



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:52 PM GMT

PDB ID : 4Y8S
Title : Yeast 20S proteasome beta2-H116D mutant in complex with Ac-LAE-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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

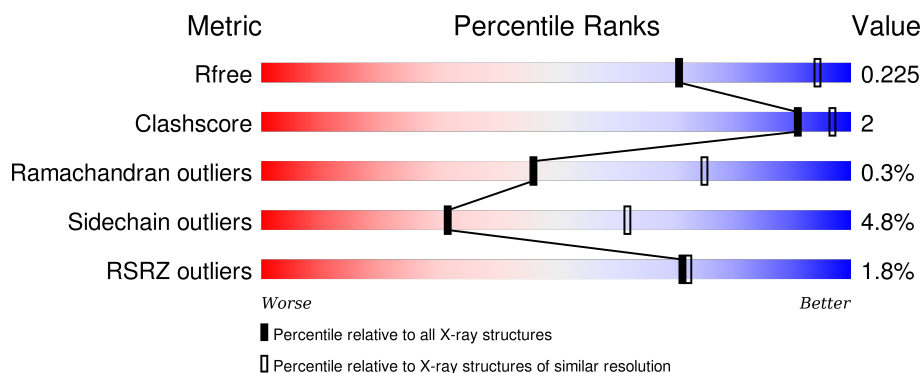
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>97%</div> <div>.</div> </div>
1	O	250	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
2	B	258	<div> <div>4%</div> <div>83%</div> <div>10% • 5%</div> </div>
2	P	258	<div> <div>3%</div> <div>84%</div> <div>10% • 5%</div> </div>
3	C	254	<div> <div>5%</div> <div>85%</div> <div>7% • 6%</div> </div>

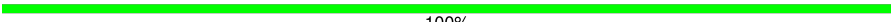
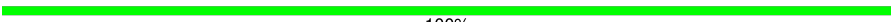


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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196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

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Mol	Chain	Length	Quality of chain
15	e	5	 100%
15	f	5	 100%
15	g	5	 100%
15	h	5	 100%

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
17	MES	K	302	-	-	-	X
17	MES	Y	302	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49825 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
			1682	1059	291	325	7			
8	V	222	Total	C	N	O	S	0	1	0
			1689	1064	293	325	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	116	ASP	HIS	engineered mutation	UNP P25043
V	116	ASP	HIS	engineered mutation	UNP P25043

- 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			
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			

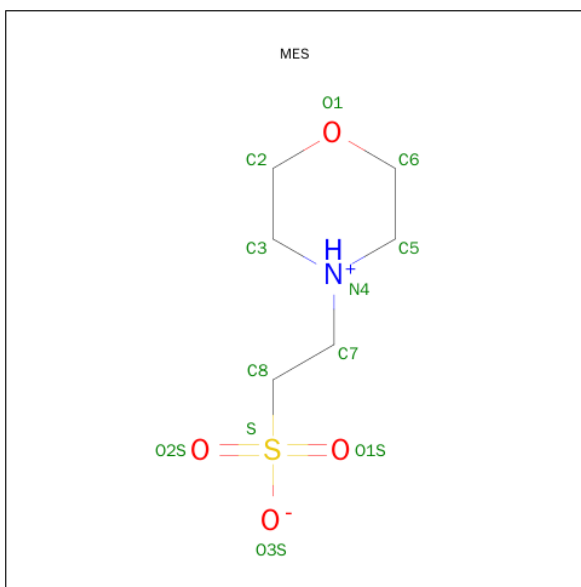
- Molecule 15 is a protein called Ac-LAE-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			29	19	3	7			
15	d	5	Total	C	N	O	0	0	0
			29	19	3	7			
15	e	5	Total	C	N	O	0	0	0
			29	19	3	7			
15	f	5	Total	C	N	O	0	0	0
			29	19	3	7			
15	g	5	Total	C	N	O	0	0	0
			29	19	3	7			
15	h	5	Total	C	N	O	0	0	0
			29	19	3	7			

- 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	H	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	Y	1	Total	Mg	0	0
			1	1		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	6	Total	O	0	0
			6	6		
18	B	13	Total	O	0	0
			13	13		
18	C	10	Total	O	0	0
			10	10		
18	D	2	Total	O	0	0
			2	2		
18	E	5	Total	O	0	0
			5	5		
18	F	13	Total	O	0	0
			13	13		
18	G	15	Total	O	0	0
			15	15		
18	H	23	Total	O	0	0
			23	23		
18	I	10	Total	O	0	0
			10	10		
18	J	11	Total	O	0	0
			11	11		

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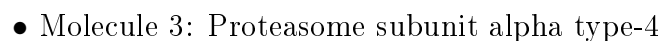
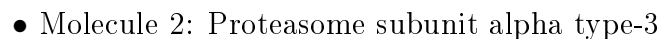
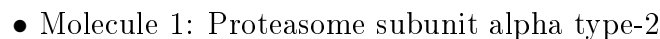
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	14	Total O 14 14	0	0
18	L	14	Total O 14 14	0	0
18	M	13	Total O 13 13	0	0
18	N	6	Total O 6 6	0	0
18	O	3	Total O 3 3	0	0
18	P	7	Total O 7 7	0	0
18	Q	8	Total O 8 8	0	0
18	R	3	Total O 3 3	0	0
18	S	4	Total O 4 4	0	0
18	T	9	Total O 9 9	0	0
18	U	21	Total O 21 21	0	0
18	V	13	Total O 13 13	0	0
18	W	8	Total O 8 8	0	0
18	X	14	Total O 14 14	0	0
18	Y	16	Total O 16 16	0	0
18	Z	20	Total O 20 20	0	0
18	a	17	Total O 17 17	0	0
18	b	11	Total O 11 11	0	0
18	c	1	Total O 1 1	0	0
18	d	1	Total O 1 1	0	0
18	e	1	Total O 1 1	0	0

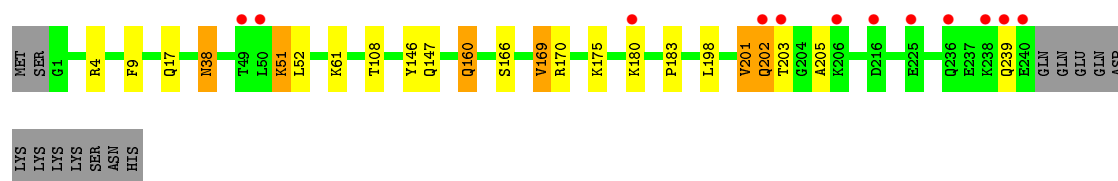
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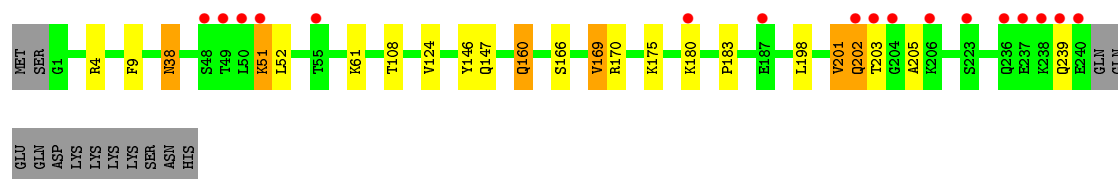
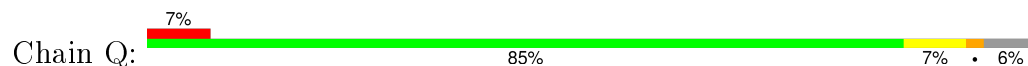
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	f	1	Total	O	0	0
			1	1		
18	g	1	Total	O	0	0
			1	1		

- Molecule 1: Proteasome subunit alpha type-2

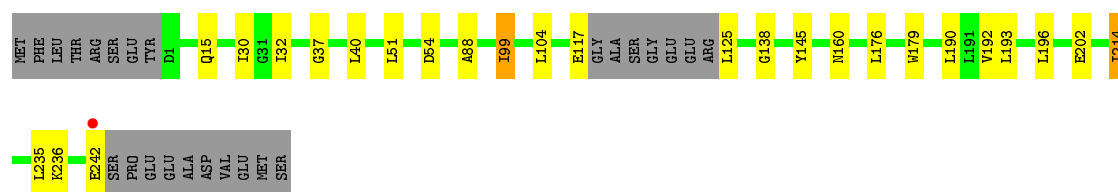
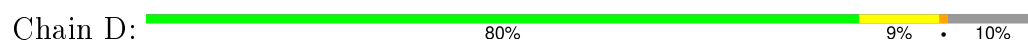




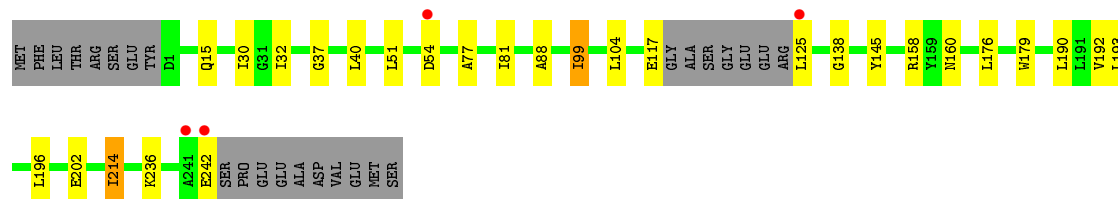
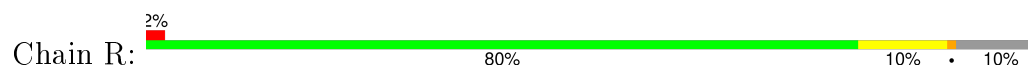
• Molecule 3: Proteasome subunit alpha type-4



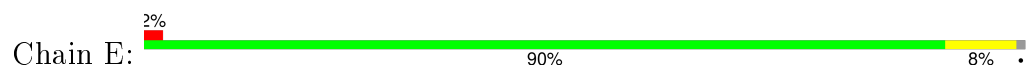
• Molecule 4: Proteasome subunit alpha type-5



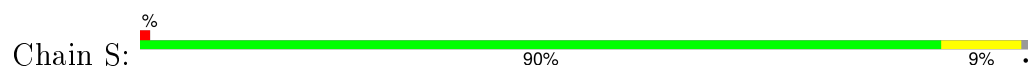
• Molecule 4: Proteasome subunit alpha type-5




• Molecule 5: Proteasome subunit alpha type-6



• Molecule 5: Proteasome subunit alpha type-6

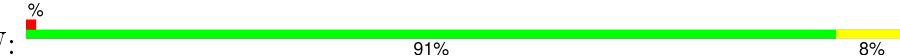


- Molecule 9: Proteasome subunit beta type-3

Chain I:  91% 9%




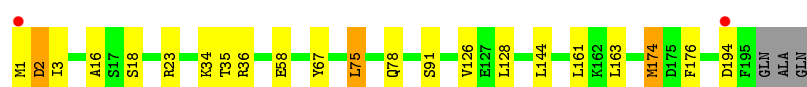
- Molecule 9: Proteasome subunit beta type-3

Chain W:  91% 8%




- Molecule 10: Proteasome subunit beta type-4

Chain J:  87% 10% ..



- Molecule 10: Proteasome subunit beta type-4

Chain X:  88% 9% ..




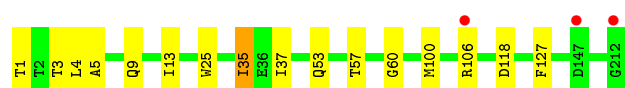
- Molecule 11: Proteasome subunit beta type-5

Chain K:  93% 6%



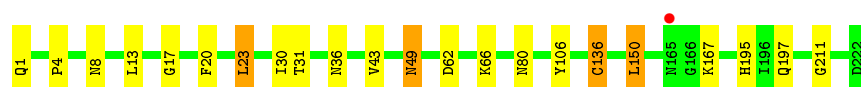
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  92% 7%




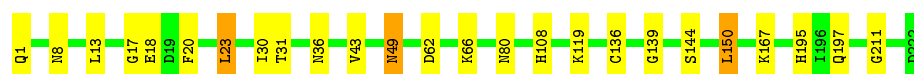
- Molecule 12: Proteasome subunit beta type-6

Chain L:  90% 8% .




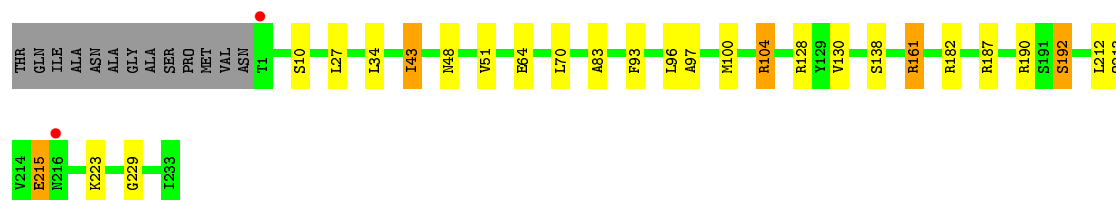
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  89% 10% .




- Molecule 13: Proteasome subunit beta type-7

Chain M:  84% 9% 5%



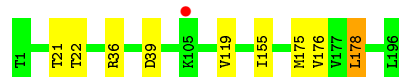
- Molecule 13: Proteasome subunit beta type-7

Chain a:  88% 7% 5%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  95% . .



- Molecule 14: Proteasome subunit beta type-1

Chain b:  97% .



- Molecule 15: Ac-LAE-ep

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAE-ep

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAE-ep

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAE-ep

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAE-ep

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAE-ep

Chain h:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.35Å 300.08Å 144.78Å 90.00° 112.99° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.70) 97.3 (15.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.188 , 0.221 0.193 , 0.225	Depositor DCC
R_{free} test set	14123 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 282450 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49825	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: MES, MG, GAU, ACE, POL

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	0.51	0/2642
1	O	0.27	0/1952	0.51	0/2642
2	B	0.27	0/1934	0.53	0/2618
2	P	0.27	0/1934	0.53	0/2618
3	C	0.28	0/1910	0.55	0/2586
3	Q	0.28	0/1910	0.55	0/2586
4	D	0.27	0/1837	0.53	0/2475
4	R	0.27	0/1837	0.53	0/2475
5	E	0.27	0/1800	0.51	0/2433
5	S	0.27	0/1800	0.51	0/2433
6	F	0.28	0/1932	0.49	0/2609
6	T	0.28	0/1932	0.49	0/2609
7	G	0.28	0/1945	0.52	0/2634
7	U	0.28	0/1945	0.52	0/2634
8	H	0.30	0/1712	0.52	0/2322
8	V	0.27	0/1723	0.56	1/2337 (0.0%)
9	I	0.27	0/1611	0.53	0/2174
9	W	0.27	0/1611	0.52	0/2174
10	J	0.27	0/1589	0.52	0/2142
10	X	0.27	0/1589	0.52	0/2142
11	K	0.29	0/1681	0.53	0/2274
11	Y	0.28	0/1681	0.53	0/2274
12	L	0.27	0/1795	0.51	0/2420
12	Z	0.29	0/1806	0.51	0/2435
13	M	0.28	0/1855	0.56	0/2514
13	a	0.28	0/1855	0.56	0/2514
14	N	0.34	0/1541	0.50	0/2087
14	b	0.32	0/1541	0.50	0/2087
15	c	1.07	0/13	1.18	0/17
15	d	1.03	0/13	1.30	0/17
15	e	0.99	0/13	0.99	0/17
15	f	0.51	0/13	1.26	0/17

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	0.72	0/13	1.18	0/17
15	h	1.09	0/13	1.23	0/17
All	All	0.28	0/50288	0.53	1/67992 (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
8	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	115	ALA	C-N-CA	5.98	136.66	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	V	115	ALA	Peptide

5.2 Too-close contacts [i](#)

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	4	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	13	0
2	P	1904	0	1904	12	0
3	C	1881	0	1895	12	0
3	Q	1881	0	1895	13	0
4	D	1813	0	1797	8	0
4	R	1813	0	1797	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1773	0	1775	5	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	7	0
8	H	1682	0	1682	6	0
8	V	1689	0	1689	4	0
9	I	1581	0	1574	10	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	11	0
10	X	1561	0	1569	10	0
11	K	1644	0	1592	8	0
11	Y	1644	0	1592	10	0
12	L	1757	0	1711	11	0
12	Z	1764	0	1718	13	0
13	M	1824	0	1832	10	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	3	0
14	b	1512	0	1478	0	0
15	c	29	0	31	0	0
15	d	29	0	31	0	0
15	e	29	0	30	0	0
15	f	29	0	31	0	0
15	g	29	0	31	0	0
15	h	29	0	31	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	Y	1	0	0	0	0
17	K	12	0	13	0	0
17	Y	12	0	13	0	0
18	A	6	0	0	0	0
18	B	13	0	0	0	0
18	C	10	0	0	0	0
18	D	2	0	0	0	0
18	E	5	0	0	0	0
18	F	13	0	0	0	0
18	G	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	23	0	0	0	0
18	I	10	0	0	0	0
18	J	11	0	0	0	0
18	K	14	0	0	0	0
18	L	14	0	0	0	0
18	M	13	0	0	0	0
18	N	6	0	0	0	0
18	O	3	0	0	0	0
18	P	7	0	0	0	0
18	Q	8	0	0	0	0
18	R	3	0	0	0	0
18	S	4	0	0	0	0
18	T	9	0	0	0	0
18	U	21	0	0	0	0
18	V	13	0	0	0	0
18	W	8	0	0	0	0
18	X	14	0	0	0	0
18	Y	16	0	0	0	0
18	Z	20	0	0	0	0
18	a	17	0	0	0	0
18	b	11	0	0	0	0
18	c	1	0	0	0	0
18	d	1	0	0	0	0
18	e	1	0	0	0	0
18	f	1	0	0	0	0
18	g	1	0	0	0	0
All	All	49825	0	49269	192	0

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

All (192) 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)
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.57	0.86
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.57	0.85
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.65	0.79
12:Z:108[B]:HIS:HD2	12:Z:139:GLY:HA3	1.48	0.79
11:K:53:GLN:O	11:K:57:THR:HG23	1.86	0.75
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.85	0.74
12:Z:108[B]:HIS:CD2	12:Z:139:GLY:HA3	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.71	0.73
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.72	0.71
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.78	0.66
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.78	0.65
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.79	0.62
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.82	0.62
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.65	0.61
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.65	0.61
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.82	0.61
7:U:23:PHE:O	7:U:26:THR:HB	2.03	0.59
7:G:23:PHE:O	7:G:26:THR:HB	2.03	0.58
8:V:116:ASP:OD2	8:V:116:ASP:C	2.44	0.56
3:C:51:LYS:O	3:C:52:LEU:HB2	2.06	0.56
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.88	0.56
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.70	0.56
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.89	0.55
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.06	0.55
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.89	0.55
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.71	0.55
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.88	0.54
10:X:1:MET:HA	10:X:34:LYS:HE3	1.90	0.54
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.89	0.54
8:H:52:THR:O	8:H:56:THR:HB	2.08	0.54
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.91	0.53
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.88	0.53
10:J:1:MET:HA	10:J:34:LYS:HE3	1.90	0.53
8:V:52:THR:O	8:V:56:THR:HB	2.09	0.53
11:Y:35:ILE:HD13	11:Y:37:ILE:HG13	1.90	0.52
12:L:8:ASN:HA	12:L:30:ILE:O	2.09	0.52
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.90	0.52
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.91	0.52
11:K:35:ILE:HD13	11:K:37:ILE:HG13	1.90	0.51
14:N:22:THR:O	14:N:22:THR:HG23	2.09	0.51
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.10	0.51
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.93	0.51
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.91	0.51
13:M:43:ILE:HG21	13:M:64:GLU:HG2	1.93	0.51
8:H:112:SER:OG	8:H:120:ASP:HB2	2.12	0.50
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.93	0.50
10:J:174:MET:HA	10:X:174:MET:HA	1.92	0.50
10:X:1:MET:HA	10:X:34:LYS:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:1:THR:CG2	11:Y:3:THR:HG23	2.42	0.50
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.42	0.50
10:J:1:MET:HA	10:J:34:LYS:CE	2.42	0.49
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.93	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.93	0.49
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.42	0.49
5:E:12:PHE:H	6:F:19:GLN:HE22	1.58	0.49
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.94	0.49
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.95	0.49
1:O:12:PHE:H	2:P:20:GLN:HE22	1.61	0.49
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.95	0.48
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.95	0.48
5:S:12:PHE:H	6:T:19:GLN:HE22	1.60	0.48
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.78	0.48
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.78	0.48
12:L:4:PRO:O	13:M:104:ARG:NH1	2.43	0.48
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.62	0.48
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.43	0.48
5:S:68:HIS:HE1	5:S:102:LEU:O	1.97	0.47
3:C:201:VAL:O	3:C:202:GLN:CB	2.62	0.47
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.97	0.47
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.50	0.47
2:P:180:LYS:O	2:P:183:MET:HB2	2.14	0.47
2:B:180:LYS:O	2:B:183:MET:HB2	2.14	0.47
5:E:68:HIS:HE1	5:E:102:LEU:O	1.96	0.47
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.63	0.47
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.97	0.47
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.79	0.47
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.50	0.47
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.96	0.47
11:K:100:MET:CE	11:K:127:PHE:HB2	2.43	0.47
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.63	0.47
3:C:201:VAL:O	3:C:202:GLN:HB2	2.14	0.46
3:C:201:VAL:HG13	3:C:202:GLN:H	1.80	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.46
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.98	0.46
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.51	0.46
11:K:5:ALA:HB3	11:K:100:MET:CE	2.41	0.46
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.51	0.46
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.98	0.46
9:W:101:PRO:HB3	9:W:126:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:VAL:HG13	3:Q:202:GLN:H	1.80	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.14	0.46
1:A:115:ALA:HB1	1:A:154:GLY:O	2.16	0.46
12:L:195:HIS:HD2	12:L:197:GLN:H	1.63	0.46
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.97	0.46
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.96	0.45
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.51	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.51	0.45
7:G:34:LEU:HD23	7:G:34:LEU:C	2.37	0.45
1:O:115:ALA:HB1	1:O:154:GLY:O	2.17	0.45
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.99	0.45
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.82	0.45
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.50	0.45
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.99	0.45
7:G:78:ILE:N	7:G:79:PRO:CD	2.80	0.45
13:M:182:ARG:NH2	13:M:215:GLU:O	2.50	0.45
9:I:101:PRO:HB3	9:I:126:ILE:CD1	2.46	0.45
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.47	0.45
7:U:34:LEU:C	7:U:34:LEU:HD23	2.37	0.45
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.52	0.45
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.52	0.45
5:E:9:THR:HG21	5:E:119:THR:HA	1.99	0.45
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.52	0.44
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.47	0.44
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.53	0.44
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.53	0.44
4:R:30:ILE:HD12	4:R:196:LEU:HG	2.00	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	0.44
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.00	0.44
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.41	0.44
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.30	0.44
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.31	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.52	0.44
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.00	0.44
11:K:1:THR:CG2	11:K:3:THR:HG23	2.48	0.44
13:M:43:ILE:HG12	13:M:51:VAL:HB	2.00	0.43
5:S:9:THR:HG21	5:S:119:THR:HA	1.99	0.43
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.83	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.00	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.43
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.83	0.43
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.67	0.43
6:T:123:ASN:HD22	6:T:123:ASN:C	2.22	0.43
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.67	0.43
1:A:12:PHE:H	2:B:20:GLN:HE22	1.67	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
2:B:12:PHE:H	3:C:17:GLN:HE22	1.67	0.43
12:L:62:ASP:O	12:L:66:LYS:HB2	2.19	0.42
13:M:93:PHE:CE2	13:M:128:ARG:HD3	2.54	0.42
10:J:3:ILE:HB	10:J:18:SER:HB3	2.01	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.01	0.42
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.84	0.42
7:U:83:ASN:C	7:U:83:ASN:HD22	2.23	0.42
3:C:9:PHE:H	4:D:15:GLN:HE22	1.67	0.42
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.02	0.42
12:Z:62:ASP:O	12:Z:66:LYS:HB2	2.19	0.42
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.52	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.01	0.42
2:B:204:ALA:O	2:B:209:ARG:NH2	2.52	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.42
4:R:77:ALA:O	4:R:81:ILE:HG12	2.20	0.42
6:F:123:ASN:C	6:F:123:ASN:HD22	2.23	0.42
2:P:204:ALA:O	2:P:209:ARG:NH2	2.53	0.42
9:I:14:MET:HB3	9:I:162:LEU:HD11	2.02	0.42
3:C:38:ASN:HD22	3:C:38:ASN:N	2.18	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.41
8:V:206:PRO:O	8:V:209:THR:OG1	2.31	0.41
14:N:155:ILE:HB	14:N:175:MET:HE1	2.02	0.41
3:C:166:SER:HA	3:C:169:VAL:HG13	2.02	0.41
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.18	0.41
2:P:57:GLU:O	2:P:61:SER:HB2	2.20	0.41
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.02	0.41
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.54	0.41
9:I:98:ARG:O	9:I:126:ILE:HD11	2.21	0.41
7:U:63:ILE:HD12	7:U:215:GLU:HG2	2.02	0.41
9:W:14:MET:HB3	9:W:162:LEU:HD11	2.03	0.41
2:B:57:GLU:O	2:B:61:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:166:SER:HA	3:Q:169:VAL:HG13	2.02	0.41
7:G:83:ASN:C	7:G:83:ASN:HD22	2.24	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.03	0.41
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.61	0.41
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	2.02	0.41
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.02	0.41
8:H:84:LYS:HG3	8:H:85:GLN:N	2.36	0.41
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.36	0.41
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.02	0.41
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.56	0.41
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.56	0.41
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.52	0.40
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.22	0.40
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.56	0.40
4:R:158:ARG:HB3	5:S:57:SER:HB3	2.03	0.40
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.56	0.40
2:B:46:ALA:HB2	2:B:212:PHE:CE1	2.57	0.40
12:Z:18:GLU:O	12:Z:119:LYS:HA	2.22	0.40
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.03	0.40
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.02	0.40
3:C:198:LEU:HA	3:C:201:VAL:HG12	2.02	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%)	237 (96%)	11 (4%)	0	100	100
1	O	248/250 (99%)	237 (96%)	11 (4%)	0	100	100
2	B	242/258 (94%)	231 (96%)	9 (4%)	2 (1%)	24	51
2	P	242/258 (94%)	231 (96%)	9 (4%)	2 (1%)	24	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	229 (96%)	4 (2%)	5 (2%)	9	23
3	Q	238/254 (94%)	229 (96%)	4 (2%)	5 (2%)	9	23
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	218 (95%)	11 (5%)	0	100	100
5	S	229/234 (98%)	218 (95%)	11 (5%)	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%)	234 (98%)	5 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	221/232 (95%)	216 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	34	63
10	X	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	34	63
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	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%)	223 (96%)	6 (3%)	2 (1%)	21	49
13	a	231/246 (94%)	223 (96%)	6 (3%)	2 (1%)	21	49
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
15	c	2/5 (40%)	2 (100%)	0	0	100	100
15	d	2/5 (40%)	2 (100%)	0	0	100	100
15	e	2/5 (40%)	2 (100%)	0	0	100	100
15	f	2/5 (40%)	2 (100%)	0	0	100	100
15	g	2/5 (40%)	2 (100%)	0	0	100	100
15	h	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6290/6644 (95%)	6083 (97%)	187 (3%)	20 (0%)	46	75

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	202	GLN
3	Q	202	GLN
2	B	51	VAL
3	C	239	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	239	GLN
10	X	2	ASP
3	C	183	PRO
3	Q	183	PRO
2	B	221	ASP
3	C	205	ALA
2	P	221	ASP
3	Q	205	ALA
13	M	83	ALA
13	a	83	ALA
3	C	201	VAL
3	Q	201	VAL
13	M	229	GLY
13	a	229	GLY

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%)	205 (98%)	4 (2%)	65	88
1	O	209/209 (100%)	205 (98%)	4 (2%)	65	88
2	B	203/216 (94%)	193 (95%)	10 (5%)	31	61
2	P	203/216 (94%)	193 (95%)	10 (5%)	31	61
3	C	212/226 (94%)	202 (95%)	10 (5%)	32	63
3	Q	212/226 (94%)	202 (95%)	10 (5%)	32	63
4	D	194/215 (90%)	180 (93%)	14 (7%)	18	41
4	R	194/215 (90%)	181 (93%)	13 (7%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	190/193 (98%)	178 (94%)	12 (6%)	22	48
5	S	190/193 (98%)	178 (94%)	12 (6%)	22	48
6	F	201/239 (84%)	188 (94%)	13 (6%)	21	46
6	T	201/239 (84%)	188 (94%)	13 (6%)	21	46
7	G	206/210 (98%)	193 (94%)	13 (6%)	22	48
7	U	206/210 (98%)	193 (94%)	13 (6%)	22	48
8	H	181/190 (95%)	175 (97%)	6 (3%)	45	76
8	V	182/190 (96%)	175 (96%)	7 (4%)	40	71
9	I	172/173 (99%)	168 (98%)	4 (2%)	58	85
9	W	172/173 (99%)	168 (98%)	4 (2%)	58	85
10	J	173/175 (99%)	163 (94%)	10 (6%)	25	52
10	X	173/175 (99%)	163 (94%)	10 (6%)	25	52
11	K	169/169 (100%)	164 (97%)	5 (3%)	48	79
11	Y	169/169 (100%)	164 (97%)	5 (3%)	48	79
12	L	185/185 (100%)	177 (96%)	8 (4%)	35	66
12	Z	186/185 (100%)	179 (96%)	7 (4%)	40	71
13	M	199/208 (96%)	185 (93%)	14 (7%)	19	42
13	a	199/208 (96%)	185 (93%)	14 (7%)	19	42
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	78
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	78
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
All	All	5320/5546 (96%)	5065 (95%)	255 (5%)	31	62

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU

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Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
2	B	50	LYS
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	119	GLN
2	B	180	LYS
2	B	183	MET
2	B	184	LYS
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	203	THR
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU

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Mol	Chain	Res	Type
5	E	71	LEU
5	E	116	GLN
5	E	118	ASN
5	E	184	ASN
5	E	188	LEU
5	E	231	LYS
6	F	14	ASP
6	F	59	LYS
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	187	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	26	THR
7	G	28	GLN
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	171	THR
7	G	181	LYS
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP

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Mol	Chain	Res	Type
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	91	SER
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
10	J	194	ASP
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	80	ASN
12	L	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	10	SER
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	190	ARG
13	M	192	SER
13	M	212	LEU
13	M	213	GLN
13	M	215	GLU
13	M	223	LYS
14	N	21	THR
14	N	36	ARG
14	N	39	ASP
14	N	119	VAL
14	N	178	LEU

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Mol	Chain	Res	Type
1	O	17	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
2	P	50	LYS
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	119	GLN
2	P	180	LYS
2	P	183	MET
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	203	THR
4	R	40	LEU
4	R	51	LEU
4	R	54	ASP
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS

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Mol	Chain	Res	Type
5	S	55	LEU
5	S	71	LEU
5	S	116	GLN
5	S	118	ASN
5	S	184	ASN
5	S	188	LEU
5	S	231	LYS
6	T	14	ASP
6	T	59	LYS
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	187	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	26	THR
7	U	28	GLN
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	171	THR
7	U	181	LYS
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	116	ASP
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU

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Mol	Chain	Res	Type
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	91	SER
10	X	144	LEU
10	X	163	LEU
10	X	174	MET
10	X	194	ASP
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	80	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	10	SER
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	138	SER
13	a	161	ARG
13	a	187	ARG
13	a	190	ARG
13	a	192	SER
13	a	212	LEU
13	a	213	GLN
13	a	215	GLU
13	a	223	LYS
14	b	21	THR
14	b	36	ARG
14	b	39	ASP
14	b	119	VAL

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Mol	Chain	Res	Type
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	30	ASN

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Mol	Chain	Res	Type
8	H	57	GLN
8	H	66	HIS
8	H	172	ASN
8	H	189	ASN
9	I	31	GLN
10	J	55	GLN
10	J	118	GLN
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	80	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
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	100	ASN
4	R	146	GLN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS

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Mol	Chain	Res	Type
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	30	ASN
8	V	57	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	31	GLN
10	X	55	GLN
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	GAU	c	4	8,15	5,8,8	1.00	0	4,9,9	1.53	1 (25%)
15	GAU	d	4	11,15	5,8,8	1.29	1 (20%)	4,9,9	1.16	0
15	GAU	e	4	15,14	5,8,8	0.99	0	4,9,9	2.13	2 (50%)
15	GAU	f	4	8,15	5,8,8	1.01	1 (20%)	4,9,9	1.92	1 (25%)
15	GAU	g	4	11,15	5,8,8	0.93	0	4,9,9	1.01	0
15	GAU	h	4	15,14	5,8,8	0.81	0	4,9,9	1.49	1 (25%)

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	GAU	c	4	8,15	-	0/5/7/7	0/0/0/0
15	GAU	d	4	11,15	-	0/5/7/7	0/0/0/0
15	GAU	e	4	15,14	-	0/5/7/7	0/0/0/0
15	GAU	f	4	8,15	-	0/5/7/7	0/0/0/0
15	GAU	g	4	11,15	-	0/5/7/7	0/0/0/0
15	GAU	h	4	15,14	-	0/5/7/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	4	GAU	C-CA	2.17	1.55	1.52
15	d	4	GAU	C-CA	2.28	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	4	GAU	CG-CB-CA	-3.37	105.40	113.80
15	e	4	GAU	CB-CA-N	-2.82	101.05	108.92
15	e	4	GAU	CG-CB-CA	-2.71	107.03	113.80
15	c	4	GAU	CB-CA-N	-2.41	102.20	108.92
15	h	4	GAU	OXT-C-CA	-2.15	106.07	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 9 ligands modelled in this entry, 7 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
17	MES	K	302	-	12,12,12	2.09	1 (8%)	15,16,16	1.77	3 (20%)
17	MES	Y	302	-	12,12,12	2.08	1 (8%)	15,16,16	1.66	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
17	MES	K	302	-	-	0/6/14/14	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	302	MES	C8-S	-6.90	1.67	1.77
17	Y	302	MES	C8-S	-6.89	1.67	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	302	MES	O1S-S-C8	2.42	108.58	106.87
17	K	302	MES	O3S-S-C8	2.45	110.09	104.99
17	Y	302	MES	O3S-S-C8	2.51	110.22	104.99
17	K	302	MES	O1S-S-C8	3.55	109.38	106.87
17	K	302	MES	O2S-S-C8	4.21	109.84	106.87
17	Y	302	MES	O2S-S-C8	4.37	109.95	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.38	6 (2%) 62 62	43, 59, 89, 130	0
1	O	250/250 (100%)	-0.32	6 (2%) 62 62	46, 67, 102, 141	0
2	B	244/258 (94%)	-0.27	10 (4%) 41 41	45, 65, 107, 150	0
2	P	244/258 (94%)	-0.21	9 (3%) 45 45	49, 69, 114, 160	0
3	C	240/254 (94%)	-0.12	12 (5%) 32 31	46, 70, 129, 157	0
3	Q	240/254 (94%)	0.09	17 (7%) 19 17	53, 81, 151, 165	0
4	D	235/260 (90%)	-0.35	1 (0%) 93 94	49, 71, 102, 135	0
4	R	235/260 (90%)	-0.27	4 (1%) 73 74	51, 72, 105, 136	0
5	E	231/234 (98%)	-0.25	5 (2%) 65 66	51, 74, 104, 154	0
5	S	231/234 (98%)	-0.19	3 (1%) 79 79	53, 78, 112, 140	0
6	F	243/288 (84%)	-0.42	3 (1%) 81 81	47, 65, 110, 134	0
6	T	243/288 (84%)	-0.31	11 (4%) 37 36	50, 71, 113, 138	0
7	G	241/252 (95%)	-0.39	4 (1%) 73 74	43, 61, 95, 138	0
7	U	241/252 (95%)	-0.41	4 (1%) 73 74	45, 62, 93, 119	0
8	H	222/232 (95%)	-0.50	2 (0%) 85 86	42, 57, 82, 107	0
8	V	222/232 (95%)	-0.46	2 (0%) 85 86	43, 59, 85, 116	0
9	I	204/205 (99%)	-0.64	1 (0%) 91 93	42, 56, 82, 106	0
9	W	204/205 (99%)	-0.57	3 (1%) 76 76	44, 59, 84, 118	0
10	J	195/198 (98%)	-0.48	2 (1%) 84 85	41, 59, 85, 121	0
10	X	195/198 (98%)	-0.50	2 (1%) 84 85	45, 61, 86, 147	0
11	K	212/212 (100%)	-0.49	0 100 100	45, 60, 89, 106	0
11	Y	212/212 (100%)	-0.43	3 (1%) 78 77	47, 63, 98, 123	0
12	L	222/222 (100%)	-0.55	1 (0%) 91 93	45, 61, 88, 109	0
12	Z	222/222 (100%)	-0.53	0 100 100	43, 60, 88, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.55	2 (0%) 85 86	41, 59, 77, 91	0
13	a	233/246 (94%)	-0.56	1 (0%) 93 94	43, 57, 76, 90	0
14	N	196/196 (100%)	-0.59	1 (0%) 91 93	42, 55, 80, 108	0
14	b	196/196 (100%)	-0.56	0 100 100	41, 56, 82, 104	0
15	c	2/5 (40%)	-1.37	0 100 100	48, 48, 48, 53	0
15	d	2/5 (40%)	-0.66	0 100 100	60, 60, 60, 61	0
15	e	2/5 (40%)	-0.65	0 100 100	45, 45, 45, 54	0
15	f	2/5 (40%)	-0.88	0 100 100	55, 55, 55, 62	0
15	g	2/5 (40%)	-0.07	0 100 100	72, 72, 72, 75	0
15	h	2/5 (40%)	-0.93	0 100 100	53, 53, 53, 57	0
All	All	6348/6644 (95%)	-0.39	115 (1%) 71 72	41, 63, 103, 165	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	206	LYS	7.4
3	Q	50	LEU	6.3
2	P	51	VAL	6.0
3	Q	206	LYS	5.9
2	P	219	ALA	5.8
2	P	218	GLY	5.6
2	B	220	ASN	5.6
3	Q	49	THR	5.6
5	E	202	ASP	5.5
3	C	49	THR	5.0
3	C	238	LYS	4.5
3	Q	236	GLN	4.5
8	V	222	ASP	4.4
3	Q	239	GLN	4.3
2	P	220	ASN	4.2
1	A	1	MET	4.2
10	J	1	MET	4.1
2	B	51	VAL	4.1
5	S	202	ASP	3.9
3	Q	240	GLU	3.9
3	Q	48	SER	3.8
9	W	1	SER	3.8
1	O	1	MET	3.8

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Mol	Chain	Res	Type	RSRZ
3	Q	238	LYS	3.7
10	X	194	ASP	3.7
10	X	1	MET	3.6
8	V	221	CYS	3.5
2	P	59	ASP	3.5
3	Q	204	GLY	3.4
2	P	221	ASP	3.4
1	A	250	LEU	3.4
3	Q	51	LYS	3.3
1	O	231	LYS	3.3
2	B	219	ALA	3.3
5	E	54	GLU	3.2
3	Q	180	LYS	3.2
2	B	218	GLY	3.2
11	Y	212	GLY	3.2
3	C	202	GLN	3.2
3	Q	237	GLU	3.1
9	I	1	SER	3.1
6	F	244	ASN	3.1
7	G	3	TYR	3.1
6	T	205	GLU	3.1
7	G	179	LYS	3.1
4	D	242	GLU	3.0
4	R	241	ALA	3.0
4	R	125	LEU	3.0
11	Y	106	ARG	3.0
3	C	236	GLN	3.0
10	J	194	ASP	3.0
13	a	1	THR	3.0
3	Q	187	GLU	2.9
7	U	222	ASP	2.9
2	B	221	ASP	2.9
6	T	243	ILE	2.9
2	B	203	SER	2.9
13	M	1	THR	2.8
1	A	249	ALA	2.8
6	T	244	ASN	2.8
1	O	249	ALA	2.8
8	H	221	CYS	2.8
5	S	54	GLU	2.7
6	T	2	THR	2.7
3	C	239	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	242	GLY	2.7
3	Q	202	GLN	2.7
1	O	52	SER	2.7
1	A	166	LYS	2.7
3	C	180	LYS	2.6
2	B	59	ASP	2.6
6	T	241	LYS	2.6
3	Q	223	SER	2.6
7	U	241	GLU	2.5
7	U	242	GLN	2.5
5	E	217	LYS	2.4
1	O	250	LEU	2.4
6	T	215	CYS	2.4
13	M	216	ASN	2.4
6	T	178	HIS	2.4
1	O	201	GLU	2.4
2	B	222	GLY	2.4
2	P	222	GLY	2.4
9	W	191	LYS	2.4
3	C	240	GLU	2.4
3	C	203	THR	2.4
2	B	50	LYS	2.3
14	N	105	LYS	2.3
3	C	225	GLU	2.3
7	G	242	GLN	2.3
3	Q	203	THR	2.3
3	C	216	ASP	2.3
5	E	233	ILE	2.3
5	S	180	LYS	2.2
1	A	248	GLU	2.2
1	A	2	THR	2.2
5	E	207	VAL	2.2
6	T	181	GLU	2.2
11	Y	147	ASP	2.2
7	G	241	GLU	2.2
6	F	215	CYS	2.1
4	R	242	GLU	2.1
6	T	166	GLN	2.1
8	H	222	ASP	2.1
6	F	181	GLU	2.1
2	P	203	SER	2.1
7	U	2	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	182	ASP	2.1
4	R	54	ASP	2.1
9	W	133	LYS	2.0
12	L	165	ASN	2.0
6	T	53	LYS	2.0
3	C	50	LEU	2.0
6	T	180	PRO	2.0
3	Q	55	THR	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. 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	GAU	h	4	9/9	0.96	0.11	-	51,52,60,67	0
15	GAU	g	4	9/9	0.96	0.13	-	64,77,81,81	0
15	GAU	c	4	9/9	0.95	0.11	-	54,58,65,68	0
15	GAU	f	4	9/9	0.94	0.14	-	55,58,65,71	0
15	GAU	d	4	9/9	0.96	0.11	-	41,57,60,61	0
15	GAU	e	4	9/9	0.97	0.10	-	49,55,61,64	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
17	MES	K	302	12/12	0.91	0.30	7.79	91,95,99,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	MES	Y	302	12/12	0.91	0.28	5.04	84,89,98,99	0
16	MG	I	301	1/1	0.96	0.14	0.18	69,69,69,69	0
16	MG	N	201	1/1	0.98	0.08	-1.62	54,54,54,54	0
16	MG	G	301	1/1	0.96	0.05	-1.86	57,57,57,57	0
16	MG	K	301	1/1	0.99	0.04	-2.11	61,61,61,61	0
16	MG	Y	301	1/1	0.98	0.03	-2.54	55,55,55,55	0
16	MG	V	301	1/1	0.99	0.03	-3.17	54,54,54,54	0
16	MG	H	301	1/1	0.97	0.17	-	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.