



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:41 PM BST

PDB ID : 4Y8Q  
Title : Yeast 20S proteasome beta7-delta7\_Cter mutant in complex with Ac-PAY-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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

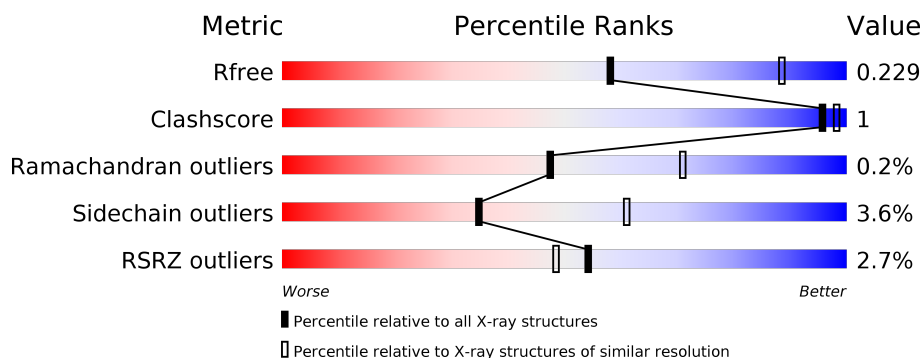
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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  $\geq 3$ , 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	<div> <div>2%</div> <div>98%</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>90%</div> <div>5% • 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>89%</div> <div>5% • 5%</div> </div>
3	C	254	<div> <div>7%</div> <div>88%</div> <div>6% • 6%</div> </div>
3	Q	254	<div> <div>9%</div> <div>89%</div> <div>• • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	239	
13	a	239	
14	N	196	
14	b	196	
15	c	5	
15	d	5	
15	e	5	

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Mol	Chain	Length	Quality of chain
15	f	5	<div><div></div><div>60%</div><div>20%</div><div>20%</div></div>

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49946 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	1	0
			1764	1120	305	335	4			
12	Z	222	Total	C	N	O	S	0	1	0
			1764	1120	305	335	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			31	22	3	6			
15	d	5	Total	C	N	O	0	0	0
			31	22	3	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	5	Total	C	N	O	0	0	0
			31	22	3	6			
15	f	5	Total	C	N	O	0	0	0
			31	22	3	6			

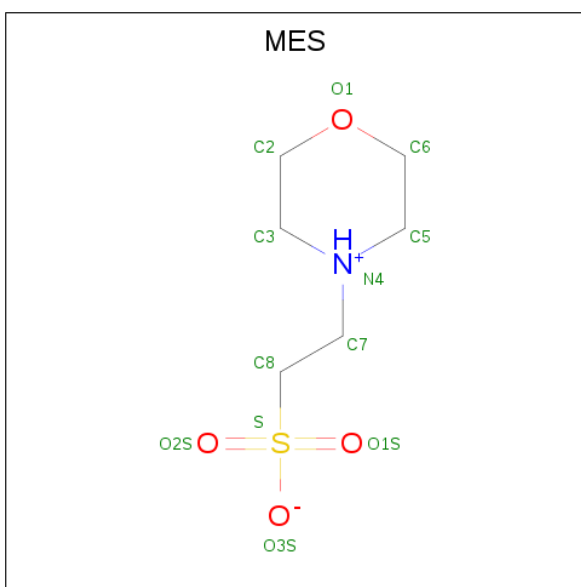
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	30	Total	O	0	0
			30	30		
19	B	27	Total	O	0	0
			27	27		
19	C	26	Total	O	0	0
			26	26		
19	D	19	Total	O	0	0
			19	19		
19	E	12	Total	O	0	0
			12	12		
19	F	17	Total	O	0	0
			17	17		
19	G	33	Total	O	0	0
			33	33		
19	H	23	Total	O	0	0
			23	23		
19	I	30	Total	O	0	0
			30	30		
19	J	30	Total	O	0	0
			30	30		

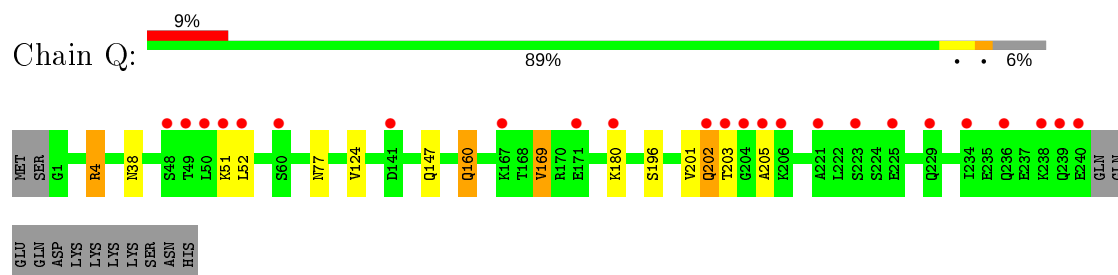
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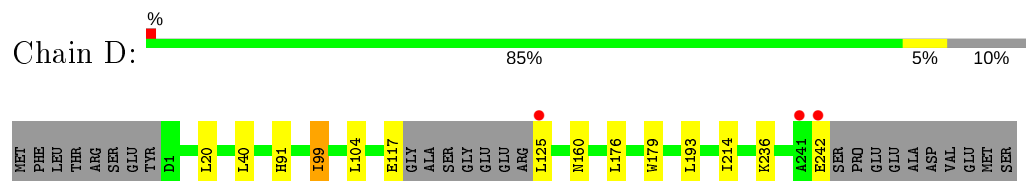
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	K	39	Total 39	O 39	0	0
19	L	31	Total 31	O 31	0	0
19	M	25	Total 25	O 25	0	0
19	N	15	Total 15	O 15	0	0
19	O	16	Total 16	O 16	0	0
19	P	14	Total 14	O 14	0	0
19	Q	12	Total 12	O 12	0	0
19	R	12	Total 12	O 12	0	0
19	S	7	Total 7	O 7	0	0
19	T	19	Total 19	O 19	0	0
19	U	34	Total 34	O 34	0	0
19	V	24	Total 24	O 24	0	0
19	W	20	Total 20	O 20	0	0
19	X	24	Total 24	O 24	0	0
19	Y	28	Total 28	O 28	0	0
19	Z	30	Total 30	O 30	0	0
19	a	32	Total 32	O 32	0	0
19	b	20	Total 20	O 20	0	0
19	d	2	Total 2	O 2	0	0
19	e	2	Total 2	O 2	0	0
19	f	2	Total 2	O 2	0	0



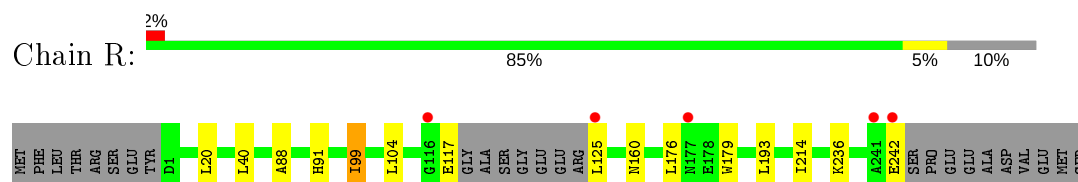
- Molecule 3: Proteasome subunit alpha type-4



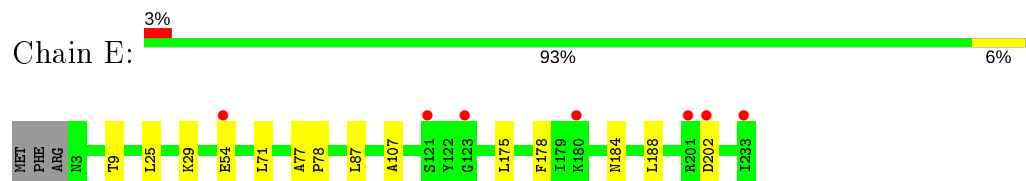
- Molecule 4: Proteasome subunit alpha type-5



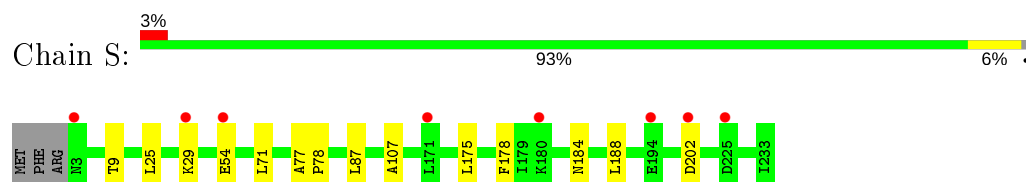
- Molecule 4: Proteasome subunit alpha type-5



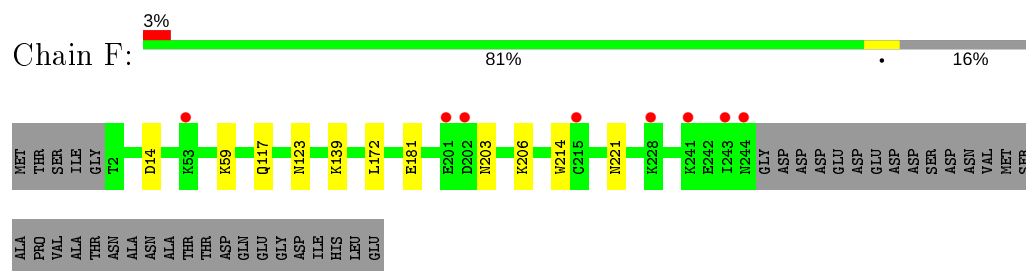
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7

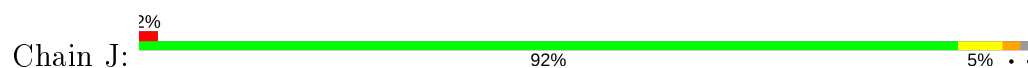


- Molecule 6: Probable proteasome subunit alpha type-7

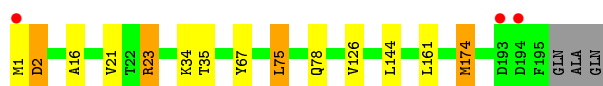
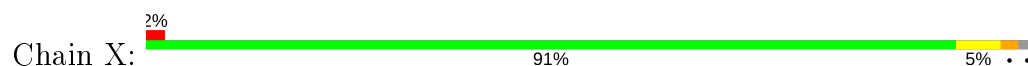




- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



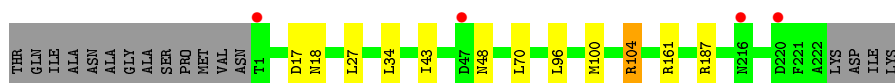
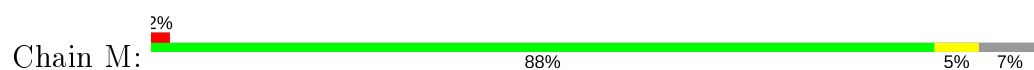
- Molecule 12: Proteasome subunit beta type-6



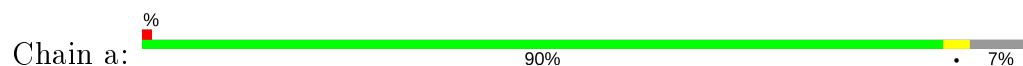
- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7



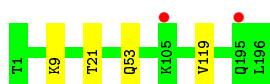
- Molecule 13: Proteasome subunit beta type-7



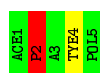
- Molecule 14: Proteasome subunit beta type-1



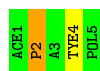
- Molecule 14: Proteasome subunit beta type-1



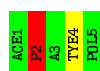
- Molecule 15: Ac-PAY-ep



- Molecule 15: Ac-PAY-ep



- Molecule 15: Ac-PAY-ep



- Molecule 15: Ac-PAY-ep



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.78Å 300.56Å 145.55Å 90.00° 113.32° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (15.00-2.60) 97.6 (15.00-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.206 , 0.228 0.209 , 0.229	Depositor DCC
$R_{free}$ test set	16001 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	49946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACE, CL, TYE, 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	0.47	0/2642
1	O	0.27	0/1952	0.47	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	0.47	0/2433
6	F	0.28	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.46	0/2609
7	G	0.28	0/1945	0.47	0/2634
7	U	0.28	0/1945	0.47	0/2634
8	H	0.33	1/1715 (0.1%)	0.58	3/2326 (0.1%)
8	V	0.36	1/1715 (0.1%)	0.59	3/2326 (0.1%)
9	I	0.31	0/1611	0.49	0/2174
9	W	0.27	0/1611	0.48	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.26	0/1589	0.49	0/2142
11	K	0.28	0/1681	0.50	0/2274
11	Y	0.28	0/1681	0.50	0/2274
12	L	0.37	2/1806 (0.1%)	0.54	2/2435 (0.1%)
12	Z	0.38	2/1806 (0.1%)	0.56	4/2435 (0.2%)
13	M	0.28	0/1766	0.51	0/2398
13	a	0.28	0/1766	0.51	0/2398
14	N	0.35	0/1541	0.50	0/2087
14	b	0.34	0/1541	0.49	0/2087
15	c	2.81	1/13 (7.7%)	2.43	1/18 (5.6%)
15	d	2.56	1/13 (7.7%)	1.34	0/18
15	e	2.64	1/13 (7.7%)	2.36	1/18 (5.6%)
15	f	2.34	1/13 (7.7%)	1.10	0/18

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.31	10/50090 (0.0%)	0.50	14/67738 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	3	ILE	C-N	-10.50	1.09	1.34
8	H	3	ILE	C-N	-8.59	1.14	1.34
15	c	2	PRO	CA-C	-7.71	1.37	1.52
15	f	2	PRO	CA-C	-7.51	1.37	1.52
12	Z	108[A]	HIS	CA-C	7.50	1.72	1.52
12	Z	108[B]	HIS	CA-C	7.50	1.72	1.52
15	e	2	PRO	CA-C	-7.35	1.38	1.52
15	d	2	PRO	CA-C	-7.19	1.38	1.52
12	L	108[A]	HIS	CA-C	6.16	1.69	1.52
12	L	108[B]	HIS	CA-C	6.16	1.69	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	2	THR	O-C-N	-12.54	102.63	122.70
8	H	2	THR	O-C-N	-11.22	104.75	122.70
8	V	2	THR	C-N-CA	8.84	143.80	121.70
8	V	2	THR	CA-C-N	8.58	136.08	117.20
8	H	2	THR	C-N-CA	8.03	141.76	121.70
8	H	2	THR	CA-C-N	7.52	133.74	117.20
12	Z	108[A]	HIS	CA-C-O	7.22	135.26	120.10
12	Z	108[B]	HIS	CA-C-O	7.22	135.26	120.10
12	L	108[A]	HIS	CA-C-O	6.26	133.24	120.10
12	L	108[B]	HIS	CA-C-O	6.26	133.24	120.10
15	c	2	PRO	CA-N-CD	-5.73	103.48	111.50
12	Z	108[A]	HIS	CA-C-N	-5.61	104.86	117.20
12	Z	108[B]	HIS	CA-C-N	-5.61	104.86	117.20
15	e	2	PRO	CA-N-CD	-5.53	103.76	111.50

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	1	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	7	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	5	0
8	H	1684	0	1687	2	0
8	V	1684	0	1687	3	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	9	0
11	K	1644	0	1592	6	0
11	Y	1644	0	1592	4	0
12	L	1764	0	1718	5	0
12	Z	1764	0	1718	7	0
13	M	1736	0	1737	4	0
13	a	1736	0	1737	0	0
14	N	1512	0	1478	3	0
14	b	1512	0	1478	0	0
15	c	31	0	28	0	0
15	d	31	0	28	0	0
15	e	31	0	28	0	0
15	f	31	0	29	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	c	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	e	12	0	13	0	0
19	A	30	0	0	0	0
19	B	27	0	0	0	0
19	C	26	0	0	0	0
19	D	19	0	0	0	0
19	E	12	0	0	0	0
19	F	17	0	0	0	0
19	G	33	0	0	0	0
19	H	23	0	0	0	0
19	I	30	0	0	0	0
19	J	30	0	0	0	0
19	K	39	0	0	0	0
19	L	31	0	0	0	0
19	M	25	0	0	0	0
19	N	15	0	0	0	0
19	O	16	0	0	0	0
19	P	14	0	0	0	0
19	Q	12	0	0	0	0
19	R	12	0	0	0	0
19	S	7	0	0	0	0
19	T	19	0	0	0	0
19	U	34	0	0	0	0
19	V	24	0	0	0	0
19	W	20	0	0	0	0
19	X	24	0	0	0	0
19	Y	28	0	0	1	0
19	Z	30	0	0	2	0
19	a	32	0	0	0	0
19	b	20	0	0	0	0
19	d	2	0	0	0	0
19	e	2	0	0	0	0
19	f	2	0	0	0	0
All	All	49946	0	49017	101	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 (101) 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)
12:Z:108[B]:HIS:CD2	19:Z:403:HOH:O	2.08	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:108[B]:HIS:HD2	19:Z:403:HOH:O	1.43	0.96
10:X:23:ARG:HD3	19:Y:401:HOH:O	1.81	0.80
10:J:1:MET:O	10:J:2:ASP:HB2	1.86	0.74
10:X:1:MET:O	10:X:2:ASP:HB2	1.87	0.73
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.78	0.66
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.79	0.65
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.85	0.58
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.85	0.58
10:J:174:MET:HA	10:X:174:MET:HA	1.86	0.56
7:G:23:PHE:O	7:G:26:THR:HB	2.08	0.54
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.90	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.53
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.91	0.53
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.91	0.52
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.76	0.50
8:H:22:GLN:HG2	8:H:27:ALA:HB2	1.93	0.50
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.92	0.50
10:X:1:MET:O	10:X:2:ASP:CB	2.59	0.50
8:V:22:GLN:HG2	8:V:27:ALA:HB2	1.93	0.50
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.94	0.49
3:C:201:VAL:O	3:C:202:GLN:CB	2.61	0.49
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.95	0.49
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.76	0.49
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.94	0.49
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.95	0.48
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.96	0.48
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.61	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.95	0.48
3:C:201:VAL:HG13	3:C:202:GLN:N	2.29	0.47
11:K:100:MET:CE	11:K:127:PHE:HB2	2.44	0.47
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.29	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.95	0.47
14:N:152:VAL:HA	14:N:175:MET:HE1	1.95	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.44	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.95	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.98	0.46
1:O:55:LEU:HB3	7:U:159:ALA:O	2.15	0.46
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.98	0.46
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.98	0.46
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.46
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.81	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.17	0.45
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.98	0.45
9:W:98:ARG:O	9:W:126:ILE:HD11	2.17	0.45
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.97	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
12:L:4:PRO:O	13:M:104:ARG:NH1	2.46	0.45
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.16	0.45
3:C:51:LYS:O	3:C:52:LEU:HB2	2.16	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
10:J:1:MET:O	10:J:2:ASP:CB	2.59	0.44
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.53	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.99	0.44
8:V:3:ILE:HG22	8:V:16:ALA:HB2	2.00	0.44
14:N:45:ARG:HD2	14:N:52:THR:HB	1.99	0.44
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.53	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.43
3:C:201:VAL:O	3:C:202:GLN:HB2	2.17	0.43
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.52	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.43
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.01	0.43
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.55	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	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
11:K:49:ALA:O	11:K:53:GLN:HB2	2.20	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.35	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.02	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.41
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.20	0.41
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.01	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
12:Z:125:PHE:HA	12:Z:130:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.41
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	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
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.56	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.51	0.41
11:K:5:ALA:HB3	11:K:100:MET:CE	2.49	0.40
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.03	0.40
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.40
13:M:17:ASP:OD1	13:M:18:ASN:N	2.54	0.40
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.40
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.03	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.03	0.40
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	242 (98%)	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%)	34	57
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34	57
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	39
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	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%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	215 (98%)	5 (2%)	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%)	29	52
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	52
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	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
12	Z	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
13	M	220/239 (92%)	214 (97%)	6 (3%)	0	100	100
13	a	220/239 (92%)	213 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	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%)	1 (50%)	0	1 (50%)	0	0
15	f	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6264/6620 (95%)	6106 (98%)	148 (2%)	10 (0%)	47	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN

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Mol	Chain	Res	Type
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
15	c	2	PRO
15	e	2	PRO
3	C	205	ALA
3	Q	205	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	67	85
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	85
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	63
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	63
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	59
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	59
4	D	194/215 (90%)	184 (95%)	10 (5%)	23	46
4	R	194/215 (90%)	184 (95%)	10 (5%)	23	46
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	55
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	55
6	F	201/239 (84%)	190 (94%)	11 (6%)	21	43
6	T	201/239 (84%)	190 (94%)	11 (6%)	21	43
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	63
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	63
8	H	181/190 (95%)	173 (96%)	8 (4%)	28	53
8	V	181/190 (95%)	173 (96%)	8 (4%)	28	53
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	75
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	62
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	62
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	61
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	61
12	L	186/185 (100%)	180 (97%)	6 (3%)	39	65
12	Z	186/185 (100%)	180 (97%)	6 (3%)	39	65
13	M	190/203 (94%)	184 (97%)	6 (3%)	39	65
13	a	190/203 (94%)	184 (97%)	6 (3%)	39	65
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	73
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	73
15	c	1/1 (100%)	0	1 (100%)	0	0
15	d	1/1 (100%)	0	1 (100%)	0	0
15	e	1/1 (100%)	0	1 (100%)	0	0
15	f	1/1 (100%)	0	1 (100%)	0	0
All	All	5300/5534 (96%)	5108 (96%)	192 (4%)	35	61

All (192) 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	79	LEU
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

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Mol	Chain	Res	Type
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
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	31	CYS
8	H	34	LEU
8	H	43	CYS

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Mol	Chain	Res	Type
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	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	53	GLN
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

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Mol	Chain	Res	Type
2	P	79	LEU
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
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

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Mol	Chain	Res	Type
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	31	CYS
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	7	ARG
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

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Mol	Chain	Res	Type
14	b	21	THR
14	b	53	GLN
14	b	119	VAL
15	c	2	PRO
15	d	2	PRO
15	e	2	PRO
15	f	2	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
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
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	6	HIS
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
8	H	57	GLN

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Mol	Chain	Res	Type
9	I	203	GLN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	79	HIS
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	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
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
8	V	57	GLN

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Mol	Chain	Res	Type
10	X	55	GLN
10	X	118	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	TYE	d	4	15,14	12,12,12	1.95	1 (8%)	13,15,15	1.45	2 (15%)
15	TYE	f	4	15,14	12,12,12	1.83	2 (16%)	13,15,15	1.32	2 (15%)
15	TYE	c	4	11,15	12,12,12	1.66	1 (8%)	13,15,15	1.47	3 (23%)
15	TYE	e	4	11,15	12,12,12	1.84	1 (8%)	13,15,15	1.46	3 (23%)

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	TYE	d	4	15,14	-	2/6/6/6	0/1/1/1
15	TYE	f	4	15,14	-	2/6/6/6	0/1/1/1
15	TYE	c	4	11,15	-	3/6/6/6	0/1/1/1
15	TYE	e	4	11,15	-	3/6/6/6	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	d	4	TYE	CB-CG	-5.88	1.37	1.51
15	e	4	TYE	CB-CG	-5.51	1.38	1.51
15	f	4	TYE	CB-CG	-5.46	1.38	1.51
15	c	4	TYE	CB-CG	-5.01	1.39	1.51
15	f	4	TYE	C-CA	2.03	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	4	TYE	CB-CA-C	-3.57	105.76	112.21
15	e	4	TYE	CB-CA-C	-2.94	106.90	112.21
15	c	4	TYE	CG-CB-CA	2.93	118.83	113.24
15	c	4	TYE	CB-CA-C	-2.91	106.95	112.21
15	f	4	TYE	CG-CB-CA	2.37	117.75	113.24
15	c	4	TYE	O-C-CA	-2.29	102.48	111.52
15	f	4	TYE	CB-CA-C	-2.28	108.08	112.21
15	d	4	TYE	CG-CB-CA	2.12	117.28	113.24
15	e	4	TYE	O-C-CA	-2.07	103.33	111.52
15	e	4	TYE	CG-CB-CA	2.04	117.13	113.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	f	4	TYE	CA-CB-CG-CD2
15	d	4	TYE	CA-CB-CG-CD2
15	f	4	TYE	CA-CB-CG-CD1
15	c	4	TYE	CA-CB-CG-CD1
15	e	4	TYE	CA-CB-CG-CD1
15	d	4	TYE	CA-CB-CG-CD1
15	c	4	TYE	CA-CB-CG-CD2
15	e	4	TYE	CA-CB-CG-CD2
15	c	4	TYE	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
15	e	4	TYE	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	c	101	-	12,12,12	2.23	1 (8%)	14,16,16	1.33	2 (14%)
18	MES	e	101	-	12,12,12	2.23	1 (8%)	14,16,16	1.34	2 (14%)

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	c	101	-	-	0/6/14/14	0/1/1/1
18	MES	e	101	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	e	101	MES	C8-S	-7.46	1.66	1.77
18	c	101	MES	C8-S	-7.45	1.66	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	e	101	MES	O2S-S-C8	2.90	110.41	106.92
18	e	101	MES	O3S-S-C8	2.73	110.19	105.77
18	c	101	MES	O3S-S-C8	2.69	110.12	105.77
18	c	101	MES	O2S-S-C8	2.31	109.70	106.92

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1
8	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	3:ILE	C	4:VAL	N	1.14
1	V	3:ILE	C	4:VAL	N	1.09

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.31	5 (2%) 65 60	40, 55, 91, 136	0
1	O	250/250 (100%)	-0.18	9 (3%) 42 35	45, 63, 107, 140	0
2	B	244/258 (94%)	-0.12	15 (6%) 21 16	41, 59, 112, 174	0
2	P	244/258 (94%)	-0.04	14 (5%) 23 18	46, 65, 114, 169	0
3	C	240/254 (94%)	-0.08	19 (7%) 12 9	42, 64, 127, 165	0
3	Q	240/254 (94%)	0.22	24 (10%) 7 4	50, 78, 160, 203	0
4	D	235/260 (90%)	-0.24	3 (1%) 77 73	47, 67, 98, 143	0
4	R	235/260 (90%)	-0.18	5 (2%) 63 58	49, 69, 107, 151	0
5	E	231/234 (98%)	-0.09	7 (3%) 50 43	49, 71, 104, 145	0
5	S	231/234 (98%)	-0.07	8 (3%) 44 36	50, 73, 112, 145	0
6	F	243/288 (84%)	-0.29	8 (3%) 46 39	41, 61, 113, 143	0
6	T	243/288 (84%)	-0.15	11 (4%) 33 26	40, 69, 118, 153	0
7	G	241/252 (95%)	-0.36	7 (2%) 51 45	39, 56, 98, 148	0
7	U	241/252 (95%)	-0.35	5 (2%) 63 58	40, 57, 91, 135	0
8	H	222/232 (95%)	-0.25	3 (1%) 75 71	43, 56, 84, 123	0
8	V	222/232 (95%)	-0.25	2 (0%) 84 82	43, 59, 90, 134	0
9	I	204/205 (99%)	-0.57	2 (0%) 82 80	37, 50, 79, 101	0
9	W	204/205 (99%)	-0.50	2 (0%) 82 80	38, 55, 84, 107	0
10	J	195/198 (98%)	-0.48	3 (1%) 73 70	38, 52, 79, 123	0
10	X	195/198 (98%)	-0.49	3 (1%) 73 70	42, 54, 80, 136	0
11	K	212/212 (100%)	-0.46	1 (0%) 91 89	40, 54, 83, 97	0
11	Y	212/212 (100%)	-0.46	1 (0%) 91 89	40, 54, 83, 109	0
12	L	222/222 (100%)	-0.49	0 100 100	40, 57, 85, 109	0
12	Z	222/222 (100%)	-0.46	2 (0%) 84 82	37, 55, 85, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	222/239 (92%)	-0.43	4 (1%) 68 64	37, 55, 83, 97	0
13	a	222/239 (92%)	-0.44	2 (0%) 84 82	38, 54, 78, 98	0
14	N	196/196 (100%)	-0.46	1 (0%) 91 89	39, 52, 82, 108	0
14	b	196/196 (100%)	-0.45	2 (1%) 82 80	40, 53, 82, 103	0
15	c	2/5 (40%)	-0.20	0 100 100	79, 79, 79, 90	0
15	d	2/5 (40%)	-0.06	0 100 100	71, 71, 71, 80	0
15	e	2/5 (40%)	0.22	0 100 100	76, 76, 76, 90	0
15	f	2/5 (40%)	-0.22	0 100 100	76, 76, 76, 87	0
All	All	6322/6620 (95%)	-0.29	168 (2%) 54 48	37, 59, 104, 203	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	8.3
3	Q	50	LEU	8.2
3	Q	49	THR	7.4
3	Q	206	LYS	7.3
1	A	1	MET	6.9
2	B	220	ASN	6.6
8	V	222	ASP	6.0
3	C	206	LYS	5.8
2	P	219	ALA	5.4
2	P	51	VAL	5.2
2	B	219	ALA	5.1
5	E	202	ASP	5.0
10	J	1	MET	4.8
3	Q	238	LYS	4.7
10	X	194	ASP	4.7
5	S	202	ASP	4.7
2	P	59	ASP	4.6
2	B	218	GLY	4.5
2	B	51	VAL	4.5
3	Q	236	GLN	4.4
13	M	220	ASP	4.4
4	D	242	GLU	4.4
2	P	218	GLY	4.3
6	T	205	GLU	4.3
1	O	249	ALA	4.2
3	Q	239	GLN	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	202	GLN	4.1
8	V	221	CYS	4.1
10	X	1	MET	4.1
3	Q	48	SER	4.1
3	C	236	GLN	4.1
3	C	49	THR	4.0
10	J	194	ASP	4.0
13	M	1	THR	4.0
3	Q	240	GLU	4.0
3	Q	51	LYS	4.0
2	B	221	ASP	4.0
2	P	220	ASN	3.9
3	Q	223	SER	3.8
2	P	221	ASP	3.8
8	H	222	ASP	3.7
13	a	220	ASP	3.7
7	U	222	ASP	3.7
3	Q	180	LYS	3.7
4	R	125	LEU	3.7
2	P	222	GLY	3.6
9	W	1	SER	3.5
2	B	217	LYS	3.4
2	B	242	GLY	3.4
3	Q	205	ALA	3.4
8	H	221	CYS	3.4
1	A	250	LEU	3.4
3	C	205	ALA	3.4
4	D	241	ALA	3.3
6	F	244	ASN	3.3
4	R	116	GLY	3.3
3	C	225	GLU	3.3
1	O	52	SER	3.2
13	a	1	THR	3.2
6	T	243	ILE	3.2
14	N	105	LYS	3.2
1	O	201	GLU	3.2
9	W	133	LYS	3.1
6	T	244	ASN	3.1
3	C	239	GLN	3.1
6	T	241	LYS	3.1
2	P	52	THR	3.0
3	C	238	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
6	T	215	CYS	3.0
3	Q	203	THR	3.0
6	F	53	LYS	3.0
6	T	204	LYS	3.0
4	R	241	ALA	3.0
1	O	2	THR	3.0
3	C	240	GLU	2.9
1	A	2	THR	2.9
2	B	59	ASP	2.9
3	Q	225	GLU	2.9
7	U	242	GLN	2.9
3	C	235	GLU	2.9
5	S	180	LYS	2.9
11	Y	212	GLY	2.8
3	Q	234	ILE	2.8
10	X	193	ASP	2.8
2	B	225	TYR	2.8
2	P	203	SER	2.8
9	I	133	LYS	2.8
5	S	194	GLU	2.8
3	C	50	LEU	2.7
6	T	2	THR	2.7
7	G	2	GLY	2.7
4	D	125	LEU	2.7
7	U	241	GLU	2.6
3	C	180	LYS	2.6
1	O	250	LEU	2.6
7	U	2	GLY	2.6
14	b	105	LYS	2.6
4	R	242	GLU	2.6
1	A	249	ALA	2.5
13	M	216	ASN	2.5
1	O	231	LYS	2.5
6	T	181	GLU	2.5
3	Q	167	LYS	2.5
9	I	1	SER	2.5
11	K	212	GLY	2.4
12	Z	210	ASP	2.4
5	E	201	ARG	2.4
3	Q	171	GLU	2.4
13	M	47	ASP	2.4
6	F	243	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	50	LYS	2.4
2	P	225	TYR	2.4
3	Q	141	ASP	2.4
7	G	181	LYS	2.4
6	T	180	PRO	2.3
5	E	121	SER	2.3
5	E	233	ILE	2.3
1	O	248	GLU	2.3
6	F	215	CYS	2.3
5	S	3	ASN	2.3
6	F	241	LYS	2.3
12	Z	1	GLN	2.3
3	C	37	LYS	2.3
4	R	177	ASN	2.2
6	F	202	ASP	2.2
3	Q	204	GLY	2.2
8	H	198	GLU	2.2
2	P	182	ASP	2.2
7	G	3	TYR	2.2
7	G	241	GLU	2.2
2	B	203	SER	2.2
5	E	54	GLU	2.2
3	C	167	LYS	2.2
6	T	166	GLN	2.2
2	P	60	THR	2.2
3	C	60	SER	2.2
7	G	188	GLU	2.2
2	P	230	LYS	2.1
3	Q	202	GLN	2.1
2	B	182	ASP	2.1
3	C	1	GLY	2.1
5	S	54	GLU	2.1
3	Q	221	ALA	2.1
3	C	179	ARG	2.1
3	C	216	ASP	2.1
5	S	171	LEU	2.1
6	F	201	GLU	2.1
2	B	52	THR	2.1
5	E	180	LYS	2.1
7	U	3	TYR	2.1
3	Q	52	LEU	2.1
2	B	230	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	201	GLU	2.1
10	J	193	ASP	2.1
2	B	50	LYS	2.0
5	E	123	GLY	2.0
5	S	225	ASP	2.0
5	S	29	LYS	2.0
6	T	53	LYS	2.0
3	Q	60	SER	2.0
3	Q	229	GLN	2.0
14	b	195	GLN	2.0
3	C	187	GLU	2.0
2	P	240	LYS	2.0
7	G	179	LYS	2.0
7	G	240	ALA	2.0
2	B	232	GLN	2.0
6	F	228	LYS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	TYE	d	4	12/12	0.96	0.17	61,71,79,81	0
15	TYE	f	4	12/12	0.96	0.18	61,75,85,85	0
15	TYE	e	4	12/12	0.96	0.17	60,79,88,89	0
15	TYE	c	4	12/12	0.97	0.18	63,73,87,87	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	MG	Z	301	1/1	0.85	0.35	74,74,74,74	0
16	MG	N	201	1/1	0.92	0.12	60,60,60,60	0
18	MES	e	101	12/12	0.92	0.20	50,76,86,87	0
18	MES	c	101	12/12	0.92	0.21	64,78,84,86	0
16	MG	L	301	1/1	0.94	0.17	63,63,63,63	0
16	MG	G	301	1/1	0.94	0.07	48,48,48,48	0
16	MG	I	301	1/1	0.97	0.21	56,56,56,56	0
16	MG	K	301	1/1	0.98	0.04	53,53,53,53	0
17	CL	U	301	1/1	0.99	0.26	30,30,30,30	0
16	MG	I	302	1/1	0.99	0.04	48,48,48,48	0
17	CL	G	302	1/1	1.00	0.16	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.