



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:42 PM GMT

PDB ID : 4Y8I
Title : Yeast 20S proteasome in complex with Ac-PLL-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

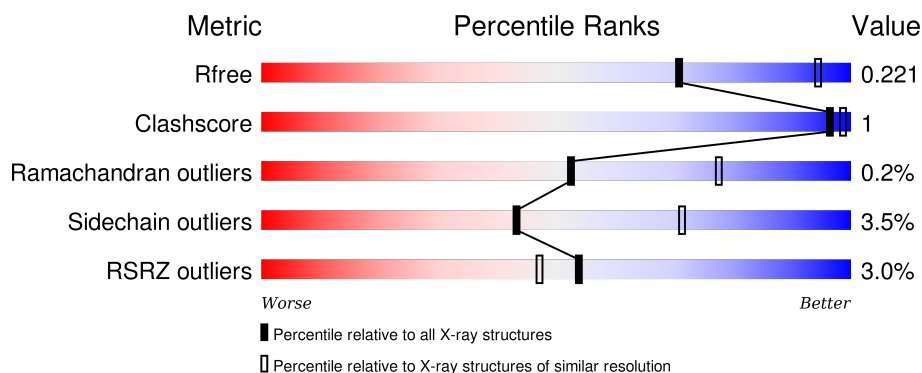
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>2%</div> <div>96%</div> <div>.</div> </div>
1	O	250	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
2	B	258	<div> <div>6%</div> <div>89%</div> <div>5% 5%</div> </div>
2	P	258	<div> <div>6%</div> <div>90%</div> <div>. . 5%</div> </div>
3	C	254	<div> <div>7%</div> <div>88%</div> <div>6% . 6%</div> </div>





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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	
15	f	5	
15	g	5	
15	h	5	

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
18	MES	K	302	-	-	-	X
18	MES	Y	301	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50137 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	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

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

- Molecule 15 is a protein called Ac-PLL-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			
15	g	5	Total	C	N	O	0	0	0
			30	22	3	5			
15	h	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	b	1	Total	Cl	0	0
			1	1		
17	N	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: 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	29	Total	O	0	0
			29	29		
19	B	21	Total	O	0	0
			21	21		
19	C	14	Total	O	0	0
			14	14		
19	D	16	Total	O	0	0
			16	16		
19	E	14	Total	O	0	0
			14	14		
19	F	17	Total	O	0	0
			17	17		
19	G	29	Total	O	0	0
			29	29		
19	H	24	Total	O	0	0
			24	24		
19	I	34	Total	O	0	0
			34	34		
19	J	22	Total	O	0	0
			22	22		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	K	21	Total 21	O 21	0	0
19	L	30	Total 30	O 30	0	0
19	M	28	Total 28	O 28	0	0
19	N	25	Total 25	O 25	0	0
19	O	19	Total 19	O 19	0	0
19	P	11	Total 11	O 11	0	0
19	Q	11	Total 11	O 11	0	0
19	R	13	Total 13	O 13	0	0
19	S	10	Total 10	O 10	0	0
19	T	14	Total 14	O 14	0	0
19	U	36	Total 36	O 36	0	0
19	V	18	Total 18	O 18	0	0
19	W	19	Total 19	O 19	0	0
19	X	28	Total 28	O 28	0	0
19	Y	25	Total 25	O 25	0	0
19	Z	28	Total 28	O 28	0	0
19	a	34	Total 34	O 34	0	0
19	b	25	Total 25	O 25	0	0
19	c	1	Total 1	O 1	0	0
19	e	2	Total 2	O 2	0	0
19	h	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

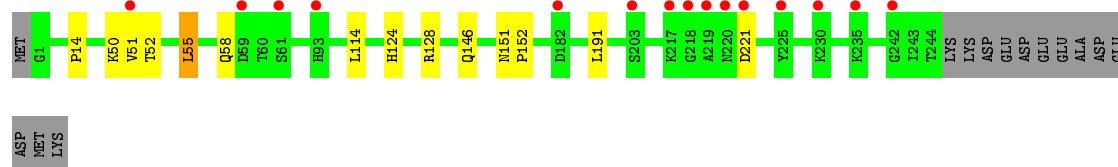
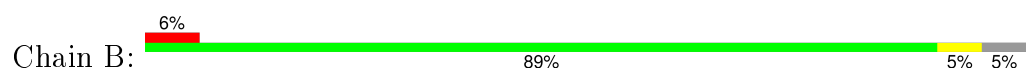
- Molecule 1: Proteasome subunit alpha type-2



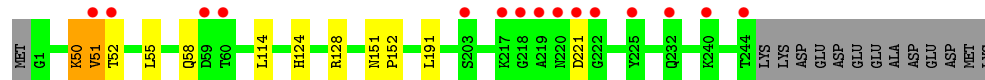
- Molecule 1: Proteasome subunit alpha type-2



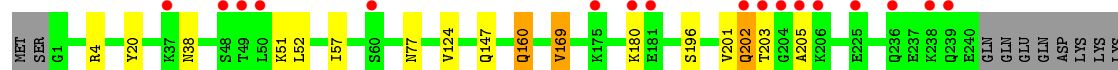
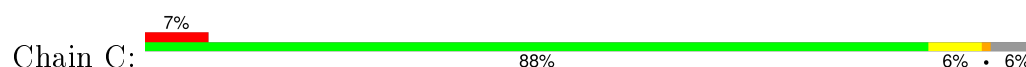
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3




- Molecule 3: Proteasome subunit alpha type-4



LYS
SER
ASN
HIS


• Molecule 3: Proteasome subunit alpha type-4

Chain Q: 

MET SER G1 R4 R38 R47 S48 T49 L50 K51 L52 S60 N77 V124 D141 Q147 Q160 V169 K175 K180 E187 S196 V201 Q202 T203 G204 A205 K206 S223 S224 E225 Q229 Y230 V231 E235 Q236 E237 K238 Q239 E240 GLN


GLU
GLN
ASP
LYS
LYS
LYS
SER
ASN
HIS

• Molecule 4: Proteasome subunit alpha type-5

Chain D: 

MET PHE LEU THR ARG SER GLU TTR D1 L20 L40 A88 H91 I99 L104 E117 GLY ALA SER GLY GLU ARG L125 L176 L193 I214 K236 E237 K238 E242 SER PRQ GLU ALA ASP VAL GLU MET SER

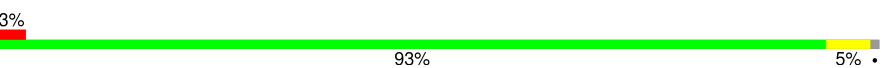
• Molecule 4: Proteasome subunit alpha type-5

Chain R: 

MET PHE LEU THR ARG SER GLU TTR D1 R2 P9 L20 L40 A88 H91 I99 L104 E117 GLY ALA SER GLY GLU ARG L125 Y159 M160 L176 M177 E178 W179 L193 E201 I214 Q217 K236 A241 E242 SER PRQ GLU ALA

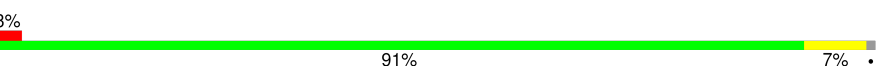
ASP
VAL
GLU
MET
SER

• Molecule 5: Proteasome subunit alpha type-6

Chain E: 


MET PHE ARG M3 T9 L25 K29 E54 L71 L87 A107 T119 Y122 L175 F178 M184 L188 K201 D202 V207 D218 I233

• Molecule 5: Proteasome subunit alpha type-6

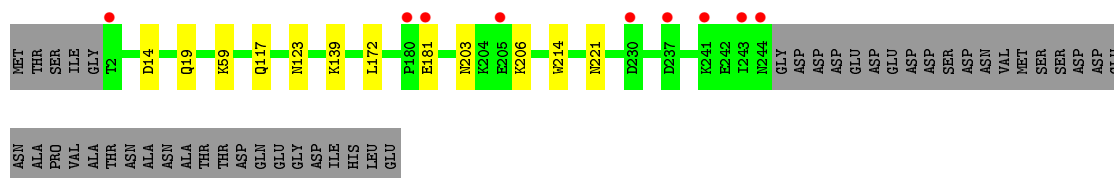
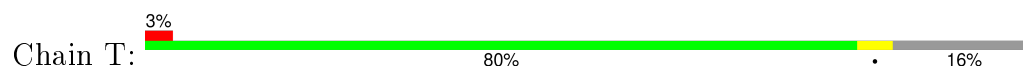
Chain S: 

MET PHE ARG M3 T9 F12 Y23 A24 L25 K29 E54 L55 S56 L71 A77 P78 L87 A107 T119 G123 R173 T174 L175 F178 I179 K180 M184 L188 D202 D218 I233

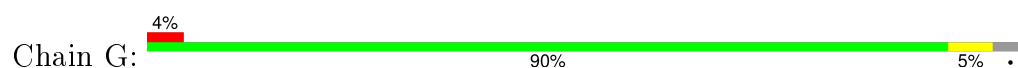
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F: 

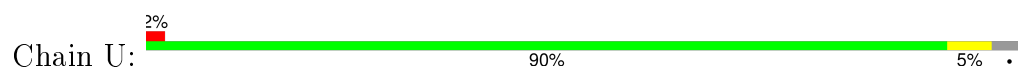
- Molecule 6: Probable proteasome subunit alpha type-7



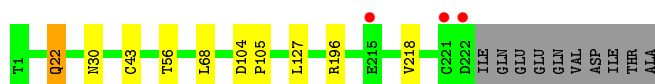
- Molecule 7: Proteasome subunit alpha type-1



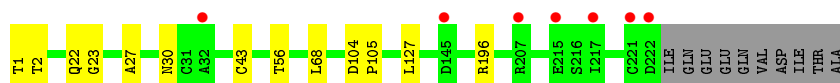
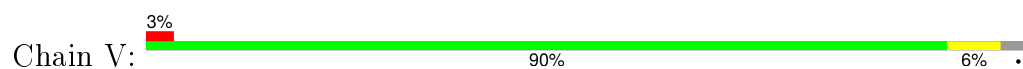
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2

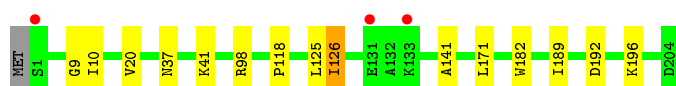


- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

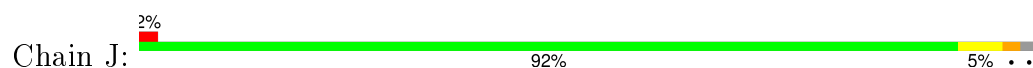




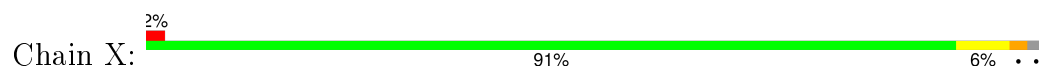
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4



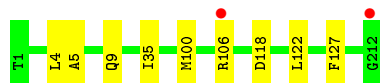
- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



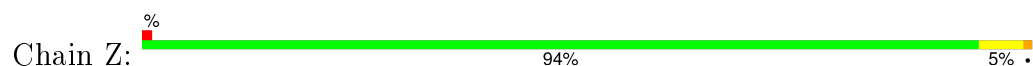
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6

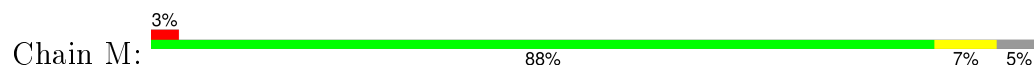


- Molecule 12: Proteasome subunit beta type-6

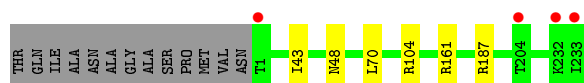
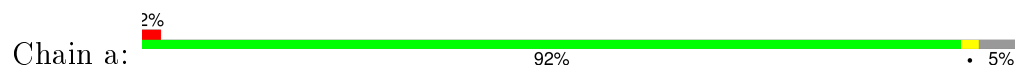




- Molecule 13: Proteasome subunit beta type-7



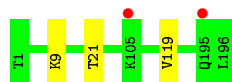
- Molecule 13: Proteasome subunit beta type-7



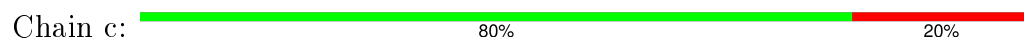
- Molecule 14: Proteasome subunit beta type-1



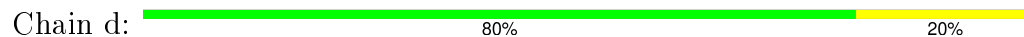
- Molecule 14: Proteasome subunit beta type-1



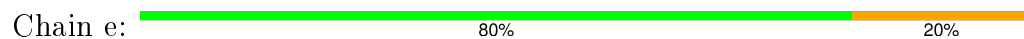
- Molecule 15: Ac-PLL-ep



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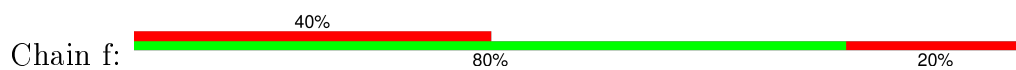


- Molecule 15: Ac-PLL-ep

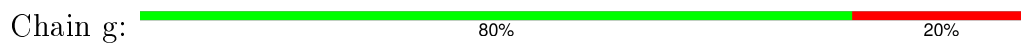




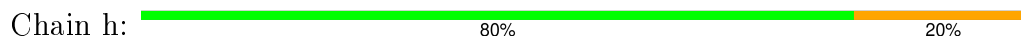
- Molecule 15: Ac-PLL-ep



- Molecule 15: Ac-PLL-ep



- Molecule 15: Ac-PLL-ep



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.82Å 298.32Å 145.62Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 14.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-2.60) 98.0 (14.99-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.199 , 0.220 0.202 , 0.221	Depositor DCC
R_{free} test set	15979 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 319589 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50137	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ACE, CL, DCL, 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	0.27	0/1952	0.48	0/2642
1	O	0.27	0/1952	0.48	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.48	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.48	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.28	0/1715	0.48	0/2326
8	V	0.29	0/1715	0.49	0/2326
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.49	0/2174
10	J	0.26	0/1589	0.49	0/2142
10	X	0.26	0/1589	0.49	0/2142
11	K	0.27	0/1681	0.49	0/2274
11	Y	0.28	0/1681	0.50	0/2274
12	L	0.27	0/1795	0.48	0/2420
12	Z	0.38	2/1806 (0.1%)	0.55	4/2435 (0.2%)
13	M	0.28	0/1855	0.51	0/2514
13	a	0.28	0/1855	0.51	0/2514
14	N	0.34	0/1541	0.49	0/2087
14	b	0.32	0/1541	0.49	0/2087
15	c	1.77	1/16 (6.2%)	2.08	1/22 (4.5%)
15	d	2.95	2/16 (12.5%)	1.46	0/22
15	e	2.47	1/16 (6.2%)	1.32	0/22
15	f	1.78	1/16 (6.2%)	1.95	1/22 (4.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	2.57	1/16 (6.2%)	1.83	0/22
15	h	2.58	1/16 (6.2%)	1.45	0/22
All	All	0.30	9/50301 (0.0%)	0.49	6/68015 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	Z	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	2	PRO	CA-C	-8.07	1.36	1.52
15	e	2	PRO	CA-C	-7.79	1.37	1.52
15	g	2	PRO	CA-C	-7.70	1.37	1.52
15	d	2	PRO	CA-C	-7.28	1.38	1.52
15	d	2	PRO	N-CD	-6.86	1.38	1.47
12	Z	108[A]	HIS	CA-C	6.80	1.70	1.52
12	Z	108[B]	HIS	CA-C	6.80	1.70	1.52
15	f	2	PRO	CA-C	-6.40	1.40	1.52
15	c	2	PRO	CA-C	-6.36	1.40	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	2	PRO	CA-N-CD	-6.87	101.88	111.50
15	f	2	PRO	CA-N-CD	-6.21	102.81	111.50
12	Z	108[A]	HIS	CA-C-N	-5.55	105.00	117.20
12	Z	108[B]	HIS	CA-C-N	-5.55	105.00	117.20
12	Z	108[A]	HIS	CA-C-O	5.53	131.71	120.10
12	Z	108[B]	HIS	CA-C-O	5.53	131.71	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	Z	108[A]	HIS	Mainchain
12	Z	108[B]	HIS	Mainchain

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	5	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1684	0	1685	4	0
8	V	1684	0	1685	4	0
9	I	1581	0	1574	10	0
9	W	1581	0	1574	10	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	8	0
11	K	1644	0	1592	6	0
11	Y	1644	0	1592	4	0
12	L	1757	0	1711	6	0
12	Z	1764	0	1718	5	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	3	0
14	b	1512	0	1478	0	0
15	c	30	0	38	0	0
15	d	30	0	37	0	0
15	e	30	0	37	0	0
15	f	30	0	39	0	0
15	g	30	0	37	0	0
15	h	30	0	37	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	K	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	29	0	0	0	0
19	B	21	0	0	0	0
19	C	14	0	0	0	0
19	D	16	0	0	0	0
19	E	14	0	0	0	0
19	F	17	0	0	0	0
19	G	29	0	0	0	0
19	H	24	0	0	0	0
19	I	34	0	0	0	0
19	J	22	0	0	0	0
19	K	21	0	0	0	0
19	L	30	0	0	0	0
19	M	28	0	0	0	0
19	N	25	0	0	0	0
19	O	19	0	0	0	0
19	P	11	0	0	0	0
19	Q	11	0	0	0	0
19	R	13	0	0	0	0
19	S	10	0	0	0	0
19	T	14	0	0	0	0
19	U	36	0	0	0	0
19	V	18	0	0	0	0
19	W	19	0	0	0	0
19	X	28	0	0	0	0
19	Y	25	0	0	0	0
19	Z	28	0	0	0	0
19	a	34	0	0	0	0
19	b	25	0	0	0	0
19	c	1	0	0	0	0
19	e	2	0	0	0	0
19	h	1	0	0	0	0
All	All	50137	0	49308	116	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 (116) 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:J:1:MET:O	10:J:2:ASP:HB2	1.86	0.73
10:X:1:MET:O	10:X:2:ASP:HB2	1.87	0.73
9:I:98:ARG:HD2	9:I:126:ILE:HD12	1.71	0.72
9:W:98:ARG:HD2	9:W:126:ILE:HD12	1.71	0.71
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.75	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.74	0.69
9:W:125:LEU:HG	9:W:126:ILE:HG22	1.80	0.64
9:W:98:ARG:CD	9:W:126:ILE:HD12	2.28	0.63
9:I:98:ARG:CD	9:I:126:ILE:HD12	2.28	0.62
9:I:125:LEU:HG	9:I:126:ILE:HG22	1.81	0.61
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.83	0.60
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.84	0.59
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.57
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.87	0.57
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.87	0.56
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.35	0.56
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.87	0.56
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.87	0.55
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.90	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.53
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.91	0.53
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.91	0.52
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.75	0.51
10:J:174:MET:HA	10:X:174:MET:HA	1.93	0.51
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.75	0.50
3:C:201:VAL:HG13	3:C:202:GLN:N	2.28	0.48
9:W:126:ILE:O	9:W:126:ILE:HG13	2.13	0.48
9:I:126:ILE:HG13	9:I:126:ILE:O	2.12	0.48
3:C:201:VAL:O	3:C:202:GLN:CB	2.62	0.48
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.48
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.28	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.48
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.62	0.48
12:L:8:ASN:HA	12:L:30:ILE:O	2.13	0.48
11:K:209:ASN:O	9:W:37:ASN:ND2	2.46	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.48
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.47
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.96	0.47
11:K:100:MET:CE	11:K:127:PHE:HB2	2.45	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.47
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.15	0.47
12:L:36:ASN:HB3	13:M:137:TYR:CD1	2.50	0.47
10:X:1:MET:O	10:X:2:ASP:CB	2.60	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.46
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.45	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.15	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.46
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.98	0.46
3:C:201:VAL:O	3:C:202:GLN:HB2	2.15	0.45
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.57	0.45
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.98	0.45
1:A:83:ARG:NH2	7:G:152:GLY:O	2.47	0.45
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.52	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.99	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.45
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.52	0.44
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.17	0.44
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.53	0.44
10:J:1:MET:O	10:J:2:ASP:CB	2.59	0.44
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.99	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.44
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.53	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.44
1:O:55:LEU:HB3	7:U:159:ALA:O	2.18	0.43
8:V:1:THR:HG22	8:V:2:THR:N	2.32	0.43
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.43
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.58	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.99	0.43
6:F:97:LYS:NZ	14:N:84:GLU:OE1	2.49	0.43
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.00	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.43
3:C:51:LYS:O	3:C:52:LEU:HB2	2.18	0.43
1:A:176:GLU:HG2	2:B:55:LEU:HD13	2.01	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.42
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.01	0.42
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.42
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.01	0.42
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.01	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.41
8:H:218:VAL:HG21	9:I:196:LYS:HB2	2.02	0.41
5:E:9:THR:HG21	5:E:119:THR:HA	2.03	0.41
8:H:22:GLN:HG3	8:H:22:GLN:O	2.19	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.02	0.41
8:V:22:GLN:O	8:V:23:GLY:C	2.56	0.41
1:A:149:GLN:O	1:A:156:TYR:HA	2.21	0.41
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.03	0.41
11:K:5:ALA:HB3	11:K:100:MET:CE	2.51	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.41
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.03	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.51	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.40
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.40
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.40
5:S:9:THR:HG21	5:S:119:THR:HA	2.03	0.40
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.56	0.40
10:J:1:MET:HA	10:J:34:LYS:CE	2.51	0.40
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.56	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%)	6 (2%)	2 (1%)	24	46
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	24	46
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	46
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	46
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%)	225 (98%)	4 (2%)	0	100	100
5	S	229/234 (98%)	225 (98%)	4 (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%)	234 (98%)	5 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	215 (98%)	5 (2%)	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%)	190 (98%)	2 (1%)	1 (0%)	34	60
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	34	60
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	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	225 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	225 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	c	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
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%)	1 (50%)	0	1 (50%)	0	0
15	g	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
15	h	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6289/6644 (95%)	6135 (98%)	141 (2%)	13 (0%)	52	77

All (13) 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
15	c	2	PRO
15	f	2	PRO
3	C	205	ALA
3	Q	205	ALA
15	g	2	PRO
2	B	221	ASP
2	P	221	ASP

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	74	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	90
2	B	203/216 (94%)	197 (97%)	6 (3%)	48	76
2	P	203/216 (94%)	197 (97%)	6 (3%)	48	76
3	C	212/226 (94%)	204 (96%)	8 (4%)	40	68
3	Q	212/226 (94%)	204 (96%)	8 (4%)	40	68
4	D	194/215 (90%)	184 (95%)	10 (5%)	29	54
4	R	194/215 (90%)	184 (95%)	10 (5%)	29	54
5	E	190/193 (98%)	182 (96%)	8 (4%)	36	65
5	S	190/193 (98%)	182 (96%)	8 (4%)	36	65
6	F	201/239 (84%)	190 (94%)	11 (6%)	27	51
6	T	201/239 (84%)	190 (94%)	11 (6%)	27	51
7	G	206/210 (98%)	199 (97%)	7 (3%)	44	72
7	U	206/210 (98%)	199 (97%)	7 (3%)	44	72
8	H	181/190 (95%)	174 (96%)	7 (4%)	39	68
8	V	181/190 (95%)	175 (97%)	6 (3%)	45	73
9	I	172/173 (99%)	167 (97%)	5 (3%)	50	77
9	W	172/173 (99%)	167 (97%)	5 (3%)	50	77
10	J	173/175 (99%)	167 (96%)	6 (4%)	43	71
10	X	173/175 (99%)	167 (96%)	6 (4%)	43	71
11	K	169/169 (100%)	164 (97%)	5 (3%)	48	76
11	Y	169/169 (100%)	164 (97%)	5 (3%)	48	76
12	L	185/185 (100%)	178 (96%)	7 (4%)	40	68
12	Z	186/185 (100%)	180 (97%)	6 (3%)	46	74
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	76
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	76
14	N	162/162 (100%)	159 (98%)	3 (2%)	65	86
14	b	162/162 (100%)	159 (98%)	3 (2%)	65	86
15	c	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	d	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	e	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	f	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	g	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	h	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	5325/5552 (96%)	5138 (96%)	187 (4%)	43	71

All (187) 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	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
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	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU

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Mol	Chain	Res	Type
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
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
7	G	125	MET
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	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
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

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Mol	Chain	Res	Type
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	150	LEU
12	L	167	LYS
13	M	43	ILE
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	119	VAL
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
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

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Mol	Chain	Res	Type
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
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	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	23	ARG
10	X	35	THR

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Mol	Chain	Res	Type
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	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
14	b	9	LYS
14	b	21	THR
14	b	119	VAL
15	c	2	PRO
15	e	2	PRO
15	f	2	PRO
15	g	2	PRO
15	h	2	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	95	GLN
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

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Mol	Chain	Res	Type
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
8	H	57	GLN
9	I	37	ASN
10	J	55	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
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN

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Mol	Chain	Res	Type
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	210	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	57	GLN
8	V	66	HIS
10	X	55	GLN
10	X	78	GLN
10	X	86	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	179	ASN

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Mol	Chain	Res	Type
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	DCL	c	4	8,15	7,7,7	0.59	0	7,8,8	1.93	2 (28%)
15	DCL	d	4	11,15	7,7,7	0.77	0	7,8,8	2.08	3 (42%)
15	DCL	e	4	15,14	7,7,7	1.24	2 (28%)	7,8,8	2.29	3 (42%)
15	DCL	f	4	8,15	7,7,7	0.38	0	7,8,8	1.98	3 (42%)
15	DCL	g	4	11,15	7,7,7	0.95	1 (14%)	7,8,8	2.10	3 (42%)
15	DCL	h	4	15,14	7,7,7	1.06	0	7,8,8	2.34	3 (42%)

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	DCL	c	4	8,15	-	0/6/6/6	0/0/0/0
15	DCL	d	4	11,15	-	0/6/6/6	0/0/0/0
15	DCL	e	4	15,14	-	0/6/6/6	0/0/0/0
15	DCL	f	4	8,15	-	0/6/6/6	0/0/0/0
15	DCL	g	4	11,15	-	0/6/6/6	0/0/0/0
15	DCL	h	4	15,14	-	0/6/6/6	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	4	DCL	OXT-C	-2.32	1.32	1.42
15	g	4	DCL	OXT-C	-2.16	1.33	1.42
15	e	4	DCL	C-CA	2.08	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	h	4	DCL	CB-CA-C	-4.54	105.41	111.67
15	e	4	DCL	CB-CA-C	-4.32	105.71	111.67
15	d	4	DCL	CB-CA-N	-3.67	98.69	108.96
15	g	4	DCL	CB-CA-N	-3.54	99.06	108.96
15	f	4	DCL	CB-CA-C	-3.40	106.97	111.67
15	h	4	DCL	CB-CA-N	-3.33	99.66	108.96
15	c	4	DCL	CB-CA-N	-3.29	99.77	108.96
15	c	4	DCL	CB-CA-C	-3.06	107.45	111.67
15	g	4	DCL	OXT-C-CA	-2.92	104.04	111.77
15	g	4	DCL	CB-CA-C	-2.90	107.66	111.67
15	e	4	DCL	OXT-C-CA	-2.86	104.20	111.77
15	d	4	DCL	CB-CA-C	-2.85	107.74	111.67
15	f	4	DCL	OXT-C-CA	-2.83	104.26	111.77
15	e	4	DCL	CB-CA-N	-2.78	101.19	108.96
15	d	4	DCL	OXT-C-CA	-2.68	104.66	111.77
15	f	4	DCL	CB-CA-N	-2.58	101.75	108.96
15	h	4	DCL	OXT-C-CA	-2.23	105.87	111.77

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	MES	K	302	-	12,12,12	2.12	1 (8%)	15,16,16	1.60	3 (20%)
18	MES	Y	301	-	12,12,12	2.10	1 (8%)	15,16,16	1.70	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	K	302	-	-	0/6/14/14	0/1/1/1
18	MES	Y	301	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	302	MES	C8-S	-7.02	1.67	1.77
18	Y	301	MES	C8-S	-6.99	1.67	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	301	MES	O3S-S-C8	2.40	109.98	104.99
18	K	302	MES	O3S-S-C8	2.46	110.10	104.99
18	Y	301	MES	O1S-S-C8	2.51	108.64	106.87
18	K	302	MES	O1S-S-C8	3.39	109.26	106.87
18	K	302	MES	O2S-S-C8	3.48	109.33	106.87
18	Y	301	MES	O2S-S-C8	4.62	110.13	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.26	5 (2%) 68 63	34, 47, 83, 127	0
1	O	250/250 (100%)	-0.18	10 (4%) 42 34	37, 53, 95, 127	0
2	B	244/258 (94%)	-0.07	15 (6%) 25 18	34, 52, 101, 154	0
2	P	244/258 (94%)	-0.05	15 (6%) 25 18	37, 55, 104, 156	0
3	C	240/254 (94%)	0.02	17 (7%) 19 13	35, 56, 120, 158	0
3	Q	240/254 (94%)	0.29	24 (10%) 9 6	39, 69, 150, 192	0
4	D	235/260 (90%)	-0.28	3 (1%) 79 75	37, 57, 90, 132	0
4	R	235/260 (90%)	-0.16	7 (2%) 54 47	41, 61, 96, 145	0
5	E	231/234 (98%)	-0.15	7 (3%) 54 47	42, 60, 94, 135	0
5	S	231/234 (98%)	-0.03	8 (3%) 48 40	39, 62, 100, 137	0
6	F	243/288 (84%)	-0.25	8 (3%) 50 43	34, 53, 103, 129	0
6	T	243/288 (84%)	-0.12	9 (3%) 45 37	29, 57, 104, 140	0
7	G	241/252 (95%)	-0.21	10 (4%) 41 33	34, 50, 90, 147	0
7	U	241/252 (95%)	-0.35	5 (2%) 67 61	35, 48, 82, 125	0
8	H	222/232 (95%)	-0.22	3 (1%) 78 74	36, 48, 76, 112	0
8	V	222/232 (95%)	-0.04	7 (3%) 51 44	36, 50, 82, 120	0
9	I	204/205 (99%)	-0.50	3 (1%) 76 71	29, 42, 71, 93	0
9	W	204/205 (99%)	-0.48	3 (1%) 76 71	30, 45, 73, 98	0
10	J	195/198 (98%)	-0.47	3 (1%) 76 71	31, 43, 68, 115	0
10	X	195/198 (98%)	-0.45	3 (1%) 76 71	33, 46, 72, 123	0
11	K	212/212 (100%)	-0.42	2 (0%) 85 83	33, 46, 71, 90	0
11	Y	212/212 (100%)	-0.51	2 (0%) 85 83	33, 44, 71, 96	0
12	L	222/222 (100%)	-0.43	1 (0%) 91 90	32, 47, 70, 97	0
12	Z	222/222 (100%)	-0.40	2 (0%) 85 83	30, 46, 73, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.31	8 (3%) 49 41	28, 46, 70, 101	0
13	a	233/246 (94%)	-0.41	4 (1%) 73 68	30, 44, 67, 85	0
14	N	196/196 (100%)	-0.56	2 (1%) 84 81	28, 40, 68, 95	0
14	b	196/196 (100%)	-0.46	2 (1%) 84 81	29, 41, 69, 92	0
15	c	2/5 (40%)	1.36	0 100 100	81, 81, 81, 82	0
15	d	2/5 (40%)	-0.33	0 100 100	67, 67, 67, 72	0
15	e	2/5 (40%)	-0.66	0 100 100	51, 51, 51, 55	0
15	f	2/5 (40%)	3.84	2 (100%) 0 0	81, 81, 81, 88	0
15	g	2/5 (40%)	-0.43	0 100 100	62, 62, 62, 67	0
15	h	2/5 (40%)	-0.69	0 100 100	54, 54, 54, 60	0
All	All	6348/6644 (95%)	-0.25	190 (2%) 54 47	28, 50, 92, 192	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.5
2	B	220	ASN	7.3
2	P	219	ALA	7.1
2	P	222	GLY	6.6
3	Q	206	LYS	6.5
1	O	1	MET	6.3
3	Q	239	GLN	6.2
3	Q	50	LEU	6.1
3	Q	238	LYS	6.1
13	M	232	LYS	6.0
13	M	233	ILE	5.8
8	V	222	ASP	5.8
8	V	221	CYS	5.6
3	Q	240	GLU	5.6
10	X	194	ASP	5.5
2	P	51	VAL	5.5
2	B	218	GLY	5.5
3	Q	49	THR	5.3
2	B	219	ALA	5.3
1	O	249	ALA	5.2
13	M	230	THR	5.2
10	J	1	MET	5.2
15	f	3	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
5	E	202	ASP	5.1
2	P	59	ASP	5.1
5	S	202	ASP	4.9
3	C	238	LYS	4.9
4	D	242	GLU	4.9
2	P	221	ASP	4.8
10	J	194	ASP	4.8
8	H	222	ASP	4.8
3	Q	51	LYS	4.7
6	F	202	ASP	4.7
11	K	212	GLY	4.7
3	C	206	LYS	4.6
13	M	231	GLN	4.6
2	B	221	ASP	4.4
13	M	229	GLY	4.4
3	C	49	THR	4.3
10	X	1	MET	4.2
2	P	220	ASN	4.2
6	F	203	ASN	4.2
3	Q	236	GLN	4.2
2	B	51	VAL	4.2
6	T	241	LYS	4.2
3	Q	205	ALA	4.2
9	I	1	SER	4.1
9	W	1	SER	4.1
7	G	242	GLN	4.0
3	Q	225	GLU	3.9
3	Q	48	SER	3.9
3	C	239	GLN	3.9
3	C	236	GLN	3.9
3	C	180	LYS	3.8
8	H	221	CYS	3.7
7	G	240	ALA	3.7
6	T	181	GLU	3.6
2	B	242	GLY	3.5
3	Q	202	GLN	3.4
6	F	244	ASN	3.4
6	T	244	ASN	3.4
5	S	54	GLU	3.4
6	T	205	GLU	3.4
13	M	216	ASN	3.4
13	a	1	THR	3.3

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Mol	Chain	Res	Type	RSRZ
5	S	233	ILE	3.3
2	P	60	THR	3.3
1	O	201	GLU	3.3
3	C	202	GLN	3.2
3	C	225	GLU	3.2
3	C	203	THR	3.2
1	A	250	LEU	3.2
11	Y	106	ARG	3.2
2	P	52	THR	3.1
2	P	218	GLY	3.1
9	W	133	LYS	3.1
12	Z	210	ASP	3.1
4	R	242	GLU	3.1
6	F	241	LYS	3.1
9	I	133	LYS	3.1
6	T	230	ASP	3.0
3	Q	223	SER	3.0
11	Y	212	GLY	3.0
2	B	182	ASP	3.0
7	U	222	ASP	2.9
14	b	195	GLN	2.9
6	T	2	THR	2.9
3	Q	141	ASP	2.9
6	F	205	GLU	2.9
7	G	3	TYR	2.9
1	A	249	ALA	2.9
10	J	193	ASP	2.9
6	T	243	ILE	2.9
4	R	241	ALA	2.9
7	U	242	GLN	2.8
13	M	1	THR	2.8
3	C	205	ALA	2.8
8	V	145	ASP	2.8
3	Q	204	GLY	2.8
1	O	52	SER	2.7
12	Z	1	GLN	2.7
1	O	231	LYS	2.7
3	C	204	GLY	2.7
7	G	181	LYS	2.7
3	C	48	SER	2.6
10	X	193	ASP	2.6
7	U	2	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
9	W	192	ASP	2.6
15	f	2	PRO	2.6
1	O	229	THR	2.6
8	V	217	ILE	2.6
2	B	59	ASP	2.6
1	O	2	THR	2.5
8	V	207	ARG	2.5
2	B	217	LYS	2.5
5	S	180	LYS	2.5
5	E	233	ILE	2.5
7	U	203	ASP	2.5
7	G	241	GLU	2.5
2	B	61	SER	2.5
3	C	37	LYS	2.5
3	Q	175	LYS	2.5
3	C	181	GLU	2.5
3	C	50	LEU	2.5
6	F	243	ILE	2.5
4	R	125	LEU	2.5
3	Q	60	SER	2.4
4	D	1	ASP	2.4
3	Q	47	ARG	2.4
5	S	173	ARG	2.4
4	D	238	LYS	2.4
2	B	230	LYS	2.4
2	B	203	SER	2.4
7	G	222	ASP	2.4
2	B	235	LYS	2.4
4	R	201	GLU	2.4
14	N	105	LYS	2.4
13	M	47	ASP	2.4
5	S	3	ASN	2.4
4	R	177	ASN	2.4
2	P	203	SER	2.3
6	T	180	PRO	2.3
1	O	182	GLU	2.3
11	K	151	GLU	2.3
14	N	195	GLN	2.3
2	P	240	LYS	2.3
6	F	53	LYS	2.3
4	R	217	GLN	2.2
8	H	215	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
7	G	188	GLU	2.2
3	C	175	LYS	2.2
1	A	201	GLU	2.2
7	U	241	GLU	2.2
9	I	131	GLU	2.2
5	E	3	ASN	2.2
6	F	2	THR	2.2
13	a	232	LYS	2.2
5	E	207	VAL	2.2
3	Q	203	THR	2.2
5	S	123	GLY	2.2
2	P	225	TYR	2.2
4	R	2	ARG	2.2
1	A	248	GLU	2.1
5	E	122	TYR	2.1
14	b	105	LYS	2.1
7	G	230	GLU	2.1
2	P	232	GLN	2.1
7	G	2	GLY	2.1
13	a	233	ILE	2.1
3	Q	187	GLU	2.1
5	E	218	ASP	2.1
5	S	218	ASP	2.1
2	P	244	THR	2.1
6	T	237	ASP	2.1
3	Q	52	LEU	2.1
3	Q	231	VAL	2.1
13	a	204	THR	2.1
1	O	53	SER	2.1
12	L	210	ASP	2.1
5	E	201	ARG	2.1
7	G	186	ASN	2.1
3	C	60	SER	2.1
8	V	215	GLU	2.1
2	B	225	TYR	2.0
1	O	50	LYS	2.0
3	Q	229	GLN	2.0
2	P	217	LYS	2.0
8	V	32	ALA	2.0
2	B	93	HIS	2.0
3	Q	235	GLU	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, 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	LLDF	B-factors(Å ²)	Q<0.9
15	DCL	h	4	8/8	0.93	0.23	-	52,62,65,66	0
15	DCL	d	4	8/8	0.94	0.23	-	59,72,74,75	0
15	DCL	g	4	8/8	0.94	0.19	-	58,68,74,77	0
15	DCL	e	4	8/8	0.93	0.20	-	50,58,60,61	0
15	DCL	c	4	8/8	0.76	0.37	-	81,82,83,86	0
15	DCL	f	4	8/8	0.82	0.35	-	84,88,89,90	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
18	MES	K	302	12/12	0.88	0.28	4.54	66,83,86,87	0
18	MES	Y	301	12/12	0.87	0.27	4.39	63,81,84,86	0
16	MG	I	301	1/1	0.98	0.21	2.57	54,54,54,54	0
16	MG	Z	301	1/1	0.95	0.19	1.43	52,52,52,52	0
17	CL	b	201	1/1	0.94	0.10	-0.88	69,69,69,69	0
16	MG	I	302	1/1	0.95	0.10	-1.23	44,44,44,44	0
16	MG	K	301	1/1	0.97	0.08	-1.51	53,53,53,53	0
16	MG	G	301	1/1	0.97	0.08	-1.55	55,55,55,55	0
16	MG	N	201	1/1	0.99	0.07	-2.17	41,41,41,41	0
17	CL	N	202	1/1	0.96	0.07	-2.71	47,47,47,47	0
16	MG	L	301	1/1	0.98	0.06	-3.59	56,56,56,56	0
17	CL	U	301	1/1	0.99	0.16	-	30,30,30,30	0
17	CL	G	302	1/1	0.99	0.13	-	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.