



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2016 – 11:25 AM EDT

PDB ID : 5LF1  
Title : Human 20S proteasome complex with Dihydroeponemycin at 2.0 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 : 2.00 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

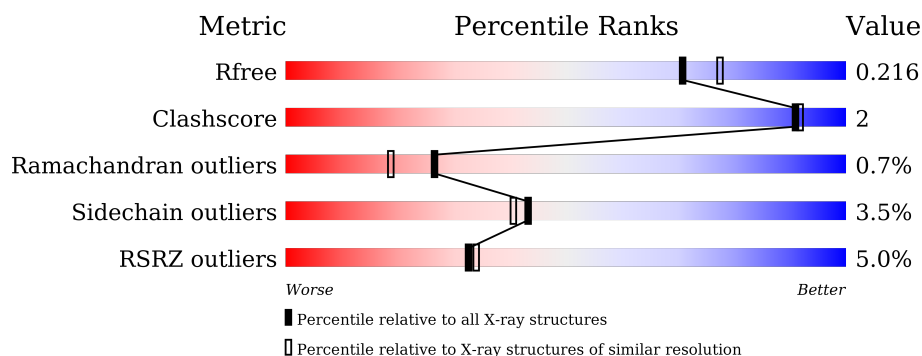
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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>3%</div> <div>88%</div> <div>9%</div> <div>...</div> </div>
1	O	234	<div> <div>14%</div> <div>90%</div> <div>6%</div> <div>...</div> </div>
2	B	261	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
2	P	261	<div> <div>15%</div> <div>84%</div> <div>8%</div> <div>5%</div> </div>
3	C	248	<div> <div>11%</div> <div>85%</div> <div>8%</div> <div>...</div> </div>
3	Q	248	<div> <div>18%</div> <div>84%</div> <div>10%</div> <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
15	CL	B	302	-	-	X	-
15	CL	D	301	-	-	-	X
15	CL	G	301	-	-	-	X
15	CL	K	305	-	-	-	X
15	CL	M	301	-	-	-	X
15	CL	Q	302	-	-	-	X
15	CL	S	301	-	-	-	X
18	1PE	H	304	-	-	-	X
18	1PE	I	303	-	-	-	X
18	1PE	L	301	-	-	-	X
18	1PE	M	304	-	-	-	X
18	1PE	W	303	-	-	-	X
18	1PE	Z	301	-	-	-	X
18	1PE	a	304	-	-	-	X
7	6V1	U	47	X	-	-	-

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 52156 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	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	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
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	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	238	Total	C	N	O	S	0	3	0
			1875	1175	340	349	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
			1545	974	269	293	9			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	P	1	Total	Cl	0	0
			1	1		
15	K	4	Total	Cl	0	0
			4	4		
15	B	2	Total	Cl	0	0
			2	2		
15	W	1	Total	Cl	0	0
			1	1		
15	N	4	Total	Cl	0	0
			4	4		
15	S	3	Total	Cl	0	0
			3	3		
15	E	4	Total	Cl	0	0
			4	4		
15	b	4	Total	Cl	0	0
			4	4		
15	V	1	Total	Cl	0	0
			1	1		
15	A	4	Total	Cl	0	0
			4	4		
15	R	2	Total	Cl	0	0
			2	2		
15	M	3	Total	Cl	0	0
			3	3		
15	D	1	Total	Cl	0	0
			1	1		
15	I	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	a	3	Total Cl 3 3	0	0
15	U	1	Total Cl 1 1	0	0
15	G	2	Total Cl 2 2	0	0
15	Q	2	Total Cl 2 2	0	0
15	H	1	Total Cl 1 1	0	0
15	C	2	Total Cl 2 2	0	0
15	O	4	Total Cl 4 4	0	0
15	Y	5	Total Cl 5 5	0	0
15	F	1	Total Cl 1 1	0	0

- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

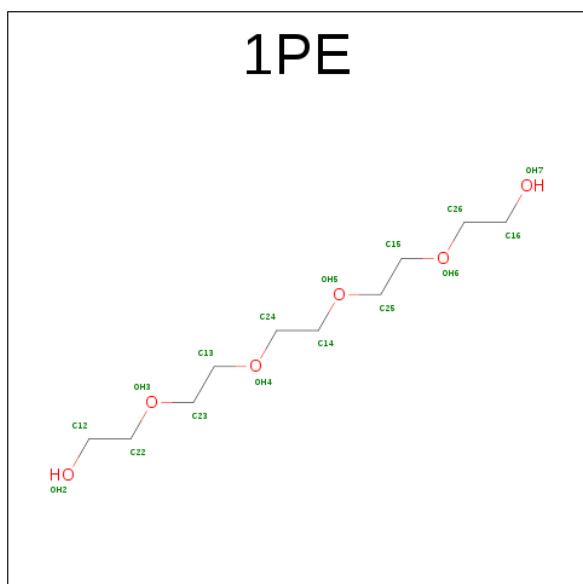
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0

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

- Molecule 18 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



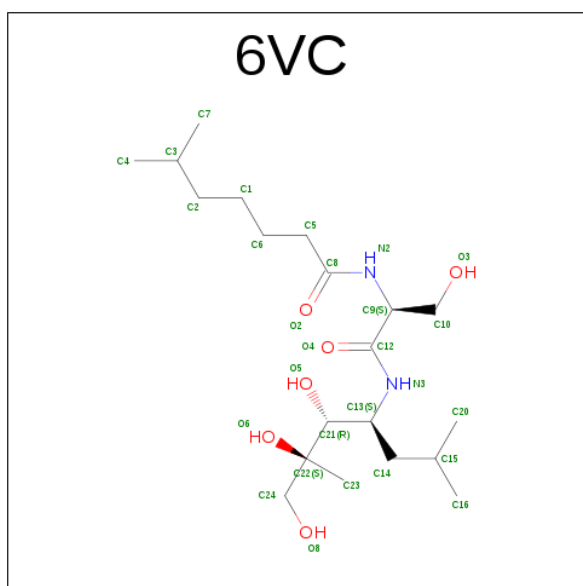
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	H	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	L	1	Total	C	O	0	0
			16	10	6		
18	M	1	Total	C	O	0	0
			16	10	6		
18	N	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	U	1	Total	C	O	0	0
			16	10	6		
18	W	1	Total	C	O	0	0
			16	10	6		
18	Z	1	Total	C	O	0	0
			16	10	6		
18	a	1	Total	C	O	0	0
			16	10	6		

- Molecule 19 is {N}-(2 {S})-1-[(2 {S},3 {R},4 {S})-2,6-dimethyl-1,2,3-tris(oxidanyl)heptan-4-yl]amino]-3-oxidanyl-1-oxidanylidene-propan-2-yl]-6-methyl-heptanamide (three-letter code: 6VC) (formula: C<sub>20</sub>H<sub>40</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	H	1	Total	C	N	O	0	0
			28	20	2	6		
19	K	1	Total	C	N	O	0	0
			28	20	2	6		
19	N	1	Total	C	N	O	0	0
			28	20	2	6		
19	V	1	Total	C	N	O	0	0
			28	20	2	6		
19	Y	1	Total	C	N	O	0	0
			28	20	2	6		
19	b	1	Total	C	N	O	0	0
			28	20	2	6		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	110	Total O 110 110	0	0
20	B	127	Total O 127 127	0	0
20	C	82	Total O 82 82	0	0
20	D	91	Total O 91 91	0	0
20	E	140	Total O 140 140	0	0
20	F	186	Total O 186 186	0	0
20	G	191	Total O 191 191	0	0
20	H	156	Total O 156 156	0	0
20	I	153	Total O 153 153	0	0
20	J	138	Total O 138 138	0	0
20	K	98	Total O 98 98	0	0
20	L	130	Total O 130 130	0	0
20	M	149	Total O 149 149	0	0
20	N	165	Total O 165 165	0	0
20	O	91	Total O 91 91	0	0
20	P	123	Total O 123 123	0	0
20	Q	75	Total O 75 75	0	0
20	R	127	Total O 127 127	0	0
20	S	122	Total O 122 122	0	0
20	T	93	Total O 93 93	0	0
20	U	112	Total O 112 112	0	0

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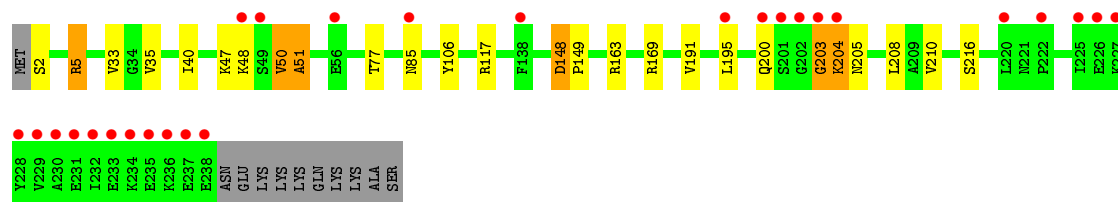
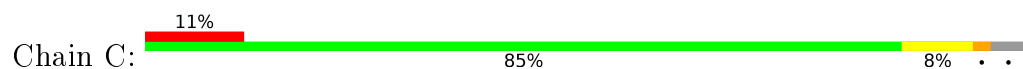
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	V	109	Total 109	O 109	0	0
20	W	116	Total 116	O 116	0	0
20	X	127	Total 127	O 127	0	0
20	Y	141	Total 141	O 141	0	0
20	Z	171	Total 171	O 171	0	0
20	a	174	Total 174	O 174	0	0
20	b	124	Total 124	O 124	0	0

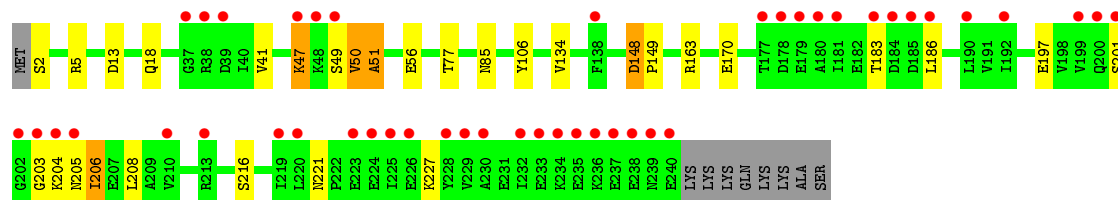
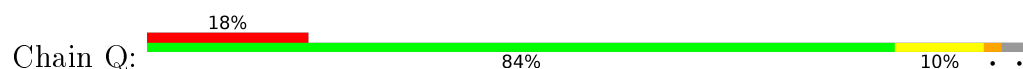




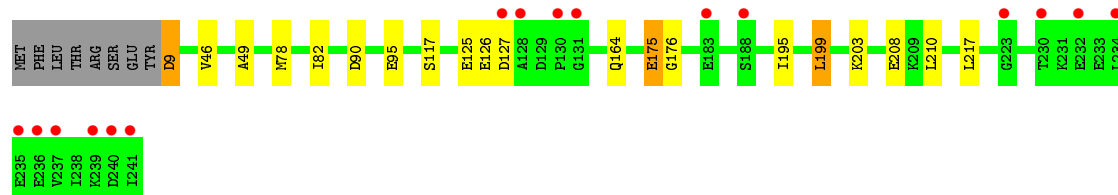
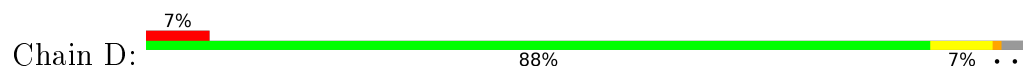
• Molecule 3: Proteasome subunit alpha type-7



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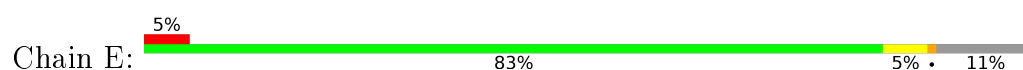
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 4: Proteasome subunit alpha type-5



• Molecule 5: Proteasome subunit alpha type-1



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

• Molecule 5: Proteasome subunit alpha type-1

Chain S: 4% 83% 6% 10%

MET F2 R3 N4 R18 E23 V29 V45 V46 V47 A48 L49 K50 A57 A56 H59 H65 R101 R122 N152 R174 L195 D204 L223 E234 G235 L236 E237 E238 E239 PRO GLN ARG LYS ALA GLN PRO ALA GLN 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 E34 V53 R65 D70 G74 L81 R85 S86 L87 R99 M105 R114 M117 D152 V156 R169 Q170 T174 K182 R187 V190 D202 E203 V204 K215 E224 V227  
R232 R240 K244 GLU ASP GLU SER GLY ASP ASP ASN MET

• Molecule 6: Proteasome subunit alpha type-3

Chain T: 7% 81% 11% 6%

MET SER SER ILE GLY G6 Y7 D17 K27 E31 E34 V53 L54 R65 D70 G74 L81 L87 R99 D113 M117 D152 V156 R169 Q170 T174 Q180 V190 K191 D202 E203 V204 K205 D206 K207 A208 F209 W215  
R223 R224 D230 E233 E236 R237 Y238 A239 K240 E241 S242 L243 K244 GLU GLU ASP GLU SER ASP ASP ASN MET

• Molecule 7: Proteasome subunit alpha type-6

Chain G: 2% 93% ..

MET S2 R3 V42 P57 I72 C78 D86 S87 R88 E108 L114 R117 V183 F187 D188 W189 T190 A198 L206 D209 R245 ASP

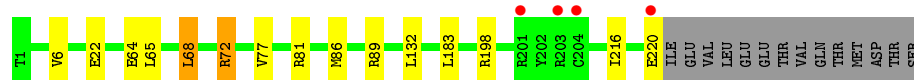
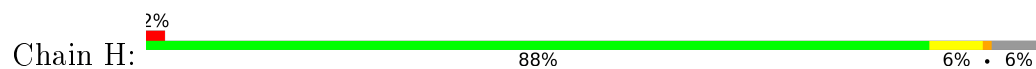
• Molecule 7: Proteasome subunit alpha type-6

Chain U: 13% 88% 7% ..

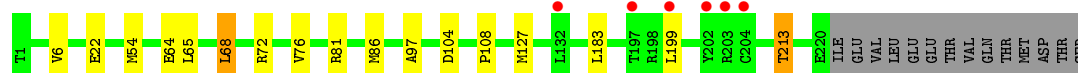
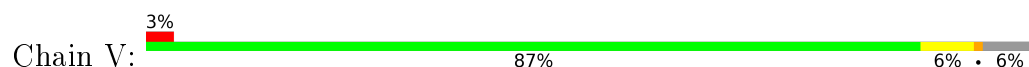
MET S2 R3 A7 R11 V42 R43 V56 P57 D58 R59 I72 C78 V79 M80 R88 V91 E108 L114 R117 I118 M138 V151 T173 E174 S177 F178 L179 V183 K186 PHE ASP TRP THR PHE GLU Q193 T194 V195 E196 T197 A198 I199  
T200 C201 L202 S203 T204 V205 L206 S207 L208 D209 F210 R211 K212 E223 L239 V240 A241 L242 A243 E244 R245 ASP



- Molecule 8: Proteasome subunit beta type-7



- Molecule 8: Proteasome subunit beta type-7



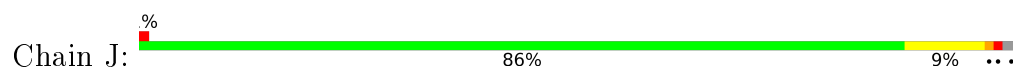
- Molecule 9: Proteasome subunit beta type-3



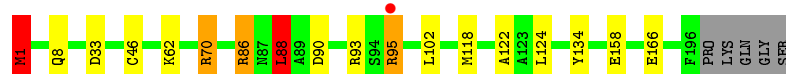
- Molecule 9: Proteasome subunit beta type-3



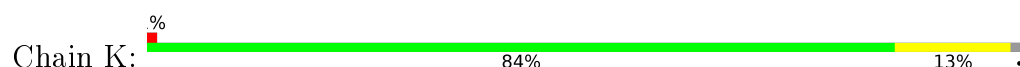
- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2

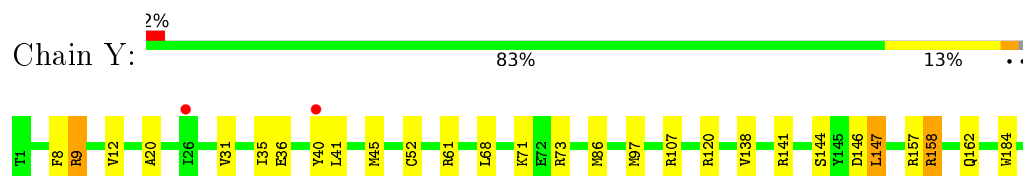


- Molecule 11: Proteasome subunit beta type-5



PRO

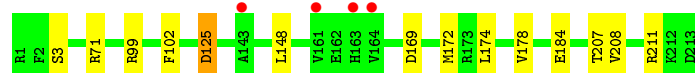
- Molecule 11: Proteasome subunit beta type-5

SER  
THR  
PRO

- Molecule 12: Proteasome subunit beta type-1



- Molecule 12: Proteasome subunit beta type-1



- Molecule 13: Proteasome subunit beta type-4



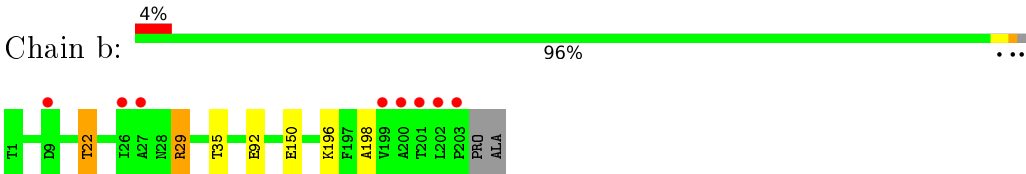
- Molecule 13: Proteasome subunit beta type-4



- 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, $\alpha$ , $\beta$ , $\gamma$	113.89Å 203.49Å 316.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.09 – 2.00 49.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (171.09-2.00) 99.5 (49.09-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.178 , 0.213 0.184 , 0.216	Depositor DCC
$R_{free}$ test set	24379 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.6	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	52156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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: MG, CL, K, 6V1, 1PE, YCM, 6VC

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	0.68	0/1833	0.82	4/2489 (0.2%)
1	O	0.60	0/1778	0.80	3/2419 (0.1%)
2	B	0.73	1/1958 (0.1%)	0.83	4/2645 (0.2%)
2	P	0.66	0/1945	0.84	4/2631 (0.2%)
3	C	0.68	0/1818	0.90	2/2469 (0.1%)
3	Q	0.67	1/1834 (0.1%)	0.87	3/2490 (0.1%)
4	D	0.70	0/1789	0.83	2/2424 (0.1%)
4	R	0.76	0/1780	0.90	3/2408 (0.1%)
5	E	0.69	0/1842	0.85	4/2493 (0.2%)
5	S	0.67	0/1901	0.84	3/2571 (0.1%)
6	F	0.79	0/1935	0.94	7/2605 (0.3%)
6	T	0.73	1/1894 (0.1%)	0.93	9/2556 (0.4%)
7	G	0.79	2/1909 (0.1%)	0.83	6/2579 (0.2%)
7	U	0.68	1/1804 (0.1%)	0.82	7/2441 (0.3%)
8	H	0.76	0/1697	1.04	10/2299 (0.4%)
8	V	0.67	0/1655	0.91	4/2251 (0.2%)
9	I	0.76	1/1648 (0.1%)	1.06	9/2219 (0.4%)
9	W	0.64	0/1630	0.97	9/2197 (0.4%)
10	J	0.73	0/1613	1.01	9/2180 (0.4%)
10	X	0.70	0/1599	0.96	7/2163 (0.3%)
11	K	0.73	0/1576	0.95	8/2131 (0.4%)
11	Y	0.80	0/1620	1.02	9/2185 (0.4%)
12	L	0.69	0/1672	0.86	3/2257 (0.1%)
12	Z	0.80	1/1675 (0.1%)	0.91	5/2257 (0.2%)
13	M	0.77	0/1728	0.91	6/2339 (0.3%)
13	a	0.82	0/1724	0.94	4/2336 (0.2%)
14	N	0.85	1/1548 (0.1%)	0.89	5/2095 (0.2%)
14	b	0.79	2/1554 (0.1%)	0.89	3/2104 (0.1%)
All	All	0.73	11/48959 (0.0%)	0.90	152/66233 (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	4
3	Q	0	2
4	D	0	4
4	R	0	2
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
13	a	0	1
All	All	1	18

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	8.64	1.35	1.25
12	Z	3	SER	CB-OG	6.72	1.50	1.42
14	N	150	GLU	CG-CD	6.05	1.61	1.51
7	G	108	GLU	CD-OE2	5.77	1.31	1.25
3	Q	13	ASP	CB-CG	5.53	1.63	1.51
9	I	105	GLU	CD-OE2	5.38	1.31	1.25
2	B	103	GLU	CD-OE1	5.38	1.31	1.25
14	b	92	GLU	CD-OE2	5.31	1.31	1.25
14	b	150	GLU	CG-CD	5.27	1.59	1.51
6	T	7	TYR	N-CA	5.23	1.56	1.46
7	U	108	GLU	CD-OE1	5.12	1.31	1.25

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	86	ARG	NE-CZ-NH2	-15.30	112.65	120.30
10	X	86	ARG	NE-CZ-NH2	-14.55	113.02	120.30
9	I	69	ARG	NE-CZ-NH1	14.17	127.39	120.30
10	J	86	ARG	NE-CZ-NH1	13.60	127.10	120.30
8	H	72	ARG	NE-CZ-NH2	-13.05	113.77	120.30
9	W	69	ARG	NE-CZ-NH1	12.84	126.72	120.30
10	X	86	ARG	NE-CZ-NH1	12.12	126.36	120.30
9	I	25[A]	ARG	NE-CZ-NH1	10.54	125.57	120.30
9	I	25[B]	ARG	NE-CZ-NH1	10.54	125.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	72	ARG	NE-CZ-NH1	9.83	125.21	120.30
9	I	69	ARG	NE-CZ-NH2	-9.62	115.49	120.30
4	R	120[A]	ALA	C-N-CA	9.47	145.39	121.70
4	R	120[B]	ALA	C-N-CA	9.47	145.39	121.70
14	b	29	ARG	NE-CZ-NH1	9.23	124.91	120.30
9	W	69	ARG	NE-CZ-NH2	-9.11	115.74	120.30
11	Y	157	ARG	NE-CZ-NH2	-8.78	115.91	120.30
9	I	16[A]	LYS	C-N-CA	8.68	143.41	121.70
9	I	16[B]	LYS	C-N-CA	8.68	143.41	121.70
11	Y	157	ARG	NE-CZ-NH1	8.65	124.63	120.30
9	W	16[A]	LYS	C-N-CA	8.65	143.32	121.70
9	W	16[B]	LYS	C-N-CA	8.65	143.32	121.70
6	F	117	MET	CG-SD-CE	8.16	113.26	100.20
7	U	88	ARG	NE-CZ-NH1	8.13	124.36	120.30
7	G	117	ARG	NE-CZ-NH1	8.06	124.33	120.30
9	W	25[A]	ARG	NE-CZ-NH1	7.90	124.25	120.30
9	W	25[B]	ARG	NE-CZ-NH1	7.90	124.25	120.30
6	T	117	MET	CG-SD-CE	7.82	112.71	100.20
2	P	96	ARG	NE-CZ-NH1	7.79	124.19	120.30
2	B	96	ARG	NE-CZ-NH1	7.73	124.16	120.30
6	T	27	MET	CG-SD-CE	7.69	112.50	100.20
11	Y	158	ARG	NE-CZ-NH1	7.56	124.08	120.30
12	Z	99	ARG	NE-CZ-NH1	7.54	124.07	120.30
12	Z	71	ARG	NE-CZ-NH2	7.26	123.93	120.30
8	H	81	ARG	NE-CZ-NH2	-7.21	116.70	120.30
12	L	99	ARG	NE-CZ-NH1	7.17	123.89	120.30
12	L	99	ARG	NE-CZ-NH2	-7.15	116.72	120.30
11	K	157	ARG	NE-CZ-NH2	-7.08	116.76	120.30
12	Z	99	ARG	NE-CZ-NH2	-7.05	116.77	120.30
13	M	151	ARG	NE-CZ-NH1	7.02	123.81	120.30
7	U	117	ARG	NE-CZ-NH1	6.87	123.74	120.30
8	V	72	ARG	NE-CZ-NH2	-6.78	116.91	120.30
5	E	122	ARG	NE-CZ-NH2	-6.74	116.93	120.30
13	a	5	MET	CG-SD-CE	6.73	110.97	100.20
7	U	88	ARG	NE-CZ-NH2	-6.67	116.97	120.30
11	K	157	ARG	NE-CZ-NH1	6.62	123.61	120.30
9	I	25[A]	ARG	NE-CZ-NH2	-6.59	117.00	120.30
9	I	25[B]	ARG	NE-CZ-NH2	-6.59	117.00	120.30
11	K	158	ARG	NE-CZ-NH2	-6.55	117.03	120.30
8	H	198	ARG	NE-CZ-NH1	6.54	123.57	120.30
11	Y	158	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	O	181	LEU	CA-CB-CG	6.49	130.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-6.47	99.10	111.40
13	M	5	MET	CG-SD-CE	6.43	110.49	100.20
10	J	88	LEU	CB-CG-CD2	6.43	121.93	111.00
1	A	219	ARG	NE-CZ-NH1	6.38	123.49	120.30
12	Z	172	MET	CG-SD-CE	-6.34	90.05	100.20
4	D	9	ASP	CB-CG-OD1	6.33	124.00	118.30
11	K	120	ARG	NE-CZ-NH1	6.33	123.47	120.30
11	K	154	ASP	CB-CG-OD2	6.33	123.99	118.30
8	V	72	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	73	LEU	CA-CB-CG	6.30	129.79	115.30
7	U	80[A]	MET	CG-SD-CE	6.30	110.27	100.20
7	U	80[B]	MET	CG-SD-CE	6.30	110.27	100.20
5	E	122	ARG	NE-CZ-NH1	6.29	123.44	120.30
5	S	122	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	B	4	ARG	NE-CZ-NH1	6.24	123.42	120.30
8	H	72	ARG	CD-NE-CZ	6.21	132.29	123.60
8	H	86	MET	CG-SD-CE	-6.18	90.31	100.20
10	J	33	ASP	CB-CG-OD1	6.15	123.83	118.30
7	G	183	VAL	CB-CA-C	-6.09	99.82	111.40
13	a	151	ARG	NE-CZ-NH1	6.07	123.33	120.30
11	Y	120	ARG	NE-CZ-NH1	6.06	123.33	120.30
6	T	70	ASP	CB-CG-OD1	6.04	123.74	118.30
2	P	6	ASP	CB-CG-OD2	6.03	123.73	118.30
14	b	22	THR	CB-CA-C	-6.02	95.34	111.60
4	R	9	ASP	CB-CG-OD1	6.00	123.70	118.30
7	G	88	ARG	NE-CZ-NH2	-6.00	117.30	120.30
9	I	134	ASP	CB-CG-OD1	5.94	123.65	118.30
6	T	169	ARG	NE-CZ-NH1	5.94	123.27	120.30
6	T	113	ASP	CB-CG-OD2	-5.94	112.96	118.30
12	L	172	MET	CG-SD-CE	-5.93	90.72	100.20
5	S	122	ARG	NE-CZ-NH1	5.92	123.26	120.30
8	H	89	ARG	NE-CZ-NH1	5.89	123.24	120.30
6	T	6	GLY	C-N-CA	5.86	136.36	121.70
1	O	73	LEU	CA-CB-CG	5.84	128.73	115.30
3	C	117	ARG	NE-CZ-NH1	5.84	123.22	120.30
13	M	99	ARG	NE-CZ-NH1	5.82	123.21	120.30
11	K	86	MET	CG-SD-CE	5.82	109.51	100.20
6	F	70	ASP	CB-CG-OD1	5.81	123.53	118.30
6	T	99	ARG	NE-CZ-NH1	5.80	123.20	120.30
11	K	158	ARG	NE-CZ-NH1	5.80	123.20	120.30
6	T	190	VAL	CB-CA-C	-5.78	100.43	111.40
2	P	96	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	182	ARG	NE-CZ-NH1	5.74	123.17	120.30
6	F	99	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	219	ARG	NE-CZ-NH2	-5.71	117.45	120.30
3	Q	5	ARG	NE-CZ-NH1	5.69	123.14	120.30
14	N	144	ARG	NE-CZ-NH1	5.65	123.13	120.30
10	X	90	ASP	CB-CG-OD1	5.65	123.39	118.30
9	W	134	ASP	CB-CG-OD1	5.58	123.32	118.30
7	G	86	ASP	CB-CG-OD1	5.55	123.30	118.30
11	K	107	ARG	NE-CZ-NH1	5.55	123.08	120.30
14	N	22	THR	CB-CA-C	-5.54	96.65	111.60
14	N	45	ARG	NE-CZ-NH1	5.53	123.06	120.30
6	F	85	ARG	NE-CZ-NH1	5.52	123.06	120.30
8	H	198	ARG	NE-CZ-NH2	-5.51	117.54	120.30
10	J	93	ARG	NE-CZ-NH1	5.51	123.06	120.30
12	Z	125	ASP	CB-CG-OD1	5.50	123.25	118.30
7	U	11	ARG	NE-CZ-NH1	5.48	123.04	120.30
10	J	86	ARG	CD-NE-CZ	5.48	131.27	123.60
6	T	7	TYR	N-CA-CB	5.45	120.41	110.60
2	B	96	ARG	NE-CZ-NH2	-5.43	117.58	120.30
7	G	117	ARG	NE-CZ-NH2	-5.39	117.61	120.30
11	Y	107	ARG	NE-CZ-NH1	5.39	123.00	120.30
10	X	70	ARG	NE-CZ-NH2	-5.38	117.61	120.30
5	S	174	ARG	NE-CZ-NH1	5.38	122.99	120.30
8	V	86	MET	CG-SD-CE	-5.37	91.61	100.20
2	B	4	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	C	5	ARG	NE-CZ-NH1	5.33	122.97	120.30
13	a	166	ARG	NE-CZ-NH2	-5.31	117.64	120.30
14	N	116	MET	CG-SD-CE	-5.27	91.77	100.20
8	V	81	ARG	NE-CZ-NH2	-5.24	117.68	120.30
13	M	166	ARG	NE-CZ-NH2	-5.22	117.69	120.30
10	X	93	ARG	NE-CZ-NH1	5.21	122.91	120.30
7	G	245	ARG	NE-CZ-NH1	5.21	122.90	120.30
9	W	25[A]	ARG	NE-CZ-NH2	-5.20	117.70	120.30
9	W	25[B]	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	17	LYS	CD-CE-NZ	5.19	123.63	111.70
6	F	85	ARG	NE-CZ-NH2	-5.18	117.71	120.30
4	D	90	ASP	CB-CG-OD2	5.18	122.96	118.30
14	N	45	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	O	73	LEU	CB-CA-C	-5.16	100.40	110.20
11	Y	61	ARG	NE-CZ-NH1	5.15	122.88	120.30
10	J	70	ARG	NE-CZ-NH2	-5.14	117.73	120.30
5	E	174	ARG	NE-CZ-NH1	5.13	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	184	ASP	CB-CG-OD1	5.13	122.91	118.30
3	Q	5	ARG	NE-CZ-NH2	-5.12	117.74	120.30
14	b	29	ARG	NE-CZ-NH2	-5.12	117.74	120.30
7	U	117	ARG	NE-CZ-NH2	-5.10	117.75	120.30
8	H	81	ARG	NE-CZ-NH1	5.09	122.84	120.30
13	M	73	ASP	CB-CG-OD1	5.08	122.87	118.30
10	X	33	ASP	CB-CG-OD1	5.07	122.86	118.30
13	M	166	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	Q	13	ASP	CB-CA-C	5.04	120.48	110.40
10	J	93	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	P	4	ARG	NE-CZ-NH1	5.03	122.82	120.30
5	E	155	ASP	CB-CG-OD1	5.03	122.82	118.30
8	H	72	ARG	CG-CD-NE	-5.03	101.25	111.80
6	F	114	ARG	NE-CZ-NH2	-5.02	117.79	120.30
11	Y	9	ARG	NE-CZ-NH1	5.02	122.81	120.30
11	Y	86	MET	CG-SD-CE	5.02	108.23	100.20
10	X	88	LEU	CB-CG-CD2	5.00	119.51	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	203	VAL	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
2	P	52	ILE	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide

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Mol	Chain	Res	Type	Group
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	9	0
1	O	1741	0	1683	5	0
2	B	1922	0	1913	5	0
2	P	1909	0	1874	11	1
3	C	1798	0	1718	17	0
3	Q	1820	0	1749	11	0
4	D	1762	0	1709	6	0
4	R	1753	0	1726	5	0
5	E	1822	0	1779	7	0
5	S	1875	0	1818	13	1
6	F	1888	0	1882	9	0
6	T	1856	0	1816	8	0
7	G	1912	0	1882	4	0
7	U	1815	0	1748	10	0
8	H	1664	0	1678	7	0
8	V	1622	0	1592	6	0
9	I	1613	0	1646	8	0
9	W	1599	0	1621	5	0
10	J	1590	0	1581	14	0
10	X	1576	0	1561	10	0
11	K	1545	0	1495	8	0
11	Y	1580	0	1555	15	0
12	L	1636	0	1625	7	0
12	Z	1642	0	1635	2	0
13	M	1692	0	1670	6	0
13	a	1688	0	1658	0	0
14	N	1519	0	1493	6	0
14	b	1524	0	1493	0	0
15	A	4	0	0	1	0
15	B	2	0	0	2	0
15	C	2	0	0	0	0
15	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	4	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	4	0	0	0	0
15	M	3	0	0	1	0
15	N	4	0	0	1	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	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	5	0	0	0	0
15	a	3	0	0	0	0
15	b	4	0	0	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	16	0	22	0	0
18	I	16	0	22	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0
18	N	16	0	22	0	0
18	U	16	0	22	0	0
18	W	16	0	22	0	0
18	Z	16	0	22	0	0
18	a	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	H	28	0	0	0	0
19	K	28	0	0	0	0
19	N	28	0	0	0	0
19	V	28	0	0	0	0
19	Y	28	0	0	0	0
19	b	28	0	0	0	0
20	A	110	0	0	1	0
20	B	127	0	0	0	0
20	C	82	0	0	1	0
20	D	91	0	0	0	0
20	E	140	0	0	3	0
20	F	186	0	0	3	0
20	G	191	0	0	2	0
20	H	156	0	0	3	0
20	I	153	0	0	1	0
20	J	138	0	0	2	0
20	K	98	0	0	0	0
20	L	130	0	0	1	0
20	M	149	0	0	0	0
20	N	165	0	0	0	0
20	O	91	0	0	1	0
20	P	123	0	0	1	0
20	Q	75	0	0	0	0
20	R	127	0	0	2	0
20	S	122	0	0	2	0
20	T	93	0	0	0	0
20	U	112	0	0	0	0
20	V	109	0	0	1	0
20	W	116	0	0	2	0
20	X	127	0	0	0	0
20	Y	141	0	0	0	0
20	Z	171	0	0	1	0
20	a	174	0	0	0	0
20	b	124	0	0	0	0
All	All	52156	0	47559	199	1

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

All (199) 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)
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.36	0.90
10:J:185:LYS:NZ	20:J:401:HOH:O	2.05	0.89
10:X:1:MET:HE1	10:X:134:TYR:H	1.40	0.87
5:E:202:GLU:OE2	20:E:401:HOH:O	1.98	0.81
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.64	0.80
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.65	0.79
11:Y:199:TYR:HA	11:Y:200:SER:HB2	1.66	0.79
9:I:35:THR:HG21	20:I:483:HOH:O	1.85	0.74
2:P:25[B]:MET:CE	2:P:25[B]:MET:HA	2.17	0.74
7:G:188:ASP:O	7:G:190:THR:HG22	1.88	0.74
11:K:35:ILE:HD11	11:K:45:MET:SD	2.29	0.73
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.06	0.73
11:Y:35:ILE:HD11	11:Y:45:MET:SD	2.29	0.73
14:N:35:THR:CG2	14:N:45:ARG:HE	2.03	0.72
8:H:77:VAL:HG12	20:H:539:HOH:O	1.88	0.71
15:R:301:CL:CL	20:R:506:HOH:O	2.44	0.71
6:F:169[A]:ARG:NH1	20:F:402:HOH:O	2.23	0.70
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.72	0.70
8:V:54:MET:HE1	20:W:477:HOH:O	1.93	0.69
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.41	0.68
5:S:65[A]:HIS:CE1	20:Z:402:HOH:O	2.46	0.68
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.28	0.67
1:O:10:THR:HG23	20:O:402:HOH:O	1.94	0.67
4:R:129:ASP:CB	4:R:130:PRO:CD	2.72	0.66
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.42	0.66
3:C:47:LYS:CB	3:C:48:LYS:HA	2.25	0.66
5:E:58:ALA:O	5:E:59:HIS:CB	2.43	0.65
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.10	0.65
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	1.98	0.64
7:U:195:VAL:O	7:U:199:ILE:HG23	1.97	0.64
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.81	0.63
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.45	0.63
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	1.99	0.63
7:U:58:ASP:O	7:U:59:LYS:CB	2.48	0.62
3:C:47:LYS:CB	3:C:48:LYS:CA	2.77	0.61
10:X:1:MET:HE1	10:X:134:TYR:N	2.14	0.61
8:H:77:VAL:CG1	20:H:539:HOH:O	2.47	0.60
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.49	0.60
15:B:301:CL:CL	15:B:302:CL:CL	2.93	0.59
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.51	0.59
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.20	0.59
11:Y:36:GLU:HG2	11:Y:184:TRP:CZ2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.83	0.59
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.33	0.59
6:F:105:ASN:ND2	20:F:404:HOH:O	2.36	0.58
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.84	0.58
10:J:99[A]:HIS:CD2	20:J:426:HOH:O	2.57	0.58
12:L:144:MET:CE	12:L:185:ARG:HB2	2.34	0.57
3:C:35:VAL:HG13	3:C:191:VAL:HG22	1.87	0.56
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.86	0.56
11:K:36:GLU:HG2	11:K:184:TRP:CZ2	2.41	0.56
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.88	0.55
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.40	0.55
11:K:141:ARG:NH1	10:X:166:GLU:OE2	2.40	0.55
11:Y:199:TYR:HA	11:Y:200:SER:CB	2.36	0.55
3:C:50:VAL:O	3:C:51:ALA:HB3	2.07	0.54
10:J:177:THR:HG22	10:J:195:SER:CB	2.37	0.54
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.89	0.54
9:W:13:MET:HE1	9:W:166:ILE:N	2.23	0.54
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.42	0.53
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.91	0.53
15:A:302:CL:CL	15:B:302:CL:CL	43.24	0.53
6:T:205:LYS:O	6:T:206:ASP:CG	2.47	0.53
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	2.09	0.53
5:S:101:ARG:NH1	20:S:404:HOH:O	2.41	0.53
7:G:117:ARG:NH2	20:G:401:HOH:O	2.28	0.52
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.75	0.52
15:M:302:CL:CL	15:N:303:CL:CL	3.02	0.52
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.92	0.52
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.91	0.52
9:W:35:THR:HG21	20:W:432:HOH:O	2.10	0.52
4:R:129:ASP:CB	4:R:130:PRO:HD2	2.40	0.52
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.92	0.51
3:C:5:ARG:NH1	4:D:125:GLU:OE2	2.40	0.51
5:E:101[A]:ARG:NH1	20:E:402:HOH:O	2.44	0.51
7:U:195:VAL:HG13	7:U:196:GLU:OE1	2.11	0.50
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.10	0.50
14:N:190:LEU:H	14:N:193:GLN:HE21	1.61	0.49
6:F:182:LYS:HE3	20:F:561:HOH:O	2.12	0.48
2:P:246:LYS:HE3	2:P:246:LYS:N	2.28	0.48
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.94	0.48
2:P:53:HIS:O	2:P:54:LYS:HB2	2.13	0.48
4:D:195:ILE:O	4:D:199:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:40:TYR:CD2	11:Y:73:ARG:CZ	2.96	0.48
20:G:464:HOH:O	8:H:72:ARG:HD3	2.13	0.48
3:C:203:GLY:CA	3:C:204:LYS:CB	2.91	0.48
6:T:170:GLN:O	6:T:174:THR:HG23	2.14	0.47
11:Y:52:CYS:SG	11:Y:97[A]:MET:HG3	2.54	0.47
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.44	0.47
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.29	0.47
7:U:118:ILE:HG21	7:U:138:MET:HE2	1.95	0.47
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.10	0.47
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.45	0.47
5:E:65:HIS:HB2	20:E:493:HOH:O	2.13	0.47
10:J:177:THR:HG22	10:J:195:SER:HB3	1.95	0.47
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.55	0.47
9:W:27:PHE:HB3	9:W:35:THR:HG22	1.97	0.47
6:F:170:GLN:O	6:F:174:THR:HG23	2.15	0.46
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.97	0.46
13:M:5:MET:HE3	14:N:116:MET:HB2	1.96	0.46
1:A:58[B]:GLU:H	1:A:58[B]:GLU:CD	2.19	0.46
3:C:33:VAL:HG21	3:C:195:LEU:HD12	1.97	0.46
11:K:52:CYS:SG	11:K:97:MET:HG3	2.55	0.46
13:M:112:ILE:HD12	13:M:112:ILE:N	2.30	0.46
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.98	0.46
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.98	0.46
5:S:18[B]:ARG:CG	5:S:23:GLU:OE2	2.64	0.46
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.46	0.46
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.96	0.46
2:B:33:THR:HB	2:B:166:ASN:O	2.15	0.46
3:C:50:VAL:O	3:C:51:ALA:CB	2.64	0.46
5:S:237:GLU:O	5:S:238:GLU:CB	2.64	0.45
8:V:213:THR:HB	9:W:198:THR:OG1	2.16	0.45
9:I:27:PHE:HB3	9:I:35:THR:HG22	1.98	0.45
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.98	0.45
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.49	0.45
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.99	0.45
7:U:80[A]:MET:HE3	7:U:91:VAL:HG23	1.98	0.45
10:X:95:ARG:HH11	10:X:95:ARG:HB2	1.82	0.45
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.98	0.45
6:T:202:ASP:OD1	6:T:204:VAL:HG12	2.16	0.45
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.99	0.45
4:R:32:LYS:HG2	20:R:506:HOH:O	2.16	0.45
11:Y:158:ARG:HE	11:Y:162:GLN:NE2	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:5:MET:HE2	14:N:116:MET:HB3	1.99	0.45
6:F:34:SER:OG	6:F:65:ARG:NH1	2.49	0.44
2:P:25[B]:MET:HE3	2:P:28:ILE:HD12	1.99	0.44
11:Y:9:ARG:NH2	11:Y:146:ASP:OD1	2.48	0.44
7:G:72:ILE:HG21	7:G:114:LEU:HD21	2.00	0.44
1:A:180:ASP:OD1	1:A:180:ASP:N	2.50	0.44
1:A:63:LYS:NZ	20:A:404:HOH:O	2.49	0.44
5:S:65[B]:HIS:CE1	5:S:223:ILE:HD12	2.53	0.44
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.99	0.44
2:P:33:THR:HB	2:P:166:ASN:O	2.17	0.44
4:D:164:GLN:OE1	5:E:58:ALA:HB2	2.17	0.44
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.99	0.44
1:A:17:LYS:HE2	1:A:22:GLU:OE2	2.18	0.44
7:G:42:VAL:HG13	7:G:198:ALA:HB2	2.00	0.44
9:I:158:ASP:OD1	9:I:161:HIS:HD2	2.00	0.44
1:O:180:ASP:N	1:O:180:ASP:OD1	2.49	0.44
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.47	0.44
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.18	0.44
12:L:43[B]:CYS:SG	20:L:401:HOH:O	2.62	0.43
5:S:49:LEU:HG	5:S:195:LEU:HD21	1.99	0.43
3:Q:85:ASN:OD1	10:X:70:ARG:NH2	2.51	0.43
11:Y:68:LEU:O	11:Y:71:LYS:CE	2.66	0.43
3:Q:106:TYR:C	3:Q:106:TYR:CD1	2.91	0.43
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.54	0.43
8:H:216:ILE:HD13	9:I:195:THR:HG23	2.00	0.43
11:K:40:TYR:CD2	11:K:73:ARG:CZ	3.01	0.43
11:K:83:LEU:HD21	11:K:99:THR:HG21	2.01	0.43
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.49	0.43
8:V:97:ALA:HB1	8:V:127[B]:MET:CE	2.49	0.43
8:V:54:MET:HE3	20:V:466:HOH:O	2.19	0.42
8:H:64:GLU:HG2	8:H:68:LEU:HD22	2.01	0.42
8:V:64:GLU:HG2	8:V:68:LEU:HD22	2.01	0.42
13:M:27:LEU:HD22	13:M:184:TYR:HB2	2.01	0.42
7:U:42:VAL:HG13	7:U:198:ALA:HB2	2.02	0.42
10:J:166:GLU:OE2	11:Y:141[A]:ARG:NH1	2.53	0.42
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.19	0.42
12:L:184:GLU:OE2	12:L:211:ARG:HD2	2.20	0.42
2:P:25[B]:MET:HE1	20:P:408:HOH:O	2.18	0.42
3:Q:204:LYS:HA	3:Q:205:ASN:C	2.40	0.42
7:U:43:ARG:HB3	7:U:151:VAL:HG13	2.01	0.42
11:Y:40:TYR:CD2	11:Y:73:ARG:NH1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:132:LEU:HD22	14:N:25:TYR:CZ	2.55	0.42
11:Y:199:TYR:CA	11:Y:200:SER:CB	2.98	0.42
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.19	0.42
3:Q:50:VAL:O	3:Q:51:ALA:CB	2.68	0.42
6:T:191:LYS:HB3	6:T:238:TYR:CD1	2.55	0.42
3:C:169:ARG:NH2	20:C:404:HOH:O	2.51	0.41
10:J:118:MET:HE2	10:J:124:LEU:HD13	2.01	0.41
10:X:118:MET:HE2	10:X:124:LEU:HD13	2.02	0.41
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.46	0.41
6:T:205:LYS:O	6:T:206:ASP:OD1	2.37	0.41
7:U:199:ILE:HD11	7:U:239:LEU:CD2	2.48	0.41
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.50	0.41
9:I:13[A]:MET:CE	9:I:162:LEU:HD12	2.51	0.41
6:T:152:ASP:OD1	6:T:156:VAL:HG12	2.21	0.41
8:H:77:VAL:HB	20:H:539:HOH:O	2.21	0.41
12:L:148:LEU:HD23	12:L:178:VAL:HG12	2.03	0.41
5:E:49:LEU:HG	5:E:195:LEU:HD21	2.02	0.41
6:F:202:ASP:OD1	6:F:204:VAL:HG22	2.20	0.41
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.56	0.41
2:B:151:ASP:HB2	2:B:152:PRO:CD	2.51	0.41
5:S:152[B]:ASN:ND2	20:S:406:HOH:O	2.53	0.41
6:T:34:SER:OG	6:T:65:ARG:NH1	2.51	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.03	0.41
10:J:27[A]:GLN:HE21	10:J:29:LYS:N	2.18	0.41
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.51	0.41
11:Y:144:SER:HB3	11:Y:147:LEU:HD13	2.03	0.40
4:D:203:LYS:HE2	4:D:210:LEU:HB3	2.02	0.40
12:L:144:MET:HE2	12:L:144:MET:HB3	1.87	0.40
13:M:5:MET:CE	14:N:116:MET:HB2	2.51	0.40
3:C:106:TYR:CD1	3:C:106:TYR:C	2.94	0.40
11:K:42:LEU:CD2	11:K:179:VAL:HG22	2.51	0.40
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:241:GLU:OE1	5:S:234:GLU:OE2[1_455]	2.09	0.11

## 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%)	221 (96%)	6 (3%)	4 (2%)	11	4
1	O	228/234 (97%)	217 (95%)	7 (3%)	4 (2%)	11	4
2	B	248/261 (95%)	238 (96%)	10 (4%)	0	100	100
2	P	248/261 (95%)	233 (94%)	11 (4%)	4 (2%)	12	5
3	C	236/248 (95%)	223 (94%)	7 (3%)	6 (2%)	7	2
3	Q	236/248 (95%)	221 (94%)	7 (3%)	8 (3%)	5	1
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	15	7
4	R	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	15	7
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	39	33
5	S	238/263 (90%)	231 (97%)	5 (2%)	2 (1%)	24	15
6	F	241/255 (94%)	239 (99%)	2 (1%)	0	100	100
6	T	239/255 (94%)	233 (98%)	3 (1%)	3 (1%)	15	7
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	3 (1%)	2 (1%)	21	13
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	5 (2%)	0	100	100
10	J	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	198/204 (97%)	195 (98%)	3 (2%)	0	100	100
11	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	34	26
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%)	210 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	2 (1%)	1 (0%)	34	26
14	b	202/205 (98%)	198 (98%)	3 (2%)	1 (0%)	34	26
All	All	6212/6458 (96%)	6040 (97%)	129 (2%)	43 (1%)	26	19

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
3	C	204	LYS
4	D	176	GLY
1	O	52	LYS
2	P	54	LYS
3	Q	206	ILE
3	Q	221	ASN
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
11	Y	200	SER
1	A	53	SER
3	C	50	VAL
4	D	175[A]	GLU
4	D	175[B]	GLU
5	E	59	HIS
14	N	198	ALA
1	O	53	SER
1	O	231	ALA
3	Q	47	LYS
3	Q	50	VAL
3	Q	201	SER
3	Q	203	GLY
5	S	236	LEU
6	T	7	TYR
1	A	176	ARG
3	C	51	ALA
3	C	200	GLN
3	C	216	SER
1	O	176	ARG
3	Q	51	ALA
3	Q	216	SER

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Mol	Chain	Res	Type
7	U	58	ASP
7	U	59	LYS
14	b	198	ALA
1	A	50	LYS
2	P	58	GLU
2	P	204	SER
6	T	208	ALA
3	C	203	GLY
2	P	52	ILE
6	T	6	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	173 (94%)	12 (6%)	21	15
1	O	176/191 (92%)	164 (93%)	12 (7%)	20	13
2	B	199/221 (90%)	192 (96%)	7 (4%)	43	40
2	P	197/221 (89%)	187 (95%)	10 (5%)	29	23
3	C	179/210 (85%)	174 (97%)	5 (3%)	51	50
3	Q	184/210 (88%)	175 (95%)	9 (5%)	31	25
4	D	189/203 (93%)	182 (96%)	7 (4%)	41	38
4	R	187/203 (92%)	184 (98%)	3 (2%)	70	73
5	E	192/223 (86%)	184 (96%)	8 (4%)	36	31
5	S	197/223 (88%)	192 (98%)	5 (2%)	55	55
6	F	199/212 (94%)	188 (94%)	11 (6%)	27	21
6	T	192/212 (91%)	181 (94%)	11 (6%)	25	19
7	G	202/207 (98%)	196 (97%)	6 (3%)	48	47
7	U	186/207 (90%)	182 (98%)	4 (2%)	60	62
8	H	181/195 (93%)	175 (97%)	6 (3%)	45	43
8	V	172/195 (88%)	164 (95%)	8 (5%)	32	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	176/174 (101%)	175 (99%)	1 (1%)	90	93
9	W	173/174 (99%)	172 (99%)	1 (1%)	90	93
10	J	166/170 (98%)	158 (95%)	8 (5%)	31	26
10	X	165/170 (97%)	159 (96%)	6 (4%)	42	39
11	K	154/159 (97%)	146 (95%)	8 (5%)	29	23
11	Y	159/159 (100%)	153 (96%)	6 (4%)	40	36
12	L	175/178 (98%)	168 (96%)	7 (4%)	38	33
12	Z	175/178 (98%)	169 (97%)	6 (3%)	44	41
13	M	180/181 (99%)	178 (99%)	2 (1%)	80	83
13	a	178/181 (98%)	173 (97%)	5 (3%)	51	50
14	N	158/159 (99%)	155 (98%)	3 (2%)	65	67
14	b	158/159 (99%)	154 (98%)	4 (2%)	55	55
All	All	5034/5366 (94%)	4853 (96%)	181 (4%)	43	39

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	VAL
1	A	69	LYS
1	A	73	LEU
1	A	142	ARG
1	A	176	ARG
1	A	180	ASP
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP
2	B	33	THR
2	B	58	GLU
2	B	190	LEU
2	B	207	SER
2	B	229	LYS
2	B	238	LYS
2	B	249	ARG
3	C	2	SER
3	C	148	ASP

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Mol	Chain	Res	Type
3	C	163	ARG
3	C	205	ASN
3	C	208	LEU
4	D	9	ASP
4	D	46	VAL
4	D	95	GLU
4	D	117	SER
4	D	126	GLU
4	D	199	LEU
4	D	208	GLU
5	E	29	VAL
5	E	61	LYS
5	E	95	SER
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	181	GLU
5	E	189	LYS
5	E	202	GLU
6	F	17	ASP
6	F	31	GLU
6	F	53	VAL
6	F	81	LEU
6	F	87	LEU
6	F	174	THR
6	F	187	ARG
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	183	VAL
7	G	190	THR
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	220	GLU
9	I	35	THR

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Mol	Chain	Res	Type
10	J	1[A]	MET
10	J	1[B]	MET
10	J	27[A]	GLN
10	J	27[B]	GLN
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	155	ARG
11	K	12	VAL
11	K	41	LEU
11	K	138	VAL
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	VAL
11	K	192	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	102	PHE
12	L	125	ASP
12	L	169	ASP
12	L	174	LEU
12	L	207	THR
13	M	100	ARG
13	M	154	LEU
14	N	22	THR
14	N	35	THR
14	N	196	LYS
1	O	10	THR
1	O	73	LEU
1	O	118	GLN
1	O	142	ARG
1	O	176	ARG
1	O	180	ASP
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	221	THR
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	190	LEU
2	P	204	SER
2	P	207	SER
2	P	235	GLN
2	P	236	LEU
2	P	246	LYS
2	P	249	ARG
3	Q	2	SER
3	Q	56	GLU
3	Q	148	ASP
3	Q	163	ARG
3	Q	170	GLU
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	227	LYS
4	R	9	ASP
4	R	46	VAL
4	R	117	SER
5	S	29	VAL
5	S	45	VAL
5	S	101	ARG
5	S	122	ARG
5	S	234	GLU
6	T	17	ASP
6	T	31	GLU
6	T	53	VAL
6	T	81	LEU
6	T	87	LEU
6	T	174	THR
6	T	190	VAL
6	T	215	TRP
6	T	223	ARG
6	T	240	LYS
6	T	241	GLU
7	U	42	VAL
7	U	78	CYS
7	U	199	ILE
7	U	206	LEU
8	V	6	VAL
8	V	22	GLU

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Mol	Chain	Res	Type
8	V	65	LEU
8	V	68	LEU
8	V	108	PRO
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	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	158	GLU
11	Y	8	PHE
11	Y	12	VAL
11	Y	41	LEU
11	Y	138	VAL
11	Y	147	LEU
11	Y	192	VAL
12	Z	102	PHE
12	Z	125	ASP
12	Z	169	ASP
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
13	a	92	LEU
13	a	100	ARG
13	a	154	LEU
13	a	198	GLU
13	a	216	SER
14	b	22	THR
14	b	29	ARG
14	b	35	THR
14	b	196	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) 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

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Mol	Chain	Res	Type
2	B	109	GLN
3	C	54	GLN
3	C	175	ASN
4	D	227	HIS
5	E	16	GLN
5	E	65	HIS
6	F	143	ASN
8	H	153	ASN
9	I	161	HIS
10	J	87	ASN
10	J	101	ASN
11	K	162	GLN
12	L	157	ASN
13	M	162	GLN
14	N	193	GLN
1	O	101	GLN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	109	GLN
2	P	146	GLN
3	Q	18	GLN
4	R	227	HIS
5	S	86	ASN
5	S	175	HIS
6	T	68	ASN
6	T	143	ASN
8	V	193	ASN
9	W	172	ASN
10	X	24	ASN
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 ⓘ

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	1.28	2 (28%)	5,10,12	1.36	1 (20%)
5	6V1	E	148	5	11,15,16	1.31	2 (18%)	11,20,22	2.74	3 (27%)
7	YCM	G	137	7	7,9,10	2.52	4 (57%)	5,10,12	5.91	3 (60%)
7	6V1	G	161	7	11,15,16	1.28	1 (9%)	11,20,22	2.71	4 (36%)
7	6V1	G	47	7	11,15,16	1.50	3 (27%)	11,20,22	3.39	3 (27%)
10	6V1	J	91	10	11,15,16	1.66	2 (18%)	11,20,22	5.63	8 (72%)
3	YCM	Q	63	3	7,9,10	1.66	2 (28%)	5,10,12	2.91	3 (60%)
5	6V1	S	148	5	11,15,16	1.45	2 (18%)	11,20,22	1.86	5 (45%)
7	YCM	U	137	7	7,9,10	1.60	1 (14%)	5,10,12	1.50	2 (40%)
7	6V1	U	161	7	11,15,16	1.52	3 (27%)	11,20,22	2.46	5 (45%)
7	6V1	U	47	7	11,15,16	1.30	1 (9%)	11,20,22	2.84	4 (36%)
10	6V1	X	91	10	11,15,16	1.66	3 (27%)	11,20,22	5.93	6 (54%)

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	-	1/6/25/27	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CB-SG	-4.55	1.72	1.81
10	J	91	6V1	C1-SG	-4.48	1.77	1.83
10	X	91	6V1	C1-SG	-4.06	1.78	1.83
7	U	137	YCM	CB-SG	-3.72	1.74	1.81
7	G	47	6V1	C2-N3	-3.35	1.33	1.38
3	Q	63	YCM	CD-SG	-3.27	1.74	1.81
5	S	148	6V1	C2-N3	-3.15	1.34	1.38
7	U	161	6V1	C2-N3	-3.09	1.34	1.38
7	G	161	6V1	C2-N3	-2.98	1.34	1.38
7	U	161	6V1	C4-N3	-2.83	1.33	1.38
7	G	47	6V1	C4-N3	-2.82	1.33	1.38
5	E	148	6V1	C4-N3	-2.55	1.34	1.38
3	Q	63	YCM	CB-SG	-2.52	1.76	1.81
5	E	148	6V1	C2-N3	-2.40	1.35	1.38
3	C	63	YCM	CB-SG	-2.31	1.76	1.81
7	U	161	6V1	C1-SG	-2.17	1.80	1.83
10	X	91	6V1	C4-N3	-2.09	1.34	1.38
3	C	63	YCM	CD-SG	-2.02	1.77	1.81
7	G	47	6V1	C5-C4	2.01	1.54	1.50
10	J	91	6V1	O7-C2	2.09	1.26	1.22
5	S	148	6V1	C5-C4	2.29	1.54	1.50
7	G	137	YCM	CD-CE	2.35	1.58	1.51
10	X	91	6V1	O7-C2	2.55	1.27	1.22
7	G	137	YCM	CD-SG	2.82	1.87	1.81
7	U	47	6V1	C1-C2	2.82	1.54	1.52
7	G	137	YCM	CE-NZ2	3.05	1.42	1.32

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	47	6V1	C5-C1-C2	-8.78	97.30	103.98
10	X	91	6V1	C6-N3-C4	-6.63	116.19	123.24
10	J	91	6V1	C6-N3-C4	-5.90	116.96	123.24
10	X	91	6V1	O7-C2-C1	-5.17	115.84	125.18
3	Q	63	YCM	CA-CB-SG	-4.56	102.06	112.84
10	X	91	6V1	O8-C4-C5	-4.46	121.40	127.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	161	6V1	C5-C1-C2	-4.39	100.64	103.98
10	J	91	6V1	O7-C2-C1	-4.23	117.55	125.18
7	G	161	6V1	C5-C1-C2	-4.22	100.78	103.98
7	U	47	6V1	C5-C1-C2	-4.15	100.82	103.98
7	G	161	6V1	O8-C4-C5	-4.06	121.94	127.38
10	J	91	6V1	O8-C4-C5	-3.62	122.53	127.38
7	U	161	6V1	O8-C4-C5	-3.37	122.86	127.38
7	G	137	YCM	OZ1-CE-CD	-3.29	113.59	120.98
5	S	148	6V1	C5-C1-C2	-3.23	101.53	103.98
5	S	148	6V1	O8-C4-C5	-2.75	123.69	127.38
7	G	47	6V1	O7-C2-C1	-2.68	120.35	125.18
5	E	148	6V1	O-C-CA	-2.61	118.72	125.72
5	E	148	6V1	C5-C1-C2	-2.52	102.06	103.98
3	Q	63	YCM	O-C-CA	-2.51	119.00	125.72
5	S	148	6V1	O-C-CA	-2.46	119.12	125.72
7	U	47	6V1	O8-C4-C5	-2.40	124.16	127.38
3	C	63	YCM	O-C-CA	-2.27	119.64	125.72
7	U	137	YCM	O-C-CA	-2.22	119.75	125.72
7	U	137	YCM	CA-CB-SG	-2.13	107.80	112.84
10	J	91	6V1	CA-CB-SG	-2.10	108.01	112.87
5	S	148	6V1	O7-C2-N3	-2.07	121.33	124.19
7	G	137	YCM	O-C-CA	-2.03	120.28	125.72
10	J	91	6V1	O-C-CA	-2.02	120.31	125.72
7	U	161	6V1	O8-C4-N3	2.04	126.44	123.91
7	U	47	6V1	C6-N3-C2	2.39	125.27	123.42
5	S	148	6V1	C6-N3-C4	2.68	126.09	123.24
7	U	161	6V1	C6-N3-C2	2.87	125.65	123.42
7	G	161	6V1	O8-C4-N3	3.41	128.15	123.91
3	Q	63	YCM	CD-CE-NZ2	3.80	119.67	115.48
7	U	161	6V1	CB-SG-C1	4.04	109.61	101.58
7	G	161	6V1	CB-SG-C1	4.75	111.02	101.58
7	G	47	6V1	CB-SG-C1	5.73	112.97	101.58
10	J	91	6V1	O7-C2-N3	6.47	133.13	124.19
10	X	91	6V1	O7-C2-N3	7.07	133.96	124.19
7	U	47	6V1	CB-SG-C1	7.27	116.03	101.58
5	E	148	6V1	C6-N3-C2	7.55	129.29	123.42
10	J	91	6V1	CB-SG-C1	8.23	117.95	101.58
10	X	91	6V1	CB-SG-C1	8.45	118.39	101.58
7	G	137	YCM	CD-CE-NZ2	12.43	129.17	115.48
10	J	91	6V1	C6-N3-C2	12.68	133.28	123.42
10	X	91	6V1	C6-N3-C2	12.80	133.38	123.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	148	6V1	C3-C6-N3-C2

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 87 ligands modelled in this entry, 72 are monoatomic - leaving 15 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
18	1PE	H	304	-	15,15,15	0.61	0	14,14,14	0.59	0
19	6VC	H	305	8	24,27,27	0.89	1 (4%)	29,36,36	1.51	5 (17%)
18	1PE	I	303	-	15,15,15	0.58	0	14,14,14	0.86	0
19	6VC	K	306	11	24,27,27	0.63	0	29,36,36	1.46	6 (20%)
18	1PE	L	301	-	15,15,15	0.63	0	14,14,14	0.65	0
18	1PE	M	304	-	15,15,15	0.64	0	14,14,14	0.36	0
18	1PE	N	305	-	15,15,15	0.54	0	14,14,14	0.55	0
19	6VC	N	307	14	24,27,27	0.80	0	29,36,36	1.69	5 (17%)
18	1PE	U	302	-	15,15,15	0.64	0	14,14,14	0.98	1 (7%)
19	6VC	V	303	8	24,27,27	0.73	0	29,36,36	1.37	4 (13%)
18	1PE	W	303	-	15,15,15	0.58	0	14,14,14	0.37	0
19	6VC	Y	306	11	24,27,27	0.92	2 (8%)	29,36,36	1.32	4 (13%)
18	1PE	Z	301	-	15,15,15	0.63	0	14,14,14	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	1PE	a	304	-	15,15,15	0.71	0	14,14,14	0.46	0
19	6VC	b	306	14	24,27,27	1.00	3 (12%)	29,36,36	2.11	9 (31%)

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
18	1PE	H	304	-	-	0/13/13/13	0/0/0/0
19	6VC	H	305	8	-	0/38/38/38	0/0/0/0
18	1PE	I	303	-	-	0/13/13/13	0/0/0/0
19	6VC	K	306	11	-	0/38/38/38	0/0/0/0
18	1PE	L	301	-	-	0/13/13/13	0/0/0/0
18	1PE	M	304	-	-	0/13/13/13	0/0/0/0
18	1PE	N	305	-	-	0/13/13/13	0/0/0/0
19	6VC	N	307	14	-	0/38/38/38	0/0/0/0
18	1PE	U	302	-	-	0/13/13/13	0/0/0/0
19	6VC	V	303	8	-	0/38/38/38	0/0/0/0
18	1PE	W	303	-	-	0/13/13/13	0/0/0/0
19	6VC	Y	306	11	-	0/38/38/38	0/0/0/0
18	1PE	Z	301	-	-	0/13/13/13	0/0/0/0
18	1PE	a	304	-	-	0/13/13/13	0/0/0/0
19	6VC	b	306	14	-	0/38/38/38	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	306	6VC	C13-N3	-2.34	1.42	1.46
19	Y	306	6VC	O4-C12	-2.07	1.19	1.23
19	b	306	6VC	C9-C12	-2.02	1.47	1.52
19	b	306	6VC	C14-C13	2.05	1.56	1.53
19	b	306	6VC	C23-C22	2.88	1.57	1.52
19	H	305	6VC	C23-C22	3.16	1.58	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	306	6VC	O3-C10-C9	-5.98	98.18	111.27
19	N	307	6VC	C10-C9-N2	-5.98	97.52	110.71
19	b	306	6VC	C1-C6-C5	-4.66	96.06	113.30
19	H	305	6VC	O3-C10-C9	-4.48	101.47	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	306	6VC	O2-C8-C5	-4.04	114.95	121.97
19	K	306	6VC	O3-C10-C9	-3.91	102.72	111.27
19	Y	306	6VC	O3-C10-C9	-3.53	103.55	111.27
19	V	303	6VC	O3-C10-C9	-3.38	103.87	111.27
19	H	305	6VC	O2-C8-C5	-3.31	116.23	121.97
19	N	307	6VC	O3-C10-C9	-3.01	104.68	111.27
19	b	306	6VC	C10-C9-C12	-2.90	102.26	110.44
19	K	306	6VC	C6-C5-C8	-2.68	106.10	113.28
19	Y	306	6VC	C10-C9-C12	-2.60	103.11	110.44
19	Y	306	6VC	O2-C8-C5	-2.55	117.55	121.97
19	V	303	6VC	C10-C9-C12	-2.45	103.54	110.44
19	K	306	6VC	C10-C9-C12	-2.41	103.65	110.44
19	V	303	6VC	O2-C8-C5	-2.39	117.83	121.97
19	K	306	6VC	O2-C8-C5	-2.37	117.86	121.97
19	H	305	6VC	C10-C9-C12	-2.28	104.03	110.44
19	b	306	6VC	C9-C12-N3	-2.11	111.88	116.80
19	N	307	6VC	O2-C8-C5	-2.11	118.31	121.97
19	N	307	6VC	C23-C22-C21	2.05	114.92	111.16
19	K	306	6VC	C1-C6-C5	2.15	121.27	113.30
19	H	305	6VC	O4-C12-N3	2.24	127.27	122.91
19	K	306	6VC	C5-C8-N2	2.34	119.78	115.85
19	b	306	6VC	C6-C1-C2	2.36	122.04	113.67
19	H	305	6VC	C10-C9-N2	2.55	116.34	110.71
19	Y	306	6VC	C5-C8-N2	2.55	120.14	115.85
19	V	303	6VC	C10-C9-N2	2.57	116.39	110.71
19	b	306	6VC	O2-C8-N2	2.88	127.80	122.96
19	b	306	6VC	C10-C9-N2	2.89	117.08	110.71
18	U	302	1PE	C26-OH6-C15	2.94	125.86	113.31
19	b	306	6VC	O4-C12-N3	3.11	128.97	122.91
19	N	307	6VC	C10-C9-C12	3.14	119.30	110.44

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	230/234 (98%)	-0.03	7 (3%) 54 55	31, 46, 82, 92	0
1	O	230/234 (98%)	0.59	32 (13%) 4 4	41, 63, 100, 120	0
2	B	248/261 (95%)	0.30	14 (5%) 28 29	35, 52, 89, 136	0
2	P	248/261 (95%)	0.77	40 (16%) 3 3	40, 61, 106, 142	0
3	C	236/248 (95%)	0.57	27 (11%) 7 7	36, 61, 100, 139	0
3	Q	238/248 (95%)	0.85	45 (18%) 2 2	34, 61, 112, 149	0
4	D	233/241 (96%)	0.26	16 (6%) 20 21	39, 58, 88, 114	0
4	R	233/241 (96%)	0.06	6 (2%) 59 60	32, 44, 71, 93	0
5	E	233/263 (88%)	0.13	13 (5%) 28 29	29, 43, 86, 100	0
5	S	237/263 (90%)	0.08	10 (4%) 40 41	34, 47, 81, 104	0
6	F	239/255 (93%)	-0.08	0 100 100	27, 36, 58, 74	0
6	T	240/255 (94%)	0.27	19 (7%) 15 16	35, 52, 85, 107	0
7	G	241/246 (97%)	0.15	6 (2%) 61 61	27, 40, 73, 101	0
7	U	235/246 (95%)	0.61	32 (13%) 4 4	42, 60, 95, 124	0
8	H	220/234 (94%)	-0.07	4 (1%) 71 72	27, 36, 66, 100	0
8	V	220/234 (94%)	0.12	6 (2%) 58 58	36, 48, 84, 97	0
9	I	204/205 (99%)	0.03	1 (0%) 91 92	29, 38, 58, 74	0
9	W	204/205 (99%)	0.08	3 (1%) 76 77	36, 50, 73, 81	0
10	J	195/201 (97%)	-0.12	3 (1%) 76 77	32, 42, 60, 76	0
10	X	195/201 (97%)	-0.06	1 (0%) 91 92	34, 44, 59, 74	0
11	K	200/204 (98%)	0.07	2 (1%) 84 84	36, 46, 71, 84	0
11	Y	201/204 (98%)	0.03	4 (1%) 68 69	28, 37, 59, 70	0
12	L	213/213 (100%)	-0.09	0 100 100	34, 49, 71, 85	0
12	Z	213/213 (100%)	0.07	4 (1%) 70 70	27, 38, 60, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	216/219 (98%)	0.11	3 (1%) 78 78	27, 39, 62, 95	0
13	a	216/219 (98%)	-0.05	3 (1%) 78 78	27, 39, 60, 82	0
14	N	202/205 (98%)	-0.05	0 100 100	27, 35, 56, 94	0
14	b	203/205 (99%)	0.15	8 (3%) 43 45	32, 41, 66, 97	0
All	All	6223/6458 (96%)	0.18	309 (4%) 32 34	27, 46, 85, 149	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	204	SER	13.9
1	O	232	ILE	11.1
4	D	241	ILE	9.8
2	P	203	VAL	8.8
3	Q	232	ILE	7.8
3	Q	238	GLU	7.6
7	G	187	PHE	7.2
3	Q	234	LYS	7.1
3	C	225	ILE	7.0
4	R	241	ILE	6.4
5	E	237	GLU	6.3
2	P	61	PHE	6.3
3	C	232	ILE	6.2
3	Q	240	GLU	6.2
3	Q	236	LYS	6.1
3	Q	202	GLY	6.1
3	Q	203	GLY	6.1
8	H	204	CYS	6.1
11	K	40	TYR	6.0
7	U	2	SER	6.0
2	P	247	ALA	6.0
3	Q	239	ASN	5.8
2	P	202	ASP	5.8
5	E	54	SER	5.7
7	G	189	TRP	5.7
1	O	201	GLN	5.6
3	C	49	SER	5.6
7	U	208	ILE	5.6
3	C	203	GLY	5.5
3	C	229	VAL	5.4
2	B	61	PHE	5.4
13	a	216	SER	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	203	VAL	5.3
7	U	206	LEU	5.3
3	Q	225	ILE	5.2
3	Q	229	VAL	5.1
3	C	202	GLY	5.1
7	U	242	LEU	5.1
2	P	234	GLU	5.0
4	R	130	PRO	4.9
14	b	203	PRO	4.9
2	P	206	LEU	4.9
2	B	248	GLU	4.9
3	Q	233	GLU	4.9
2	P	205	LYS	4.8
8	H	203	ARG	4.8
3	Q	237	GLU	4.7
8	V	203	ARG	4.7
3	C	201	SER	4.7
11	Y	40	TYR	4.7
6	T	208	ALA	4.6
7	U	3	ARG	4.6
3	Q	48	LYS	4.6
8	V	199	LEU	4.6
2	B	204	SER	4.5
1	A	230	ALA	4.5
3	C	48	LYS	4.5
1	A	231	ALA	4.4
5	E	52	ALA	4.4
4	D	237	VAL	4.4
1	A	232	ILE	4.3
4	D	240	ASP	4.3
2	P	249	ARG	4.3
1	O	192	LEU	4.2
3	Q	201	SER	4.2
2	B	247	ALA	4.2
5	E	235	GLY	4.2
7	G	188	ASP	4.1
7	U	243	ALA	4.1
3	C	234	LYS	4.1
10	J	1[A]	MET	4.1
1	O	199	GLU	4.0
6	T	207	LYS	4.0
5	S	239	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
3	Q	223	GLU	4.0
3	Q	226	GLU	4.0
3	Q	192	ILE	3.9
3	C	233	GLU	3.9
2	P	220	ASN	3.9
5	S	57	ALA	3.9
1	O	181	LEU	3.9
2	P	244	GLU	3.9
1	O	200	GLY	3.8
3	Q	179	GLU	3.8
3	C	230	ALA	3.7
4	D	234	LEU	3.7
2	B	205	LYS	3.7
3	Q	230	ALA	3.6
1	O	229	LEU	3.6
7	U	204	THR	3.6
4	R	128	ALA	3.6
1	O	177	TYR	3.6
1	O	184	GLU	3.6
2	P	246	LYS	3.6
1	O	40	ALA	3.5
3	C	236	LYS	3.5
7	U	199	ILE	3.5
8	V	202	TYR	3.5
6	T	204	VAL	3.5
3	C	138	PHE	3.5
5	S	2	PHE	3.5
6	T	205	LYS	3.5
7	U	177	SER	3.5
4	D	127	ASP	3.5
3	C	195	LEU	3.5
6	T	206	ASP	3.5
7	U	58	ASP	3.5
12	Z	161	VAL	3.5
3	Q	200	GLN	3.5
1	O	176	ARG	3.5
10	X	95	ARG	3.5
9	W	113	PRO	3.4
4	D	239	LYS	3.4
2	P	230	GLN	3.4
7	U	240	VAL	3.4
3	Q	181	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
7	U	207	SER	3.3
2	P	243	GLU	3.3
14	b	199	VAL	3.3
6	T	5	THR	3.3
2	P	201	MET	3.3
4	R	127	ASP	3.3
1	O	198	PHE	3.3
3	Q	47	LYS	3.3
2	P	233	VAL	3.3
1	O	225	VAL	3.3
8	H	201	ARG	3.2
3	C	200	GLN	3.2
3	C	228	TYR	3.2
1	O	186	ALA	3.2
2	P	177	GLN	3.2
7	U	245	ARG	3.2
6	T	209	PHE	3.2
5	S	3	ARG	3.1
6	T	203	GLU	3.1
1	O	223	THR	3.1
7	U	183	VAL	3.1
1	O	157	TRP	3.1
2	P	52	ILE	3.1
7	U	212	PRO	3.1
5	E	56	LEU	3.1
4	R	131	GLY	3.0
3	Q	180	ALA	3.0
7	U	196	GLU	3.0
2	B	202	ASP	3.0
13	M	215	ILE	3.0
6	T	243	LEU	3.0
7	U	178	PHE	3.0
12	Z	164	VAL	3.0
2	P	200	THR	3.0
1	O	3	ARG	2.9
2	P	248	GLU	2.9
1	O	187	ILE	2.9
2	P	197	LEU	2.9
1	O	182	GLU	2.9
1	O	59	ARG	2.9
2	P	51	ASN	2.9
3	Q	199	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	237	ILE	2.9
14	b	26	ILE	2.9
4	D	130	PRO	2.9
1	O	228	TYR	2.9
2	P	241	GLU	2.9
7	U	56	VAL	2.9
2	P	237	ILE	2.9
3	Q	37	GLY	2.8
5	S	174	ARG	2.8
7	G	209	ASP	2.8
2	P	55	LEU	2.8
2	B	242	GLU	2.8
2	P	58	GLU	2.8
3	C	238	GLU	2.8
14	b	200	ALA	2.8
3	C	220	LEU	2.8
3	C	237	GLU	2.8
4	D	131	GLY	2.8
5	E	202	GLU	2.8
7	U	57	PRO	2.8
2	P	178	ASP	2.8
3	Q	178	ASP	2.8
5	E	53	GLN	2.7
13	M	216	SER	2.7
3	C	222	PRO	2.7
6	T	237	LYS	2.7
11	K	145	TYR	2.7
7	U	209	ASP	2.7
4	D	236	GLU	2.7
6	T	241	GLU	2.7
7	U	205	VAL	2.7
2	B	249	ARG	2.7
4	D	188	SER	2.7
4	D	235	GLU	2.7
3	Q	220	LEU	2.7
11	Y	200	SER	2.6
4	D	232	GLU	2.6
8	V	197	THR	2.6
2	B	206	LEU	2.6
2	P	207	SER	2.6
3	C	227	LYS	2.6
1	O	227	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
6	T	54	LEU	2.6
2	P	199	LYS	2.6
3	Q	213	ARG	2.6
5	E	218	ASP	2.6
4	D	128	ALA	2.6
6	T	240	LYS	2.6
8	V	204	CYS	2.6
5	S	18[A]	ARG	2.5
2	B	241	GLU	2.5
7	G	57	PRO	2.5
3	Q	185	ASP	2.5
2	P	53	HIS	2.5
3	Q	204	LYS	2.5
7	G	3	ARG	2.5
9	W	116	PHE	2.5
10	J	95	ARG	2.5
3	Q	228	TYR	2.5
13	M	33	LEU	2.5
1	O	195	LYS	2.5
7	U	200	THR	2.5
7	U	223	GLU	2.5
11	Y	201	GLY	2.4
1	O	172	PHE	2.4
3	Q	138	PHE	2.4
3	Q	205	ASN	2.4
5	S	238	GLU	2.4
13	a	194	GLU	2.4
6	T	233	GLU	2.4
7	U	174	GLU	2.4
7	U	179	LEU	2.4
5	E	201	ALA	2.4
1	O	191	ILE	2.4
6	T	236	GLU	2.4
2	P	180	LYS	2.4
3	Q	49	SER	2.4
3	C	56	GLU	2.3
2	P	240	HIS	2.3
3	Q	38	ARG	2.3
3	Q	183	THR	2.3
5	S	204	ASP	2.3
2	P	219	GLU	2.3
3	Q	235	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	230	THR	2.3
6	T	180	GLN	2.3
5	E	59	HIS	2.3
3	Q	184	ASP	2.3
7	U	195	VAL	2.3
3	C	226	GLU	2.3
4	D	183	GLU	2.3
7	U	210	PHE	2.3
3	Q	224	GLU	2.3
6	T	230	ASP	2.3
2	B	243	GLU	2.3
2	B	245	ALA	2.3
5	E	58	ALA	2.3
3	Q	219	ILE	2.3
3	C	231	GLU	2.2
4	D	223	GLY	2.2
1	O	50	LYS	2.2
6	T	202	ASP	2.2
9	W	192	ASP	2.2
1	A	198	PHE	2.2
2	P	211	VAL	2.2
2	P	187	LYS	2.2
3	Q	190	LEU	2.2
2	P	183	GLU	2.2
12	Z	163	HIS	2.2
8	V	132	LEU	2.2
2	P	30	HIS	2.2
2	P	198	ASN	2.2
1	A	229	LEU	2.2
3	Q	186	LEU	2.2
1	A	3	ARG	2.2
7	U	7	ALA	2.2
14	b	201	THR	2.2
3	C	235	GLU	2.1
3	Q	210	VAL	2.1
5	S	4	ASN	2.1
2	P	235	GLN	2.1
7	U	173	THR	2.1
1	O	138	TRP	2.1
3	Q	39	ASP	2.1
4	R	240	ASP	2.1
3	C	204	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
7	U	202	LEU	2.1
14	b	202	LEU	2.1
5	E	234	GLU	2.1
11	Y	26	ILE	2.1
5	S	235	GLY	2.1
1	O	41	ASN	2.1
3	C	85[A]	ASN	2.1
3	Q	177	THR	2.1
5	E	203	GLN	2.1
8	H	220	GLU	2.1
1	O	168	ASN	2.1
6	T	6	GLY	2.1
2	P	56	LEU	2.0
9	I	179	VAL	2.0
10	J	185	LYS	2.0
7	U	186	LYS	2.0
13	a	215	ILE	2.0
12	Z	143	ALA	2.0
14	b	27	ALA	2.0
1	A	199	GLU	2.0
14	b	9	ASP	2.0
1	O	202	MET	2.0
1	O	194	LEU	2.0
7	U	198	ALA	2.0
1	O	180	ASP	2.0

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

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	0.88	0.16	-	33,39,51,53	0
3	YCM	Q	63	10/11	0.91	0.13	-	51,54,64,67	0
7	6V1	G	47	15/16	0.90	0.20	-	39,61,64,65	0
10	6V1	J	91	15/16	0.91	0.21	-	33,53,58,59	0
7	6V1	U	161	15/16	0.92	0.12	-	53,73,78,78	0
3	YCM	C	63	10/11	0.88	0.12	-	55,56,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	6V1	E	148	15/16	0.90	0.17	-	32,54,64,65	0
7	YCM	U	137	10/11	0.82	0.18	-	51,59,75,76	0
7	6V1	U	47	15/16	0.78	0.38	-	72,103,109,110	0
7	6V1	G	161	15/16	0.92	0.17	-	33,51,57,58	0
10	6V1	X	91	15/16	0.91	0.22	-	36,54,57,61	0
5	6V1	S	148	15/16	0.87	0.20	-	37,63,68,70	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( $\text{\AA}^2$ )	Q<0.9
18	1PE	H	304	16/16	0.77	0.28	14.89	58,69,77,79	0
15	CL	K	305	1/1	0.95	0.23	13.11	65,65,65,65	0
15	CL	S	301	1/1	0.98	0.31	8.14	64,64,64,64	0
18	1PE	I	303	16/16	0.88	0.21	7.07	55,58,68,71	0
18	1PE	Z	301	16/16	0.84	0.20	4.77	57,66,72,73	0
18	1PE	M	304	16/16	0.66	0.34	4.38	78,83,97,98	0
15	CL	M	301	1/1	0.95	0.22	4.14	56,56,56,56	0
15	CL	Q	302	1/1	0.90	0.23	3.82	64,64,64,64	0
18	1PE	W	303	16/16	0.82	0.25	3.52	59,64,71,74	0
18	1PE	L	301	16/16	0.75	0.21	3.16	60,70,74,76	0
18	1PE	a	304	16/16	0.71	0.26	3.11	66,70,86,87	0
15	CL	D	301	1/1	0.91	0.22	2.53	69,69,69,69	0
15	CL	G	301	1/1	0.98	0.18	2.46	48,48,48,48	0
15	CL	A	304	1/1	0.97	0.14	1.46	57,57,57,57	0
18	1PE	N	305	16/16	0.91	0.15	1.43	41,49,62,64	0
19	6VC	N	307	28/28	0.95	0.17	1.26	25,29,49,52	0
18	1PE	U	302	16/16	0.88	0.17	1.07	46,56,73,75	0
15	CL	N	301	1/1	0.99	0.15	0.88	35,35,35,35	0
19	6VC	V	303	28/28	0.92	0.14	0.73	42,45,60,61	0
19	6VC	K	306	28/28	0.96	0.14	0.52	36,39,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	a	301	1/1	0.97	0.13	0.37	59,59,59,59	0
19	6VC	Y	306	28/28	0.96	0.15	0.36	27,29,51,56	0
15	CL	U	301	1/1	0.98	0.12	-0.08	54,54,54,54	0
19	6VC	b	306	28/28	0.96	0.15	-0.11	31,34,55,56	0
19	6VC	H	305	28/28	0.95	0.11	-0.12	33,37,55,60	0
15	CL	A	301	1/1	0.99	0.11	-0.13	52,52,52,52	0
15	CL	C	301	1/1	0.94	0.10	-0.23	60,60,60,60	0
15	CL	S	302	1/1	0.99	0.13	-0.38	63,63,63,63	0
15	CL	N	304	1/1	0.96	0.13	-0.57	52,52,52,52	0
15	CL	b	304	1/1	0.98	0.11	-0.58	42,42,42,42	0
15	CL	O	301	1/1	0.96	0.10	-0.59	55,55,55,55	0
15	CL	F	301	1/1	0.97	0.11	-0.76	51,51,51,51	0
15	CL	G	302	1/1	0.97	0.11	-0.81	60,60,60,60	0
15	CL	N	303	1/1	0.98	0.11	-1.14	56,56,56,56	0
15	CL	Y	303	1/1	0.95	0.09	-1.28	64,64,64,64	0
15	CL	Y	304	1/1	0.96	0.08	-1.56	57,57,57,57	0
15	CL	b	303	1/1	0.97	0.07	-1.72	56,56,56,56	0
15	CL	b	302	1/1	0.97	0.09	-1.88	55,55,55,55	0
15	CL	B	302	1/1	0.91	0.11	-2.08	57,57,57,57	0
15	CL	K	303	1/1	0.94	0.07	-2.36	69,69,69,69	0
17	MG	I	301	1/1	0.96	0.08	-2.80	33,33,33,33	0
16	K	Z	302	1/1	0.99	0.08	-2.92	39,39,39,39	0
15	CL	S	303	1/1	0.96	0.06	-3.73	55,55,55,55	0
15	CL	E	304	1/1	0.94	0.09	-3.86	63,63,63,63	0
17	MG	W	301	1/1	0.96	0.06	-3.91	38,38,38,38	0
17	MG	H	302	1/1	0.98	0.05	-3.94	33,33,33,33	0
16	K	N	306	1/1	0.99	0.08	-4.28	38,38,38,38	0
17	MG	L	303	1/1	0.97	0.04	-4.90	37,37,37,37	0
16	K	L	302	1/1	0.96	0.04	-5.00	47,47,47,47	0
17	MG	I	304	1/1	0.97	0.07	-5.65	30,30,30,30	0
16	K	G	303	1/1	0.98	0.05	-5.83	33,33,33,33	0
15	CL	E	301	1/1	0.98	0.05	-5.95	61,61,61,61	0
17	MG	K	301	1/1	0.98	0.08	-6.37	36,36,36,36	0
16	K	U	303	1/1	0.98	0.06	-6.91	41,41,41,41	0
16	K	b	305	1/1	0.96	0.07	-7.27	41,41,41,41	0
15	CL	N	302	1/1	0.99	0.06	-	45,45,45,45	0
15	CL	a	302	1/1	0.98	0.08	-	43,43,43,43	0
17	MG	X	301	1/1	0.98	0.11	-	49,49,49,49	0
17	MG	V	301	1/1	0.93	0.24	-	58,58,58,58	0
15	CL	H	303	1/1	0.97	0.07	-	53,53,53,53	0
15	CL	Y	302	1/1	0.98	0.15	-	59,59,59,59	0
15	CL	M	302	1/1	0.99	0.07	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CL	O	302	1/1	0.95	0.09	-	63,63,63,63	0
15	CL	O	303	1/1	0.81	0.25	-	87,87,87,87	0
15	CL	O	304	1/1	0.90	0.07	-	67,67,67,67	0
15	CL	K	302	1/1	0.97	0.07	-	42,42,42,42	0
15	CL	I	302	1/1	0.91	0.08	-	48,48,48,48	0
15	CL	a	303	1/1	0.95	0.08	-	60,60,60,60	0
17	MG	J	301	1/1	0.97	0.05	-	48,48,48,48	0
15	CL	B	301	1/1	0.96	0.07	-	41,41,41,41	0
15	CL	A	303	1/1	0.97	0.08	-	50,50,50,50	0
15	CL	M	303	1/1	0.91	0.10	-	59,59,59,59	0
15	CL	E	302	1/1	0.97	0.05	-	55,55,55,55	0
15	CL	A	302	1/1	0.94	0.10	-	64,64,64,64	0
17	MG	H	301	1/1	0.95	0.17	-	57,57,57,57	0
15	CL	R	301	1/1	0.92	0.09	-	58,58,58,58	0
15	CL	C	302	1/1	0.95	0.16	-	71,71,71,71	0
15	CL	P	301	1/1	0.98	0.07	-	53,53,53,53	0
15	CL	Y	301	1/1	1.00	0.09	-	38,38,38,38	0
15	CL	W	302	1/1	0.97	0.07	-	54,54,54,54	0
15	CL	R	302	1/1	0.96	0.17	-	57,57,57,57	0
15	CL	b	301	1/1	0.98	0.06	-	45,45,45,45	0
15	CL	V	302	1/1	0.93	0.10	-	59,59,59,59	0
15	CL	Y	305	1/1	0.91	0.23	-	63,63,63,63	0
15	CL	Q	301	1/1	0.93	0.17	-	67,67,67,67	0
15	CL	K	304	1/1	0.93	0.15	-	60,60,60,60	0
15	CL	E	303	1/1	0.90	0.16	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.