



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:08 PM GMT

PDB ID : 4NO8  
Title : yCP in complex with Z-Leu-Leu-Leu-ketoamide  
Authors : Stein, M.L.; Cui, H.; Beck, P.; Dubiella, C.; Voss, C.; Krueger, A.; Schmidt, B.; Groll, M.  
Deposited on : 2013-11-19  
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](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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

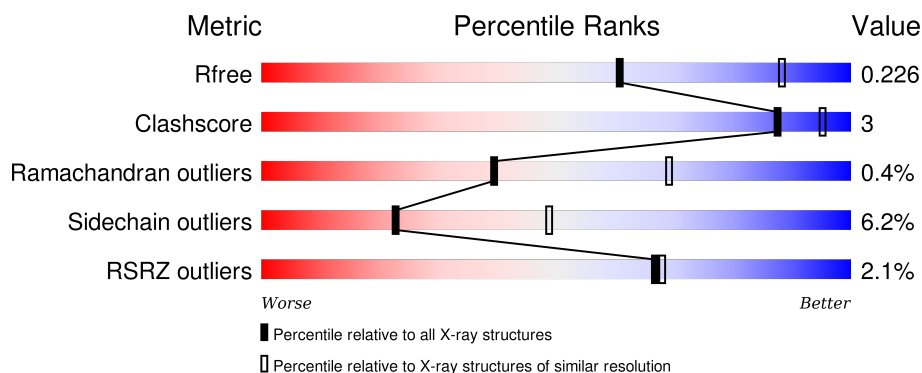
# 1 Overall quality at a glance

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  $\geq 3$ , 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>3%</div> <div>94%</div> <div>5%</div> </div>
1	O	250	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
2	B	258	<div> <div>5%</div> <div>81%</div> <div>12%</div> <div>5%</div> </div>
2	P	258	<div> <div>5%</div> <div>81%</div> <div>12%</div> <div>5%</div> </div>
3	C	254	<div> <div>5%</div> <div>80%</div> <div>12%</div> <div>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	MG	I	301	-	-	-	X
15	MG	N	201	-	-	-	X
16	2LV	K	301	-	-	-	X
16	2LV	Y	301	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49878 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

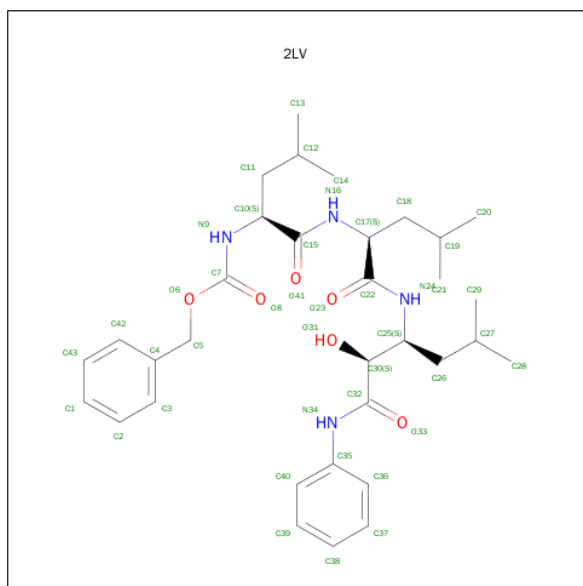
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		

- Molecule 16 is N-[(BENZYLOXY)CARBONYL]-L-LEUCYL-N-[(2S,3S)-2-HYDROXY-5-METHYL-1-OXO-1-(PHENYLAMINO)HEXAN-3-YL]-L-LEUCINAMIDE (three-letter code: 2LV) (formula:  $C_{33}H_{48}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			43	33	4	6		
16	Y	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 17 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	18	Total O 18 18	0	0
17	B	11	Total O 11 11	0	0
17	C	19	Total O 19 19	0	0
17	D	10	Total O 10 10	0	0
17	E	15	Total O 15 15	0	0
17	F	18	Total O 18 18	0	0
17	G	21	Total O 21 21	0	0
17	H	13	Total O 13 13	0	0
17	I	14	Total O 14 14	0	0
17	J	35	Total O 35 35	0	0
17	K	17	Total O 17 17	0	0
17	L	21	Total O 21 21	0	0
17	M	22	Total O 22 22	0	0
17	N	20	Total O 20 20	0	0
17	O	13	Total O 13 13	0	0
17	P	13	Total O 13 13	0	0
17	Q	12	Total O 12 12	0	0
17	R	12	Total O 12 12	0	0
17	S	8	Total O 8 8	0	0
17	T	12	Total O 12 12	0	0
17	U	19	Total O 19 19	0	0
17	V	17	Total O 17 17	0	0

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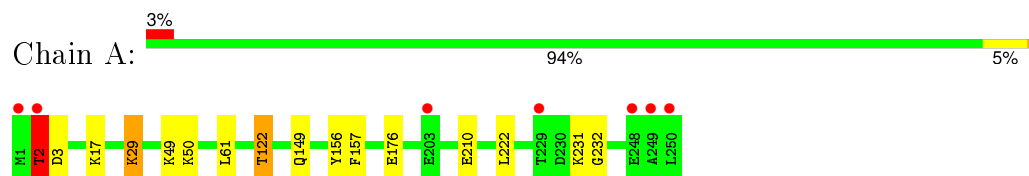
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	17	Total 17	O 17	0	0
17	X	21	Total 21	O 21	0	0
17	Y	13	Total 13	O 13	0	0
17	Z	24	Total 24	O 24	0	0
17	a	29	Total 29	O 29	0	0
17	b	24	Total 24	O 24	0	0

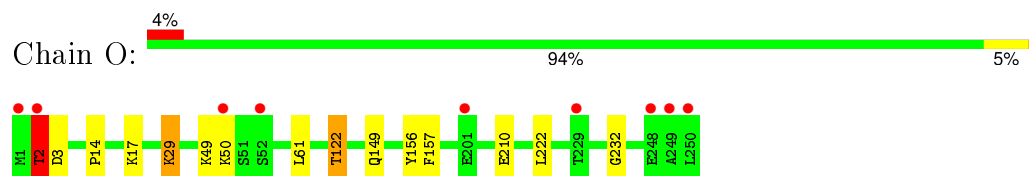
### 3 Residue-property plots [i](#)

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

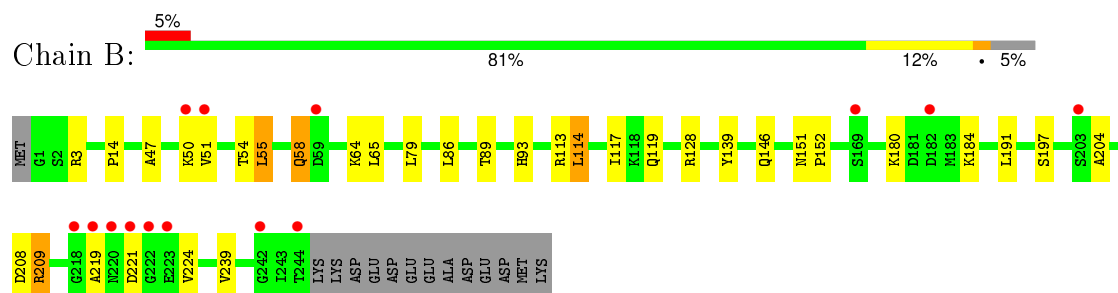
- Molecule 1: Proteasome subunit alpha type-2



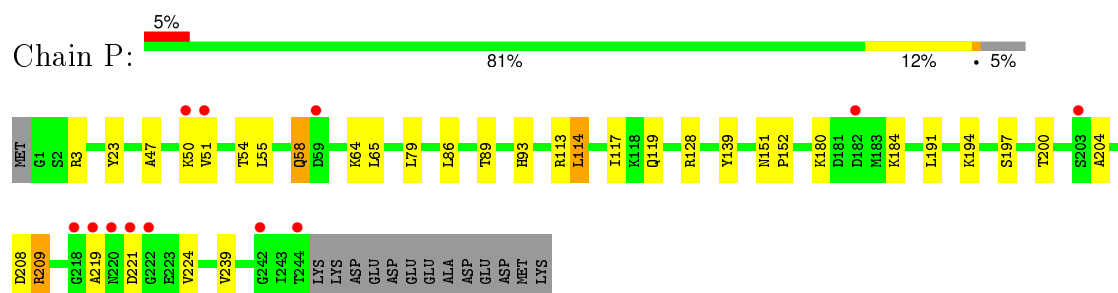
- Molecule 1: Proteasome subunit alpha type-2



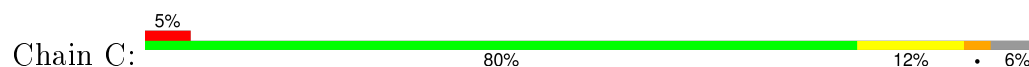
- Molecule 2: Proteasome subunit alpha type-3

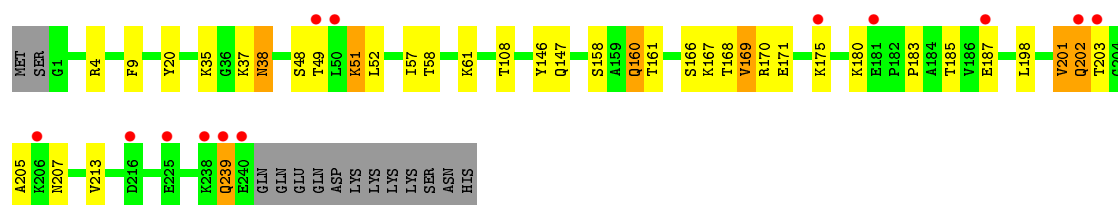


- Molecule 2: Proteasome subunit alpha type-3

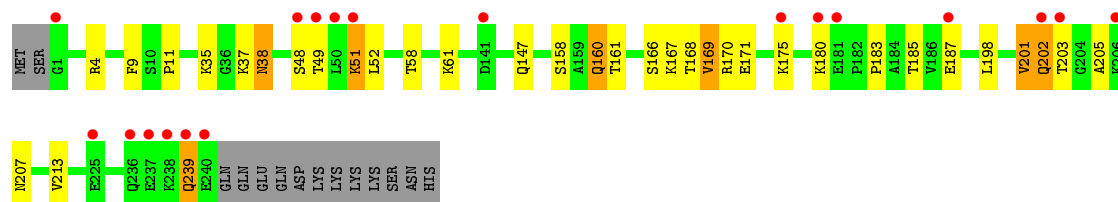
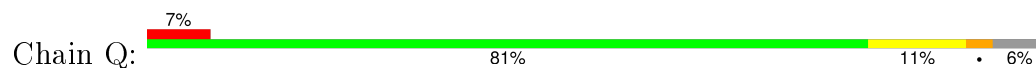


- Molecule 3: Proteasome subunit alpha type-4

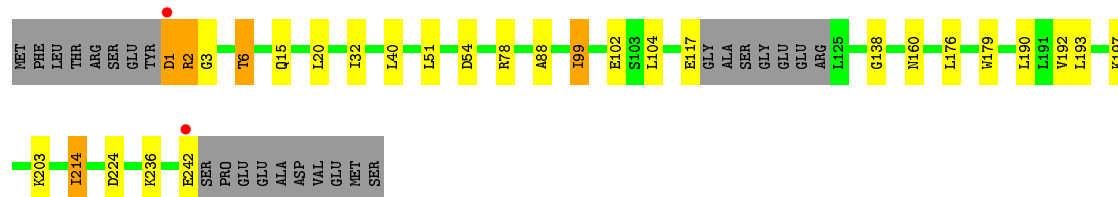
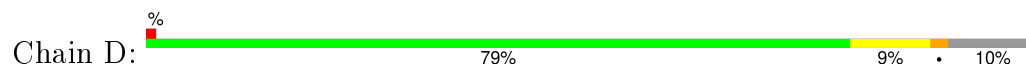




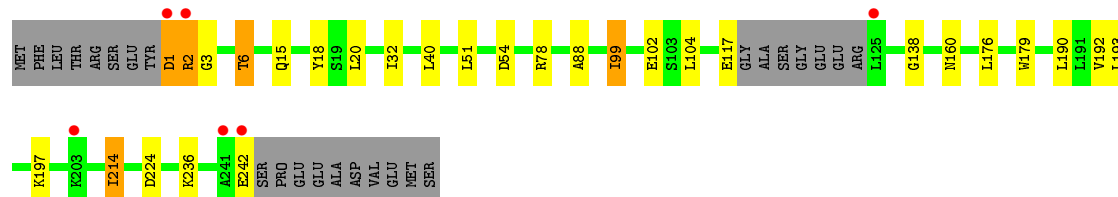
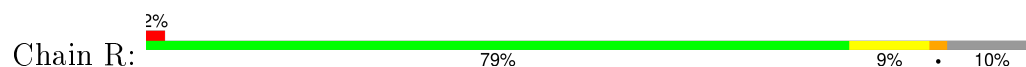
• Molecule 3: Proteasome subunit alpha type-4



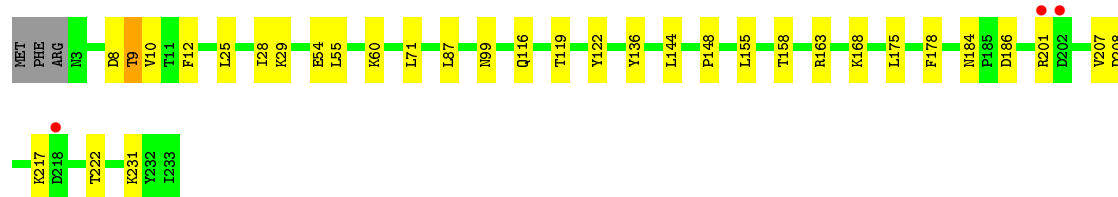
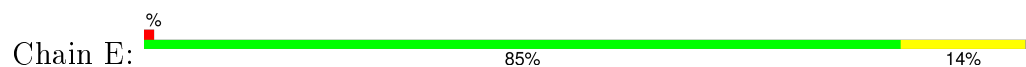
• Molecule 4: Proteasome subunit alpha type-5



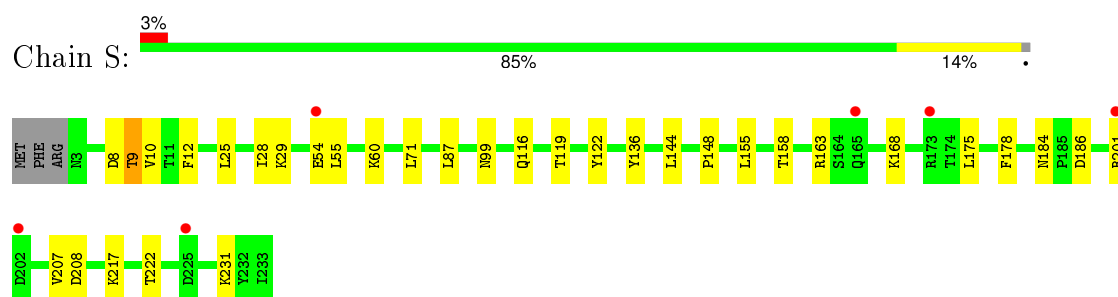
• Molecule 4: Proteasome subunit alpha type-5



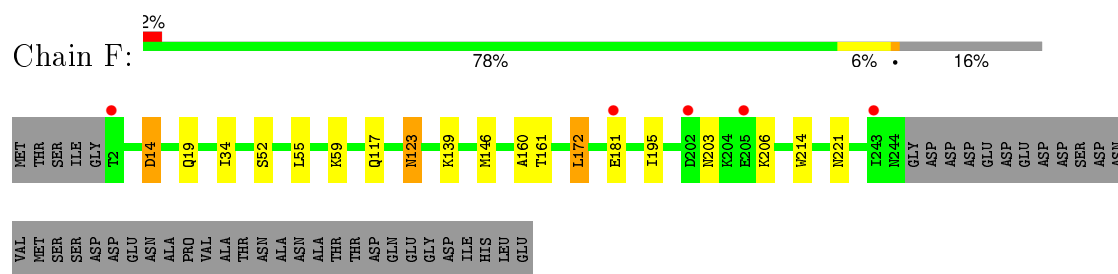
• Molecule 5: Proteasome subunit alpha type-6



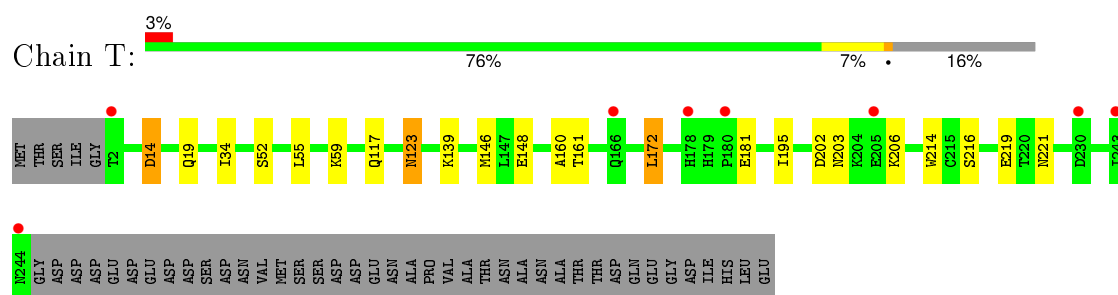
• Molecule 5: Proteasome subunit alpha type-6



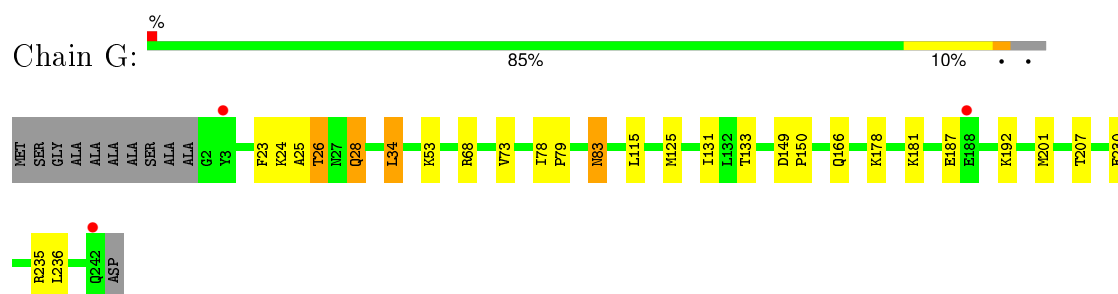
- Molecule 6: Probable proteasome subunit alpha type-7



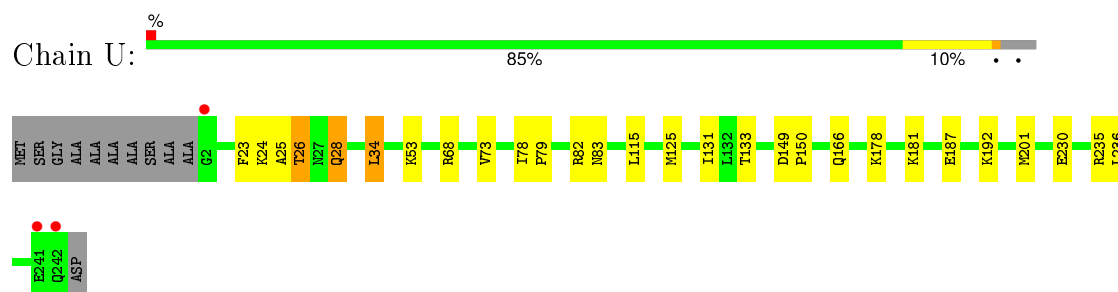
- Molecule 6: Probable proteasome subunit alpha type-7



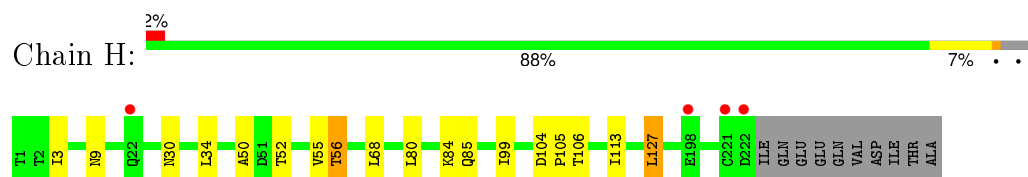
- Molecule 7: Proteasome subunit alpha type-1



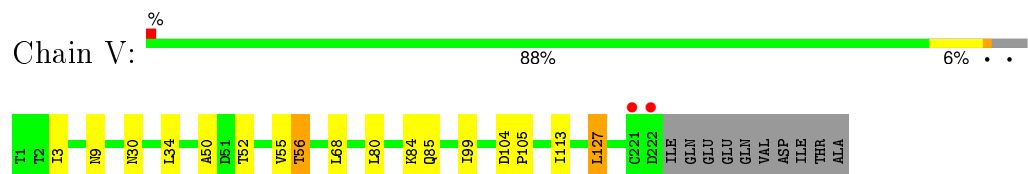
- Molecule 7: Proteasome subunit alpha type-1



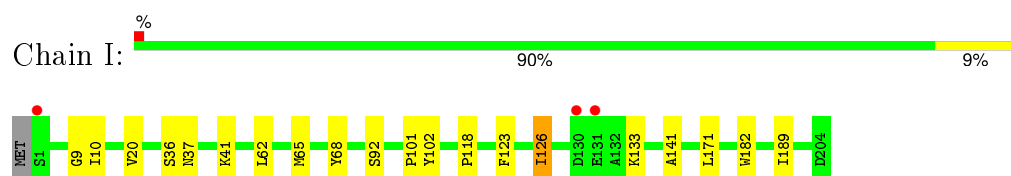
- Molecule 8: Proteasome subunit beta type-2



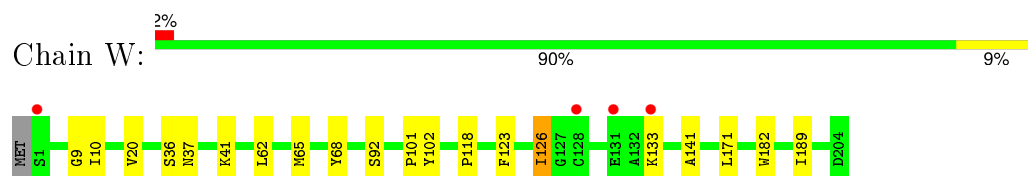
- Molecule 8: Proteasome subunit beta type-2



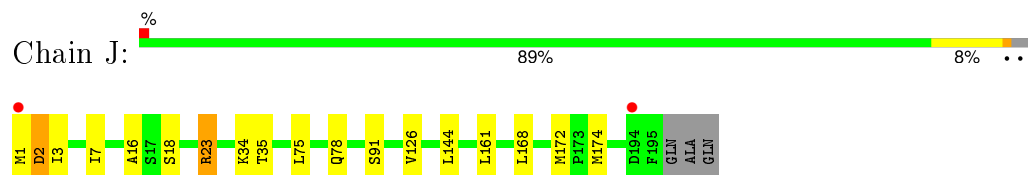
- Molecule 9: Proteasome subunit beta type-3



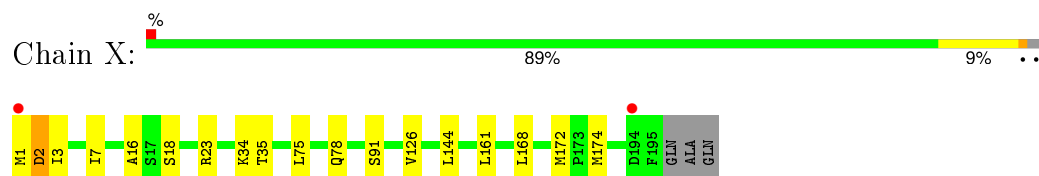
- Molecule 9: Proteasome subunit beta type-3



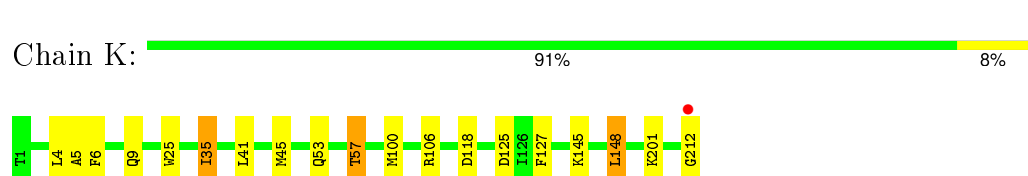
- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4

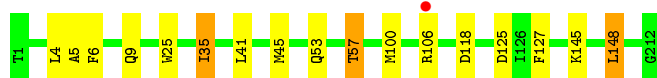


- Molecule 11: Proteasome subunit beta type-5




- Molecule 11: Proteasome subunit beta type-5

Chain Y:  92% 7%




- Molecule 12: Proteasome subunit beta type-6

Chain L:  87% 12%




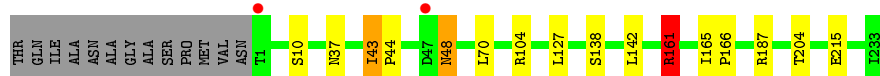
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  87% 12%



- Molecule 13: Proteasome subunit beta type-7

Chain M:  88% 5% 5%



- Molecule 13: Proteasome subunit beta type-7

Chain a:  90% 5%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  93% 6%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.15Å 300.35Å 144.83Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-2.70) 97.4 (14.99-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.193 , 0.217 0.200 , 0.226	Depositor DCC
$R_{free}$ test set	13978 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 279566 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	49878	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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, 2LV

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	0.28	0/1952	0.52	0/2642
1	O	0.28	0/1952	0.52	0/2642
2	B	0.28	0/1934	0.55	0/2618
2	P	0.28	0/1934	0.55	0/2618
3	C	0.29	0/1910	0.56	0/2586
3	Q	0.29	0/1910	0.56	0/2586
4	D	0.28	0/1837	0.54	0/2475
4	R	0.28	0/1837	0.54	0/2475
5	E	0.28	0/1800	0.54	0/2433
5	S	0.28	0/1800	0.53	0/2433
6	F	0.28	0/1932	0.50	0/2609
6	T	0.28	0/1932	0.50	0/2609
7	G	0.28	0/1945	0.52	0/2634
7	U	0.28	0/1945	0.52	0/2634
8	H	0.26	0/1715	0.51	0/2326
8	V	0.26	0/1715	0.51	0/2326
9	I	0.28	0/1611	0.52	0/2174
9	W	0.29	0/1611	0.52	0/2174
10	J	0.27	0/1589	0.54	0/2142
10	X	0.28	0/1589	0.54	0/2142
11	K	0.28	0/1681	0.53	0/2274
11	Y	0.28	0/1681	0.53	0/2274
12	L	0.27	0/1795	0.52	0/2420
12	Z	0.28	0/1795	0.52	0/2420
13	M	0.29	0/1855	0.57	1/2514 (0.0%)
13	a	0.28	0/1855	0.57	1/2514 (0.0%)
14	N	0.27	0/1541	0.50	0/2087
14	b	0.26	0/1541	0.50	0/2087
All	All	0.28	0/50194	0.53	2/67868 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	161	ARG	NE-CZ-NH1	5.53	123.06	120.30
13	a	161	ARG	NE-CZ-NH1	5.48	123.04	120.30

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	8	0
1	O	1915	0	1929	8	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	13	1
3	C	1881	0	1895	18	0
3	Q	1881	0	1895	16	0
4	D	1813	0	1797	8	1
4	R	1813	0	1797	10	0
5	E	1773	0	1775	9	0
5	S	1773	0	1775	9	0
6	F	1892	0	1883	8	0
6	T	1892	0	1883	11	0
7	G	1907	0	1901	12	0
7	U	1907	0	1901	11	0
8	H	1684	0	1688	8	0
8	V	1684	0	1688	7	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	9	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	8	0
11	K	1644	0	1594	9	0
11	Y	1644	0	1594	8	0
12	L	1757	0	1711	15	0
12	Z	1757	0	1711	15	0
13	M	1824	0	1832	5	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	6	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	K	43	0	47	0	0
16	Y	43	0	47	0	0
17	A	18	0	0	0	0
17	B	11	0	0	0	0
17	C	19	0	0	0	0
17	D	10	0	0	0	0
17	E	15	0	0	0	0
17	F	18	0	0	0	0
17	G	21	0	0	0	0
17	H	13	0	0	0	0
17	I	14	0	0	0	0
17	J	35	0	0	0	0
17	K	17	0	0	1	0
17	L	21	0	0	0	0
17	M	22	0	0	0	0
17	N	20	0	0	0	0
17	O	13	0	0	0	0
17	P	13	0	0	0	0
17	Q	12	0	0	0	0
17	R	12	0	0	0	0
17	S	8	0	0	0	0
17	T	12	0	0	2	0
17	U	19	0	0	0	0
17	V	17	0	0	0	0
17	W	17	0	0	0	0
17	X	21	0	0	0	0
17	Y	13	0	0	0	0
17	Z	24	0	0	0	0
17	a	29	0	0	0	0
17	b	24	0	0	0	0
All	All	49878	0	49160	240	1

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 3.

All (240) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.54	0.90
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.62	0.81
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.62	0.81
11:K:53:GLN:O	11:K:57:THR:HG23	1.84	0.78
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.85	0.75
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.70	0.72
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.40	0.69
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.74	0.69
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.40	0.68
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.60	0.67
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.60	0.66
3:C:51:LYS:O	3:C:52:LEU:HB2	1.97	0.65
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.97	0.63
10:J:23:ARG:HD3	17:K:401:HOH:O	1.98	0.63
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.82	0.62
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.82	0.62
14:N:20:THR:HG22	14:N:31:THR:OG1	2.00	0.61
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.65	0.61
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.66	0.61
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.83	0.60
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.84	0.60
11:K:100:MET:CE	11:K:127:PHE:HB2	2.30	0.60
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.84	0.59
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.30	0.59
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.65	0.59
2:B:204:ALA:O	2:B:209:ARG:NH2	2.36	0.59
3:C:201:VAL:O	3:C:202:GLN:HB2	2.03	0.59
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.83	0.58
2:P:204:ALA:O	2:P:209:ARG:NH2	2.36	0.58
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.03	0.57
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.88	0.56
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.87	0.56
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.89	0.55
6:F:146:MET:HE1	6:F:161:THR:HB	1.88	0.55
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.22	0.55
6:F:14:ASP:N	6:F:14:ASP:OD2	2.39	0.55
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.72	0.55
3:C:201:VAL:HG13	3:C:202:GLN:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.89	0.54
4:D:3:GLY:O	4:D:6:THR:OG1	2.23	0.54
5:E:9:THR:HG21	5:E:119:THR:HA	1.90	0.54
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.43	0.54
3:C:202:GLN:HG3	3:C:203:THR:H	1.73	0.54
5:S:9:THR:HG21	5:S:119:THR:HA	1.90	0.54
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.43	0.53
6:T:19:GLN:NE2	17:T:304:HOH:O	2.41	0.53
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.73	0.53
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.73	0.53
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.90	0.53
12:L:164:THR:O	12:L:167:LYS:HB2	2.08	0.53
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.91	0.53
14:N:35:THR:HG21	14:N:45:ARG:HE	1.74	0.53
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.39	0.53
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.91	0.52
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.89	0.52
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.90	0.52
4:R:3:GLY:O	4:R:6:THR:OG1	2.22	0.52
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.92	0.52
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.92	0.52
5:E:155:LEU:HD13	5:E:158:THR:HB	1.91	0.52
12:Z:164:THR:O	12:Z:167:LYS:HB2	2.09	0.52
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.90	0.52
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.92	0.52
14:N:20:THR:CG2	14:N:28:ASN:HB3	2.40	0.51
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.92	0.51
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.92	0.51
2:P:86:LEU:HB3	2:P:114:LEU:HD21	1.92	0.51
2:B:86:LEU:HB3	2:B:114:LEU:HD21	1.92	0.51
7:U:23:PHE:O	7:U:26:THR:HB	2.11	0.51
10:X:1:MET:HA	10:X:34:LYS:HE3	1.92	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.10	0.51
6:F:146:MET:CE	6:F:161:THR:HB	2.41	0.51
6:T:146:MET:CE	6:T:161:THR:HB	2.41	0.51
10:J:1:MET:HA	10:J:34:LYS:HE3	1.92	0.51
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.92	0.50
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.92	0.50
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.93	0.50
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.77	0.50
14:N:35:THR:CG2	14:N:45:ARG:HE	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.94	0.50
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.77	0.50
5:S:155:LEU:HD13	5:S:158:THR:HB	1.92	0.50
12:L:8:ASN:HA	12:L:30:ILE:O	2.12	0.49
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.47	0.49
5:S:12:PHE:H	6:T:19:GLN:HE22	1.59	0.49
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.93	0.49
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.47	0.49
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.47	0.49
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.94	0.49
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.47	0.49
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.12	0.49
1:O:29:LYS:HA	1:O:29:LYS:HE2	1.95	0.49
6:T:14:ASP:N	6:T:14:ASP:OD2	2.38	0.49
1:A:29:LYS:HA	1:A:29:LYS:HE2	1.95	0.48
5:E:12:PHE:H	6:F:19:GLN:HE22	1.61	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.96	0.48
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.96	0.48
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.95	0.47
4:R:99:ILE:HD13	4:R:104:LEU:HB2	1.96	0.47
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.97	0.47
4:D:99:ILE:HD13	4:D:104:LEU:HB2	1.96	0.47
12:L:164:THR:O	12:L:165:ASN:HB3	2.15	0.47
6:T:146:MET:HE1	6:T:161:THR:HB	1.96	0.47
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.97	0.47
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.97	0.47
3:Q:160:GLN:HE21	3:Q:161:THR:H	1.63	0.46
8:V:99:ILE:HG13	8:V:127:LEU:HD22	1.97	0.46
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.45	0.46
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.50	0.46
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.50	0.46
12:Z:164:THR:O	12:Z:165:ASN:HB3	2.14	0.46
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.50	0.46
1:A:149:GLN:O	1:A:156:TYR:HA	2.16	0.46
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.96	0.46
3:C:160:GLN:HE21	3:C:161:THR:H	1.64	0.46
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.51	0.46
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.51	0.46
2:B:3:ARG:NH1	5:E:122:TYR:OH	2.48	0.46
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.45
7:G:187:GLU:CG	7:G:192:LYS:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:123:ASN:C	6:F:123:ASN:HD22	2.20	0.45
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.64	0.45
7:G:34:LEU:HD23	7:G:34:LEU:C	2.37	0.45
10:X:1:MET:HA	10:X:34:LYS:CE	2.47	0.45
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.47	0.45
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.47	0.45
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.87	0.45
1:O:49:LYS:HG3	1:O:210:GLU:HB2	1.99	0.45
14:N:9:LYS:HA	14:N:9:LYS:HD3	1.75	0.45
8:H:99:ILE:HG13	8:H:127:LEU:HD22	1.99	0.45
3:Q:166:SER:HA	3:Q:169:VAL:HG13	1.98	0.45
5:E:163:ARG:HD3	5:E:201:ARG:NH1	2.32	0.45
7:U:187:GLU:CG	7:U:192:LYS:HB2	2.47	0.44
5:S:163:ARG:HD3	5:S:201:ARG:NH1	2.32	0.44
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.99	0.44
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.99	0.44
11:K:35:ILE:HB	11:K:45:MET:HE3	1.99	0.44
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.47	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.44
4:R:1:ASP:O	4:R:2:ARG:HB2	2.16	0.44
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.33	0.44
10:J:1:MET:HA	10:J:34:LYS:CE	2.47	0.44
6:T:123:ASN:HD22	6:T:123:ASN:C	2.20	0.44
1:A:222:LEU:HD13	1:A:232:GLY:HA2	2.00	0.44
7:U:73:VAL:HG12	7:U:133:THR:HB	1.99	0.44
7:U:34:LEU:C	7:U:34:LEU:HD23	2.38	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.44
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.53	0.43
8:V:52:THR:O	8:V:56:THR:HB	2.19	0.43
12:L:147:MET:N	12:L:148:PRO:HD2	2.33	0.43
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.47	0.43
6:T:146:MET:HE2	6:T:148:GLU:OE2	2.18	0.43
1:A:49:LYS:HG3	1:A:210:GLU:HB2	1.99	0.43
3:C:166:SER:HA	3:C:169:VAL:HG13	1.99	0.43
1:O:222:LEU:HD13	1:O:232:GLY:HA2	2.00	0.43
10:J:3:ILE:HD13	10:J:168:LEU:HD13	2.00	0.43
9:I:62:LEU:HD21	9:I:102:TYR:CD2	2.52	0.43
9:W:62:LEU:HD21	9:W:102:TYR:CD2	2.52	0.43
12:L:161:GLU:HB3	12:L:164:THR:HG21	2.00	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.54	0.43
10:X:3:ILE:HD13	10:X:168:LEU:HD13	2.01	0.43
1:O:2:THR:HG22	1:O:3:ASP:H	1.84	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.43
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.43
7:G:73:VAL:HG12	7:G:133:THR:HB	2.00	0.43
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.54	0.43
3:Q:201:VAL:HG21	3:Q:207:ASN:HB3	2.01	0.42
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.19	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
4:D:1:ASP:O	4:D:2:ARG:HB2	2.18	0.42
3:C:168:THR:O	3:C:171:GLU:HB3	2.19	0.42
12:Z:161:GLU:HB3	12:Z:164:THR:HG21	2.01	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.42
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.54	0.42
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.42
3:C:201:VAL:HG21	3:C:207:ASN:HB3	2.01	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
8:V:84:LYS:HG3	8:V:85:GLN:N	2.35	0.42
5:S:155:LEU:CD2	6:T:55:LEU:HD23	2.50	0.42
7:U:25:ALA:O	7:U:28:GLN:HB2	2.20	0.42
5:E:155:LEU:CD2	6:F:55:LEU:HD23	2.50	0.42
7:G:73:VAL:CG1	7:G:133:THR:HB	2.50	0.42
7:G:25:ALA:O	7:G:28:GLN:HB2	2.19	0.42
13:M:48:ASN:H	13:M:48:ASN:HD22	1.65	0.42
2:P:58:GLN:NE2	2:P:208:ASP:HA	2.35	0.42
10:J:3:ILE:HB	10:J:18:SER:HB3	2.02	0.42
10:J:168:LEU:O	10:J:172:MET:HB2	2.20	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.41
10:X:3:ILE:HB	10:X:18:SER:HB3	2.01	0.41
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.51	0.41
12:Z:134:GLU:OE1	12:Z:137:ARG:NH2	2.53	0.41
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.50	0.41
3:C:51:LYS:HA	3:C:51:LYS:HE3	2.02	0.41
7:U:73:VAL:CG1	7:U:133:THR:HB	2.50	0.41
3:C:38:ASN:N	3:C:38:ASN:HD22	2.18	0.41
3:C:9:PHE:H	4:D:15:GLN:HE22	1.69	0.41
3:C:198:LEU:HA	3:C:201:VAL:HG12	2.03	0.41
10:X:168:LEU:O	10:X:172:MET:HB2	2.20	0.41
1:A:2:THR:HG22	1:A:3:ASP:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.41
8:H:52:THR:O	8:H:56:THR:HB	2.20	0.41
2:P:3:ARG:NH1	5:S:122:TYR:OH	2.54	0.41
7:G:83:ASN:C	7:G:83:ASN:HD22	2.24	0.41
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.31	0.41
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.03	0.41
12:L:134:GLU:OE1	12:L:137:ARG:NH2	2.52	0.41
2:B:58:GLN:NE2	2:B:208:ASP:HA	2.35	0.41
11:K:6:PHE:HA	11:K:125:ASP:O	2.20	0.41
10:J:7:ILE:HD12	10:J:161:LEU:HD13	2.03	0.41
8:H:104:ASP:OD1	8:H:106:THR:HB	2.20	0.41
4:R:1:ASP:HB3	4:R:2:ARG:H	1.72	0.41
17:T:301:HOH:O	7:U:82:ARG:HD2	2.21	0.41
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	2.02	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.41
11:K:25:TRP:CH2	12:L:144:SER:HA	2.56	0.41
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.69	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
10:X:7:ILE:HD12	10:X:161:LEU:HD13	2.03	0.40
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.03	0.40
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.04	0.40
11:Y:35:ILE:HB	11:Y:45:MET:HE3	2.02	0.40
9:I:65:MET:O	9:I:68:TYR:HB3	2.22	0.40
9:W:65:MET:O	9:W:68:TYR:HB3	2.21	0.40
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.33	0.40
12:Z:161:GLU:HB3	12:Z:164:THR:CG2	2.51	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	0.40
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.18	0.40
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.04	0.40
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.51	0.40
8:H:84:LYS:HG3	8:H:85:GLN:N	2.35	0.40
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.51	0.40
3:Q:51:LYS:HA	3:Q:51:LYS:HE3	2.02	0.40
7:G:83:ASN:ND2	7:G:83:ASN:C	2.75	0.40
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.04	0.40
11:K:201:LYS:HE2	11:K:212:GLY:HA2	2.04	0.40
12:L:195:HIS:HD2	12:L:197:GLN:H	1.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:LYS:NZ	2:P:200:THR:O[2_555]	2.18	0.02

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	69
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	69
2	B	242/258 (94%)	231 (96%)	8 (3%)	3 (1%)	16	39
2	P	242/258 (94%)	231 (96%)	8 (3%)	3 (1%)	16	39
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%)	226 (98%)	4 (2%)	1 (0%)	39	69
4	R	231/260 (89%)	226 (98%)	4 (2%)	1 (0%)	39	69
5	E	229/234 (98%)	215 (94%)	14 (6%)	0	100	100
5	S	229/234 (98%)	215 (94%)	14 (6%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
7	U	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
8	H	220/232 (95%)	211 (96%)	8 (4%)	1 (0%)	34	63
8	V	220/232 (95%)	212 (96%)	7 (3%)	1 (0%)	34	63
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	34	63
10	X	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	34	63
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6276/6614 (95%)	6064 (97%)	188 (3%)	24 (0%)	39	69

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
3	Q	202	GLN
2	B	219	ALA
3	C	205	ALA
4	D	2	ARG
2	P	219	ALA
3	Q	205	ALA
4	R	2	ARG
10	J	2	ASP
10	X	2	ASP
2	B	221	ASP
2	P	221	ASP
3	C	239	GLN
3	Q	239	GLN
8	V	9	ASN
3	C	201	VAL
8	H	9	ASN
3	Q	201	VAL
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%)	201 (96%)	8 (4%)	40	71
1	O	209/209 (100%)	202 (97%)	7 (3%)	45	76
2	B	203/216 (94%)	189 (93%)	14 (7%)	19	43
2	P	203/216 (94%)	188 (93%)	15 (7%)	17	39
3	C	212/226 (94%)	194 (92%)	18 (8%)	13	30
3	Q	212/226 (94%)	194 (92%)	18 (8%)	13	30
4	D	194/215 (90%)	176 (91%)	18 (9%)	11	25
4	R	194/215 (90%)	176 (91%)	18 (9%)	11	25
5	E	190/193 (98%)	170 (90%)	20 (10%)	8	19
5	S	190/193 (98%)	170 (90%)	20 (10%)	8	19
6	F	201/239 (84%)	189 (94%)	12 (6%)	24	50
6	T	201/239 (84%)	188 (94%)	13 (6%)	21	46
7	G	206/210 (98%)	189 (92%)	17 (8%)	14	31
7	U	206/210 (98%)	190 (92%)	16 (8%)	16	35
8	H	181/190 (95%)	175 (97%)	6 (3%)	45	76
8	V	181/190 (95%)	175 (97%)	6 (3%)	45	76
9	I	172/173 (99%)	165 (96%)	7 (4%)	37	69
9	W	172/173 (99%)	165 (96%)	7 (4%)	37	69
10	J	173/175 (99%)	165 (95%)	8 (5%)	33	64
10	X	173/175 (99%)	165 (95%)	8 (5%)	33	64
11	K	169/169 (100%)	161 (95%)	8 (5%)	32	63
11	Y	169/169 (100%)	161 (95%)	8 (5%)	32	63
12	L	185/185 (100%)	176 (95%)	9 (5%)	31	61
12	Z	185/185 (100%)	176 (95%)	9 (5%)	31	61
13	M	199/208 (96%)	188 (94%)	11 (6%)	27	55
13	a	199/208 (96%)	188 (94%)	11 (6%)	27	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	153 (94%)	9 (6%)	26	54
14	b	162/162 (100%)	153 (94%)	9 (6%)	26	54
All	All	5312/5540 (96%)	4982 (94%)	330 (6%)	23	49

All (330) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	29	LYS
1	A	50	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	231	LYS
2	B	50	LYS
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	65	LEU
2	B	79	LEU
2	B	114	LEU
2	B	119	GLN
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	197	SER
2	B	209	ARG
2	B	239	VAL
3	C	4	ARG
3	C	37	LYS
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	51	LYS
3	C	58	THR
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL

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Mol	Chain	Res	Type
3	C	175	LYS
3	C	180	LYS
3	C	185	THR
3	C	187	GLU
3	C	213	VAL
3	C	239	GLN
4	D	1	ASP
4	D	6	THR
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	78	ARG
4	D	99	ILE
4	D	102	GLU
4	D	117	GLU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	197	LYS
4	D	214	ILE
4	D	224	ASP
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	54	GLU
5	E	55	LEU
5	E	60	LYS
5	E	71	LEU
5	E	87	LEU
5	E	99	ASN
5	E	116	GLN
5	E	144	LEU
5	E	168	LYS
5	E	184	ASN
5	E	186	ASP
5	E	207	VAL
5	E	208	ASP

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Mol	Chain	Res	Type
5	E	222	THR
5	E	231	LYS
6	F	14	ASP
6	F	52	SER
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	34	LEU
7	G	53	LYS
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	178	LYS
7	G	181	LYS
7	G	201	MET
7	G	207	THR
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
9	I	37	ASN
9	I	92	SER
9	I	123	PHE
9	I	126	ILE
9	I	133	LYS

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Mol	Chain	Res	Type
9	I	171	LEU
9	I	182	TRP
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	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	41	LEU
11	K	57	THR
11	K	106	ARG
11	K	118	ASP
11	K	148	LEU
12	L	1	GLN
12	L	3	ASN
12	L	11	THR
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
12	L	214	LYS
13	M	10	SER
13	M	37	ASN
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	204	THR
13	M	215	GLU
14	N	9	LYS
14	N	20	THR
14	N	36	ARG
14	N	48	SER

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Mol	Chain	Res	Type
14	N	104	ASP
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	17	LYS
1	O	29	LYS
1	O	50	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	65	LEU
2	P	79	LEU
2	P	114	LEU
2	P	119	GLN
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	197	SER
2	P	209	ARG
2	P	239	VAL
3	Q	4	ARG
3	Q	37	LYS
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	51	LYS
3	Q	58	THR
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	167	LYS
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	185	THR

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Mol	Chain	Res	Type
3	Q	187	GLU
3	Q	213	VAL
3	Q	239	GLN
4	R	1	ASP
4	R	6	THR
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	54	ASP
4	R	78	ARG
4	R	99	ILE
4	R	102	GLU
4	R	117	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	197	LYS
4	R	214	ILE
4	R	224	ASP
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
5	S	54	GLU
5	S	55	LEU
5	S	60	LYS
5	S	71	LEU
5	S	87	LEU
5	S	99	ASN
5	S	116	GLN
5	S	144	LEU
5	S	168	LYS
5	S	184	ASN
5	S	186	ASP
5	S	207	VAL
5	S	208	ASP
5	S	222	THR
5	S	231	LYS
6	T	14	ASP

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Mol	Chain	Res	Type
6	T	52	SER
6	T	59	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	202	ASP
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	24	LYS
7	U	26	THR
7	U	28	GLN
7	U	34	LEU
7	U	53	LYS
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	178	LYS
7	U	181	LYS
7	U	201	MET
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
9	W	37	ASN
9	W	92	SER
9	W	123	PHE
9	W	126	ILE
9	W	133	LYS
9	W	171	LEU
9	W	182	TRP
10	X	2	ASP

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Mol	Chain	Res	Type
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	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	41	LEU
11	Y	57	THR
11	Y	106	ARG
11	Y	118	ASP
11	Y	148	LEU
12	Z	1	GLN
12	Z	3	ASN
12	Z	11	THR
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	214	LYS
13	a	10	SER
13	a	37	ASN
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	204	THR
13	a	215	GLU
14	b	9	LYS
14	b	20	THR
14	b	36	ARG
14	b	48	SER
14	b	104	ASP
14	b	115	LEU
14	b	119	VAL

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Mol	Chain	Res	Type
14	b	144	GLU
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) 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	102	ASN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	38	ASN
3	C	77	ASN
3	C	92	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	59	GLN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	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

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Mol	Chain	Res	Type
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
8	H	57	GLN
8	H	66	HIS
8	H	165	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	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	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	119	GLN
2	P	123	GLN
2	P	155	ASN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN

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Mol	Chain	Res	Type
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	57	GLN
8	V	66	HIS
8	V	165	ASN
9	W	31	GLN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
10	X	118	GLN
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	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	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 10 ligands modelled in this entry, 8 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	$\# Z  > 2$
16	2LV	K	301	11	44,44,44	1.03	2 (4%)	57,58,58	1.09	4 (7%)
16	2LV	Y	301	11	44,44,44	1.02	2 (4%)	57,58,58	1.13	5 (8%)

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
16	2LV	K	301	11	-	0/49/49/49	0/2/2/2
16	2LV	Y	301	11	-	0/49/49/49	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	2LV	C5-C4	-4.41	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	2LV	C5-C4	-4.34	1.40	1.50
16	K	301	2LV	C35-N34	-3.79	1.34	1.41
16	Y	301	2LV	C35-N34	-3.61	1.34	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	301	2LV	C35-N34-C32	-3.53	121.06	127.40
16	Y	301	2LV	C35-N34-C32	-3.25	121.55	127.40
16	Y	301	2LV	O8-C7-N9	-2.66	120.22	124.86
16	K	301	2LV	O8-C7-N9	-2.60	120.32	124.86
16	Y	301	2LV	C27-C26-C25	-2.57	109.83	115.51
16	K	301	2LV	C27-C26-C25	-2.43	110.14	115.51
16	Y	301	2LV	O6-C7-O8	-2.03	120.04	124.22
16	K	301	2LV	O6-C7-N9	3.91	119.21	110.54
16	Y	301	2LV	O6-C7-N9	4.14	119.73	110.54

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%)	-0.34	7 (2%) 56 57	35, 50, 87, 127	0
1	O	250/250 (100%)	-0.28	9 (3%) 46 46	38, 56, 95, 122	0
2	B	244/258 (94%)	-0.12	14 (5%) 27 26	37, 58, 104, 162	0
2	P	244/258 (94%)	-0.14	12 (4%) 33 32	39, 57, 106, 164	0
3	C	240/254 (94%)	-0.09	13 (5%) 29 28	33, 58, 113, 142	0
3	Q	240/254 (94%)	0.14	19 (7%) 15 13	40, 69, 136, 148	0
4	D	235/260 (90%)	-0.33	2 (0%) 85 86	34, 57, 86, 128	0
4	R	235/260 (90%)	-0.28	6 (2%) 59 59	41, 63, 94, 125	0
5	E	231/234 (98%)	-0.28	3 (1%) 79 79	36, 62, 91, 135	0
5	S	231/234 (98%)	-0.11	6 (2%) 59 59	41, 68, 101, 130	0
6	F	243/288 (84%)	-0.36	5 (2%) 67 68	34, 57, 94, 142	0
6	T	243/288 (84%)	-0.24	8 (3%) 50 50	40, 62, 103, 124	0
7	G	241/252 (95%)	-0.38	3 (1%) 81 81	29, 52, 84, 122	0
7	U	241/252 (95%)	-0.33	3 (1%) 81 81	34, 54, 86, 115	0
8	H	222/232 (95%)	-0.37	4 (1%) 71 72	34, 50, 75, 134	0
8	V	222/232 (95%)	-0.33	2 (0%) 85 86	38, 52, 79, 141	0
9	I	204/205 (99%)	-0.50	3 (1%) 76 76	31, 49, 81, 119	0
9	W	204/205 (99%)	-0.49	4 (1%) 68 69	32, 49, 85, 117	0
10	J	195/198 (98%)	-0.47	2 (1%) 84 85	32, 49, 75, 122	0
10	X	195/198 (98%)	-0.46	2 (1%) 84 85	35, 50, 73, 133	0
11	K	212/212 (100%)	-0.48	1 (0%) 91 93	33, 48, 74, 97	0
11	Y	212/212 (100%)	-0.48	1 (0%) 91 93	35, 51, 79, 103	0
12	L	222/222 (100%)	-0.52	0 100 100	32, 50, 74, 94	0
12	Z	222/222 (100%)	-0.46	1 (0%) 91 93	31, 52, 78, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.49	2 (0%) 85 86	32, 50, 71, 97	0
13	a	233/246 (94%)	-0.51	1 (0%) 93 94	34, 48, 68, 80	0
14	N	196/196 (100%)	-0.54	1 (0%) 91 93	27, 45, 69, 97	0
14	b	196/196 (100%)	-0.53	2 (1%) 84 85	29, 47, 73, 103	0
All	All	6336/6614 (95%)	-0.34	136 (2%) 67 68	27, 54, 93, 164	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	10.3
8	V	222	ASP	8.9
2	B	220	ASN	7.6
2	B	218	GLY	7.1
8	V	221	CYS	6.9
2	B	219	ALA	6.9
3	C	206	LYS	6.9
2	P	220	ASN	6.7
3	Q	240	GLU	5.8
3	Q	49	THR	5.8
2	P	218	GLY	5.6
5	S	202	ASP	5.6
2	B	221	ASP	5.6
2	P	59	ASP	5.1
8	H	222	ASP	5.0
3	Q	238	LYS	4.9
2	B	51	VAL	4.8
9	W	1	SER	4.8
3	Q	50	LEU	4.8
6	F	202	ASP	4.5
1	A	1	MET	4.5
8	H	221	CYS	4.5
1	A	2	THR	4.4
2	B	222	GLY	4.4
3	C	238	LYS	4.4
3	Q	206	LYS	4.4
2	P	221	ASP	4.3
3	Q	203	THR	4.0
7	U	2	GLY	4.0
1	O	249	ALA	3.9
3	Q	239	GLN	3.8
3	Q	48	SER	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	49	THR	3.7
7	U	242	GLN	3.7
3	Q	236	GLN	3.7
2	P	51	VAL	3.6
3	C	202	GLN	3.6
2	P	222	GLY	3.6
10	X	194	ASP	3.6
1	O	52	SER	3.6
5	E	202	ASP	3.5
3	C	240	GLU	3.4
1	O	1	MET	3.4
13	M	47	ASP	3.4
3	C	239	GLN	3.4
9	I	1	SER	3.3
4	D	242	GLU	3.2
4	R	125	LEU	3.2
6	T	243	ILE	3.2
3	Q	202	GLN	3.1
5	S	54	GLU	3.1
1	O	248	GLU	3.1
9	I	131	GLU	3.1
6	F	205	GLU	3.0
2	B	50	LYS	3.0
2	P	203	SER	2.9
7	G	242	GLN	2.9
6	T	230	ASP	2.9
9	W	133	LYS	2.9
7	U	241	GLU	2.8
2	B	182	ASP	2.8
14	b	195	GLN	2.8
6	T	2	THR	2.8
3	C	50	LEU	2.8
2	B	242	GLY	2.8
6	T	244	ASN	2.7
14	b	105	LYS	2.7
5	E	201	ARG	2.7
5	S	173	ARG	2.7
10	J	194	ASP	2.7
1	O	201	GLU	2.6
9	W	131	GLU	2.6
6	F	181	GLU	2.6
1	O	2	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	248	GLU	2.6
1	A	250	LEU	2.5
13	a	1	THR	2.5
2	P	50	LYS	2.5
3	C	175	LYS	2.5
4	R	241	ALA	2.5
8	H	198	GLU	2.5
5	S	225	ASP	2.5
4	R	203	LYS	2.4
11	Y	106	ARG	2.4
3	Q	1	GLY	2.4
3	Q	180	LYS	2.4
1	A	249	ALA	2.4
3	C	203	THR	2.4
4	R	1	ASP	2.3
1	O	250	LEU	2.3
6	T	205	GLU	2.3
1	O	50	LYS	2.3
10	X	1	MET	2.3
5	E	218	ASP	2.3
11	K	212	GLY	2.3
2	B	223	GLU	2.3
4	R	2	ARG	2.3
6	T	178	HIS	2.3
2	P	242	GLY	2.3
6	T	166	GLN	2.3
8	H	22	GLN	2.3
6	F	243	ILE	2.2
3	Q	187	GLU	2.2
1	A	203	GLU	2.2
4	R	242	GLU	2.2
2	B	59	ASP	2.2
12	Z	210	ASP	2.2
3	C	181	GLU	2.2
3	C	216	ASP	2.2
9	I	130	ASP	2.2
13	M	1	THR	2.2
10	J	1	MET	2.2
3	C	187	GLU	2.2
3	C	225	GLU	2.2
3	Q	237	GLU	2.1
2	P	182	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	S	201	ARG	2.1
3	Q	51	LYS	2.1
1	A	229	THR	2.1
5	S	165	GLN	2.1
3	Q	175	LYS	2.1
3	Q	225	GLU	2.1
4	D	1	ASP	2.0
2	B	203	SER	2.0
6	F	2	THR	2.0
7	G	188	GLU	2.0
7	G	3	TYR	2.0
2	B	244	THR	2.0
9	W	128	CYS	2.0
3	Q	181	GLU	2.0
3	Q	141	ASP	2.0
6	T	180	PRO	2.0
2	B	169	SER	2.0
14	N	181	ALA	2.0
1	O	229	THR	2.0
2	P	244	THR	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	MG	I	301	1/1	0.97	0.30	4.98	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	N	201	1/1	0.91	0.17	3.56	63,63,63,63	0
16	2LV	Y	301	43/43	0.82	0.25	2.88	70,101,114,117	0
16	2LV	K	301	43/43	0.86	0.24	2.74	66,98,117,130	0
15	MG	G	301	1/1	0.91	0.15	0.26	59,59,59,59	0
15	MG	Z	301	1/1	0.98	0.11	-0.87	58,58,58,58	0
15	MG	Y	302	1/1	0.98	0.09	-1.18	55,55,55,55	0
15	MG	K	302	1/1	0.94	0.08	-1.35	58,58,58,58	0
15	MG	V	301	1/1	0.96	0.05	-3.17	59,59,59,59	0
15	MG	H	301	1/1	0.95	0.14	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.