



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:43 am GMT

PDB ID : 4Y8O  
Title : Yeast 20S proteasome beta7-delta7\_Cter mutant in complex with Ac-PAF-ep  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-02-16  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

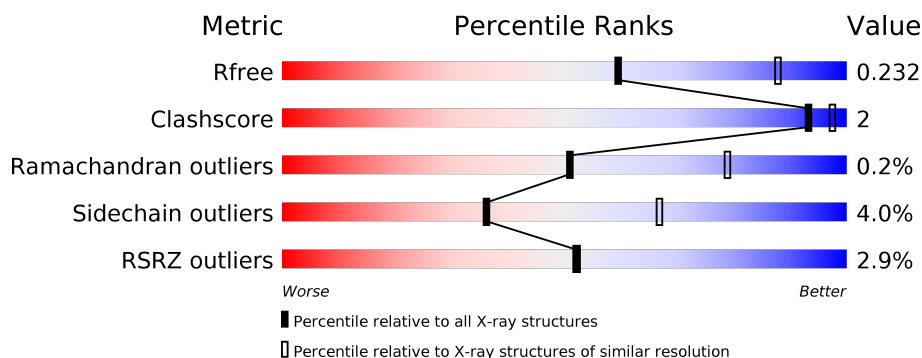
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	O	250	<div> <div>4%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>
2	B	258	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
2	P	258	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
3	C	254	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
3	Q	254	<div> <div>9%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>


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Mol	Chain	Length	Quality of chain
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	239	
13	a	239	
14	N	196	
14	b	196	
15	c	5	
15	d	5	
15	e	5	

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Mol	Chain	Length	Quality of chain
15	f	5	 <div>80%20%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MG	I	301	-	-	-	X
16	MG	Z	301	-	-	-	X
18	MES	K	302	-	-	-	X
18	MES	e	101	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49748 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	1	0
			1764	1120	305	335	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1736	1098	297	334	7			
13	a	222	Total	C	N	O	S	0	0	0
			1736	1098	297	334	7			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			30	22	3	5			
15	d	5	Total	C	N	O	0	0	0
			30	22	3	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	5	Total	C	N	O	0	0	0
			30	22	3	5			
15	f	5	Total	C	N	O	0	0	0
			30	22	3	5			

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

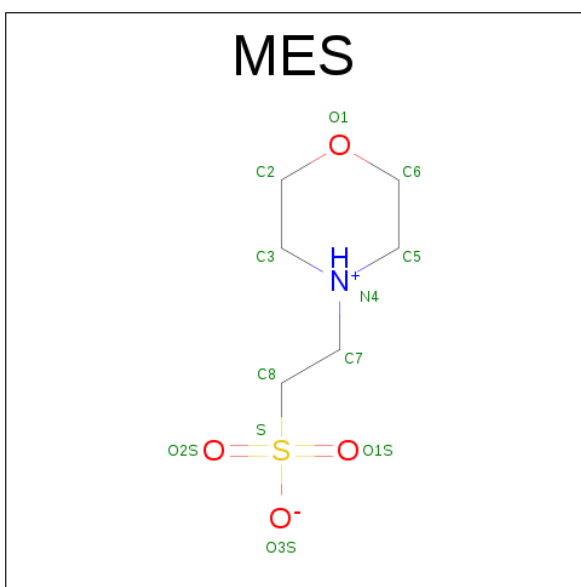
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	I	2	Total	Mg	0	0
			2	2		
16	Z	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	L	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	e	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	24	Total	O	0	0
			24	24		
19	B	21	Total	O	0	0
			21	21		
19	C	11	Total	O	0	0
			11	11		
19	D	11	Total	O	0	0
			11	11		
19	E	8	Total	O	0	0
			8	8		
19	F	13	Total	O	0	0
			13	13		
19	G	20	Total	O	0	0
			20	20		
19	H	20	Total	O	0	0
			20	20		
19	I	17	Total	O	0	0
			17	17		
19	J	17	Total	O	0	0
			17	17		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	28	Total O 28 28	0	0
19	L	21	Total O 21 21	0	0
19	M	12	Total O 12 12	0	0
19	N	13	Total O 13 13	0	0
19	O	13	Total O 13 13	0	0
19	P	10	Total O 10 10	0	0
19	Q	7	Total O 7 7	0	0
19	R	8	Total O 8 8	0	0
19	S	8	Total O 8 8	0	0
19	T	17	Total O 17 17	0	0
19	U	24	Total O 24 24	0	0
19	V	18	Total O 18 18	0	0
19	W	22	Total O 22 22	0	0
19	X	26	Total O 26 26	0	0
19	Y	16	Total O 16 16	0	0
19	Z	20	Total O 20 20	0	0
19	a	25	Total O 25 25	0	0
19	b	10	Total O 10 10	0	0
19	c	1	Total O 1 1	0	0
19	d	2	Total O 2 2	0	0
19	e	3	Total O 3 3	0	0

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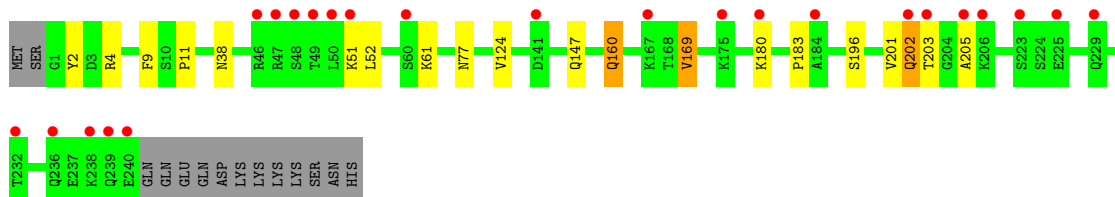
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	f	2	Total	O	0	0
			2	2		




GLN  
GLN  
GLN  
GLN  
ASP  
LYS  
LYS  
LYS  
LYS  
SER  
ASN  
HIS

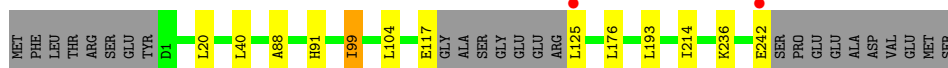
• Molecule 3: Proteasome subunit alpha type-4

Chain Q: 




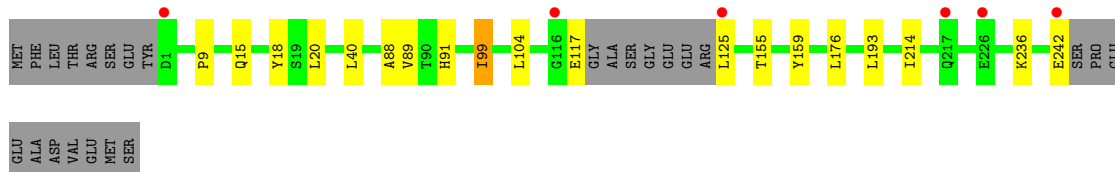
• Molecule 4: Proteasome subunit alpha type-5

Chain D: 

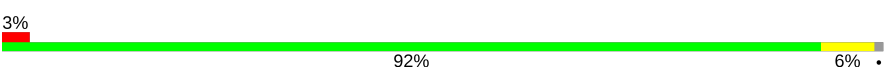


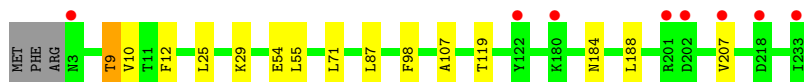
• Molecule 4: Proteasome subunit alpha type-5

Chain R: 

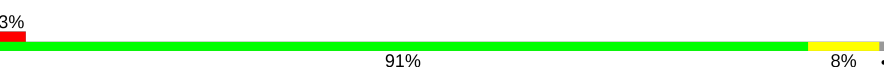


• Molecule 5: Proteasome subunit alpha type-6

Chain E: 




• Molecule 5: Proteasome subunit alpha type-6

Chain S: 

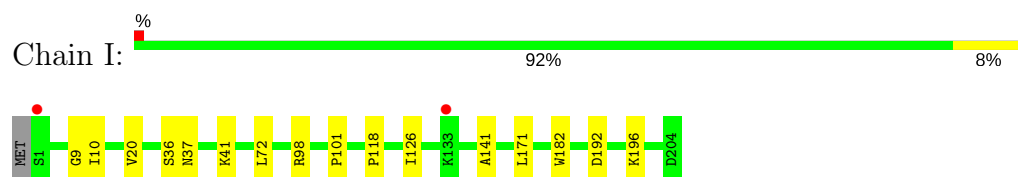


• Molecule 6: Probable proteasome subunit alpha type-7

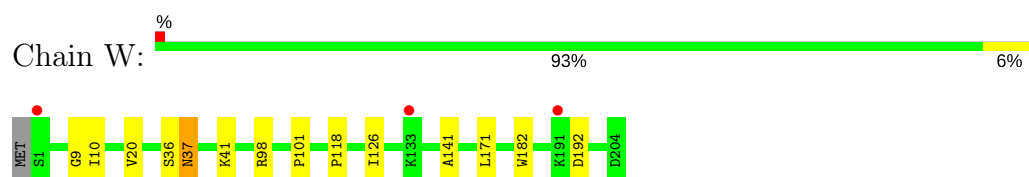
Chain F: 



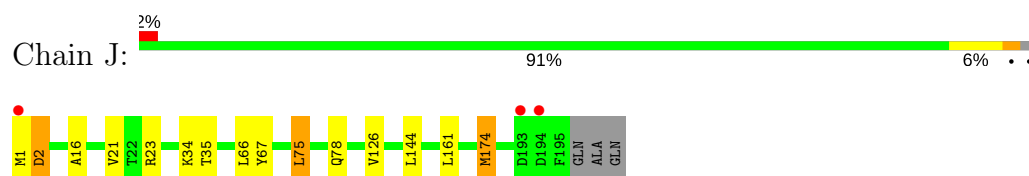
- Molecule 9: Proteasome subunit beta type-3



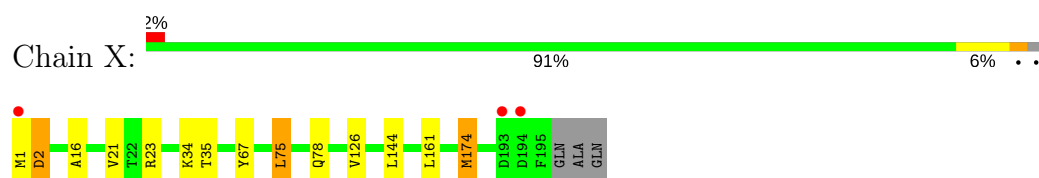
- Molecule 9: Proteasome subunit beta type-3



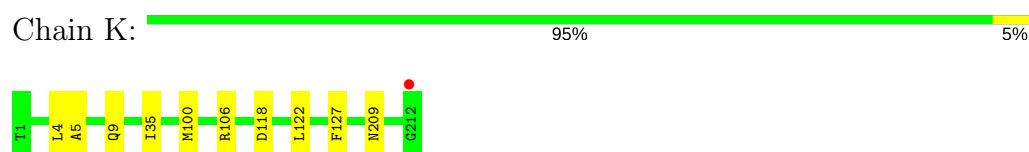
- Molecule 10: Proteasome subunit beta type-4



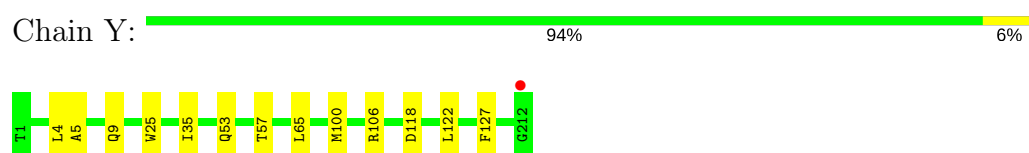
- Molecule 10: Proteasome subunit beta type-4



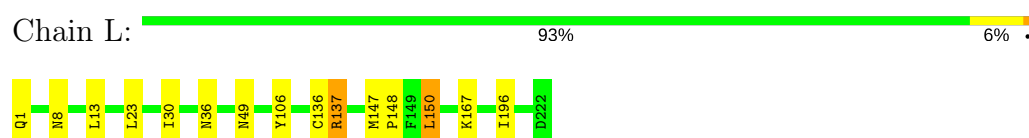
- Molecule 11: Proteasome subunit beta type-5



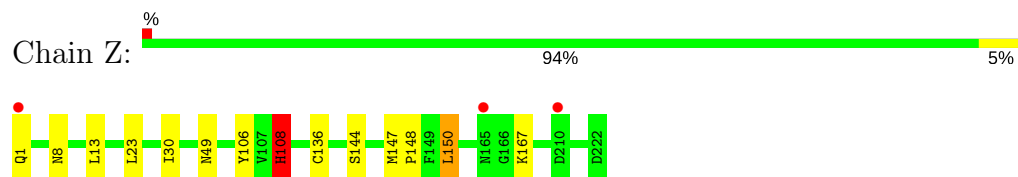
- Molecule 11: Proteasome subunit beta type-5



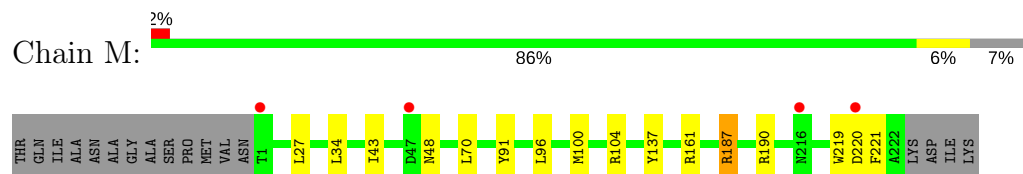
- Molecule 12: Proteasome subunit beta type-6



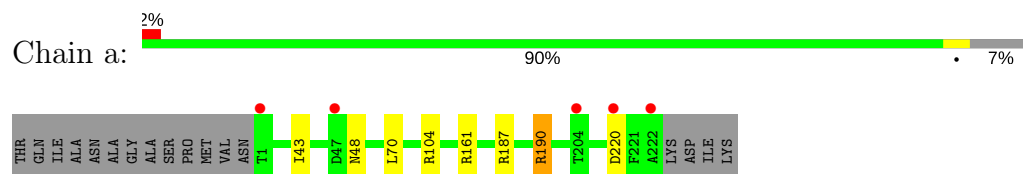
- Molecule 12: Proteasome subunit beta type-6



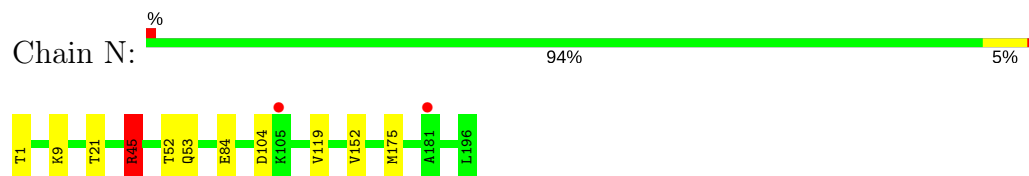
- Molecule 13: Proteasome subunit beta type-7



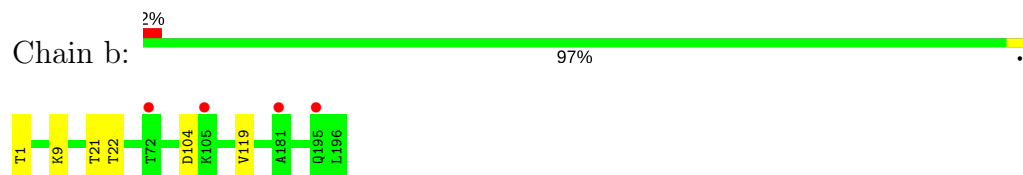
- Molecule 13: Proteasome subunit beta type-7



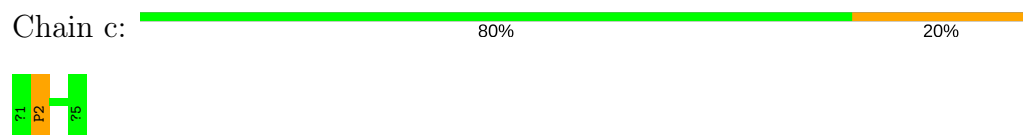
- Molecule 14: Proteasome subunit beta type-1



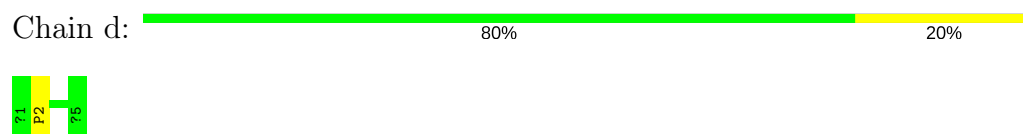
- Molecule 14: Proteasome subunit beta type-1



- Molecule 15: Ac-PAF-ep




- Molecule 15: Ac-PAF-ep




- Molecule 15: Ac-PAF-ep



Chain e:  80% 20%



- Molecule 15: Ac-PAF-ep

Chain f:  80% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.39Å 298.81Å 146.44Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (15.00-2.70) 96.5 (15.00-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.209 , 0.231 0.210 , 0.232	Depositor DCC
$R_{free}$ test set	14107 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	49748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, ACE, CL, PHL, POL, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.29	0/1952	0.49	0/2642
1	O	0.28	0/1952	0.48	0/2642
2	B	0.29	0/1934	0.50	0/2618
2	P	0.29	0/1934	0.50	0/2618
3	C	0.29	0/1910	0.51	0/2586
3	Q	0.29	0/1910	0.51	0/2586
4	D	0.28	0/1837	0.49	0/2475
4	R	0.28	0/1837	0.49	0/2475
5	E	0.28	0/1800	0.48	0/2433
5	S	0.28	0/1800	0.48	0/2433
6	F	0.29	0/1932	0.46	0/2609
6	T	0.28	0/1932	0.46	0/2609
7	G	0.29	0/1945	0.48	0/2634
7	U	0.29	0/1945	0.48	0/2634
8	H	0.32	0/1715	0.50	0/2326
8	V	0.32	0/1715	0.53	0/2326
9	I	0.29	0/1611	0.49	0/2174
9	W	0.29	0/1611	0.49	0/2174
10	J	0.28	0/1589	0.50	0/2142
10	X	0.28	0/1589	0.50	0/2142
11	K	0.29	0/1681	0.51	0/2274
11	Y	0.29	0/1681	0.52	0/2274
12	L	0.31	0/1795	0.49	0/2420
12	Z	0.39	2/1806 (0.1%)	0.59	4/2435 (0.2%)
13	M	0.36	0/1766	0.58	2/2398 (0.1%)
13	a	0.34	0/1766	0.60	2/2398 (0.1%)
14	N	0.33	0/1541	0.73	4/2087 (0.2%)
14	b	0.35	0/1541	0.50	1/2087 (0.0%)
15	c	2.89	1/13 (7.7%)	1.93	0/18
15	d	1.97	1/13 (7.7%)	0.91	0/18
15	e	2.95	1/13 (7.7%)	2.73	1/18 (5.6%)
15	f	1.97	1/13 (7.7%)	0.94	0/18

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.31	6/50079 (0.0%)	0.52	14/67723 (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
14	N	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	2	PRO	CA-C	-7.91	1.37	1.52
15	c	2	PRO	CA-C	-7.85	1.37	1.52
12	Z	108[A]	HIS	CA-C	7.54	1.72	1.52
12	Z	108[B]	HIS	CA-C	7.54	1.72	1.52
15	f	2	PRO	CA-C	-6.62	1.39	1.52
15	d	2	PRO	CA-C	-6.59	1.39	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	45	ARG	NE-CZ-NH2	-17.95	111.33	120.30
14	N	45	ARG	NE-CZ-NH1	12.19	126.39	120.30
13	a	190	ARG	NE-CZ-NH2	11.37	125.98	120.30
14	N	45	ARG	CD-NE-CZ	10.05	137.67	123.60
13	M	190	ARG	NE-CZ-NH2	10.03	125.31	120.30
12	Z	108[A]	HIS	CA-C-O	8.46	137.86	120.10
12	Z	108[B]	HIS	CA-C-O	8.46	137.86	120.10
13	a	190	ARG	NE-CZ-NH1	-8.27	116.16	120.30
15	e	2	PRO	CA-N-CD	-7.42	101.11	111.50
12	Z	108[A]	HIS	CA-C-N	-6.38	103.16	117.20
12	Z	108[B]	HIS	CA-C-N	-6.38	103.16	117.20
13	M	190	ARG	NE-CZ-NH1	-6.08	117.26	120.30
14	N	1	THR	N-CA-C	5.45	125.72	111.00
14	b	1	THR	N-CA-C	5.41	125.60	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	45	ARG	Sidechain

## 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	8	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	10	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	9	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	8	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	8	0
8	H	1684	0	1688	11	0
8	V	1684	0	1688	10	0
9	I	1581	0	1574	10	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	8	0
11	K	1644	0	1592	5	0
11	Y	1644	0	1592	7	0
12	L	1757	0	1711	7	0
12	Z	1764	0	1718	5	0
13	M	1736	0	1737	12	0
13	a	1736	0	1737	0	0
14	N	1512	0	1478	4	0
14	b	1512	0	1478	0	0
15	c	30	0	30	0	0
15	d	30	0	30	0	0
15	e	30	0	29	0	0
15	f	30	0	30	0	0
16	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	U	1	0	0	0	0
18	K	12	0	13	0	0
18	e	12	0	13	0	0
19	A	24	0	0	0	0
19	B	21	0	0	0	0
19	C	11	0	0	0	0
19	D	11	0	0	0	0
19	E	8	0	0	0	0
19	F	13	0	0	0	0
19	G	20	0	0	0	0
19	H	20	0	0	0	0
19	I	17	0	0	0	0
19	J	17	0	0	0	0
19	K	28	0	0	0	0
19	L	21	0	0	0	0
19	M	12	0	0	0	0
19	N	13	0	0	0	0
19	O	13	0	0	0	0
19	P	10	0	0	0	0
19	Q	7	0	0	0	0
19	R	8	0	0	0	0
19	S	8	0	0	0	0
19	T	17	0	0	1	0
19	U	24	0	0	0	0
19	V	18	0	0	0	0
19	W	22	0	0	0	0
19	X	26	0	0	0	0
19	Y	16	0	0	0	0
19	Z	20	0	0	0	0
19	a	25	0	0	0	0
19	b	10	0	0	0	0
19	c	1	0	0	0	0
19	d	2	0	0	0	0
19	e	3	0	0	0	0
19	f	2	0	0	0	0
All	All	49748	0	49018	142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:O	10:X:2:ASP:HB2	1.87	0.74
10:J:1:MET:O	10:J:2:ASP:HB2	1.88	0.72
13:M:219:TRP:O	13:M:221:PHE:N	2.23	0.70
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.79	0.65
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.79	0.65
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.82	0.62
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.81	0.62
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.81	0.62
8:H:22:GLN:HG2	8:H:27:ALA:HB2	1.82	0.61
8:V:22:GLN:HG2	8:V:27:ALA:HB2	1.82	0.60
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.83	0.60
8:H:119:THR:H	14:N:53:GLN:HE22	1.52	0.58
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.58
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.85	0.58
7:G:23:PHE:O	7:G:26:THR:HB	2.04	0.58
13:M:219:TRP:C	13:M:221:PHE:H	2.08	0.57
14:N:45:ARG:HD2	14:N:52:THR:HB	1.88	0.56
6:T:215:CYS:HB3	19:T:310:HOH:O	2.05	0.56
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.88	0.56
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.88	0.55
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.89	0.54
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.07	0.54
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.37	0.54
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.89	0.54
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.71	0.54
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.72	0.54
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.90	0.53
1:O:55:LEU:HB3	7:U:159:ALA:O	2.09	0.53
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.91	0.53
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.53
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.75	0.52
14:N:152:VAL:HA	14:N:175:MET:HE1	1.91	0.52
10:J:1:MET:O	10:J:2:ASP:CB	2.58	0.52
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.74	0.52
5:S:12:PHE:H	6:T:19:GLN:HE22	1.57	0.52
10:X:1:MET:O	10:X:2:ASP:CB	2.58	0.52
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:NH2	7:G:152:GLY:O	2.41	0.51
10:J:174:MET:HA	10:X:174:MET:HA	1.93	0.50
13:M:221:PHE:HD2	13:M:221:PHE:O	1.94	0.50
13:M:221:PHE:CD2	13:M:221:PHE:C	2.85	0.50
11:K:209:ASN:O	9:W:37:ASN:ND2	2.44	0.50
6:F:97:LYS:NZ	14:N:84:GLU:OE1	2.41	0.50
8:V:114:HIS:HD2	8:V:116:HIS:H	1.60	0.49
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.49
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.94	0.49
11:K:100:MET:CE	11:K:127:PHE:HB2	2.43	0.49
5:E:12:PHE:H	6:F:19:GLN:HE22	1.61	0.49
3:C:201:VAL:HG13	3:C:202:GLN:N	2.28	0.49
8:H:114:HIS:HD2	8:H:116:HIS:H	1.60	0.48
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.28	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.95	0.48
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.42	0.48
3:C:201:VAL:O	3:C:202:GLN:CB	2.62	0.48
12:L:36:ASN:HB3	13:M:137:TYR:CD1	2.49	0.48
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.48
1:A:7:PHE:HB3	3:C:2:TYR:CE1	2.49	0.48
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.62	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.48
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.44	0.48
8:H:3:ILE:HG12	8:H:127:LEU:O	2.15	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
8:H:218:VAL:HG21	9:I:196:LYS:HB2	1.95	0.47
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.15	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.98	0.46
9:W:98:ARG:O	9:W:126:ILE:HD11	2.16	0.46
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.51	0.46
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.96	0.46
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.51	0.46
3:C:201:VAL:O	3:C:202:GLN:HB2	2.15	0.46
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.99	0.45
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.52	0.45
8:H:81:GLN:OE1	8:H:84:LYS:NZ	2.50	0.45
5:E:9:THR:HG21	5:E:119:THR:HA	1.99	0.45
13:M:221:PHE:O	13:M:221:PHE:CD2	2.70	0.45
9:I:98:ARG:O	9:I:126:ILE:HD11	2.17	0.45
12:L:8:ASN:HA	12:L:30:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.45
8:V:112:SER:O	8:V:119:THR:HA	2.16	0.44
1:O:7:PHE:HB3	3:Q:2:TYR:CE1	2.52	0.44
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.52	0.44
1:A:14:PRO:HA	2:B:23:TYR:CD1	2.53	0.44
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.99	0.44
5:S:9:THR:HG21	5:S:119:THR:HA	1.99	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.44
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.53	0.44
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.53	0.44
12:L:137:ARG:HA	12:L:137:ARG:HD3	1.72	0.43
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.44	0.43
1:A:149:GLN:O	1:A:156:TYR:HA	2.18	0.43
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.66	0.43
5:S:18:LEU:HD21	6:T:126:ARG:HD2	2.01	0.43
1:O:61:LEU:HB2	7:U:155:VAL:HG23	1.99	0.43
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.43
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.43
5:E:98:PHE:O	13:M:91:TYR:HA	2.18	0.43
8:V:81:GLN:OE1	8:V:84:LYS:NZ	2.52	0.43
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.33	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.43
3:C:92:GLN:HG3	10:J:66:LEU:HB2	2.00	0.43
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.43
2:P:1:GLY:HA3	5:S:122:TYR:CD1	2.54	0.43
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.43
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.54	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.43
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.42
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.01	0.42
13:M:221:PHE:O	8:V:123:TYR:HE2	2.01	0.42
1:A:23:TYR:CD1	7:G:12:PRO:HA	2.54	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
12:L:36:ASN:HB3	13:M:137:TYR:CE1	2.54	0.42
8:H:19:ARG:NH1	8:H:167:LEU:O	2.53	0.42
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.02	0.42
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.02	0.42
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:HA	10:J:34:LYS:CE	2.50	0.42
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.01	0.42
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.01	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.49	0.41
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.41
12:L:196:ILE:HB	8:V:167:LEU:HB3	2.02	0.41
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.02	0.41
4:R:89:VAL:HG11	11:Y:65:LEU:HG	2.02	0.41
4:R:155:THR:HG23	5:S:59:GLN:HE22	1.86	0.41
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.02	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.84	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.84	0.41
8:V:19:ARG:NH1	8:V:167:LEU:O	2.53	0.41
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.03	0.41
6:T:228:LYS:HE3	6:T:228:LYS:HB2	1.82	0.41
8:V:52:THR:O	8:V:56:THR:HB	2.21	0.41
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.21	0.40
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.02	0.40
2:B:95:GLN:HG3	9:I:72:LEU:HG	2.02	0.40
1:O:54:PRO:HG2	7:U:174:GLU:HG2	2.03	0.40
8:H:52:THR:O	8:H:56:THR:HB	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	248/250 (99%)	242 (98%)	5 (2%)	1 (0%)	38 66
1	O	248/250 (99%)	241 (97%)	6 (2%)	1 (0%)	38 66
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	38 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	38	66
3	C	238/254 (94%)	229 (96%)	6 (2%)	3 (1%)	14	35
3	Q	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	14	35
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	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%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	32	60
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	32	60
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
13	M	220/239 (92%)	214 (97%)	5 (2%)	1 (0%)	32	60
13	a	220/239 (92%)	214 (97%)	5 (2%)	1 (0%)	32	60
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
15	c	2/5 (40%)	2 (100%)	0	0	100	100
15	d	2/5 (40%)	2 (100%)	0	0	100	100
15	e	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
15	f	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6263/6620 (95%)	6100 (97%)	148 (2%)	15 (0%)	51	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
13	M	220	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
13	a	220	ASP
15	e	2	PRO
3	C	205	ALA
3	Q	205	ALA
1	A	3	ASP
1	O	3	ASP
3	C	183	PRO
3	Q	183	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	71	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	71	90
2	B	203/216 (94%)	195 (96%)	8 (4%)	37	68
2	P	203/216 (94%)	195 (96%)	8 (4%)	37	68
3	C	212/226 (94%)	203 (96%)	9 (4%)	34	65
3	Q	212/226 (94%)	203 (96%)	9 (4%)	34	65
4	D	194/215 (90%)	184 (95%)	10 (5%)	27	55
4	R	194/215 (90%)	184 (95%)	10 (5%)	27	55
5	E	190/193 (98%)	180 (95%)	10 (5%)	26	54
5	S	190/193 (98%)	180 (95%)	10 (5%)	26	54
6	F	201/239 (84%)	190 (94%)	11 (6%)	25	52
6	T	201/239 (84%)	190 (94%)	11 (6%)	25	52
7	G	206/210 (98%)	198 (96%)	8 (4%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	206/210 (98%)	198 (96%)	8 (4%)	37	68
8	H	181/190 (95%)	169 (93%)	12 (7%)	19	43
8	V	181/190 (95%)	168 (93%)	13 (7%)	17	39
9	I	172/173 (99%)	168 (98%)	4 (2%)	56	84
9	W	172/173 (99%)	168 (98%)	4 (2%)	56	84
10	J	173/175 (99%)	167 (96%)	6 (4%)	41	72
10	X	173/175 (99%)	167 (96%)	6 (4%)	41	72
11	K	169/169 (100%)	164 (97%)	5 (3%)	46	76
11	Y	169/169 (100%)	164 (97%)	5 (3%)	46	76
12	L	185/185 (100%)	177 (96%)	8 (4%)	33	64
12	Z	186/185 (100%)	177 (95%)	9 (5%)	30	59
13	M	190/203 (94%)	184 (97%)	6 (3%)	44	75
13	a	190/203 (94%)	183 (96%)	7 (4%)	39	70
14	N	162/162 (100%)	158 (98%)	4 (2%)	53	82
14	b	162/162 (100%)	157 (97%)	5 (3%)	45	75
15	c	1/1 (100%)	0	1 (100%)	0	0
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
All	All	5299/5534 (96%)	5085 (96%)	214 (4%)	36	67

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	191	LEU

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Mol	Chain	Res	Type
3	C	4	ARG
3	C	38	ASN
3	C	61	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	40	LEU
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
6	F	14	ASP
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU

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Mol	Chain	Res	Type
7	G	125	MET
7	G	154	TYR
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	31	CYS
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	84	LYS
8	H	120	ASP
8	H	127	LEU
8	H	185	GLU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	136	CYS
12	L	137	ARG
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE

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Mol	Chain	Res	Type
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	21	THR
14	N	104	ASP
14	N	119	VAL
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	61	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	40	LEU
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	10	VAL
5	S	25	LEU

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Mol	Chain	Res	Type
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
6	T	14	ASP
6	T	59	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	154	TYR
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	3	ILE
8	V	22	GLN
8	V	30	ASN
8	V	31	CYS
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	84	LYS
8	V	120	ASP
8	V	127	LEU
8	V	185	GLU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP

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Mol	Chain	Res	Type
9	W	192	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	108[A]	HIS
12	Z	108[B]	HIS
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	190	ARG
14	b	9	LYS
14	b	21	THR
14	b	22	THR
14	b	104	ASP
14	b	119	VAL
15	c	2	PRO
15	e	2	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN

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Mol	Chain	Res	Type
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	6	HIS
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
8	H	30	ASN
8	H	57	GLN
8	H	114	HIS
8	H	189	ASN
10	J	55	GLN
10	J	118	GLN
11	K	85	ASN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	70	ASN
12	L	158	ASN
13	M	18	ASN

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Mol	Chain	Res	Type
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	53	GLN
1	O	94	HIS
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	92	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
8	V	30	ASN
8	V	57	GLN
8	V	66	HIS
8	V	114	HIS
8	V	165	ASN
8	V	189	ASN
8	V	200	GLN

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Mol	Chain	Res	Type
10	X	55	GLN
10	X	65	GLN
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	79	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN
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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	PHL	c	4	11,15	11,11,11	1.78	1 (9%)	11,13,13	1.44	2 (18%)
15	PHL	d	4	15,14	11,11,11	1.48	1 (9%)	11,13,13	1.63	3 (27%)
15	PHL	e	4	11,15	11,11,11	1.77	2 (18%)	11,13,13	1.53	2 (18%)
15	PHL	f	4	15,14	11,11,11	1.47	1 (9%)	11,13,13	1.65	3 (27%)

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	PHL	c	4	11,15	-	0/6/6/6	0/1/1/1
15	PHL	d	4	15,14	-	0/6/6/6	0/1/1/1
15	PHL	e	4	11,15	-	0/6/6/6	0/1/1/1
15	PHL	f	4	15,14	-	0/6/6/6	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	PHL	CB-CG	-5.28	1.38	1.51
15	e	4	PHL	CB-CG	-5.14	1.39	1.51
15	d	4	PHL	CB-CG	-4.31	1.41	1.51
15	f	4	PHL	CB-CG	-4.29	1.41	1.51
15	e	4	PHL	O-C	-2.04	1.33	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	4	PHL	CB-CA-C	-3.10	106.08	112.16
15	f	4	PHL	CB-CA-C	-3.09	106.10	112.16
15	f	4	PHL	CB-CG-CD2	-2.89	115.07	120.91
15	d	4	PHL	CB-CG-CD2	-2.85	115.15	120.91
15	e	4	PHL	O-C-CA	-2.18	103.49	111.47
15	c	4	PHL	O-C-CA	-2.05	103.98	111.47
15	c	4	PHL	CG-CB-CA	2.46	117.85	113.27
15	e	4	PHL	CG-CB-CA	2.52	117.97	113.27
15	d	4	PHL	CB-CG-CD1	2.94	126.84	120.91
15	f	4	PHL	CB-CG-CD1	3.01	126.99	120.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 9 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	2.13	1 (8%)	14,16,16	1.62	3 (21%)
18	MES	e	101	-	12,12,12	2.11	1 (8%)	14,16,16	1.64	3 (21%)

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	e	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	K	302	MES	C8-S	-7.11	1.66	1.77
18	e	101	MES	C8-S	-7.03	1.67	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	e	101	MES	O1S-S-C8	2.30	108.77	106.79
18	K	302	MES	O1S-S-C8	2.59	109.02	106.79
18	K	302	MES	O2S-S-C8	2.78	109.18	106.79
18	e	101	MES	O3S-S-C8	3.19	109.98	106.06
18	K	302	MES	O3S-S-C8	3.79	110.71	106.06
18	e	101	MES	O2S-S-C8	3.83	110.08	106.79

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.15	8 (3%)	48	48	42, 55, 90, 132	0
1	O	250/250 (100%)	-0.09	11 (4%)	35	33	45, 63, 106, 135	0
2	B	244/258 (94%)	-0.04	13 (5%)	27	25	41, 60, 111, 169	0
2	P	244/258 (94%)	-0.00	14 (5%)	24	23	45, 63, 109, 167	0
3	C	240/254 (94%)	0.05	17 (7%)	17	14	44, 64, 128, 159	0
3	Q	240/254 (94%)	0.32	24 (10%)	8	6	47, 76, 153, 192	0
4	D	235/260 (90%)	-0.20	2 (0%)	84	85	44, 63, 96, 137	0
4	R	235/260 (90%)	-0.06	6 (2%)	56	56	52, 70, 104, 149	0
5	E	231/234 (98%)	-0.06	8 (3%)	44	44	49, 66, 97, 145	0
5	S	231/234 (98%)	0.03	7 (3%)	51	50	47, 69, 106, 144	0
6	F	243/288 (84%)	-0.14	10 (4%)	38	36	41, 62, 108, 137	0
6	T	243/288 (84%)	0.01	12 (4%)	30	29	41, 64, 111, 144	0
7	G	241/252 (95%)	-0.13	8 (3%)	47	46	40, 57, 99, 150	0
7	U	241/252 (95%)	-0.29	6 (2%)	58	58	42, 56, 88, 131	0
8	H	222/232 (95%)	-0.11	4 (1%)	69	70	43, 56, 85, 126	0
8	V	222/232 (95%)	-0.02	5 (2%)	61	61	43, 58, 85, 129	0
9	I	204/205 (99%)	-0.45	2 (0%)	82	82	38, 51, 78, 101	0
9	W	204/205 (99%)	-0.36	3 (1%)	74	75	39, 54, 81, 106	0
10	J	195/198 (98%)	-0.33	3 (1%)	74	75	41, 52, 78, 127	0
10	X	195/198 (98%)	-0.30	3 (1%)	74	75	41, 54, 78, 134	0
11	K	212/212 (100%)	-0.38	1 (0%)	90	92	39, 52, 76, 95	0
11	Y	212/212 (100%)	-0.34	1 (0%)	90	92	41, 53, 82, 106	0
12	L	222/222 (100%)	-0.36	0	100	100	41, 55, 79, 102	0
12	Z	222/222 (100%)	-0.24	3 (1%)	75	76	41, 55, 84, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	222/239 (92%)	-0.32	4 (1%) 69 70	38, 54, 78, 95	0
13	a	222/239 (92%)	-0.33	5 (2%) 61 61	38, 52, 76, 94	0
14	N	196/196 (100%)	-0.36	2 (1%) 82 82	38, 50, 77, 105	0
14	b	196/196 (100%)	-0.33	4 (2%) 65 66	37, 50, 80, 100	0
15	c	2/5 (40%)	-0.56	0 100 100	73, 73, 73, 83	0
15	d	2/5 (40%)	-0.12	0 100 100	64, 64, 64, 71	0
15	e	2/5 (40%)	0.11	0 100 100	71, 71, 71, 85	0
15	f	2/5 (40%)	-0.03	0 100 100	67, 67, 67, 77	0
All	All	6322/6620 (95%)	-0.17	186 (2%) 52 52	37, 58, 100, 192	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	8.5
3	Q	50	LEU	7.0
2	B	218	GLY	6.9
10	X	1	MET	6.8
5	E	202	ASP	6.8
3	Q	49	THR	5.9
10	X	194	ASP	5.8
3	Q	206	LYS	5.7
2	B	220	ASN	5.7
2	P	219	ALA	5.5
1	A	1	MET	5.5
3	C	206	LYS	5.5
5	S	202	ASP	5.3
2	B	242	GLY	5.2
1	O	249	ALA	5.1
10	J	1	MET	5.1
10	J	194	ASP	5.0
2	B	219	ALA	4.9
8	V	222	ASP	4.9
11	Y	212	GLY	4.9
2	P	221	ASP	4.7
3	Q	240	GLU	4.6
2	P	59	ASP	4.6
3	C	180	LYS	4.5
8	H	222	ASP	4.5
3	Q	238	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
3	Q	236	GLN	4.4
6	F	202	ASP	4.4
13	M	220	ASP	4.4
3	Q	225	GLU	4.4
3	C	49	THR	4.3
8	V	221	CYS	4.2
4	D	242	GLU	4.1
11	K	212	GLY	4.1
2	B	51	VAL	4.0
3	C	239	GLN	4.0
2	B	59	ASP	3.8
2	P	51	VAL	3.8
3	Q	239	GLN	3.8
8	H	221	CYS	3.8
7	G	2	GLY	3.8
1	O	2	THR	3.8
3	C	202	GLN	3.8
3	C	236	GLN	3.7
9	W	1	SER	3.7
9	I	133	LYS	3.6
2	P	222	GLY	3.5
4	D	125	LEU	3.5
6	F	203	ASN	3.5
13	M	1	THR	3.5
3	Q	48	SER	3.4
13	a	1	THR	3.4
1	A	249	ALA	3.4
2	P	220	ASN	3.4
3	C	225	GLU	3.4
3	C	50	LEU	3.4
6	T	241	LYS	3.3
7	G	241	GLU	3.3
13	a	220	ASP	3.3
6	T	244	ASN	3.3
3	Q	184	ALA	3.3
7	U	222	ASP	3.2
6	T	181	GLU	3.2
2	B	221	ASP	3.2
3	Q	229	GLN	3.2
2	P	218	GLY	3.1
3	Q	205	ALA	3.1
3	Q	51	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	238	LYS	3.1
7	G	181	LYS	3.1
7	G	188	GLU	3.1
1	O	231	LYS	3.1
9	W	133	LYS	3.1
7	G	3	TYR	3.0
3	Q	202	GLN	3.0
3	Q	223	SER	3.0
6	F	205	GLU	3.0
1	A	201	GLU	3.0
7	U	241	GLU	3.0
4	R	242	GLU	2.9
14	N	105	LYS	2.9
1	O	201	GLU	2.9
6	T	180	PRO	2.9
6	F	244	ASN	2.9
8	V	217	ILE	2.8
6	T	2	THR	2.8
2	P	225	TYR	2.8
4	R	217	GLN	2.8
6	F	181	GLU	2.8
7	U	242	GLN	2.8
1	A	250	LEU	2.8
12	Z	210	ASP	2.8
6	T	215	CYS	2.8
2	B	52	THR	2.8
5	E	207	VAL	2.7
7	G	68	ARG	2.7
13	M	47	ASP	2.7
6	T	205	GLU	2.7
1	A	248	GLU	2.7
7	G	242	GLN	2.7
10	J	193	ASP	2.6
14	b	105	LYS	2.6
2	B	203	SER	2.6
2	P	50	LYS	2.6
3	C	175	LYS	2.6
7	U	2	GLY	2.6
6	F	241	LYS	2.6
3	Q	175	LYS	2.5
6	T	217	LEU	2.5
8	V	215	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
5	S	3	ASN	2.5
3	C	205	ALA	2.5
6	T	178	HIS	2.5
5	E	3	ASN	2.5
6	T	204	LYS	2.5
7	U	181	LYS	2.5
7	G	240	ALA	2.5
6	F	243	ILE	2.5
2	P	182	ASP	2.5
14	N	181	ALA	2.4
3	C	37	LYS	2.4
5	E	218	ASP	2.4
2	P	52	THR	2.4
4	R	125	LEU	2.4
3	Q	47	ARG	2.4
6	T	53	LYS	2.4
2	B	235	LYS	2.4
1	A	231	LYS	2.3
2	P	203	SER	2.3
8	V	196	ARG	2.3
5	S	180	LYS	2.3
6	F	53	LYS	2.3
8	H	204	LYS	2.3
3	C	240	GLU	2.3
1	O	245	ASP	2.3
1	O	52	SER	2.3
1	O	182	GLU	2.3
2	B	230	LYS	2.3
4	R	116	GLY	2.2
4	R	226	GLU	2.2
3	Q	180	LYS	2.2
5	E	180	LYS	2.2
3	Q	141	ASP	2.2
9	W	191	LYS	2.2
2	B	239	VAL	2.2
13	a	222	ALA	2.2
3	Q	203	THR	2.2
1	A	245	ASP	2.2
3	C	235	GLU	2.2
3	Q	167	LYS	2.2
3	Q	46	ARG	2.2
10	X	193	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
5	S	54	GLU	2.2
9	I	1	SER	2.2
2	P	60	THR	2.2
1	O	50	LYS	2.2
2	B	93	HIS	2.2
3	C	167	LYS	2.1
1	O	248	GLU	2.1
3	Q	60	SER	2.1
1	O	250	LEU	2.1
6	T	230	ASP	2.1
3	Q	232	THR	2.1
5	E	201	ARG	2.1
5	S	233	ILE	2.1
13	a	47	ASP	2.1
3	C	187	GLU	2.1
12	Z	1	GLN	2.1
12	Z	165	ASN	2.1
2	P	186	ASP	2.1
6	F	215	CYS	2.1
14	b	181	ALA	2.1
14	b	195	GLN	2.1
3	C	51	LYS	2.1
5	E	233	ILE	2.1
14	b	72	THR	2.1
4	R	1	ASP	2.1
5	S	218	ASP	2.1
13	M	216	ASN	2.1
8	H	215	GLU	2.1
6	F	177	ASP	2.0
13	a	204	THR	2.0
5	E	122	TYR	2.0
7	U	3	TYR	2.0
5	S	194	GLU	2.0
1	A	14	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	PHL	c	4	11/11	0.97	0.20	-	57,64,82,82	0
15	PHL	d	4	11/11	0.97	0.20	-	57,65,71,73	0
15	PHL	e	4	11/11	0.98	0.16	-	63,70,81,81	0
15	PHL	f	4	11/11	0.97	0.20	-	59,66,75,75	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	MG	Z	301	1/1	0.97	0.37	9.03	60,60,60,60	0
16	MG	I	301	1/1	0.94	0.27	4.46	61,61,61,61	0
18	MES	e	101	12/12	0.91	0.26	3.09	58,88,96,97	0
18	MES	K	302	12/12	0.92	0.23	2.90	64,89,94,97	0
16	MG	L	301	1/1	0.95	0.18	1.48	63,63,63,63	0
16	MG	N	201	1/1	0.95	0.12	-0.31	62,62,62,62	0
16	MG	I	302	1/1	0.98	0.12	-0.75	53,53,53,53	0
16	MG	G	301	1/1	0.95	0.09	-0.87	50,50,50,50	0
16	MG	K	301	1/1	0.98	0.06	-2.18	61,61,61,61	0
17	CL	U	301	1/1	0.97	0.20	-	30,30,30,30	0
17	CL	G	302	1/1	0.93	0.20	-	30,30,30,30	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.