



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2016 – 11:37 PM EDT

PDB ID : 5LEX  
Title : Native human 20S proteasome in Mg-Acetate at 2.2 Angstrom  
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.  
Deposited on : 2016-06-30  
Resolution : 2.20 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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-20027939

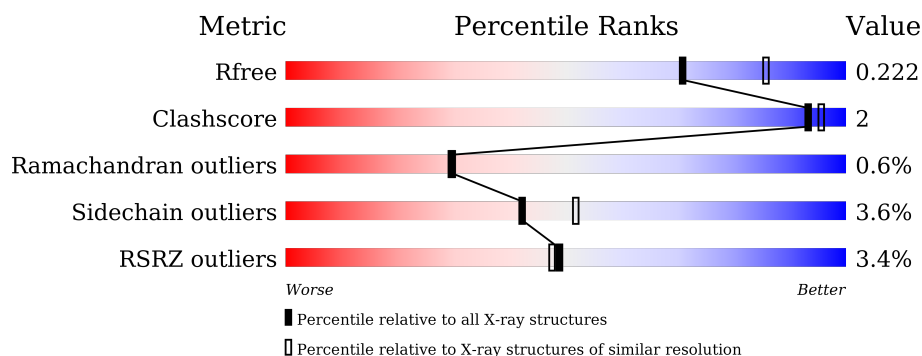
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



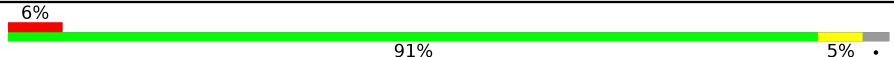
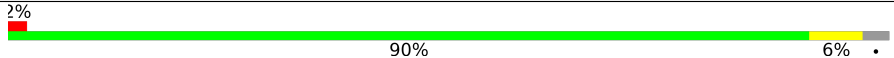




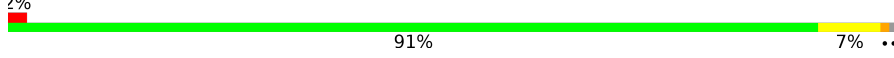
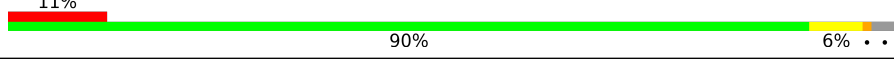
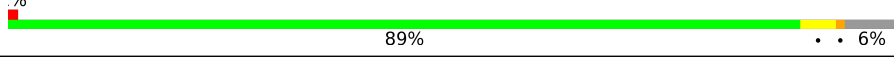
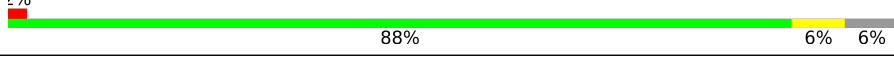
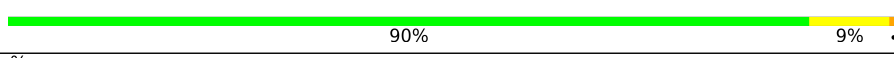
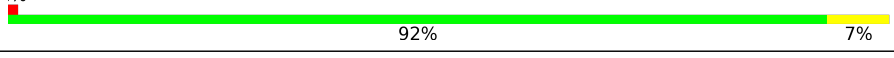
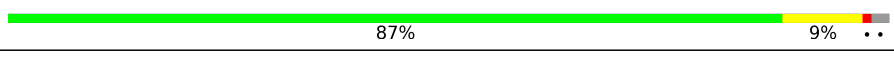
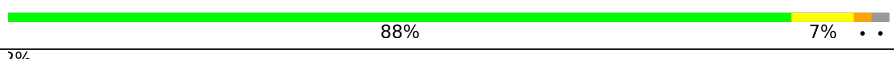
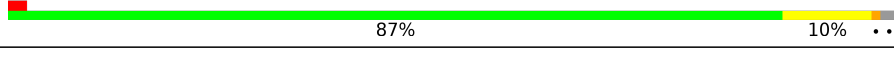
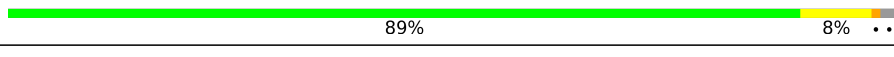
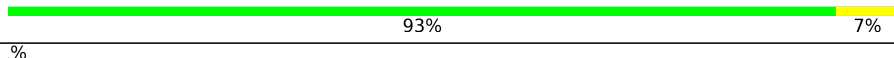
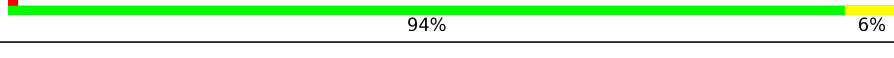
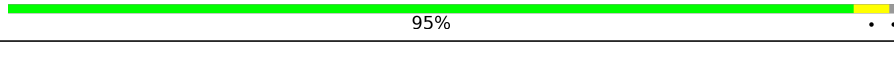
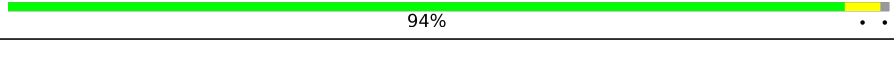
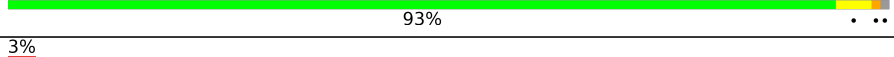
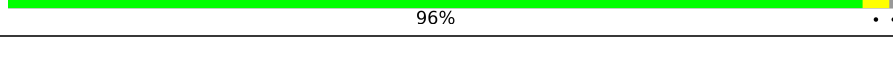
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	234	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	O	234	<div> <div>8%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</div> </div> </div>
2	B	261	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
2	P	261	<div> <div>11%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>5%</div> </div> </div>
3	C	248	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>..</div> </div> </div>
3	Q	248	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	205	
14	b	205	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	1PE	H	302	-	-	-	X
17	1PE	I	302	-	-	-	X
17	1PE	K	302	-	-	-	X
17	1PE	L	301	-	-	-	X
17	1PE	W	302	-	-	-	X
17	1PE	Z	301	-	-	-	X
17	1PE	a	301	-	-	-	X
7	6V1	U	47	X	-	-	-

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 51579 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	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1922	1217	331	363	11			
2	P	247	Total	C	N	O	S	0	2	0
			1898	1200	321	366	11			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	2	0
			1797	1120	320	352	5			
3	Q	234	Total	C	N	O	S	0	0	0
			1796	1123	315	353	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	1	0
			1822	1144	325	342	11			
5	S	236	Total	C	N	O	S	0	3	0
			1853	1160	335	347	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	148	6V1	CYS	conflict	UNP P25786
S	148	6V1	CYS	conflict	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	239	Total	C	N	O	S	0	4	0
			1888	1198	325	353	12			
6	T	240	Total	C	N	O	S	0	1	0
			1856	1178	315	351	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	2	0
			1912	1214	321	364	13			
7	U	238	Total	C	N	O	S	0	1	0
			1815	1147	304	350	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	47	6V1	CYS	conflict	UNP P60900
G	161	6V1	CYS	conflict	UNP P60900
U	47	6V1	CYS	conflict	UNP P60900
U	161	6V1	CYS	conflict	UNP P60900

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	2	0
			1664	1047	284	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1622	1023	269	318	12			

- 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	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			
10	X	196	Total	C	N	O	S	0	2	0
			1576	1012	267	287	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	91	6V1	CYS	conflict	UNP P49721
X	91	6V1	CYS	conflict	UNP P49721

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	0	0
			1551	977	272	293	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1570	991	278	291	10			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1636	1038	277	310	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1642	1041	280	310	11			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- Molecule 15 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	K	0	0
			1	1		
15	b	1	Total	K	0	0
			1	1		
15	Z	1	Total	K	0	0
			1	1		
15	N	1	Total	K	0	0
			1	1		
15	U	1	Total	K	0	0
			1	1		
15	L	1	Total	K	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	H	1	Total	Mg	0	0
			1	1		
16	I	2	Total	Mg	0	0
			2	2		
16	V	1	Total	Mg	0	0
			1	1		
16	W	1	Total	Mg	0	0
			1	1		

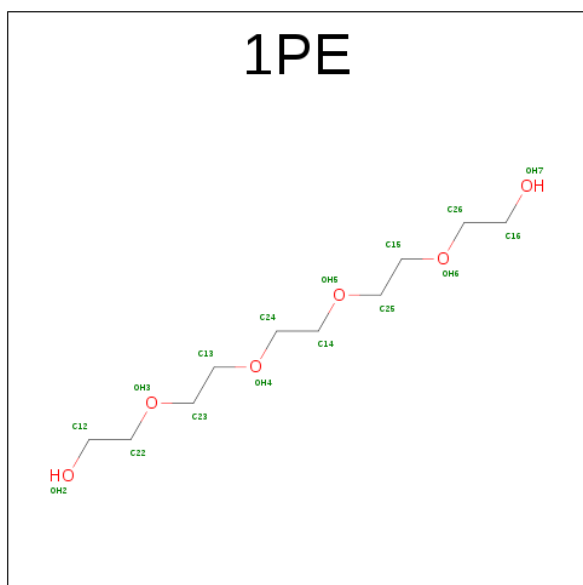
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	X	1	Total	Mg	0	0
			1	1		
16	L	1	Total	Mg	0	0
			1	1		

- Molecule 17 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	H	1	Total	C	O	0	0
			16	10	6		
17	I	1	Total	C	O	0	0
			16	10	6		
17	K	1	Total	C	O	0	0
			16	10	6		
17	L	1	Total	C	O	0	0
			16	10	6		
17	N	1	Total	C	O	0	0
			16	10	6		
17	W	1	Total	C	O	0	0
			16	10	6		
17	Z	1	Total	C	O	0	0
			16	10	6		
17	a	1	Total	C	O	0	0
			16	10	6		
17	b	1	Total	C	O	0	0
			16	10	6		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	106	Total O 106 106	0	0
18	B	126	Total O 126 126	0	0
18	C	59	Total O 59 59	0	0
18	D	80	Total O 80 80	0	0
18	E	128	Total O 128 128	0	0
18	F	175	Total O 175 175	0	0
18	G	165	Total O 165 165	0	0
18	H	151	Total O 151 151	0	0
18	I	145	Total O 145 145	0	0
18	J	122	Total O 122 122	0	0
18	K	96	Total O 96 96	0	0
18	L	115	Total O 115 115	0	0
18	M	143	Total O 143 143	0	0
18	N	160	Total O 160 160	0	0
18	O	78	Total O 78 78	0	0
18	P	104	Total O 104 104	0	0
18	Q	62	Total O 62 62	0	0
18	R	112	Total O 112 112	0	0
18	S	114	Total O 114 114	0	0
18	T	83	Total O 83 83	0	0
18	U	90	Total O 90 90	0	0

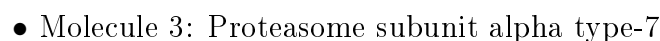
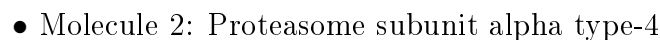
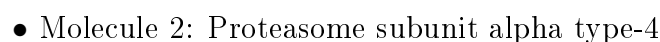
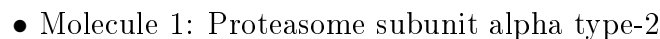
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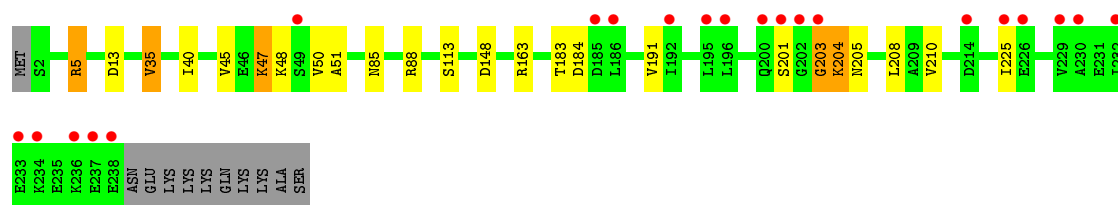
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	V	102	Total 102	O 102	0	0
18	W	101	Total 101	O 101	0	0
18	X	110	Total 110	O 110	0	0
18	Y	140	Total 140	O 140	0	0
18	Z	169	Total 169	O 169	0	0
18	a	173	Total 173	O 173	0	0
18	b	122	Total 122	O 122	0	0

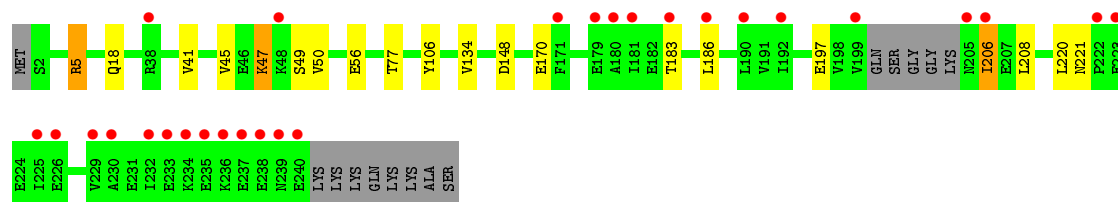
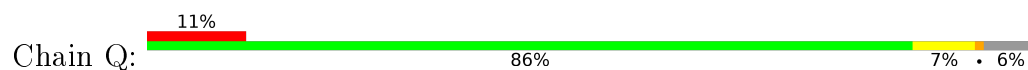


- Molecule 1: Proteasome subunit alpha type-2

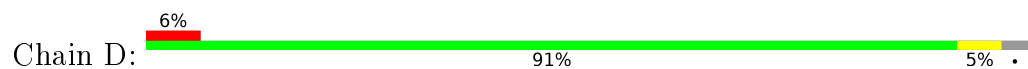




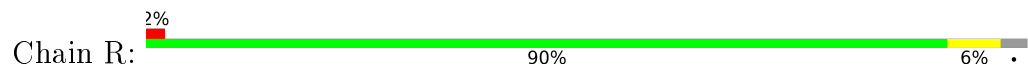
• Molecule 3: Proteasome subunit alpha type-7



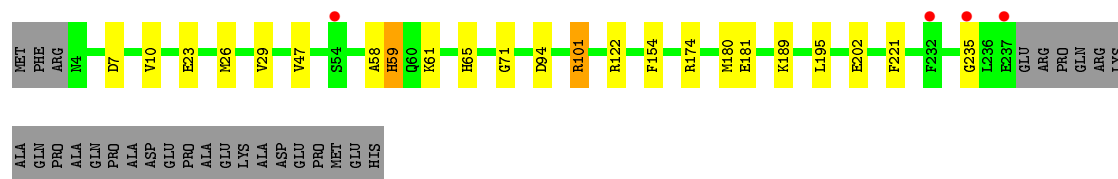
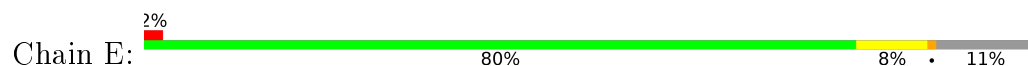
• Molecule 4: Proteasome subunit alpha type-5



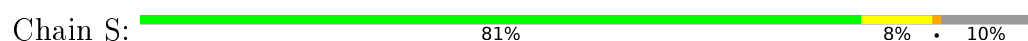
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 5: Proteasome subunit alpha type-1




• Molecule 5: Proteasome subunit alpha type-1



PRO  
ALA  
ASP  
GLU  
PRO  
ALA  
GLU  
LYS  
ALA  
ASP  
GLU  
PRO  
MET  
GLU  
HIS


• Molecule 6: Proteasome subunit alpha type-3

Chain F:  82% 11% • 6%

MET SER SER ILE GLY THR G6 D17 E31 S34 S62 N63 K64 R65 G74 L81 S86 L87 M117 F131 D152 V156 A168 R169 R187 V190 V200 D206 W215 L219 H224 V227 R232 K237 K240 E241 S242

L243 K244 GLU ASP GLU SER ASP ASP ASN MET

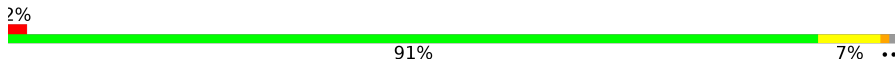
• Molecule 6: Proteasome subunit alpha type-3

Chain T:  4% 80% 13% • 6%

MET SER SER ILE GLY T5 G6 Y7 D17 E31 S34 D43 S62 N63 K64 R65 G74 L81 A82 D83 S86 L87 R99 M117 F131 F135 S139 I151 D152 V156 A168 R169 K173 Q180 V190 V200 H201 D202 E203 V204

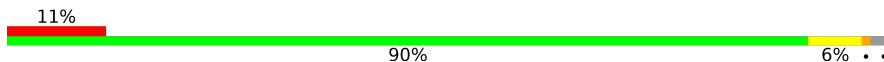
K205 D206 K207 A208 F209 E210 W215 V216 H224 K237 K240 S242 L243 K244 GLU ASP GLU SER ASP ASP ASN MET

• Molecule 7: Proteasome subunit alpha type-6

Chain G:  2% 91% 7% ••

MET S2 R11 V42 R43 I72 C78 D86 S87 R88 R95 E108 L114 R117 L140 I141 E145 V151 T173 V183 K184 K185 K186 F187 D188 W189 L206 E244 R245 ASP


• Molecule 7: Proteasome subunit alpha type-6

Chain U:  11% 90% 6% ••

MET S2 R3 A7 V42 R43 V51 P57 D68 K59 I72 C78 V79 M80 V91 L114 R117 L140 S177 F178 L179 V183 K186 PHE ASP TRP PHE GLU Q193 T194 V195 A198 I199 T200 C201 L202 S203 T204 V205 L206 S207 I208 D209 F210 K211

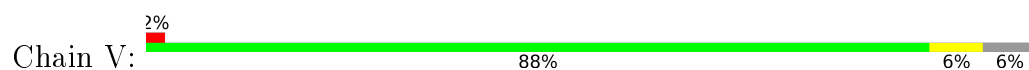
P212 E223 I235 L239 A241 L242 A243 E244 R245 ASP

• Molecule 8: Proteasome subunit beta type-7

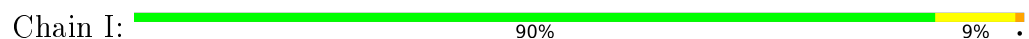
Chain H:  89% •• 6%

T1 V6 E22 L65 L68 R72 R75 R89 L132 L183 T197 R201 C204 T208 L219 E220 ILE GLU VAL LEU GLU THR VAL GLN THR MET ASP THR SER

• Molecule 8: Proteasome subunit beta type-7



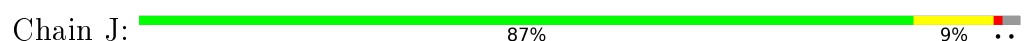
- Molecule 9: Proteasome subunit beta type-3



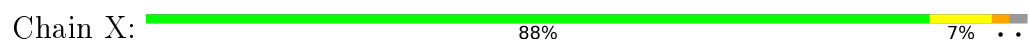
- Molecule 9: Proteasome subunit beta type-3



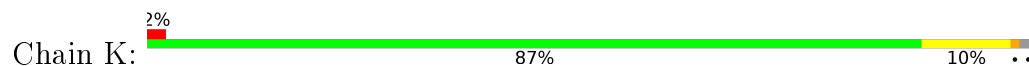
- Molecule 10: Proteasome subunit beta type-2



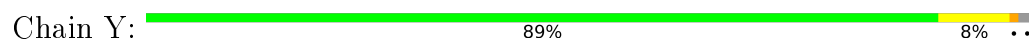
- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



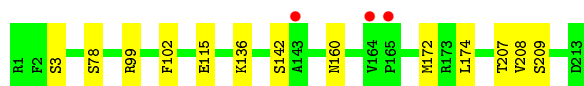
- Molecule 12: Proteasome subunit beta type-1

Chain L:  93% 7%



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  94% 6%



- Molecule 13: Proteasome subunit beta type-4

Chain M:  95%



- Molecule 13: Proteasome subunit beta type-4

Chain a:  94%



- Molecule 14: Proteasome subunit beta type-6

Chain N:  93%



- Molecule 14: Proteasome subunit beta type-6

Chain b:  96% 3%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.86Å 203.15Å 316.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.89 – 2.20 49.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (170.89-2.20) 98.8 (49.06-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.177 , 0.221 0.180 , 0.222	Depositor DCC
$R_{free}$ test set	18235 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	51579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YCM, MG, K, 6V1, 1PE

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	0.75	0/1833	0.83	2/2489 (0.1%)
1	O	0.64	0/1778	0.80	3/2419 (0.1%)
2	B	0.75	0/1958	0.87	3/2645 (0.1%)
2	P	0.71	1/1934 (0.1%)	0.89	4/2617 (0.2%)
3	C	0.77	1/1817 (0.1%)	0.92	6/2467 (0.2%)
3	Q	0.74	0/1809	0.90	2/2455 (0.1%)
4	D	0.77	1/1789 (0.1%)	0.87	3/2424 (0.1%)
4	R	0.87	1/1780 (0.1%)	0.93	2/2408 (0.1%)
5	E	0.79	0/1842	0.89	6/2493 (0.2%)
5	S	0.79	1/1878 (0.1%)	0.93	5/2541 (0.2%)
6	F	0.86	0/1935	0.94	2/2605 (0.1%)
6	T	0.85	2/1894 (0.1%)	0.95	8/2556 (0.3%)
7	G	0.87	4/1909 (0.2%)	0.89	9/2579 (0.3%)
7	U	0.73	0/1804	0.83	4/2441 (0.2%)
8	H	0.89	1/1697 (0.1%)	1.00	5/2299 (0.2%)
8	V	0.72	0/1655	0.89	2/2251 (0.1%)
9	I	0.82	2/1648 (0.1%)	1.00	10/2219 (0.5%)
9	W	0.64	0/1630	0.89	4/2197 (0.2%)
10	J	0.79	0/1613	0.95	5/2180 (0.2%)
10	X	0.71	0/1599	0.93	5/2163 (0.2%)
11	K	0.74	0/1582	0.95	7/2138 (0.3%)
11	Y	0.87	0/1610	1.01	8/2172 (0.4%)
12	L	0.75	0/1672	0.87	3/2257 (0.1%)
12	Z	0.93	4/1675 (0.2%)	0.93	3/2257 (0.1%)
13	M	0.84	0/1728	0.95	4/2339 (0.2%)
13	a	0.93	0/1724	0.98	6/2336 (0.3%)
14	N	0.93	2/1548 (0.1%)	0.90	3/2095 (0.1%)
14	b	0.85	0/1554	0.90	2/2104 (0.1%)
All	All	0.80	20/48895 (0.0%)	0.91	126/66146 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	2
3	Q	0	2
4	D	0	2
4	R	0	1
5	E	0	1
6	F	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
13	a	0	1
All	All	1	16

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	9.95	1.36	1.25
12	Z	78	SER	CB-OG	-7.27	1.32	1.42
12	Z	3	SER	CB-OG	7.13	1.51	1.42
3	C	113	SER	CB-OG	-6.78	1.33	1.42
4	R	25	GLU	CD-OE1	6.50	1.32	1.25
5	S	7	ASP	CB-CG	-6.28	1.38	1.51
6	T	7	TYR	N-CA	6.27	1.58	1.46
9	I	77	GLU	CD-OE1	6.17	1.32	1.25
14	N	150	GLU	CG-CD	5.82	1.60	1.51
12	Z	142	SER	CB-OG	-5.77	1.34	1.42
7	G	189	TRP	CB-CG	5.77	1.60	1.50
7	G	108	GLU	CD-OE2	5.73	1.31	1.25
7	G	78	CYS	CB-SG	-5.63	1.72	1.81
14	N	24	SER	CB-OG	-5.44	1.35	1.42
9	I	105	GLU	CD-OE2	5.25	1.31	1.25
4	D	127	ASP	CB-CG	5.22	1.62	1.51
2	P	103	GLU	CD-OE2	5.18	1.31	1.25
12	Z	115	GLU	CD-OE2	5.16	1.31	1.25
6	T	210	GLU	CD-OE2	5.04	1.31	1.25
8	H	22	GLU	CD-OE1	5.01	1.31	1.25

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	72	ARG	NE-CZ-NH2	-11.14	114.73	120.30
10	J	86	ARG	NE-CZ-NH1	10.75	125.67	120.30
10	X	86	ARG	NE-CZ-NH1	10.29	125.44	120.30
10	J	86	ARG	NE-CZ-NH2	-10.14	115.23	120.30
10	X	86	ARG	NE-CZ-NH2	-9.82	115.39	120.30
4	R	120[A]	ALA	C-N-CA	9.69	145.93	121.70
4	R	120[B]	ALA	C-N-CA	9.69	145.93	121.70
12	Z	99	ARG	NE-CZ-NH2	-9.03	115.79	120.30
9	I	69	ARG	NE-CZ-NH1	8.87	124.74	120.30
9	W	16[A]	LYS	C-N-CA	8.80	143.69	121.70
9	W	16[B]	LYS	C-N-CA	8.80	143.69	121.70
9	I	16[A]	LYS	C-N-CA	8.44	142.79	121.70
9	I	16[B]	LYS	C-N-CA	8.44	142.79	121.70
2	B	96	ARG	NE-CZ-NH1	8.35	124.47	120.30
12	Z	99	ARG	NE-CZ-NH1	8.26	124.43	120.30
2	P	96	ARG	NE-CZ-NH1	8.11	124.35	120.30
11	Y	158	ARG	NE-CZ-NH2	-8.02	116.29	120.30
9	W	69	ARG	NE-CZ-NH1	7.97	124.29	120.30
5	S	122	ARG	NE-CZ-NH1	7.96	124.28	120.30
6	T	117	MET	CG-SD-CE	7.87	112.80	100.20
7	G	11	ARG	NE-CZ-NH1	7.85	124.22	120.30
11	Y	157	ARG	NE-CZ-NH2	-7.82	116.39	120.30
6	F	117	MET	CG-SD-CE	7.70	112.51	100.20
11	Y	157	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	219	ARG	NE-CZ-NH1	7.53	124.06	120.30
12	L	99	ARG	NE-CZ-NH1	7.49	124.05	120.30
8	H	72	ARG	NE-CZ-NH1	7.43	124.02	120.30
5	S	122	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	O	181	LEU	CA-CB-CG	7.20	131.86	115.30
3	Q	5	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	B	96	ARG	NE-CZ-NH2	-7.16	116.72	120.30
5	E	122	ARG	NE-CZ-NH2	-7.13	116.73	120.30
11	Y	158	ARG	NE-CZ-NH1	7.07	123.83	120.30
12	L	99	ARG	NE-CZ-NH2	-7.06	116.77	120.30
9	I	25[A]	ARG	NE-CZ-NH1	6.82	123.71	120.30
9	I	25[B]	ARG	NE-CZ-NH1	6.82	123.71	120.30
8	V	72	ARG	NE-CZ-NH1	6.81	123.71	120.30
11	K	42	LEU	CA-CB-CG	6.80	130.95	115.30
1	A	219	ARG	NE-CZ-NH2	-6.79	116.90	120.30
14	N	116	MET	CG-SD-CE	-6.78	89.35	100.20
7	U	117	ARG	NE-CZ-NH1	6.64	123.62	120.30
7	G	86	ASP	CB-CG-OD1	6.56	124.20	118.30
3	C	5	ARG	NE-CZ-NH2	-6.54	117.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	172	MET	CG-SD-CE	-6.50	89.81	100.20
13	M	99	ARG	NE-CZ-NH1	6.48	123.54	120.30
10	X	70	ARG	NE-CZ-NH2	-6.37	117.11	120.30
8	V	72	ARG	NE-CZ-NH2	-6.36	117.12	120.30
14	b	116	MET	CG-SD-CE	-6.31	90.10	100.20
7	G	117	ARG	NE-CZ-NH1	6.28	123.44	120.30
11	K	157	ARG	NE-CZ-NH1	6.23	123.42	120.30
13	a	166	ARG	NE-CZ-NH2	-6.15	117.22	120.30
6	F	190	VAL	CB-CA-C	-6.12	99.77	111.40
13	M	151	ARG	NE-CZ-NH1	6.09	123.35	120.30
5	E	7	ASP	CB-CG-OD1	-6.09	112.82	118.30
11	K	157	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	Q	5	ARG	NE-CZ-NH1	6.04	123.32	120.30
5	S	7	ASP	CB-CG-OD1	-6.03	112.87	118.30
6	T	43	ASP	CB-CG-OD2	6.03	123.73	118.30
2	B	4	ARG	NE-CZ-NH1	6.03	123.31	120.30
13	a	79	ASP	CB-CG-OD1	6.00	123.70	118.30
5	E	122	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	P	4	ARG	NE-CZ-NH1	5.99	123.29	120.30
11	K	107	ARG	NE-CZ-NH1	5.96	123.28	120.30
11	K	120	ARG	NE-CZ-NH1	5.92	123.26	120.30
12	L	172	MET	CG-SD-CE	-5.91	90.74	100.20
7	U	117	ARG	NE-CZ-NH2	-5.91	117.34	120.30
4	D	127	ASP	CB-CG-OD1	5.86	123.57	118.30
4	D	175[A]	GLU	N-CA-C	-5.83	95.25	111.00
4	D	175[B]	GLU	N-CA-C	-5.83	95.25	111.00
1	O	219	ARG	NE-CZ-NH1	5.80	123.20	120.30
8	H	75	ARG	NE-CZ-NH2	-5.77	117.41	120.30
2	P	3	ARG	NE-CZ-NH1	5.77	123.19	120.30
7	G	117	ARG	NE-CZ-NH2	-5.74	117.43	120.30
13	a	100	ARG	NE-CZ-NH2	-5.72	117.44	120.30
14	N	45	ARG	NE-CZ-NH1	5.72	123.16	120.30
14	N	144	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	P	96	ARG	NE-CZ-NH2	-5.67	117.46	120.30
11	Y	61	ARG	NE-CZ-NH1	5.67	123.13	120.30
7	G	183	VAL	CB-CA-C	-5.62	100.71	111.40
3	C	5	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	O	219	ARG	NE-CZ-NH2	-5.59	117.50	120.30
9	W	197	ARG	NE-CZ-NH1	5.59	123.09	120.30
6	T	7	TYR	N-CA-CB	5.53	120.55	110.60
3	C	88	ARG	NE-CZ-NH1	5.53	123.06	120.30
10	J	88	LEU	CB-CG-CD2	5.53	120.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	67	LEU	CA-CB-CG	5.52	128.00	115.30
5	E	174	ARG	NE-CZ-NH1	5.50	123.05	120.30
7	G	11	ARG	NE-CZ-NH2	-5.48	117.56	120.30
9	I	150	GLU	CG-CD-OE1	5.47	129.25	118.30
11	K	69	ARG	NE-CZ-NH1	5.47	123.04	120.30
10	X	85	ARG	NE-CZ-NH1	5.47	123.04	120.30
5	E	94	ASP	CB-CG-OD2	5.46	123.22	118.30
10	J	70	ARG	NE-CZ-NH2	-5.46	117.57	120.30
11	K	166	ARG	NE-CZ-NH1	5.46	123.03	120.30
6	T	6	GLY	C-N-CA	5.42	135.26	121.70
11	Y	120	ARG	NE-CZ-NH1	5.42	123.01	120.30
9	I	150	GLU	CG-CD-OE2	-5.40	107.50	118.30
13	a	99	ARG	NE-CZ-NH1	5.39	122.99	120.30
14	b	29	ARG	CB-CA-C	-5.38	99.64	110.40
6	T	169	ARG	NE-CZ-NH1	5.38	122.99	120.30
13	M	79	ASP	CB-CG-OD1	5.35	123.12	118.30
7	G	86	ASP	CB-CG-OD2	-5.34	113.49	118.30
9	I	197	ARG	NE-CZ-NH1	5.34	122.97	120.30
11	Y	107	ARG	NE-CZ-NH1	5.33	122.97	120.30
7	G	95	ARG	NE-CZ-NH2	-5.31	117.64	120.30
6	T	83	ASP	CB-CG-OD2	5.29	123.06	118.30
7	U	80[A]	MET	CG-SD-CE	5.29	108.66	100.20
7	U	80[B]	MET	CG-SD-CE	5.29	108.66	100.20
9	I	203	MET	CG-SD-CE	5.24	108.58	100.20
5	E	94	ASP	CB-CG-OD1	-5.23	113.60	118.30
8	H	89	ARG	NE-CZ-NH1	5.21	122.91	120.30
3	C	163	ARG	NE-CZ-NH1	5.20	122.90	120.30
8	H	72	ARG	CD-NE-CZ	5.19	130.87	123.60
6	T	190	VAL	CB-CA-C	-5.19	101.54	111.40
7	G	11	ARG	CD-NE-CZ	5.17	130.85	123.60
5	S	174	ARG	NE-CZ-NH1	5.13	122.87	120.30
5	S	89	ARG	NE-CZ-NH2	-5.10	117.75	120.30
6	T	99	ARG	NE-CZ-NH1	5.09	122.85	120.30
10	J	85	ARG	NE-CZ-NH2	-5.07	117.76	120.30
3	C	85[A]	ASN	CB-CA-C	5.07	120.54	110.40
3	C	85[B]	ASN	CB-CA-C	5.07	120.54	110.40
13	M	94	ARG	NE-CZ-NH2	-5.07	117.77	120.30
11	Y	154	ASP	CB-CG-OD2	-5.06	113.75	118.30
13	a	37	ARG	NE-CZ-NH2	-5.05	117.77	120.30
9	I	69	ARG	NE-CZ-NH2	-5.05	117.78	120.30
10	X	19	ARG	NE-CZ-NH2	-5.01	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
5	E	235	GLY	Peptide
6	F	206	ASP	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	245	ALA	Peptide
2	P	54	LYS	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
10	X	102	LEU	Peptide
13	a	215	ILE	Peptide

## 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	1788	0	1761	8	0
1	O	1741	0	1683	8	0
2	B	1922	0	1913	2	0
2	P	1898	0	1861	11	0
3	C	1797	0	1714	11	0
3	Q	1796	0	1733	7	0
4	D	1762	0	1709	3	0
4	R	1753	0	1726	5	0
5	E	1822	0	1779	8	0
5	S	1853	0	1796	13	0
6	F	1888	0	1882	12	0
6	T	1856	0	1816	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1912	0	1882	7	0
7	U	1815	0	1748	7	0
8	H	1664	0	1681	4	0
8	V	1622	0	1595	5	0
9	I	1613	0	1646	9	0
9	W	1599	0	1621	7	0
10	J	1590	0	1581	13	0
10	X	1576	0	1561	10	0
11	K	1551	0	1509	6	0
11	Y	1570	0	1550	6	0
12	L	1636	0	1625	6	0
12	Z	1642	0	1635	2	0
13	M	1692	0	1670	1	0
13	a	1688	0	1658	0	0
14	N	1519	0	1496	4	0
14	b	1524	0	1496	0	0
15	G	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	U	1	0	0	0	0
15	Z	1	0	0	0	0
15	b	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	X	1	0	0	0	0
17	H	16	0	22	0	0
17	I	16	0	22	0	0
17	K	16	0	22	0	0
17	L	16	0	22	0	0
17	N	16	0	22	0	0
17	W	16	0	22	0	0
17	Z	16	0	22	0	0
17	a	16	0	22	0	0
17	b	16	0	22	0	0
18	A	106	0	0	0	0
18	B	126	0	0	0	0
18	C	59	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	D	80	0	0	0	0
18	E	128	0	0	2	0
18	F	175	0	0	4	0
18	G	165	0	0	3	0
18	H	151	0	0	1	0
18	I	145	0	0	1	0
18	J	122	0	0	2	0
18	K	96	0	0	0	0
18	L	115	0	0	0	0
18	M	143	0	0	0	0
18	N	160	0	0	0	0
18	O	78	0	0	1	0
18	P	104	0	0	1	0
18	Q	62	0	0	0	0
18	R	112	0	0	0	0
18	S	114	0	0	6	0
18	T	83	0	0	1	0
18	U	90	0	0	0	0
18	V	102	0	0	2	0
18	W	101	0	0	0	0
18	X	110	0	0	0	0
18	Y	140	0	0	0	0
18	Z	169	0	0	1	0
18	a	173	0	0	0	0
18	b	122	0	0	0	0
All	All	51579	0	47525	174	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 (174) 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:K:9:ARG:NH2	11:K:146:ASP:OD1	1.96	0.98
5:S:204:ASP:OD1	18:S:301:HOH:O	1.91	0.86
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.42	0.83
10:X:1:MET:HE1	10:X:134:TYR:H	1.46	0.79
5:S:152[B]:ASN:OD1	18:S:302:HOH:O	2.01	0.79
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.67	0.77
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.66	0.76
5:S:65[A]:HIS:CE1	18:S:304:HOH:O	2.39	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:58:ALA:O	5:E:59:HIS:CB	2.35	0.74
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.23	0.72
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.19	0.72
10:J:185:LYS:NZ	18:J:401:HOH:O	2.21	0.71
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.07	0.70
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	1.91	0.70
12:L:144:MET:CE	12:L:185:ARG:HB2	2.23	0.68
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.34	0.68
5:S:86:ASN:ND2	18:S:303:HOH:O	2.27	0.68
10:X:1:MET:HE1	10:X:134:TYR:N	2.10	0.67
7:U:195:VAL:O	7:U:199:ILE:HG23	1.93	0.67
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.78	0.65
10:J:99[A]:HIS:CD2	18:J:421:HOH:O	2.50	0.63
6:F:169[A]:ARG:NH1	18:F:301:HOH:O	2.26	0.63
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.78	0.63
5:S:65[A]:HIS:ND1	18:S:304:HOH:O	2.31	0.63
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.82	0.62
6:T:6:GLY:HA3	6:T:7:TYR:CD2	2.33	0.62
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.81	0.61
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	1.83	0.60
10:X:95:ARG:HB2	10:X:95:ARG:HH11	1.67	0.60
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.35	0.59
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.50	0.59
5:E:101[A]:ARG:NH1	18:E:301:HOH:O	2.36	0.58
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.69	0.57
9:W:13:MET:HE1	9:W:166:ILE:N	2.19	0.57
12:Z:136:LYS:NZ	18:Z:401:HOH:O	2.38	0.57
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.20	0.57
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.87	0.57
2:P:8:ARG:NH2	3:Q:5:ARG:HD2	2.20	0.56
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.87	0.56
18:H:527:HOH:O	12:Z:160:ASN:CB	2.54	0.55
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.54	0.55
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.88	0.55
2:P:53:HIS:O	2:P:54:LYS:HB2	2.08	0.54
9:W:13:MET:HE2	9:W:166:ILE:HB	1.88	0.54
5:E:65:HIS:HB2	18:E:416:HOH:O	2.08	0.53
2:P:25[B]:MET:CE	2:P:25[B]:MET:HA	2.37	0.53
3:C:47:LYS:HA	3:C:205:ASN:HB3	1.89	0.53
4:R:129:ASP:CB	4:R:130:PRO:CD	2.87	0.53
1:O:10:THR:HG23	18:O:302:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.91	0.53
9:I:35:THR:HG21	18:I:409:HOH:O	2.08	0.52
7:U:80[A]:MET:HE3	7:U:91:VAL:HG23	1.91	0.52
5:E:23:GLU:HA	5:E:26:MET:HE2	1.91	0.52
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.40	0.52
18:G:529:HOH:O	8:H:72:ARG:HD3	2.10	0.51
5:S:101:ARG:NH1	18:S:306:HOH:O	2.44	0.51
5:E:23:GLU:HA	5:E:26:MET:CE	2.42	0.50
6:F:117:MET:HG3	18:F:444:HOH:O	2.12	0.50
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.42	0.50
8:H:132:LEU:HD22	14:N:25:TYR:CZ	2.47	0.50
7:U:51:VAL:HG12	7:U:198:ALA:HB1	1.94	0.49
5:S:238:GLU:CB	5:S:239:ARG:C	2.80	0.49
6:F:237:LYS:O	6:F:241:GLU:HG3	2.12	0.49
6:T:202:ASP:O	6:T:205:LYS:O	2.30	0.49
10:J:182:ILE:CD1	10:J:191:LEU:HD11	2.42	0.49
2:P:8:ARG:HH21	3:Q:5:ARG:HD2	1.77	0.49
10:X:118:MET:HE2	10:X:124:LEU:HD13	1.95	0.49
14:N:35:THR:CG2	14:N:45:ARG:HE	2.25	0.49
11:K:12:VAL:HG13	11:K:179:VAL:HB	1.95	0.49
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	1.95	0.49
11:Y:40:TYR:HB3	11:Y:73:ARG:NH1	2.27	0.49
10:J:101:ASN:HB3	10:J:132:HIS:CE1	2.48	0.48
7:G:244:GLU:O	7:G:245:ARG:CG	2.61	0.48
6:T:7:TYR:N	18:T:301:HOH:O	2.32	0.48
6:T:87:LEU:HD13	6:T:131:PHE:CE1	2.49	0.48
2:B:8:ARG:NH2	3:C:5:ARG:HD2	2.29	0.48
1:O:49:LYS:O	1:O:51:GLN:N	2.47	0.48
4:R:91:LYS:HG2	4:R:119:LEU:HD11	1.95	0.48
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.96	0.48
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.94	0.48
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.95	0.47
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.97	0.47
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.97	0.47
11:K:40:TYR:HB3	11:K:73:ARG:NH1	2.30	0.47
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.33	0.47
9:I:146:TYR:O	9:I:150:GLU:HB2	2.15	0.46
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.55	0.46
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.16	0.46
10:X:1:MET:HE2	10:X:1:MET:HB3	1.87	0.46
8:V:57:GLN:NE2	18:V:402:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:O	1:A:51:GLN:N	2.49	0.46
6:T:152:ASP:OD1	6:T:156:VAL:HG12	2.14	0.46
5:S:154:PHE:HD2	6:T:63:ASN:HD21	1.64	0.46
7:U:58:ASP:O	7:U:59:LYS:CB	2.64	0.46
3:C:203:GLY:CA	3:C:204:LYS:CB	2.94	0.46
6:F:219:LEU:HD22	18:F:401:HOH:O	2.14	0.46
9:W:146:TYR:O	9:W:150:GLU:HB2	2.15	0.46
9:I:158:ASP:OD1	9:I:161:HIS:CD2	2.69	0.45
8:H:132:LEU:HD22	14:N:25:TYR:CE2	2.51	0.45
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.98	0.45
3:C:47:LYS:CB	3:C:48:LYS:C	2.85	0.45
11:Y:37:ILE:O	11:Y:38:ASN:HB3	2.16	0.45
1:A:198:PHE:O	1:A:199:GLU:CB	2.65	0.45
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.99	0.45
3:C:35:VAL:CG1	3:C:191:VAL:CG2	2.95	0.45
12:L:144:MET:HE3	12:L:185:ARG:HB2	1.99	0.45
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.63	0.45
1:O:73:LEU:CD2	1:O:135:ILE:HG12	2.48	0.44
2:P:25[B]:MET:HA	2:P:25[B]:MET:HE2	2.00	0.44
8:V:213:THR:HB	9:W:198:THR:OG1	2.17	0.44
4:D:91:LYS:HG2	4:D:119:LEU:HD11	1.98	0.44
7:G:72:ILE:HG21	7:G:114:LEU:HD21	2.00	0.44
1:O:230:ALA:O	1:O:231:ALA:CB	2.66	0.44
4:R:196:LYS:HE3	4:R:240:ASP:HB3	1.99	0.44
3:C:47:LYS:CB	3:C:48:LYS:O	2.65	0.44
6:T:34:SER:OG	6:T:65:ARG:NH1	2.49	0.44
3:C:35:VAL:CG1	3:C:191:VAL:HG22	2.48	0.43
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.99	0.43
1:A:73:LEU:CD2	1:A:135:ILE:HG12	2.48	0.43
2:B:33:THR:HB	2:B:166:ASN:O	2.19	0.43
5:E:71:GLY:HA3	5:E:221:PHE:CZ	2.53	0.43
5:E:154:PHE:CD2	6:F:63:ASN:OD1	2.71	0.43
10:J:118:MET:HE2	10:J:124:LEU:HD13	2.01	0.43
6:F:87:LEU:HD13	6:F:131:PHE:CE2	2.53	0.43
6:F:34:SER:OG	6:F:65:ARG:NH1	2.49	0.43
2:P:155:ASN:ND2	18:P:301:HOH:O	2.41	0.43
7:G:141:ILE:HG22	7:G:151:VAL:HG22	2.01	0.43
1:O:79:GLY:O	1:O:82:TYR:HB3	2.19	0.43
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.52	0.43
2:P:197:LEU:HB3	2:P:201:MET:HE3	2.00	0.43
2:P:246:LYS:N	2:P:246:LYS:HE3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:13[A]:MET:HE1	9:I:166:ILE:CA	2.49	0.42
9:I:204:ASP:HB3	11:Y:192:VAL:HG11	2.01	0.42
5:S:71:GLY:HA3	5:S:221:PHE:CZ	2.55	0.42
1:O:165:ASN:OD1	1:O:168:ASN:HB2	2.20	0.42
6:T:205:LYS:O	6:T:206:ASP:CG	2.57	0.42
11:K:37:ILE:O	11:K:38:ASN:HB3	2.19	0.42
6:T:173:LYS:HB3	6:T:173:LYS:HE2	1.72	0.42
6:F:169[B]:ARG:NH2	18:F:307:HOH:O	2.52	0.42
7:G:145:GLU:CB	18:G:506:HOH:O	2.67	0.42
8:H:204:CYS:SG	8:H:208:THR:HG21	2.60	0.42
12:L:145:LEU:HD22	12:L:178:VAL:HB	2.01	0.42
1:A:79:GLY:O	1:A:82:TYR:HB3	2.20	0.41
10:J:1[A]:MET:CE	10:J:134:TYR:H	2.23	0.41
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.50	0.41
7:G:117:ARG:NH2	18:G:406:HOH:O	2.54	0.41
2:P:33:THR:HB	2:P:166:ASN:O	2.20	0.41
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.51	0.41
6:F:168:ALA:HB1	6:F:200:VAL:HB	2.03	0.41
7:G:244:GLU:O	7:G:245:ARG:HG2	2.21	0.41
11:K:133:VAL:HG21	10:X:137:PHE:HB3	2.03	0.41
8:V:153:ASN:HB2	18:V:441:HOH:O	2.20	0.41
10:X:1:MET:C	10:X:1:MET:HE3	2.41	0.41
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.56	0.41
3:Q:106:TYR:C	3:Q:106:TYR:CD1	2.94	0.41
6:T:43:ASP:OD1	6:T:43:ASP:N	2.53	0.41
9:W:141:CYS:HB3	9:W:177:ASP:HB2	2.03	0.41
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.51	0.41
10:J:1[A]:MET:HB3	10:J:1[A]:MET:HE2	1.87	0.41
1:A:114:ALA:HB1	1:A:152:GLY:O	2.21	0.41
12:L:148:LEU:HD23	12:L:178:VAL:HG12	2.03	0.41
3:C:183:THR:OG1	3:C:184:ASP:N	2.54	0.40
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.56	0.40
6:T:139:SER:HA	6:T:216:VAL:HG11	2.03	0.40
8:V:97:ALA:HB1	8:V:127[B]:MET:CE	2.52	0.40
3:C:5:ARG:HD3	4:D:125:GLU:OE2	2.21	0.40
9:I:111:LEU:HD23	9:I:118:PRO:HA	2.02	0.40
9:W:111:LEU:HD23	9:W:118:PRO:HA	2.03	0.40
6:T:135:PHE:CE1	6:T:151:ILE:HD13	2.56	0.40
6:T:168:ALA:HB1	6:T:200:VAL:HB	2.03	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	231/234 (99%)	222 (96%)	5 (2%)	4 (2%)	11	7
1	O	228/234 (97%)	217 (95%)	6 (3%)	5 (2%)	8	4
2	B	248/261 (95%)	240 (97%)	7 (3%)	1 (0%)	39	42
2	P	247/261 (95%)	234 (95%)	8 (3%)	5 (2%)	9	5
3	C	236/248 (95%)	224 (95%)	7 (3%)	5 (2%)	9	5
3	Q	229/248 (92%)	217 (95%)	8 (4%)	4 (2%)	11	7
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	15	11
4	R	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	11	7
5	E	232/263 (88%)	225 (97%)	6 (3%)	1 (0%)	39	42
5	S	236/263 (90%)	229 (97%)	5 (2%)	2 (1%)	24	22
6	F	241/255 (94%)	232 (96%)	8 (3%)	1 (0%)	39	42
6	T	239/255 (94%)	227 (95%)	9 (4%)	3 (1%)	15	11
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
8	H	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
8	V	220/234 (94%)	214 (97%)	6 (3%)	0	100	100
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	3 (2%)	2 (1%)	19	16
10	J	195/201 (97%)	191 (98%)	4 (2%)	0	100	100
10	X	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
11	K	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
11	Y	200/204 (98%)	197 (98%)	3 (2%)	0	100	100
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	208 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	216/219 (99%)	207 (96%)	9 (4%)	0	100	100
14	N	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
14	b	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	6200/6458 (96%)	6021 (97%)	139 (2%)	40 (1%)	30	29

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	53	SER
3	C	47	LYS
5	E	59	HIS
1	O	50	LYS
1	O	53	SER
2	P	54	LYS
2	P	247	ALA
3	Q	47	LYS
3	Q	206	ILE
4	R	128	ALA
4	R	130	PRO
4	R	132	ALA
5	S	238	GLU
6	T	7	TYR
1	A	52	LYS
1	A	176	ARG
3	C	204	LYS
4	D	175[A]	GLU
4	D	175[B]	GLU
4	D	176	GLY
6	F	62	SER
1	O	52	LYS
1	O	176	ARG
1	O	231	ALA
4	R	129	ASP
6	T	208	ALA
2	P	245	ALA
3	Q	221	ASN
5	S	236	LEU
6	T	62	SER
3	C	50	VAL
3	C	51	ALA

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Mol	Chain	Res	Type
3	C	203	GLY
2	P	52	ILE
3	Q	50	VAL
9	W	16[A]	LYS
9	W	16[B]	LYS
2	P	204	SER
2	B	203	VAL

### 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	185/191 (97%)	173 (94%)	12 (6%)	21	23
1	O	176/191 (92%)	167 (95%)	9 (5%)	29	34
2	B	199/221 (90%)	193 (97%)	6 (3%)	48	60
2	P	196/221 (89%)	184 (94%)	12 (6%)	23	26
3	C	179/210 (85%)	172 (96%)	7 (4%)	39	48
3	Q	183/210 (87%)	175 (96%)	8 (4%)	35	42
4	D	189/203 (93%)	184 (97%)	5 (3%)	54	66
4	R	187/203 (92%)	184 (98%)	3 (2%)	70	82
5	E	192/223 (86%)	183 (95%)	9 (5%)	32	39
5	S	195/223 (87%)	189 (97%)	6 (3%)	47	59
6	F	199/212 (94%)	188 (94%)	11 (6%)	27	30
6	T	192/212 (91%)	183 (95%)	9 (5%)	32	39
7	G	202/207 (98%)	194 (96%)	8 (4%)	38	47
7	U	186/207 (90%)	181 (97%)	5 (3%)	52	64
8	H	181/195 (93%)	175 (97%)	6 (3%)	45	56
8	V	172/195 (88%)	163 (95%)	9 (5%)	29	33
9	I	176/174 (101%)	174 (99%)	2 (1%)	80	89
9	W	173/174 (99%)	172 (99%)	1 (1%)	90	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	166/170 (98%)	158 (95%)	8 (5%)	31	37
10	X	165/170 (97%)	157 (95%)	8 (5%)	31	37
11	K	155/159 (98%)	146 (94%)	9 (6%)	25	28
11	Y	158/159 (99%)	154 (98%)	4 (2%)	55	67
12	L	175/178 (98%)	167 (95%)	8 (5%)	33	40
12	Z	175/178 (98%)	170 (97%)	5 (3%)	50	62
13	M	180/181 (99%)	178 (99%)	2 (1%)	80	89
13	a	178/181 (98%)	174 (98%)	4 (2%)	60	72
14	N	158/159 (99%)	155 (98%)	3 (2%)	65	77
14	b	158/159 (99%)	153 (97%)	5 (3%)	46	57
All	All	5030/5366 (94%)	4846 (96%)	184 (4%)	42	50

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	51	GLN
1	A	53	SER
1	A	61	VAL
1	A	73	LEU
1	A	142	ARG
1	A	164	LYS
1	A	174	GLU
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
2	B	33	THR
2	B	70	GLU
2	B	173	SER
2	B	190	LEU
2	B	229	LYS
2	B	249	ARG
3	C	13	ASP
3	C	35	VAL
3	C	45	VAL
3	C	148	ASP
3	C	201	SER

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Mol	Chain	Res	Type
3	C	208	LEU
3	C	225	ILE
4	D	9	ASP
4	D	32	LYS
4	D	46	VAL
4	D	126	GLU
4	D	199	LEU
5	E	10	VAL
5	E	29	VAL
5	E	61	LYS
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	180	MET
5	E	181	GLU
5	E	189	LYS
5	E	202	GLU
6	F	17	ASP
6	F	31	GLU
6	F	81	LEU
6	F	86	SER
6	F	87	LEU
6	F	187	ARG
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	242	SER
6	F	244	LYS
7	G	11	ARG
7	G	42	VAL
7	G	43	ARG
7	G	78	CYS
7	G	88	ARG
7	G	173	THR
7	G	183	VAL
7	G	206	LEU
8	H	6	VAL
8	H	22	GLU
8	H	65	LEU
8	H	68	LEU
8	H	183	LEU
8	H	197	THR
9	I	35	THR

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Mol	Chain	Res	Type
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	8	GLN
10	J	18	ASP
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	155	ARG
11	K	8	PHE
11	K	12	VAL
11	K	42	LEU
11	K	91	LYS
11	K	138	VAL
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	102	PHE
12	L	142	SER
12	L	163	HIS
12	L	174	LEU
12	L	207	THR
12	L	209	SER
13	M	100	ARG
13	M	154	LEU
14	N	35	THR
14	N	84	LYS
14	N	196	LYS
1	O	10	THR
1	O	53	SER
1	O	73	LEU
1	O	142	ARG
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER

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Mol	Chain	Res	Type
2	P	33	THR
2	P	70	GLU
2	P	124	PHE
2	P	173	SER
2	P	177	GLN
2	P	190	LEU
2	P	204	SER
2	P	230	GLN
2	P	235	GLN
2	P	246	LYS
3	Q	45	VAL
3	Q	56	GLU
3	Q	148	ASP
3	Q	170	GLU
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	220	LEU
4	R	9	ASP
4	R	46	VAL
4	R	65	GLU
5	S	10	VAL
5	S	29	VAL
5	S	45	VAL
5	S	78	THR
5	S	101	ARG
5	S	234	GLU
6	T	17	ASP
6	T	31	GLU
6	T	81	LEU
6	T	86	SER
6	T	87	LEU
6	T	190	VAL
6	T	215	TRP
6	T	240	LYS
6	T	242	SER
7	U	42	VAL
7	U	43	ARG
7	U	78	CYS
7	U	199	ILE
7	U	206	LEU
8	V	6	VAL

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Mol	Chain	Res	Type
8	V	22	GLU
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	183	LEU
8	V	199	LEU
8	V	213	THR
9	W	35	THR
10	X	1	MET
10	X	8	GLN
10	X	27	GLN
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	174	ASN
10	X	182	ILE
11	Y	8	PHE
11	Y	12	VAL
11	Y	138	VAL
11	Y	147	LEU
12	Z	102	PHE
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
12	Z	209	SER
13	a	92	LEU
13	a	94	ARG
13	a	100	ARG
13	a	154	LEU
14	b	35	THR
14	b	84	LYS
14	b	92	GLU
14	b	196	LYS
14	b	202	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	108	GLN
1	A	206	ASN

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Mol	Chain	Res	Type
2	B	40	ASN
2	B	109	GLN
5	E	65	HIS
8	H	153	ASN
9	I	161	HIS
10	J	101	ASN
10	J	132	HIS
12	L	77	HIS
12	L	157	ASN
13	M	47	ASN
14	N	193	GLN
1	O	101	GLN
1	O	118	GLN
1	O	206	ASN
2	P	109	GLN
2	P	142	HIS
2	P	146	GLN
3	Q	18	GLN
3	Q	239	ASN
5	S	86	ASN
6	T	68	ASN
6	T	143	ASN
9	W	172	ASN
10	X	24	ASN
10	X	63	ASN
10	X	82	ASN
10	X	174	ASN
11	Y	162	GLN
12	Z	79	ASN
12	Z	157	ASN
13	a	47	ASN
13	a	89	HIS
14	b	193	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	YCM	C	63	3	7,9,10	1.47	1 (14%)	5,10,12	1.54	1 (20%)
5	6V1	E	148	5	11,15,16	1.29	1 (9%)	11,20,22	1.67	3 (27%)
7	YCM	G	137	7	7,9,10	1.63	1 (14%)	5,10,12	3.02	2 (40%)
7	6V1	G	161	7	11,15,16	1.18	1 (9%)	11,20,22	3.23	6 (54%)
7	6V1	G	47	7	11,15,16	1.29	2 (18%)	11,20,22	2.56	2 (18%)
10	6V1	J	91	10	11,15,16	1.77	3 (27%)	11,20,22	4.20	8 (72%)
3	YCM	Q	63	3	7,9,10	1.12	0	5,10,12	2.13	2 (40%)
5	6V1	S	148	5	11,15,16	1.50	3 (27%)	11,20,22	2.43	6 (54%)
7	YCM	U	137	7	7,9,10	1.45	1 (14%)	5,10,12	2.87	2 (40%)
7	6V1	U	161	7	11,15,16	1.79	3 (27%)	11,20,22	2.38	5 (45%)
7	6V1	U	47	7	11,15,16	1.44	2 (18%)	11,20,22	4.49	3 (27%)
10	6V1	X	91	10	11,15,16	1.67	3 (27%)	11,20,22	4.41	8 (72%)

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
3	YCM	C	63	3	-	0/6/8/10	0/0/0/0
5	6V1	E	148	5	-	0/6/25/27	0/1/1/1
7	YCM	G	137	7	-	0/6/8/10	0/0/0/0
7	6V1	G	161	7	-	0/6/25/27	0/1/1/1
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
10	6V1	J	91	10	-	0/6/25/27	0/1/1/1
3	YCM	Q	63	3	-	0/6/8/10	0/0/0/0
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1
7	YCM	U	137	7	-	0/6/8/10	0/0/0/0
7	6V1	U	161	7	-	0/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	0/6/25/27	0/1/1/1
10	6V1	X	91	10	-	0/6/25/27	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	C1-SG	-4.37	1.77	1.83
7	U	161	6V1	C1-SG	-3.90	1.78	1.83
10	X	91	6V1	C1-SG	-3.66	1.78	1.83
7	G	137	YCM	CB-SG	-3.15	1.75	1.81
5	S	148	6V1	C2-N3	-3.10	1.34	1.38
3	C	63	YCM	CB-SG	-3.03	1.75	1.81
7	U	137	YCM	CB-SG	-2.98	1.75	1.81
7	U	161	6V1	C2-N3	-2.83	1.34	1.38
10	J	91	6V1	C4-N3	-2.80	1.33	1.38
7	G	47	6V1	C2-N3	-2.59	1.35	1.38
10	X	91	6V1	C4-N3	-2.45	1.34	1.38
7	U	47	6V1	C4-N3	-2.18	1.34	1.38
5	S	148	6V1	C1-SG	-2.13	1.80	1.83
7	G	47	6V1	C5-C4	2.08	1.54	1.50
10	J	91	6V1	O7-C2	2.11	1.26	1.22
7	U	47	6V1	C1-C2	2.18	1.54	1.52
10	X	91	6V1	O7-C2	2.23	1.26	1.22
7	G	161	6V1	C1-C2	2.28	1.54	1.52
5	S	148	6V1	C5-C4	2.48	1.54	1.50
7	U	161	6V1	C1-C2	2.71	1.54	1.52
5	E	148	6V1	C5-C4	2.78	1.55	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	47	6V1	C5-C1-C2	-8.36	97.62	103.98
7	G	161	6V1	O8-C4-C5	-5.31	120.26	127.38
7	U	161	6V1	O8-C4-C5	-5.24	120.36	127.38
10	X	91	6V1	C6-N3-C4	-4.75	118.19	123.24
7	G	161	6V1	C5-C1-C2	-4.49	100.56	103.98
10	J	91	6V1	C6-N3-C4	-4.42	118.54	123.24
10	X	91	6V1	O7-C2-C1	-4.10	117.78	125.18
10	J	91	6V1	O7-C2-C1	-3.95	118.05	125.18
3	Q	63	YCM	CA-CB-SG	-3.77	103.93	112.84
7	G	137	YCM	CA-CB-SG	-3.19	105.30	112.84
7	U	137	YCM	CA-CB-SG	-3.13	105.45	112.84
5	S	148	6V1	O7-C2-N3	-3.07	119.94	124.19
5	S	148	6V1	C6-N3-C2	-2.91	121.15	123.42
10	X	91	6V1	C5-C1-C2	-2.85	101.81	103.98
10	X	91	6V1	O8-C4-C5	-2.83	123.59	127.38
5	S	148	6V1	C5-C1-C2	-2.79	101.86	103.98
5	E	148	6V1	CA-CB-SG	-2.77	106.46	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	161	6V1	O7-C2-C1	-2.71	120.29	125.18
10	J	91	6V1	O8-C4-C5	-2.55	123.96	127.38
3	C	63	YCM	O-C-CA	-2.39	119.31	125.72
3	Q	63	YCM	O-C-CA	-2.38	119.33	125.72
10	X	91	6V1	CA-CB-SG	-2.37	107.39	112.87
7	G	47	6V1	C5-C1-C2	-2.29	102.24	103.98
10	J	91	6V1	C5-C1-C2	-2.26	102.26	103.98
5	E	148	6V1	O-C-CA	-2.25	119.70	125.72
5	S	148	6V1	O-C-CA	-2.23	119.73	125.72
5	S	148	6V1	O8-C4-C5	-2.16	124.48	127.38
10	J	91	6V1	O-C-CA	-2.13	120.00	125.72
7	U	161	6V1	O-C-CA	-2.01	120.34	125.72
7	U	161	6V1	C6-N3-C4	2.02	125.39	123.24
7	U	161	6V1	O8-C4-N3	3.02	127.67	123.91
5	E	148	6V1	C6-N3-C4	3.05	126.49	123.24
7	G	161	6V1	CB-SG-C1	3.61	108.76	101.58
7	U	47	6V1	C6-N3-C2	3.69	126.28	123.42
7	U	161	6V1	CB-SG-C1	3.88	109.29	101.58
7	G	161	6V1	C6-N3-C2	4.14	126.63	123.42
7	G	161	6V1	O8-C4-N3	4.53	129.53	123.91
5	S	148	6V1	C6-N3-C4	4.69	128.23	123.24
10	X	91	6V1	O7-C2-N3	5.00	131.09	124.19
10	J	91	6V1	O7-C2-N3	5.03	131.14	124.19
7	U	137	YCM	CD-CE-NZ2	5.13	121.13	115.48
10	X	91	6V1	CB-SG-C1	5.25	112.03	101.58
7	G	137	YCM	CD-CE-NZ2	5.48	121.52	115.48
10	J	91	6V1	CB-SG-C1	5.85	113.22	101.58
7	G	47	6V1	CB-SG-C1	7.32	116.15	101.58
10	J	91	6V1	C6-N3-C2	8.91	130.34	123.42
10	X	91	6V1	C6-N3-C2	9.78	131.02	123.42
7	U	47	6V1	CB-SG-C1	11.08	123.61	101.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 15 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
17	1PE	H	302	-	15,15,15	0.66	0	14,14,14	0.75	0
17	1PE	I	302	-	15,15,15	0.72	0	14,14,14	0.87	0
17	1PE	K	302	-	15,15,15	0.81	0	14,14,14	0.79	0
17	1PE	L	301	-	15,15,15	0.66	0	14,14,14	0.44	0
17	1PE	N	301	-	15,15,15	0.59	0	14,14,14	0.56	0
17	1PE	W	302	-	15,15,15	0.76	0	14,14,14	0.44	0
17	1PE	Z	301	-	15,15,15	0.65	0	14,14,14	0.47	0
17	1PE	a	301	-	15,15,15	0.55	0	14,14,14	0.56	0
17	1PE	b	301	-	15,15,15	0.74	0	14,14,14	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	1PE	H	302	-	-	0/13/13/13	0/0/0/0
17	1PE	I	302	-	-	0/13/13/13	0/0/0/0
17	1PE	K	302	-	-	0/13/13/13	0/0/0/0
17	1PE	L	301	-	-	0/13/13/13	0/0/0/0
17	1PE	N	301	-	-	0/13/13/13	0/0/0/0
17	1PE	W	302	-	-	0/13/13/13	0/0/0/0
17	1PE	Z	301	-	-	0/13/13/13	0/0/0/0
17	1PE	a	301	-	-	0/13/13/13	0/0/0/0
17	1PE	b	301	-	-	0/13/13/13	0/0/0/0

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	230/234 (98%)	-0.23	5 (2%) 65 64	45, 65, 103, 119	0
1	O	230/234 (98%)	0.20	19 (8%) 14 13	57, 83, 127, 149	0
2	B	248/261 (95%)	-0.01	12 (4%) 34 34	50, 71, 121, 170	0
2	P	247/261 (94%)	0.45	29 (11%) 6 6	54, 82, 143, 180	0
3	C	236/248 (95%)	0.34	21 (8%) 12 11	51, 84, 136, 178	0
3	Q	233/248 (93%)	0.51	28 (12%) 6 5	48, 79, 144, 195	0
4	D	233/241 (96%)	0.09	15 (6%) 23 22	54, 80, 113, 148	0
4	R	233/241 (96%)	-0.25	5 (2%) 67 65	41, 58, 91, 128	0
5	E	233/263 (88%)	-0.22	4 (1%) 73 72	44, 59, 107, 130	0
5	S	235/263 (89%)	-0.40	1 (0%) 93 93	43, 58, 92, 139	0
6	F	239/255 (93%)	-0.35	0 100 100	40, 53, 79, 98	0
6	T	240/255 (94%)	-0.05	10 (4%) 40 39	46, 66, 107, 139	0
7	G	241/246 (97%)	-0.03	6 (2%) 61 60	40, 58, 106, 158	0
7	U	235/246 (95%)	0.31	27 (11%) 6 6	56, 78, 116, 155	0
8	H	220/234 (94%)	-0.46	2 (0%) 85 85	37, 48, 81, 110	0
8	V	220/234 (94%)	-0.18	4 (1%) 71 70	45, 65, 105, 130	0
9	I	204/205 (99%)	-0.18	0 100 100	39, 51, 76, 97	0
9	W	204/205 (99%)	-0.17	3 (1%) 76 75	50, 68, 101, 115	0
10	J	195/201 (97%)	-0.44	1 (0%) 91 91	42, 57, 77, 96	0
10	X	195/201 (97%)	-0.34	1 (0%) 91 91	46, 59, 80, 97	0
11	K	200/204 (98%)	-0.10	5 (2%) 61 60	51, 64, 93, 107	0
11	Y	199/204 (97%)	-0.25	1 (0%) 91 91	39, 49, 73, 83	0
12	L	213/213 (100%)	-0.32	0 100 100	45, 67, 95, 112	0
12	Z	213/213 (100%)	-0.24	3 (1%) 78 77	35, 48, 75, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	M	216/219 (98%)	-0.14	1 (0%)	91	91	37, 52, 81, 124	0
13	a	216/219 (98%)	-0.35	1 (0%)	91	91	34, 48, 75, 105	0
14	N	202/205 (98%)	-0.38	1 (0%)	91	91	37, 45, 70, 120	0
14	b	203/205 (99%)	-0.11	6 (2%)	54	53	41, 52, 82, 126	0
All	All	6213/6458 (96%)	-0.11	211 (3%)	49	47	34, 62, 110, 195	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	187	PHE	11.8
2	P	204	SER	11.7
3	Q	232	ILE	9.7
1	O	232	ILE	7.9
7	G	188	ASP	7.8
4	D	241	ILE	7.5
3	Q	238	GLU	7.5
4	D	131	GLY	7.4
3	Q	234	LYS	7.0
4	R	131	GLY	6.8
8	V	203	ARG	6.2
3	Q	229	VAL	5.8
14	b	203	PRO	5.7
3	Q	236	LYS	5.6
3	C	234	LYS	5.5
3	C	232	ILE	5.3
4	D	237	VAL	5.2
7	G	189	TRP	5.2
2	P	203	VAL	5.2
3	C	225	ILE	5.1
2	P	61	PHE	5.1
4	R	130	PRO	5.0
3	C	229	VAL	5.0
3	Q	192	ILE	4.9
7	U	212	PRO	4.9
3	C	201	SER	4.8
3	Q	225	ILE	4.8
2	P	233	VAL	4.7
7	U	206	LEU	4.6
3	Q	239	ASN	4.6
1	O	50	LYS	4.5
6	T	208	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
3	Q	48	LYS	4.5
1	A	230	ALA	4.5
2	P	234	GLU	4.4
2	B	205	LYS	4.4
1	O	177	TYR	4.4
2	B	61	PHE	4.4
7	U	242	LEU	4.3
1	O	192	LEU	4.2
2	P	206	LEU	4.2
5	E	237	GLU	4.1
8	V	202	TYR	4.1
3	C	236	LYS	4.1
7	G	185	LYS	4.1
2	B	204	SER	4.0
3	Q	237	GLU	4.0
7	U	200	THR	4.0
13	a	216	SER	3.9
2	P	230	GLN	3.9
1	O	229	LEU	3.9
1	O	225	VAL	3.8
4	D	234	LEU	3.8
3	Q	181	ILE	3.8
3	C	230	ALA	3.7
2	P	246	LYS	3.7
6	T	207	LYS	3.7
2	P	244	GLU	3.7
1	O	199	GLU	3.7
3	Q	240	GLU	3.7
4	D	130	PRO	3.7
11	K	11	GLY	3.7
2	P	237	ILE	3.7
10	J	1[A]	MET	3.7
2	P	202	ASP	3.6
3	Q	233	GLU	3.6
3	Q	186	LEU	3.6
14	b	202	LEU	3.6
2	P	247	ALA	3.6
7	U	207	SER	3.6
3	Q	226	GLU	3.6
7	U	243	ALA	3.6
7	U	179	LEU	3.5
7	U	198	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	249	ARG	3.5
7	U	183	VAL	3.4
3	C	49	SER	3.4
7	U	204	THR	3.4
1	O	228	TYR	3.4
2	P	220	ASN	3.4
6	T	204	VAL	3.4
3	Q	206	ILE	3.4
14	N	201	THR	3.3
1	O	223	THR	3.3
11	Y	40	TYR	3.2
8	V	199	LEU	3.2
7	U	199	ILE	3.2
7	U	208	ILE	3.2
3	C	233	GLU	3.2
3	Q	171	PHE	3.2
2	B	248	GLU	3.2
7	U	235	ILE	3.1
2	P	205	LYS	3.1
6	T	243	LEU	3.1
3	C	200	GLN	3.0
3	Q	222	PRO	3.0
6	T	203	GLU	3.0
4	D	188	SER	3.0
7	U	202	LEU	3.0
2	P	243	GLU	3.0
2	B	206	LEU	3.0
3	C	192	ILE	3.0
3	C	203	GLY	3.0
3	C	238	GLU	2.9
4	D	232	GLU	2.9
3	C	195	LEU	2.9
4	D	240	ASP	2.9
5	E	232	PHE	2.9
6	T	180	GLN	2.9
7	G	186	LYS	2.9
3	Q	199	VAL	2.9
2	P	236	LEU	2.9
3	Q	179	GLU	2.9
4	D	236	GLU	2.9
4	D	239	LYS	2.8
2	B	203	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	227	ASP	2.8
11	K	9	ARG	2.8
2	P	53	HIS	2.8
1	A	232	ILE	2.8
2	B	247	ALA	2.8
2	P	200	THR	2.8
1	O	200	GLY	2.8
2	B	244	GLU	2.8
6	T	206	ASP	2.7
7	U	2	SER	2.7
6	T	209	PHE	2.7
7	G	183	VAL	2.7
4	D	230	THR	2.7
2	B	202	ASP	2.7
1	O	176	ARG	2.7
3	C	202	GLY	2.7
5	S	239	ARG	2.7
2	P	177	GLN	2.6
2	P	58	GLU	2.6
4	D	223	GLY	2.6
9	W	17	ASN	2.6
11	K	145	TYR	2.6
12	Z	164	VAL	2.6
4	D	183	GLU	2.6
3	Q	190	LEU	2.6
1	O	202	MET	2.6
11	K	40	TYR	2.6
5	E	235	GLY	2.6
3	C	237	GLU	2.5
3	Q	205	ASN	2.5
7	U	3	ARG	2.5
12	Z	165	PRO	2.5
2	P	55	LEU	2.5
10	X	95	ARG	2.5
7	U	178	PHE	2.5
3	Q	180	ALA	2.5
14	b	201	THR	2.5
4	D	190	THR	2.5
1	O	201	GLN	2.5
7	U	177	SER	2.5
7	U	7	ALA	2.5
1	O	181	LEU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	198	PHE	2.4
14	b	198	ALA	2.4
7	U	223	GLU	2.4
1	O	220	LEU	2.4
3	C	214	ASP	2.4
1	A	175	LYS	2.4
7	U	209	ASP	2.4
6	T	205	LYS	2.4
14	b	26	ILE	2.4
3	Q	38	ARG	2.4
11	K	89	GLN	2.4
1	O	191	ILE	2.3
7	U	240	VAL	2.3
7	U	57	PRO	2.3
12	Z	143	ALA	2.3
7	U	210	PHE	2.3
2	P	242	GLU	2.3
3	Q	235	GLU	2.3
5	E	54	SER	2.3
7	U	203	SER	2.3
9	W	116	PHE	2.3
4	D	222	PRO	2.3
2	B	245	ALA	2.3
3	C	196	LEU	2.3
7	U	201	CYS	2.3
1	O	184	GLU	2.2
1	A	231	ALA	2.2
3	C	186	LEU	2.2
13	M	33	LEU	2.2
14	b	199	VAL	2.2
3	Q	223	GLU	2.2
4	R	241	ILE	2.2
8	V	217	THR	2.2
2	P	197	LEU	2.2
8	H	219	LEU	2.2
3	Q	230	ALA	2.2
2	B	237	ILE	2.2
6	T	237	LYS	2.1
2	P	35	LEU	2.1
2	P	179	TYR	2.1
4	R	127	ASP	2.1
3	Q	183	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	241	GLU	2.1
2	P	189	ALA	2.1
2	P	211	VAL	2.1
4	R	186	HIS	2.1
7	U	239	LEU	2.1
2	P	248	GLU	2.1
3	C	226	GLU	2.0
3	C	185	ASP	2.0
9	W	113	PRO	2.0
8	H	201	ARG	2.0
1	O	186	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
7	YCM	G	137	10/11	0.94	0.14	-	48,54,74,76	0
3	YCM	Q	63	10/11	0.93	0.13	-	71,74,78,80	0
7	6V1	G	47	15/16	0.91	0.17	-	55,85,90,94	0
10	6V1	J	91	15/16	0.94	0.16	-	45,65,72,74	0
7	6V1	U	161	15/16	0.92	0.09	-	70,91,97,99	0
3	YCM	C	63	10/11	0.91	0.12	-	74,78,93,96	0
5	6V1	E	148	15/16	0.88	0.18	-	47,66,73,74	0
7	YCM	U	137	10/11	0.89	0.17	-	65,76,92,93	0
7	6V1	U	47	15/16	0.78	0.29	-	97,136,140,141	0
7	6V1	G	161	15/16	0.94	0.17	-	47,69,76,77	0
10	6V1	X	91	15/16	0.93	0.14	-	48,69,75,77	0
5	6V1	S	148	15/16	0.90	0.14	-	45,73,78,79	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
17	1PE	I	302	16/16	0.77	0.26	10.40	76,85,93,93	0
17	1PE	H	302	16/16	0.82	0.24	8.33	65,87,100,103	0
17	1PE	W	302	16/16	0.73	0.34	7.44	79,90,95,97	0
17	1PE	L	301	16/16	0.69	0.34	4.50	93,97,105,106	0
17	1PE	Z	301	16/16	0.87	0.20	3.00	64,87,93,98	0
17	1PE	a	301	16/16	0.84	0.25	2.86	75,87,106,107	0
17	1PE	K	302	16/16	0.70	0.23	2.49	72,86,101,101	0
17	1PE	b	301	16/16	0.91	0.16	1.62	58,68,96,96	0
17	1PE	N	301	16/16	0.90	0.14	1.62	54,62,75,78	0
15	K	L	302	1/1	0.93	0.10	-1.19	74,74,74,74	0
15	K	G	301	1/1	0.90	0.09	-1.36	64,64,64,64	0
15	K	U	301	1/1	0.87	0.09	-1.80	64,64,64,64	0
16	MG	H	301	1/1	0.92	0.07	-1.90	47,47,47,47	0
15	K	Z	302	1/1	0.94	0.07	-2.35	70,70,70,70	0
16	MG	L	303	1/1	0.97	0.07	-2.57	53,53,53,53	0
16	MG	I	301	1/1	0.97	0.10	-2.68	46,46,46,46	0
16	MG	W	301	1/1	0.96	0.06	-3.98	52,52,52,52	0
16	MG	K	301	1/1	0.93	0.05	-5.37	53,53,53,53	0
15	K	b	302	1/1	0.98	0.06	-5.62	63,63,63,63	0
16	MG	I	303	1/1	0.98	0.07	-5.87	45,45,45,45	0
15	K	N	302	1/1	0.94	0.04	-8.23	58,58,58,58	0
16	MG	X	301	1/1	0.81	0.09	-	69,69,69,69	0
16	MG	V	301	1/1	0.96	0.09	-	63,63,63,63	0
16	MG	J	301	1/1	0.98	0.08	-	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.