



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 09:16 pm GMT

PDB ID : 5LE5  
Title : Native human 20S proteasome at 1.8 Angstrom  
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.  
Deposited on : 2016-06-29  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

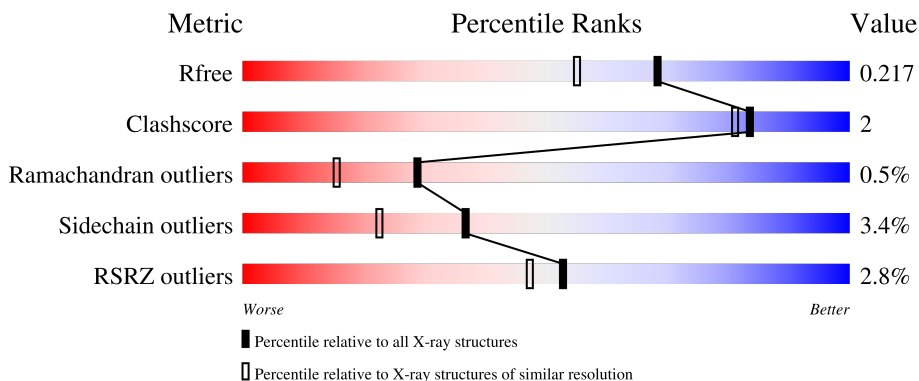
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



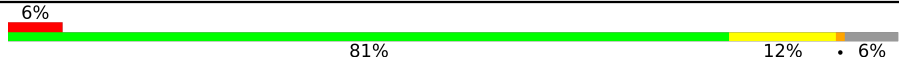
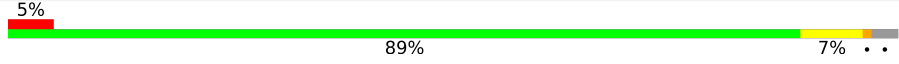
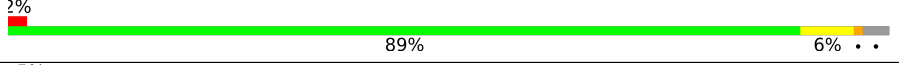



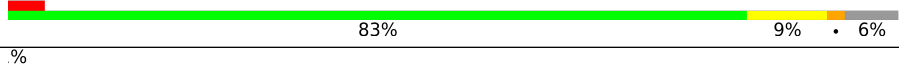
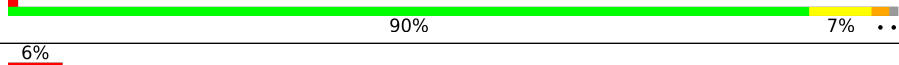
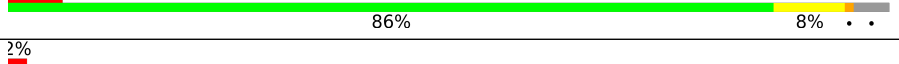


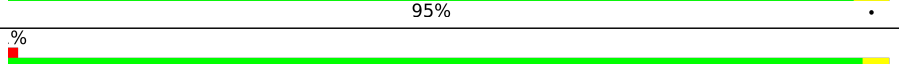
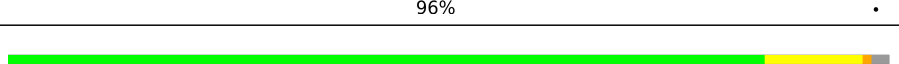
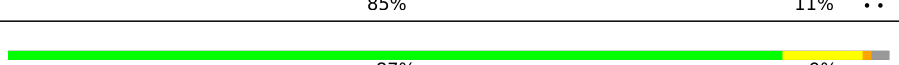
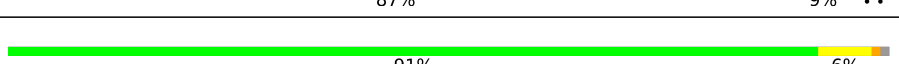
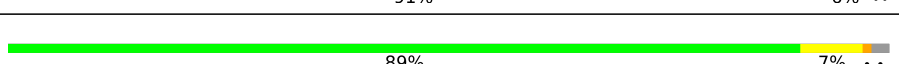
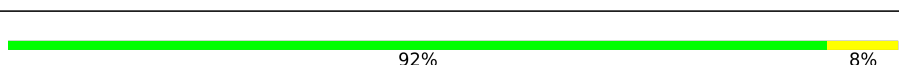
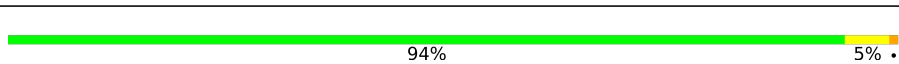
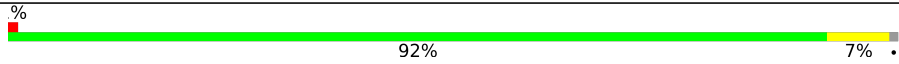
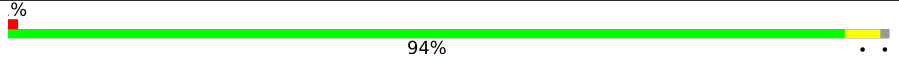
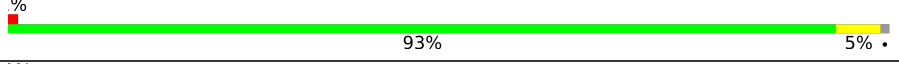
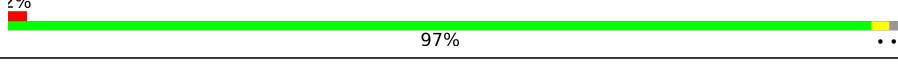

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	234	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      89%      8%    ..</p>
1	O	234	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">7%      87%      9%    ...</p>
2	B	261	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      88%      6%    . 5%</p>
2	P	261	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">7%      84%      8%    .. 5%</p>
3	C	248	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">8%      80%      15%    ..</p>

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Mol	Chain	Length	Quality of chain
3	Q	248	 6% 81% 12% 6%
4	D	241	 5% 89% 7% 6%
4	R	241	 2% 89% 6% 6%
5	E	263	 5% 81% 8% 11%
5	S	263	 3% 83% 7% 10%
6	F	255	 0% 84% 8% 6%
6	T	255	 4% 83% 9% 6%
7	G	246	 0% 90% 7% 6%
7	U	246	 6% 86% 8% 6%
8	H	234	 2% 87% 7% 6%
8	V	234	 3% 85% 8% 6%
9	I	205	 0% 95% 6% 0%
9	W	205	 0% 96% 5% 0%
10	J	201	 0% 85% 11% 6%
10	X	201	 0% 87% 9% 6%
11	K	204	 0% 91% 6% 6%
11	Y	204	 0% 89% 7% 6%
12	L	213	 0% 92% 8% 0%
12	Z	213	 0% 94% 5% 6%
13	M	219	 0% 92% 7% 6%
13	a	219	 0% 94% 6% 6%
14	N	205	 0% 93% 5% 6%
14	b	205	 2% 97% 6% 6%

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
7	6V1	U	47	X	-	-	-

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 52161 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
			Total	C	N	O	S			
1	A	230	Total	C	N	O	S	0	2	0
			1799	1151	307	335	6			
1	O	230	Total	C	N	O	S	0	0	0
			1779	1136	301	336	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	Total	C	N	O	S	0	1	0
			1942	1226	332	373	11			
2	P	247	Total	C	N	O	S	0	2	0
			1919	1211	326	371	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	Total	C	N	O	S	0	0	0
			1836	1152	328	351	5			
3	Q	234	Total	C	N	O	S	0	0	0
			1821	1143	319	354	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	233	Total	C	N	O	S	0	2	0
			1783	1118	294	360	11			
4	R	233	Total	C	N	O	S	0	1	0
			1773	1115	295	352	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	234	Total 1833	C 1150	N 328	O 344	S 11	0	0	0
5	S	238	Total 1880	C 1179	N 339	O 351	S 11	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	239	Total 1890	C 1200	N 323	O 355	S 12	0	4	0
6	T	240	Total 1867	C 1186	N 320	O 349	S 12	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	244	Total 1928	C 1223	N 322	O 370	S 13	0	2	0
7	U	235	Total 1820	C 1151	N 306	O 350	S 13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	220	Total 1672	C 1053	N 286	O 320	S 13	0	2	0
8	V	220	Total 1655	C 1042	N 278	O 322	S 13	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	Total 1633	C 1039	N 274	O 301	S 19	0	6	0
9	W	204	Total 1604	C 1021	N 269	O 295	S 19	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	196	Total 1585	C 1017	N 268	O 290	S 10	0	2	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1590	1019	270	291	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1543	974	267	293	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1564	988	275	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
			1656	1048	283	314	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1644	1043	281	309	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	0	0
			1687	1064	291	320	12			
13	a	216	Total	C	N	O	S	0	1	0
			1688	1065	291	320	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
			1515	951	258	293	13			
14	b	203	Total	C	N	O	S	0	1	0
			1526	958	259	296	13			

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	4	Total	Cl	0	0
			4	4		
15	B	2	Total	Cl	0	0
			2	2		

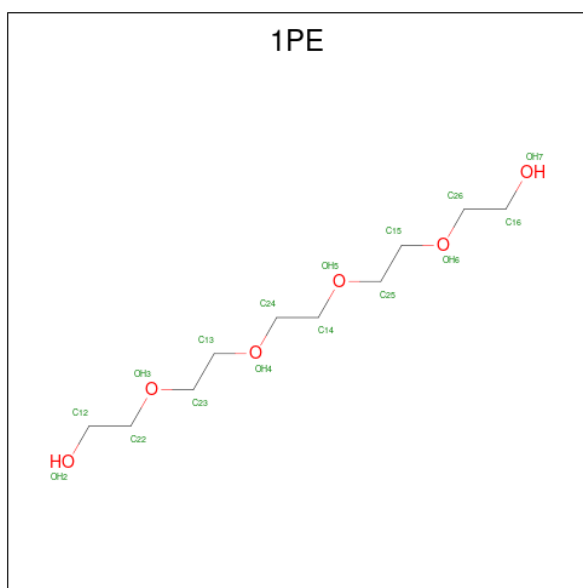
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	2	Total 2	Cl 2	0	0
15	D	2	Total 2	Cl 2	0	0
15	E	3	Total 3	Cl 3	0	0
15	F	1	Total 1	Cl 1	0	0
15	G	2	Total 2	Cl 2	0	0
15	H	2	Total 2	Cl 2	0	0
15	I	1	Total 1	Cl 1	0	0
15	K	4	Total 4	Cl 4	0	0
15	M	4	Total 4	Cl 4	0	0
15	N	3	Total 3	Cl 3	0	0
15	O	4	Total 4	Cl 4	0	0
15	P	1	Total 1	Cl 1	0	0
15	Q	2	Total 2	Cl 2	0	0
15	R	2	Total 2	Cl 2	0	0
15	S	3	Total 3	Cl 3	0	0
15	U	1	Total 1	Cl 1	0	0
15	V	2	Total 2	Cl 2	0	0
15	W	1	Total 1	Cl 1	0	0
15	Y	5	Total 5	Cl 5	0	0
15	a	3	Total 3	Cl 3	0	0
15	b	3	Total 3	Cl 3	0	0



- Molecule 16 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



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

- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total K 1 1	0	0
17	L	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	N	1	Total K 1 1	0	0
17	U	1	Total K 1 1	0	0
17	Z	1	Total K 1 1	0	0
17	b	1	Total K 1 1	0	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	112	Total O 112 112	0	0
19	B	123	Total O 123 123	0	0
19	C	75	Total O 75 75	0	0
19	D	83	Total O 83 83	0	0
19	E	134	Total O 134 134	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	F	189	Total 189	O 189	0	0
19	G	190	Total 190	O 190	0	0
19	H	151	Total 151	O 151	0	0
19	I	149	Total 149	O 149	0	0
19	J	127	Total 127	O 127	0	0
19	K	108	Total 108	O 108	0	0
19	L	115	Total 115	O 115	0	0
19	M	155	Total 155	O 155	0	0
19	N	164	Total 164	O 164	0	0
19	O	85	Total 85	O 85	0	0
19	P	111	Total 111	O 111	0	0
19	Q	66	Total 66	O 66	0	0
19	R	126	Total 126	O 126	0	0
19	S	115	Total 115	O 115	0	0
19	T	85	Total 85	O 85	0	0
19	U	100	Total 100	O 100	0	0
19	V	108	Total 108	O 108	0	0
19	W	117	Total 117	O 117	0	0
19	X	120	Total 120	O 120	0	0
19	Y	145	Total 145	O 145	0	0
19	Z	168	Total 168	O 168	0	0

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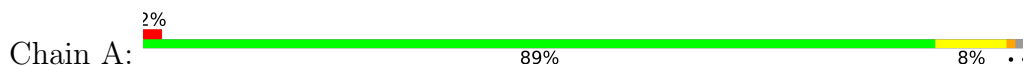
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
19	a	164	Total 164	O 164	0	0
19	b	127	Total 127	O 127	0	0

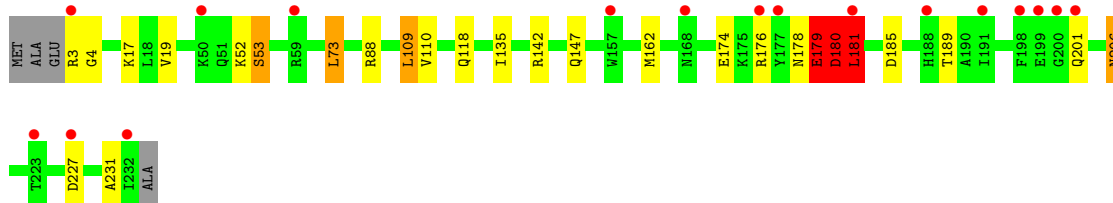
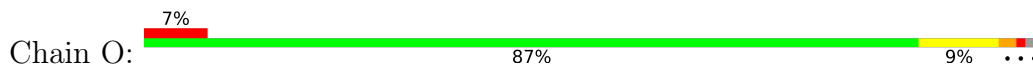
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

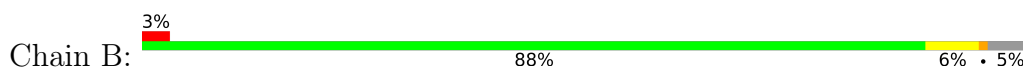
- Molecule 1: Proteasome subunit alpha type-2



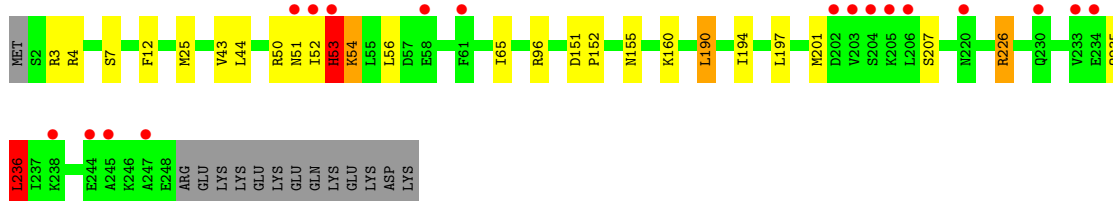
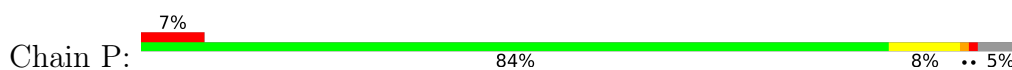
- Molecule 1: Proteasome subunit alpha type-2



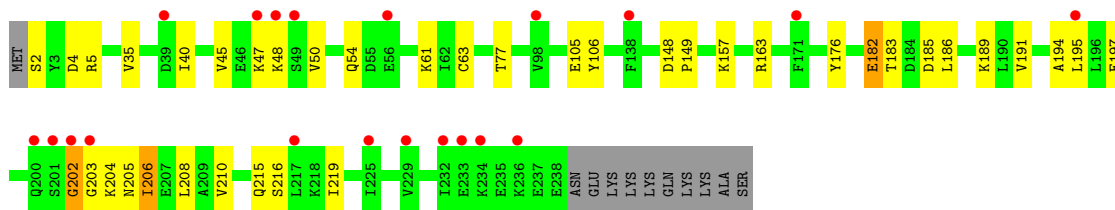
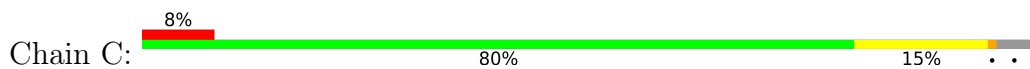
- Molecule 2: Proteasome subunit alpha type-4



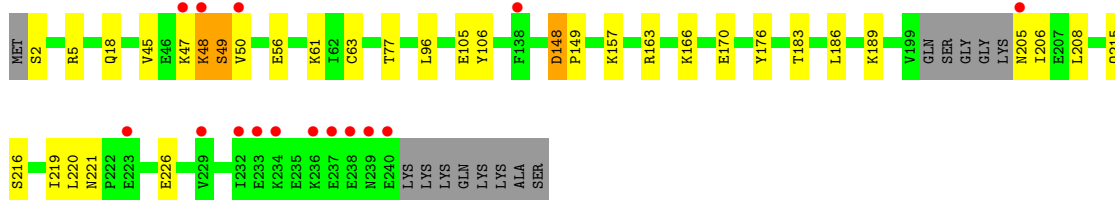
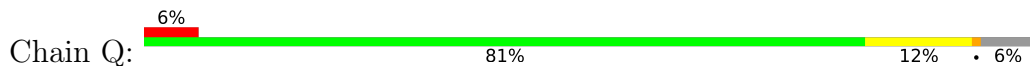
- Molecule 2: Proteasome subunit alpha type-4



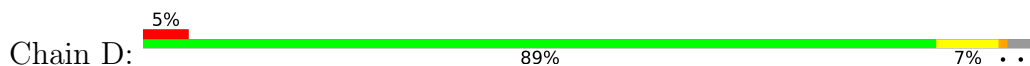
- Molecule 3: Proteasome subunit alpha type-7



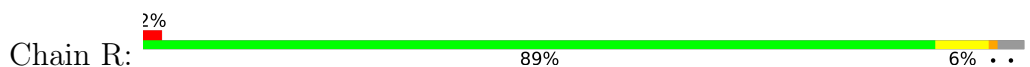
- Molecule 3: Proteasome subunit alpha type-7



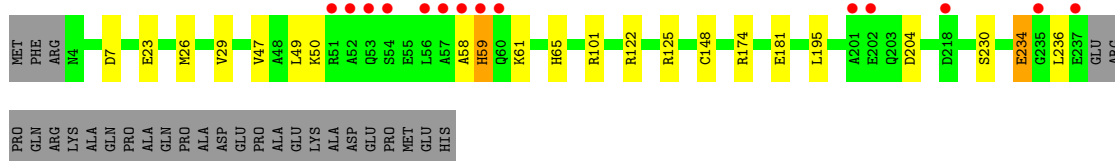
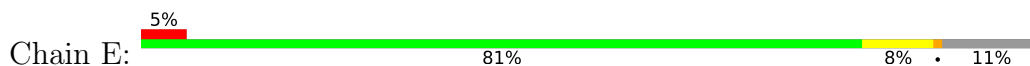
- Molecule 4: Proteasome subunit alpha type-5



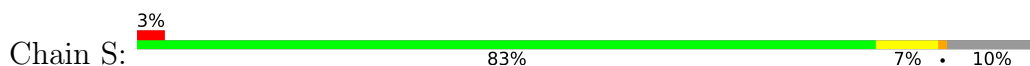
- Molecule 4: Proteasome subunit alpha type-5

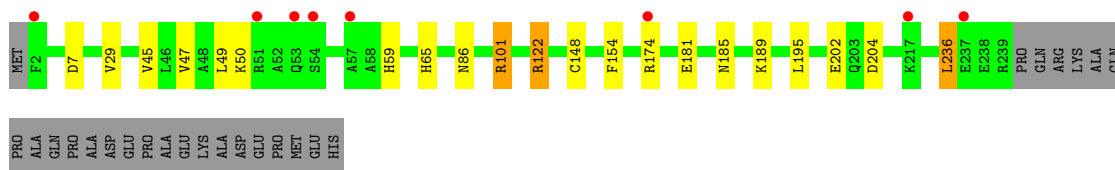


- Molecule 5: Proteasome subunit alpha type-1

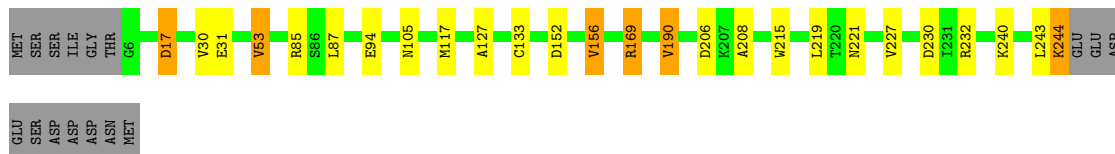
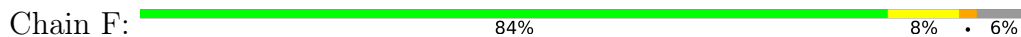


- Molecule 5: Proteasome subunit alpha type-1

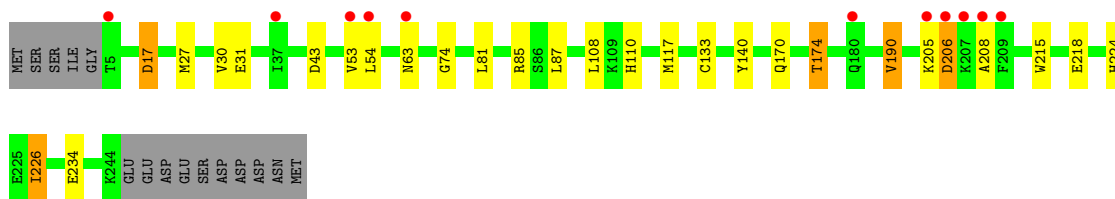
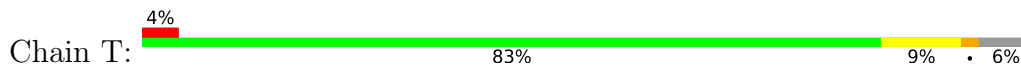




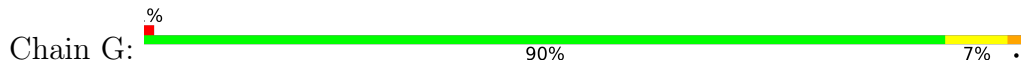
• Molecule 6: Proteasome subunit alpha type-3



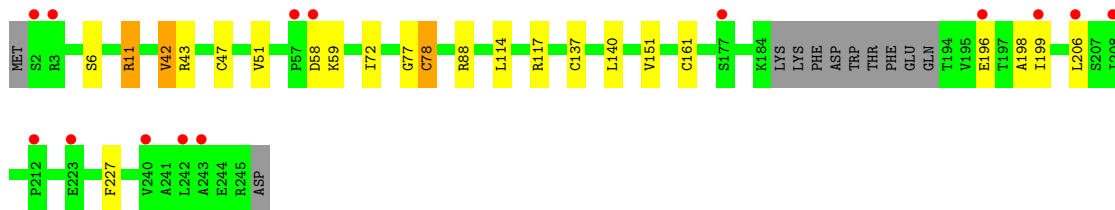
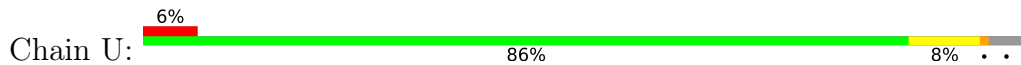
• Molecule 6: Proteasome subunit alpha type-3



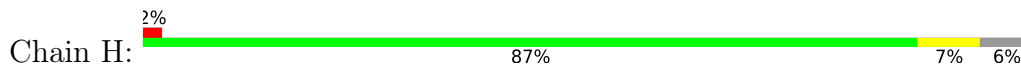
• Molecule 7: Proteasome subunit alpha type-6

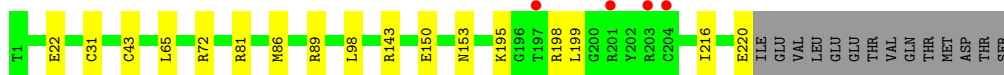


• Molecule 7: Proteasome subunit alpha type-6

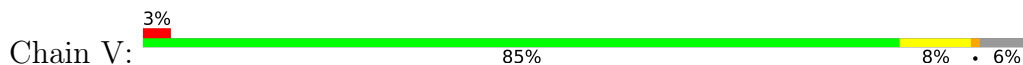


• Molecule 8: Proteasome subunit beta type-7





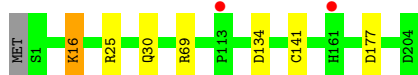
- Molecule 8: Proteasome subunit beta type-7



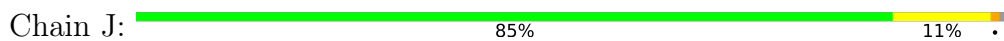
- Molecule 9: Proteasome subunit beta type-3



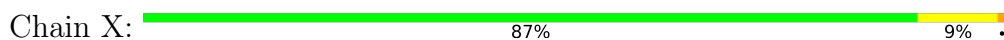
- Molecule 9: Proteasome subunit beta type-3



- 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



- Molecule 12: Proteasome subunit beta type-1



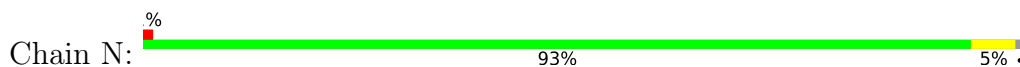
- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.44Å 202.77Å 316.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.66 – 1.80 106.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (170.66-1.80) 99.9 (106.77-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.182 , 0.212 0.190 , 0.217	Depositor DCC
$R_{free}$ test set	33208 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtrriage
Anisotropy	0.231	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52161	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: YCM, K, MG, CL, 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	0.73	1/1844 (0.1%)	0.82	1/2500 (0.0%)
1	O	0.64	0/1818	0.86	5/2467 (0.2%)
2	B	0.81	2/1975 (0.1%)	0.94	4/2665 (0.2%)
2	P	0.75	0/1955	0.90	6/2642 (0.2%)
3	C	1.16	3/1851 (0.2%)	0.91	3/2502 (0.1%)
3	Q	0.79	1/1835 (0.1%)	0.89	2/2485 (0.1%)
4	D	0.76	1/1810 (0.1%)	0.91	4/2448 (0.2%)
4	R	0.81	0/1800	0.94	4/2431 (0.2%)
5	E	0.75	1/1851 (0.1%)	0.91	3/2502 (0.1%)
5	S	0.71	0/1908	0.91	6/2577 (0.2%)
6	F	0.91	1/1937 (0.1%)	1.01	9/2607 (0.3%)
6	T	0.77	0/1905	0.96	8/2567 (0.3%)
7	G	0.91	1/1925 (0.1%)	0.92	8/2598 (0.3%)
7	U	0.69	0/1806	0.84	4/2438 (0.2%)
8	H	0.85	1/1705 (0.1%)	0.98	6/2307 (0.3%)
8	V	0.68	0/1688	0.90	4/2288 (0.2%)
9	I	0.82	0/1668	0.97	5/2247 (0.2%)
9	W	0.68	0/1636	1.00	9/2205 (0.4%)
10	J	0.95	3/1605 (0.2%)	0.99	2/2170 (0.1%)
10	X	0.84	2/1613 (0.1%)	0.98	8/2180 (0.4%)
11	K	0.79	0/1574	1.00	7/2128 (0.3%)
11	Y	0.85	0/1604	1.04	10/2165 (0.5%)
12	L	0.73	1/1692 (0.1%)	0.87	3/2281 (0.1%)
12	Z	0.84	2/1677 (0.1%)	1.06	4/2260 (0.2%)
13	M	0.82	1/1720 (0.1%)	0.97	4/2328 (0.2%)
13	a	0.86	0/1724	0.98	7/2334 (0.3%)
14	N	0.94	4/1544 (0.3%)	0.94	4/2090 (0.2%)
14	b	0.86	4/1556 (0.3%)	0.91	2/2107 (0.1%)
All	All	0.82	29/49226 (0.1%)	0.94	142/66519 (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	1
3	C	0	1
3	Q	0	2
4	D	0	3
7	U	1	0
9	I	0	1
10	X	0	1
12	Z	0	1
All	All	1	10

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	182	GLU	CG-CD	27.93	1.93	1.51
3	C	182	GLU	CD-OE2	-24.47	0.98	1.25
7	G	108	GLU	CD-OE1	14.97	1.42	1.25
3	Q	189	LYS	C-O	11.20	1.44	1.23
14	b	150	GLU	CD-OE1	9.45	1.36	1.25
10	J	10	PRO	C-O	-7.39	1.08	1.23
6	F	94	GLU	CD-OE2	-6.78	1.18	1.25
12	Z	3	SER	CB-OG	6.71	1.50	1.42
8	H	31	CYS	CB-SG	-6.65	1.71	1.82
14	b	150	GLU	CD-OE2	6.58	1.32	1.25
2	B	188	SER	CB-OG	6.52	1.50	1.42
10	J	154	GLU	CA-C	6.26	1.69	1.52
10	J	155	ARG	N-CA	-6.22	1.33	1.46
14	N	24	SER	CB-OG	-6.13	1.34	1.42
12	Z	142	SER	CB-OG	-6.03	1.34	1.42
12	L	142	SER	CB-OG	-5.95	1.34	1.42
3	C	189	LYS	C-O	5.82	1.34	1.23
1	A	3	ARG	CZ-NH2	5.63	1.40	1.33
14	b	150	GLU	CG-CD	5.62	1.60	1.51
10	X	152	SER	CB-OG	5.54	1.49	1.42
14	N	92	GLU	CD-OE1	5.47	1.31	1.25
2	B	168	SER	CB-OG	-5.47	1.35	1.42
14	N	92	GLU	CB-CG	5.45	1.62	1.52
14	N	92	GLU	CG-CD	5.34	1.59	1.51
13	M	119	GLU	CD-OE2	5.31	1.31	1.25
14	b	181	GLU	C-O	5.25	1.33	1.23
10	X	184	ASP	CG-OD1	5.25	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	25	GLU	CD-OE1	5.15	1.31	1.25
5	E	7	ASP	CB-CG	-5.08	1.41	1.51

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	99	ARG	NE-CZ-NH2	-17.26	111.67	120.30
12	Z	99	ARG	NE-CZ-NH1	16.34	128.47	120.30
9	W	69	ARG	NE-CZ-NH1	14.69	127.64	120.30
9	W	69	ARG	NE-CZ-NH2	-12.94	113.83	120.30
13	M	151	ARG	NE-CZ-NH1	11.86	126.23	120.30
7	U	88	ARG	NE-CZ-NH1	10.81	125.70	120.30
11	Y	157	ARG	NE-CZ-NH2	-10.75	114.92	120.30
9	I	25[A]	ARG	NE-CZ-NH2	-10.68	114.96	120.30
9	I	25[B]	ARG	NE-CZ-NH2	-10.68	114.96	120.30
11	Y	157	ARG	NE-CZ-NH1	10.58	125.59	120.30
6	T	27	MET	CG-SD-CE	10.38	116.82	100.20
7	G	88	ARG	NE-CZ-NH1	-10.35	115.13	120.30
11	K	86	MET	CG-SD-CE	10.00	116.20	100.20
4	D	120[A]	ALA	C-N-CA	9.77	146.12	121.70
4	D	120[B]	ALA	C-N-CA	9.77	146.12	121.70
13	a	151	ARG	NE-CZ-NH1	9.57	125.08	120.30
13	a	5	MET	CG-SD-CE	9.55	115.48	100.20
4	R	120[A]	ALA	C-N-CA	9.55	145.58	121.70
4	R	120[B]	ALA	C-N-CA	9.55	145.58	121.70
11	K	157	ARG	NE-CZ-NH2	-9.48	115.56	120.30
13	M	151	ARG	NE-CZ-NH2	-9.42	115.59	120.30
10	X	1	MET	CB-CG-SD	-9.32	84.45	112.40
9	I	25[A]	ARG	NE-CZ-NH1	9.17	124.89	120.30
9	I	25[B]	ARG	NE-CZ-NH1	9.17	124.89	120.30
11	K	157	ARG	NE-CZ-NH1	8.95	124.78	120.30
11	Y	71	LYS	CD-CE-NZ	8.51	131.27	111.70
5	E	122	ARG	NE-CZ-NH2	-8.44	116.08	120.30
9	W	16[A]	LYS	C-N-CA	8.42	142.75	121.70
9	W	16[B]	LYS	C-N-CA	8.42	142.75	121.70
7	G	117	ARG	NE-CZ-NH1	8.26	124.43	120.30
12	Z	125	ASP	CB-CG-OD1	8.21	125.69	118.30
8	H	86	MET	CG-SD-CE	-7.78	87.75	100.20
6	F	117	MET	CG-SD-CE	7.78	112.65	100.20
5	E	122	ARG	NE-CZ-NH1	7.65	124.12	120.30
7	G	183	VAL	CB-CA-C	-7.64	96.88	111.40
8	H	81	ARG	NE-CZ-NH2	-7.56	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	151	ARG	NE-CZ-NH2	-7.55	116.52	120.30
2	B	96	ARG	NE-CZ-NH1	7.51	124.06	120.30
7	U	88	ARG	NE-CZ-NH2	-7.46	116.57	120.30
6	T	117	MET	CG-SD-CE	7.45	112.12	100.20
1	O	73	LEU	CA-CB-CG	7.41	132.33	115.30
2	B	4	ARG	NE-CZ-NH1	7.38	123.99	120.30
5	S	122	ARG	NE-CZ-NH2	-7.34	116.63	120.30
6	F	190	VAL	CB-CA-C	-7.27	97.59	111.40
6	F	169	ARG	NE-CZ-NH2	-7.25	116.67	120.30
2	P	96	ARG	NE-CZ-NH1	7.23	123.92	120.30
8	V	86	MET	CG-SD-CE	-7.18	88.72	100.20
11	Y	158	ARG	NE-CZ-NH1	7.12	123.86	120.30
9	W	25[A]	ARG	NE-CZ-NH2	-7.05	116.77	120.30
9	W	25[B]	ARG	NE-CZ-NH2	-7.05	116.77	120.30
10	X	70	ARG	NE-CZ-NH1	6.95	123.78	120.30
6	F	206	ASP	CB-CG-OD1	-6.95	112.05	118.30
5	S	101	ARG	NE-CZ-NH2	6.75	123.68	120.30
12	Z	99	ARG	CD-NE-CZ	6.70	132.98	123.60
7	U	117	ARG	NE-CZ-NH1	6.69	123.64	120.30
14	N	45	ARG	NE-CZ-NH1	6.67	123.64	120.30
9	W	25[A]	ARG	NE-CZ-NH1	6.67	123.64	120.30
9	W	25[B]	ARG	NE-CZ-NH1	6.67	123.64	120.30
10	J	90	ASP	CB-CG-OD1	6.66	124.29	118.30
10	X	184	ASP	CB-CG-OD2	-6.65	112.31	118.30
13	M	180	ASP	CB-CG-OD2	6.58	124.22	118.30
6	F	85	ARG	NE-CZ-NH2	-6.57	117.02	120.30
8	H	89	ARG	NE-CZ-NH1	6.57	123.58	120.30
6	F	17	ASP	CB-CG-OD1	-6.56	112.40	118.30
2	P	4	ARG	NE-CZ-NH1	6.44	123.52	120.30
6	F	169	ARG	NE-CZ-NH1	6.43	123.51	120.30
10	X	90	ASP	CB-CG-OD1	6.41	124.07	118.30
2	B	4	ARG	NE-CZ-NH2	-6.35	117.13	120.30
6	T	43	ASP	CB-CG-OD2	6.31	123.98	118.30
3	C	182	GLU	CG-CD-OE2	-6.24	105.82	118.30
6	T	190	VAL	CB-CA-C	-6.23	99.56	111.40
5	S	7	ASP	CB-CG-OD1	-6.21	112.71	118.30
6	F	206	ASP	CB-CG-OD2	6.20	123.88	118.30
10	X	19	ARG	NE-CZ-NH1	6.18	123.39	120.30
5	S	122	ARG	NE-CZ-NH1	6.16	123.38	120.30
12	L	125	ASP	CB-CG-OD1	6.10	123.79	118.30
6	T	108	LEU	CB-CG-CD2	6.04	121.27	111.00
11	K	42	LEU	CB-CG-CD1	6.04	121.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	ARG	NE-CZ-NH2	-6.02	117.29	120.30
6	T	17	ASP	CB-CG-OD1	-5.98	112.92	118.30
8	H	198	ARG	NE-CZ-NH1	5.98	123.29	120.30
8	H	198	ARG	NE-CZ-NH2	-5.96	117.32	120.30
8	H	72	ARG	NE-CZ-NH2	-5.95	117.33	120.30
9	I	134	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	219	ARG	NE-CZ-NH1	5.83	123.22	120.30
9	W	134	ASP	CB-CG-OD1	5.81	123.53	118.30
2	P	4	ARG	NE-CZ-NH2	-5.81	117.40	120.30
5	S	236	LEU	N-CA-C	-5.79	95.36	111.00
11	K	107	ARG	NE-CZ-NH1	5.76	123.18	120.30
6	F	156	VAL	CG1-CB-CG2	-5.75	101.69	110.90
10	X	184	ASP	CB-CG-OD1	5.74	123.46	118.30
14	N	6	VAL	CB-CA-C	-5.72	100.53	111.40
2	P	236	LEU	CA-CB-CG	5.71	128.43	115.30
14	b	6	VAL	CB-CA-C	-5.71	100.55	111.40
4	D	168	ARG	NE-CZ-NH1	5.70	123.15	120.30
11	Y	107	ARG	NE-CZ-NH1	5.63	123.11	120.30
4	D	9	ASP	CB-CG-OD1	5.60	123.34	118.30
14	N	92	GLU	OE1-CD-OE2	-5.58	116.61	123.30
6	T	226	ILE	CB-CA-C	-5.58	100.45	111.60
1	O	88	ARG	NE-CZ-NH1	5.55	123.07	120.30
7	G	245	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	O	181	LEU	CA-CB-CG	5.54	128.04	115.30
7	G	88	ARG	CG-CD-NE	-5.54	100.18	111.80
13	a	44	ARG	NE-CZ-NH1	5.52	123.06	120.30
13	a	43	MET	CG-SD-CE	-5.52	91.37	100.20
7	G	108	GLU	CG-CD-OE2	-5.51	107.27	118.30
11	Y	141[A]	ARG	NE-CZ-NH1	5.50	123.05	120.30
11	Y	141[B]	ARG	NE-CZ-NH1	5.50	123.05	120.30
5	E	174	ARG	NE-CZ-NH1	5.49	123.05	120.30
6	T	85	ARG	NE-CZ-NH2	-5.46	117.57	120.30
7	G	11	ARG	CG-CD-NE	5.46	123.26	111.80
12	L	99	ARG	NE-CZ-NH2	5.45	123.02	120.30
11	Y	158	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	P	226	ARG	NE-CZ-NH2	5.44	123.02	120.30
13	a	180	ASP	CB-CG-OD1	5.43	123.19	118.30
1	O	109	LEU	CA-CB-CG	-5.41	102.86	115.30
11	Y	115	ASP	CB-CG-OD2	5.40	123.16	118.30
11	Y	58	LEU	CB-CG-CD1	5.37	120.13	111.00
5	S	174	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	C	182	GLU	OE1-CD-OE2	5.32	129.68	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	52	ASP	CB-CG-OD2	-5.31	113.52	118.30
8	V	145	ASP	CB-CG-OD1	5.30	123.07	118.30
14	b	45	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	Q	5	ARG	NE-CZ-NH1	5.24	122.92	120.30
7	G	108	GLU	OE1-CD-OE2	5.23	129.57	123.30
2	B	43	VAL	CB-CA-C	-5.21	101.50	111.40
11	K	141	ARG	NE-CZ-NH1	5.20	122.90	120.30
8	V	81	ARG	NE-CZ-NH2	-5.16	117.72	120.30
4	R	168	ARG	NE-CZ-NH2	-5.16	117.72	120.30
3	Q	5	ARG	NE-CZ-NH2	-5.16	117.72	120.30
13	M	171	ARG	NE-CZ-NH1	5.12	122.86	120.30
14	N	89	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	O	73	LEU	CB-CA-C	-5.11	100.50	110.20
11	K	12	VAL	CG1-CB-CG2	5.09	119.05	110.90
4	R	9	ASP	CB-CG-OD1	5.09	122.88	118.30
10	J	33	ASP	CB-CG-OD1	5.08	122.87	118.30
10	X	155	ARG	CB-CA-C	-5.07	100.26	110.40
3	C	185	ASP	CB-CG-OD1	5.06	122.86	118.30
12	L	99	ARG	NE-CZ-NH1	-5.05	117.78	120.30
8	V	184	ASP	CB-CG-OD1	-5.04	113.77	118.30
7	U	11	ARG	NE-CZ-NH1	5.01	122.81	120.30
13	a	154	LEU	CB-CG-CD1	5.01	119.51	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	202	GLY	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,Peptide
9	I	78[B]	GLY	Peptide
2	P	54	LYS	Peptide
3	Q	220	LEU	Peptide
3	Q	49	SER	Peptide
10	X	10	PRO	Mainchain
12	Z	99	ARG	Sidechain



## 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	1799	0	1793	8	0
1	O	1779	0	1747	13	0
2	B	1942	0	1938	6	0
2	P	1919	0	1895	16	0
3	C	1836	0	1821	20	0
3	Q	1821	0	1788	12	0
4	D	1783	0	1751	6	0
4	R	1773	0	1760	9	0
5	E	1833	0	1797	8	0
5	S	1880	0	1850	10	0
6	F	1890	0	1886	11	0
6	T	1867	0	1847	8	0
7	G	1928	0	1905	10	0
7	U	1820	0	1792	10	0
8	H	1672	0	1703	5	0
8	V	1655	0	1661	9	0
9	I	1633	0	1660	4	0
9	W	1604	0	1626	3	0
10	J	1585	0	1568	19	0
10	X	1590	0	1580	7	0
11	K	1543	0	1495	4	0
11	Y	1564	0	1539	9	0
12	L	1656	0	1655	7	0
12	Z	1644	0	1644	3	0
13	M	1687	0	1666	4	0
13	a	1688	0	1666	0	0
14	N	1515	0	1492	2	0
14	b	1526	0	1503	0	0
15	A	4	0	0	0	0
15	B	2	0	0	1	0
15	C	2	0	0	0	0
15	D	2	0	0	0	0
15	E	3	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	2	0	0	1	0
15	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	4	0	0	0	0
15	M	4	0	0	1	0
15	N	3	0	0	0	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	2	0	0	1	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	2	0	0	0	0
15	W	1	0	0	0	0
15	Y	5	0	0	1	0
15	a	3	0	0	0	0
15	b	3	0	0	0	0
16	G	16	0	22	1	0
16	I	32	0	44	0	0
16	L	16	0	22	0	0
16	W	16	0	22	0	0
16	Z	16	0	22	0	0
16	a	16	0	22	0	0
16	b	32	0	44	0	0
17	G	1	0	0	0	0
17	L	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	Z	1	0	0	0	0
17	b	1	0	0	0	0
18	H	2	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	K	1	0	0	0	0
18	L	1	0	0	0	0
18	V	1	0	0	0	0
18	W	1	0	0	0	0
18	X	1	0	0	0	0
19	A	112	0	0	1	0
19	B	123	0	0	0	0
19	C	75	0	0	0	0
19	D	83	0	0	0	0
19	E	134	0	0	1	0
19	F	189	0	0	5	0
19	G	190	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	H	151	0	0	2	0
19	I	149	0	0	1	0
19	J	127	0	0	1	0
19	K	108	0	0	0	0
19	L	115	0	0	1	0
19	M	155	0	0	0	0
19	N	164	0	0	0	0
19	O	85	0	0	1	0
19	P	111	0	0	1	0
19	Q	66	0	0	0	0
19	R	126	0	0	2	0
19	S	115	0	0	3	0
19	T	85	0	0	1	0
19	U	100	0	0	0	0
19	V	108	0	0	2	0
19	W	117	0	0	3	0
19	X	120	0	0	1	0
19	Y	145	0	0	0	0
19	Z	168	0	0	0	0
19	a	164	0	0	0	0
19	b	127	0	0	0	0
All	All	52161	0	48226	213	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 (213) 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)
3:C:182:GLU:CD	3:C:182:GLU:CG	1.93	1.34
10:J:1:MET:HG3	10:J:134:TYR:CD2	1.92	1.04
10:J:183:ILE:O	10:J:184:ASP:OD1	1.83	0.97
9:I:16[A]:LYS:O	19:I:401:HOH:O	1.85	0.95
10:J:1:MET:HG3	10:J:134:TYR:HD2	1.36	0.91
2:P:155:ASN:OD1	3:Q:77:THR:OG1	1.89	0.88
10:J:153:ARG:NH2	10:J:184:ASP:OD2	2.11	0.84
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.61	0.82
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.62	0.80
5:S:65[A]:HIS:CE1	19:S:401:HOH:O	2.34	0.80
7:G:192:GLU:OE2	19:G:401:HOH:O	2.01	0.77
4:R:129:ASP:CB	4:R:130:PRO:HD3	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:194:ILE:CD1	2:P:236:LEU:HB3	2.15	0.77
3:C:35:VAL:HG13	3:C:191:VAL:HG22	1.68	0.75
15:R:301:CL:CL	19:R:515:HOH:O	2.42	0.75
2:P:52:ILE:O	2:P:53:HIS:HB2	1.87	0.75
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.04	0.74
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.35	0.74
10:J:1:MET:CG	10:J:134:TYR:CD2	2.71	0.73
1:O:73:LEU:CD2	1:O:135:ILE:HG12	2.19	0.73
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.71	0.73
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.38	0.72
1:A:3:ARG:HG2	6:F:127:ALA:HB2	1.71	0.71
10:J:99[A]:HIS:CD2	19:J:408:HOH:O	2.45	0.69
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.74	0.68
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.74	0.68
10:J:153:ARG:NH1	10:J:184:ASP:OD2	2.28	0.67
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.40	0.66
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.77	0.65
1:O:181:LEU:CD2	1:O:185:ASP:HB2	2.27	0.64
12:L:144:MET:CE	12:L:185:ARG:HB2	2.29	0.63
9:W:16[B]:LYS:NZ	19:W:401:HOH:O	2.30	0.63
8:H:153:ASN:ND2	19:H:401:HOH:O	2.30	0.63
10:J:153:ARG:CZ	10:J:184:ASP:OD2	2.47	0.63
8:H:143:ARG:NH2	8:H:150:GLU:OE1	2.29	0.62
8:V:54:MET:HE1	19:W:495:HOH:O	2.00	0.61
10:J:183:ILE:C	10:J:184:ASP:OD1	2.39	0.61
10:J:182:ILE:CD1	10:J:191:LEU:HD11	2.31	0.61
2:P:25[B]:MET:HE1	19:P:433:HOH:O	1.99	0.61
1:O:180:ASP:N	1:O:180:ASP:OD1	2.34	0.60
3:Q:157:LYS:HB3	3:Q:176:TYR:CE2	2.37	0.60
10:J:12:TYR:CB	10:J:184:ASP:OD1	2.51	0.59
3:Q:157:LYS:HB3	3:Q:176:TYR:CZ	2.38	0.59
6:T:205:LYS:O	6:T:206:ASP:CG	2.41	0.58
16:G:303:1PE:H222	19:G:457:HOH:O	2.02	0.58
5:S:65[A]:HIS:ND1	19:S:401:HOH:O	2.32	0.58
10:J:12:TYR:HB2	10:J:184:ASP:OD1	2.05	0.56
3:C:182:GLU:CG	3:C:182:GLU:OE2	2.40	0.56
2:P:25[B]:MET:HA	2:P:25[B]:MET:CE	2.36	0.56
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.86	0.55
2:P:194:ILE:HD12	2:P:236:LEU:HB3	1.88	0.55
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.71	0.55
7:U:58:ASP:O	7:U:59:LYS:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.06	0.55
12:L:72:LEU:HD22	12:L:83:MET:SD	2.47	0.55
10:X:1:MET:HG2	10:X:134:TYR:H	1.71	0.55
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.37	0.55
3:Q:47:LYS:O	3:Q:48:LYS:CB	2.53	0.55
3:C:195:LEU:HD22	3:C:206:ILE:HG13	1.88	0.55
6:T:87:LEU:HD12	6:T:133[A]:CYS:SG	2.46	0.55
2:P:25[B]:MET:HA	2:P:25[B]:MET:HE2	1.89	0.54
4:R:129:ASP:CB	4:R:130:PRO:CD	2.85	0.54
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	2.07	0.54
2:P:194:ILE:HD13	2:P:236:LEU:HB3	1.89	0.54
6:F:87:LEU:HD12	6:F:133[A]:CYS:SG	2.48	0.54
15:H:304:CL:CL	19:H:533:HOH:O	2.55	0.54
5:S:185:ASN:HD21	5:S:189:LYS:HE2	1.72	0.54
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.48	0.53
12:Z:72:LEU:HD22	12:Z:83:MET:SD	2.48	0.53
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.91	0.53
14:N:190:LEU:H	14:N:193:GLN:HE21	1.57	0.53
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.91	0.52
13:M:112:ILE:HD12	13:M:112:ILE:N	2.25	0.52
7:U:43:ARG:HB3	7:U:151:VAL:HG13	1.91	0.52
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.91	0.51
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.93	0.51
3:Q:183:THR:HG23	3:Q:186:LEU:H	1.75	0.51
11:Y:141[A]:ARG:NE	11:Y:141[A]:ARG:HA	2.25	0.51
3:C:47:LYS:HB2	3:C:205:ASN:HB3	1.93	0.51
10:J:147:TYR:CE1	10:J:148:THR:C	2.85	0.51
1:O:181:LEU:HD21	1:O:185:ASP:HB2	1.92	0.51
3:C:157:LYS:HB3	3:C:176:TYR:CE2	2.46	0.50
7:G:43:ARG:HB3	7:G:151:VAL:HG23	1.93	0.50
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.94	0.50
11:K:176:LEU:HD23	11:K:187:VAL:HG22	1.93	0.50
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.94	0.50
1:A:221:THR:HG21	19:A:509:HOH:O	2.12	0.50
10:J:182:ILE:HD12	10:J:191:LEU:HD11	1.93	0.50
15:M:302:CL:CL	15:M:303:CL:CL	3.04	0.50
8:V:201:ARG:NH1	19:V:401:HOH:O	2.39	0.50
4:D:164:GLN:OE1	5:E:58:ALA:HB2	2.12	0.49
5:S:185:ASN:ND2	5:S:189:LYS:HE2	2.27	0.49
10:X:49:GLU:O	10:X:53:THR:HG23	2.13	0.49
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:195:LYS:HD2	12:Z:184:GLU:HG3	1.95	0.49
4:R:213:THR:HG22	4:R:231:LYS:HE3	1.95	0.49
3:C:40:ILE:HD11	3:C:210:VAL:CG1	2.42	0.49
3:C:203:GLY:HA3	3:C:206:ILE:HG22	1.94	0.49
6:F:105:ASN:ND2	19:F:405:HOH:O	2.44	0.49
7:G:192:GLU:HG3	19:G:401:HOH:O	2.12	0.49
6:F:169:ARG:NH1	19:F:406:HOH:O	2.46	0.49
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.94	0.48
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.53	0.48
7:G:88:ARG:NH1	19:G:406:HOH:O	2.46	0.48
3:C:182:GLU:CD	3:C:182:GLU:CB	2.76	0.48
6:T:170:GLN:O	6:T:174:THR:HG22	2.14	0.48
6:F:221:ASN:HB2	19:F:566:HOH:O	2.12	0.48
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.96	0.48
8:H:216:ILE:HD13	9:I:195:THR:HG23	1.94	0.48
11:K:141:ARG:HA	11:K:141:ARG:NE	2.28	0.48
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.10	0.48
2:B:194:ILE:HD12	2:B:236:LEU:HB3	1.96	0.47
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.44	0.47
11:Y:158:ARG:HE	11:Y:162:GLN:NE2	2.08	0.47
12:L:81:LYS:NZ	19:L:401:HOH:O	2.46	0.47
10:J:49:GLU:O	10:J:53:THR:HG23	2.14	0.47
1:A:206:ASN:C	1:A:206:ASN:HD22	2.18	0.47
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.96	0.47
11:Y:186[A]:ARG:HE	11:Y:186[A]:ARG:HB2	1.58	0.47
7:G:11:ARG:HG2	7:G:11:ARG:HH11	1.80	0.47
5:S:86:ASN:ND2	19:S:403:HOH:O	2.48	0.47
5:S:49:LEU:HG	5:S:195:LEU:HD21	1.96	0.46
5:E:230:SER:O	5:E:234:GLU:HG2	2.14	0.46
6:F:30:VAL:HG22	6:F:133[A]:CYS:HA	1.98	0.46
4:R:204:GLN:NE2	19:R:403:HOH:O	2.47	0.46
6:T:140:TYR:CZ	6:T:218:GLU:HG2	2.50	0.46
5:E:23:GLU:HA	5:E:26:MET:HE2	1.96	0.46
2:P:197:LEU:HB3	2:P:201:MET:HE3	1.96	0.46
9:I:141:CYS:HB3	9:I:177:ASP:HB2	1.97	0.46
12:L:159:GLN:HG3	8:V:210:ALA:HB2	1.98	0.46
3:Q:96:LEU:HD13	10:X:62:LYS:HG2	1.98	0.46
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.42	0.45
10:J:137:PHE:HB3	11:Y:133:VAL:HG21	1.98	0.45
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.46	0.45
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ILE:CD1	2:B:236:LEU:HB3	2.46	0.45
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.50	0.45
2:B:248:GLU:N	2:B:248:GLU:OE1	2.50	0.45
5:S:154:PHE:HD2	6:T:63:ASN:HD21	1.65	0.45
5:E:50:LYS:HB3	5:E:59:HIS:HB3	1.98	0.45
1:O:179:GLU:O	1:O:181:LEU:N	2.50	0.45
8:V:64:GLU:HG2	8:V:68:LEU:HD22	1.99	0.44
6:F:219:LEU:HD22	19:F:525:HOH:O	2.17	0.44
1:O:17:LYS:HE2	1:O:19:VAL:HG12	1.99	0.44
3:C:194:ALA:O	3:C:197:GLU:HB2	2.17	0.44
3:Q:45:VAL:HG21	3:Q:61:LYS:HB2	1.99	0.44
7:G:72:ILE:HG21	7:G:114:LEU:HD21	2.00	0.44
4:R:78:MET:HG3	4:R:82:ILE:HD12	2.00	0.44
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.98	0.44
11:K:133:VAL:HG21	10:X:137:PHE:HB3	2.00	0.44
1:O:206:ASN:C	1:O:206:ASN:HD22	2.21	0.44
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.91	0.44
7:U:58:ASP:O	7:U:59:LYS:CB	2.65	0.44
8:V:143:ARG:HE	8:V:143:ARG:HB2	1.67	0.44
15:B:301:CL:CL	15:B:302:CL:CL	3.10	0.43
5:E:65:HIS:HB2	19:E:494:HOH:O	2.17	0.43
6:T:30:VAL:HG22	6:T:133[A]:CYS:HA	1.99	0.43
2:P:52:ILE:O	2:P:53:HIS:CB	2.64	0.43
4:R:96:THR:HG22	4:R:112:VAL:HG22	2.00	0.43
4:R:199:LEU:HD12	4:R:237:VAL:HG12	2.01	0.43
11:Y:68:LEU:O	11:Y:71:LYS:CE	2.66	0.43
4:D:127:ASP:HB3	5:E:125:ARG:HD3	2.00	0.43
8:V:153:ASN:HB2	19:V:493:HOH:O	2.18	0.43
5:S:189:LYS:HG2	5:S:236:LEU:HD13	2.01	0.43
7:G:49[B]:VAL:HG22	7:G:219:VAL:HG12	2.00	0.43
2:P:50:ARG:O	2:P:52:ILE:N	2.52	0.43
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.49	0.43
7:U:6:SER:OG	7:U:11:ARG:NH1	2.45	0.43
8:V:97:ALA:HB1	8:V:127[B]:MET:CE	2.49	0.42
3:C:183:THR:HG23	3:C:186:LEU:H	1.84	0.42
1:O:109:LEU:O	1:O:109:LEU:HG	2.16	0.42
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.19	0.42
5:E:49:LEU:HG	5:E:195:LEU:HD21	2.00	0.42
9:I:116:PHE:CD2	9:I:191:LYS:HE3	2.54	0.42
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.42
3:C:4:ASP:O	4:D:125:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:199:LEU:HD12	4:R:237:VAL:CG1	2.49	0.42
1:A:164:LYS:HE2	1:A:164:LYS:HB3	1.81	0.42
3:C:5:ARG:NH1	4:D:125:GLU:OE2	2.44	0.42
7:U:43:ARG:HB3	7:U:151:VAL:CG1	2.50	0.42
7:U:77:GLY:HA3	7:U:227:PHE:CD1	2.55	0.42
2:P:51:ASN:HB3	2:P:56:LEU:HD13	2.02	0.42
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.20	0.42
2:P:190:LEU:HG	2:P:236:LEU:HD21	2.01	0.42
6:T:110:HIS:HD2	19:T:364:HOH:O	2.03	0.41
6:F:243:LEU:O	6:F:244:LYS:C	2.57	0.41
19:F:448:HOH:O	7:G:88:ARG:HD2	2.20	0.41
8:H:43:CYS:SG	8:H:98:LEU:HB3	2.60	0.41
7:U:42:VAL:HG13	7:U:198:ALA:HB2	2.02	0.41
10:X:132:HIS:HD2	19:X:488:HOH:O	2.03	0.41
1:O:181:LEU:HD23	1:O:185:ASP:HB2	2.00	0.41
2:B:160:LYS:HE2	2:B:181:GLU:HG3	2.02	0.41
6:F:53:VAL:HG12	6:F:208:ALA:HB3	2.03	0.41
9:W:141:CYS:HB3	9:W:177:ASP:HB2	2.02	0.41
9:W:30:GLN:NE2	19:W:403:HOH:O	2.45	0.41
10:X:62:LYS:HA	10:X:62:LYS:HD3	1.81	0.41
7:G:192:GLU:OE1	7:G:193:GLN:OE1	2.39	0.41
11:Y:1:THR:HB	15:Y:301:CL:CL	2.58	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.03	0.41
12:L:144:MET:HE2	12:L:144:MET:HB3	1.90	0.41
12:L:184:GLU:OE2	12:L:211:ARG:HD2	2.21	0.41
3:Q:183:THR:HG22	3:Q:186:LEU:HD22	2.02	0.41
7:U:51:VAL:HG12	7:U:198:ALA:HB1	2.03	0.41
11:Y:9:ARG:NH2	11:Y:146:ASP:OD1	2.53	0.41
3:C:45:VAL:HG21	3:C:61:LYS:HB2	2.04	0.40
10:J:155:ARG:HD2	10:J:155:ARG:HA	1.95	0.40
3:C:106:TYR:CD1	3:C:106:TYR:C	2.94	0.40
13:M:27:LEU:HD22	13:M:184:TYR:HB2	2.02	0.40
10:J:62:LYS:HD3	10:J:62:LYS:HA	1.84	0.40
13:M:92:LEU:O	13:M:96:MET:HG2	2.22	0.40
1:O:227:ASP:HB2	19:O:471:HOH:O	2.20	0.40
4:D:203:LYS:HE2	4:D:210:LEU:HB3	2.03	0.40
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.56	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/234 (98%)	220 (96%)	6 (3%)	4 (2%)	9	2
1	O	228/234 (97%)	214 (94%)	7 (3%)	7 (3%)	4	0
2	B	247/261 (95%)	238 (96%)	9 (4%)	0	100	100
2	P	247/261 (95%)	234 (95%)	11 (4%)	2 (1%)	19	7
3	C	234/248 (94%)	224 (96%)	6 (3%)	4 (2%)	9	2
3	Q	229/248 (92%)	218 (95%)	6 (3%)	5 (2%)	6	1
4	D	233/241 (97%)	223 (96%)	6 (3%)	4 (2%)	9	2
4	R	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	12	3
5	E	231/263 (88%)	226 (98%)	4 (2%)	1 (0%)	34	21
5	S	238/263 (90%)	234 (98%)	4 (2%)	0	100	100
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100	100
6	T	239/255 (94%)	233 (98%)	4 (2%)	2 (1%)	19	7
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	228/246 (93%)	224 (98%)	4 (2%)	0	100	100
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	215 (98%)	4 (2%)	1 (0%)	29	15
9	I	208/205 (102%)	204 (98%)	4 (2%)	0	100	100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100	100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
11	K	199/204 (98%)	195 (98%)	4 (2%)	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	214/219 (98%)	208 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	6196/6458 (96%)	6031 (97%)	132 (2%)	33 (0%)	29	15

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
4	D	127	ASP
4	D	176	GLY
1	O	52	LYS
1	O	53	SER
1	O	179	GLU
1	O	180	ASP
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
3	C	50	VAL
4	D	175[A]	GLU
4	D	175[B]	GLU
5	E	59	HIS
1	O	4	GLY
1	O	231	ALA
2	P	53	HIS
2	P	54	LYS
3	Q	48	LYS
1	A	50	LYS
3	C	48	LYS
3	C	202	GLY
3	C	216	SER
3	Q	49	SER
3	Q	216	SER
6	T	208	ALA
8	V	203	ARG
1	A	201	GLN
3	Q	50	VAL
1	O	201	GLN
6	T	206	ASP
3	Q	221	ASN

### 5.3.2 Protein sidechains [i](#)

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	188/191 (98%)	177 (94%)	11 (6%)	19	7
1	O	184/191 (96%)	172 (94%)	12 (6%)	17	6
2	B	205/221 (93%)	198 (97%)	7 (3%)	37	22
2	P	201/221 (91%)	190 (94%)	11 (6%)	21	8
3	C	189/210 (90%)	181 (96%)	8 (4%)	30	15
3	Q	189/210 (90%)	176 (93%)	13 (7%)	15	5
4	D	194/203 (96%)	187 (96%)	7 (4%)	35	20
4	R	192/203 (95%)	189 (98%)	3 (2%)	62	54
5	E	195/223 (87%)	188 (96%)	7 (4%)	35	20
5	S	201/223 (90%)	194 (96%)	7 (4%)	36	21
6	F	200/212 (94%)	192 (96%)	8 (4%)	31	16
6	T	194/212 (92%)	184 (95%)	10 (5%)	23	10
7	G	206/207 (100%)	201 (98%)	5 (2%)	49	36
7	U	192/207 (93%)	187 (97%)	5 (3%)	46	32
8	H	183/195 (94%)	179 (98%)	4 (2%)	52	39
8	V	180/195 (92%)	172 (96%)	8 (4%)	28	14
9	I	178/174 (102%)	178 (100%)	0	100	100
9	W	174/174 (100%)	174 (100%)	0	100	100
10	J	166/170 (98%)	160 (96%)	6 (4%)	35	20
10	X	168/170 (99%)	164 (98%)	4 (2%)	49	36
11	K	153/159 (96%)	144 (94%)	9 (6%)	19	7
11	Y	157/159 (99%)	152 (97%)	5 (3%)	39	25
12	L	179/178 (101%)	170 (95%)	9 (5%)	24	10
12	Z	176/178 (99%)	171 (97%)	5 (3%)	43	30
13	M	179/181 (99%)	175 (98%)	4 (2%)	52	39
13	a	179/181 (99%)	174 (97%)	5 (3%)	43	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	157/159 (99%)	155 (99%)	2 (1%)	69	62
14	b	159/159 (100%)	158 (99%)	1 (1%)	86	84
All	All	5118/5366 (95%)	4942 (97%)	176 (3%)	37	22

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	53	SER
1	A	61	VAL
1	A	73	LEU
1	A	142	ARG
1	A	164	LYS
1	A	176	ARG
1	A	178	ASN
1	A	189	THR
1	A	206	ASN
1	A	227	ASP
2	B	43	VAL
2	B	65	ILE
2	B	190	LEU
2	B	204	SER
2	B	207	SER
2	B	229	LYS
2	B	249	ARG
3	C	2	SER
3	C	54	GLN
3	C	105	GLU
3	C	163	ARG
3	C	206	ILE
3	C	208	LEU
3	C	215	GLN
3	C	219	ILE
4	D	46	VAL
4	D	95	GLU
4	D	126	GLU
4	D	129	ASP
4	D	187	LYS
4	D	199	LEU
4	D	217	LEU
5	E	29	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	61	LYS
5	E	101	ARG
5	E	181	GLU
5	E	204	ASP
5	E	234	GLU
5	E	236	LEU
6	F	17	ASP
6	F	31	GLU
6	F	53	VAL
6	F	190	VAL
6	F	215	TRP
6	F	230	ASP
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	146	GLU
7	G	183	VAL
7	G	206	LEU
8	H	22	GLU
8	H	65	LEU
8	H	199	LEU
8	H	220	GLU
10	J	1	MET
10	J	27	GLN
10	J	62	LYS
10	J	86	ARG
10	J	155	ARG
10	J	185	LYS
11	K	12	VAL
11	K	42	LEU
11	K	58	LEU
11	K	106	LYS
11	K	141	ARG
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	VAL
12	L	1	ARG
12	L	3[A]	SER
12	L	3[B]	SER
12	L	72	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	L	102	PHE
12	L	163	HIS
12	L	169	ASP
12	L	174	LEU
12	L	207	THR
13	M	100	ARG
13	M	154	LEU
13	M	155	GLU
13	M	216	SER
14	N	196	LYS
14	N	202	LEU
1	O	3	ARG
1	O	53	SER
1	O	118	GLN
1	O	142	ARG
1	O	174	GLU
1	O	176	ARG
1	O	178	ASN
1	O	179	GLU
1	O	180	ASP
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
2	P	7[A]	SER
2	P	7[B]	SER
2	P	43	VAL
2	P	53	HIS
2	P	65	ILE
2	P	160	LYS
2	P	190	LEU
2	P	207	SER
2	P	226	ARG
2	P	235	GLN
2	P	236	LEU
3	Q	2	SER
3	Q	56	GLU
3	Q	105	GLU
3	Q	148	ASP
3	Q	163	ARG
3	Q	166	LYS
3	Q	170	GLU
3	Q	205	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	206	ILE
3	Q	208	LEU
3	Q	215	GLN
3	Q	219	ILE
3	Q	226	GLU
4	R	46	VAL
4	R	130	PRO
4	R	217	LEU
5	S	29	VAL
5	S	45	VAL
5	S	101	ARG
5	S	122	ARG
5	S	181	GLU
5	S	202	GLU
5	S	204	ASP
6	T	17	ASP
6	T	31	GLU
6	T	53	VAL
6	T	54	LEU
6	T	81	LEU
6	T	174	THR
6	T	190	VAL
6	T	215	TRP
6	T	226	ILE
6	T	234	GLU
7	U	42	VAL
7	U	78	CYS
7	U	196	GLU
7	U	199	ILE
7	U	206	LEU
8	V	22	GLU
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	201	ARG
8	V	205	GLU
8	V	220	GLU
10	X	62	LYS
10	X	86	ARG
10	X	95	ARG
10	X	174	ASN

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Mol	Chain	Res	Type
11	Y	58	LEU
11	Y	89	GLN
11	Y	141[A]	ARG
11	Y	141[B]	ARG
11	Y	147	LEU
12	Z	72	LEU
12	Z	102	PHE
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
13	a	71	VAL
13	a	92	LEU
13	a	100	ARG
13	a	154	LEU
13	a	216	SER
14	b	196	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
2	B	102	GLN
2	B	109	GLN
4	D	227	HIS
5	E	65	HIS
6	F	143	ASN
7	G	193	GLN
8	H	116	HIS
8	H	153	ASN
9	I	161	HIS
10	J	101	ASN
12	L	152	GLN
12	L	157	ASN
13	M	47	ASN
13	M	162	GLN
14	N	193	GLN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN

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Mol	Chain	Res	Type
2	P	109	GLN
3	Q	18	GLN
3	Q	239	ASN
4	R	204	GLN
4	R	227	HIS
5	S	86	ASN
5	S	185	ASN
6	T	63	ASN
6	T	143	ASN
7	U	128	ASN
8	V	116	HIS
8	V	153	ASN
9	W	172	ASN
10	X	24	ASN
10	X	132	HIS
10	X	174	ASN
11	Y	162	GLN
12	Z	79	ASN
12	Z	157	ASN
13	a	89	HIS
13	a	162	GLN
14	b	193	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](#)

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
7	6V1	G	161	7	12,15,16	1.93	4 (33%)	9,20,22	2.13	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	6V1	E	148	5	12,15,16	1.79	4 (33%)	9,20,22	3.07	3 (33%)
7	YCM	U	137	7	7,9,10	1.25	1 (14%)	4,10,12	1.92	2 (50%)
7	6V1	G	47	7	12,15,16	3.22	5 (41%)	9,20,22	2.27	3 (33%)
10	6V1	X	91	10	12,15,16	2.73	4 (33%)	9,20,22	5.55	7 (77%)
3	YCM	C	63	3	7,9,10	1.07	1 (14%)	4,10,12	0.73	0
10	6V1	J	91	10	12,15,16	2.43	2 (16%)	9,20,22	5.84	7 (77%)
7	6V1	U	47	7	12,15,16	2.14	2 (16%)	9,20,22	3.01	3 (33%)
5	6V1	S	148	5	12,15,16	1.88	2 (16%)	9,20,22	3.32	5 (55%)
3	YCM	Q	63	3	7,9,10	1.64	1 (14%)	4,10,12	3.94	3 (75%)
7	YCM	G	137	7	7,9,10	2.19	3 (42%)	4,10,12	2.50	3 (75%)
7	6V1	U	161	7	12,15,16	1.85	4 (33%)	9,20,22	2.47	4 (44%)

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
7	6V1	G	161	7	-	1/6/25/27	0/1/1/1
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1
7	YCM	U	137	7	-	1/6/8/10	-
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
3	YCM	C	63	3	-	1/6/8/10	-
10	6V1	J	91	10	-	3/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	2/6/25/27	0/1/1/1
5	6V1	S	148	5	-	2/6/25/27	0/1/1/1
3	YCM	Q	63	3	-	3/6/8/10	-
7	YCM	G	137	7	-	2/6/8/10	-
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-8.11	1.73	1.82
10	X	91	6V1	C1-SG	-7.84	1.74	1.83
10	J	91	6V1	C1-SG	-7.47	1.75	1.83
7	U	47	6V1	CB-SG	-6.21	1.75	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	148	6V1	CB-SG	-4.55	1.77	1.82
7	G	47	6V1	C4-N3	-4.28	1.31	1.38
5	E	148	6V1	CB-SG	-4.11	1.77	1.82
7	G	47	6V1	C1-SG	3.95	1.87	1.83
3	Q	63	YCM	CD-SG	-3.70	1.72	1.81
7	G	47	6V1	C2-N3	-3.63	1.33	1.38
7	G	137	YCM	CE-NZ2	3.55	1.44	1.32
10	X	91	6V1	CB-SG	-3.47	1.78	1.82
5	S	148	6V1	C2-N3	-3.45	1.33	1.38
7	G	161	6V1	CB-SG	-3.29	1.78	1.82
7	G	161	6V1	C2-N3	-3.20	1.34	1.38
7	U	161	6V1	C1-SG	-3.15	1.79	1.83
7	U	161	6V1	CB-SG	-3.14	1.78	1.82
7	G	161	6V1	C1-SG	-3.14	1.79	1.83
7	U	161	6V1	C4-N3	-3.14	1.33	1.38
7	G	137	YCM	CD-SG	2.91	1.89	1.81
7	G	137	YCM	CB-SG	-2.81	1.69	1.80
7	U	161	6V1	C2-N3	-2.74	1.34	1.38
7	G	47	6V1	C5-C4	2.71	1.54	1.50
7	G	161	6V1	C4-N3	-2.71	1.34	1.38
10	X	91	6V1	O7-C2	2.68	1.27	1.22
7	U	47	6V1	C4-N3	-2.66	1.34	1.38
5	E	148	6V1	C4-N3	-2.54	1.34	1.38
5	E	148	6V1	C1-SG	-2.42	1.80	1.83
10	J	91	6V1	CB-SG	-2.41	1.79	1.82
5	E	148	6V1	C2-N3	-2.36	1.35	1.38
3	C	63	YCM	CD-SG	-2.17	1.76	1.81
10	X	91	6V1	C4-N3	-2.14	1.35	1.38
7	U	137	YCM	CA-N	-2.06	1.41	1.48

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	91	6V1	C5-C4-N3	10.03	114.04	108.13
10	J	91	6V1	C6-N3-C2	9.25	135.09	123.36
10	X	91	6V1	C5-C4-N3	9.05	113.46	108.13
10	X	91	6V1	C6-N3-C2	8.49	134.12	123.36
3	Q	63	YCM	CE-CD-SG	-6.49	94.49	113.59
10	X	91	6V1	O7-C2-N3	6.20	131.72	124.14
5	S	148	6V1	C5-C4-N3	6.11	111.73	108.13
10	J	91	6V1	C2-N3-C4	-5.90	109.54	113.04
5	E	148	6V1	C5-C4-N3	5.84	111.57	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	47	6V1	C5-C4-N3	5.80	111.55	108.13
10	J	91	6V1	C6-N3-C4	-5.60	115.29	122.59
5	S	148	6V1	C2-N3-C4	-5.46	109.80	113.04
7	U	47	6V1	C2-N3-C4	-5.36	109.86	113.04
10	X	91	6V1	C2-N3-C4	-5.32	109.89	113.04
10	X	91	6V1	C6-N3-C4	-5.17	115.85	122.59
10	J	91	6V1	O7-C2-N3	5.10	130.38	124.14
5	E	148	6V1	C2-N3-C4	-4.89	110.14	113.04
7	G	47	6V1	C2-N3-C4	-4.86	110.15	113.04
5	S	148	6V1	C6-N3-C2	4.40	128.94	123.36
7	G	161	6V1	O8-C4-N3	4.15	128.51	123.92
10	X	91	6V1	O8-C4-C5	-4.13	121.23	127.24
7	U	161	6V1	C2-N3-C4	-4.03	110.65	113.04
10	J	91	6V1	O8-C4-C5	-4.02	121.39	127.24
5	E	148	6V1	C6-N3-C2	4.00	128.43	123.36
7	U	161	6V1	C5-C4-N3	3.80	110.37	108.13
3	Q	63	YCM	CA-CB-SG	-3.32	101.60	113.74
7	G	137	YCM	CE-CD-SG	3.23	123.10	113.59
7	U	161	6V1	O8-C4-C5	-3.19	122.59	127.24
10	X	91	6V1	C3-C6-N3	3.17	122.01	111.65
10	J	91	6V1	C3-C6-N3	3.13	121.89	111.65
7	G	161	6V1	O8-C4-C5	-3.11	122.71	127.24
3	Q	63	YCM	CB-SG-CD	2.90	131.39	104.44
7	U	47	6V1	O8-C4-C5	-2.88	123.05	127.24
7	U	161	6V1	O8-C4-N3	2.81	127.03	123.92
7	G	47	6V1	O7-C2-N3	-2.69	120.85	124.14
7	G	137	YCM	CA-CB-SG	-2.64	104.06	113.74
7	U	137	YCM	CA-CB-SG	-2.43	104.84	113.74
7	U	137	YCM	CE-CD-SG	2.41	120.69	113.59
5	S	148	6V1	O8-C4-C5	-2.40	123.75	127.24
7	G	161	6V1	O7-C2-N3	2.21	126.84	124.14
7	G	47	6V1	O8-C4-C5	2.14	130.36	127.24
5	S	148	6V1	C3-C6-N3	2.11	118.57	111.65
7	G	137	YCM	OZ1-CE-NZ2	-2.02	116.99	122.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	63	YCM	CE-CD-SG-CB
5	E	148	6V1	C3-C6-N3-C2
5	E	148	6V1	C3-C6-N3-C4
7	G	137	YCM	CE-CD-SG-CB
7	G	137	YCM	SG-CD-CE-NZ2
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2
5	S	148	6V1	C3-C6-N3-C2
5	S	148	6V1	C3-C6-N3-C4
7	U	47	6V1	C3-C6-N3-C2
7	U	47	6V1	C3-C6-N3-C4
7	U	137	YCM	CE-CD-SG-CB
10	X	91	6V1	C3-C6-N3-C2
10	X	91	6V1	C3-C6-N3-C4
7	G	161	6V1	N-CA-CB-SG
7	U	161	6V1	N-CA-CB-SG
10	J	91	6V1	CA-CB-SG-C1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 73 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	$\# Z  > 2$
16	1PE	W	303	-	15,15,15	0.56	0	14,14,14	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	1PE	a	304	-	15,15,15	0.53	0	14,14,14	0.57	0
16	1PE	G	303	-	15,15,15	0.57	0	14,14,14	0.70	0
16	1PE	Z	301	-	15,15,15	0.62	0	14,14,14	0.62	0
16	1PE	b	505	-	15,15,15	0.66	0	14,14,14	0.39	0
16	1PE	I	304	-	15,15,15	0.53	0	14,14,14	0.64	0
16	1PE	b	504	-	15,15,15	0.61	0	14,14,14	0.77	0
16	1PE	I	303	-	15,15,15	0.55	0	14,14,14	0.86	1 (7%)
16	1PE	L	301	-	15,15,15	0.61	0	14,14,14	0.73	1 (7%)

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	1PE	W	303	-	-	6/13/13/13	-
16	1PE	a	304	-	-	4/13/13/13	-
16	1PE	G	303	-	-	3/13/13/13	-
16	1PE	Z	301	-	-	6/13/13/13	-
16	1PE	b	505	-	-	9/13/13/13	-
16	1PE	I	304	-	-	5/13/13/13	-
16	1PE	b	504	-	-	5/13/13/13	-
16	1PE	I	303	-	-	8/13/13/13	-
16	1PE	L	301	-	-	6/13/13/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	303	1PE	C25-OH5-C14	2.12	122.49	113.29
16	L	301	1PE	C26-OH6-C15	2.11	122.45	113.29

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	I	304	1PE	C24-C14-OH5-C25
16	I	303	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
16	b	505	1PE	OH5-C14-C24-OH4
16	L	301	1PE	OH6-C15-C25-OH5
16	W	303	1PE	OH6-C15-C25-OH5
16	Z	301	1PE	OH6-C15-C25-OH5
16	L	301	1PE	C16-C26-OH6-C15
16	G	303	1PE	C13-C23-OH3-C22
16	b	504	1PE	OH6-C15-C25-OH5
16	a	304	1PE	OH4-C13-C23-OH3
16	I	304	1PE	OH4-C13-C23-OH3
16	L	301	1PE	OH5-C14-C24-OH4
16	Z	301	1PE	C16-C26-OH6-C15
16	a	304	1PE	OH5-C14-C24-OH4
16	b	505	1PE	OH4-C13-C23-OH3
16	I	303	1PE	OH6-C15-C25-OH5
16	b	504	1PE	OH4-C13-C23-OH3
16	I	303	1PE	OH2-C12-C22-OH3
16	a	304	1PE	OH7-C16-C26-OH6
16	b	505	1PE	OH7-C16-C26-OH6
16	Z	301	1PE	OH4-C13-C23-OH3
16	b	505	1PE	OH6-C15-C25-OH5
16	G	303	1PE	OH7-C16-C26-OH6
16	b	504	1PE	C24-C14-OH5-C25
16	L	301	1PE	C25-C15-OH6-C26
16	I	303	1PE	OH4-C13-C23-OH3
16	I	303	1PE	C14-C24-OH4-C13
16	L	301	1PE	C13-C23-OH3-C22
16	W	303	1PE	C13-C23-OH3-C22
16	W	303	1PE	C23-C13-OH4-C24
16	b	505	1PE	C12-C22-OH3-C23
16	b	505	1PE	C23-C13-OH4-C24
16	W	303	1PE	C14-C24-OH4-C13
16	I	303	1PE	C24-C14-OH5-C25
16	I	304	1PE	C23-C13-OH4-C24
16	W	303	1PE	C24-C14-OH5-C25
16	Z	301	1PE	C15-C25-OH5-C14
16	G	303	1PE	OH2-C12-C22-OH3
16	a	304	1PE	C25-C15-OH6-C26
16	I	304	1PE	OH7-C16-C26-OH6
16	b	505	1PE	OH2-C12-C22-OH3
16	W	303	1PE	C12-C22-OH3-C23
16	b	505	1PE	C14-C24-OH4-C13
16	Z	301	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
16	b	504	1PE	C14-C24-OH4-C13
16	I	303	1PE	C25-C15-OH6-C26
16	I	303	1PE	C12-C22-OH3-C23
16	Z	301	1PE	OH2-C12-C22-OH3
16	b	505	1PE	C15-C25-OH5-C14
16	L	301	1PE	OH2-C12-C22-OH3
16	I	304	1PE	OH6-C15-C25-OH5
16	b	504	1PE	C13-C23-OH3-C22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	303	1PE	1	0

## 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 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%)	-0.11	4 (1%) 70 66	27, 42, 75, 87	0
1	O	230/234 (98%)	0.34	17 (7%) 14 11	36, 56, 92, 119	0
2	B	248/261 (95%)	0.11	9 (3%) 42 37	31, 48, 85, 130	0
2	P	247/261 (94%)	0.25	18 (7%) 15 11	35, 53, 91, 133	0
3	C	236/248 (95%)	0.47	20 (8%) 10 8	32, 57, 97, 128	0
3	Q	233/248 (93%)	0.28	15 (6%) 19 15	31, 54, 95, 127	0
4	D	233/241 (96%)	0.23	13 (5%) 24 19	35, 55, 85, 106	0
4	R	233/241 (96%)	-0.11	5 (2%) 63 59	29, 40, 62, 82	0
5	E	233/263 (88%)	0.09	14 (6%) 21 17	25, 39, 82, 98	0
5	S	237/263 (90%)	-0.05	8 (3%) 45 39	31, 43, 72, 94	0
6	F	239/255 (93%)	-0.15	0 100 100	22, 32, 52, 72	0
6	T	240/255 (94%)	0.17	11 (4%) 32 26	32, 49, 79, 105	0
7	G	241/246 (97%)	-0.10	3 (1%) 79 76	23, 35, 65, 89	0
7	U	232/246 (94%)	0.23	14 (6%) 21 17	38, 56, 86, 122	0
8	H	220/234 (94%)	-0.00	4 (1%) 68 64	25, 32, 62, 87	0
8	V	220/234 (94%)	-0.07	6 (2%) 54 49	34, 44, 78, 100	0
9	I	204/205 (99%)	-0.25	0 100 100	25, 32, 51, 64	0
9	W	204/205 (99%)	-0.22	2 (0%) 82 80	32, 44, 66, 72	0
10	J	195/201 (97%)	-0.16	1 (0%) 91 89	28, 38, 55, 70	0
10	X	195/201 (97%)	-0.22	0 100 100	30, 38, 54, 69	0
11	K	201/204 (98%)	-0.28	0 100 100	32, 41, 65, 90	0
11	Y	199/204 (97%)	-0.26	0 100 100	26, 33, 51, 62	0
12	L	213/213 (100%)	-0.11	0 100 100	29, 45, 65, 83	0
12	Z	213/213 (100%)	-0.16	1 (0%) 91 89	24, 34, 55, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	-0.10	2 (0%) 84 82	24, 35, 59, 94	0
13	a	216/219 (98%)	-0.14	2 (0%) 84 82	24, 36, 57, 82	0
14	N	202/205 (98%)	-0.08	3 (1%) 73 70	23, 32, 52, 91	0
14	b	203/205 (99%)	-0.13	4 (1%) 65 61	30, 38, 63, 90	0
All	All	6213/6458 (96%)	-0.01	176 (2%) 53 47	22, 42, 78, 133	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	232	ILE	13.9
2	B	203	VAL	10.3
4	D	241	ILE	9.3
2	P	204	SER	9.0
2	P	203	VAL	9.0
5	E	54	SER	8.7
3	C	138	PHE	8.4
3	C	49	SER	7.0
2	P	61	PHE	6.8
5	E	52	ALA	6.8
7	U	2	SER	6.6
4	R	131	GLY	6.4
3	Q	238	GLU	6.2
2	P	205	LYS	6.0
3	Q	48	LYS	5.9
4	R	130	PRO	5.9
7	G	187	PHE	5.7
8	V	199	LEU	5.6
14	N	202	LEU	5.5
8	V	203	ARG	5.5
2	B	61	PHE	5.4
3	C	200	GLN	5.4
6	T	208	ALA	5.3
2	P	234	GLU	5.2
3	Q	232	ILE	5.1
14	b	199	VAL	5.1
3	C	225	ILE	5.0
8	H	204	CYS	5.0
3	Q	234	LYS	4.9
8	V	204	CYS	4.6
6	T	54	LEU	4.6
5	E	58	ALA	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	202	ASP	4.6
5	E	56	LEU	4.5
1	O	201	GLN	4.4
3	Q	240	GLU	4.4
3	C	48	LYS	4.3
7	G	188	ASP	4.3
13	M	215	ILE	4.3
5	E	201	ALA	4.3
7	U	58	ASP	4.2
4	D	130	PRO	4.2
3	C	201	SER	4.2
1	A	231	ALA	4.2
2	P	247	ALA	4.2
4	R	241	ILE	4.1
14	b	203	PRO	4.1
3	Q	138	PHE	4.0
5	E	59	HIS	4.0
5	E	53	GLN	4.0
7	U	57	PRO	4.0
14	b	200	ALA	4.0
13	a	215	ILE	3.9
2	B	204	SER	3.9
10	J	184	ASP	3.8
12	Z	161	VAL	3.8
3	C	236	LYS	3.7
3	Q	236	LYS	3.7
5	S	53	GLN	3.7
3	C	232	ILE	3.7
7	U	3	ARG	3.6
13	a	216	SER	3.6
2	P	230	GLN	3.6
14	N	199	VAL	3.6
1	O	50	LYS	3.5
13	M	216	SER	3.5
1	O	188	HIS	3.4
5	E	235	GLY	3.4
2	P	202	ASP	3.4
6	T	5	THR	3.4
4	R	127	ASP	3.4
7	G	189	TRP	3.4
2	P	53	HIS	3.4
4	D	131	GLY	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	183	GLU	3.3
1	A	232	ILE	3.3
3	Q	233	GLU	3.3
3	C	229	VAL	3.3
5	S	2	PHE	3.2
7	U	242	LEU	3.2
5	E	202	GLU	3.2
8	H	197	THR	3.2
6	T	206	ASP	3.2
2	P	58	GLU	3.2
7	U	206	LEU	3.2
5	S	174	ARG	3.2
6	T	207	LYS	3.2
5	S	237	GLU	3.1
2	B	205	LYS	3.1
2	B	247	ALA	3.1
3	Q	205	ASN	3.1
5	E	57	ALA	3.1
1	O	199	GLU	3.0
6	T	209	PHE	3.0
1	O	176	ARG	3.0
1	O	200	GLY	3.0
5	S	57	ALA	3.0
4	D	127	ASP	3.0
2	P	245	ALA	3.0
7	U	212	PRO	3.0
2	P	52	ILE	2.9
8	H	201	ARG	2.9
6	T	205	LYS	2.9
1	A	3	ARG	2.9
3	Q	239	ASN	2.9
8	V	197	THR	2.9
4	D	237	VAL	2.9
4	D	234	LEU	2.8
1	O	177	TYR	2.8
5	E	51	ARG	2.8
3	C	203	GLY	2.8
1	O	181	LEU	2.7
3	C	195	LEU	2.7
1	O	157	TRP	2.7
5	E	218	ASP	2.7
3	C	56	GLU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	S	54	SER	2.7
3	Q	47	LYS	2.7
2	P	220	ASN	2.7
7	U	208	ILE	2.7
5	S	51	ARG	2.7
2	B	248	GLU	2.7
4	D	239	LYS	2.6
4	D	240	ASP	2.6
5	E	60	GLN	2.6
5	E	237	GLU	2.6
6	T	180	GLN	2.6
8	V	198	ARG	2.6
1	O	3	ARG	2.6
3	C	234	LYS	2.5
3	Q	223	GLU	2.5
1	O	59	ARG	2.5
3	Q	50	VAL	2.5
4	R	128	ALA	2.5
14	N	198	ALA	2.5
4	D	223	GLY	2.5
8	H	203	ARG	2.5
1	A	230	ALA	2.5
3	C	171	PHE	2.5
2	P	238	LYS	2.4
4	D	129	ASP	2.4
7	U	243	ALA	2.4
7	U	240	VAL	2.4
14	b	201	THR	2.4
3	C	202	GLY	2.4
3	C	39	ASP	2.4
2	P	51	ASN	2.4
3	C	98	VAL	2.3
3	Q	229	VAL	2.3
6	T	53	VAL	2.3
3	C	217	LEU	2.3
9	W	161	HIS	2.3
4	D	232	GLU	2.3
7	U	223	GLU	2.3
2	P	206	LEU	2.3
4	D	188	SER	2.3
8	V	201	ARG	2.3
6	T	63	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
6	T	37	ILE	2.2
3	C	233	GLU	2.2
3	Q	237	GLU	2.2
2	B	241	GLU	2.2
1	O	191	ILE	2.2
2	B	206	LEU	2.2
1	O	198	PHE	2.2
5	S	217	LYS	2.2
2	P	244	GLU	2.1
1	O	223	THR	2.1
7	U	199	ILE	2.1
1	O	168	ASN	2.1
3	C	47	LYS	2.1
7	U	177	SER	2.1
2	P	233	VAL	2.0
9	W	113	PRO	2.0
7	U	196	GLU	2.0
1	O	227	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	6V1	U	47	15/16	0.83	0.29	64,96,103,104	0
7	YCM	U	137	10/11	0.83	0.15	46,54,72,72	0
3	YCM	C	63	10/11	0.87	0.11	48,50,59,60	0
7	YCM	G	137	10/11	0.89	0.12	27,34,48,49	0
5	6V1	S	148	15/16	0.89	0.18	35,56,62,64	0
5	6V1	E	148	15/16	0.89	0.15	29,45,55,55	0
7	6V1	G	47	15/16	0.89	0.17	33,52,55,55	0
3	YCM	Q	63	10/11	0.90	0.09	45,48,59,60	0
10	6V1	J	91	15/16	0.90	0.19	31,44,50,50	0
10	6V1	X	91	15/16	0.92	0.16	32,47,53,53	0
7	6V1	U	161	15/16	0.94	0.11	48,62,69,70	0
7	6V1	G	161	15/16	0.94	0.12	28,44,50,52	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
18	MG	H	301	1/1	0.71	0.10	45,45,45,45	0
18	MG	V	301	1/1	0.74	0.18	48,48,48,48	0
16	1PE	a	304	16/16	0.78	0.22	57,62,69,71	0
15	CL	b	502	1/1	0.79	0.10	59,59,59,59	0
16	1PE	b	505	16/16	0.79	0.23	64,67,78,78	0
15	CL	O	303	1/1	0.80	0.37	74,74,74,74	0
16	1PE	I	304	16/16	0.80	0.25	48,61,71,75	0
16	1PE	L	301	16/16	0.84	0.17	49,62,66,69	0
16	1PE	W	303	16/16	0.84	0.14	55,58,64,66	0
16	1PE	b	504	16/16	0.85	0.13	41,50,67,68	0
16	1PE	I	303	16/16	0.85	0.14	48,52,60,68	0
16	1PE	Z	301	16/16	0.86	0.14	51,61,64,64	0
15	CL	M	302	1/1	0.86	0.18	62,62,62,62	0
15	CL	C	302	1/1	0.87	0.15	63,63,63,63	0
15	CL	H	303	1/1	0.88	0.11	51,51,51,51	0
18	MG	X	301	1/1	0.89	0.07	44,44,44,44	0
16	1PE	G	303	16/16	0.91	0.12	34,42,51,56	0
15	CL	A	302	1/1	0.91	0.07	61,61,61,61	0
15	CL	K	304	1/1	0.91	0.15	52,52,52,52	0
15	CL	V	303	1/1	0.91	0.09	59,59,59,59	0
18	MG	J	301	1/1	0.91	0.06	41,41,41,41	0
15	CL	Y	305	1/1	0.91	0.09	54,54,54,54	0
15	CL	K	305	1/1	0.91	0.29	60,60,60,60	0
15	CL	D	302	1/1	0.92	0.10	53,53,53,53	0
15	CL	C	301	1/1	0.92	0.11	56,56,56,56	0
15	CL	O	304	1/1	0.92	0.14	55,55,55,55	0
15	CL	V	302	1/1	0.92	0.10	50,50,50,50	0
15	CL	M	301	1/1	0.92	0.18	52,52,52,52	0
15	CL	G	302	1/1	0.93	0.05	56,56,56,56	0
18	MG	K	301	1/1	0.93	0.07	33,33,33,33	0
15	CL	S	302	1/1	0.93	0.12	54,54,54,54	0
15	CL	Y	304	1/1	0.93	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	P	301	1/1	0.94	0.06	45,45,45,45	0
15	CL	B	302	1/1	0.94	0.17	54,54,54,54	0
15	CL	F	301	1/1	0.94	0.06	46,46,46,46	0
15	CL	E	303	1/1	0.95	0.15	54,54,54,54	0
15	CL	A	301	1/1	0.95	0.07	45,45,45,45	0
15	CL	O	301	1/1	0.95	0.05	49,49,49,49	0
15	CL	Y	303	1/1	0.95	0.06	56,56,56,56	0
17	K	b	506	1/1	0.95	0.07	38,38,38,38	0
15	CL	O	302	1/1	0.96	0.07	59,59,59,59	0
15	CL	E	302	1/1	0.96	0.07	49,49,49,49	0
15	CL	D	301	1/1	0.96	0.19	61,61,61,61	0
15	CL	I	302	1/1	0.96	0.06	40,40,40,40	0
15	CL	a	301	1/1	0.96	0.13	53,53,53,53	0
17	K	U	302	1/1	0.96	0.06	38,38,38,38	0
15	CL	a	303	1/1	0.96	0.08	52,52,52,52	0
15	CL	Q	302	1/1	0.96	0.21	54,54,54,54	0
18	MG	I	301	1/1	0.96	0.08	29,29,29,29	0
15	CL	R	302	1/1	0.96	0.15	48,48,48,48	0
15	CL	S	301	1/1	0.96	0.29	59,59,59,59	0
15	CL	M	304	1/1	0.96	0.04	49,49,49,49	0
18	MG	W	301	1/1	0.96	0.07	34,34,34,34	0
15	CL	B	301	1/1	0.96	0.09	37,37,37,37	0
15	CL	Q	301	1/1	0.97	0.16	62,62,62,62	0
15	CL	S	303	1/1	0.97	0.06	48,48,48,48	0
15	CL	N	501	1/1	0.97	0.07	42,42,42,42	0
15	CL	a	302	1/1	0.97	0.06	42,42,42,42	0
15	CL	K	303	1/1	0.97	0.12	62,62,62,62	0
15	CL	b	501	1/1	0.97	0.07	44,44,44,44	0
18	MG	L	303	1/1	0.97	0.08	33,33,33,33	0
15	CL	W	302	1/1	0.97	0.05	49,49,49,49	0
15	CL	K	302	1/1	0.97	0.07	41,41,41,41	0
17	K	N	504	1/1	0.97	0.06	37,37,37,37	0
15	CL	Y	301	1/1	0.98	0.09	33,33,33,33	0
15	CL	U	301	1/1	0.98	0.10	51,51,51,51	0
17	K	L	302	1/1	0.98	0.05	42,42,42,42	0
15	CL	G	301	1/1	0.98	0.10	41,41,41,41	0
15	CL	R	301	1/1	0.98	0.09	50,50,50,50	0
15	CL	b	503	1/1	0.98	0.07	44,44,44,44	0
15	CL	A	304	1/1	0.98	0.12	52,52,52,52	0
15	CL	N	503	1/1	0.99	0.06	40,40,40,40	0
15	CL	A	303	1/1	0.99	0.07	42,42,42,42	0
18	MG	H	302	1/1	0.99	0.05	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	M	303	1/1	0.99	0.05	38,38,38,38	0
18	MG	I	305	1/1	0.99	0.07	26,26,26,26	0
15	CL	E	301	1/1	0.99	0.08	54,54,54,54	0
17	K	G	304	1/1	0.99	0.07	28,28,28,28	0
15	CL	H	304	1/1	0.99	0.06	47,47,47,47	0
15	CL	N	502	1/1	0.99	0.05	43,43,43,43	0
15	CL	Y	302	1/1	0.99	0.07	47,47,47,47	0
17	K	Z	302	1/1	0.99	0.06	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.