



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:53 PM GMT

PDB ID : 4YA1  
Title : Yeast 20S proteasome beta2-H116N mutant  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2015-02-17  
Resolution : 2.90 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : unknown  
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

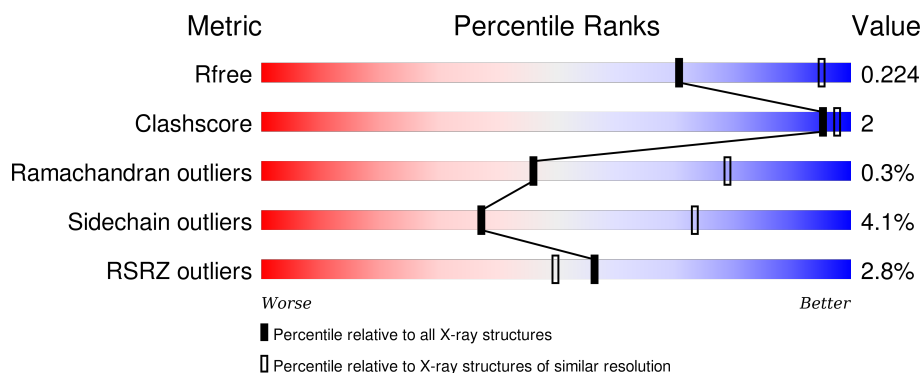
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
1	O	250	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
2	B	258	<div> <div>3%</div> <div>86%</div> <div>8% • 5%</div> </div>
2	P	258	<div> <div>3%</div> <div>86%</div> <div>7% • 5%</div> </div>
3	C	254	<div> <div>5%</div> <div>84%</div> <div>9% • 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	

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
15	CL	C	301	-	-	X	X
16	MG	I	301	-	-	-	X
16	MG	Z	301	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49723 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	226	Total	C	N	O	S	0	0	0
			1717	1080	297	333	7			
8	V	226	Total	C	N	O	S	0	0	0
			1717	1080	297	333	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	116	ASN	HIS	engineered mutation	UNP P25043
V	116	ASN	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	0	0
			1757	1115	303	335	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Cl 1 1	0	0
15	a	1	Total Cl 1 1	0	0
15	C	1	Total Cl 1 1	0	0
15	M	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	K	1	Total Mg 1 1	0	0
16	H	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0
16	Y	1	Total Mg 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	7	Total O 7 7	0	0
17	B	10	Total O 10 10	0	0
17	C	9	Total O 9 9	0	0
17	D	8	Total O 8 8	0	0
17	E	10	Total O 10 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	F	7	Total 7	O 7	0	0
17	G	15	Total 15	O 15	0	0
17	H	13	Total 13	O 13	0	0
17	I	10	Total 10	O 10	0	0
17	J	9	Total 9	O 9	0	0
17	K	15	Total 15	O 15	0	0
17	L	23	Total 23	O 23	0	0
17	M	20	Total 20	O 20	0	0
17	N	14	Total 14	O 14	0	0
17	O	12	Total 12	O 12	0	0
17	P	11	Total 11	O 11	0	0
17	Q	14	Total 14	O 14	0	0
17	R	7	Total 7	O 7	0	0
17	S	7	Total 7	O 7	0	0
17	T	12	Total 12	O 12	0	0
17	U	10	Total 10	O 10	0	0
17	V	12	Total 12	O 12	0	0
17	W	14	Total 14	O 14	0	0
17	X	12	Total 12	O 12	0	0
17	Y	24	Total 24	O 24	0	0
17	Z	11	Total 11	O 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	a	16	Total	O	0	0
			16	16		
17	b	16	Total	O	0	0
			16	16		

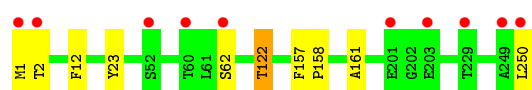
### 3 Residue-property plots [i](#)

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

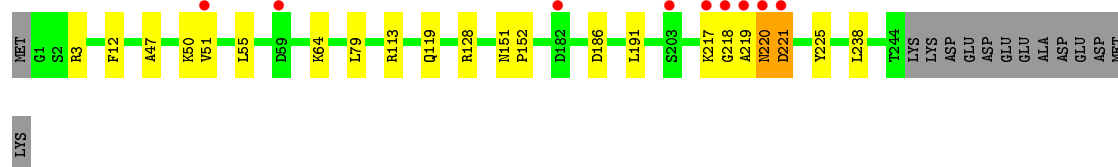
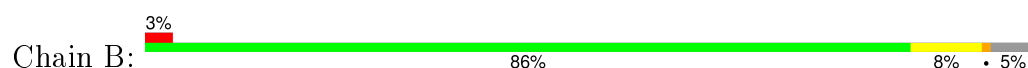
- Molecule 1: Proteasome subunit alpha type-2



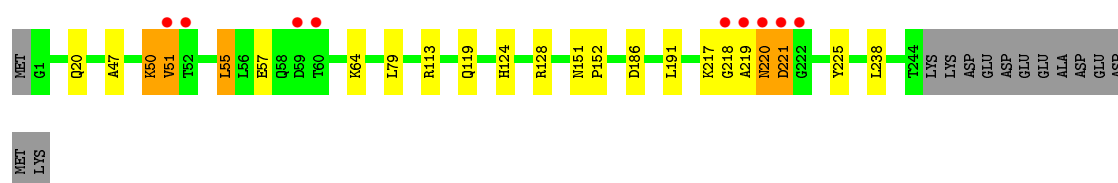
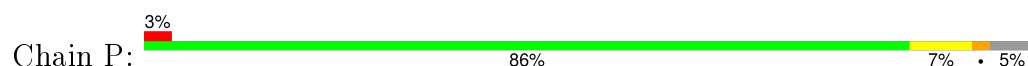
- Molecule 1: Proteasome subunit alpha type-2



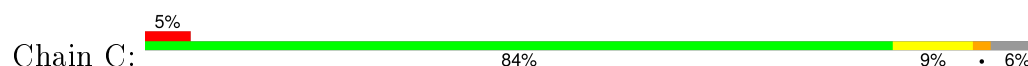
- Molecule 2: Proteasome subunit alpha type-3

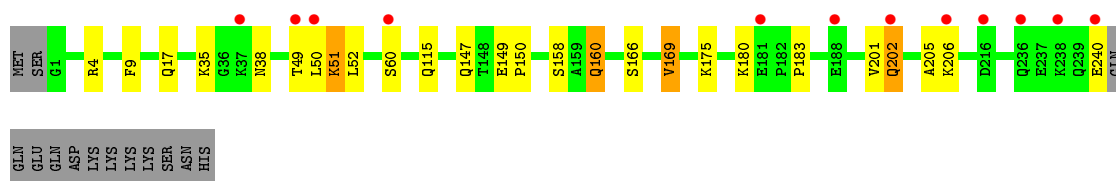


- Molecule 2: Proteasome subunit alpha type-3

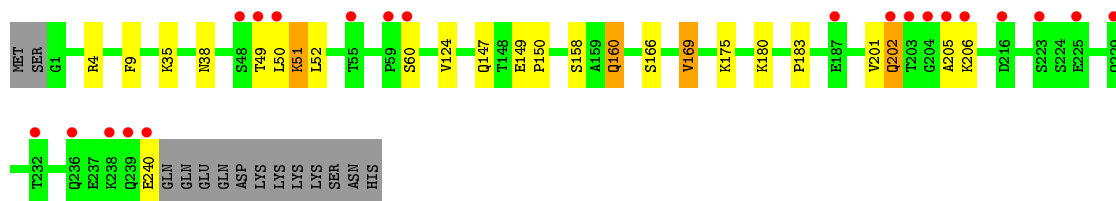
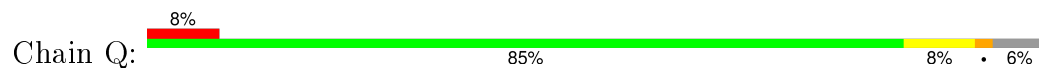


- Molecule 3: Proteasome subunit alpha type-4

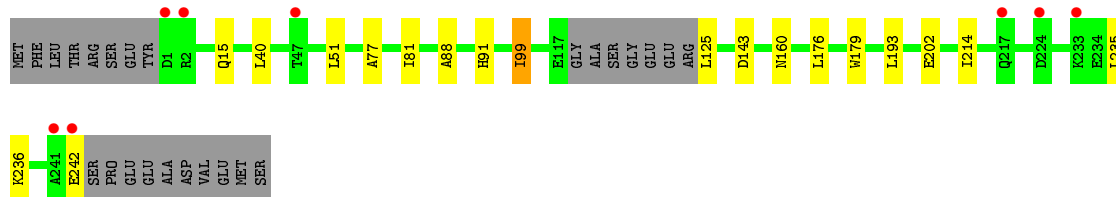
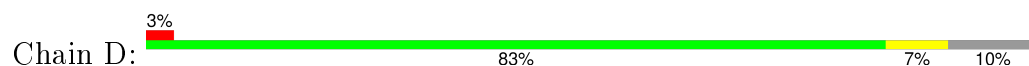




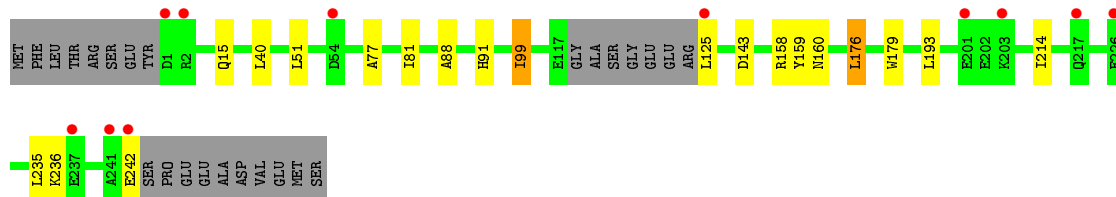
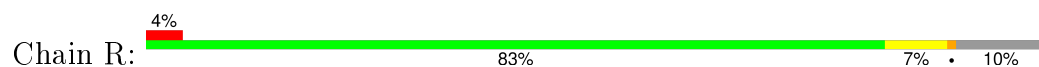
• Molecule 3: Proteasome subunit alpha type-4



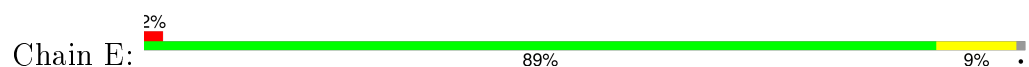
• Molecule 4: Proteasome subunit alpha type-5



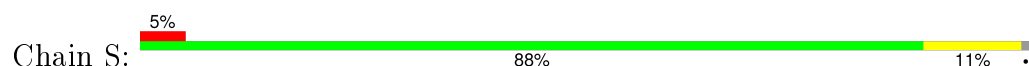
• Molecule 4: Proteasome subunit alpha type-5

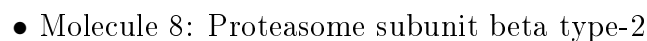
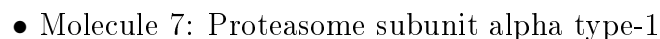
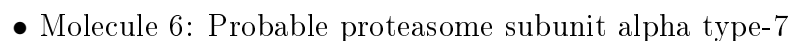
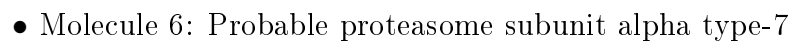


• Molecule 5: Proteasome subunit alpha type-6



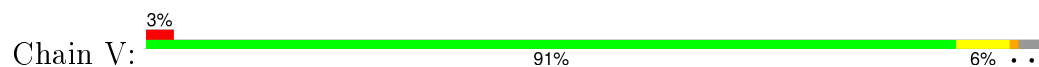
• Molecule 5: Proteasome subunit alpha type-6



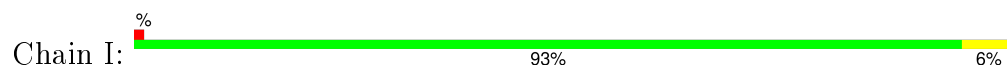




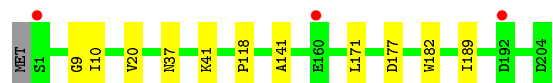
- Molecule 8: Proteasome subunit beta type-2



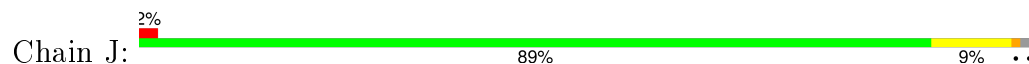
- Molecule 9: Proteasome subunit beta type-3



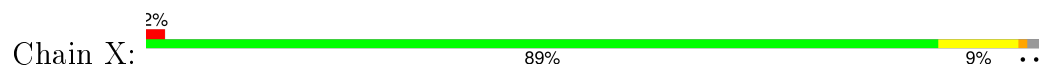
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5





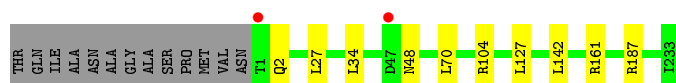
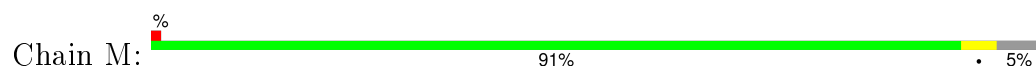
- Molecule 12: Proteasome subunit beta type-6



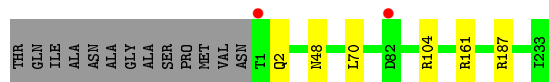
- Molecule 12: Proteasome subunit beta type-6



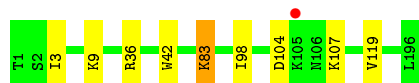
- Molecule 13: Proteasome subunit beta type-7



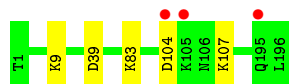
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.86Å 302.06Å 144.23Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (15.00-2.90) 92.3 (15.00-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.198 , 0.218 0.205 , 0.224	Depositor DCC
$R_{free}$ test set	10734 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 214679 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	49723	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL

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	0.28	0/1934	0.50	0/2618
2	P	0.27	0/1934	0.51	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	0.48	0/2433
5	S	0.26	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.46	0/2609
6	T	0.26	0/1932	0.46	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.27	0/1747	0.48	0/2369
8	V	0.26	0/1747	0.47	0/2369
9	I	0.27	0/1611	0.48	0/2174
9	W	0.28	0/1611	0.49	0/2174
10	J	0.26	0/1589	0.49	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.26	0/1681	0.49	1/2274 (0.0%)
11	Y	0.26	0/1681	0.49	1/2274 (0.0%)
12	L	0.27	0/1795	0.48	0/2420
12	Z	0.27	0/1795	0.48	0/2420
13	M	0.27	0/1855	0.51	0/2514
13	a	0.27	0/1855	0.51	0/2514
14	N	0.30	0/1541	0.49	0/2087
14	b	0.29	0/1541	0.48	0/2087
All	All	0.27	0/50258	0.49	2/67954 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	LEU	CA-CB-CG	5.14	127.12	115.30
11	Y	4	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	6	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	12	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	9	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	9	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	8	0
7	U	1907	0	1901	8	0
8	H	1717	0	1718	12	0
8	V	1717	0	1718	10	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	12	0
10	X	1561	0	1569	11	0
11	K	1644	0	1595	6	0
11	Y	1644	0	1595	6	0
12	L	1757	0	1711	1	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
15	C	1	0	0	2	0
15	G	1	0	0	0	0
15	M	1	0	0	0	0
15	a	1	0	0	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	W	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	A	7	0	0	0	0
17	B	10	0	0	0	0
17	C	9	0	0	0	0
17	D	8	0	0	0	0
17	E	10	0	0	0	0
17	F	7	0	0	0	0
17	G	15	0	0	0	0
17	H	13	0	0	0	0
17	I	10	0	0	0	0
17	J	9	0	0	0	0
17	K	15	0	0	0	0
17	L	23	0	0	0	0
17	M	20	0	0	0	0
17	N	14	0	0	0	0
17	O	12	0	0	0	0
17	P	11	0	0	0	0
17	Q	14	0	0	0	0
17	R	7	0	0	0	0
17	S	7	0	0	1	0
17	T	12	0	0	0	0
17	U	10	0	0	0	0
17	V	12	0	0	0	0
17	W	14	0	0	0	0
17	X	12	0	0	0	0
17	Y	24	0	0	0	0
17	Z	11	0	0	0	0
17	a	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	b	16	0	0	0	0
All	All	49723	0	49128	154	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 (154) 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)
8:H:52:THR:O	8:H:56:THR:OG1	1.95	0.84
8:V:52:THR:O	8:V:56:THR:OG1	1.96	0.84
2:B:12:PHE:H	3:C:17:GLN:HE22	1.47	0.62
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.49	0.60
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.02	0.59
3:C:51:LYS:O	3:C:52:LEU:HB2	2.02	0.59
4:R:176:LEU:HD11	5:S:54:GLU:HB2	1.85	0.57
3:C:115:GLN:O	15:C:301:CL:CL	2.61	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.55
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.42	0.55
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.72	0.55
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.55
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.73	0.53
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.38	0.53
14:N:3:ILE:HD12	14:N:98:ILE:HD12	1.90	0.53
2:P:217:LYS:C	2:P:219:ALA:H	2.12	0.53
3:C:201:VAL:O	3:C:202:GLN:CB	2.56	0.53
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.45	0.53
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
2:B:217:LYS:C	2:B:219:ALA:H	2.12	0.52
5:E:12:PHE:H	6:F:19:GLN:HE22	1.59	0.51
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.93	0.51
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.93	0.51
5:S:12:PHE:H	6:T:19:GLN:HE22	1.58	0.50
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.58	0.50
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.94	0.50
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.93	0.50
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.94	0.50
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
8:H:116:ASN:N	8:H:116:ASN:HD22	2.10	0.49
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.95	0.49
10:J:25:ILE:O	10:X:139:TYR:OH	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.49
8:V:116:ASN:N	8:V:116:ASN:HD22	2.11	0.48
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.48
3:C:35:LYS:HG2	3:C:158:SER:O	2.14	0.48
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.95	0.48
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.79	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.95	0.48
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.96	0.47
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.96	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.13	0.47
7:U:73:VAL:HG12	7:U:133:THR:HB	1.95	0.47
7:U:23:PHE:O	7:U:26:THR:HB	2.15	0.47
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.96	0.47
7:G:73:VAL:HG12	7:G:133:THR:HB	1.95	0.47
7:G:23:PHE:O	7:G:26:THR:HB	2.14	0.47
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.45	0.47
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.97	0.47
8:H:112:SER:OG	8:H:120:ASP:HB2	2.15	0.47
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.47
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.96	0.47
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.15	0.47
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.97	0.47
8:H:116:ASN:HD22	8:H:116:ASN:H	1.61	0.46
10:X:1:MET:CB	10:X:34:LYS:HE3	2.45	0.46
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.98	0.46
1:O:158:PRO:HB2	2:P:57:GLU:HB3	1.97	0.46
10:J:139:TYR:OH	10:X:25:ILE:O	2.33	0.46
10:J:1:MET:CB	10:J:34:LYS:HE3	2.45	0.46
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.97	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.97	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.46
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.96	0.46
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.45	0.46
8:V:116:ASN:ND2	8:V:116:ASN:H	2.14	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.97	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.46
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.97	0.46
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.97	0.46
8:V:116:ASN:H	8:V:116:ASN:HD22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.97	0.46
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.56	0.46
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.97	0.45
8:H:116:ASN:ND2	8:H:116:ASN:H	2.14	0.45
8:V:112:SER:OG	8:V:120:ASP:HB2	2.17	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.57	0.45
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.98	0.45
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.52	0.45
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.99	0.45
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.45
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.52	0.45
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.99	0.45
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.52	0.45
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.99	0.45
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.99	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.44
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.47	0.44
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.99	0.44
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.48	0.44
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.47	0.44
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.48	0.44
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.00	0.44
3:C:9:PHE:H	4:D:15:GLN:HE22	1.64	0.44
10:J:168:LEU:O	10:J:172:MET:HB2	2.18	0.43
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.00	0.43
4:R:77:ALA:O	4:R:81:ILE:HG12	2.18	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
3:C:150:PRO:O	15:C:301:CL:CL	2.73	0.43
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.01	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.43
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.43
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.83	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.53	0.43
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.48	0.43
4:R:158:ARG:HB3	5:S:57:SER:HB3	2.01	0.43
3:Q:166:SER:HA	3:Q:169:VAL:HG13	2.01	0.43
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.00	0.42
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.01	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.00	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.42
5:S:147:GLN:HG2	17:S:307:HOH:O	2.17	0.42
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.01	0.42
3:C:166:SER:HA	3:C:169:VAL:HG13	2.00	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.01	0.42
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
10:X:168:LEU:O	10:X:172:MET:HB2	2.20	0.41
4:D:77:ALA:O	4:D:81:ILE:HG12	2.19	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.41
5:E:68:HIS:HE1	5:E:102:LEU:O	2.02	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
2:P:220:ASN:O	2:P:221:ASP:HB2	2.21	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.50	0.41
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.03	0.41
1:O:161:ALA:O	2:P:55:LEU:HD23	2.20	0.41
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.02	0.41
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.03	0.41
7:U:63:ILE:HD12	7:U:215:GLU:HG2	2.01	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
2:B:220:ASN:O	2:B:221:ASP:HB2	2.21	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
14:N:83:LYS:HG3	14:N:119:VAL:HG22	2.02	0.41
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.51	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.03	0.41
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.03	0.41
10:X:119:ILE:HG12	10:X:125:LYS:HG3	2.03	0.41
1:O:12:PHE:H	2:P:20:GLN:HE22	1.68	0.41
9:I:98:ARG:O	9:I:126:ILE:HD11	2.20	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.40
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.03	0.40
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.03	0.40
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.04	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%)	238 (96%)	9 (4%)	1 (0%)	39	74
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	39	74
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	11	38
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	11	38
3	C	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	15	46
3	Q	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	15	46
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	239 (100%)	0	0	100	100
7	U	239/252 (95%)	239 (100%)	0	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6284/6614 (95%)	6136 (98%)	132 (2%)	16 (0%)	46	79

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
2	B	218	GLY
2	B	220	ASN
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	65	89
1	O	209/209 (100%)	205 (98%)	4 (2%)	65	89
2	B	203/216 (94%)	195 (96%)	8 (4%)	39	75
2	P	203/216 (94%)	195 (96%)	8 (4%)	39	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	212/226 (94%)	199 (94%)	13 (6%)	23	56
3	Q	212/226 (94%)	199 (94%)	13 (6%)	23	56
4	D	194/215 (90%)	182 (94%)	12 (6%)	23	55
4	R	194/215 (90%)	183 (94%)	11 (6%)	25	59
5	E	190/193 (98%)	178 (94%)	12 (6%)	22	54
5	S	190/193 (98%)	178 (94%)	12 (6%)	22	54
6	F	201/239 (84%)	191 (95%)	10 (5%)	30	65
6	T	201/239 (84%)	191 (95%)	10 (5%)	30	65
7	G	206/210 (98%)	195 (95%)	11 (5%)	28	63
7	U	206/210 (98%)	195 (95%)	11 (5%)	28	63
8	H	185/190 (97%)	180 (97%)	5 (3%)	52	84
8	V	185/190 (97%)	179 (97%)	6 (3%)	46	81
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	91
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	91
10	J	173/175 (99%)	169 (98%)	4 (2%)	58	87
10	X	173/175 (99%)	169 (98%)	4 (2%)	58	87
11	K	169/169 (100%)	159 (94%)	10 (6%)	24	58
11	Y	169/169 (100%)	159 (94%)	10 (6%)	24	58
12	L	185/185 (100%)	178 (96%)	7 (4%)	40	76
12	Z	185/185 (100%)	178 (96%)	7 (4%)	40	76
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	83
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	83
14	N	162/162 (100%)	158 (98%)	4 (2%)	55	85
14	b	162/162 (100%)	157 (97%)	5 (3%)	47	82
All	All	5320/5540 (96%)	5101 (96%)	219 (4%)	37	73

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS

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Mol	Chain	Res	Type
2	B	55	LEU
2	B	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	50	LEU
3	C	51	LYS
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	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	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL

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Mol	Chain	Res	Type
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	178	LYS
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	116	ASN
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	57	THR
11	K	69	ARG
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP

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Mol	Chain	Res	Type
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
12	L	161	GLU
13	M	2	GLN
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	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	50	LEU
3	Q	51	LYS
3	Q	60	SER
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS

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Mol	Chain	Res	Type
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG

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Mol	Chain	Res	Type
7	U	125	MET
7	U	178	LYS
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	116	ASN
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	57	THR
11	Y	69	ARG
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	161	GLU
13	a	2	GLN
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	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) 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
2	B	176	GLN
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	120	GLN
5	E	151	ASN
5	E	184	ASN
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

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Mol	Chain	Res	Type
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	116	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	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
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	146	GLN

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Mol	Chain	Res	Type
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	66	HIS
8	V	116	ASN
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
10	X	146	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	95	HIS
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN

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Mol	Chain	Res	Type
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	161	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 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%)	-0.23	11 (4%) 38 32	32, 45, 78, 118	0
1	O	250/250 (100%)	-0.18	10 (4%) 42 35	36, 51, 95, 125	0
2	B	244/258 (94%)	-0.13	9 (3%) 45 38	31, 50, 92, 142	0
2	P	244/258 (94%)	-0.11	9 (3%) 45 38	37, 53, 95, 140	0
3	C	240/254 (94%)	-0.05	12 (5%) 32 26	34, 56, 113, 135	0
3	Q	240/254 (94%)	0.22	21 (8%) 12 8	41, 68, 145, 171	0
4	D	235/260 (90%)	-0.21	8 (3%) 49 41	37, 56, 87, 123	0
4	R	235/260 (90%)	-0.11	11 (4%) 35 29	38, 60, 102, 139	0
5	E	231/234 (98%)	-0.12	5 (2%) 65 60	36, 59, 98, 143	0
5	S	231/234 (98%)	0.12	11 (4%) 34 28	41, 69, 112, 160	0
6	F	243/288 (84%)	-0.28	8 (3%) 50 42	35, 52, 100, 128	0
6	T	243/288 (84%)	-0.10	10 (4%) 41 34	40, 64, 113, 143	0
7	G	241/252 (95%)	-0.35	2 (0%) 87 86	29, 48, 79, 129	0
7	U	241/252 (95%)	-0.22	7 (2%) 55 49	36, 52, 81, 126	0
8	H	226/232 (97%)	-0.25	8 (3%) 48 40	27, 43, 75, 144	0
8	V	226/232 (97%)	-0.22	8 (3%) 48 40	32, 45, 75, 150	0
9	I	204/205 (99%)	-0.54	2 (0%) 84 82	30, 41, 66, 86	0
9	W	204/205 (99%)	-0.51	3 (1%) 76 74	30, 41, 69, 97	0
10	J	195/198 (98%)	-0.40	4 (2%) 67 62	28, 44, 68, 125	0
10	X	195/198 (98%)	-0.39	3 (1%) 76 74	30, 44, 68, 129	0
11	K	212/212 (100%)	-0.37	1 (0%) 91 90	26, 43, 63, 83	0
11	Y	212/212 (100%)	-0.45	1 (0%) 91 90	33, 44, 66, 89	0
12	L	222/222 (100%)	-0.42	2 (0%) 85 84	29, 44, 73, 109	0
12	Z	222/222 (100%)	-0.44	1 (0%) 91 90	30, 44, 73, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.48	2 (0%)	85 84	28, 44, 66, 84	0
13	a	233/246 (94%)	-0.47	2 (0%)	85 84	28, 42, 62, 79	0
14	N	196/196 (100%)	-0.52	1 (0%)	91 90	27, 39, 65, 92	0
14	b	196/196 (100%)	-0.51	3 (1%)	76 74	30, 40, 66, 98	0
All	All	6344/6614 (95%)	-0.27	175 (2%)	56 50	26, 49, 94, 171	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	10.1
3	Q	49	THR	8.3
2	B	221	ASP	6.3
8	V	222	ASP	6.3
5	S	202	ASP	5.9
8	V	226	GLU	5.9
3	Q	50	LEU	5.7
8	H	224	GLN	5.5
8	H	226	GLU	5.5
2	P	219	ALA	5.4
1	O	2	THR	5.2
2	P	220	ASN	5.0
2	P	221	ASP	4.9
1	A	2	THR	4.8
3	C	206	LYS	4.8
5	E	202	ASP	4.8
8	H	222	ASP	4.7
2	B	219	ALA	4.7
2	B	51	VAL	4.6
8	V	225	GLU	4.6
2	B	220	ASN	4.6
9	W	1	SER	4.6
8	V	223	ILE	4.6
4	R	241	ALA	4.5
7	U	242	GLN	4.2
10	X	1	MET	4.2
14	b	195	GLN	4.2
8	H	223	ILE	4.1
3	Q	239	GLN	4.1
3	C	49	THR	4.1
8	H	221	CYS	4.1
1	O	1	MET	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	H	225	GLU	4.0
12	L	174	TYR	4.0
8	V	221	CYS	3.9
2	P	51	VAL	3.9
1	O	62	SER	3.9
10	J	1	MET	3.8
3	Q	236	GLN	3.8
3	Q	187	GLU	3.7
4	R	1	ASP	3.7
7	U	222	ASP	3.7
1	A	1	MET	3.7
1	A	62	SER	3.6
10	X	194	ASP	3.6
5	S	52	ALA	3.6
3	Q	223	SER	3.5
2	P	218	GLY	3.5
12	Z	174	TYR	3.5
7	U	153	TYR	3.5
5	S	227	GLU	3.5
6	T	201	GLU	3.4
2	P	59	ASP	3.4
2	B	218	GLY	3.4
6	F	205	GLU	3.3
3	Q	202	GLN	3.3
3	Q	203	THR	3.3
1	A	249	ALA	3.3
2	B	203	SER	3.2
3	Q	60	SER	3.2
3	Q	205	ALA	3.1
11	Y	212	GLY	3.1
1	O	249	ALA	3.1
14	N	105	LYS	3.1
9	W	192	ASP	3.1
10	J	193	ASP	3.0
4	D	241	ALA	3.0
6	F	51	THR	3.0
7	U	206	GLY	3.0
1	A	248	GLU	3.0
8	V	219	ASN	3.0
8	H	219	ASN	2.9
3	Q	204	GLY	2.9
1	O	201	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
4	R	242	GLU	2.9
3	Q	48	SER	2.9
3	Q	232	THR	2.9
5	S	173	ARG	2.9
6	T	181	GLU	2.9
13	a	1	THR	2.9
14	b	105	LYS	2.9
8	V	145	ASP	2.9
4	R	201	GLU	2.9
6	T	244	ASN	2.8
3	Q	238	LYS	2.8
4	D	1	ASP	2.8
4	R	217	GLN	2.8
7	G	222	ASP	2.8
5	E	54	GLU	2.7
3	Q	55	THR	2.7
3	Q	216	ASP	2.7
14	b	104	ASP	2.7
9	I	1	SER	2.7
3	C	60	SER	2.7
3	C	216	ASP	2.7
3	Q	240	GLU	2.7
7	G	242	GLN	2.7
6	F	244	ASN	2.6
5	S	180	LYS	2.6
2	P	222	GLY	2.6
3	C	181	GLU	2.6
6	T	51	THR	2.6
3	C	240	GLU	2.6
4	R	203	LYS	2.6
1	O	203	GLU	2.6
3	C	238	LYS	2.6
6	T	178	HIS	2.5
5	E	227	GLU	2.5
1	A	52	SER	2.5
4	D	47	THR	2.4
1	O	52	SER	2.4
5	S	165	GLN	2.4
6	T	241	LYS	2.4
1	A	229	THR	2.4
2	B	59	ASP	2.4
3	Q	225	GLU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	50	LEU	2.4
13	M	1	THR	2.4
8	H	198	GLU	2.4
1	A	201	GLU	2.4
5	S	226	GLY	2.4
13	M	47	ASP	2.3
1	O	250	LEU	2.3
3	C	236	GLN	2.3
5	S	201	ARG	2.3
1	A	203	GLU	2.3
6	F	29	ASN	2.3
9	I	192	ASP	2.3
5	S	183	GLY	2.3
6	F	2	THR	2.3
5	E	233	ILE	2.3
11	K	212	GLY	2.3
4	R	226	GLU	2.3
6	T	166	GLN	2.3
3	Q	206	LYS	2.2
3	Q	229	GLN	2.2
6	T	215	CYS	2.2
10	J	24	GLY	2.2
1	A	59	GLU	2.2
7	U	188	GLU	2.2
4	R	2	ARG	2.2
10	X	72	ASP	2.2
4	D	233	LYS	2.2
6	F	204	LYS	2.2
5	S	194	GLU	2.2
4	D	2	ARG	2.2
6	T	206	LYS	2.2
7	U	183	ASP	2.2
1	O	60	THR	2.2
4	R	125	LEU	2.2
7	U	230	GLU	2.2
9	W	160	GLU	2.1
4	R	54	ASP	2.1
3	C	37	LYS	2.1
5	E	201	ARG	2.1
5	S	51	ASN	2.1
2	P	60	THR	2.1
4	D	224	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	217	GLN	2.1
12	L	165	ASN	2.1
4	D	242	GLU	2.1
6	T	230	ASP	2.1
3	Q	59	PRO	2.1
2	P	52	THR	2.1
13	a	82	ASP	2.1
4	R	237	GLU	2.1
6	F	181	GLU	2.1
3	C	202	GLN	2.1
6	F	166	GLN	2.0
1	O	229	THR	2.0
2	B	217	LYS	2.0
2	B	182	ASP	2.0
3	C	188	GLU	2.0
10	J	194	ASP	2.0
1	A	61	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	CL	C	301	1/1	0.91	0.40	10.17	30,30,30,30	0
16	MG	Z	301	1/1	0.86	0.28	4.43	59,59,59,59	0
16	MG	I	301	1/1	0.98	0.22	2.25	51,51,51,51	0
16	MG	W	301	1/1	0.98	0.16	1.29	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	MG	V	301	1/1	0.99	0.15	0.71	48,48,48,48	0
16	MG	G	301	1/1	0.94	0.13	-0.49	36,36,36,36	0
16	MG	K	301	1/1	0.96	0.10	-1.08	41,41,41,41	0
16	MG	Y	301	1/1	0.95	0.08	-1.91	40,40,40,40	0
16	MG	N	201	1/1	0.98	0.07	-1.98	42,42,42,42	0
15	CL	M	301	1/1	0.96	0.08	-2.03	30,30,30,30	0
15	CL	a	301	1/1	0.97	0.13	-	30,30,30,30	0
15	CL	G	302	1/1	0.90	0.20	-	30,30,30,30	0
16	MG	H	301	1/1	0.83	0.14	-	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.