



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 PM UTC

PDB ID : 4Y8G / pdb_00004y8g
Title : Yeast 20S proteasome in complex with N3-APnLL-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

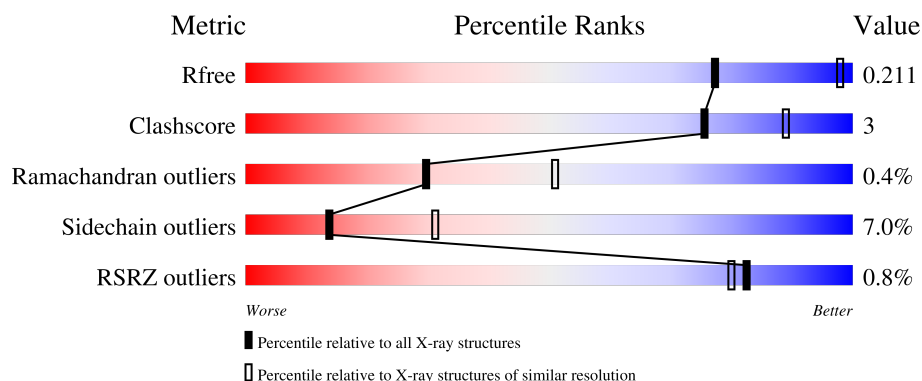
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0% 91% 7% •
1	O	250	91% 7% •
2	B	258	2% 79% 14% • 5%
2	P	258	2% 79% 14% • 5%
3	C	254	2% 81% 11% • 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	83% 17%
15	f	6	83% 17%
15	g	6	33% 50% 17%
15	h	6	67% 17% 17%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50001 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-APnLL-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	6	Total	C	N	O	0	0	0
			38	25	7	6			
15	d	6	Total	C	N	O	0	0	0
			38	25	7	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	6	Total	C	N	O	0	0	0
			38	25	7	6			
15	f	6	Total	C	N	O	0	0	0
			38	25	7	6			
15	g	6	Total	C	N	O	0	0	0
			38	25	7	6			
15	h	6	Total	C	N	O	0	0	0
			38	25	7	6			

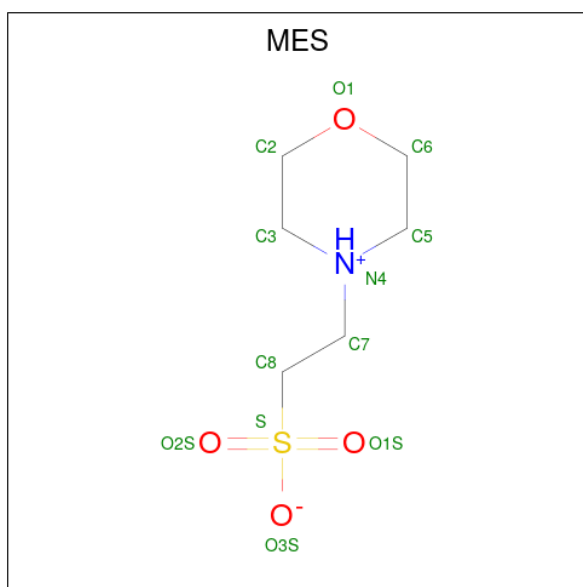
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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	1	Total	Mg	0	0
			1	1		
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	Y	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	19	Total	O	0	0
			19	19		
19	B	17	Total	O	0	0
			17	17		
19	C	12	Total	O	0	0
			12	12		
19	D	7	Total	O	0	0
			7	7		
19	E	9	Total	O	0	0
			9	9		
19	F	16	Total	O	0	0
			16	16		
19	G	26	Total	O	0	0
			26	26		
19	H	20	Total	O	0	0
			20	20		
19	I	12	Total	O	0	0
			12	12		
19	J	15	Total	O	0	0
			15	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	16	Total O 16 16	0	0
19	L	23	Total O 23 23	0	0
19	M	20	Total O 20 20	0	0
19	N	17	Total O 17 17	0	0
19	O	8	Total O 8 8	0	0
19	P	11	Total O 11 11	0	0
19	Q	11	Total O 11 11	0	0
19	R	13	Total O 13 13	0	0
19	S	7	Total O 7 7	0	0
19	T	11	Total O 11 11	0	0
19	U	16	Total O 16 16	0	0
19	V	18	Total O 18 18	0	0
19	W	9	Total O 9 9	0	0
19	X	15	Total O 15 15	0	0
19	Y	14	Total O 14 14	0	0
19	Z	23	Total O 23 23	0	0
19	a	30	Total O 30 30	0	0
19	b	17	Total O 17 17	0	0
19	c	3	Total O 3 3	0	0
19	e	1	Total O 1 1	0	0
19	f	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	h	4	Total	O	0	0
			4	4		

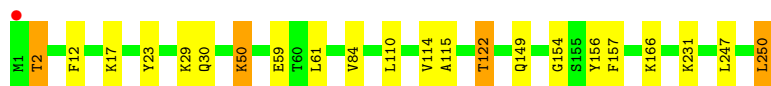
3 Residue-property plots [i](#)

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.

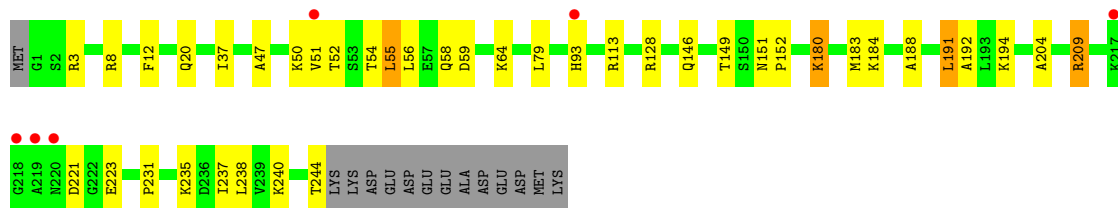
- Molecule 1: Proteasome subunit alpha type-2



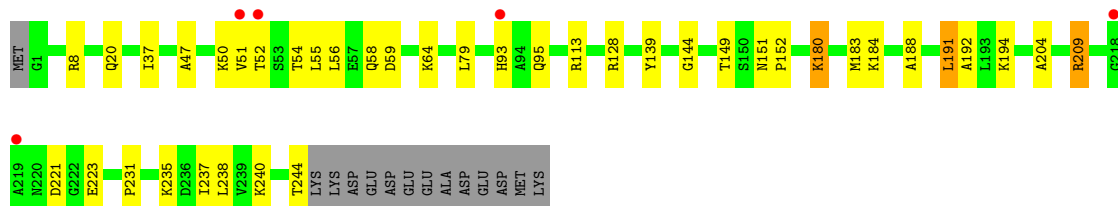
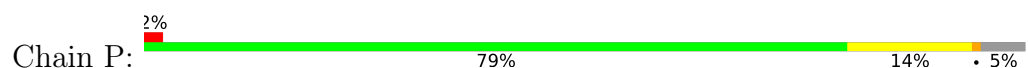
- Molecule 1: Proteasome subunit alpha type-2



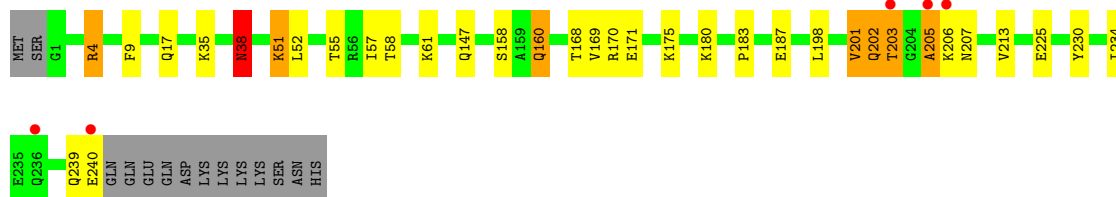
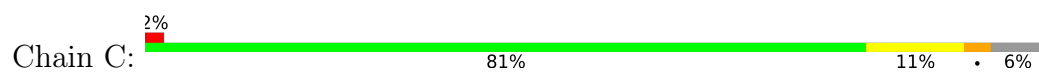
- Molecule 2: Proteasome subunit alpha type-3



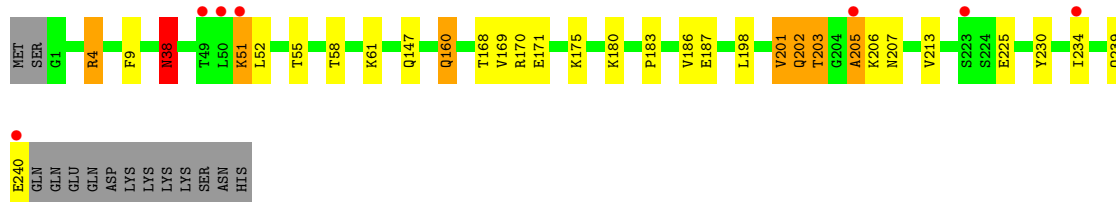
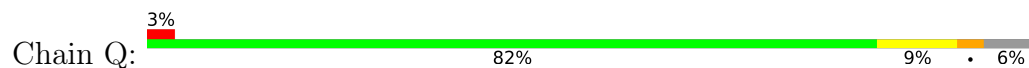
- Molecule 2: Proteasome subunit alpha type-3



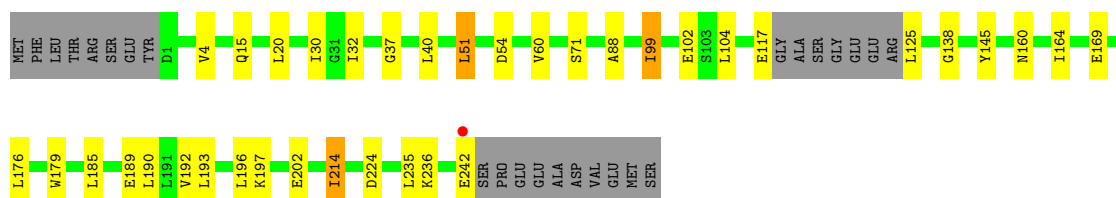
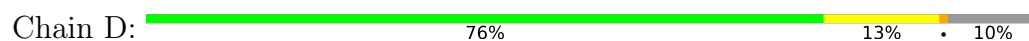
- Molecule 3: Proteasome subunit alpha type-4



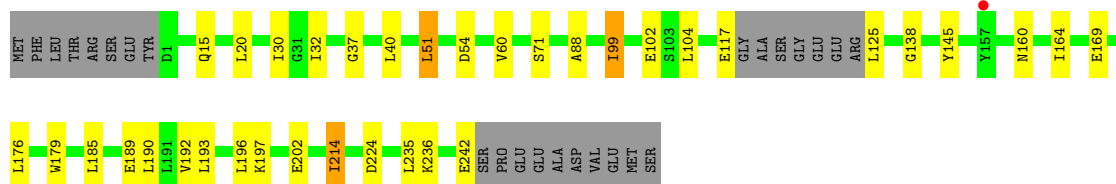
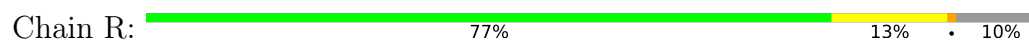
- Molecule 3: Proteasome subunit alpha type-4



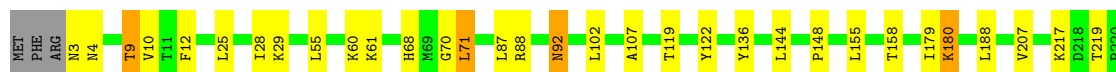
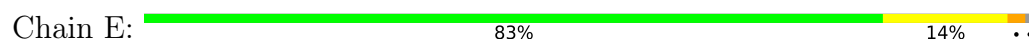
- Molecule 4: Proteasome subunit alpha type-5

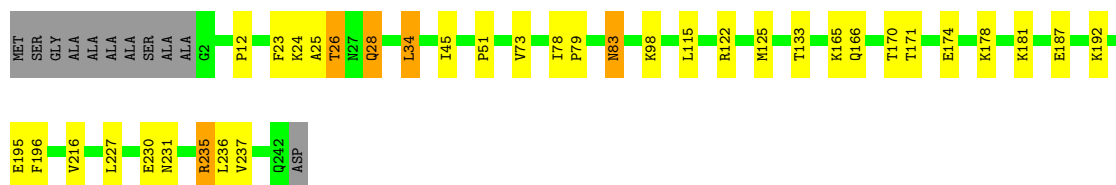


- Molecule 4: Proteasome subunit alpha type-5



- Molecule 5: Proteasome subunit alpha type-6





• Molecule 8: Proteasome subunit beta type-2

Chain H: 87% 8% . .



• Molecule 8: Proteasome subunit beta type-2

Chain V: 88% 7% . .



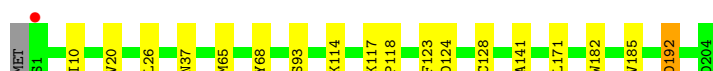
• Molecule 9: Proteasome subunit beta type-3

Chain I: 92% 7%



• Molecule 9: Proteasome subunit beta type-3

Chain W: 91% 8%



• Molecule 10: Proteasome subunit beta type-4

Chain J: 90% 7% . .



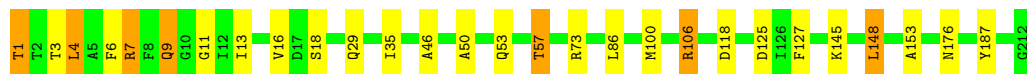
• Molecule 10: Proteasome subunit beta type-4

Chain X: 90% 7% . .



- Molecule 11: Proteasome subunit beta type-5

Chain K:  87% 10% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  90% 8% .



- Molecule 12: Proteasome subunit beta type-6

Chain L:  89% 9% .



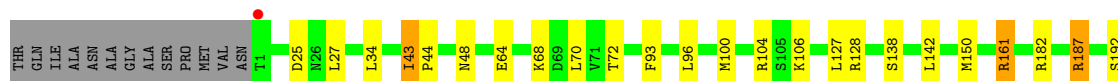
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  89% 9% .



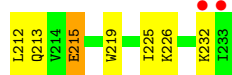
- Molecule 13: Proteasome subunit beta type-7

Chain M:  81% 12% . 5%



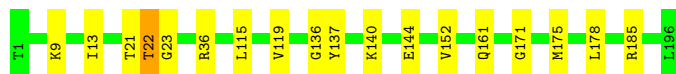
- Molecule 13: Proteasome subunit beta type-7

Chain a:  83% 11% . 5%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  91% 9%



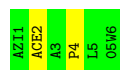
- Molecule 14: Proteasome subunit beta type-1

Chain b:  91% 9%

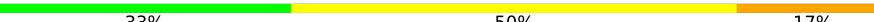


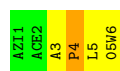
- Molecule 15: N3-APnLL-ep

Chain c:  67% 33%



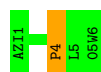
- Molecule 15: N3-APnLL-ep

Chain d:  33% 50% 17%



- Molecule 15: N3-APnLL-ep

Chain e:  83% 17%

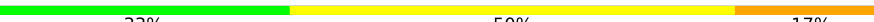


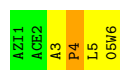
- Molecule 15: N3-APnLL-ep

Chain f:  83% 17%



- Molecule 15: N3-APnLL-ep

Chain g:  33% 50% 17%



- Molecule 15: N3-APnLL-ep



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.23Å 300.48Å 145.71Å 90.00° 113.18° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.60) 98.2 (15.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.208 0.195 , 0.211	Depositor DCC
R_{free} test set	16141 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50001	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/1952	0.75	0/2642
1	O	0.40	0/1952	0.75	0/2642
2	B	0.40	0/1934	0.76	0/2618
2	P	0.40	0/1934	0.76	0/2618
3	C	0.41	0/1910	0.80	1/2586 (0.0%)
3	Q	0.41	0/1910	0.80	1/2586 (0.0%)
4	D	0.39	0/1837	0.71	0/2475
4	R	0.40	0/1837	0.72	0/2475
5	E	0.40	0/1800	0.74	1/2433 (0.0%)
5	S	0.39	0/1800	0.75	1/2433 (0.0%)
6	F	0.41	0/1932	0.73	0/2609
6	T	0.40	0/1932	0.73	0/2609
7	G	0.40	0/1945	0.73	0/2634
7	U	0.39	0/1945	0.72	0/2634
8	H	0.39	0/1715	0.70	0/2326
8	V	0.40	1/1715 (0.1%)	0.70	0/2326
9	I	0.39	0/1611	0.73	0/2174
9	W	0.39	0/1611	0.73	0/2174
10	J	0.38	0/1589	0.70	0/2142
10	X	0.38	0/1589	0.70	0/2142
11	K	0.63	2/1681 (0.1%)	0.73	0/2274
11	Y	0.40	1/1681 (0.1%)	0.71	0/2274
12	L	0.38	0/1795	0.69	0/2420
12	Z	0.40	0/1795	0.69	0/2420
13	M	0.40	0/1855	0.71	0/2514
13	a	0.40	0/1855	0.71	0/2514
14	N	0.48	0/1541	0.77	1/2087 (0.0%)
14	b	0.49	0/1541	0.76	1/2087 (0.0%)
15	c	1.83	1/13 (7.7%)	1.88	1/18 (5.6%)
15	d	2.75	1/13 (7.7%)	1.20	0/18
15	e	2.69	1/13 (7.7%)	1.50	0/18
15	f	2.35	1/13 (7.7%)	1.32	0/18

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	2.53	1/13 (7.7%)	1.25	0/18
15	h	2.47	1/13 (7.7%)	1.08	0/18
All	All	0.42	10/50272 (0.0%)	0.73	7/67976 (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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	d	4	PRO	CA-C	-7.95	1.36	1.52
15	g	4	PRO	CA-C	-7.54	1.37	1.52
15	e	4	PRO	CA-C	-7.17	1.37	1.52
15	h	4	PRO	CA-C	-7.03	1.38	1.52
15	f	4	PRO	CA-C	-6.87	1.38	1.52
11	K	1	THR	CB-OG1	-6.81	1.32	1.43
11	K	11	GLY	C-O	-6.22	1.20	1.24
15	c	4	PRO	CA-C	-6.16	1.40	1.52
8	V	1	THR	CB-OG1	-5.86	1.34	1.43
11	Y	1	THR	CB-OG1	-5.43	1.35	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.32	116.95	110.82
3	C	201	VAL	N-CA-C	6.20	116.84	110.82
14	N	23	GLY	N-CA-C	-5.93	104.16	111.45
15	c	4	PRO	CA-N-CD	-5.61	104.15	112.00
14	b	24	ALA	N-CA-C	-5.44	106.01	113.30
5	S	180	LYS	CG-CD-CE	5.05	122.93	111.30
5	E	180	LYS	CG-CD-CE	5.02	122.85	111.30

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	9	0
1	O	1915	0	1929	9	0
2	B	1904	0	1904	20	0
2	P	1904	0	1904	18	0
3	C	1881	0	1895	18	0
3	Q	1881	0	1895	15	0
4	D	1813	0	1797	13	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	9	0
6	T	1892	0	1883	9	0
7	G	1907	0	1901	13	0
7	U	1907	0	1901	14	0
8	H	1684	0	1685	8	0
8	V	1684	0	1685	5	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	8	0
11	K	1644	0	1592	18	0
11	Y	1644	0	1592	12	0
12	L	1757	0	1711	13	0
12	Z	1757	0	1711	13	0
13	M	1824	0	1832	14	0
13	a	1824	0	1832	11	0
14	N	1512	0	1478	11	0
14	b	1512	0	1478	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	c	38	0	35	2	0
15	d	38	0	35	2	0
15	e	38	0	35	0	0
15	f	38	0	35	1	0
15	g	38	0	35	2	0
15	h	38	0	35	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	1	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	K	12	0	13	1	0
18	Y	12	0	13	0	0
19	A	19	0	0	0	0
19	B	17	0	0	0	0
19	C	12	0	0	0	0
19	D	7	0	0	0	0
19	E	9	0	0	0	0
19	F	16	0	0	0	0
19	G	26	0	0	0	0
19	H	20	0	0	1	0
19	I	12	0	0	0	0
19	J	15	0	0	0	0
19	K	16	0	0	0	0
19	L	23	0	0	0	0
19	M	20	0	0	0	0
19	N	17	0	0	1	0
19	O	8	0	0	0	0
19	P	11	0	0	0	0
19	Q	11	0	0	0	0
19	R	13	0	0	0	0
19	S	7	0	0	0	0
19	T	11	0	0	0	0
19	U	16	0	0	0	0
19	V	18	0	0	0	0
19	W	9	0	0	0	0
19	X	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	14	0	0	0	0
19	Z	23	0	0	0	0
19	a	30	0	0	0	0
19	b	17	0	0	0	0
19	c	3	0	0	0	0
19	e	1	0	0	0	0
19	f	2	0	0	0	0
19	h	4	0	0	0	0
All	All	50001	0	49286	298	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 (298) 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	1.56	0.88
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.55	0.88
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.83	0.78
11:K:53:GLN:O	11:K:57:THR:HG23	1.86	0.75
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.53	0.73
19:H:311:HOH:O	17:N:202:CL:CL	2.44	0.73
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.54	0.72
8:H:22:GLN:HE22	15:c:2:ACE:C	1.98	0.71
3:C:201:VAL:O	3:C:202:GLN:HB2	1.91	0.71
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.92	0.70
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.74	0.69
3:C:51:LYS:O	3:C:52:LEU:HB2	1.91	0.69
3:Q:201:VAL:O	3:Q:202:GLN:HB2	1.91	0.69
3:C:202:GLN:HG3	3:C:203:THR:H	1.56	0.69
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.56	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.75	0.69
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.24	0.68
7:G:23:PHE:O	7:G:26:THR:HB	1.95	0.66
11:K:100:MET:CE	11:K:127:PHE:HB2	2.25	0.66
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.77	0.66
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.78	0.65
7:U:23:PHE:O	7:U:26:THR:HB	1.97	0.65
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.80	0.63
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.80	0.61
5:S:12:PHE:H	6:T:19:GLN:HE22	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.50	0.59
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.68	0.59
11:K:100:MET:HE3	11:K:127:PHE:CB	2.30	0.59
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.68	0.59
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.59
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.29	0.59
3:C:201:VAL:O	3:C:202:GLN:CB	2.50	0.58
14:b:152:VAL:HA	14:b:175:MET:HE1	1.85	0.58
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.68	0.58
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.68	0.58
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.86	0.57
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.85	0.57
8:H:52:THR:O	8:H:56:THR:HB	2.06	0.56
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.86	0.56
6:F:123:ASN:C	6:F:123:ASN:HD22	2.14	0.56
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.88	0.56
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.88	0.55
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.53	0.55
5:E:12:PHE:H	6:F:19:GLN:HE22	1.54	0.55
6:T:123:ASN:C	6:T:123:ASN:HD22	2.14	0.55
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.72	0.55
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.53	0.55
8:V:52:THR:O	8:V:56:THR:HB	2.06	0.55
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.21	0.55
11:K:106:ARG:HH11	11:K:106:ARG:HB3	1.72	0.55
11:Y:106:ARG:HH11	11:Y:106:ARG:HB3	1.72	0.54
2:B:183:MET:HE1	2:B:191:LEU:HD12	1.89	0.54
2:P:183:MET:HE1	2:P:191:LEU:HD12	1.90	0.54
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.89	0.54
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.90	0.54
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.89	0.54
7:G:34:LEU:C	7:G:34:LEU:HD23	2.33	0.54
3:C:230:TYR:O	3:C:234:ILE:HG13	2.07	0.54
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.90	0.53
3:Q:230:TYR:O	3:Q:234:ILE:HG13	2.07	0.53
6:T:31:THR:HB	6:T:47:GLU:HG2	1.91	0.53
10:X:1:MET:HA	10:X:34:LYS:CE	2.38	0.53
10:J:1:MET:HA	10:J:34:LYS:HE3	1.90	0.53
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.08	0.53
12:L:8:ASN:HA	12:L:30:ILE:O	2.08	0.53
6:F:31:THR:HB	6:F:47:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.44	0.53
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.90	0.53
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.91	0.52
10:J:1:MET:HA	10:J:34:LYS:CE	2.39	0.52
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.91	0.52
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.75	0.52
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.45	0.52
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.90	0.52
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.75	0.52
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.90	0.52
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.52
7:U:34:LEU:C	7:U:34:LEU:HD23	2.34	0.52
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.91	0.52
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.45	0.52
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.92	0.52
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.92	0.51
10:X:1:MET:HA	10:X:34:LYS:HE3	1.90	0.51
13:M:150:MET:HE1	13:M:187:ARG:HG2	1.93	0.51
8:H:22:GLN:NE2	15:c:2:ACE:O	2.41	0.51
11:Y:49:ALA:HA	15:g:6:05W:H17	1.93	0.51
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.93	0.51
14:N:22:THR:HG23	14:N:22:THR:O	2.10	0.51
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.92	0.50
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.93	0.50
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.41	0.50
18:K:302:MES:O1S	15:d:6:05W:H28	2.12	0.50
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.60	0.50
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.77	0.50
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.93	0.50
2:B:204:ALA:O	2:B:209:ARG:NH2	2.45	0.50
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.93	0.50
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.93	0.50
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.47	0.50
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.50
2:P:204:ALA:O	2:P:209:ARG:NH2	2.45	0.50
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.93	0.50
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.47	0.49
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.77	0.49
4:R:51:LEU:C	4:R:51:LEU:HD12	2.38	0.49
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.94	0.49
9:W:124:ASP:OD2	15:f:4:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.48	0.49
11:K:9:GLN:NE2	11:K:148:LEU:O	2.45	0.49
14:b:22:THR:HG23	14:b:22:THR:O	2.13	0.49
3:C:51:LYS:HD2	3:C:51:LYS:HA	1.71	0.49
11:K:4:LEU:C	11:K:4:LEU:CD2	2.86	0.49
5:S:68:HIS:HE1	5:S:102:LEU:O	1.95	0.49
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.93	0.49
5:E:68:HIS:HE1	5:E:102:LEU:O	1.96	0.48
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.95	0.48
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.77	0.48
5:E:9:THR:HG21	5:E:119:THR:HA	1.96	0.48
8:V:84:LYS:HG3	8:V:85:GLN:N	2.28	0.48
4:R:185:LEU:O	4:R:189:GLU:HG3	2.14	0.48
4:D:51:LEU:HD12	4:D:51:LEU:C	2.37	0.48
8:H:50:ALA:HB3	9:I:126:ILE:HD12	1.95	0.48
2:B:3:ARG:NH1	5:E:122:TYR:OH	2.47	0.48
1:O:12:PHE:H	2:P:20:GLN:HE22	1.62	0.48
2:P:180:LYS:O	2:P:183:MET:HB2	2.14	0.47
7:U:73:VAL:HG12	7:U:133:THR:HB	1.96	0.47
2:P:183:MET:HE2	2:P:188:ALA:HA	1.96	0.47
4:D:185:LEU:O	4:D:189:GLU:HG3	2.15	0.47
6:F:194:LYS:HD3	6:F:242:GLU:HG3	1.97	0.47
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.96	0.47
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.41	0.47
2:B:237:ILE:HD12	2:B:240:LYS:HE3	1.96	0.47
9:I:65:MET:HE1	9:I:93:SER:HB3	1.97	0.47
6:T:194:LYS:HD3	6:T:242:GLU:HG3	1.97	0.47
7:G:73:VAL:HG12	7:G:133:THR:HB	1.96	0.47
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.47
5:S:9:THR:HG21	5:S:119:THR:HA	1.96	0.47
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.44	0.47
8:H:84:LYS:HG3	8:H:85:GLN:N	2.28	0.47
14:N:137:TYR:CE1	14:b:140:LYS:HG3	2.50	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.46
2:B:180:LYS:O	2:B:183:MET:HB2	2.14	0.46
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.97	0.46
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.28	0.46
7:U:45:ILE:HG22	7:U:216:VAL:HG13	1.97	0.46
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.96	0.46
1:O:149:GLN:O	1:O:156:TYR:HA	2.16	0.46
3:Q:51:LYS:HD2	3:Q:51:LYS:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.97	0.46
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.97	0.46
2:B:183:MET:HE2	2:B:188:ALA:HA	1.96	0.46
3:C:38:ASN:N	3:C:38:ASN:HD22	2.14	0.46
2:P:237:ILE:HD12	2:P:240:LYS:HE3	1.96	0.46
4:R:99:ILE:HD13	4:R:104:LEU:HB2	1.98	0.46
7:G:45:ILE:HG22	7:G:216:VAL:HG13	1.97	0.46
2:P:59:ASP:HB3	2:P:231:PRO:HG2	1.98	0.46
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.41	0.46
6:F:146:MET:HE3	6:F:161:THR:HB	1.97	0.46
13:M:43:ILE:HG21	13:M:64:GLU:HG2	1.97	0.46
6:T:146:MET:HE3	6:T:161:THR:HB	1.97	0.46
1:A:149:GLN:O	1:A:156:TYR:HA	2.16	0.46
1:A:247:LEU:O	1:A:250:LEU:HB2	2.16	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.45
4:D:99:ILE:HD13	4:D:104:LEU:HB2	1.98	0.45
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.98	0.45
11:K:4:LEU:C	11:K:4:LEU:HD22	2.42	0.45
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.14	0.45
2:B:59:ASP:HB3	2:B:231:PRO:HG2	1.98	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.45
11:K:1:THR:HG21	11:K:46:ALA:HB2	1.99	0.45
13:a:43:ILE:HG21	13:a:64:GLU:HG2	1.98	0.45
1:O:247:LEU:O	1:O:250:LEU:HB2	2.16	0.45
7:G:196:PHE:CD1	7:G:196:PHE:C	2.95	0.45
11:K:86:LEU:C	11:K:86:LEU:HD13	2.42	0.45
9:W:65:MET:HE1	9:W:93:SER:HB3	1.97	0.45
13:M:182:ARG:NH2	13:M:215:GLU:O	2.50	0.45
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.30	0.44
11:K:7:ARG:HG2	11:K:7:ARG:HH11	1.82	0.44
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.90	0.44
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.18	0.44
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.53	0.44
6:T:34:ILE:HG22	6:T:160:ALA:HB2	2.00	0.44
7:U:196:PHE:CD1	7:U:196:PHE:C	2.95	0.44
13:a:182:ARG:NH2	13:a:215:GLU:O	2.50	0.44
11:K:18:SER:OG	11:K:29:GLN:O	2.35	0.44
1:A:50:LYS:O	1:A:50:LYS:HG3	2.18	0.44
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.53	0.44
5:E:155:LEU:HD13	5:E:158:THR:HB	2.00	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
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.33	0.43
7:U:83:ASN:C	7:U:83:ASN:ND2	2.76	0.43
14:N:140:LYS:HG3	14:b:137:TYR:CE1	2.53	0.43
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.48	0.43
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.53	0.43
7:G:83:ASN:C	7:G:83:ASN:ND2	2.76	0.43
11:K:50:ALA:CB	12:L:128:VAL:HG23	2.49	0.43
2:P:37:ILE:HD12	2:P:192:ALA:HB2	2.00	0.43
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.53	0.43
5:S:155:LEU:HD13	5:S:158:THR:HB	2.00	0.43
5:S:98:PHE:O	13:a:91:TYR:HA	2.17	0.43
3:C:202:GLN:CG	3:C:203:THR:H	2.26	0.43
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.48	0.43
11:K:13:ILE:HG13	11:K:153:ALA:HB1	1.99	0.43
5:S:226:GLY:O	5:S:229:VAL:HG22	2.18	0.43
5:E:226:GLY:O	5:E:229:VAL:HG22	2.19	0.43
6:T:238:PHE:O	6:T:242:GLU:HG2	2.19	0.43
6:F:34:ILE:HG22	6:F:160:ALA:HB2	2.00	0.43
13:M:187:ARG:HG3	14:b:25:TYR:CE1	2.53	0.43
11:Y:30:THR:OG1	12:Z:132:GLU:OE2	2.28	0.43
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.54	0.43
2:B:93:HIS:CG	2:B:113:ARG:HE	2.37	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.43
3:C:168:THR:O	3:C:171:GLU:HB3	2.19	0.43
10:J:3:ILE:HB	10:J:18:SER:HB3	2.00	0.43
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.43
2:B:37:ILE:HD12	2:B:192:ALA:HB2	2.01	0.42
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.54	0.42
1:O:50:LYS:O	1:O:50:LYS:HG3	2.18	0.42
13:a:93:PHE:CE2	13:a:128:ARG:HD3	2.54	0.42
1:A:110:LEU:O	1:A:114:VAL:HG23	2.19	0.42
13:M:93:PHE:CE2	13:M:128:ARG:HD3	2.53	0.42
15:d:3:ALA:HA	15:d:4:PRO:HD3	1.78	0.42
15:g:3:ALA:HA	15:g:4:PRO:HD3	1.84	0.42
2:B:12:PHE:H	3:C:17:GLN:HE22	1.67	0.42
6:F:238:PHE:O	6:F:242:GLU:HG2	2.19	0.42
7:G:170:THR:O	7:G:174:GLU:HG3	2.20	0.42
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.54	0.42
7:U:227:LEU:HB3	7:U:231:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:3:THR:HB	11:K:16:VAL:HG12	2.01	0.42
2:P:93:HIS:CG	2:P:113:ARG:HE	2.37	0.42
10:X:3:ILE:HB	10:X:18:SER:HB3	2.00	0.42
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.49	0.42
7:G:25:ALA:O	7:G:28:GLN:HB2	2.19	0.42
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.02	0.42
7:U:170:THR:O	7:U:174:GLU:HG3	2.20	0.42
1:A:12:PHE:H	2:B:20:GLN:HE22	1.68	0.42
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.02	0.42
7:G:83:ASN:C	7:G:83:ASN:HD22	2.28	0.42
7:U:25:ALA:O	7:U:28:GLN:HB2	2.20	0.42
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.55	0.42
3:C:35:LYS:HG2	3:C:158:SER:O	2.20	0.42
3:Q:205:ALA:C	3:Q:207:ASN:H	2.28	0.42
3:C:9:PHE:H	4:D:15:GLN:HE22	1.68	0.41
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.53	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.41
13:a:25:ASP:HA	13:a:195:PHE:CB	2.50	0.41
1:A:115:ALA:HB1	1:A:154:GLY:O	2.20	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.41
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.02	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.41
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.03	0.41
1:O:115:ALA:HB1	1:O:154:GLY:O	2.20	0.41
7:U:83:ASN:C	7:U:83:ASN:HD22	2.28	0.41
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.50	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
14:N:185:ARG:NH1	19:N:301:HOH:O	2.48	0.41
5:S:71:LEU:C	5:S:71:LEU:HD23	2.45	0.41
7:G:227:LEU:HB3	7:G:231:ASN:HB2	2.01	0.41
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.56	0.41
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.60	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.41
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.60	0.41
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.03	0.41
12:L:195:HIS:HD2	12:L:197:GLN:H	1.69	0.41
14:N:13:ILE:HG21	14:N:175:MET:CE	2.51	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.56	0.41
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.69	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.41
14:N:22:THR:O	14:N:22:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.50	0.41
13:M:25:ASP:HA	13:M:195:PHE:CB	2.50	0.41
1:O:110:LEU:O	1:O:114:VAL:HG23	2.21	0.41
3:C:205:ALA:C	3:C:207:ASN:H	2.28	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.41
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.56	0.41
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.55	0.41
13:a:27:LEU:HB2	13:a:192:SER:HB3	2.02	0.41
5:E:88:ARG:O	5:E:92:ASN:HB2	2.21	0.41
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.03	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.56	0.41
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.55	0.40
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.56	0.40
4:D:71:SER:HB3	4:D:164:ILE:HD12	2.03	0.40
11:Y:116:ASP:OD1	11:Y:116:ASP:C	2.64	0.40
4:D:4:VAL:HG13	4:D:15:GLN:HG3	2.03	0.40
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.03	0.40
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.55	0.40
11:K:6:PHE:HA	11:K:125:ASP:O	2.21	0.40
8:V:8:PHE:O	8:V:9:ASN:C	2.65	0.40
9:W:123:PHE:HA	9:W:128:CYS:O	2.22	0.40
5:E:71:LEU:HD23	5:E:71:LEU:C	2.46	0.40
8:H:8:PHE:O	8:H:9:ASN:C	2.65	0.40
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.57	0.40
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.30	0.40
4:R:71:SER:HB3	4:R:164:ILE:HD12	2.03	0.40
6:T:165:ARG:HG2	6:T:166:GLN:N	2.37	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	34
1	O	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	16	34
2	B	242/258 (94%)	230 (95%)	9 (4%)	3 (1%)	10	23
2	P	242/258 (94%)	230 (95%)	9 (4%)	3 (1%)	10	23
3	C	238/254 (94%)	227 (95%)	6 (2%)	5 (2%)	5	11
3	Q	238/254 (94%)	227 (95%)	6 (2%)	5 (2%)	5	11
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%)	218 (95%)	11 (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%)	235 (98%)	3 (1%)	1 (0%)	30	51
7	U	239/252 (95%)	235 (98%)	3 (1%)	1 (0%)	30	51
8	H	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	24	46
8	V	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	24	46
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	46
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	46
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	24	46
12	L	220/222 (99%)	215 (98%)	5 (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%)	225 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
15	c	2/6 (33%)	2 (100%)	0	0	100	100
15	d	2/6 (33%)	2 (100%)	0	0	100	100
15	e	2/6 (33%)	2 (100%)	0	0	100	100
15	f	2/6 (33%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	g	2/6 (33%)	2 (100%)	0	0	100	100
15	h	2/6 (33%)	2 (100%)	0	0	100	100
All	All	6288/6650 (95%)	6084 (97%)	177 (3%)	27 (0%)	30	51

All (27) 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	Y	9	GLN
2	B	221	ASP
3	C	183	PRO
2	P	221	ASP
3	Q	183	PRO
3	C	206	LYS
3	Q	206	LYS
7	U	51	PRO
1	A	166	LYS
7	G	51	PRO
1	O	166	LYS

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	40
1	O	209/209 (100%)	197 (94%)	12 (6%)	18	40
2	B	203/216 (94%)	187 (92%)	16 (8%)	11	26
2	P	203/216 (94%)	187 (92%)	16 (8%)	11	26
3	C	212/226 (94%)	195 (92%)	17 (8%)	11	25
3	Q	212/226 (94%)	194 (92%)	18 (8%)	10	22
4	D	194/215 (90%)	174 (90%)	20 (10%)	7	15
4	R	194/215 (90%)	174 (90%)	20 (10%)	7	15
5	E	190/193 (98%)	172 (90%)	18 (10%)	8	18
5	S	190/193 (98%)	172 (90%)	18 (10%)	8	18
6	F	201/239 (84%)	182 (90%)	19 (10%)	8	18
6	T	201/239 (84%)	182 (90%)	19 (10%)	8	18
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%)	171 (94%)	10 (6%)	19	41
8	V	181/190 (95%)	172 (95%)	9 (5%)	22	46
9	I	172/173 (99%)	166 (96%)	6 (4%)	32	59
9	W	172/173 (99%)	166 (96%)	6 (4%)	32	59
10	J	173/175 (99%)	166 (96%)	7 (4%)	28	55
10	X	173/175 (99%)	166 (96%)	7 (4%)	28	55
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	43
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	54
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	47
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	47
13	M	199/208 (96%)	183 (92%)	16 (8%)	11	25
13	a	199/208 (96%)	183 (92%)	16 (8%)	11	25
14	N	162/162 (100%)	154 (95%)	8 (5%)	22	47
14	b	162/162 (100%)	154 (95%)	8 (5%)	22	47
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	e	1/1 (100%)	0	1 (100%)	0	0
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%)	0	1 (100%)	0	0
All	All	5318/5546 (96%)	4948 (93%)	370 (7%)	14	31

All (370) 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	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	209	ARG
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

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Mol	Chain	Res	Type
3	C	58	THR
3	C	61	LYS
3	C	147	GLN
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

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Mol	Chain	Res	Type
5	E	71	LEU
5	E	92	ASN
5	E	144	LEU
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	94	SER
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

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Mol	Chain	Res	Type
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
7	G	237	VAL
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
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	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	7	ARG
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	13	LEU
12	L	23	LEU
12	L	49	ASN
12	L	66	LYS
12	L	136	CYS

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	P	56	LEU
2	P	58	GLN
2	P	79	LEU
2	P	149	THR
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	209	ARG
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	186	VAL
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

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Mol	Chain	Res	Type
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
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	94	SER
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	118	ASP
11	Y	148	LEU
12	Z	1	GLN
12	Z	13	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	66	LYS
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

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Mol	Chain	Res	Type
15	e	4	PRO
15	h	4	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) 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
2	B	124	HIS
2	B	146	GLN
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	17	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	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	165	GLN
5	E	184	ASN

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Mol	Chain	Res	Type
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
8	H	66	HIS
8	H	86	HIS
8	H	116	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	63	ASN
10	J	10	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	112	ASN
10	J	146	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	153	GLN

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Mol	Chain	Res	Type
12	L	158	ASN
13	M	48	ASN
13	M	62	HIS
13	M	102	GLN
13	M	179	ASN
14	N	38	HIS
14	N	69	GLN
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
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	115	GLN
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	91	HIS
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	90	GLN
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN

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Mol	Chain	Res	Type
5	S	151	ASN
5	S	165	GLN
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	116	HIS
8	V	141	HIS
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	24	ASN
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

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Mol	Chain	Res	Type
12	Z	80	ASN
12	Z	153	GLN
12	Z	159	GLN
12	Z	165	ASN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	179	ASN
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 ⓘ

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	NLE	f	5	15	6,7,8	0.80	0	2,7,9	0.86	0
15	NLE	c	5	15	6,7,8	0.73	0	2,7,9	1.20	0
15	NLE	d	5	15	6,7,8	1.55	1 (16%)	2,7,9	1.00	0
15	NLE	h	5	15	6,7,8	0.97	1 (16%)	2,7,9	0.75	0
15	NLE	e	5	15	6,7,8	0.67	0	2,7,9	0.56	0
15	NLE	g	5	15	6,7,8	1.22	1 (16%)	2,7,9	0.72	0

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	NLE	f	5	15	-	2/5/6/8	-
15	NLE	c	5	15	-	1/5/6/8	-
15	NLE	d	5	15	-	0/5/6/8	-
15	NLE	h	5	15	-	2/5/6/8	-
15	NLE	e	5	15	-	2/5/6/8	-
15	NLE	g	5	15	-	1/5/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	d	5	NLE	CB-CA	-3.49	1.48	1.53
15	g	5	NLE	CB-CA	-2.55	1.49	1.53
15	h	5	NLE	CB-CA	-2.09	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	h	5	NLE	CA-CB-CG-CD
15	f	5	NLE	CA-CB-CG-CD
15	h	5	NLE	CE-CD-CG-CB
15	e	5	NLE	CE-CD-CG-CB
15	c	5	NLE	CA-CB-CG-CD
15	e	5	NLE	CA-CB-CG-CD
15	g	5	NLE	CE-CD-CG-CB
15	f	5	NLE	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	MES	K	302	-	12,12,12	2.26	1 (8%)	15,16,16	1.20	2 (13%)
18	MES	Y	301	-	12,12,12	2.26	1 (8%)	15,16,16	1.14	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	Y	301	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	301	MES	C8-S	-7.51	1.67	1.77
18	K	302	MES	C8-S	-7.47	1.67	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	301	MES	O2S-S-C8	2.19	110.03	106.73
18	K	302	MES	O3S-S-C8	2.08	110.08	106.00
18	K	302	MES	O1S-S-C8	2.07	109.86	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	302	MES	1	0

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, 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%)	-0.37	2 (0%) 82 80	37, 55, 88, 132	0
1	O	250/250 (100%)	-0.32	1 (0%) 88 86	40, 62, 101, 137	0
2	B	244/258 (94%)	-0.19	6 (2%) 58 52	39, 60, 107, 154	0
2	P	244/258 (94%)	-0.13	5 (2%) 65 60	43, 63, 109, 159	0
3	C	240/254 (94%)	-0.20	5 (2%) 63 58	40, 62, 127, 149	0
3	Q	240/254 (94%)	0.08	7 (2%) 53 48	44, 75, 152, 173	0
4	D	235/260 (90%)	-0.23	1 (0%) 88 86	42, 66, 99, 149	0
4	R	235/260 (90%)	-0.17	1 (0%) 88 86	46, 68, 107, 155	0
5	E	231/234 (98%)	-0.21	0 100 100	46, 68, 100, 140	0
5	S	231/234 (98%)	-0.02	2 (0%) 81 78	46, 71, 112, 150	0
6	F	243/288 (84%)	-0.22	2 (0%) 82 80	40, 61, 113, 141	0
6	T	243/288 (84%)	-0.21	5 (2%) 63 58	40, 63, 110, 154	0
7	G	241/252 (95%)	-0.28	1 (0%) 88 86	34, 56, 93, 141	0
7	U	241/252 (95%)	-0.39	0 100 100	39, 56, 90, 115	0
8	H	222/232 (95%)	-0.38	0 100 100	39, 53, 80, 120	0
8	V	222/232 (95%)	-0.34	0 100 100	40, 56, 82, 134	0
9	I	204/205 (99%)	-0.54	0 100 100	36, 51, 78, 102	0
9	W	204/205 (99%)	-0.52	1 (0%) 87 85	34, 52, 83, 114	0
10	J	195/198 (98%)	-0.44	1 (0%) 87 85	34, 53, 81, 137	0
10	X	195/198 (98%)	-0.50	1 (0%) 87 85	37, 54, 82, 146	0
11	K	212/212 (100%)	-0.48	0 100 100	39, 53, 82, 107	0
11	Y	212/212 (100%)	-0.41	1 (0%) 87 85	41, 54, 83, 108	0
12	L	222/222 (100%)	-0.48	0 100 100	38, 55, 82, 101	0
12	Z	222/222 (100%)	-0.46	0 100 100	37, 53, 81, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.44	2 (0%) 81 78	38, 53, 78, 114	0
13	a	233/246 (94%)	-0.45	3 (1%) 75 71	36, 51, 76, 118	0
14	N	196/196 (100%)	-0.50	0 100 100	36, 49, 77, 106	0
14	b	196/196 (100%)	-0.47	1 (0%) 87 85	36, 49, 77, 102	0
15	c	2/6 (33%)	0.19	0 100 100	61, 61, 61, 69	0
15	d	2/6 (33%)	-0.61	0 100 100	60, 60, 60, 69	0
15	e	2/6 (33%)	-0.62	0 100 100	49, 49, 49, 56	0
15	f	2/6 (33%)	0.79	0 100 100	65, 65, 65, 70	0
15	g	2/6 (33%)	-0.41	0 100 100	61, 61, 61, 71	0
15	h	2/6 (33%)	-0.72	0 100 100	51, 51, 51, 56	0
All	All	6348/6650 (95%)	-0.32	48 (0%) 82 80	34, 58, 101, 173	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	1	MET	5.7
10	X	1	MET	5.3
3	Q	50	LEU	4.7
13	a	233	ILE	3.7
2	B	218	GLY	3.6
1	A	1	MET	3.4
7	G	2	GLY	3.4
6	F	202	ASP	3.2
5	S	225	ASP	3.2
2	B	51	VAL	3.0
1	O	1	MET	2.8
3	Q	234	ILE	2.8
13	M	1	THR	2.8
2	P	51	VAL	2.8
3	Q	240	GLU	2.8
6	T	178	HIS	2.7
4	D	242	GLU	2.7
6	F	215	CYS	2.7
3	Q	51	LYS	2.6
3	Q	49	THR	2.6
2	B	219	ALA	2.6
2	P	52	THR	2.5
13	a	1	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	93	HIS	2.5
2	P	93	HIS	2.5
2	P	219	ALA	2.5
6	T	244	ASN	2.5
14	b	103	ASP	2.5
11	Y	212	GLY	2.5
2	B	220	ASN	2.4
3	C	206	LYS	2.4
2	B	217	LYS	2.3
4	R	157	TYR	2.3
1	A	201	GLU	2.3
3	C	205	ALA	2.3
13	M	233	ILE	2.3
9	W	1	SER	2.3
6	T	241	LYS	2.2
6	T	205	GLU	2.2
2	P	218	GLY	2.2
13	a	232	LYS	2.2
3	C	236	GLN	2.2
3	C	203	THR	2.1
6	T	204	LYS	2.1
3	Q	223	SER	2.1
3	Q	205	ALA	2.1
3	C	240	GLU	2.0
5	S	52	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	NLE	e	5	8/9	0.91	0.12	39,42,48,49	0
15	NLE	f	5	8/9	0.91	0.11	63,65,68,72	0
15	NLE	c	5	8/9	0.94	0.10	56,58,69,76	0
15	NLE	h	5	8/9	0.95	0.08	44,49,54,56	0
15	NLE	d	5	8/9	0.96	0.08	46,49,56,58	0
15	NLE	g	5	8/9	0.97	0.05	44,45,50,50	0

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
18	MES	K	302	12/12	0.87	0.14	74,84,94,100	0
18	MES	Y	301	12/12	0.89	0.13	71,79,90,92	0
16	MG	I	301	1/1	0.94	0.10	56,56,56,56	0
16	MG	N	201	1/1	0.94	0.07	52,52,52,52	0
17	CL	N	202	1/1	0.95	0.22	30,30,30,30	0
16	MG	K	301	1/1	0.96	0.11	58,58,58,58	0
17	CL	b	201	1/1	0.96	0.26	30,30,30,30	0
16	MG	G	301	1/1	0.96	0.04	55,55,55,55	0
16	MG	Z	301	1/1	0.96	0.05	56,56,56,56	0
17	CL	G	302	1/1	0.97	0.19	30,30,30,30	0
16	MG	L	301	1/1	0.97	0.06	67,67,67,67	0
17	CL	U	301	1/1	0.97	0.20	30,30,30,30	0
16	MG	I	302	1/1	0.99	0.04	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.