



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:18 PM UTC

PDB ID : 4Y77 / pdb_00004y77
Title : Yeast 20S proteasome in complex with Ac-LAF-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-13
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

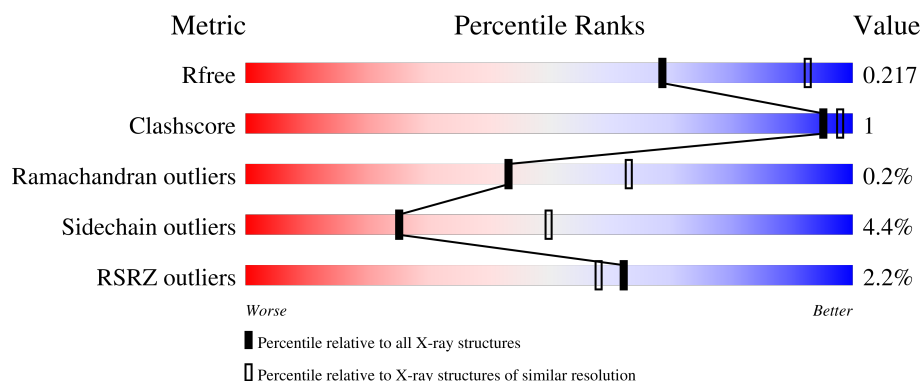
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	250	0% 97% •
1	O	250	2% 96% •
2	B	258	4% 88% 5% • 5%
2	P	258	4% 89% 5% • 5%
3	C	254	4% 87% 6% • 6%

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

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Mol	Chain	Length	Quality of chain
15	e	5	80% 20%
15	f	5	20% 80% 20%
15	g	5	80% 20%
15	h	5	60% 40%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50341 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	1	0
			1691	1066	295	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	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			
13	a	223	Total	C	N	O	S	0	0	0
			1745	1104	299	335	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-LAF-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			31	23	3	5			
15	d	5	Total	C	N	O	0	0	0
			31	23	3	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	5	Total	C	N	O	0	0	0
			31	23	3	5			
15	f	5	Total	C	N	O	0	0	0
			31	23	3	5			
15	g	5	Total	C	N	O	0	0	0
			31	23	3	5			
15	h	5	Total	C	N	O	0	0	0
			31	23	3	5			

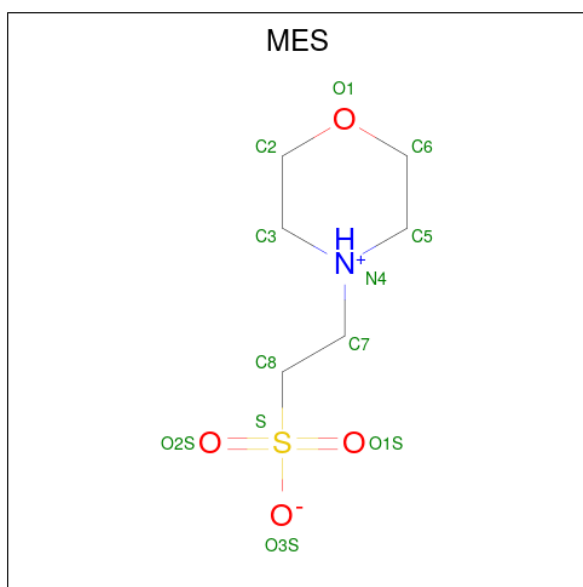
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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	U	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	43	Total	O	0	0
			43	43		
19	B	33	Total	O	0	0
			33	33		
19	C	24	Total	O	0	0
			24	24		
19	D	24	Total	O	0	0
			24	24		
19	E	15	Total	O	0	0
			15	15		
19	F	32	Total	O	0	0
			32	32		
19	G	43	Total	O	0	0
			43	43		
19	H	40	Total	O	0	0
			40	40		
19	I	49	Total	O	0	0
			49	49		
19	J	42	Total	O	0	0
			42	42		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	57	Total O 57 57	0	0
19	L	42	Total O 42 42	0	0
19	M	30	Total O 30 30	0	0
19	N	29	Total O 29 29	0	0
19	O	26	Total O 26 26	0	0
19	P	23	Total O 23 23	0	0
19	Q	13	Total O 13 13	0	0
19	R	18	Total O 18 18	0	0
19	S	13	Total O 13 13	0	0
19	T	24	Total O 24 24	0	0
19	U	36	Total O 36 36	0	0
19	V	34	Total O 34 34	0	0
19	W	40	Total O 40 40	0	0
19	X	47	Total O 47 47	0	0
19	Y	50	Total O 50 50	0	0
19	Z	47	Total O 47 47	0	0
19	a	47	Total O 47 47	0	0
19	b	38	Total O 38 38	0	0
19	c	3	Total O 3 3	0	0
19	d	1	Total O 1 1	0	0
19	e	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	f	1	Total 1	O 1	0	0
19	g	2	Total 2	O 2	0	0
19	h	2	Total 2	O 2	0	0

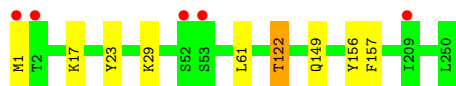
3 Residue-property plots [i](#)

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

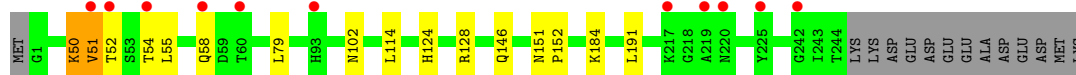
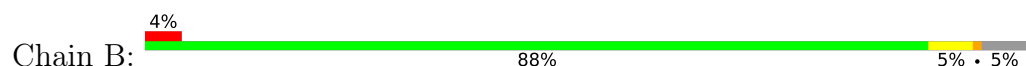
- Molecule 1: Proteasome subunit alpha type-2



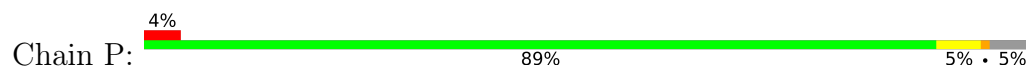
- Molecule 1: Proteasome subunit alpha type-2



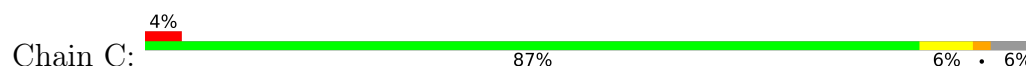
- Molecule 2: Proteasome subunit alpha type-3



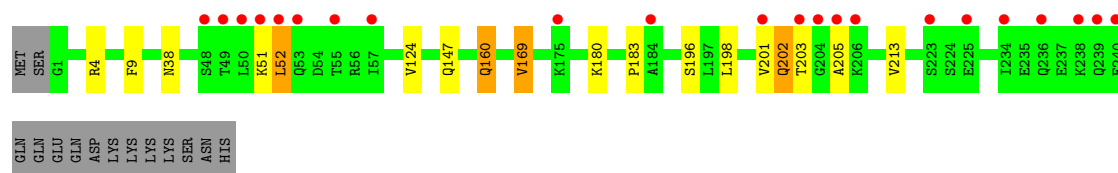
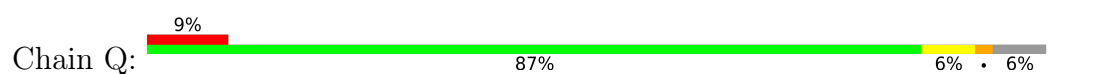
- Molecule 2: Proteasome subunit alpha type-3



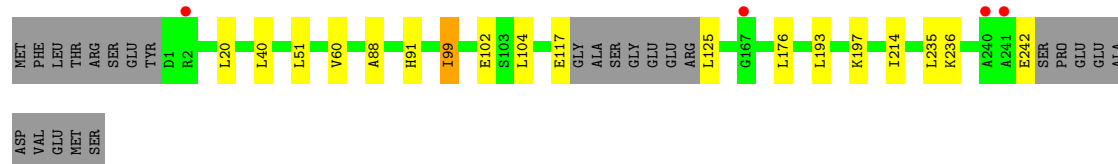
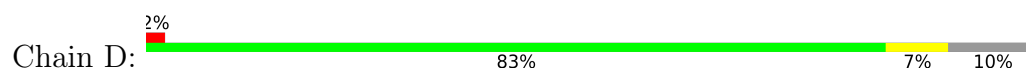
- Molecule 3: Proteasome subunit alpha type-4



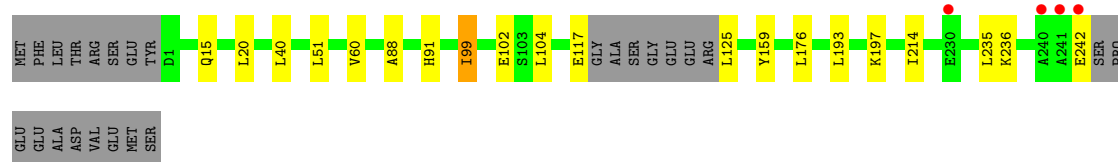
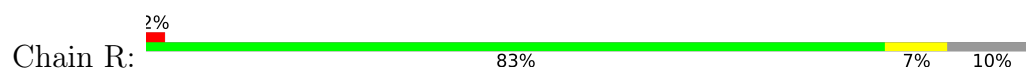
- Molecule 3: Proteasome subunit alpha type-4



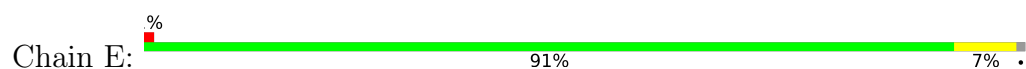
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 4: Proteasome subunit alpha type-5



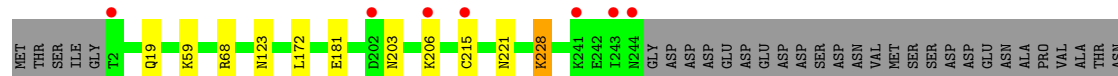
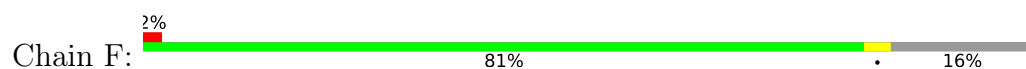
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 5: Proteasome subunit alpha type-6



• Molecule 6: Probable proteasome subunit alpha type-7



ALA
ASN
ALA
THR
THR
ASP
GLN
GLY
GLY
ASP
ILE
HIS
LEU
GLU

- Molecule 6: Probable proteasome subunit alpha type-7

Chain T: 5% 81% 16%

MET THR SER ILE GLY T2 D14 Q19 K53 L54 L55 K59 R63 N123 L172 H178 E181 G182 L183 N203 K204 E205 K206 D207 F208 N221 K228 A235 F238 L243 N244 GLY ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP VAL MET

SER SER ASP ASP GLU ALA PRO VAL ALA THR ASN ALA THR THR ASP GLN GLY ILE HIS LEU GLU

- Molecule 7: Proteasome subunit alpha type-1

Chain G: 2% 90% 6%

MET SER GLY ALA ALA ALA SER ALA ALA G2 Y3 F23 T26 T78 P79 N83 L115 M125 I131 Q166 T171 S180 K181 E187 K192 R235 L236 A240 E241 Q242 ASP

- Molecule 7: Proteasome subunit alpha type-1

Chain U: 0% 90% 5%

MET SER GLY ALA ALA ALA SER ALA ALA G2 P12 F23 K24 A25 T26 T78 P79 N83 L115 M125 I131 Q166 T171 K181 D222 R235 L236 Q242 ASP

- Molecule 8: Proteasome subunit beta type-2

Chain H: 2% 90% 5%

T1 Q22 N30 L34 H35 C43 T52 T56 L68 D104 P105 D120 L127 R196 V212 C221 D222 ILE GLN GLU GLU VAL ASP ILE THR ALA

- Molecule 8: Proteasome subunit beta type-2

Chain V: 2% 91% 5%

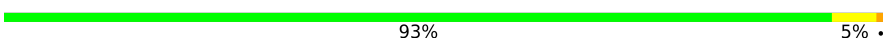
T1 H9 Q22 G31 L34 C43 A50 T56 L68 D104 P105 L127 R196 C221 D222 ILE GLN GLU GLU VAL ASP ILE THR ALA

- Molecule 9: Proteasome subunit beta type-3

Chain I: 92% 7%

MET S1 G9 I10 V20 S36 N37 K41 R93 P101 P118 I126 A141 L171 V182 I189 K190 K191 D192 D204

- Molecule 9: Proteasome subunit beta type-3

Chain W:  93% 5% .



- Molecule 10: Proteasome subunit beta type-4

Chain J:  91% 6% ..

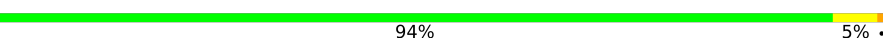


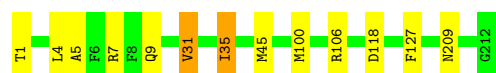
- Molecule 10: Proteasome subunit beta type-4

Chain X:  91% 6% ..

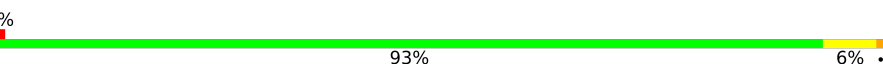


- Molecule 11: Proteasome subunit beta type-5

Chain K:  94% 5% .

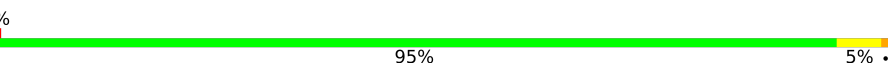


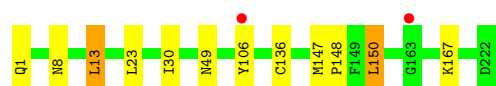
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  93% 6% .

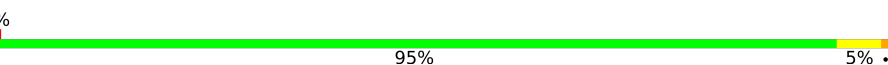


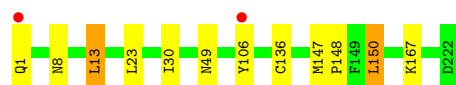
- Molecule 12: Proteasome subunit beta type-6

Chain L:  95% 5% .



- Molecule 12: Proteasome subunit beta type-6

Chain Z:  95% 5% .



- Molecule 13: Proteasome subunit beta type-7

Chain M:  85% 5% 9%

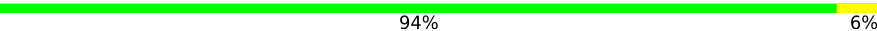


- Molecule 13: Proteasome subunit beta type-7

Chain a:  84% 7% 9%

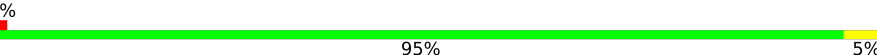


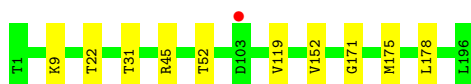
- Molecule 14: Proteasome subunit beta type-1

Chain N:  94% 6%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  95% 5%



- Molecule 15: Ac-LAF-ep

Chain c:  80% 20%



- Molecule 15: Ac-LAF-ep

Chain d:  80% 20%

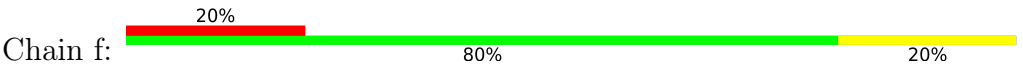


- Molecule 15: Ac-LAF-ep

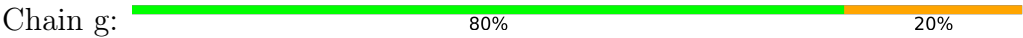
Chain e:  80% 20%



- Molecule 15: Ac-LAF-ep



● Molecule 15: Ac-LAF-ep



● Molecule 15: Ac-LAF-ep



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.45Å 300.30Å 145.22Å 90.00° 112.90° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.50) 97.7 (15.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.199 , 0.215 0.202 , 0.217	Depositor DCC
R_{free} test set	17933 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50341	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: CL, MG, POL, PHL, MES, ACE

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	0.68	0/2642
1	O	0.40	0/1952	0.69	0/2642
2	B	0.40	0/1934	0.68	0/2618
2	P	0.40	0/1934	0.68	0/2618
3	C	0.41	0/1910	0.71	0/2586
3	Q	0.41	0/1910	0.71	0/2586
4	D	0.40	0/1837	0.65	0/2475
4	R	0.40	0/1837	0.65	0/2475
5	E	0.40	0/1800	0.67	0/2433
5	S	0.40	0/1800	0.67	0/2433
6	F	0.40	0/1932	0.70	0/2609
6	T	0.40	0/1932	0.70	0/2609
7	G	0.40	0/1945	0.67	0/2634
7	U	0.40	0/1945	0.67	0/2634
8	H	0.53	1/1715 (0.1%)	0.69	0/2326
8	V	0.43	1/1726 (0.1%)	0.67	0/2341
9	I	0.38	0/1611	0.67	0/2174
9	W	0.39	0/1611	0.69	0/2174
10	J	0.39	0/1589	0.66	0/2142
10	X	0.38	0/1589	0.66	0/2142
11	K	0.41	0/1681	0.67	1/2274 (0.0%)
11	Y	0.41	0/1681	0.68	1/2274 (0.0%)
12	L	0.38	0/1795	0.65	0/2420
12	Z	0.41	0/1795	0.65	0/2420
13	M	0.42	0/1783	0.69	1/2420 (0.0%)
13	a	0.42	0/1775	0.69	1/2409 (0.0%)
14	N	0.50	1/1541 (0.1%)	0.72	1/2087 (0.0%)
14	b	0.49	0/1541	0.72	0/2087
15	c	0.90	0/13	1.12	0/17
15	d	1.27	0/13	1.07	0/17
15	e	1.34	0/13	1.25	0/17
15	f	0.75	0/13	1.09	0/17

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	1.35	0/13	1.01	0/17
15	h	1.09	0/13	1.06	0/17
All	All	0.41	3/50131 (0.0%)	0.68	5/67786 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	1	THR	CB-OG1	-5.46	1.35	1.43
8	H	1	THR	CB-OG1	-5.23	1.35	1.43
14	N	1	THR	CB-OG1	-5.10	1.35	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35	ARG	N-CA-C	7.38	119.11	111.14
13	M	35	ARG	N-CA-C	6.77	119.66	111.40
11	Y	1	THR	N-CA-C	5.67	126.87	111.00
11	K	1	THR	N-CA-C	5.21	125.57	111.00
14	N	1	THR	N-CA-C	5.15	125.42	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1773	0	1775	6	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1684	0	1685	3	0
8	V	1691	0	1692	4	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	9	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	8	0
11	K	1644	0	1592	6	0
11	Y	1644	0	1592	6	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	3	0
13	M	1753	0	1754	5	0
13	a	1745	0	1750	4	0
14	N	1512	0	1478	3	0
14	b	1512	0	1478	4	0
15	c	31	0	34	0	0
15	d	31	0	33	1	0
15	e	31	0	34	0	0
15	f	31	0	34	0	0
15	g	31	0	33	1	0
15	h	31	0	34	1	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	U	1	0	0	0	0
18	K	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	43	0	0	0	0
19	B	33	0	0	0	0
19	C	24	0	0	0	0
19	D	24	0	0	0	0
19	E	15	0	0	0	0
19	F	32	0	0	1	0
19	G	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	H	40	0	0	0	0
19	I	49	0	0	0	0
19	J	42	0	0	1	0
19	K	57	0	0	0	0
19	L	42	0	0	0	0
19	M	30	0	0	0	0
19	N	29	0	0	0	0
19	O	26	0	0	0	0
19	P	23	0	0	0	0
19	Q	13	0	0	0	0
19	R	18	0	0	0	0
19	S	13	0	0	0	0
19	T	24	0	0	0	0
19	U	36	0	0	0	0
19	V	34	0	0	0	0
19	W	40	0	0	0	0
19	X	47	0	0	0	0
19	Y	50	0	0	0	0
19	Z	47	0	0	0	0
19	a	47	0	0	0	0
19	b	38	0	0	0	0
19	c	3	0	0	0	0
19	d	1	0	0	0	0
19	e	1	0	0	0	0
19	f	1	0	0	0	0
19	g	2	0	0	0	0
19	h	2	0	0	0	0
All	All	50341	0	49125	121	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 1.

All (121) 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:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.64	0.80
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.63	0.79
10:J:1:MET:O	10:J:2:ASP:HB2	1.85	0.75
10:X:1:MET:O	10:X:2:ASP:HB2	1.86	0.75
8:V:50:ALA:HB3	9:W:126:ILE:HD12	1.73	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.76	0.66
14:b:152:VAL:HA	14:b:175:MET:HE1	1.81	0.62
11:Y:31:VAL:HG11	15:g:4:PHL:CE1	2.30	0.62
14:N:152:VAL:HA	14:N:175:MET:HE1	1.82	0.61
11:K:31:VAL:HG11	15:d:4:PHL:CE1	2.30	0.61
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.83	0.61
8:V:50:ALA:CB	9:W:126:ILE:HD12	2.30	0.61
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.83	0.61
13:M:35:ARG:HD2	13:M:36:PHE:CZ	2.41	0.56
7:G:23:PHE:O	7:G:26:THR:HB	2.07	0.55
7:U:23:PHE:O	7:U:26:THR:HB	2.07	0.55
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.07	0.55
3:C:51:LYS:O	3:C:52:LEU:HB2	2.07	0.54
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.73	0.54
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.73	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.51
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.38	0.51
8:H:35:HIS:CB	8:H:56:THR:HG21	2.41	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
8:V:50:ALA:HB3	9:W:126:ILE:CD1	2.40	0.50
3:C:201:VAL:O	3:C:202:GLN:CB	2.60	0.50
10:J:1:MET:O	10:J:2:ASP:CB	2.59	0.50
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.94	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.49
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.60	0.49
3:C:201:VAL:HG13	3:C:202:GLN:N	2.28	0.49
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.95	0.48
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.28	0.48
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.79	0.48
10:J:93:ARG:NH1	19:J:201:HOH:O	2.43	0.47
10:J:174:MET:HA	10:X:174:MET:HA	1.96	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.95	0.47
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
12:L:8:ASN:HA	12:L:30:ILE:O	2.15	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.47
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.15	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.47
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.47
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.50	0.46
10:X:1:MET:O	10:X:2:ASP:CB	2.59	0.46
9:I:98:ARG:O	9:I:126:ILE:HD11	2.15	0.46
5:E:9:THR:HG21	5:E:119:THR:HA	1.98	0.46
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.98	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
3:C:201:VAL:O	3:C:202:GLN:HB2	2.15	0.46
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.98	0.46
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.98	0.46
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.98	0.46
5:S:12:PHE:H	6:T:19:GLN:HE22	1.63	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.45
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.51	0.45
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.99	0.45
6:F:215:CYS:HB3	19:F:305:HOH:O	2.17	0.45
11:K:100:MET:CE	11:K:127:PHE:HB2	2.39	0.45
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.16	0.45
6:F:228:LYS:HE3	6:F:228:LYS:HB2	1.83	0.45
5:S:9:THR:HG21	5:S:119:THR:HA	1.98	0.45
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.46	0.45
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.47	0.45
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.52	0.45
5:E:12:PHE:H	6:F:19:GLN:HE22	1.64	0.44
8:H:52:THR:O	8:H:56:THR:HB	2.17	0.44
11:K:5:ALA:HB3	11:K:100:MET:CE	2.48	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.44
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.00	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.44
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.99	0.44
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.00	0.43
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.48	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.00	0.43
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.54	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.00	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.00	0.43
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.01	0.43
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.43
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.54	0.43
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.01	0.43
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:209:ASN:O	9:W:37:ASN:ND2	2.52	0.43
10:J:1:MET:HA	10:J:34:LYS:CE	2.49	0.42
10:X:1:MET:HA	10:X:34:LYS:CE	2.48	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.54	0.42
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.01	0.42
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.01	0.42
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.55	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.20	0.41
14:b:45:ARG:HD2	14:b:52:THR:HB	2.01	0.41
11:K:35:ILE:HB	11:K:45:MET:HE3	2.02	0.41
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	2.02	0.41
14:b:22:THR:HB	15:h:2:LEU:HD23	2.02	0.41
3:C:198:LEU:HA	3:C:201:VAL:HG12	2.02	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
14:N:45:ARG:HD2	14:N:52:THR:HB	2.01	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.01	0.41
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.20	0.41
7:G:187:GLU:HG2	7:G:192:LYS:HB2	2.02	0.41
6:T:228:LYS:HB2	6:T:228:LYS:HE3	1.83	0.41
10:X:119:ILE:HG12	10:X:125:LYS:HG3	2.02	0.41
13:a:96:LEU:O	13:a:100:MET:HG2	2.20	0.41
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.03	0.40
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.98	0.40
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.03	0.40
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.69	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	0.40
10:J:1:MET:HA	10:J:34:LYS:HE3	2.04	0.40
11:Y:35:ILE:HB	11:Y:45:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	49
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	49
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	18
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	18
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%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	221/232 (95%)	214 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	43
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	43
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	222/246 (90%)	216 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	221/246 (90%)	216 (98%)	5 (2%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	c	2/5 (40%)	2 (100%)	0	0	100	100
15	d	2/5 (40%)	2 (100%)	0	0	100	100
15	e	2/5 (40%)	2 (100%)	0	0	100	100
15	f	2/5 (40%)	2 (100%)	0	0	100	100
15	g	2/5 (40%)	2 (100%)	0	0	100	100
15	h	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6270/6644 (94%)	6115 (98%)	145 (2%)	10 (0%)	43	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
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%)	203 (97%)	6 (3%)	37	65
1	O	209/209 (100%)	203 (97%)	6 (3%)	37	65
2	B	203/216 (94%)	193 (95%)	10 (5%)	22	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	203/216 (94%)	193 (95%)	10 (5%)	22	45
3	C	212/226 (94%)	203 (96%)	9 (4%)	26	52
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	52
4	D	194/215 (90%)	179 (92%)	15 (8%)	12	25
4	R	194/215 (90%)	179 (92%)	15 (8%)	12	25
5	E	190/193 (98%)	179 (94%)	11 (6%)	18	38
5	S	190/193 (98%)	180 (95%)	10 (5%)	20	42
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	49
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	49
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	50
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	50
8	H	181/190 (95%)	173 (96%)	8 (4%)	25	50
8	V	182/190 (96%)	175 (96%)	7 (4%)	29	56
9	I	172/173 (99%)	165 (96%)	7 (4%)	27	53
9	W	172/173 (99%)	165 (96%)	7 (4%)	27	53
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	65
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	65
11	K	169/169 (100%)	162 (96%)	7 (4%)	27	53
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	53
12	L	185/185 (100%)	177 (96%)	8 (4%)	26	51
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	51
13	M	192/208 (92%)	184 (96%)	8 (4%)	26	52
13	a	191/208 (92%)	183 (96%)	8 (4%)	26	52
14	N	162/162 (100%)	157 (97%)	5 (3%)	35	62
14	b	162/162 (100%)	158 (98%)	4 (2%)	42	69
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5304/5546 (96%)	5073 (96%)	231 (4%)	25 50

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	17	LYS
1	A	29	LYS
1	A	61	LEU
1	A	122	THR
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	102	ASN
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	52	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
3	C	213	VAL
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	102	GLU
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	197	LYS
4	D	214	ILE

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Mol	Chain	Res	Type
4	D	235	LEU
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	174	THR
5	E	188	LEU
5	E	207	VAL
5	E	231	LYS
6	F	59	LYS
6	F	68	ARG
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	221	ASN
6	F	228	LYS
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	171	THR
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	20	VAL
9	I	37	ASN

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Mol	Chain	Res	Type
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
9	I	191	LYS
9	I	192	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	13	LEU
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	35	ARG
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
13	M	212	LEU
13	M	223	LYS
14	N	9	LYS
14	N	22	THR
14	N	31	THR
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	17	LYS
1	O	29	LYS
1	O	61	LEU

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Mol	Chain	Res	Type
1	O	122	THR
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	102	ASN
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	52	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
3	Q	213	VAL
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	102	GLU
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	197	LYS
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU

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Mol	Chain	Res	Type
5	S	71	LEU
5	S	188	LEU
5	S	207	VAL
5	S	231	LYS
6	T	59	LYS
6	T	68	ARG
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	221	ASN
6	T	228	LYS
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	171	THR
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	20	VAL
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
9	W	191	LYS
9	W	192	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU

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Mol	Chain	Res	Type
11	Y	7	ARG
11	Y	9	GLN
11	Y	31	VAL
11	Y	35	ILE
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	13	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
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	187	ARG
13	a	204	THR
13	a	212	LEU
13	a	223	LYS
14	b	9	LYS
14	b	31	THR
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
2	B	176	GLN
2	B	232	GLN
3	C	38	ASN
3	C	77	ASN
3	C	115	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN

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Mol	Chain	Res	Type
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	106	GLN
4	D	217	GLN
4	D	225	ASN
5	E	68	HIS
5	E	85	ASN
5	E	92	ASN
5	E	99	ASN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	165	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	123	ASN
7	G	28	GLN
7	G	30	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	22	GLN
8	H	30	ASN
8	H	57	GLN
8	H	86	HIS
8	H	189	ASN
8	H	194	ASN
9	I	37	ASN
9	I	88	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN

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Mol	Chain	Res	Type
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	36	ASN
12	L	70	ASN
12	L	76	HIS
12	L	79	HIS
12	L	80	ASN
12	L	165	ASN
12	L	197	GLN
13	M	2	GLN
13	M	26	ASN
13	M	102	GLN
13	M	108	ASN
14	N	38	HIS
14	N	53	GLN
14	N	141	ASN
1	O	30	GLN
1	O	143	ASN
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
2	P	226	GLN
2	P	232	GLN
3	Q	38	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	160	ASN
4	R	217	GLN
4	R	225	ASN
5	S	68	HIS
5	S	85	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	147	GLN
5	S	151	ASN
5	S	165	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
7	U	28	GLN
7	U	30	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
8	V	57	GLN
8	V	86	HIS
8	V	194	ASN
9	W	37	ASN
9	W	88	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	79	HIS
12	Z	158	ASN
12	Z	165	ASN
12	Z	197	GLN
13	a	2	GLN
13	a	102	GLN
13	a	108	ASN

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Mol	Chain	Res	Type
14	b	38	HIS
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	PHL	h	4	14,15	11,11,11	1.96	1 (9%)	11,13,13	1.94	3 (27%)
15	PHL	d	4	15,11	11,11,11	1.72	1 (9%)	11,13,13	1.69	3 (27%)
15	PHL	f	4	15,8	11,11,11	1.67	1 (9%)	11,13,13	1.46	2 (18%)
15	PHL	g	4	15,11	11,11,11	1.80	1 (9%)	11,13,13	1.52	3 (27%)
15	PHL	e	4	14,15	11,11,11	1.95	1 (9%)	11,13,13	1.53	2 (18%)
15	PHL	c	4	15,8	11,11,11	1.67	1 (9%)	11,13,13	1.50	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	h	4	14,15	-	4/6/6/6	0/1/1/1
15	PHL	d	4	15,11	-	2/6/6/6	0/1/1/1
15	PHL	f	4	15,8	-	4/6/6/6	0/1/1/1
15	PHL	g	4	15,11	-	2/6/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PHL	e	4	14,15	-	3/6/6/6	0/1/1/1
15	PHL	c	4	15,8	-	4/6/6/6	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	4	PHL	CB-CG	-5.97	1.37	1.51
15	e	4	PHL	CB-CG	-5.77	1.37	1.51
15	g	4	PHL	CB-CG	-5.46	1.38	1.51
15	c	4	PHL	CB-CG	-5.45	1.38	1.51
15	f	4	PHL	CB-CG	-5.34	1.38	1.51
15	d	4	PHL	CB-CG	-5.12	1.39	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	h	4	PHL	CB-CA-C	-3.69	105.55	112.21
15	h	4	PHL	CG-CB-CA	3.62	120.19	113.23
15	e	4	PHL	CB-CA-C	-3.33	106.19	112.21
15	d	4	PHL	CG-CB-CA	3.26	119.50	113.23
15	g	4	PHL	CB-CA-C	-3.06	106.68	112.21
15	d	4	PHL	CB-CA-C	-3.03	106.72	112.21
15	c	4	PHL	CB-CA-C	-3.01	106.77	112.21
15	f	4	PHL	CB-CA-C	-2.84	107.07	112.21
15	g	4	PHL	CG-CB-CA	2.33	117.72	113.23
15	f	4	PHL	O-C-CA	-2.32	102.61	111.52
15	c	4	PHL	O-C-CA	-2.19	103.09	111.52
15	g	4	PHL	O-C-CA	-2.17	103.17	111.52
15	d	4	PHL	O-C-CA	-2.16	103.20	111.52
15	c	4	PHL	CG-CB-CA	2.11	117.30	113.23
15	e	4	PHL	CG-CB-CA	2.11	117.28	113.23
15	h	4	PHL	CB-CG-CD1	-2.03	117.13	120.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	d	4	PHL	CA-CB-CG-CD1
15	d	4	PHL	CA-CB-CG-CD2
15	g	4	PHL	CA-CB-CG-CD1
15	g	4	PHL	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
15	c	4	PHL	CA-CB-CG-CD2
15	c	4	PHL	CA-CB-CG-CD1
15	f	4	PHL	N-CA-CB-CG
15	h	4	PHL	N-CA-CB-CG
15	e	4	PHL	CA-CB-CG-CD2
15	f	4	PHL	CA-CB-CG-CD2
15	e	4	PHL	CA-CB-CG-CD1
15	f	4	PHL	CA-CB-CG-CD1
15	h	4	PHL	CA-CB-CG-CD1
15	h	4	PHL	CA-CB-CG-CD2
15	c	4	PHL	C-CA-CB-CG
15	f	4	PHL	C-CA-CB-CG
15	h	4	PHL	C-CA-CB-CG
15	c	4	PHL	N-CA-CB-CG
15	e	4	PHL	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	d	4	PHL	1	0
15	g	4	PHL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	Y	301	-	12,12,12	2.30	1 (8%)	15,16,16	1.09	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	MES	K	302	-	12,12,12	2.31	1 (8%)	15,16,16	1.09	2 (13%)

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	Y	301	-	-	0/6/14/14	0/1/1/1
18	MES	K	302	-	-	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	-7.74	1.66	1.77
18	Y	301	MES	C8-S	-7.72	1.66	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	302	MES	O3S-S-C8	2.41	110.72	106.00
18	Y	301	MES	O2S-S-C8	2.30	110.21	106.73
18	Y	301	MES	O3S-S-C8	2.28	110.46	106.00
18	K	302	MES	O2S-S-C8	2.02	109.78	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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%)	-0.17	3 (1%) 76 73	35, 50, 89, 128	0
1	O	250/250 (100%)	-0.10	5 (2%) 65 61	41, 57, 102, 132	0
2	B	244/258 (94%)	-0.00	11 (4%) 38 33	36, 54, 108, 166	0
2	P	244/258 (94%)	0.10	11 (4%) 38 33	40, 57, 110, 166	0
3	C	240/254 (94%)	0.00	11 (4%) 37 33	35, 57, 121, 159	0
3	Q	240/254 (94%)	0.50	22 (9%) 14 13	45, 75, 157, 213	0
4	D	235/260 (90%)	-0.04	4 (1%) 69 65	41, 61, 94, 141	0
4	R	235/260 (90%)	0.11	4 (1%) 69 65	46, 65, 103, 153	0
5	E	231/234 (98%)	0.03	2 (0%) 81 78	44, 65, 99, 140	0
5	S	231/234 (98%)	0.45	14 (6%) 27 23	46, 74, 118, 155	0
6	F	243/288 (84%)	-0.06	7 (2%) 53 49	40, 60, 110, 142	0
6	T	243/288 (84%)	0.38	14 (5%) 29 25	40, 72, 125, 164	0
7	G	241/252 (95%)	-0.07	5 (2%) 63 59	36, 52, 96, 150	0
7	U	241/252 (95%)	-0.10	3 (1%) 76 73	39, 55, 89, 140	0
8	H	222/232 (95%)	-0.02	5 (2%) 61 57	36, 51, 78, 121	0
8	V	222/232 (95%)	-0.02	4 (1%) 67 64	30, 54, 78, 132	1 (0%)
9	I	204/205 (99%)	-0.44	1 (0%) 87 85	31, 44, 73, 95	0
9	W	204/205 (99%)	-0.35	0 100 100	32, 47, 77, 100	0
10	J	195/198 (98%)	-0.39	1 (0%) 87 85	32, 44, 70, 117	0
10	X	195/198 (98%)	-0.37	2 (1%) 79 76	35, 47, 73, 125	0
11	K	212/212 (100%)	-0.43	0 100 100	31, 45, 69, 90	0
11	Y	212/212 (100%)	-0.34	2 (0%) 81 78	34, 47, 74, 99	0
12	L	222/222 (100%)	-0.34	2 (0%) 81 78	33, 49, 75, 101	0
12	Z	222/222 (100%)	-0.26	2 (0%) 81 78	35, 49, 77, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	224/246 (91%)	-0.29	1 (0%) 88 86	30, 49, 74, 94	0
13	a	223/246 (90%)	-0.33	1 (0%) 88 86	32, 49, 73, 93	0
14	N	196/196 (100%)	-0.35	0 100 100	32, 45, 73, 100	0
14	b	196/196 (100%)	-0.32	1 (0%) 87 85	33, 46, 75, 96	0
15	c	2/5 (40%)	1.33	0 100 100	67, 67, 67, 69	0
15	d	2/5 (40%)	0.65	0 100 100	62, 62, 62, 71	0
15	e	2/5 (40%)	-0.01	0 100 100	53, 53, 53, 64	0
15	f	2/5 (40%)	2.03	1 (50%) 0 0	70, 70, 70, 76	0
15	g	2/5 (40%)	0.68	0 100 100	62, 62, 62, 73	0
15	h	2/5 (40%)	0.03	0 100 100	56, 56, 56, 68	0
All	All	6329/6644 (95%)	-0.10	139 (2%) 62 58	30, 54, 101, 213	1 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	7.1
10	X	1	MET	6.6
2	B	219	ALA	6.3
3	Q	50	LEU	6.2
10	J	1	MET	6.2
3	Q	205	ALA	5.0
3	Q	49	THR	4.9
2	B	51	VAL	4.8
13	a	1	THR	4.7
1	A	1	MET	4.6
1	O	1	MET	4.2
13	M	1	THR	4.1
3	Q	51	LYS	4.0
6	T	243	ILE	4.0
8	V	222	ASP	4.0
2	P	51	VAL	3.9
4	D	240	ALA	3.9
3	Q	234	ILE	3.8
6	T	178	HIS	3.6
3	Q	240	GLU	3.6
2	P	52	THR	3.6
2	P	218	GLY	3.6
4	D	241	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
8	H	222	ASP	3.4
11	Y	212	GLY	3.4
7	U	242	GLN	3.3
6	T	14	ASP	3.2
3	Q	203	THR	3.2
2	P	220	ASN	3.2
3	C	205	ALA	3.2
2	B	220	ASN	3.2
6	T	204	LYS	3.1
5	S	52	ALA	3.1
5	S	233	ILE	3.1
3	Q	52	LEU	2.9
5	E	122	TYR	2.9
4	D	167	GLY	2.9
6	F	243	ILE	2.9
3	Q	184	ALA	2.9
2	P	244	THR	2.8
6	F	215	CYS	2.8
3	Q	225	GLU	2.8
3	C	203	THR	2.8
3	C	240	GLU	2.8
6	F	244	ASN	2.7
15	f	3	ALA	2.7
12	L	163	GLY	2.7
1	A	249	ALA	2.7
1	A	201	GLU	2.7
6	T	205	GLU	2.7
3	Q	239	GLN	2.7
4	R	241	ALA	2.7
4	R	242	GLU	2.7
6	T	2	THR	2.7
2	P	222	GLY	2.6
8	V	31	CYS	2.6
3	Q	238	LYS	2.6
8	H	221	CYS	2.6
6	F	202	ASP	2.5
7	U	222	ASP	2.5
3	Q	57	ILE	2.5
4	D	2	ARG	2.5
3	Q	175	LYS	2.5
4	R	240	ALA	2.5
6	T	235	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
7	U	24	LYS	2.4
3	C	236	GLN	2.4
3	Q	48	SER	2.4
5	S	175	LEU	2.4
6	T	183	LEU	2.4
3	Q	223	SER	2.4
1	O	209	ILE	2.4
8	H	212	VAL	2.4
3	C	48	SER	2.4
9	I	1	SER	2.4
2	P	93	HIS	2.4
7	G	240	ALA	2.4
3	Q	55	THR	2.3
5	S	56	SER	2.3
7	G	180	SER	2.3
2	B	58	GLN	2.3
5	S	218	ASP	2.3
6	T	53	LYS	2.3
8	V	9	ASN	2.3
3	C	53	GLN	2.3
3	C	206	LYS	2.3
5	S	122	TYR	2.3
1	O	2	THR	2.3
2	B	54	THR	2.3
1	O	53	SER	2.3
5	S	48	LEU	2.3
5	E	123	GLY	2.3
3	C	238	LYS	2.3
14	b	103	ASP	2.3
8	V	221	CYS	2.3
2	B	52	THR	2.2
1	O	52	SER	2.2
2	P	225	TYR	2.2
5	S	58	TYR	2.2
8	H	120	ASP	2.2
3	Q	201	VAL	2.2
3	Q	206	LYS	2.2
2	P	54	THR	2.2
6	F	241	LYS	2.2
6	T	244	ASN	2.2
3	Q	236	GLN	2.2
8	H	1	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	242	GLY	2.2
6	F	206	LYS	2.2
5	S	207	VAL	2.1
2	B	60	THR	2.1
2	P	60	THR	2.1
3	C	52	LEU	2.1
2	B	217	LYS	2.1
5	S	209	ASN	2.1
7	G	2	GLY	2.1
12	L	106	TYR	2.1
10	X	194	ASP	2.1
5	S	49	LYS	2.1
3	Q	53	GLN	2.1
5	S	51	ASN	2.1
3	Q	204	GLY	2.1
6	F	2	THR	2.1
5	S	179	ILE	2.1
6	T	208	PHE	2.1
6	T	238	PHE	2.1
3	C	49	THR	2.1
11	Y	1	THR	2.1
3	C	51	LYS	2.1
7	G	3	TYR	2.1
12	Z	1	GLN	2.0
12	Z	106	TYR	2.0
4	R	230	GLU	2.0
6	T	54	LEU	2.0
6	T	55	LEU	2.0
7	G	181	LYS	2.0
5	S	177	THR	2.0
2	B	93	HIS	2.0
2	B	225	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	PHL	f	4	11/11	0.85	0.17	73,79,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	PHL	c	4	11/11	0.86	0.16	72,77,80,80	0
15	PHL	h	4	11/11	0.93	0.12	57,59,64,64	0
15	PHL	g	4	11/11	0.94	0.12	64,68,73,75	0
15	PHL	d	4	11/11	0.94	0.13	60,63,73,73	0
15	PHL	e	4	11/11	0.95	0.10	54,57,60,60	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($\text{\AA}^2$)	Q<0.9
18	MES	Y	301	12/12	0.92	0.15	50,80,84,86	0
18	MES	K	302	12/12	0.93	0.14	48,80,87,89	0
16	MG	I	301	1/1	0.93	0.14	61,61,61,61	0
16	MG	Z	301	1/1	0.94	0.08	65,65,65,65	0
17	CL	G	302	1/1	0.95	0.15	30,30,30,30	0
17	CL	U	301	1/1	0.96	0.14	30,30,30,30	0
16	MG	K	301	1/1	0.96	0.10	42,42,42,42	0
16	MG	L	301	1/1	0.96	0.08	49,49,49,49	0
16	MG	I	302	1/1	0.98	0.07	43,43,43,43	0
16	MG	N	201	1/1	0.99	0.02	41,41,41,41	0
16	MG	G	301	1/1	0.99	0.08	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.