



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 06:57 PM UTC

PDB ID : 9QBO / pdb\_00009qbo  
Title : Yeast 20S proteasome mutant: beta5\_G128V (b5-propeptide in trans) in complex with MG132  
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.  
Deposited on : 2025-03-03  
Resolution : 2.80 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

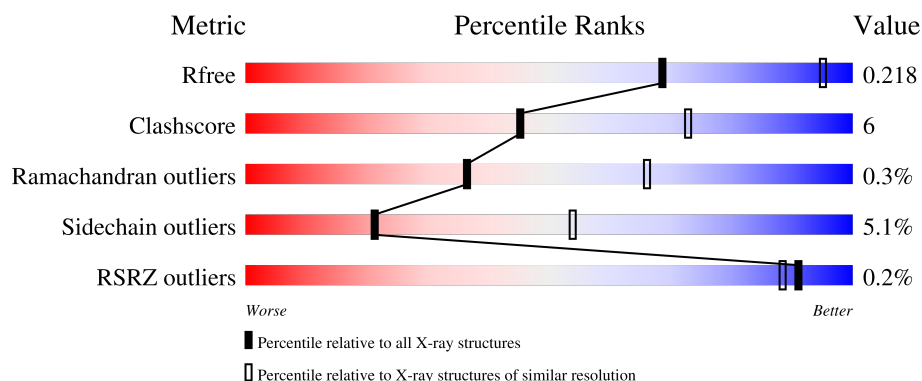
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	250	<div><div></div><div>95%</div><div>.</div></div>
1	O	250	<div><div></div><div>93%</div><div>6%</div></div>
2	B	258	<div><div></div><div>84%</div><div>10%</div><div>5%</div></div>
2	P	258	<div><div></div><div>84%</div><div>9%</div><div>5%</div></div>
3	C	254	<div><div></div><div>85%</div><div>7%</div><div>6%</div></div>





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Mol	Chain	Length	Quality of chain
3	Q	254	% 
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	231	
8	V	231	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	% 
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	195	
14	b	195	
15	f	4	
15	g	4	

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Mol	Chain	Length	Quality of chain
15	h	4	
15	i	4	
15	j	4	
15	k	4	

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
16	SO4	G	303	-	-	-	X
16	SO4	U	302	-	-	-	X

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 49864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			
8	V	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	130	VAL	GLY	engineered mutation	UNP P30656
Y	130	VAL	GLY	engineered mutation	UNP P30656

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	1	0
			1832	1159	315	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

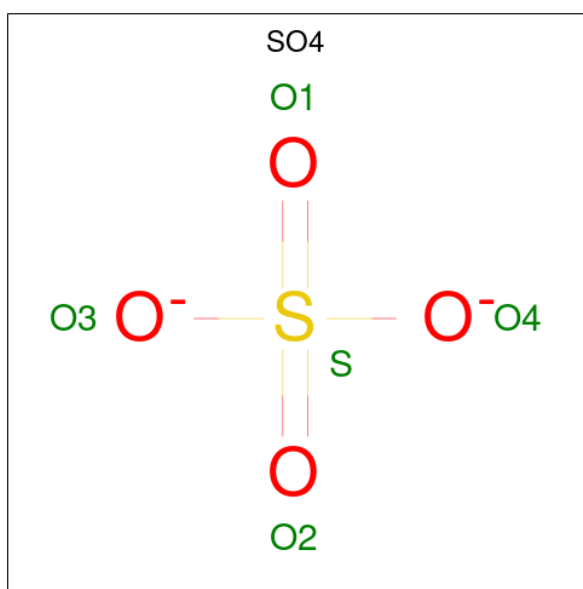
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			

- Molecule 15 is a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZ

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	f	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	g	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	h	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	i	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	j	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	k	4	Total	C	N	O	0	0	0
			41	30	4	7			

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	O	S	0	0
			5	4	1		
16	G	1	Total	O	S	0	0
			5	4	1		
16	P	1	Total	O	S	0	0
			5	4	1		
16	U	1	Total	O	S	0	0
			5	4	1		

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

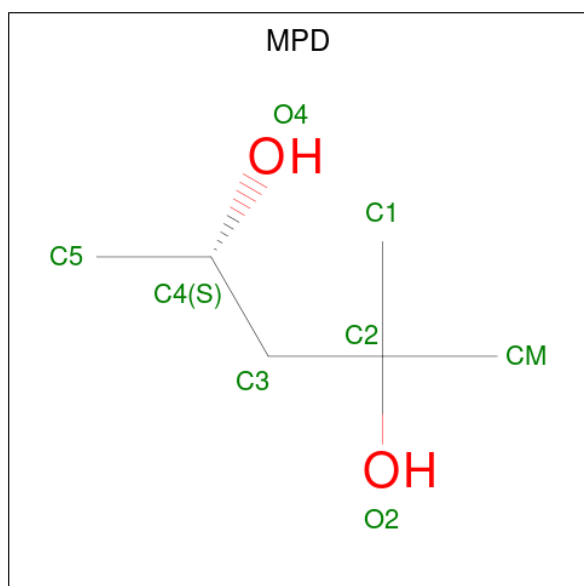


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total Mg 1 1	0	0
17	N	1	Total Mg 1 1	0	0

- Molecule 18 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

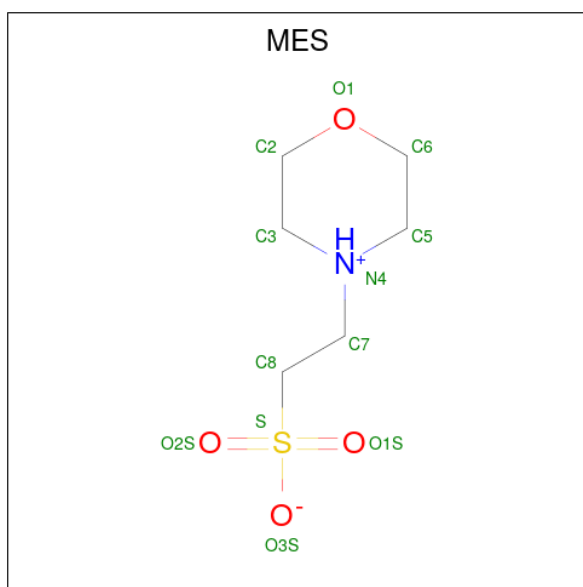
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	1	Total Cl 1 1	0	0
18	N	1	Total Cl 1 1	0	0
18	U	1	Total Cl 1 1	0	0
18	b	1	Total Cl 1 1	0	0

- Molecule 19 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	1	Total C O 8 6 2	0	0
19	a	1	Total C O 8 6 2	0	0

- Molecule 20 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
20	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	8	Total	O	0	0
			8	8		
21	B	10	Total	O	0	0
			10	10		
21	C	6	Total	O	0	0
			6	6		
21	D	4	Total	O	0	0
			4	4		
21	E	5	Total	O	0	0
			5	5		
21	F	10	Total	O	0	0
			10	10		
21	G	8	Total	O	0	0
			8	8		
21	H	8	Total	O	0	0
			8	8		
21	I	8	Total	O	0	0
			8	8		
21	J	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	3	Total O 3 3	0	0
21	L	11	Total O 11 11	0	0
21	M	15	Total O 15 15	0	0
21	N	9	Total O 9 9	0	0
21	O	2	Total O 2 2	0	0
21	P	6	Total O 6 6	0	0
21	Q	4	Total O 4 4	0	0
21	R	9	Total O 9 9	0	0
21	S	1	Total O 1 1	0	0
21	T	8	Total O 8 8	0	0
21	U	10	Total O 10 10	0	0
21	V	5	Total O 5 5	0	0
21	W	4	Total O 4 4	0	0
21	X	10	Total O 10 10	0	0
21	Y	7	Total O 7 7	0	0
21	Z	5	Total O 5 5	0	0
21	a	18	Total O 18 18	0	0
21	b	10	Total O 10 10	0	0
21	f	1	Total O 1 1	0	0
21	h	1	Total O 1 1	0	0
21	k	2	Total O 2 2	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.

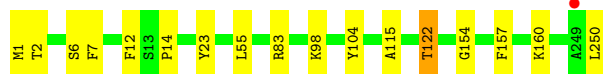
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  95%




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  93% 6%




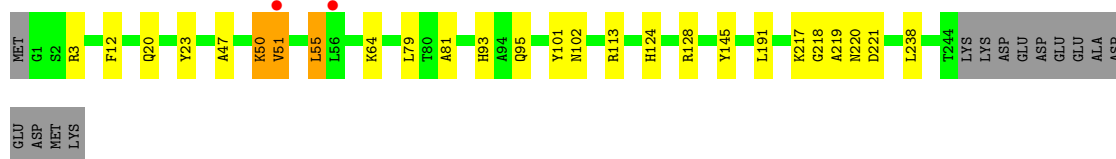
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  84% 10% 5%




- Molecule 2: Proteasome subunit alpha type-3

Chain P:  84% 9% 5%

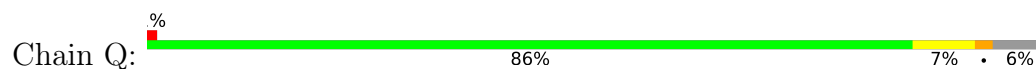


- Molecule 3: Proteasome subunit alpha type-4

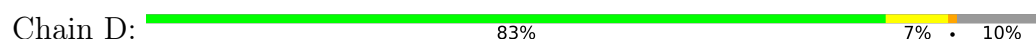
Chain C:  85% 7% 6%



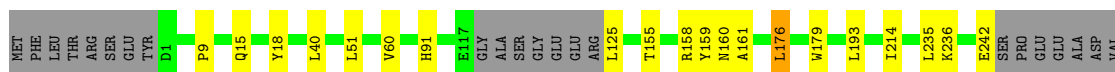
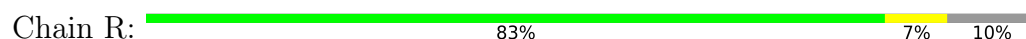
- Molecule 3: Proteasome subunit alpha type-4



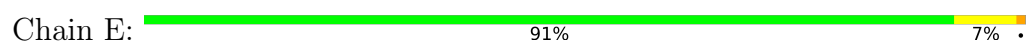
- Molecule 4: Proteasome subunit alpha type-5



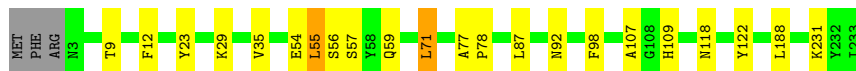
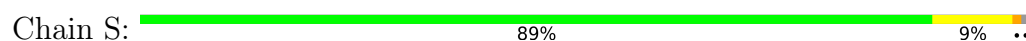
- Molecule 4: Proteasome subunit alpha type-5



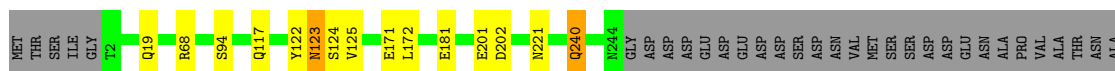
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6




- Molecule 6: Probable proteasome subunit alpha type-7



ASN  
ALA  
THR  
THR  
ASP  
GLN  
GLU  
GLY  
GLY  
HIS  
LEU  
GLU

- Molecule 6: Probable proteasome subunit alpha type-7

Chain T:  79% 5% 16%

MET THR SER ILE ALA THR T2 Q19 R68 L77 R62 S94 Q117 Y122 N123 S124 G155 E171 L172 E181 E201 N221 Q240 Y244 GLY ASP ASP ASP GLU ASP ASP ASP ASP ASP ASP VAL MET SER SER ASP ASP GLU ASN ALA PRO VAL


ALA THR ASN ALA ALA THR THR ASP GLN GLU ASP ILE HIS LEU GLU

- Molecule 7: Proteasome subunit alpha type-1

Chain G:  87% 8% . .

MET SER GLY ALA ALA ALA SER ALA ALA G2 E13 F23 T26 L34 F64 R68 M72 V73 V74 P79 N83 N114 L115 R122 M125 K165 Q166 Q167 T171 L205 E208 R235 L236 Q242 ASP

- Molecule 7: Proteasome subunit alpha type-1

Chain U:  87% 8% . .


MET SER GLY ALA ALA ALA SER ALA ALA G2 P12 E13 F23 T26 L34 T59 R63 I78 P79 N83 N114 L115 R122 M125 A159 K165 Q166 Q167 T171 L205 E208 K223 R235 L236 Q242 ASP

- Molecule 8: Proteasome subunit beta type-2

Chain H:  86% 10% . .

T2 R19 K33 L34 S38 A50 V55 L68 L80 Y97 L98 D104 P105 L110 F111 S112 I113 H114 T119 L125 S126 L127 I163 V164 N165 D166 G170 N194 V195 R196 L213 K214 E215 I223 E226 GLN VAL ASP ILE ALA


- Molecule 8: Proteasome subunit beta type-2

Chain V:  84% 11% . .

T2 R19 K33 L34 S38 A50 V55 L68 L80 L83 Y97 L98 D104 P105 I113 H114 S118 T119 L125 S126 L127 S131 L132 I163 V164 N165 D166 L167 G170 N194 V195 R196 V212 L213 K214 E215 I223 E226 GLN VAL


ASP  
ILE  
THR  
ALA

- Molecule 9: Proteasome subunit beta type-3

Chain I:  86% 12% .

MET S1 N7 G8 G9 I10 V20 G29 G34 N37 K41 A56 T57 D59 N71 E77 P101 P118 F123 I126 G127 C128 A141 E150 L171 R176 W182 G183 R197 K200 M201 R202 Q203 D204

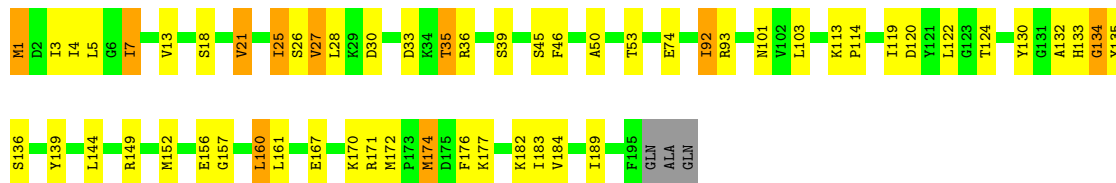
- Molecule 9: Proteasome subunit beta type-3

Chain W:  87% 11% .



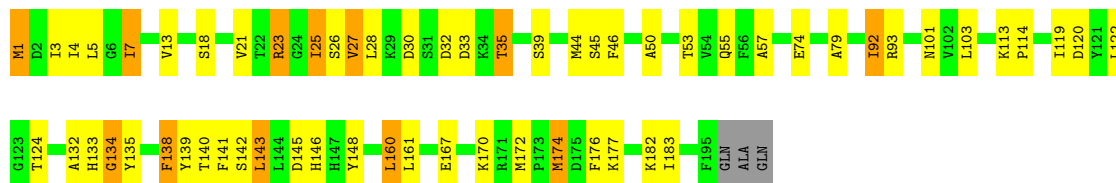
- Molecule 10: Proteasome subunit beta type-4

Chain J:  70% 24% 5% .



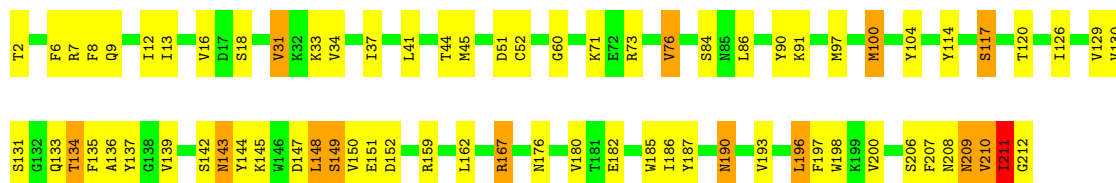
- Molecule 10: Proteasome subunit beta type-4

Chain X:  68% 24% 6% .



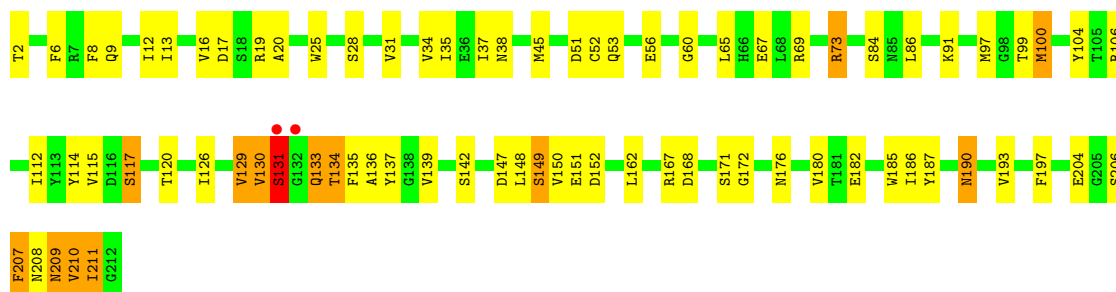
- Molecule 11: Proteasome subunit beta type-5

Chain K:  65% 28% 6% .

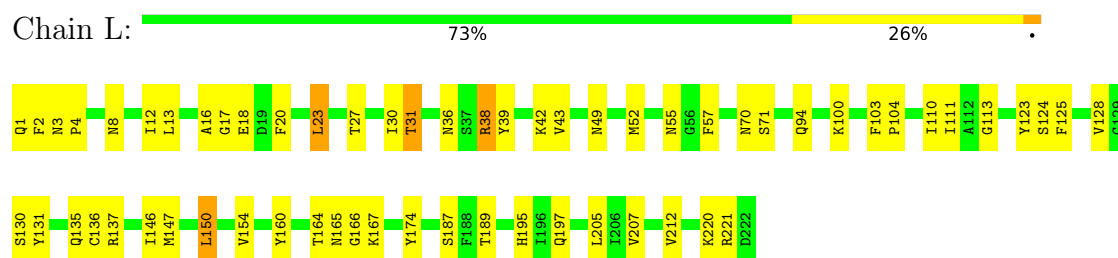


- Molecule 11: Proteasome subunit beta type-5

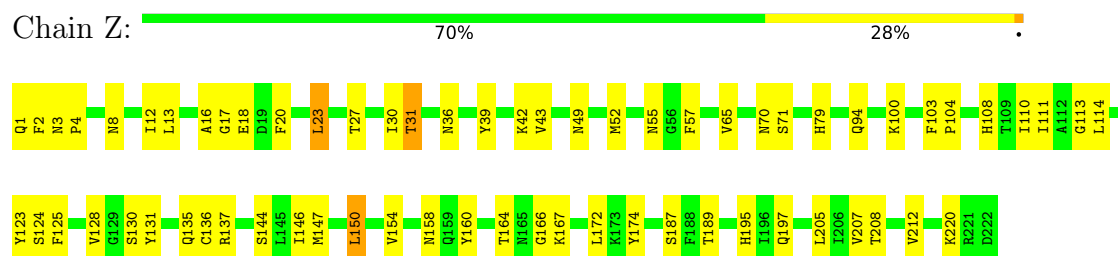
Chain Y:  63% 30% 6% .



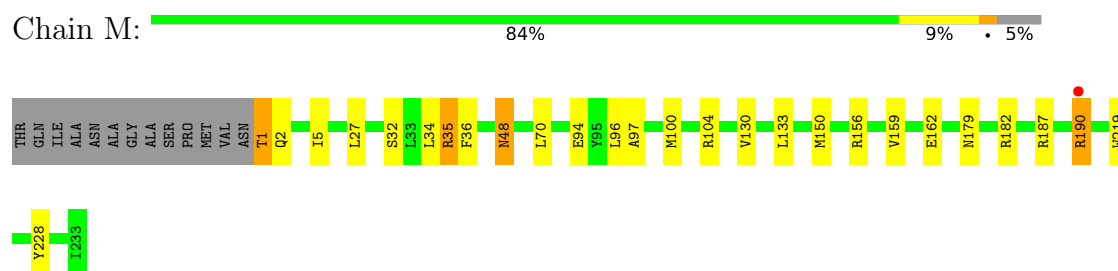
- Molecule 12: Proteasome subunit beta type-6



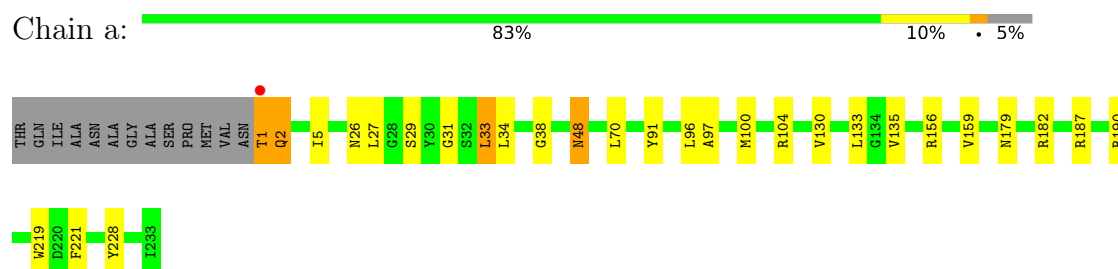
- Molecule 12: Proteasome subunit beta type-6



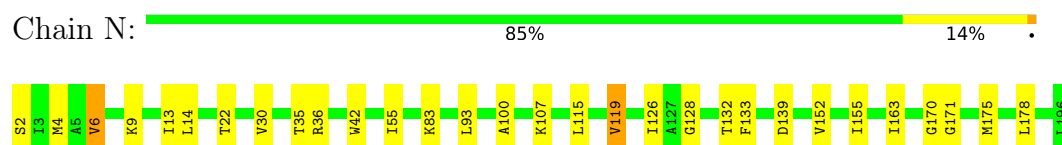
- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7




- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



Chain b:  84% 15%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain f:  25% 25% 50%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain g:  50% 25% 25%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain h:  50% 25% 25%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain i:  25% 25% 50%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain j:  50% 25% 25%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain k:  50% 25% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.19Å 298.96Å 146.78Å 90.00° 112.98° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.80) 97.8 (15.00-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.174 , 0.212 0.170 , 0.218	Depositor DCC
$R_{free}$ test set	13019 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	1.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 72.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	49864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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, A1I48, SO4, MPD, MES, P6S, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.03	0/1952	1.42	0/2642
1	O	1.03	0/1952	1.43	0/2642
2	B	1.04	0/1934	1.44	0/2618
2	P	1.04	0/1934	1.44	0/2618
3	C	1.04	0/1910	1.47	0/2586
3	Q	1.05	0/1910	1.47	0/2586
4	D	1.04	0/1837	1.48	0/2475
4	R	1.04	0/1837	1.48	0/2475
5	E	1.04	0/1800	1.44	2/2433 (0.1%)
5	S	1.04	0/1800	1.45	2/2433 (0.1%)
6	F	1.03	0/1932	1.45	0/2609
6	T	1.04	0/1932	1.46	2/2609 (0.1%)
7	G	1.02	0/1945	1.42	0/2634
7	U	1.03	0/1945	1.42	0/2634
8	H	1.01	0/1743	1.40	0/2363
8	V	1.02	0/1743	1.40	0/2363
9	I	1.03	0/1611	1.41	2/2174 (0.1%)
9	W	1.04	0/1611	1.42	2/2174 (0.1%)
10	J	0.96	0/1589	1.36	2/2142 (0.1%)
10	X	0.94	0/1589	1.33	2/2142 (0.1%)
11	K	0.96	0/1677	1.37	0/2269
11	Y	0.95	0/1677	1.39	0/2269
12	L	0.95	0/1795	1.35	0/2420
12	Z	0.95	0/1795	1.35	0/2420
13	M	1.05	0/1866	1.42	2/2528 (0.1%)
13	a	1.03	0/1855	1.40	0/2514
14	N	1.01	0/1534	1.40	1/2077 (0.0%)
14	b	1.01	0/1534	1.40	1/2077 (0.0%)
15	f	0.74	0/15	0.82	0/19
15	g	1.79	0/15	1.34	0/19
15	h	0.79	0/15	0.86	0/19
15	i	0.75	0/15	0.70	0/19

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	j	0.85	0/15	0.81	0/19
15	k	0.86	0/15	0.96	0/19
All	All	1.02	0/50329	1.42	18/68040 (0.0%)

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
15	f	0	1
15	g	0	1
15	h	0	1
15	i	0	1
15	j	0	1
15	k	0	1
All	All	0	6

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	190[A]	ARG	CA-C-O	8.32	130.02	119.95
13	M	190[B]	ARG	CA-C-O	8.32	130.02	119.95
9	I	183	GLY	CA-C-O	-5.76	118.47	122.22
9	W	183	GLY	CA-C-O	-5.70	118.34	122.45
10	X	134	GLY	CA-C-N	5.35	127.45	120.28
10	X	134	GLY	C-N-CA	5.35	127.45	120.28
9	I	9	GLY	CA-C-O	-5.35	118.00	122.33
14	N	128	GLY	CA-C-O	-5.34	118.31	122.52
10	J	134	GLY	CA-C-N	5.30	127.39	120.28
10	J	134	GLY	C-N-CA	5.30	127.39	120.28
5	S	35	VAL	CA-C-N	5.27	125.23	121.65
5	S	35	VAL	C-N-CA	5.27	125.23	121.65
5	E	35	VAL	CA-C-N	5.26	125.23	121.65
5	E	35	VAL	C-N-CA	5.26	125.23	121.65
9	W	9	GLY	CA-C-O	-5.12	118.18	122.33
14	b	128	GLY	CA-C-O	-5.04	118.54	122.52
6	T	77	LEU	CA-C-N	5.00	124.33	120.33
6	T	77	LEU	C-N-CA	5.00	124.33	120.33

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	f	3	LEU	Peptide
15	g	3	LEU	Peptide
15	h	3	LEU	Peptide
15	i	3	LEU	Peptide
15	j	3	LEU	Peptide
15	k	3	LEU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	7	0
1	O	1915	0	1929	15	0
2	B	1904	0	1904	26	0
2	P	1904	0	1904	20	0
3	C	1881	0	1895	15	0
3	Q	1881	0	1895	15	0
4	D	1813	0	1797	11	0
4	R	1813	0	1797	12	0
5	E	1773	0	1775	20	0
5	S	1773	0	1775	20	0
6	F	1892	0	1883	13	0
6	T	1892	0	1883	6	0
7	G	1907	0	1901	13	0
7	U	1907	0	1901	14	0
8	H	1712	0	1709	26	0
8	V	1712	0	1709	27	0
9	I	1581	0	1574	27	0
9	W	1581	0	1574	24	0
10	J	1561	0	1569	61	0
10	X	1561	0	1569	67	0
11	K	1640	0	1591	69	0
11	Y	1640	0	1591	70	0
12	L	1757	0	1711	45	0
12	Z	1757	0	1711	47	0
13	M	1832	0	1845	21	0
13	a	1824	0	1832	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1505	0	1471	19	0
14	b	1505	0	1471	18	0
15	f	41	0	21	1	0
15	g	41	0	21	1	0
15	h	41	0	21	0	0
15	i	41	0	21	1	0
15	j	41	0	21	0	0
15	k	41	0	21	0	0
16	B	5	0	0	0	0
16	G	5	0	0	1	0
16	P	5	0	0	0	0
16	U	5	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
18	G	1	0	0	0	0
18	N	1	0	0	0	0
18	U	1	0	0	0	0
18	b	1	0	0	0	0
19	K	8	0	14	3	0
19	a	8	0	14	0	0
20	M	12	0	13	1	0
20	a	12	0	13	0	0
21	A	8	0	0	0	0
21	B	10	0	0	0	0
21	C	6	0	0	0	0
21	D	4	0	0	0	0
21	E	5	0	0	0	0
21	F	10	0	0	0	0
21	G	8	0	0	0	0
21	H	8	0	0	0	0
21	I	8	0	0	0	0
21	J	6	0	0	0	0
21	K	3	0	0	0	0
21	L	11	0	0	0	0
21	M	15	0	0	0	0
21	N	9	0	0	0	0
21	O	2	0	0	0	0
21	P	6	0	0	0	0
21	Q	4	0	0	0	0
21	R	9	0	0	0	0
21	S	1	0	0	0	0
21	T	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	10	0	0	0	0
21	V	5	0	0	0	0
21	W	4	0	0	0	0
21	X	10	0	0	1	0
21	Y	7	0	0	0	0
21	Z	5	0	0	0	0
21	a	18	0	0	1	0
21	b	10	0	0	0	0
21	f	1	0	0	0	0
21	h	1	0	0	0	0
21	k	2	0	0	0	0
All	All	49864	0	49275	584	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 6.

All (584) 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)
12:L:31:THR:HG22	12:L:36:ASN:HD21	1.11	1.13
12:Z:31:THR:HG22	12:Z:36:ASN:HD21	0.93	1.05
11:Y:129:VAL:HG22	11:Y:134:THR:HG23	1.39	1.02
11:K:167:ARG:NH2	9:W:182:TRP:HH2	1.57	1.01
12:Z:31:THR:HG22	12:Z:36:ASN:ND2	1.75	1.01
2:B:1:GLY:HA2	6:F:123:ASN:HD22	1.26	0.97
10:X:28:LEU:O	11:Y:136:ALA:HB2	1.65	0.97
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.44	0.96
11:K:129:VAL:HG22	11:K:134:THR:HG23	1.44	0.96
11:K:167:ARG:NH2	9:W:182:TRP:CH2	2.33	0.96
8:H:97:TYR:CE2	8:H:114:HIS:CD2	2.58	0.91
8:H:97:TYR:HE2	8:H:114:HIS:CD2	1.87	0.91
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.38	0.88
12:L:31:THR:HG22	12:L:36:ASN:ND2	1.86	0.88
1:O:12:PHE:H	2:P:20:GLN:HE22	1.18	0.88
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.39	0.87
10:X:28:LEU:HD21	11:Y:134:THR:HB	1.57	0.87
11:K:167:ARG:HH21	9:W:182:TRP:HH2	1.19	0.85
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	1.84	0.85
2:B:1:GLY:C	6:F:123:ASN:ND2	2.34	0.85
2:B:12:PHE:H	3:C:17:GLN:HE22	1.25	0.84
2:B:1:GLY:HA2	6:F:123:ASN:ND2	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLY:C	6:F:123:ASN:HD21	1.84	0.84
11:Y:210:VAL:HG12	11:Y:211:ILE:H	1.46	0.81
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.45	0.81
10:X:28:LEU:CD2	11:Y:134:THR:HB	2.11	0.80
3:C:9:PHE:H	4:D:15:GLN:HE22	1.31	0.79
11:K:167:ARG:HD2	10:X:145:ASP:OD2	1.83	0.78
1:A:12:PHE:H	2:B:20:GLN:HE22	1.30	0.77
2:B:1:GLY:CA	6:F:123:ASN:ND2	2.48	0.77
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.33	0.77
11:K:18:SER:O	11:K:31:VAL:HG23	1.85	0.76
5:S:12:PHE:H	6:T:19:GLN:HE22	1.31	0.76
11:Y:129:VAL:CG2	11:Y:134:THR:HG23	2.14	0.76
11:K:210:VAL:O	11:K:211:ILE:HB	1.85	0.76
11:Y:129:VAL:HG22	11:Y:134:THR:CG2	2.16	0.73
9:I:37:ASN:OD1	11:Y:209:ASN:ND2	2.23	0.71
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.37	0.71
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.24	0.70
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.56	0.70
8:V:98:LEU:HB2	8:V:113:ILE:HG23	1.74	0.70
13:a:31:GLY:C	13:a:190:ARG:HH21	1.99	0.70
2:B:3:ARG:CB	5:E:122:TYR:OH	2.39	0.70
10:J:152:MET:HE1	10:J:157:GLY:HA2	1.72	0.70
8:V:97:TYR:HE2	8:V:114:HIS:CE1	2.10	0.70
8:V:132:LEU:HD12	8:V:132:LEU:N	2.08	0.69
2:B:3:ARG:HB2	5:E:122:TYR:OH	1.93	0.69
5:E:12:PHE:H	6:F:19:GLN:HE22	1.39	0.69
12:L:2:PHE:HB3	13:M:1:THR:OG1	1.93	0.69
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.22	0.69
10:X:138:PHE:H	10:X:138:PHE:HD2	1.40	0.68
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.92	0.67
11:Y:73:ARG:HH22	11:Y:106:ARG:HG2	1.60	0.67
11:Y:19:ARG:NH1	11:Y:171:SER:O	2.28	0.67
8:H:97:TYR:HE2	8:H:114:HIS:NE2	1.93	0.67
10:J:139:TYR:CE2	10:J:167:GLU:HB3	2.30	0.67
11:K:129:VAL:HG22	11:K:134:THR:CG2	2.22	0.66
11:Y:97:MET:N	11:Y:117:SER:OG	2.28	0.66
11:K:176:ASN:ND2	11:K:190:ASN:HB2	2.10	0.66
8:V:132:LEU:HD12	8:V:132:LEU:H	1.61	0.66
11:Y:129:VAL:CG2	11:Y:134:THR:CG2	2.73	0.66
8:H:213:LEU:CD1	9:I:200:LYS:HB2	2.26	0.65
10:X:30:ASP:N	10:X:30:ASP:OD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.44	0.65
11:Y:176:ASN:ND2	11:Y:190:ASN:HB2	2.12	0.65
10:J:177:LYS:NZ	10:X:170:LYS:O	2.22	0.65
11:Y:99:THR:HG22	11:Y:115:VAL:O	1.97	0.65
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.79	0.65
11:K:209:ASN:C	11:K:209:ASN:ND2	2.55	0.64
8:H:98:LEU:HB2	8:H:113:ILE:HG23	1.79	0.64
11:K:176:ASN:HD21	11:K:190:ASN:HB2	1.63	0.64
11:Y:133:GLN:HB3	11:Y:135:PHE:CE1	2.32	0.64
11:Y:209:ASN:ND2	11:Y:209:ASN:C	2.55	0.64
10:J:50:ALA:O	11:K:91:LYS:NZ	2.30	0.64
6:T:123:ASN:HD22	6:T:124:SER:N	1.95	0.64
13:M:32:SER:HA	13:M:190[B]:ARG:NH2	2.12	0.64
10:X:28:LEU:HD21	11:Y:134:THR:CB	2.28	0.64
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.45	0.63
10:J:139:TYR:CD1	10:J:139:TYR:C	2.72	0.63
11:K:167:ARG:HD3	10:X:141:PHE:HB3	1.80	0.63
10:X:26:SER:HB3	11:Y:133:GLN:HG3	1.80	0.62
11:Y:197:PHE:HZ	11:Y:210:VAL:HG21	1.64	0.62
11:K:197:PHE:HZ	11:K:210:VAL:HG21	1.65	0.62
11:K:114:TYR:CE1	11:K:134:THR:HG21	2.34	0.62
11:K:159:ARG:NH2	10:X:146:HIS:HD2	1.97	0.62
11:K:209:ASN:C	11:K:209:ASN:HD22	2.08	0.62
11:Y:209:ASN:C	11:Y:209:ASN:HD22	2.08	0.62
13:a:2:GLN:NE2	21:a:401:HOH:O	2.32	0.62
11:K:209:ASN:ND2	9:W:37:ASN:OD1	2.30	0.62
4:D:88:ALA:HA	4:D:99:ILE:HD12	1.82	0.62
11:K:97:MET:N	11:K:117:SER:OG	2.31	0.62
7:U:23:PHE:O	7:U:26:THR:HB	1.99	0.61
11:Y:104:TYR:CD1	11:Y:182:GLU:HA	2.35	0.61
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.97	0.61
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.82	0.61
11:K:114:TYR:CZ	11:K:134:THR:HG21	2.36	0.61
6:T:123:ASN:HD22	6:T:123:ASN:C	2.08	0.61
11:K:159:ARG:HH21	10:X:146:HIS:HD2	1.47	0.61
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.47	0.61
6:F:122:TYR:CE1	7:G:125:MET:HE3	2.36	0.61
10:J:25:ILE:HD12	10:J:25:ILE:O	2.00	0.61
9:I:56:ALA:HB3	10:J:124:THR:HG23	1.83	0.60
10:X:138:PHE:HB3	21:X:209:HOH:O	2.00	0.60
8:H:97:TYR:CE2	8:H:114:HIS:HD2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.32	0.60
11:K:33:LYS:NZ	15:g:4:A1I48:OG1	2.34	0.60
7:G:23:PHE:O	7:G:26:THR:HB	2.02	0.60
11:Y:114:TYR:CZ	11:Y:134:THR:HG21	2.37	0.60
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.32	0.60
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.84	0.60
10:J:139:TYR:HE2	10:J:167:GLU:HB3	1.66	0.60
11:K:159:ARG:NH2	10:X:146:HIS:CD2	2.70	0.60
14:b:152:VAL:HA	14:b:175:MET:HE1	1.83	0.60
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.83	0.59
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.84	0.59
10:J:152:MET:CE	10:J:157:GLY:HA2	2.31	0.59
11:Y:2:THR:N	11:Y:17:ASP:OD1	2.35	0.59
9:I:58:ASP:OD2	10:J:93:ARG:NH2	2.35	0.59
9:W:58:ASP:OD2	10:X:93:ARG:NH2	2.36	0.59
11:K:104:TYR:CD1	11:K:182:GLU:HA	2.37	0.59
11:K:210:VAL:HG12	11:K:211:ILE:H	1.67	0.59
11:Y:176:ASN:HD21	11:Y:190:ASN:HB2	1.66	0.59
14:N:152:VAL:HA	14:N:175:MET:HE1	1.84	0.59
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.83	0.59
12:L:164:THR:O	12:L:167:LYS:HG2	2.02	0.59
8:H:97:TYR:CD2	8:H:114:HIS:HD2	2.21	0.58
12:L:12:ILE:HD13	12:L:55:ASN:HB2	1.85	0.58
2:P:93:HIS:ND1	2:P:113:ARG:HG2	2.18	0.58
10:J:170:LYS:O	10:X:177:LYS:NZ	2.27	0.58
11:K:9:GLN:HG2	11:K:147:ASP:HA	1.86	0.58
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.39	0.58
2:B:2:SER:N	6:F:123:ASN:HD21	2.01	0.58
11:Y:114:TYR:CE1	11:Y:134:THR:HG21	2.38	0.58
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.29	0.58
12:L:16:ALA:O	12:L:135:GLN:NE2	2.35	0.57
12:Z:2:PHE:HB3	13:a:1:THR:OG1	2.04	0.57
12:Z:124:SER:HB2	12:Z:137:ARG:HG2	1.86	0.57
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.38	0.57
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.86	0.57
10:J:27:VAL:HG12	10:J:27:VAL:O	2.04	0.57
12:Z:12:ILE:HD13	12:Z:55:ASN:HB2	1.86	0.57
12:Z:136:CYS:SG	12:Z:154:VAL:HG11	2.44	0.57
11:Y:9:GLN:HG2	11:Y:147:ASP:HA	1.87	0.57
12:Z:52:MET:HG3	12:Z:111:ILE:HG22	1.86	0.57
11:K:206:SER:O	11:K:208:ASN:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:97:TYR:CD2	8:H:114:HIS:CD2	2.93	0.57
11:K:86:LEU:C	11:K:86:LEU:HD13	2.29	0.57
12:L:52:MET:HG3	12:L:111:ILE:HG22	1.86	0.57
11:Y:28:SER:HB3	11:Y:31:VAL:HG23	1.87	0.57
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.85	0.57
10:X:138:PHE:CD2	10:X:138:PHE:N	2.73	0.56
11:Y:209:ASN:C	11:Y:210:VAL:O	2.47	0.56
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.86	0.56
12:Z:207:VAL:HG22	12:Z:212:VAL:HG22	1.87	0.56
12:L:207:VAL:HG22	12:L:212:VAL:HG22	1.88	0.56
8:V:196:ARG:HH21	9:W:150:GLU:HG3	1.70	0.56
11:Y:210:VAL:HG12	11:Y:211:ILE:N	2.20	0.56
8:H:196:ARG:HH21	9:I:150:GLU:HG3	1.70	0.56
13:a:5:ILE:HG21	14:b:115:LEU:HB2	1.87	0.56
11:K:129:VAL:CG2	11:K:134:THR:HG23	2.29	0.56
10:J:28:LEU:HD21	11:K:134:THR:HB	1.87	0.56
12:L:124:SER:HB2	12:L:137:ARG:HG2	1.88	0.56
12:L:160:TYR:CG	12:L:166:GLY:HA2	2.41	0.56
9:W:56:ALA:HB3	10:X:124:THR:HG23	1.88	0.56
12:Z:146:ILE:HG23	12:Z:187:SER:HB3	1.88	0.56
2:B:93:HIS:ND1	2:B:113:ARG:HG2	2.20	0.56
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.04	0.56
11:Y:197:PHE:CZ	11:Y:210:VAL:HG21	2.41	0.56
11:K:197:PHE:CZ	11:K:210:VAL:HG21	2.41	0.55
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.06	0.55
12:L:146:ILE:HG23	12:L:187:SER:HB3	1.88	0.55
12:L:165:ASN:C	12:L:165:ASN:HD22	2.14	0.55
13:M:150:MET:HG2	8:V:132:LEU:HB3	1.88	0.55
8:V:215:GLU:OE2	9:W:197:ARG:NE	2.31	0.55
11:Y:130:VAL:O	11:Y:131:SER:C	2.50	0.55
10:X:27:VAL:HG12	10:X:27:VAL:O	2.06	0.55
11:K:41:LEU:HD21	11:K:76:VAL:HG13	1.88	0.55
1:A:97:TYR:OH	9:I:77:GLU:OE2	2.25	0.54
11:K:196:LEU:HD22	11:K:200:VAL:HG23	1.88	0.54
11:Y:104:TYR:CE1	11:Y:182:GLU:HA	2.42	0.54
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.71	0.54
11:Y:131:SER:HB2	11:Y:168:ASP:OD2	2.08	0.54
12:Z:164:THR:O	12:Z:167:LYS:HG2	2.07	0.54
10:J:139:TYR:HD1	10:J:139:TYR:O	1.90	0.54
11:K:212:GLY:HA2	8:V:213:LEU:HD13	1.89	0.54
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:5:ILE:HG21	14:N:115:LEU:HB2	1.88	0.54
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.90	0.54
2:P:217:LYS:C	2:P:219:ALA:H	2.16	0.53
10:X:26:SER:HB2	11:Y:134:THR:O	2.08	0.53
12:L:136:CYS:SG	12:L:154:VAL:HG11	2.48	0.53
7:G:64:PHE:HA	16:G:303:SO4:O3	2.07	0.53
11:K:209:ASN:O	11:K:210:VAL:O	2.25	0.53
12:Z:160:TYR:CG	12:Z:166:GLY:HA2	2.43	0.53
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.08	0.53
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.43	0.53
8:H:213:LEU:HD13	9:I:200:LYS:CA	2.39	0.53
10:X:1:MET:N	10:X:174:MET:HG3	2.24	0.53
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.89	0.53
10:J:21:VAL:HG12	10:J:28:LEU:HB2	1.90	0.53
9:I:182:TRP:HH2	11:Y:167:ARG:HH11	1.56	0.53
10:J:136:SER:HA	10:J:172:MET:HE3	1.90	0.53
5:E:92:ASN:CG	12:L:70:ASN:HD21	2.16	0.53
8:H:194:ASN:HB3	12:Z:220:LYS:HE3	1.90	0.53
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.90	0.53
12:Z:57:PHE:HZ	13:a:133:LEU:HB3	1.73	0.53
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.06	0.53
11:K:180:VAL:HG22	11:K:185:TRP:HB3	1.91	0.53
13:M:32:SER:HA	13:M:190[B]:ARG:HH21	1.74	0.53
11:Y:180:VAL:HG22	11:Y:185:TRP:HB3	1.90	0.53
11:Y:206:SER:O	11:Y:208:ASN:N	2.42	0.53
2:B:217:LYS:C	2:B:219:ALA:H	2.16	0.53
12:Z:16:ALA:O	12:Z:135:GLN:NE2	2.38	0.53
12:L:8:ASN:HA	12:L:30:ILE:O	2.08	0.52
11:K:104:TYR:CE1	11:K:182:GLU:HA	2.43	0.52
8:V:97:TYR:CE2	8:V:114:HIS:ND1	2.77	0.52
3:C:35:LYS:HG2	3:C:158:SER:O	2.09	0.52
10:X:45:SER:OG	10:X:103:LEU:HB2	2.10	0.52
12:Z:43:VAL:HG12	12:Z:205:LEU:HD22	1.91	0.52
10:J:1:MET:N	10:J:174:MET:HG3	2.23	0.52
10:J:13:VAL:HG23	10:J:114:PRO:HB2	1.90	0.52
10:X:13:VAL:HG23	10:X:114:PRO:HB2	1.90	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.52
7:U:83:ASN:C	7:U:83:ASN:HD22	2.18	0.52
11:Y:129:VAL:HG12	11:Y:129:VAL:O	2.08	0.52
7:G:83:ASN:C	7:G:83:ASN:HD22	2.18	0.52
10:J:18:SER:HB2	10:J:176:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.18	0.52
5:S:98:PHE:O	13:a:91:TYR:HA	2.10	0.52
11:Y:65:LEU:O	11:Y:69:ARG:HG3	2.09	0.52
12:L:220:LYS:HE3	8:V:194:ASN:HB3	1.90	0.52
1:O:12:PHE:N	2:P:20:GLN:HE22	1.98	0.52
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.44	0.51
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.75	0.51
12:Z:30:ILE:HD12	12:Z:30:ILE:C	2.35	0.51
8:V:132:LEU:H	8:V:132:LEU:CD1	2.22	0.51
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.51
10:X:143:LEU:HD12	10:X:143:LEU:C	2.36	0.51
8:V:97:TYR:HE2	8:V:114:HIS:ND1	2.07	0.51
8:V:213:LEU:HD23	9:W:200:LYS:HB2	1.92	0.51
10:X:119:ILE:HA	10:X:124:THR:O	2.11	0.51
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.45	0.51
12:L:57:PHE:HZ	13:M:133:LEU:HB3	1.74	0.51
10:X:5:LEU:HD21	10:X:140:THR:HG21	1.92	0.51
10:J:26:SER:HB2	11:K:134:THR:O	2.10	0.51
8:H:213:LEU:HD13	9:I:200:LYS:HB2	1.92	0.51
1:O:7:PHE:HB3	3:Q:2:TYR:CE1	2.46	0.51
10:J:39:SER:OG	10:J:74:GLU:OE1	2.24	0.50
10:X:33:ASP:OD2	10:X:182:LYS:NZ	2.44	0.50
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.11	0.50
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.76	0.50
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.91	0.50
10:J:45:SER:OG	10:J:103:LEU:HB2	2.11	0.50
10:J:139:TYR:C	10:J:139:TYR:HD1	2.19	0.50
11:K:143:ASN:OD1	11:K:143:ASN:N	2.44	0.50
12:L:164:THR:HB	12:L:167:LYS:HB2	1.94	0.50
10:X:35:THR:HG21	10:X:182:LYS:NZ	2.27	0.50
3:C:38:ASN:C	3:C:38:ASN:HD22	2.19	0.50
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.59	0.50
12:L:12:ILE:HG13	12:L:110:ILE:HD12	1.94	0.50
12:L:18:GLU:HG3	12:L:174:TYR:CE2	2.47	0.50
12:L:30:ILE:HD12	12:L:30:ILE:C	2.36	0.50
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.09	0.50
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.47	0.50
10:X:28:LEU:HD23	11:Y:134:THR:HB	1.92	0.50
8:H:213:LEU:CD1	9:I:200:LYS:CB	2.90	0.49
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.94	0.49
8:H:19:ARG:NH1	8:H:167:LEU:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:27:VAL:CG1	11:K:137:TYR:HE1	2.25	0.49
4:R:158:ARG:HB3	5:S:57:SER:HB3	1.94	0.49
12:Z:100:LYS:O	12:Z:104:PRO:HA	2.12	0.49
10:X:5:LEU:HD23	10:X:132:ALA:HB2	1.94	0.49
12:Z:12:ILE:HG13	12:Z:110:ILE:HD12	1.93	0.49
10:J:33:ASP:OD2	10:J:182:LYS:NZ	2.46	0.49
10:J:139:TYR:CD1	10:J:139:TYR:O	2.66	0.49
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.48	0.49
12:L:94:GLN:NE2	12:L:131:TYR:HD1	2.10	0.49
4:R:155:THR:HG23	5:S:59:GLN:HE22	1.77	0.49
11:K:210:VAL:HG12	11:K:211:ILE:N	2.27	0.49
12:L:100:LYS:O	12:L:104:PRO:HA	2.13	0.49
4:R:159:TYR:HA	5:S:56:SER:HA	1.95	0.49
12:Z:94:GLN:NE2	12:Z:131:TYR:HD1	2.10	0.49
10:J:5:LEU:HD23	10:J:132:ALA:HB2	1.95	0.49
8:V:132:LEU:N	8:V:132:LEU:CD1	2.76	0.48
13:M:162:GLU:HB2	20:M:301:MES:O2S	2.13	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.95	0.48
10:J:119:ILE:HA	10:J:124:THR:O	2.14	0.48
9:I:203:GLN:HG3	11:Y:197:PHE:CE2	2.49	0.48
10:J:1:MET:HE1	10:J:135:TYR:H	1.79	0.48
10:J:35:THR:HG21	10:J:182:LYS:NZ	2.29	0.48
10:X:143:LEU:HD12	10:X:143:LEU:O	2.14	0.48
11:Y:100:MET:HB2	11:Y:100:MET:HE2	1.70	0.48
11:Y:210:VAL:CG1	11:Y:211:ILE:H	2.22	0.48
5:S:71:LEU:HD22	5:S:71:LEU:C	2.38	0.48
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.12	0.48
8:V:97:TYR:HB3	8:V:127:LEU:HD23	1.95	0.48
11:K:97:MET:H	11:K:117:SER:HG	1.61	0.48
12:L:38:ARG:NH1	12:L:221:ARG:O	2.46	0.48
2:P:3:ARG:HB2	5:S:122:TYR:OH	2.14	0.48
7:U:78:ILE:N	7:U:79:PRO:CD	2.77	0.48
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.96	0.47
9:I:7:ASN:HA	9:I:29:GLY:O	2.13	0.47
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.96	0.47
8:V:97:TYR:CE2	8:V:114:HIS:CE1	2.96	0.47
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.62	0.47
5:E:71:LEU:C	5:E:71:LEU:HD22	2.39	0.47
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.78	0.47
7:G:78:ILE:N	7:G:79:PRO:CD	2.77	0.47
10:J:28:LEU:CD2	11:K:134:THR:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:28:LEU:O	11:K:136:ALA:HB2	2.15	0.47
10:J:35:THR:HG21	10:J:182:LYS:HZ2	1.79	0.47
11:K:90:TYR:HH	19:K:301:MPD:HO2	1.60	0.47
2:P:3:ARG:CB	5:S:122:TYR:OH	2.62	0.47
10:J:172:MET:HB3	10:J:174:MET:SD	2.55	0.47
13:M:159:VAL:HG23	13:M:159:VAL:O	2.15	0.47
11:Y:19:ARG:NH1	11:Y:172:GLY:HA3	2.30	0.47
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.96	0.47
12:Z:164:THR:HB	12:Z:167:LYS:HB2	1.96	0.47
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.96	0.47
6:F:123:ASN:ND2	6:F:123:ASN:C	2.72	0.47
10:J:35:THR:HG21	10:J:182:LYS:HD2	1.96	0.47
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.97	0.47
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.97	0.47
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.63	0.47
12:Z:18:GLU:HG3	12:Z:174:TYR:CE2	2.49	0.47
10:J:1:MET:HE2	10:J:1:MET:HB3	1.62	0.47
7:U:78:ILE:HG22	7:U:79:PRO:HD3	1.97	0.47
4:D:155:THR:HG23	5:E:59:GLN:HE22	1.79	0.47
10:X:35:THR:HG21	10:X:182:LYS:HD2	1.95	0.47
11:K:162:LEU:CD1	11:K:193:VAL:HG13	2.45	0.47
11:Y:130:VAL:O	11:Y:131:SER:O	2.33	0.47
14:b:55:ILE:HD11	14:b:93:LEU:HD13	1.97	0.47
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.50	0.46
1:O:6:SER:OG	3:Q:2:TYR:HA	2.16	0.46
10:X:172:MET:HB3	10:X:174:MET:SD	2.54	0.46
4:R:91:HIS:CE1	12:Z:79:HIS:NE2	2.83	0.46
9:W:7:ASN:HA	9:W:29:GLY:O	2.15	0.46
10:X:7:ILE:CG2	10:X:161:LEU:HD13	2.45	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.46
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.15	0.46
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.50	0.46
11:Y:162:LEU:CD1	11:Y:193:VAL:HG13	2.44	0.46
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.15	0.46
11:K:6:PHE:HB3	11:K:126:ILE:HD12	1.96	0.46
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.98	0.46
10:J:46:PHE:HD1	10:J:53:THR:HB	1.80	0.46
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.98	0.46
5:E:71:LEU:C	5:E:71:LEU:CD2	2.89	0.46
10:J:101:ASN:OD1	10:J:120:ASP:HA	2.16	0.46
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:160:LYS:N	2:P:55:LEU:O	2.41	0.46
8:H:215:GLU:OE2	9:I:197:ARG:NE	2.35	0.46
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.98	0.46
1:O:55:LEU:HB3	7:U:159:ALA:O	2.16	0.46
9:W:101:PRO:O	10:X:93:ARG:NH1	2.49	0.46
11:Y:51:ASP:HB3	11:Y:97:MET:HE2	1.98	0.46
5:S:71:LEU:C	5:S:71:LEU:CD2	2.88	0.46
14:b:4:MET:HB3	14:b:126:ILE:HG22	1.98	0.46
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.51	0.46
1:O:14:PRO:HA	2:P:23:TYR:CE1	2.51	0.46
10:X:139:TYR:CE2	10:X:167:GLU:HB3	2.51	0.46
14:N:35:THR:HG21	13:a:228:TYR:CE2	2.36	0.45
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.98	0.45
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.28	0.45
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.51	0.45
14:b:163:ILE:HG23	14:b:170:GLY:HA2	1.98	0.45
11:K:8:PHE:CE1	11:K:13:ILE:HG12	2.51	0.45
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.46	0.45
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.65	0.45
11:K:97:MET:HE3	11:K:97:MET:HB2	1.72	0.45
13:M:96:LEU:O	13:M:100:MET:HG2	2.17	0.45
4:R:161:ALA:HB3	5:S:55:LEU:HG	1.97	0.45
11:Y:6:PHE:HB3	11:Y:126:ILE:HD12	1.98	0.45
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.46	0.45
9:I:34:GLY:O	11:Y:167:ARG:NH1	2.48	0.45
9:I:182:TRP:HH2	11:Y:167:ARG:NH1	2.13	0.45
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.98	0.45
13:a:96:LEU:O	13:a:100:MET:HG2	2.16	0.45
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.98	0.45
11:K:197:PHE:CE2	9:W:203:GLN:HG3	2.51	0.45
10:X:1:MET:H2	10:X:174:MET:HG3	1.81	0.45
14:b:6:VAL:HG23	14:b:155:ILE:HD11	1.99	0.45
10:J:152:MET:CE	10:J:157:GLY:CA	2.94	0.45
10:X:5:LEU:CD2	10:X:140:THR:HG21	2.47	0.45
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.99	0.45
11:K:145:LYS:O	11:K:148:LEU:HD13	2.16	0.45
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.99	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.99	0.45
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.16	0.45
4:D:88:ALA:HA	4:D:99:ILE:CD1	2.45	0.45
12:L:43:VAL:HG12	12:L:205:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:147:MET:HE3	9:W:176:ARG:NH2	2.31	0.45
13:M:35:ARG:HD2	13:M:36:PHE:CZ	2.52	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.99	0.45
9:I:171:LEU:HB3	12:Z:158:ASN:ND2	2.31	0.45
10:J:7:ILE:CG2	10:J:161:LEU:HD13	2.47	0.45
11:K:44:THR:HG21	11:K:100:MET:HE2	2.00	0.45
1:O:98:LYS:HE3	1:O:104:TYR:CZ	2.52	0.45
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.17	0.45
5:S:92:ASN:CG	12:Z:70:ASN:HD21	2.25	0.45
10:X:160:LEU:HD12	10:X:160:LEU:O	2.17	0.45
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.99	0.44
9:I:101:PRO:O	10:J:93:ARG:NH1	2.50	0.44
10:J:160:LEU:HD12	10:J:160:LEU:O	2.17	0.44
11:K:167:ARG:CZ	9:W:182:TRP:HH2	2.26	0.44
13:a:159:VAL:HG23	13:a:159:VAL:O	2.16	0.44
3:C:201:VAL:O	3:C:202:GLN:CB	2.65	0.44
7:G:78:ILE:HG22	7:G:79:PRO:HD3	1.98	0.44
12:L:2:PHE:HB3	13:M:1:THR:HG1	1.83	0.44
10:X:1:MET:HE1	10:X:135:TYR:H	1.81	0.44
11:Y:8:PHE:CE1	11:Y:13:ILE:HG12	2.52	0.44
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.53	0.44
9:I:176:ARG:NH2	12:Z:147:MET:HE3	2.33	0.44
11:Y:97:MET:H	11:Y:117:SER:HG	1.61	0.44
11:K:90:TYR:OH	19:K:301:MPD:O2	2.30	0.44
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.65	0.44
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.32	0.44
14:N:13:ILE:HG21	14:N:175:MET:HE2	2.00	0.44
8:H:110:LEU:HG	8:H:125:LEU:HD12	2.00	0.44
14:b:19:ARG:NH1	14:b:167:GLY:O	2.42	0.44
14:N:139:ASP:OD2	14:b:164:LYS:NZ	2.50	0.44
10:J:152:MET:CE	10:J:157:GLY:N	2.81	0.43
12:L:165:ASN:HD21	8:V:212:VAL:H	1.66	0.43
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.00	0.43
8:H:50:ALA:HB3	9:I:126:ILE:HD12	1.99	0.43
11:K:7:ARG:O	11:K:144:TYR:OH	2.24	0.43
11:K:16:VAL:HG21	11:K:34:VAL:HG23	2.00	0.43
10:X:7:ILE:HD11	10:X:148:TYR:HD1	1.83	0.43
10:X:46:PHE:HD1	10:X:53:THR:HB	1.83	0.43
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	2.00	0.43
13:a:33:LEU:HD12	13:a:34:LEU:N	2.33	0.43
12:L:94:GLN:NE2	12:L:131:TYR:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:115:ALA:HB1	1:O:154:GLY:O	2.19	0.43
8:V:50:ALA:HB3	9:W:126:ILE:HD12	1.99	0.43
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.43
11:Y:149:SER:HB2	11:Y:152:ASP:HB2	2.00	0.43
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.51	0.43
14:b:13:ILE:HG21	14:b:175:MET:HE2	2.00	0.43
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.01	0.43
8:H:80:LEU:HD11	8:H:119:THR:CG2	2.48	0.43
10:J:3:ILE:HD11	10:J:174:MET:HE2	2.00	0.43
10:J:35:THR:CG2	10:J:182:LYS:HZ2	2.32	0.43
10:J:184:VAL:HG22	10:J:189:ILE:HG12	2.01	0.43
12:L:111:ILE:HG12	12:L:123:TYR:HB2	2.00	0.43
14:N:6:VAL:HG23	14:N:155:ILE:HD11	2.01	0.43
5:S:77:ALA:N	5:S:78:PRO:CD	2.82	0.43
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.00	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.43
10:X:1:MET:HE1	10:X:134:GLY:HA3	1.99	0.43
7:G:83:ASN:C	7:G:83:ASN:ND2	2.76	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.54	0.43
10:X:92:ILE:HG21	10:X:122:LEU:HA	1.99	0.43
1:A:98:LYS:HE3	1:A:104:TYR:CZ	2.53	0.43
10:J:152:MET:HE3	10:J:156:GLU:C	2.44	0.43
12:Z:100:LYS:HE3	12:Z:103:PHE:O	2.19	0.43
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.54	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43
12:L:113:GLY:HA2	12:L:207:VAL:HG11	2.00	0.43
7:U:83:ASN:C	7:U:83:ASN:ND2	2.75	0.43
14:b:14:LEU:HD11	14:b:100:ALA:HB3	2.00	0.43
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.66	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.43
10:J:30:ASP:OD1	10:J:30:ASP:N	2.51	0.43
11:K:198:TRP:CE2	9:W:200:LYS:HE3	2.54	0.43
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.54	0.43
10:X:3:ILE:HD11	10:X:174:MET:HE2	2.01	0.43
11:Y:35:ILE:HG21	11:Y:56:GLU:HB3	2.00	0.43
11:Y:206:SER:O	11:Y:207:PHE:C	2.62	0.43
2:B:1:GLY:HA2	6:F:123:ASN:O	2.18	0.42
12:L:100:LYS:HE3	12:L:103:PHE:O	2.19	0.42
8:V:33:LYS:NZ	15:i:4:A1I48:OG1	2.50	0.42
8:H:33:LYS:NZ	15:f:4:A1I48:OG1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:123:PHE:HA	9:I:128:CYS:O	2.18	0.42
10:J:36:ARG:HD3	10:J:36:ARG:HA	1.84	0.42
10:J:46:PHE:CD1	10:J:53:THR:HB	2.55	0.42
10:X:101:ASN:OD1	10:X:120:ASP:HA	2.19	0.42
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.85	0.42
9:I:58:ASP:CG	10:J:93:ARG:NH2	2.78	0.42
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.55	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.02	0.42
10:X:50:ALA:HB1	11:Y:120:THR:OG1	2.19	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.18	0.42
10:J:92:ILE:HG21	10:J:122:LEU:HA	2.01	0.42
11:K:149:SER:HB2	11:K:152:ASP:HB2	2.01	0.42
8:V:19:ARG:NH1	8:V:167:LEU:O	2.52	0.42
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.54	0.42
3:C:51:LYS:O	3:C:52:LEU:HB2	2.19	0.42
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.08	0.42
7:U:34:LEU:C	7:U:34:LEU:HD23	2.44	0.42
9:W:123:PHE:HA	9:W:128:CYS:O	2.19	0.42
10:X:39:SER:OG	10:X:74:GLU:OE1	2.22	0.42
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.66	0.42
2:B:10:THR:O	3:C:125:ARG:HB3	2.19	0.42
2:P:101:TYR:O	10:X:79:ALA:HA	2.19	0.42
6:T:122:TYR:CE1	7:U:125:MET:HE3	2.55	0.42
12:L:27:THR:HB	12:L:39:TYR:HA	2.02	0.42
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.78	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.01	0.42
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.02	0.42
7:U:68:ARG:O	7:U:223:LYS:HA	2.19	0.42
9:W:58:ASP:CG	10:X:93:ARG:NH2	2.78	0.42
10:X:4:ILE:HD11	10:X:133:HIS:CD2	2.55	0.42
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	2.02	0.42
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.18	0.42
7:G:34:LEU:C	7:G:34:LEU:HD23	2.45	0.42
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.19	0.42
10:X:55:GLN:HE21	10:X:55:GLN:HB3	1.70	0.42
11:Y:129:VAL:HG23	11:Y:134:THR:HG22	2.01	0.42
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.50	0.41
11:K:129:VAL:CG2	11:K:134:THR:CG2	2.94	0.41
1:O:154:GLY:C	2:P:81:ALA:HB2	2.45	0.41
3:Q:156:SER:O	4:R:51:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:H3	10:J:174:MET:HG3	1.84	0.41
10:X:21:VAL:HG23	10:X:32:ASP:HB2	2.02	0.41
10:X:44:MET:HE1	10:X:57:ALA:HA	2.02	0.41
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.51	0.41
4:D:176:LEU:HD22	5:E:55:LEU:HD22	2.03	0.41
5:E:10:VAL:CG2	6:F:125:VAL:C	2.93	0.41
8:H:213:LEU:HD13	9:I:200:LYS:CB	2.48	0.41
10:J:1:MET:HE1	10:J:134:GLY:HA3	2.02	0.41
10:J:130:TYR:HB2	10:J:144:LEU:HD13	2.01	0.41
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.36	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.41
10:X:4:ILE:HD11	10:X:133:HIS:HD2	1.85	0.41
12:Z:94:GLN:NE2	12:Z:131:TYR:CD1	2.88	0.41
12:Z:111:ILE:HG12	12:Z:123:TYR:HB2	2.03	0.41
13:a:48:ASN:C	13:a:48:ASN:HD22	2.29	0.41
11:K:2:THR:HA	11:K:129:VAL:O	2.20	0.41
13:a:31:GLY:O	13:a:190:ARG:NH2	2.53	0.41
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.69	0.41
13:M:48:ASN:C	13:M:48:ASN:ND2	2.77	0.41
8:V:80:LEU:CD2	8:V:119:THR:HG21	2.50	0.41
11:Y:12:ILE:HD13	11:Y:112:ILE:HG12	2.03	0.41
11:Y:97:MET:N	11:Y:117:SER:HG	2.17	0.41
12:Z:27:THR:HB	12:Z:39:TYR:HA	2.02	0.41
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.34	0.41
12:L:195:HIS:HD2	12:L:197:GLN:H	1.67	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.02	0.41
14:b:36:ARG:HG3	14:b:42:TRP:CZ2	2.56	0.41
3:C:29:THR:OG1	3:C:61:LYS:NZ	2.52	0.41
14:N:30:VAL:HG11	13:a:221:PHE:CE2	2.55	0.41
10:X:4:ILE:O	10:X:4:ILE:HG13	2.21	0.41
10:X:23:ARG:O	10:X:23:ARG:HG3	2.19	0.41
2:B:217:LYS:C	2:B:219:ALA:N	2.79	0.41
10:J:4:ILE:O	10:J:4:ILE:HG13	2.20	0.41
10:J:26:SER:HA	11:K:135:PHE:CE2	2.55	0.41
10:J:174:MET:HA	10:X:174:MET:HA	2.03	0.41
13:M:48:ASN:C	13:M:48:ASN:HD22	2.28	0.41
14:N:132:THR:O	14:b:133:PHE:HA	2.21	0.41
4:R:176:LEU:HD11	5:S:54:GLU:HB2	2.02	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.02	0.41
10:X:3:ILE:N	10:X:3:ILE:HD12	2.36	0.41
10:X:5:LEU:HD23	10:X:132:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:ALA:HB1	11:K:120:THR:OG1	2.21	0.41
12:L:160:TYR:CD2	12:L:166:GLY:HA2	2.56	0.41
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.69	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.41
12:Z:57:PHE:CE1	13:a:135:VAL:CG2	3.04	0.41
19:K:301:MPD:HM1	19:K:301:MPD:H4	1.98	0.40
10:X:27:VAL:CG1	11:Y:137:TYR:HE1	2.34	0.40
12:Z:114:LEU:HD11	12:Z:208:THR:C	2.46	0.40
13:a:48:ASN:C	13:a:48:ASN:ND2	2.78	0.40
5:E:99:ASN:HB2	13:M:94:GLU:HG2	2.03	0.40
10:J:27:VAL:HG11	11:K:137:TYR:HE1	1.86	0.40
11:K:18:SER:C	11:K:31:VAL:HG23	2.44	0.40
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.87	0.40
10:X:27:VAL:HG12	11:Y:137:TYR:HE1	1.86	0.40
10:X:35:THR:HG21	10:X:182:LYS:HZ2	1.84	0.40
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.70	0.40
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.19	0.40
8:V:213:LEU:CD2	9:W:200:LYS:HB2	2.51	0.40
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.02	0.40
6:F:240:GLN:HA	6:F:240:GLN:HE21	1.85	0.40
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.51	0.40
10:J:4:ILE:HD11	10:J:133:HIS:CD2	2.56	0.40
10:X:25:ILE:O	10:X:25:ILE:CG1	2.70	0.40
10:X:46:PHE:CD1	10:X:53:THR:HB	2.57	0.40
13:a:26:ASN:O	13:a:38:GLY:N	2.55	0.40
2:P:50:LYS:O	2:P:51:VAL:C	2.64	0.40
8:V:55:VAL:HG13	8:V:83:LEU:CD2	2.51	0.40
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.52	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	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	60
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	60
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	25
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	25
3	C	238/254 (94%)	232 (98%)	4 (2%)	2 (1%)	16	44
3	Q	238/254 (94%)	232 (98%)	4 (2%)	2 (1%)	16	44
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	223/231 (96%)	218 (98%)	5 (2%)	0	100	100
8	V	223/231 (96%)	218 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	209/211 (99%)	200 (96%)	6 (3%)	3 (1%)	9	30
11	Y	209/211 (99%)	200 (96%)	5 (2%)	4 (2%)	6	22
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
13	a	231/246 (94%)	225 (97%)	6 (3%)	0	100	100
14	N	193/195 (99%)	190 (98%)	3 (2%)	0	100	100
14	b	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100
15	g	1/4 (25%)	1 (100%)	0	0	100	100
15	h	1/4 (25%)	1 (100%)	0	0	100	100
15	i	1/4 (25%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	j	1/4 (25%)	1 (100%)	0	0	100	100
15	k	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6285/6632 (95%)	6127 (98%)	137 (2%)	21 (0%)	36	66

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
11	K	207	PHE
11	K	210	VAL
11	K	211	ILE
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
11	Y	207	PHE
11	Y	210	VAL
1	A	2	THR
2	B	218	GLY
2	B	220	ASN
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
11	Y	131	SER
11	Y	211	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	50	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	72
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	72
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	57
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	57
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	53
4	R	194/215 (90%)	185 (95%)	9 (5%)	24	58
5	E	190/193 (98%)	183 (96%)	7 (4%)	30	65
5	S	190/193 (98%)	183 (96%)	7 (4%)	30	65
6	F	201/239 (84%)	189 (94%)	12 (6%)	17	47
6	T	201/239 (84%)	191 (95%)	10 (5%)	22	54
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	59
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	59
8	H	184/189 (97%)	176 (96%)	8 (4%)	26	60
8	V	184/189 (97%)	173 (94%)	11 (6%)	17	47
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	83
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	83
10	J	173/175 (99%)	160 (92%)	13 (8%)	12	37
10	X	173/175 (99%)	159 (92%)	14 (8%)	11	33
11	K	169/169 (100%)	145 (86%)	24 (14%)	3	12
11	Y	169/169 (100%)	147 (87%)	22 (13%)	4	14
12	L	185/185 (100%)	174 (94%)	11 (6%)	18	48
12	Z	185/185 (100%)	172 (93%)	13 (7%)	14	40
13	M	200/208 (96%)	193 (96%)	7 (4%)	32	67
13	a	199/208 (96%)	191 (96%)	8 (4%)	28	63
14	N	161/161 (100%)	154 (96%)	7 (4%)	26	60
14	b	161/161 (100%)	154 (96%)	7 (4%)	26	60
15	f	2/2 (100%)	0	2 (100%)	0	0
15	g	2/2 (100%)	2 (100%)	0	100	100
15	h	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	i	2/2 (100%)	0	2 (100%)	0	0
15	j	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	k	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	5329/5548 (96%)	5058 (95%)	271 (5%)	21	54

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	52	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	40	LEU
4	D	60	VAL
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	118	ASN
5	E	188	LEU

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Mol	Chain	Res	Type
5	E	231	LYS
6	F	68	ARG
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	124	SER
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	34	LEU
8	H	38	SER
8	H	55	VAL
8	H	68	LEU
8	H	113	ILE
8	H	127	LEU
8	H	196	ARG
8	H	215	GLU
9	I	37	ASN
9	I	171	LEU
9	I	202	ARG
10	J	1	MET
10	J	7	ILE
10	J	21	VAL
10	J	25	ILE
10	J	27	VAL
10	J	35	THR
10	J	92	ILE
10	J	113	LYS
10	J	149	ARG

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Mol	Chain	Res	Type
10	J	160	LEU
10	J	171	ARG
10	J	174	MET
10	J	183	ILE
11	K	31	VAL
11	K	71	LYS
11	K	73	ARG
11	K	76	VAL
11	K	84	SER
11	K	100	MET
11	K	117	SER
11	K	130	VAL
11	K	131	SER
11	K	133	GLN
11	K	134	THR
11	K	139	VAL
11	K	142	SER
11	K	143	ASN
11	K	148	LEU
11	K	149	SER
11	K	150	VAL
11	K	151	GLU
11	K	167	ARG
11	K	186	ILE
11	K	190	ASN
11	K	196	LEU
11	K	209	ASN
11	K	211	ILE
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	38	ARG
12	L	42	LYS
12	L	49	ASN
12	L	71	SER
12	L	128	VAL
12	L	130	SER
12	L	150	LEU
12	L	189	THR
13	M	1	THR
13	M	2	GLN
13	M	35	ARG

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Mol	Chain	Res	Type
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	2	SER
14	N	6	VAL
14	N	9	LYS
14	N	22	THR
14	N	107	LYS
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	40	LEU
4	R	60	VAL
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS

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Mol	Chain	Res	Type
5	S	55	LEU
5	S	71	LEU
5	S	118	ASN
5	S	188	LEU
5	S	231	LYS
6	T	68	ARG
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	34	LEU
8	V	38	SER
8	V	55	VAL
8	V	68	LEU
8	V	80	LEU
8	V	113	ILE
8	V	118	SER
8	V	125	LEU
8	V	127	LEU
8	V	131	SER
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	202	ARG
10	X	1	MET
10	X	7	ILE
10	X	23	ARG
10	X	25	ILE

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Mol	Chain	Res	Type
10	X	27	VAL
10	X	35	THR
10	X	92	ILE
10	X	113	LYS
10	X	138	PHE
10	X	142	SER
10	X	143	LEU
10	X	160	LEU
10	X	174	MET
10	X	183	ILE
11	Y	38	ASN
11	Y	53	GLN
11	Y	67	GLU
11	Y	73	ARG
11	Y	84	SER
11	Y	100	MET
11	Y	117	SER
11	Y	129	VAL
11	Y	130	VAL
11	Y	131	SER
11	Y	133	GLN
11	Y	134	THR
11	Y	139	VAL
11	Y	142	SER
11	Y	148	LEU
11	Y	149	SER
11	Y	150	VAL
11	Y	151	GLU
11	Y	186	ILE
11	Y	190	ASN
11	Y	204	GLU
11	Y	209	ASN
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	42	LYS
12	Z	49	ASN
12	Z	65	VAL
12	Z	71	SER
12	Z	108	HIS
12	Z	128	VAL
12	Z	130	SER

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Mol	Chain	Res	Type
12	Z	150	LEU
12	Z	172	LEU
12	Z	189	THR
13	a	1	THR
13	a	2	GLN
13	a	29	SER
13	a	33	LEU
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	2	SER
14	b	6	VAL
14	b	9	LYS
14	b	22	THR
14	b	107	LYS
14	b	119	VAL
14	b	178	LEU
15	f	2	LEU
15	f	3	LEU
15	h	3	LEU
15	i	2	LEU
15	i	3	LEU
15	j	3	LEU
15	k	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN

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Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	225	ASN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	143	HIS
6	F	191	GLN
6	F	203	ASN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	231	ASN
8	H	30	ASN
8	H	35	HIS
8	H	66	HIS
8	H	114	HIS
8	H	189	ASN
8	H	200	GLN
8	H	219	ASN
9	I	37	ASN
9	I	88	GLN

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Mol	Chain	Res	Type
9	I	168	GLN
9	I	172	ASN
10	J	10	GLN
10	J	55	GLN
10	J	78	GLN
10	J	118	GLN
10	J	191	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	179	HIS
11	K	190	ASN
11	K	191	HIS
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	80	ASN
12	L	94	GLN
12	L	108	HIS
12	L	152	ASN
12	L	159	GLN
12	L	165	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN

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Mol	Chain	Res	Type
3	Q	38	ASN
3	Q	77	ASN
3	Q	115	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	176	ASN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	59	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	140	ASN
6	T	143	HIS
6	T	191	GLN
6	T	203	ASN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	231	ASN
8	V	30	ASN

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Mol	Chain	Res	Type
8	V	189	ASN
8	V	200	GLN
8	V	219	ASN
9	W	37	ASN
9	W	44	HIS
9	W	168	GLN
9	W	203	GLN
10	X	10	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	118	GLN
10	X	146	HIS
10	X	191	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	190	ASN
11	Y	191	HIS
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	94	GLN
12	Z	159	GLN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	179	ASN
14	b	69	GLN
14	b	141	ASN
14	b	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z  > 2$
15	A1I48	k	4	15,14	12,14,15	1.50	1 (8%)	10,18,20	1.34	1 (10%)
15	A1I48	f	4	15,8	12,14,15	1.48	1 (8%)	10,18,20	1.41	2 (20%)
15	A1I48	h	4	15,14	12,14,15	1.52	1 (8%)	10,18,20	1.36	1 (10%)
15	A1I48	g	4	15,11	12,14,15	0.75	0	10,18,20	1.49	2 (20%)
15	A1I48	j	4	15,11	12,14,15	1.42	1 (8%)	10,18,20	1.47	2 (20%)
15	A1I48	i	4	15,8	12,14,15	1.47	1 (8%)	10,18,20	1.44	2 (20%)

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
15	A1I48	k	4	15,14	-	4/15/18/20	-
15	A1I48	f	4	15,8	-	4/15/18/20	-
15	A1I48	h	4	15,14	-	4/15/18/20	-
15	A1I48	g	4	15,11	-	4/15/18/20	-
15	A1I48	j	4	15,11	-	5/15/18/20	-
15	A1I48	i	4	15,8	-	4/15/18/20	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	4	A1I48	CA-N2	-4.75	1.33	1.47
15	k	4	A1I48	CA-N2	-4.70	1.34	1.47
15	f	4	A1I48	CA-N2	-4.60	1.34	1.47
15	i	4	A1I48	CA-N2	-4.54	1.34	1.47
15	j	4	A1I48	CA-N2	-4.31	1.35	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	4	A1I48	C22-OG1-CB	-3.05	111.00	115.27
15	h	4	A1I48	CB-CA-N2	-2.92	95.08	114.17
15	i	4	A1I48	CB-CA-N2	-2.81	95.78	114.17
15	f	4	A1I48	CB-CA-N2	-2.77	96.06	114.17
15	k	4	A1I48	CB-CA-N2	-2.73	96.32	114.17
15	j	4	A1I48	CB-CA-N2	-2.48	97.96	114.17
15	j	4	A1I48	CG2-CB-CA	2.43	117.98	113.26
15	g	4	A1I48	OG1-CB-CA	2.35	113.10	107.06
15	i	4	A1I48	CG2-CB-CA	2.11	117.37	113.26
15	f	4	A1I48	CG2-CB-CA	2.03	117.21	113.26

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	f	4	A1I48	O23-C22-OG1-CB
15	f	4	A1I48	O-C-CA-CB
15	g	4	A1I48	O23-C22-OG1-CB
15	g	4	A1I48	C-CA-CB-CG2
15	g	4	A1I48	C-CA-CB-OG1
15	h	4	A1I48	O23-C22-OG1-CB
15	i	4	A1I48	O23-C22-OG1-CB
15	i	4	A1I48	O-C-CA-CB
15	j	4	A1I48	O23-C22-OG1-CB
15	j	4	A1I48	C-CA-CB-CG2
15	j	4	A1I48	C-CA-CB-OG1
15	k	4	A1I48	O23-C22-OG1-CB
15	g	4	A1I48	N2-CA-CB-CG2
15	f	4	A1I48	C-CA-CB-CG2
15	h	4	A1I48	C-CA-CB-CG2
15	i	4	A1I48	C-CA-CB-CG2
15	k	4	A1I48	C-CA-CB-CG2
15	f	4	A1I48	C-CA-CB-OG1
15	i	4	A1I48	C-CA-CB-OG1
15	h	4	A1I48	O-C-CA-CB
15	j	4	A1I48	CA-CB-OG1-C22
15	k	4	A1I48	O-C-CA-CB
15	h	4	A1I48	C-CA-CB-OG1
15	j	4	A1I48	N2-CA-CB-CG2
15	k	4	A1I48	C-CA-CB-OG1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	f	4	A1I48	1	0
15	g	4	A1I48	1	0
15	i	4	A1I48	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z  > 2$
19	MPD	a	302	-	7,7,7	0.14	0	9,10,10	0.36	0
20	MES	a	301	-	12,12,12	0.65	0	15,16,16	0.39	0
16	SO4	U	302	-	4,4,4	0.55	0	6,6,6	0.15	0
16	SO4	G	303	-	4,4,4	0.60	0	6,6,6	0.22	0
16	SO4	P	301	-	4,4,4	0.34	0	6,6,6	0.08	0
19	MPD	K	301	-	7,7,7	0.17	0	9,10,10	0.46	0
16	SO4	B	301	-	4,4,4	0.34	0	6,6,6	0.08	0
20	MES	M	301	-	12,12,12	0.66	0	15,16,16	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MPD	K	301	-	-	2/5/5/5	-
19	MPD	a	302	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	MES	M	301	-	-	4/6/14/14	0/1/1/1
20	MES	a	301	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	K	301	MPD	C2-C3-C4-O4
19	K	301	MPD	C2-C3-C4-C5
20	M	301	MES	C7-C8-S-O3S
20	M	301	MES	N4-C7-C8-S
20	M	301	MES	C7-C8-S-O1S
20	M	301	MES	C7-C8-S-O2S

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	303	SO4	1	0
19	K	301	MPD	3	0
20	M	301	MES	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	250/250 (100%)	-0.62	0 100 100	56, 72, 105, 140	0
1	O	250/250 (100%)	-0.64	1 (0%) 88 84	59, 79, 120, 156	0
2	B	244/258 (94%)	-0.44	1 (0%) 88 84	54, 76, 128, 181	0
2	P	244/258 (94%)	-0.55	2 (0%) 82 75	60, 79, 123, 164	0
3	C	240/254 (94%)	-0.59	0 100 100	58, 81, 141, 156	0
3	Q	240/254 (94%)	-0.48	2 (0%) 82 75	60, 91, 159, 182	0
4	D	235/260 (90%)	-0.62	0 100 100	60, 82, 116, 132	0
4	R	235/260 (90%)	-0.59	0 100 100	61, 85, 120, 139	0
5	E	231/234 (98%)	-0.55	0 100 100	62, 85, 122, 158	0
5	S	231/234 (98%)	-0.51	0 100 100	63, 93, 135, 149	0
6	F	243/288 (84%)	-0.67	0 100 100	55, 77, 119, 144	0
6	T	243/288 (84%)	-0.59	0 100 100	55, 84, 129, 141	0
7	G	241/252 (95%)	-0.69	0 100 100	53, 71, 106, 154	0
7	U	241/252 (95%)	-0.68	0 100 100	58, 75, 110, 144	0
8	H	225/231 (97%)	-0.67	1 (0%) 88 84	51, 67, 102, 156	0
8	V	225/231 (97%)	-0.65	1 (0%) 88 84	53, 70, 104, 171	0
9	I	204/205 (99%)	-0.77	0 100 100	51, 68, 93, 119	0
9	W	204/205 (99%)	-0.83	0 100 100	52, 70, 98, 124	0
10	J	195/198 (98%)	-0.71	0 100 100	51, 75, 106, 132	0
10	X	195/198 (98%)	-0.76	0 100 100	55, 76, 107, 135	0
11	K	211/211 (100%)	-0.61	0 100 100	55, 75, 116, 139	0
11	Y	211/211 (100%)	-0.62	2 (0%) 81 74	60, 75, 119, 134	0
12	L	222/222 (100%)	-0.76	0 100 100	54, 72, 110, 122	0
12	Z	222/222 (100%)	-0.78	0 100 100	55, 72, 110, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.68	1 (0%) 88 84	52, 68, 93, 109	1 (0%)
13	a	233/246 (94%)	-0.77	1 (0%) 88 84	50, 67, 91, 104	0
14	N	195/195 (100%)	-0.81	0 100 100	48, 62, 92, 115	0
14	b	195/195 (100%)	-0.77	0 100 100	51, 64, 94, 119	0
15	f	2/4 (50%)	0.08	0 100 100	84, 84, 84, 84	0
15	g	2/4 (50%)	-0.50	0 100 100	76, 76, 76, 78	0
15	h	2/4 (50%)	-0.59	0 100 100	70, 70, 70, 73	0
15	i	2/4 (50%)	0.44	0 100 100	90, 90, 90, 91	0
15	j	2/4 (50%)	-0.58	0 100 100	82, 82, 82, 83	0
15	k	2/4 (50%)	-0.75	0 100 100	66, 66, 66, 70	0
All	All	6350/6632 (95%)	-0.65	12 (0%) 91 88	48, 75, 120, 182	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	218	GLY	3.7
3	Q	50	LEU	3.4
13	a	1	THR	3.1
13	M	190[A]	ARG	3.1
8	H	223	ILE	2.7
8	V	223	ILE	2.6
3	Q	205	ALA	2.2
11	Y	131	SER	2.2
2	P	56	LEU	2.2
11	Y	132	GLY	2.1
1	O	249	ALA	2.1
2	P	51	VAL	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. 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
15	A1I48	j	4	15/16	0.96	0.08	68,79,83,83	0
15	A1I48	k	4	15/16	0.96	0.08	64,68,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	A1I48	h	4	15/16	0.97	0.08	58,66,77,83	0
15	A1I48	i	4	15/16	0.97	0.08	65,73,79,85	0
15	A1I48	f	4	15/16	0.97	0.09	65,76,84,86	0
15	A1I48	g	4	15/16	0.97	0.07	70,75,77,80	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
16	SO4	U	302	5/5	0.75	0.46	20,20,20,20	0
20	MES	M	301	12/12	0.75	0.17	135,172,177,179	0
16	SO4	G	303	5/5	0.79	0.44	20,20,20,20	0
18	CL	N	202	1/1	0.80	0.35	30,30,30,30	0
18	CL	b	201	1/1	0.82	0.40	30,30,30,30	0
20	MES	a	301	12/12	0.85	0.13	141,166,174,180	0
19	MPD	a	302	8/8	0.87	0.16	109,120,134,137	0
19	MPD	K	301	8/8	0.92	0.14	90,99,105,105	0
18	CL	U	301	1/1	0.95	0.06	101,101,101,101	0
18	CL	G	302	1/1	0.95	0.08	93,93,93,93	0
16	SO4	P	301	5/5	0.96	0.12	127,131,143,145	0
16	SO4	B	301	5/5	0.96	0.16	123,128,147,161	0
17	MG	G	301	1/1	0.97	0.06	94,94,94,94	0
17	MG	N	201	1/1	0.97	0.11	125,125,125,125	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.