)	-0.06	7 (2%) 53 49	32, 52, 101, 129	0
6	T	243/288 (84%)	-0.05	9 (3%) 45 40	32, 54, 100, 142	0
7	G	241/252 (95%)	-0.05	6 (2%) 58 54	26, 48, 83, 132	0
7	U	241/252 (95%)	-0.16	3 (1%) 76 73	33, 50, 82, 107	0
8	H	222/232 (95%)	-0.29	1 (0%) 87 85	31, 45, 70, 111	0
8	V	222/232 (95%)	-0.20	3 (1%) 73 70	33, 49, 73, 130	0
9	I	204/205 (99%)	-0.46	2 (0%) 79 76	29, 42, 67, 94	0
9	W	204/205 (99%)	-0.43	1 (0%) 87 85	26, 44, 74, 106	0
10	J	195/198 (98%)	-0.37	1 (0%) 87 85	27, 45, 72, 130	0
10	X	195/198 (98%)	-0.35	2 (1%) 79 76	31, 48, 73, 140	0
11	K	212/212 (100%)	-0.32	0 100 100	30, 44, 72, 96	0
11	Y	212/212 (100%)	-0.40	0 100 100	33, 45, 74, 99	0
12	L	222/222 (100%)	-0.40	1 (0%) 87 85	30, 46, 73, 90	0
12	Z	222/222 (100%)	-0.41	0 100 100	30, 45, 73, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.36	3 (1%) 75 71	29, 44, 67, 104	0
13	a	233/246 (94%)	-0.33	3 (1%) 75 71	29, 43, 67, 108	0
14	N	196/196 (100%)	-0.44	1 (0%) 87 85	27, 40, 66, 96	0
14	b	196/196 (100%)	-0.39	1 (0%) 87 85	28, 41, 67, 95	0
15	c	3/6 (50%)	1.46	1 (33%) 1 1	53, 53, 55, 65	0
15	d	3/6 (50%)	-0.19	0 100 100	41, 41, 50, 60	0
15	e	3/6 (50%)	-0.48	0 100 100	33, 33, 40, 47	0
15	f	3/6 (50%)	1.65	1 (33%) 1 1	61, 61, 61, 64	0
15	g	3/6 (50%)	-0.25	0 100 100	38, 38, 54, 63	0
15	h	3/6 (50%)	-0.35	0 100 100	41, 41, 44, 49	0
All	All	6354/6650 (95%)	-0.17	112 (1%) 67 64	26, 50, 93, 165	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	1	MET	6.5
3	Q	50	LEU	5.9
10	X	1	MET	5.6
2	P	218	GLY	4.5
1	A	1	MET	4.5
2	P	219	ALA	4.5
2	B	218	GLY	4.3
13	a	233	ILE	4.0
13	M	1	THR	4.0
1	O	1	MET	3.8
2	P	51	VAL	3.8
2	B	219	ALA	3.8
3	Q	51	LYS	3.6
3	Q	205	ALA	3.5
2	B	51	VAL	3.4
13	a	1	THR	3.4
3	Q	240	GLU	3.4
3	C	236	GLN	3.3
14	b	103	ASP	3.1
6	T	215	CYS	3.1
9	W	1	SER	3.1
6	T	204	LYS	3.0
15	c	3	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	2	THR	3.0
3	Q	234	ILE	2.9
3	Q	223	SER	2.9
1	A	2	THR	2.9
6	T	178	HIS	2.9
2	B	220	ASN	2.9
6	T	244	ASN	2.9
4	D	242	GLU	2.9
2	B	52	THR	2.9
6	T	205	GLU	2.9
3	C	203	THR	2.8
6	F	2	THR	2.8
6	F	215	CYS	2.8
6	F	202	ASP	2.8
6	F	244	ASN	2.8
6	T	243	ILE	2.8
6	T	2	THR	2.8
3	C	239	GLN	2.8
13	M	233	ILE	2.8
7	U	24	LYS	2.8
13	a	232	LYS	2.8
1	O	53	SER	2.7
3	C	206	LYS	2.7
2	B	93	HIS	2.7
1	A	201	GLU	2.7
14	N	103	ASP	2.6
3	Q	49	THR	2.6
7	G	242	GLN	2.6
2	P	93	HIS	2.6
1	A	62	SER	2.6
2	B	217	LYS	2.6
4	R	242	GLU	2.6
9	I	1	SER	2.6
4	D	241	ALA	2.5
12	L	136	CYS	2.5
5	E	122	TYR	2.5
3	Q	204	GLY	2.5
3	C	51	LYS	2.5
8	V	9	ASN	2.5
3	Q	238	LYS	2.4
3	Q	227	ILE	2.4
4	R	157	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	52	THR	2.4
7	U	242	GLN	2.4
7	G	181	LYS	2.4
7	G	2	GLY	2.4
8	H	222	ASP	2.4
3	Q	175	LYS	2.4
4	D	240	ALA	2.4
7	G	12	PRO	2.3
6	F	203	ASN	2.3
2	P	58	GLN	2.3
6	T	183	LEU	2.3
10	X	194	ASP	2.3
4	D	167	GLY	2.3
3	C	205	ALA	2.3
2	P	199	THR	2.3
5	S	233	ILE	2.3
3	C	240	GLU	2.3
2	B	50	LYS	2.2
5	E	204	SER	2.2
1	A	249	ALA	2.2
3	Q	184	ALA	2.2
5	S	209	ASN	2.2
7	G	17	TYR	2.2
3	Q	222	LEU	2.2
15	f	5	ALA	2.2
5	S	122	TYR	2.2
7	G	165	LYS	2.2
13	M	232	LYS	2.2
2	P	202	SER	2.1
1	O	61	LEU	2.1
2	B	222	GLY	2.1
8	V	222	ASP	2.1
5	S	96	LEU	2.1
2	B	235	LYS	2.1
5	E	209	ASN	2.1
2	B	60	THR	2.1
2	P	244	THR	2.1
9	I	191	LYS	2.1
7	U	203	ASP	2.1
8	V	216	SER	2.1
2	P	60	THR	2.0
2	B	58	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
6	F	201	GLU	2.0
6	T	241	LYS	2.0
2	P	40	SER	2.0
3	Q	230	TYR	2.0
6	F	178	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	MG	N	202	1/1	0.85	0.11	59,59,59,59	0
16	MG	Z	301	1/1	0.90	0.07	56,56,56,56	0
18	MES	K	302	12/12	0.90	0.14	63,72,75,78	0
18	MES	g	101	12/12	0.93	0.12	59,68,73,76	0
16	MG	I	301	1/1	0.94	0.10	58,58,58,58	0
16	MG	L	301	1/1	0.96	0.08	55,55,55,55	0
17	CL	b	201	1/1	0.96	0.19	30,30,30,30	0
16	MG	G	301	1/1	0.97	0.06	41,41,41,41	0
16	MG	N	201	1/1	0.97	0.05	45,45,45,45	0
17	CL	U	301	1/1	0.97	0.12	30,30,30,30	0
17	CL	N	203	1/1	0.98	0.12	30,30,30,30	0
17	CL	G	302	1/1	0.99	0.11	30,30,30,30	0
16	MG	I	302	1/1	0.99	0.04	46,46,46,46	0
16	MG	K	301	1/1	0.99	0.06	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.