



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:55 PM GMT

PDB ID : 4X6Z  
Title : Yeast 20S proteasome in complex with PR-VI modulator  
Authors : Rostankowski, R.; Witkowska, J.; Borek, D.; Otwinowski, Z.; Jankowska, E.  
Deposited on : 2014-12-09  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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-20026982

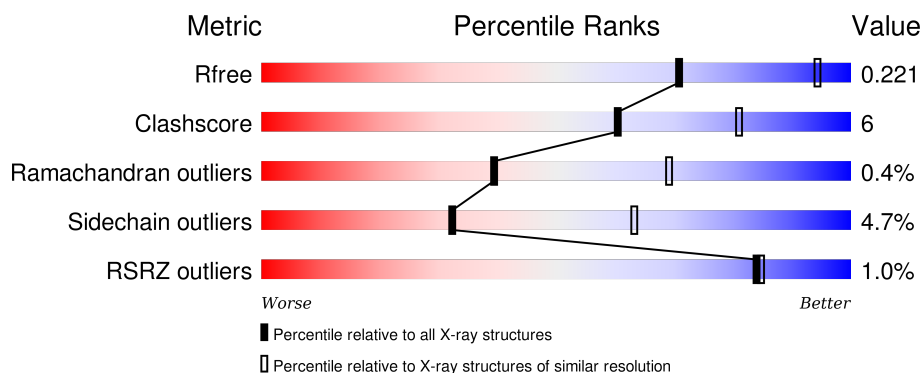
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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











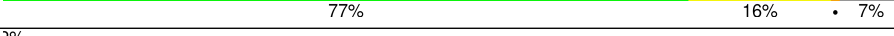

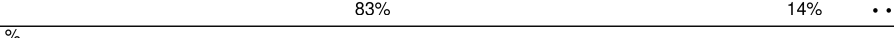
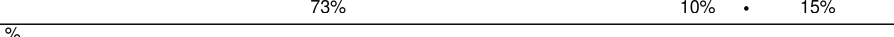

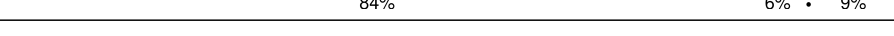


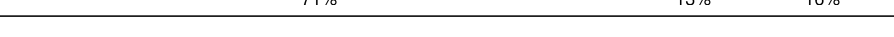

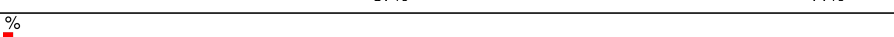






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	1	241	<div> <div></div> <div>79% 12% • 8%</div> </div>
1	M	241	<div> <div>%</div> <div>76% 15% • 8%</div> </div>
2	2	266	<div> <div></div> <div>72% 14% • 12%</div> </div>
2	N	266	<div> <div></div> <div>73% 14% • 12%</div> </div>
3	A	252	<div> <div>%</div> <div>83% 12% • •</div> </div>

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Mol	Chain	Length	Quality of chain
3	O	252	
4	B	250	
4	P	250	
5	C	258	
5	Q	258	
6	D	254	
6	R	254	
7	E	260	
7	S	260	
8	F	234	
8	T	234	
9	G	288	
9	U	288	
10	H	215	
10	V	215	
11	I	261	
11	W	261	
12	J	205	
12	X	205	
13	K	198	
13	Y	198	
14	L	287	
14	Z	287	
15	a	13	
15	e	13	

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	MPD	1	301	-	-	-	X
16	MPD	L	301	-	-	-	X
16	MPD	M	301	-	-	-	X
16	MPD	V	201	-	-	X	X
16	MPD	Z	301	-	-	-	X
17	GOL	1	303	-	-	-	X
17	GOL	2	303	-	-	-	X
17	GOL	A	302	-	-	-	X
17	GOL	A	304	-	-	-	X
17	GOL	D	301	-	-	-	X
17	GOL	E	301	-	-	-	X
17	GOL	F	304	-	-	-	X
17	GOL	H	201	-	-	-	X
17	GOL	I	301	-	-	-	X
17	GOL	I	302	-	-	-	X
17	GOL	K	201	-	-	-	X
17	GOL	L	302	-	-	-	X
17	GOL	L	303	-	-	-	X
17	GOL	M	302	-	-	-	X
17	GOL	M	303	-	-	-	X
17	GOL	N	303	-	-	-	X
17	GOL	O	301	-	-	-	X
17	GOL	O	302	-	-	-	X
17	GOL	S	301	-	-	-	X
17	GOL	T	302	-	-	-	X
17	GOL	V	203	-	-	-	X
17	GOL	W	301	-	-	-	X
17	GOL	X	202	-	-	-	X
17	GOL	Z	303	-	-	-	X
17	GOL	Z	304	-	-	-	X
18	MG	V	206	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50245 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 beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	222	Total	C	N	O	S	0	1	0
			1765	1120	306	335	4			
1	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	233	Total	C	N	O	S	0	1	0
			1833	1159	313	354	7			
2	N	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 3 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	242	Total	C	N	O	S	0	0	0
			1916	1218	321	369	8			
3	O	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	248	Total	C	N	O	S	0	0	0
			1898	1208	313	374	3			
4	P	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- Molecule 5 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
5	Q	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 6 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
6	R	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
7	S	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 8 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			
8	T	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

- Molecule 9 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
9	U	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 10 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	196	Total	C	N	O	S	0	1	0
			1523	961	254	301	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	V	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	221	Total	C	N	O	S	0	1	0
			1685	1065	292	321	7			
11	W	220	Total	C	N	O	S	0	2	0
			1683	1063	293	321	6			

- Molecule 12 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
12	X	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			
13	Y	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			

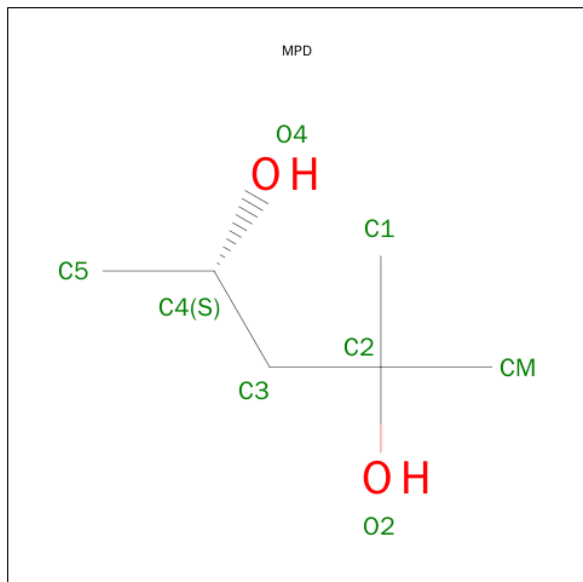
- Molecule 14 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
14	Z	212	Total	C	N	O	S	0	1	0
			1650	1049	281	313	7			

- Molecule 15 is a protein called synthetic peptide (polymer).

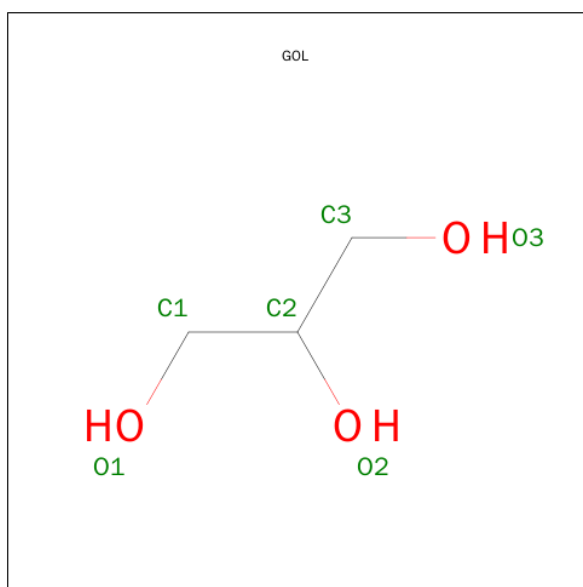
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	a	3	Total	C	N	O	0	0	0
			27	17	6	4			
15	e	3	Total	C	N	O	0	0	0
			27	17	6	4			

- Molecule 16 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	1	1	Total	C	O	0	0
			8	6	2		
16	2	1	Total	C	O	0	0
			8	6	2		
16	L	1	Total	C	O	0	0
			8	6	2		
16	M	1	Total	C	O	0	0
			8	6	2		
16	N	1	Total	C	O	0	0
			8	6	2		
16	T	1	Total	C	O	0	0
			8	6	2		
16	V	1	Total	C	O	0	0
			8	6	2		
16	X	1	Total	C	O	0	0
			8	6	2		
16	Z	1	Total	C	O	0	0
			8	6	2		

- Molecule 17 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	1	1	Total	C	O	0	0
			6	3	3		
17	1	1	Total	C	O	0	0
			6	3	3		
17	2	1	Total	C	O	0	0
			6	3	3		
17	2	1	Total	C	O	0	0
			6	3	3		
17	A	1	Total	C	O	0	0
			6	3	3		
17	A	1	Total	C	O	0	0
			6	3	3		
17	A	1	Total	C	O	0	0
			6	3	3		
17	A	1	Total	C	O	0	0
			6	3	3		
17	D	1	Total	C	O	0	0
			6	3	3		
17	E	1	Total	C	O	0	0
			6	3	3		
17	F	1	Total	C	O	0	0
			6	3	3		
17	F	1	Total	C	O	0	0
			6	3	3		
17	F	1	Total	C	O	0	0
			6	3	3		
17	F	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	G	1	Total 6	C 3	O 3	0	0
17	G	1	Total 6	C 3	O 3	0	0
17	H	1	Total 6	C 3	O 3	0	0
17	I	1	Total 6	C 3	O 3	0	0
17	I	1	Total 6	C 3	O 3	0	0
17	J	1	Total 6	C 3	O 3	0	0
17	K	1	Total 6	C 3	O 3	0	0
17	L	1	Total 6	C 3	O 3	0	0
17	L	1	Total 6	C 3	O 3	0	0
17	M	1	Total 6	C 3	O 3	0	0
17	M	1	Total 6	C 3	O 3	0	0
17	N	1	Total 6	C 3	O 3	0	0
17	N	1	Total 6	C 3	O 3	0	0
17	O	1	Total 6	C 3	O 3	0	0
17	O	1	Total 6	C 3	O 3	0	0
17	S	1	Total 6	C 3	O 3	0	0
17	T	1	Total 6	C 3	O 3	0	0
17	V	1	Total 6	C 3	O 3	0	0
17	V	1	Total 6	C 3	O 3	0	0
17	W	1	Total 6	C 3	O 3	0	0
17	X	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	Z	1	Total	C	O	0	0
			6	3	3		
17	Z	1	Total	C	O	0	0
			6	3	3		
17	Z	1	Total	C	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	P	1	Total	Mg	0	0
			1	1		
18	K	2	Total	Mg	0	0
			2	2		
18	B	1	Total	Mg	0	0
			1	1		
18	W	1	Total	Mg	0	0
			1	1		
18	N	4	Total	Mg	0	0
			4	4		
18	X	3	Total	Mg	0	0
			3	3		
18	2	5	Total	Mg	0	0
			5	5		
18	S	2	Total	Mg	0	0
			2	2		
18	J	6	Total	Mg	0	0
			6	6		
18	V	4	Total	Mg	0	0
			4	4		
18	R	3	Total	Mg	0	0
			3	3		
18	M	4	Total	Mg	0	0
			4	4		
18	1	1	Total	Mg	0	0
			1	1		
18	D	1	Total	Mg	0	0
			1	1		
18	Z	2	Total	Mg	0	0
			2	2		
18	L	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	Q	2	Total 2	Mg 2	0	0
18	H	4	Total 4	Mg 4	0	0
18	C	2	Total 2	Mg 2	0	0
18	T	2	Total 2	Mg 2	0	0
18	O	1	Total 1	Mg 1	0	0
18	Y	2	Total 2	Mg 2	0	0
18	F	1	Total 1	Mg 1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	1	14	Total 14	O 14	0	0
19	2	20	Total 20	O 20	0	0
19	A	13	Total 13	O 13	0	0
19	B	16	Total 16	O 16	0	0
19	C	5	Total 5	O 5	0	0
19	D	10	Total 10	O 10	0	0
19	E	11	Total 11	O 11	0	0
19	F	9	Total 9	O 9	0	0
19	G	14	Total 14	O 14	0	0
19	H	17	Total 17	O 17	0	0
19	I	15	Total 15	O 15	0	0
19	J	13	Total 13	O 13	0	0

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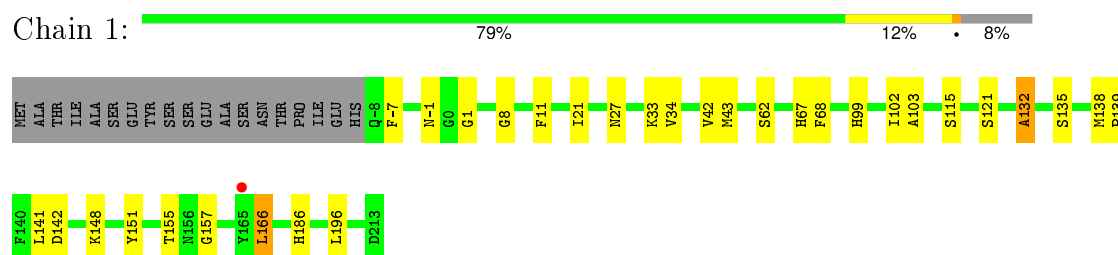
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	K	11	Total 11	O 11	0	0
19	L	14	Total 14	O 14	0	0
19	M	9	Total 9	O 9	0	0
19	N	15	Total 15	O 15	0	0
19	O	14	Total 14	O 14	0	0
19	P	13	Total 13	O 13	0	0
19	Q	13	Total 13	O 13	0	0
19	R	11	Total 11	O 11	0	0
19	S	10	Total 10	O 10	0	0
19	T	8	Total 8	O 8	0	0
19	U	17	Total 17	O 17	0	0
19	V	17	Total 17	O 17	0	0
19	W	12	Total 12	O 12	0	0
19	X	9	Total 9	O 9	0	0
19	Y	14	Total 14	O 14	0	0
19	Z	15	Total 15	O 15	0	0

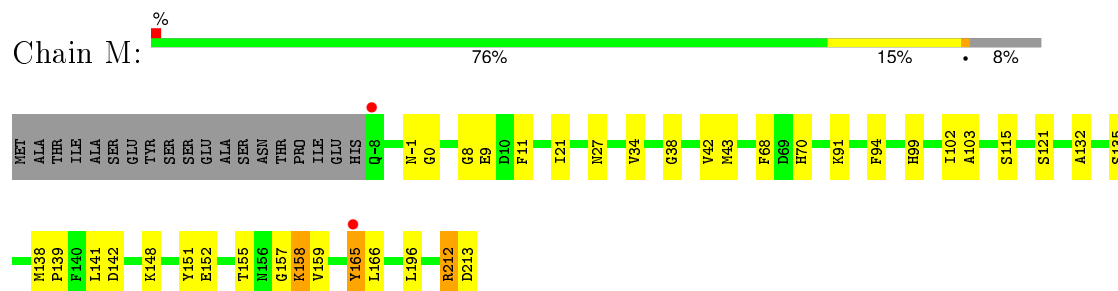
### 3 Residue-property plots [i](#)

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

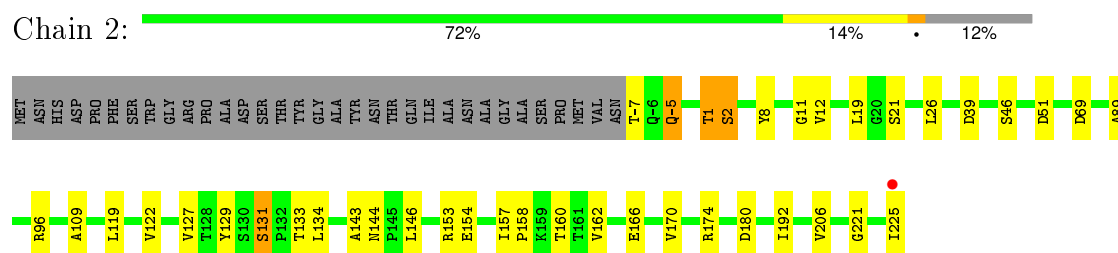
#### • Molecule 1: Proteasome subunit beta type-6



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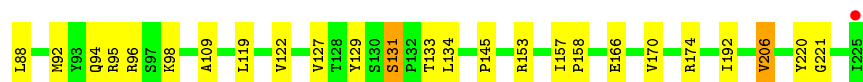


#### • Molecule 2: Proteasome subunit beta type-7

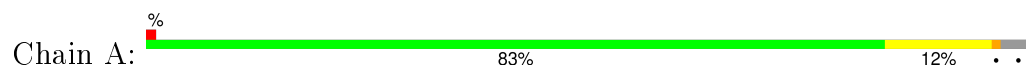


#### • Molecule 2: Proteasome subunit beta type-7

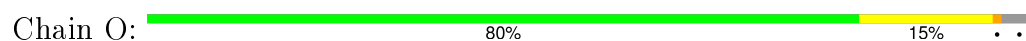




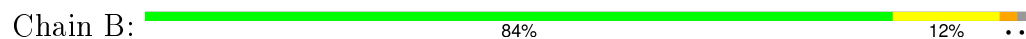
• Molecule 3: Proteasome subunit alpha type-1



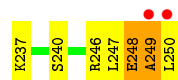
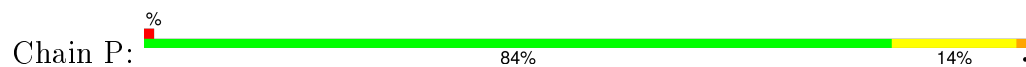
• Molecule 3: Proteasome subunit alpha type-1



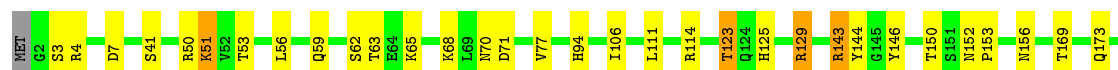
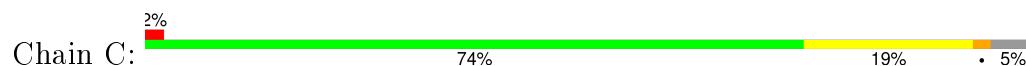
• Molecule 4: Proteasome subunit alpha type-2



• Molecule 4: Proteasome subunit alpha type-2

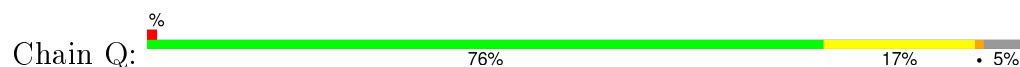


• Molecule 5: Proteasome subunit alpha type-3

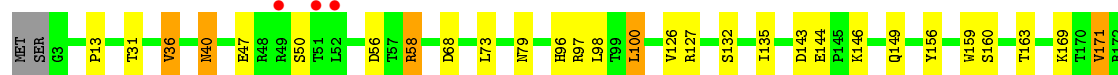
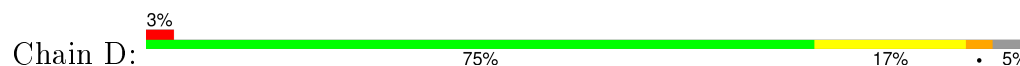




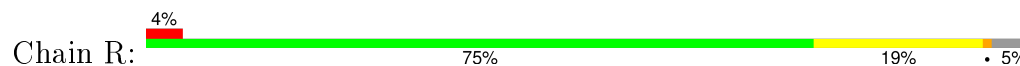
• Molecule 5: Proteasome subunit alpha type-3



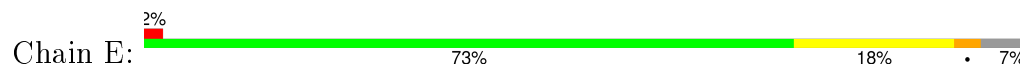
• Molecule 6: Proteasome subunit alpha type-4



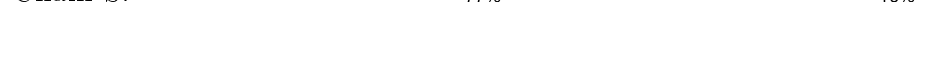
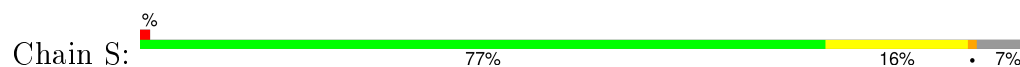
• Molecule 6: Proteasome subunit alpha type-4

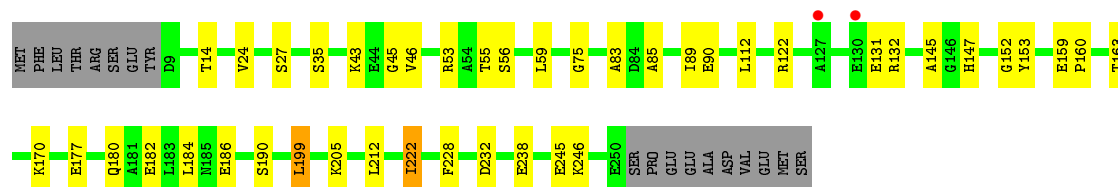


• Molecule 7: Proteasome subunit alpha type-5

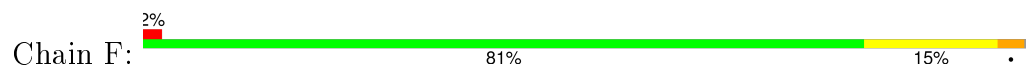


• Molecule 7: Proteasome subunit alpha type-5

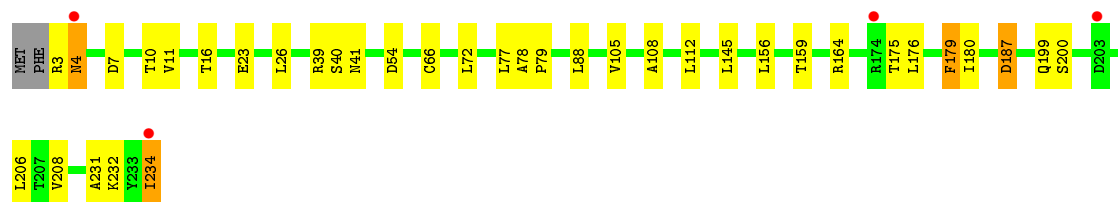
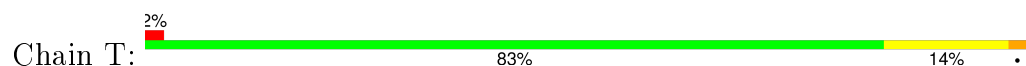




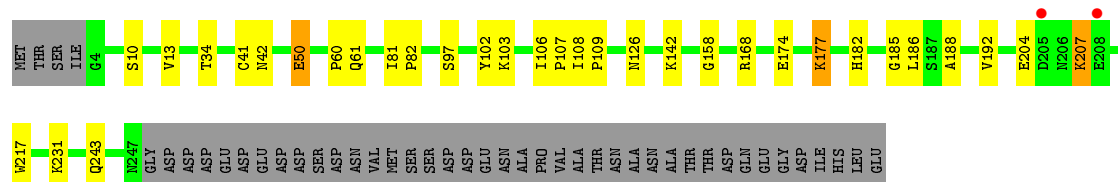
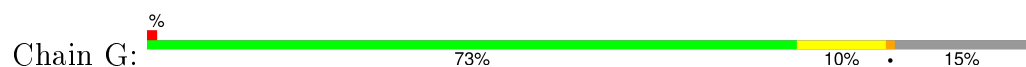
• Molecule 8: Proteasome subunit alpha type-6



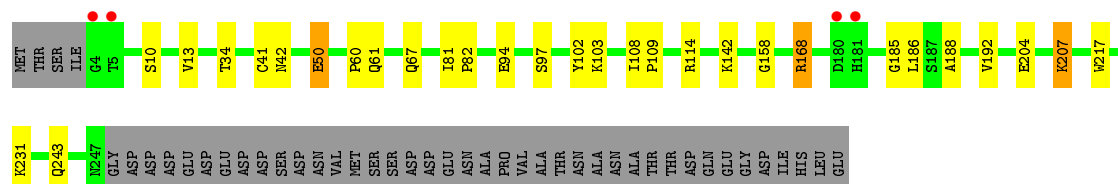
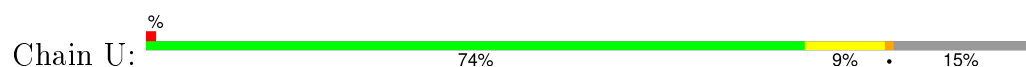
• Molecule 8: Proteasome subunit alpha type-6




• Molecule 9: Probable proteasome subunit alpha type-7

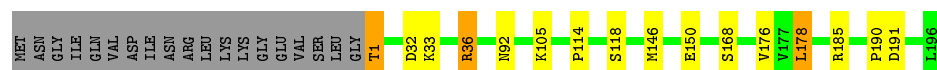


• Molecule 9: Probable proteasome subunit alpha type-7




• Molecule 10: Proteasome subunit beta type-1

Chain H: 



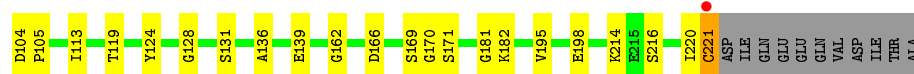
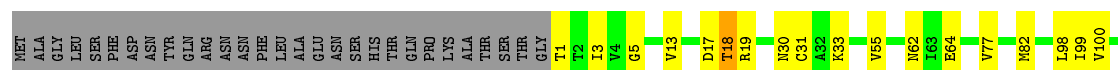
- Molecule 10: Proteasome subunit beta type-1

Chain V: 



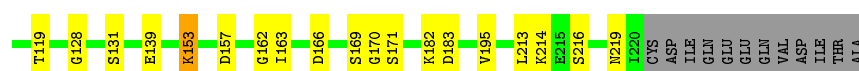
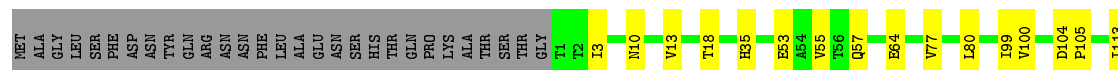
- Molecule 11: Proteasome subunit beta type-2

Chain I: 




- Molecule 11: Proteasome subunit beta type-2

Chain W: 




- Molecule 12: Proteasome subunit beta type-3

Chain J: 




- Molecule 12: Proteasome subunit beta type-3

Chain X: 

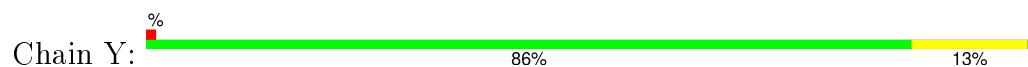


- Molecule 13: Proteasome subunit beta type-4

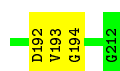
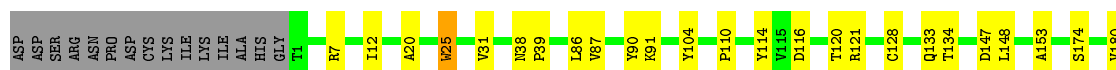
Chain K: 



- Molecule 13: Proteasome subunit beta type-4



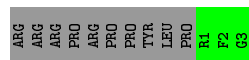
- Molecule 14: Proteasome subunit beta type-5



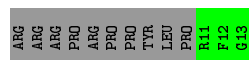
- Molecule 14: Proteasome subunit beta type-5



- Molecule 15: synthetic peptide (polymer)



- Molecule 15: synthetic peptide (polymer)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.35Å 300.79Å 144.58Å 90.00° 112.11° 90.00°	Depositor
Resolution (Å)	49.46 – 2.70 49.46 – 2.70	Depositor EDS
% Data completeness (in resolution range)	68.3 (49.46-2.70) 68.4 (49.46-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.177 , 0.222 0.181 , 0.221	Depositor DCC
$R_{free}$ test set	9928 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 35.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 196842 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50245	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, MPD

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	1	0.72	0/1806	0.83	0/2434
1	M	0.74	0/1795	0.86	2/2420 (0.1%)
2	2	0.78	0/1864	0.92	0/2526
2	N	0.78	0/1855	0.91	2/2514 (0.1%)
3	A	0.79	1/1954 (0.1%)	0.87	0/2645
3	O	0.77	0/1945	0.87	0/2634
4	B	0.74	0/1935	0.85	1/2621 (0.0%)
4	P	0.68	0/1944	0.83	0/2632
5	C	0.75	0/1934	0.92	2/2618 (0.1%)
5	Q	0.74	0/1934	0.91	1/2618 (0.0%)
6	D	0.66	0/1919	0.83	1/2598 (0.0%)
6	R	0.64	0/1919	0.81	0/2598
7	E	0.70	0/1886	0.88	1/2541 (0.0%)
7	S	0.65	0/1886	0.86	0/2541
8	F	0.65	0/1811	0.80	0/2447
8	T	0.64	0/1811	0.83	1/2447 (0.0%)
9	G	0.70	0/1936	0.81	0/2614
9	U	0.70	0/1936	0.81	0/2614
10	H	0.80	0/1552	0.86	0/2101
10	V	0.81	0/1541	0.87	0/2087
11	I	0.74	0/1720	0.87	0/2333
11	W	0.74	0/1721	0.86	1/2334 (0.0%)
12	J	0.77	0/1611	0.90	4/2174 (0.2%)
12	X	0.78	1/1611 (0.1%)	0.89	4/2174 (0.2%)
13	K	0.76	0/1598	0.88	0/2154
13	Y	0.74	0/1598	0.87	0/2154
14	L	0.77	1/1681 (0.1%)	0.83	0/2274
14	Z	0.77	0/1690	0.86	0/2286
15	a	0.65	0/27	1.31	0/32
15	e	0.85	0/27	1.30	0/32
All	All	0.73	3/50447 (0.0%)	0.86	20/68197 (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
11	I	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	X	196	ASP	CB-CG	5.80	1.64	1.51
14	L	25	TRP	CB-CG	-5.67	1.40	1.50
3	A	128	TYR	C-O	5.00	1.32	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	X	19	ARG	NE-CZ-NH2	-7.73	116.44	120.30
12	J	19	ARG	NE-CZ-NH1	7.57	124.08	120.30
12	X	19	ARG	NE-CZ-NH1	7.16	123.88	120.30
12	J	19	ARG	NE-CZ-NH2	-6.68	116.96	120.30
5	Q	143	ARG	NE-CZ-NH1	6.01	123.31	120.30
8	T	7	ASP	CB-CG-OD1	6.01	123.71	118.30
5	C	7	ASP	CB-CG-OD1	5.92	123.62	118.30
12	X	71	ARG	NE-CZ-NH2	-5.91	117.34	120.30
12	J	59	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	N	95	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	M	38	GLY	N-CA-C	5.64	127.20	113.10
11	W	183	ASP	CB-CG-OD2	-5.50	113.35	118.30
6	D	100	LEU	CA-CB-CG	5.49	127.92	115.30
1	M	212	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	N	95	ARG	NE-CZ-NH2	-5.22	117.69	120.30
7	E	72	ARG	NE-CZ-NH1	5.18	122.89	120.30
12	X	196	ASP	CB-CG-OD1	5.14	122.92	118.30
5	C	129	ARG	NE-CZ-NH1	5.08	122.84	120.30
4	B	201	GLU	OE1-CD-OE2	5.06	129.37	123.30
12	J	59	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	I	181	GLY	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	1	1765	0	1724	18	0
1	M	1757	0	1711	23	0
2	2	1833	0	1837	29	0
2	N	1824	0	1832	19	0
3	A	1916	0	1905	13	0
3	O	1907	0	1901	18	0
4	B	1898	0	1906	23	0
4	P	1907	0	1917	24	0
5	C	1904	0	1901	41	0
5	Q	1904	0	1901	37	0
6	D	1890	0	1900	33	0
6	R	1890	0	1900	35	0
7	E	1861	0	1836	35	0
7	S	1861	0	1836	24	0
8	F	1784	0	1788	28	0
8	T	1784	0	1788	22	0
9	G	1896	0	1886	23	0
9	U	1896	0	1886	18	0
10	H	1523	0	1493	9	0
10	V	1512	0	1481	21	0
11	I	1685	0	1693	19	0
11	W	1683	0	1692	18	0
12	J	1581	0	1574	8	0
12	X	1581	0	1574	10	0
13	K	1570	0	1577	10	0
13	Y	1570	0	1577	10	0
14	L	1644	0	1595	15	0
14	Z	1650	0	1603	15	0
15	a	27	0	27	0	0
15	e	27	0	24	0	0
16	1	8	0	14	0	0
16	2	8	0	14	1	0
16	L	8	0	14	0	0
16	M	8	0	14	0	0
16	N	8	0	14	1	0
16	T	8	0	14	0	0
16	V	8	0	14	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	X	8	0	14	3	0
16	Z	8	0	14	2	0
17	1	12	0	16	0	0
17	2	12	0	16	0	0
17	A	24	0	32	0	0
17	D	6	0	8	2	0
17	E	6	0	8	0	0
17	F	24	0	32	0	0
17	G	12	0	16	0	0
17	H	6	0	8	0	0
17	I	12	0	16	0	0
17	J	6	0	8	0	0
17	K	6	0	8	0	0
17	L	12	0	16	0	0
17	M	12	0	16	0	0
17	N	12	0	16	0	0
17	O	12	0	16	0	0
17	S	6	0	8	0	0
17	T	6	0	8	0	0
17	V	12	0	16	0	0
17	W	6	0	8	0	0
17	X	6	0	8	0	0
17	Z	18	0	24	0	0
18	1	1	0	0	0	0
18	2	5	0	0	0	0
18	B	1	0	0	0	0
18	C	2	0	0	0	0
18	D	1	0	0	0	0
18	F	1	0	0	0	0
18	H	4	0	0	0	0
18	J	6	0	0	0	0
18	K	2	0	0	0	0
18	L	2	0	0	0	0
18	M	4	0	0	0	0
18	N	4	0	0	0	0
18	O	1	0	0	0	0
18	P	1	0	0	0	0
18	Q	2	0	0	0	0
18	R	3	0	0	0	0
18	S	2	0	0	0	0
18	T	2	0	0	0	0
18	V	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	1	0	0	0	0
18	X	3	0	0	0	0
18	Y	2	0	0	0	0
18	Z	2	0	0	0	0
19	1	14	0	0	1	0
19	2	20	0	0	1	0
19	A	13	0	0	0	0
19	B	16	0	0	1	0
19	C	5	0	0	0	0
19	D	10	0	0	0	0
19	E	11	0	0	1	0
19	F	9	0	0	0	0
19	G	14	0	0	1	0
19	H	17	0	0	0	0
19	I	15	0	0	0	0
19	J	13	0	0	0	0
19	K	11	0	0	0	0
19	L	14	0	0	0	0
19	M	9	0	0	1	0
19	N	15	0	0	0	0
19	O	14	0	0	0	0
19	P	13	0	0	1	0
19	Q	13	0	0	0	0
19	R	11	0	0	0	0
19	S	10	0	0	1	0
19	T	8	0	0	0	0
19	U	17	0	0	1	0
19	V	17	0	0	0	0
19	W	12	0	0	2	0
19	X	9	0	0	0	0
19	Y	14	0	0	0	0
19	Z	15	0	0	0	0
All	All	50245	0	49695	555	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 (555) 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)
6:R:197:ARG:CG	6:R:236:ILE:HD11	1.80	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:232:TYR:O	6:D:236:ILE:HG12	1.54	1.06
6:D:238:GLN:N	6:D:238:GLN:OE1	1.97	0.97
6:R:197:ARG:HG2	6:R:236:ILE:HD11	1.45	0.93
6:R:197:ARG:HG3	6:R:236:ILE:CD1	2.01	0.91
10:V:129:SER:H	16:V:201:MPD:H12	1.38	0.89
6:R:197:ARG:HG3	6:R:236:ILE:HD11	1.52	0.87
6:D:50:SER:HB3	6:D:209:ASN:HD21	1.40	0.87
10:V:1:THR:HB	10:V:33:LYS:NZ	1.96	0.80
10:H:1:THR:HB	10:H:33:LYS:NZ	1.95	0.80
5:C:51:LYS:O	5:C:53:THR:HG23	1.82	0.80
7:E:125:GLU:O	7:E:126:GLY:O	2.00	0.79
10:V:47:GLY:H	16:V:201:MPD:HM3	1.49	0.77
10:H:1:THR:HB	10:H:33:LYS:HZ2	1.49	0.77
8:T:164:ARG:O	8:T:200:SER:HB2	1.88	0.73
2:N:-5:GLN:HG3	2:N:-5:GLN:O	1.88	0.73
5:Q:83:ASP:OD2	5:Q:129:ARG:NH1	2.22	0.73
1:1:-7:PHE:HA	19:1:405:HOH:O	1.89	0.72
2:2:1:THR:HG22	2:2:2:SER:N	2.05	0.72
7:S:122:ARG:HH22	7:S:131:GLU:HG3	1.54	0.72
2:2:-5:GLN:O	2:2:-5:GLN:HG3	1.89	0.71
9:U:94:GLU:HG2	9:U:114:ARG:HB3	1.72	0.71
8:F:198:SER:HA	8:F:201:LEU:HD21	1.71	0.71
11:W:80:LEU:HD12	11:W:113:ILE:HD11	1.71	0.71
10:V:1:THR:HG23	16:V:201:MPD:HM2	1.72	0.71
1:M:91:LYS:HE2	1:M:94:PHE:O	1.91	0.70
8:F:201:LEU:HD23	8:F:201:LEU:N	2.05	0.70
5:C:230:PHE:HE2	5:C:238:ILE:CD1	2.04	0.70
4:B:37:ILE:HG23	4:B:44:VAL:HG13	1.74	0.70
10:V:1:THR:HB	10:V:33:LYS:HZ2	1.55	0.70
10:V:129:SER:H	16:V:201:MPD:C1	2.05	0.69
10:V:47:GLY:H	16:V:201:MPD:CM	2.06	0.68
9:G:204:GLU:HG2	9:G:207:LYS:CE	2.24	0.68
6:D:50:SER:CB	6:D:209:ASN:HD21	2.07	0.67
4:P:201:GLU:N	4:P:201:GLU:OE2	2.28	0.67
8:T:164:ARG:O	8:T:200:SER:CB	2.43	0.66
5:C:4:ARG:NH1	7:E:10:ARG:HA	2.09	0.66
5:C:230:PHE:HE2	5:C:238:ILE:HD11	1.58	0.66
2:2:1:THR:HG21	2:2:180:ASP:OD2	1.96	0.66
9:G:204:GLU:HG2	9:G:207:LYS:HE3	1.78	0.66
4:P:160:LYS:HG3	5:Q:56:LEU:O	1.97	0.65
10:V:1:THR:HG23	16:V:201:MPD:CM	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1:THR:CG2	2:2:2:SER:H	2.09	0.64
2:2:1:THR:HG22	2:2:2:SER:H	1.63	0.64
1:M:151:TYR:CD2	1:M:157:GLY:HA2	2.33	0.64
11:I:18:THR:HG22	11:I:31:CYS:O	1.98	0.64
9:G:182:HIS:NE2	19:G:413:HOH:O	2.30	0.63
9:U:94:GLU:CG	9:U:114:ARG:HD2	2.29	0.63
6:R:197:ARG:CG	6:R:236:ILE:CD1	2.60	0.63
5:C:230:PHE:CE2	5:C:238:ILE:CD1	2.81	0.63
10:V:129:SER:N	16:V:201:MPD:H12	2.10	0.63
6:R:237:GLU:O	6:R:238:GLN:HB3	1.99	0.62
7:S:45:GLY:HA2	7:S:153:TYR:CE1	2.34	0.62
4:P:196:LEU:O	4:P:200:VAL:HG23	1.99	0.62
3:A:176:GLN:OE1	3:A:180:THR:HG23	1.98	0.62
10:V:1:THR:CG2	16:V:201:MPD:HM2	2.30	0.61
14:L:25:TRP:CZ3	1:M:135:SER:HA	2.35	0.60
10:V:1:THR:N	16:V:201:MPD:H11	2.16	0.60
17:D:301:GOL:H2	7:E:86:ARG:HB3	1.84	0.60
9:U:168:ARG:HD2	19:U:314:HOH:O	2.00	0.60
6:R:205:THR:HB	6:R:209:ASN:HD22	1.65	0.60
5:C:125:HIS:HB3	6:D:126:VAL:HG12	1.84	0.60
2:2:225:ILE:HD11	10:H:36[B]:ARG:NH1	2.17	0.60
8:F:206:LEU:O	8:F:234:ILE:HD11	2.02	0.60
7:E:45:GLY:HA2	7:E:153:TYR:CE1	2.37	0.59
5:C:143:ARG:HD3	5:C:144:TYR:CE2	2.37	0.59
5:C:111:LEU:HD23	5:C:111:LEU:C	2.23	0.59
8:F:198:SER:O	8:F:200:SER:N	2.34	0.59
11:W:57:GLN:HG3	16:X:201:MPD:H11	1.83	0.59
1:I:151:TYR:CD2	1:I:157:GLY:HA2	2.37	0.58
13:K:2:ILE:HB	13:K:17:SER:HB3	1.85	0.58
10:V:1:THR:HG23	16:V:201:MPD:H11	1.85	0.58
7:E:131:GLU:OE1	7:E:131:GLU:N	2.37	0.58
8:T:206:LEU:O	8:T:234:ILE:HD11	2.04	0.58
2:2:1:THR:CG2	2:2:2:SER:N	2.62	0.58
11:W:113:ILE:HG13	11:W:119:THR:HG22	1.84	0.58
5:Q:111:LEU:HD23	5:Q:111:LEU:C	2.23	0.58
4:B:196:LEU:O	4:B:200:VAL:HG12	2.04	0.57
6:D:50:SER:HB3	6:D:209:ASN:ND2	2.16	0.57
8:T:232:LYS:HD3	8:T:232:LYS:C	2.24	0.57
4:B:122:THR:CG2	5:C:129:ARG:HH21	2.18	0.57
5:Q:235:ILE:HA	5:Q:238:ILE:HG22	1.86	0.57
9:U:243:GLN:HA	9:U:243:GLN:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:34:GLY:O	7:E:35:SER:O	2.23	0.56
5:C:123:THR:HG23	6:D:127:ARG:HH21	1.69	0.56
11:W:10:ASN:HA	19:W:407:HOH:O	2.05	0.56
7:E:129:GLY:CA	7:E:130:GLU:C	2.73	0.56
9:G:243:GLN:OE1	9:G:243:GLN:HA	2.05	0.56
11:W:163:ILE:HG23	11:W:170:GLY:HA2	1.88	0.56
10:V:1:THR:HG23	16:V:201:MPD:C1	2.35	0.56
6:D:96:HIS:CD2	6:D:100:LEU:HD23	2.41	0.56
13:Y:2:ILE:HB	13:Y:17:SER:HB3	1.87	0.56
8:T:232:LYS:HD3	8:T:232:LYS:O	2.06	0.55
5:C:244:ILE:O	5:C:244:ILE:HG22	2.06	0.55
9:G:61:GLN:HA	9:G:61:GLN:NE2	2.22	0.55
1:1:135:SER:HA	14:Z:25:TRP:CZ3	2.41	0.55
2:2:131:SER:HB3	2:2:133:THR:O	2.06	0.55
10:V:1:THR:HB	10:V:33:LYS:HZ3	1.68	0.55
9:U:94:GLU:HG3	9:U:114:ARG:HD2	1.88	0.55
1:1:34:VAL:HG12	1:1:196:LEU:HD22	1.89	0.55
8:F:39:ARG:NH1	8:F:40:SER:O	2.40	0.55
2:N:12:VAL:HG21	2:N:109:ALA:HB1	1.89	0.55
4:B:160:LYS:HG3	5:C:56:LEU:O	2.07	0.55
11:W:35:HIS:CE1	11:W:53:GLU:OE1	2.60	0.55
4:P:104:TYR:OH	11:W:64:GLU:OE1	2.25	0.55
19:M:405:HOH:O	16:N:301:MPD:HM3	2.07	0.54
6:R:157:SER:HB2	7:S:59:LEU:HD11	1.88	0.54
2:2:12:VAL:HG21	2:2:109:ALA:HB1	1.89	0.54
2:N:131:SER:HB3	2:N:133:THR:O	2.08	0.54
2:2:119:LEU:HG	2:2:134:LEU:HD12	1.89	0.54
5:Q:244:ILE:HG22	5:Q:244:ILE:O	2.08	0.54
6:R:31:THR:HB	6:R:47:GLU:HG3	1.90	0.54
5:Q:184:MET:HE3	5:Q:188:ASP:HB3	1.90	0.54
17:D:301:GOL:H2	7:E:86:ARG:CB	2.38	0.54
8:T:39:ARG:NH1	8:T:40:SER:O	2.41	0.54
13:K:15:ALA:HB2	13:K:160:LEU:HD21	1.89	0.54
11:W:153:LYS:HE2	11:W:157:ASP:OD1	2.07	0.54
7:E:24:VAL:O	7:E:27:SER:HB3	2.09	0.53
13:Y:15:ALA:HB2	13:Y:160:LEU:HD21	1.91	0.53
14:L:148:LEU:HD23	14:L:153:ALA:HA	1.90	0.53
14:L:133:GLN:HG3	14:L:134:THR:N	2.23	0.53
3:A:158:ASP:HB2	3:A:159:PRO:CD	2.39	0.53
1:M:9:GLU:HG3	1:M:165:TYR:CD2	2.43	0.53
7:S:24:VAL:O	7:S:27:SER:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:232:LYS:C	8:F:232:LYS:HD3	2.29	0.53
8:T:164:ARG:HB3	8:T:200:SER:HB2	1.90	0.53
8:F:232:LYS:O	8:F:232:LYS:HD3	2.08	0.53
1:I:21:ILE:C	1:I:21:ILE:HD12	2.29	0.53
9:G:174:GLU:O	9:G:177:LYS:HB2	2.08	0.53
8:F:188:GLU:OE1	8:F:188:GLU:HA	2.08	0.53
11:I:18:THR:HG21	11:I:30:ASN:OD1	2.09	0.53
2:N:119:LEU:HG	2:N:134:LEU:HD12	1.90	0.53
3:O:158:ASP:HB2	3:O:159:PRO:CD	2.38	0.53
1:M:34:VAL:HG12	1:M:196:LEU:HD22	1.91	0.53
6:D:187:THR:HB	6:D:190:GLU:H	1.74	0.52
5:Q:156:ASN:OD1	6:R:79:ASN:HB2	2.09	0.52
5:C:210:ARG:HB3	5:C:210:ARG:NH1	2.24	0.52
14:L:25:TRP:CH2	1:M:135:SER:HA	2.44	0.52
6:D:31:THR:HB	6:D:47:GLU:HG3	1.91	0.52
3:O:196:GLU:HG2	3:O:201:LYS:HB2	1.92	0.52
9:U:42:ASN:HD22	9:U:185:GLY:HA3	1.74	0.52
4:B:4:ARG:HH12	7:E:127:ALA:CB	2.23	0.52
6:R:187:THR:HB	6:R:190:GLU:H	1.75	0.52
6:D:40:ASN:N	6:D:40:ASN:ND2	2.57	0.52
4:B:35:LEU:C	4:B:35:LEU:HD12	2.30	0.52
14:Z:148:LEU:HD23	14:Z:153:ALA:HA	1.91	0.52
14:Z:20:ALA:HB2	14:Z:31:VAL:HG21	1.92	0.52
9:G:42:ASN:HD22	9:G:185:GLY:HA3	1.75	0.52
1:M:155:THR:HG21	1:M:159:VAL:HB	1.92	0.51
14:Z:7:ARG:NH1	14:Z:110:PRO:O	2.43	0.51
7:S:112:LEU:C	7:S:112:LEU:HD13	2.31	0.51
10:H:1:THR:HB	10:H:33:LYS:HZ3	1.73	0.51
9:G:204:GLU:HG2	9:G:207:LYS:HE2	1.90	0.51
13:K:148:ARG:O	13:K:151:MET:HG3	2.11	0.51
4:B:176:GLU:HG3	5:C:56:LEU:HD22	1.93	0.51
5:Q:143:ARG:HD3	5:Q:144:TYR:CE2	2.45	0.51
5:C:184:MET:HE3	5:C:188:ASP:HB3	1.93	0.51
7:S:122:ARG:HH22	7:S:131:GLU:CG	2.24	0.51
5:C:152:ASN:HB2	5:C:153:PRO:CD	2.41	0.51
14:Z:38:ASN:HB2	14:Z:39:PRO:HD2	1.92	0.51
11:I:98:LEU:HB2	11:I:113:ILE:CG2	2.41	0.51
2:2:19:LEU:HD21	2:2:26:LEU:HD22	1.92	0.51
6:R:68:ASP:OD2	6:R:97:ARG:NH1	2.43	0.50
10:V:128:GLY:HA2	16:V:201:MPD:H13	1.94	0.50
4:P:176:GLU:HG3	5:Q:56:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:80:GLN:OE1	16:X:201:MPD:HM3	2.12	0.50
1:I:138:MET:N	1:I:139:PRO:CD	2.75	0.50
9:G:34:THR:HB	9:G:50:GLU:HG2	1.93	0.50
7:S:159:GLU:HB3	7:S:160:PRO:CD	2.41	0.50
3:O:48:LYS:HE2	3:O:195:ASN:OD1	2.12	0.50
6:R:234:THR:O	6:R:237:GLU:O	2.30	0.50
12:J:36:HIS:HB3	12:J:41:PHE:CD2	2.47	0.50
4:B:62:SER:HA	19:B:411:HOH:O	2.10	0.50
1:M:21:ILE:HD12	1:M:21:ILE:C	2.31	0.50
14:L:20:ALA:HB2	14:L:31:VAL:HG21	1.92	0.49
8:F:23:GLU:HA	8:F:26:LEU:HD12	1.94	0.49
8:T:179:PHE:CD1	8:T:180:ILE:N	2.80	0.49
3:O:205:PHE:CD1	3:O:205:PHE:C	2.85	0.49
5:C:68:LYS:HG3	5:C:227:GLN:OE1	2.12	0.49
7:E:112:LEU:C	7:E:112:LEU:HD13	2.33	0.49
7:S:53:ARG:O	7:S:53:ARG:HG2	2.12	0.49
5:Q:210:ARG:HB3	5:Q:210:ARG:NH1	2.27	0.49
4:P:119:GLN:O	4:P:122:THR:HB	2.13	0.49
8:T:23:GLU:HA	8:T:26:LEU:HD12	1.95	0.49
2:2:225:ILE:OXT	10:H:185:ARG:NE	2.44	0.49
4:B:15:SER:OG	4:B:17:LYS:HG2	2.12	0.49
4:P:15:SER:OG	4:P:17:LYS:HG2	2.12	0.49
11:I:3:ILE:HG13	11:I:99:ILE:HD12	1.94	0.49
6:R:236:ILE:O	6:R:239:GLU:HB3	2.12	0.49
10:V:1:THR:H3	16:V:201:MPD:H11	1.77	0.49
2:2:160:THR:HA	19:2:419:HOH:O	2.13	0.49
8:F:231:ALA:HA	8:F:234:ILE:HG22	1.95	0.49
5:Q:68:LYS:HG3	5:Q:227:GLN:OE1	2.13	0.49
4:B:104:TYR:OH	11:I:64:GLU:OE1	2.30	0.49
6:R:178:ASN:OD1	6:R:197:ARG:NH2	2.46	0.49
10:H:32:ASP:OD2	10:H:185:ARG:NH2	2.46	0.49
6:D:68:ASP:CG	6:D:97:ARG:HH21	2.14	0.49
7:S:222:ILE:O	7:S:222:ILE:HG13	2.13	0.49
1:I:27:ASN:HB3	2:2:129:TYR:CE1	2.48	0.49
6:D:232:TYR:O	6:D:236:ILE:CG1	2.44	0.48
5:C:143:ARG:HD3	5:C:144:TYR:CD2	2.48	0.48
11:W:128:GLY:O	11:W:131:SER:HB2	2.13	0.48
14:L:38:ASN:HB2	14:L:39:PRO:HD2	1.95	0.48
1:M:138:MET:N	1:M:139:PRO:CD	2.75	0.48
5:C:70:ASN:OD1	5:C:71:ASP:N	2.46	0.48
5:Q:152:ASN:HB2	5:Q:153:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:114:PRO:HD2	10:H:118:SER:O	2.14	0.48
8:F:105:VAL:HG12	8:F:145:LEU:HD22	1.94	0.48
7:E:222:ILE:HG13	7:E:222:ILE:O	2.13	0.48
2:N:19:LEU:HD21	2:N:26:LEU:HD22	1.95	0.48
9:U:34:THR:HB	9:U:50:GLU:HG2	1.95	0.48
10:V:176:VAL:HG12	10:V:178:LEU:HD13	1.95	0.48
8:T:72:LEU:C	8:T:72:LEU:HD12	2.33	0.48
13:Y:7:ARG:HH11	13:Y:7:ARG:HG2	1.79	0.48
8:F:156:LEU:HD13	8:F:159:THR:HB	1.95	0.48
4:B:122:THR:HG23	5:C:129:ARG:HH21	1.79	0.48
5:C:94:HIS:HB2	5:C:114:ARG:NH1	2.28	0.48
2:2:39:ASP:OD1	2:2:39:ASP:N	2.44	0.48
4:P:4:ARG:HB3	5:Q:3:SER:OG	2.13	0.48
5:Q:125:HIS:HB3	6:R:126:VAL:HG12	1.96	0.48
10:V:32:ASP:OD2	10:V:185:ARG:NH2	2.46	0.48
7:S:112:LEU:O	7:S:112:LEU:HD13	2.13	0.48
6:R:197:ARG:HG3	6:R:236:ILE:HD12	1.92	0.47
1:1:142:ASP:O	1:1:148:LYS:HB2	2.14	0.47
5:Q:59:GLN:OE1	5:Q:209:ASP:HA	2.15	0.47
7:E:85:ALA:O	7:E:89:ILE:HG12	2.14	0.47
5:C:181:LYS:HG3	5:C:184:MET:HG3	1.96	0.47
10:H:176:VAL:HG12	10:H:178:LEU:HD13	1.95	0.47
1:1:8:GLY:HA3	1:1:11:PHE:CE1	2.49	0.47
11:W:139:GLU:HA	11:W:139:GLU:OE1	2.14	0.47
7:S:85:ALA:O	7:S:89:ILE:HG12	2.14	0.47
11:I:17:ASP:HB2	11:I:170:GLY:HA3	1.96	0.47
5:C:152:ASN:HB2	5:C:153:PRO:HD2	1.96	0.47
14:Z:12:ILE:HB	14:Z:180:VAL:HB	1.96	0.47
7:S:43:LYS:HD2	7:S:43:LYS:N	2.30	0.47
4:P:194:LEU:HD21	4:P:250:LEU:HB3	1.96	0.47
2:N:122:VAL:HA	2:N:127:VAL:O	2.15	0.47
8:T:231:ALA:HA	8:T:234:ILE:HG22	1.96	0.47
7:E:34:GLY:C	7:E:35:SER:O	2.53	0.47
6:D:216:LYS:HE2	6:D:220:ASP:OD2	2.14	0.47
6:R:238:GLN:O	6:R:238:GLN:HG2	2.15	0.47
7:E:112:LEU:O	7:E:112:LEU:HD13	2.14	0.47
11:I:17:ASP:OD2	11:I:170:GLY:HA2	2.14	0.47
5:Q:52:VAL:HG13	5:Q:53:THR:N	2.30	0.47
14:L:7:ARG:NH1	14:L:110:PRO:O	2.46	0.47
1:M:142:ASP:O	1:M:148:LYS:HB2	2.15	0.47
2:N:157:ILE:HB	2:N:158:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:106:PRO:HG2	4:B:109:LEU:HB2	1.95	0.47
7:E:212:LEU:C	7:E:212:LEU:HD23	2.35	0.47
5:Q:187:ASP:HA	5:Q:190:ILE:HD12	1.96	0.47
8:T:156:LEU:HD13	8:T:159:THR:HB	1.97	0.47
7:S:186:GLU:HB3	7:S:199:LEU:HD21	1.97	0.47
6:D:144:GLU:HG3	6:D:146:LYS:HE2	1.97	0.47
5:Q:181:LYS:HG3	5:Q:184:MET:HG3	1.96	0.47
1:M:155:THR:O	1:M:158:LYS:HD2	2.15	0.47
7:S:75:GLY:HA3	7:S:228:PHE:CD2	2.50	0.47
2:N:174:ARG:HA	2:N:206:VAL:HG21	1.97	0.47
8:F:66:CYS:SG	8:F:88:LEU:HD23	2.55	0.47
1:M:8:GLY:HA3	1:M:11:PHE:CE1	2.51	0.47
6:R:189:GLU:HG2	6:R:232:TYR:OH	2.15	0.47
3:A:205:PHE:C	3:A:205:PHE:CD1	2.89	0.47
5:Q:169:THR:O	5:Q:173:GLN:HB2	2.14	0.47
6:D:238:GLN:O	6:D:239:GLU:HG3	2.15	0.46
4:P:106:PRO:HG2	4:P:109:LEU:HB2	1.97	0.46
10:V:114:PRO:HD2	10:V:118:SER:O	2.15	0.46
5:Q:9:ARG:HD3	6:R:6:ARG:NH1	2.31	0.46
11:I:128:GLY:O	11:I:131:SER:HB2	2.14	0.46
1:I:1:GLY:HA2	1:I:33:LYS:NZ	2.30	0.46
5:Q:70:ASN:OD1	5:Q:71:ASP:N	2.47	0.46
5:C:187:ASP:HA	5:C:190:ILE:HD12	1.97	0.46
12:X:2:ILE:HG21	12:X:133:ALA:HB3	1.96	0.46
11:W:104:ASP:HB2	11:W:105:PRO:HD2	1.97	0.46
2:2:122:VAL:HA	2:2:127:VAL:O	2.16	0.46
11:W:219:ASN:HA	19:W:404:HOH:O	2.15	0.46
11:W:3:ILE:HG13	11:W:99:ILE:HD12	1.96	0.46
3:O:189:SER:O	3:O:190:LYS:HB2	2.15	0.46
9:U:60:PRO:O	9:U:61:GLN:HB2	2.15	0.46
4:B:4:ARG:HB3	5:C:3:SER:OG	2.15	0.46
5:Q:94:HIS:HB2	5:Q:114:ARG:NH1	2.30	0.46
14:L:12:ILE:HB	14:L:180:VAL:HB	1.96	0.46
1:M:27:ASN:HB3	2:N:129:TYR:CE1	2.50	0.46
2:N:220:TYR:N	2:N:221:GLY:HA2	2.30	0.46
6:D:238:GLN:O	6:D:239:GLU:CG	2.64	0.46
12:J:2:ILE:HG21	12:J:133:ALA:HB3	1.98	0.46
2:N:11:GLY:HA3	2:N:192:ILE:O	2.15	0.46
9:G:60:PRO:O	9:G:61:GLN:HB2	2.16	0.46
8:T:105:VAL:HG12	8:T:145:LEU:HD22	1.96	0.46
7:S:46:VAL:HG11	7:S:145:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:148:ARG:O	13:Y:151:MET:HG3	2.16	0.46
4:B:119:GLN:O	4:B:122:THR:HB	2.16	0.46
7:E:248:ALA:O	7:E:249:ALA:HB2	2.16	0.46
6:D:160:SER:HB3	6:D:179:TYR:CE1	2.51	0.46
3:O:176:GLN:NE2	3:O:176:GLN:O	2.48	0.46
8:F:143:HIS:CD2	8:F:155:GLU:OE2	2.69	0.46
1:I:135:SER:HA	14:Z:25:TRP:CH2	2.52	0.45
3:O:248:ILE:O	3:O:251:GLN:NE2	2.49	0.45
7:E:46:VAL:HG11	7:E:145:ALA:HB1	1.98	0.45
14:Z:174:SER:HA	14:Z:193:VAL:HG23	1.97	0.45
2:2:157:ILE:HB	2:2:158:PRO:HD3	1.97	0.45
5:Q:235:ILE:HA	5:Q:238:ILE:CG2	2.46	0.45
11:I:19:ARG:HB3	11:I:170:GLY:HA2	1.98	0.45
7:E:75:GLY:HA3	7:E:228:PHE:CD2	2.51	0.45
5:C:156:ASN:OD1	6:D:79:ASN:HB2	2.15	0.45
3:A:68:THR:HG21	9:G:158:GLY:HA3	1.97	0.45
7:E:53:ARG:O	7:E:53:ARG:HG2	2.17	0.45
8:F:72:LEU:C	8:F:72:LEU:HD12	2.36	0.45
6:R:177:LYS:HG3	6:R:178:ASN:HD22	1.82	0.45
2:2:11:GLY:HA3	2:2:192:ILE:O	2.17	0.45
4:B:205:ASN:OD1	4:B:205:ASN:C	2.54	0.45
2:2:174:ARG:HA	2:2:206:VAL:HG21	1.99	0.45
2:N:39:ASP:OD1	2:N:39:ASP:N	2.45	0.45
4:P:49:LYS:HE3	4:P:207:ASP:O	2.17	0.45
4:B:37:ILE:HG23	4:B:44:VAL:CG1	2.46	0.45
1:M:213:ASP:O	11:W:163:ILE:O	2.35	0.45
9:G:102:TYR:O	9:G:103:LYS:HB3	2.16	0.45
3:O:185:HIS:CD2	3:O:209:HIS:CE1	3.04	0.45
14:L:86:LEU:C	14:L:86:LEU:HD13	2.37	0.45
6:D:197:ARG:HG3	6:D:236:ILE:HD12	1.99	0.45
12:X:100:VAL:O	12:X:112:ILE:HA	2.16	0.45
7:S:170:LYS:HA	7:S:180:GLN:OE1	2.17	0.45
14:Z:86:LEU:C	14:Z:86:LEU:HD13	2.37	0.45
12:J:194:ARG:NH1	12:J:196:ASP:OD2	2.50	0.45
4:B:149:GLN:O	4:B:156:TYR:HA	2.17	0.45
9:G:204:GLU:HA	9:G:207:LYS:HG2	1.98	0.45
7:E:129:GLY:HA3	7:E:130:GLU:C	2.36	0.45
8:T:66:CYS:SG	8:T:88:LEU:HD23	2.56	0.45
14:Z:47:GLY:H	16:Z:301:MPD:H11	1.82	0.45
3:A:92:ASN:C	3:A:92:ASN:OD1	2.55	0.45
7:E:43:LYS:N	7:E:43:LYS:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:160:SER:HB3	6:R:179:TYR:CE1	2.52	0.45
9:U:94:GLU:HG3	9:U:114:ARG:HH11	1.82	0.45
4:B:5:TYR:OH	9:G:126:ASN:ND2	2.50	0.45
1:M:152:GLU:HA	1:M:152:GLU:OE2	2.16	0.45
5:C:228:LYS:HE2	5:C:234:GLU:OE1	2.17	0.44
7:E:180:GLN:NE2	8:F:54:ASP:OD1	2.49	0.44
5:C:4:ARG:HG2	8:F:123:TYR:OH	2.16	0.44
2:2:157:ILE:N	2:2:158:PRO:CD	2.80	0.44
3:O:83:VAL:HG22	3:O:141:LEU:HD12	1.99	0.44
5:C:146:TYR:OH	5:C:218:LYS:N	2.49	0.44
4:P:205:ASN:OD1	4:P:205:ASN:C	2.55	0.44
1:1:67:HIS:O	1:1:68:PHE:C	2.56	0.44
7:S:83:ALA:HB3	19:S:403:HOH:O	2.17	0.44
4:P:246:ARG:O	4:P:249:ALA:HB3	2.18	0.44
19:E:410:HOH:O	1:M:70:HIS:CD2	2.69	0.44
7:E:125:GLU:O	7:E:126:GLY:C	2.53	0.44
1:M:9:GLU:HG3	1:M:165:TYR:CE2	2.53	0.44
1:M:-1:ASN:O	1:M:0:GLY:O	2.36	0.44
8:F:197:ILE:O	8:F:201:LEU:HD21	2.18	0.44
5:Q:244:ILE:O	5:Q:245:THR:HG23	2.17	0.44
9:G:108:ILE:N	9:G:109:PRO:CD	2.80	0.44
4:B:49:LYS:HE3	4:B:207:ASP:O	2.18	0.44
4:B:2:THR:O	4:B:2:THR:HG22	2.17	0.44
6:R:233:VAL:O	6:R:236:ILE:HG22	2.17	0.44
5:C:181:LYS:O	5:C:184:MET:HG3	2.17	0.44
7:S:182:GLU:O	7:S:186:GLU:HG2	2.18	0.44
3:O:245:LEU:O	3:O:248:ILE:HG13	2.18	0.44
12:X:36:HIS:HB3	12:X:41:PHE:CD2	2.52	0.44
4:P:61:LEU:HA	4:P:61:LEU:HD23	1.80	0.44
5:C:196:THR:O	5:C:200:THR:HB	2.18	0.44
14:L:174:SER:HA	14:L:193:VAL:HG23	2.00	0.44
5:Q:147:GLN:HG2	6:R:59:ILE:HG21	1.99	0.44
5:Q:150:THR:O	5:Q:157:TYR:HA	2.17	0.44
8:F:187:ASP:OD1	8:F:187:ASP:N	2.50	0.44
8:F:112:LEU:HA	8:F:112:LEU:HD23	1.82	0.44
16:X:201:MPD:O4	16:X:201:MPD:HM1	2.18	0.43
7:S:147:HIS:CE1	7:S:152:GLY:HA2	2.53	0.43
12:X:22:SER:O	12:X:23:GLN:HB2	2.18	0.43
4:B:227:ILE:HG22	4:B:229:THR:HG23	2.00	0.43
5:C:59:GLN:OE1	5:C:209:ASP:HA	2.18	0.43
9:U:10:SER:HB3	9:U:13:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:111:ASN:O	13:Y:112:LYS:HD2	2.18	0.43
6:R:148:TYR:CE1	6:R:158:SER:HB3	2.54	0.43
16:Z:301:MPD:H52	16:Z:301:MPD:H12	2.00	0.43
6:D:159:TRP:CZ2	7:E:59:LEU:HD13	2.53	0.43
8:F:89:ARG:NH1	1:M:68:PHE:HB3	2.34	0.43
14:L:90:TYR:O	14:L:91:LYS:C	2.56	0.43
11:I:104:ASP:HB2	11:I:105:PRO:HD2	1.99	0.43
6:D:13:PRO:HA	7:E:26:TYR:CD1	2.53	0.43
5:Q:152:ASN:HB2	5:Q:153:PRO:HD2	2.01	0.43
8:T:72:LEU:O	8:T:72:LEU:HD12	2.18	0.43
5:C:65:LYS:HE3	5:C:77:VAL:O	2.19	0.43
8:T:175:THR:O	8:T:176:LEU:C	2.57	0.43
3:A:83:VAL:HG22	3:A:141:LEU:HD12	1.99	0.43
11:I:1:THR:OG1	11:I:33:LYS:NZ	2.44	0.43
1:1:42:VAL:CG2	1:1:103:ALA:HB3	2.49	0.43
11:W:213:LEU:HD21	12:X:192:LYS:HD3	1.99	0.43
1:M:42:VAL:CG2	1:M:103:ALA:HB3	2.48	0.43
12:X:6:MET:HB3	12:X:127:PHE:HB3	2.01	0.43
11:I:139:GLU:OE1	11:I:139:GLU:HA	2.18	0.43
6:D:237:GLU:HB3	6:D:238:GLN:OE1	2.18	0.43
5:C:210:ARG:HB3	5:C:210:ARG:HH11	1.82	0.43
8:T:179:PHE:C	8:T:179:PHE:CD1	2.92	0.43
8:F:78:ALA:HB3	8:F:79:PRO:HD3	2.00	0.43
2:2:166:GLU:O	2:2:170:VAL:HG23	2.18	0.43
5:C:244:ILE:O	5:C:245:THR:HG23	2.19	0.43
9:G:61:GLN:HA	9:G:61:GLN:HE21	1.84	0.43
8:F:72:LEU:O	8:F:72:LEU:HD12	2.19	0.43
13:K:111:ASN:O	13:K:112:LYS:HD2	2.18	0.43
1:1:-1:ASN:HA	1:1:21:ILE:O	2.19	0.43
6:R:39:LYS:HG3	6:R:186:ALA:HA	2.01	0.43
4:P:227:ILE:HG22	4:P:229:THR:HG23	2.00	0.43
5:Q:106:ILE:HG23	5:Q:106:ILE:O	2.19	0.43
2:2:1:THR:O	2:2:46:SER:HB3	2.19	0.43
5:Q:181:LYS:O	5:Q:184:MET:HG3	2.19	0.43
3:A:245:LEU:O	3:A:248:ILE:HG13	2.18	0.43
7:E:182:GLU:O	7:E:186:GLU:HG2	2.19	0.43
2:N:61:ASP:O	2:N:65:GLU:HG3	2.19	0.43
7:S:212:LEU:HD23	7:S:212:LEU:C	2.39	0.43
4:P:199:SER:O	19:P:403:HOH:O	2.20	0.43
5:C:50:ARG:HH12	5:C:62:SER:HB3	1.84	0.43
5:C:228:LYS:CE	5:C:234:GLU:OE1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:94:GLN:HG2	2:N:98:LYS:HE3	2.01	0.42
11:I:162:GLY:O	11:I:166:ASP:HB3	2.19	0.42
6:D:169:LYS:O	6:D:173:GLU:HG2	2.19	0.42
9:U:41:CYS:HB2	9:U:186:LEU:O	2.18	0.42
1:1:141:LEU:O	1:1:142:ASP:C	2.56	0.42
6:D:56:ASP:OD1	6:D:58:ARG:HG3	2.19	0.42
10:V:36:ARG:NH1	10:V:60:GLN:HE21	2.16	0.42
9:U:188:ALA:O	9:U:192:VAL:HG23	2.19	0.42
12:J:12:VAL:CG1	12:J:110:PRO:HB3	2.49	0.42
4:B:235:PHE:C	4:B:235:PHE:CD1	2.92	0.42
5:Q:185:LYS:CG	5:Q:186:VAL:N	2.82	0.42
3:O:100:GLU:HG2	3:O:120:ARG:HG2	2.00	0.42
14:L:192:ASP:OD1	14:L:194:GLY:N	2.52	0.42
13:Y:3:ILE:O	13:Y:131:ALA:HA	2.19	0.42
4:B:59:GLU:H	4:B:59:GLU:CD	2.23	0.42
3:O:92:ASN:C	3:O:92:ASN:OD1	2.57	0.42
14:Z:114:TYR:O	14:Z:121:ARG:HA	2.19	0.42
12:J:22:SER:O	12:J:23:GLN:HB2	2.18	0.42
7:E:186:GLU:HB3	7:E:199:LEU:HD21	2.00	0.42
3:O:133:TYR:HB3	4:P:5:TYR:CD1	2.55	0.42
10:H:146:MET:HE3	10:H:150:GLU:HB3	2.02	0.42
9:U:102:TYR:O	9:U:103:LYS:HB3	2.19	0.42
1:1:43:MET:HG3	1:1:102:ILE:HG22	2.02	0.42
2:N:-7:THR:HG21	2:N:51:ASP:OD2	2.19	0.42
7:E:126:GLY:O	7:E:127:ALA:HB2	2.19	0.42
8:F:175:THR:O	8:F:176:LEU:C	2.57	0.42
6:D:73:LEU:HD12	6:D:135:ILE:HG12	2.01	0.42
6:R:53:LYS:HA	6:R:53:LYS:HD3	1.72	0.42
5:C:218:LYS:HB3	5:C:218:LYS:HE3	1.82	0.42
9:G:188:ALA:O	9:G:192:VAL:HG23	2.20	0.42
6:R:73:LEU:HD12	6:R:135:ILE:HG12	2.00	0.42
3:A:96:ARG:O	3:A:100:GLU:HG2	2.20	0.42
6:R:178:ASN:HD22	6:R:178:ASN:N	2.17	0.42
9:G:61:GLN:NE2	9:G:61:GLN:CA	2.82	0.42
5:Q:50:ARG:HH12	5:Q:62:SER:HB3	1.85	0.42
2:N:166:GLU:O	2:N:170:VAL:HG23	2.20	0.42
2:2:154:GLU:HB2	16:2:301:MPD:HM1	2.02	0.42
2:2:146:LEU:HD11	11:I:136:ALA:HB1	2.01	0.42
14:L:114:TYR:O	14:L:121:ARG:HA	2.20	0.42
9:G:81:ILE:HB	9:G:82:PRO:HD3	2.00	0.42
14:L:116:ASP:OD1	14:L:120:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:68:THR:HG21	9:U:158:GLY:HA3	2.01	0.42
8:F:167:GLY:HA3	8:F:199:GLN:O	2.20	0.42
5:Q:143:ARG:HD3	5:Q:144:TYR:CD2	2.55	0.42
8:F:199:GLN:NE2	8:F:199:GLN:N	2.68	0.42
2:N:88:LEU:O	2:N:92:MET:HG2	2.20	0.42
3:O:87:ILE:N	3:O:88:PRO:CD	2.82	0.42
3:A:189:SER:O	3:A:190:LYS:HB2	2.19	0.42
6:D:240:LYS:HD3	6:D:240:LYS:HA	1.87	0.42
2:2:69:ASP:OD2	9:U:67:GLN:HG2	2.20	0.42
3:O:115:ASP:HB3	3:O:155:TYR:CE1	2.55	0.42
2:N:35:ILE:HD13	2:N:56:GLU:HG2	2.02	0.42
13:K:3:ILE:O	13:K:131:ALA:HA	2.20	0.42
13:Y:138:TYR:CE2	13:Y:171:MET:HG3	2.55	0.42
10:V:4:MET:HB3	10:V:126:ILE:HG22	2.01	0.42
12:J:6:MET:HB3	12:J:127:PHE:HB3	2.02	0.41
14:Z:192:ASP:OD1	14:Z:194:GLY:N	2.53	0.41
13:Y:91:ILE:HD13	13:Y:120:TYR:O	2.20	0.41
8:T:112:LEU:HD23	8:T:112:LEU:HA	1.83	0.41
12:J:115:PHE:N	12:J:115:PHE:CD2	2.88	0.41
11:I:62:ASN:HB3	11:I:82:MET:HE1	2.02	0.41
7:S:45:GLY:HA2	7:S:153:TYR:CD1	2.55	0.41
6:R:149:GLN:O	6:R:156:TYR:HA	2.20	0.41
9:G:10:SER:HB3	9:G:13:VAL:CG2	2.50	0.41
5:Q:196:THR:O	5:Q:200:THR:HB	2.20	0.41
7:S:90:GLU:OE1	14:Z:69:ARG:HD2	2.20	0.41
13:K:70:GLU:HA	13:K:70:GLU:OE1	2.21	0.41
8:T:78:ALA:HB3	8:T:79:PRO:HD3	2.01	0.41
11:I:62:ASN:HB2	11:I:82:MET:HE2	2.03	0.41
9:U:81:ILE:HB	9:U:82:PRO:HD3	2.02	0.41
12:X:47:LEU:HG	12:X:49:THR:HG22	2.02	0.41
3:A:54:ILE:HD12	3:A:206:ALA:HB1	2.03	0.41
5:C:106:ILE:HG23	5:C:106:ILE:O	2.20	0.41
7:E:205:LYS:HB3	7:E:205:LYS:HE2	1.83	0.41
3:A:87:ILE:N	3:A:88:PRO:CD	2.83	0.41
6:R:49:ARG:HG3	6:R:166:ARG:HH22	1.85	0.41
1:M:141:LEU:O	1:M:142:ASP:C	2.58	0.41
11:I:5:GLY:O	11:I:124:TYR:HA	2.20	0.41
1:1:132:ALA:HB1	1:1:186:HIS:CE1	2.54	0.41
8:T:3:ARG:HA	8:T:4:ASN:HA	1.74	0.41
6:D:149:GLN:O	6:D:156:TYR:HA	2.20	0.41
8:F:225:TYR:C	8:F:226:ASP:OD1	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:237:LYS:HE2	4:P:237:LYS:HB3	1.93	0.41
12:X:115:PHE:CD2	12:X:115:PHE:N	2.88	0.41
5:C:230:PHE:CE2	5:C:238:ILE:HD11	2.47	0.41
2:2:89:ALA:HA	2:2:122:VAL:HG21	2.03	0.41
11:I:220:ILE:O	11:I:221:CYS:C	2.57	0.41
2:2:-7:THR:HG21	2:2:51:ASP:OD2	2.21	0.41
1:M:43:MET:HG3	1:M:102:ILE:HG22	2.03	0.41
6:D:174:PHE:CD1	6:D:174:PHE:C	2.94	0.41
9:U:204:GLU:HA	9:U:207:LYS:HB3	2.02	0.41
3:O:54:ILE:HD12	3:O:206:ALA:HB1	2.02	0.41
4:P:122:THR:CG2	5:Q:129:ARG:HH22	2.33	0.41
12:X:12:VAL:CG1	12:X:110:PRO:HB3	2.51	0.41
6:D:163:THR:HG21	6:D:171:VAL:HG22	2.03	0.41
3:A:196:GLU:OE2	3:A:201:LYS:HB2	2.19	0.41
1:1:166:LEU:N	1:1:166:LEU:HD12	2.35	0.41
11:W:80:LEU:CD1	11:W:113:ILE:HD11	2.47	0.41
1:M:165:TYR:CD1	1:M:165:TYR:N	2.88	0.41
11:I:113:ILE:HD12	11:I:119:THR:HG22	2.02	0.41
7:E:67:ILE:HD12	7:E:218:GLN:HG2	2.03	0.41
11:W:18:THR:OG1	11:W:171:SER:HB2	2.21	0.41
8:T:187:ASP:N	8:T:187:ASP:OD1	2.53	0.41
6:D:181:ARG:NH1	7:E:57:PRO:O	2.54	0.41
6:R:177:LYS:HG3	6:R:178:ASN:ND2	2.36	0.41
6:R:230:ASN:OD1	6:R:234:THR:HG23	2.20	0.41
6:D:241:GLN:HG3	6:D:242:GLU:N	2.36	0.41
5:Q:65:LYS:HE3	5:Q:77:VAL:O	2.21	0.41
7:E:167:TYR:CZ	7:E:170:LYS:HD3	2.56	0.41
11:W:162:GLY:O	11:W:166:ASP:HB3	2.21	0.41
7:S:222:ILE:HG22	7:S:228:PHE:HD2	1.86	0.41
7:E:168:ASN:HB3	7:E:187:TRP:CE2	2.56	0.41
3:A:115:ASP:HB3	3:A:155:TYR:CE1	2.56	0.41
13:K:48:GLU:O	13:K:52:THR:HG23	2.21	0.41
9:G:106:ILE:HA	9:G:107:PRO:HD3	1.93	0.41
4:P:247:LEU:HD23	4:P:247:LEU:HA	1.86	0.41
9:U:108:ILE:N	9:U:109:PRO:CD	2.84	0.41
8:F:198:SER:HA	8:F:201:LEU:CD2	2.48	0.40
6:R:158:SER:O	7:S:59:LEU:HD12	2.21	0.40
5:Q:52:VAL:CG1	5:Q:53:THR:N	2.84	0.40
2:N:157:ILE:N	2:N:158:PRO:CD	2.84	0.40
14:Z:193:VAL:HG12	14:Z:193:VAL:O	2.21	0.40
13:K:100:ASN:HB3	13:K:132:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:41:CYS:HB2	9:G:186:LEU:O	2.21	0.40
9:G:177:LYS:HA	9:G:177:LYS:HD3	1.87	0.40
14:Z:9:GLN:OE1	14:Z:148:LEU:O	2.40	0.40
4:P:227:ILE:CG2	4:P:229:THR:HG23	2.51	0.40
13:K:22:ARG:HH21	14:L:120:THR:HG1	1.62	0.40
7:E:214:GLU:HG3	7:E:233:ASN:HB3	2.02	0.40
6:R:236:ILE:HG23	6:R:237:GLU:N	2.36	0.40
8:T:88:LEU:HD11	8:T:108:ALA:HB1	2.03	0.40
2:2:8:TYR:CE2	2:2:162:VAL:HB	2.57	0.40
2:2:143:ALA:O	2:2:144:ASN:C	2.59	0.40
6:D:36:VAL:CG1	6:D:195:THR:OG1	2.69	0.40
13:Y:48:GLU:O	13:Y:52:THR:HG23	2.22	0.40
5:C:169:THR:O	5:C:173:GLN:HB2	2.21	0.40
4:P:149:GLN:O	4:P:156:TYR:HA	2.21	0.40
5:Q:210:ARG:HB3	5:Q:210:ARG:HH11	1.85	0.40
13:Y:91:ILE:HA	13:Y:91:ILE:HD12	1.93	0.40
13:K:38:SER:HB2	13:K:39:PRO:CD	2.52	0.40
4:P:35:LEU:C	4:P:35:LEU:HD12	2.41	0.40
4:P:248:GLU:OE1	4:P:248:GLU:N	2.54	0.40
12:J:42:LEU:HD12	12:J:99:VAL:O	2.22	0.40
3:O:112:MET:HA	3:O:113:PRO:HD3	1.91	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	1	221/241 (92%)	205 (93%)	15 (7%)	1 (0%)	34	63
1	M	220/241 (91%)	202 (92%)	17 (8%)	1 (0%)	34	63
2	2	232/266 (87%)	219 (94%)	12 (5%)	1 (0%)	39	69
2	N	231/266 (87%)	217 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	240/252 (95%)	235 (98%)	4 (2%)	1 (0%)	39	69
3	O	239/252 (95%)	235 (98%)	3 (1%)	1 (0%)	39	69
4	B	246/250 (98%)	231 (94%)	14 (6%)	1 (0%)	39	69
4	P	247/250 (99%)	233 (94%)	13 (5%)	1 (0%)	39	69
5	C	242/258 (94%)	228 (94%)	14 (6%)	0	100	100
5	Q	242/258 (94%)	230 (95%)	12 (5%)	0	100	100
6	D	239/254 (94%)	229 (96%)	9 (4%)	1 (0%)	39	69
6	R	239/254 (94%)	226 (95%)	12 (5%)	1 (0%)	39	69
7	E	240/260 (92%)	228 (95%)	9 (4%)	3 (1%)	15	37
7	S	240/260 (92%)	227 (95%)	11 (5%)	2 (1%)	24	51
8	F	230/234 (98%)	211 (92%)	16 (7%)	3 (1%)	15	37
8	T	230/234 (98%)	214 (93%)	15 (6%)	1 (0%)	39	69
9	G	242/288 (84%)	228 (94%)	13 (5%)	1 (0%)	39	69
9	U	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
10	H	195/215 (91%)	187 (96%)	8 (4%)	0	100	100
10	V	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
11	I	220/261 (84%)	211 (96%)	8 (4%)	1 (0%)	34	63
11	W	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
12	J	202/205 (98%)	186 (92%)	14 (7%)	2 (1%)	19	45
12	X	202/205 (98%)	189 (94%)	11 (5%)	2 (1%)	19	45
13	K	194/198 (98%)	188 (97%)	5 (3%)	1 (0%)	34	63
13	Y	194/198 (98%)	186 (96%)	7 (4%)	1 (0%)	34	63
14	L	210/287 (73%)	204 (97%)	6 (3%)	0	100	100
14	Z	211/287 (74%)	202 (96%)	9 (4%)	0	100	100
15	a	1/13 (8%)	1 (100%)	0	0	100	100
15	e	1/13 (8%)	0	1 (100%)	0	100	100
All	All	6306/6964 (91%)	5985 (95%)	295 (5%)	26 (0%)	39	69

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	239	GLU
7	E	35	SER

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Mol	Chain	Res	Type
7	E	249	ALA
4	P	249	ALA
6	R	239	GLU
7	E	126	GLY
8	F	200	SER
11	I	171	SER
12	J	92	GLY
13	K	8	VAL
7	S	35	SER
7	S	246	LYS
12	X	92	GLY
13	Y	8	VAL
12	J	23	GLN
8	T	199	GLN
1	1	132	ALA
3	A	114	CYS
8	F	199	GLN
1	M	132	ALA
3	O	114	CYS
12	X	23	GLN
2	2	221	GLY
8	F	4	ASN
9	G	207	LYS
4	B	232	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	1	186/201 (92%)	180 (97%)	6 (3%)	46	77
1	M	185/201 (92%)	178 (96%)	7 (4%)	40	71
2	2	200/224 (89%)	193 (96%)	7 (4%)	43	74
2	N	199/224 (89%)	191 (96%)	8 (4%)	38	69
3	A	207/210 (99%)	197 (95%)	10 (5%)	31	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	206/210 (98%)	196 (95%)	10 (5%)	31	61
4	B	207/209 (99%)	193 (93%)	14 (7%)	20	43
4	P	208/209 (100%)	196 (94%)	12 (6%)	25	52
5	C	203/216 (94%)	192 (95%)	11 (5%)	27	56
5	Q	203/216 (94%)	196 (97%)	7 (3%)	44	75
6	D	213/226 (94%)	203 (95%)	10 (5%)	32	63
6	R	213/226 (94%)	199 (93%)	14 (7%)	21	45
7	E	198/215 (92%)	185 (93%)	13 (7%)	21	45
7	S	198/215 (92%)	184 (93%)	14 (7%)	18	41
8	F	191/193 (99%)	181 (95%)	10 (5%)	29	58
8	T	191/193 (99%)	180 (94%)	11 (6%)	25	52
9	G	201/239 (84%)	194 (96%)	7 (4%)	43	74
9	U	201/239 (84%)	194 (96%)	7 (4%)	43	74
10	H	163/178 (92%)	154 (94%)	9 (6%)	27	55
10	V	162/178 (91%)	155 (96%)	7 (4%)	35	66
11	I	181/214 (85%)	169 (93%)	12 (7%)	21	45
11	W	181/214 (85%)	171 (94%)	10 (6%)	27	55
12	J	172/173 (99%)	168 (98%)	4 (2%)	58	85
12	X	172/173 (99%)	165 (96%)	7 (4%)	37	69
13	K	174/175 (99%)	166 (95%)	8 (5%)	33	64
13	Y	174/175 (99%)	166 (95%)	8 (5%)	33	64
14	L	169/235 (72%)	165 (98%)	4 (2%)	57	85
14	Z	170/235 (72%)	164 (96%)	6 (4%)	43	74
15	a	2/12 (17%)	2 (100%)	0	100	100
15	e	2/12 (17%)	2 (100%)	0	100	100
All	All	5332/5840 (91%)	5079 (95%)	253 (5%)	32	63

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	62	SER
1	1	99	HIS
1	1	115	SER

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Mol	Chain	Res	Type
1	1	121	SER
1	1	155	THR
1	1	166	LEU
2	2	-5	GLN
2	2	1	THR
2	2	2	SER
2	2	21	SER
2	2	96	ARG
2	2	131	SER
2	2	153	ARG
3	A	17	THR
3	A	42	SER
3	A	92	ASN
3	A	134	MET
3	A	141	LEU
3	A	163	TYR
3	A	175	GLN
3	A	198	SER
3	A	232	LYS
3	A	240	ASN
4	B	2	THR
4	B	6	SER
4	B	30	GLN
4	B	37	ILE
4	B	51	SER
4	B	108	LYS
4	B	109	LEU
4	B	122	THR
4	B	157	PHE
4	B	184	GLU
4	B	200	VAL
4	B	229	THR
4	B	231	LYS
4	B	240	SER
5	C	41	SER
5	C	51	LYS
5	C	63	THR
5	C	123	THR
5	C	143	ARG
5	C	150	THR
5	C	185	LYS
5	C	200	THR

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Mol	Chain	Res	Type
5	C	202	ASP
5	C	207	THR
5	C	242	THR
6	D	36	VAL
6	D	40	ASN
6	D	58	ARG
6	D	98	LEU
6	D	132	SER
6	D	143	ASP
6	D	171	VAL
6	D	187	THR
6	D	224	LEU
6	D	230	ASN
7	E	10	ARG
7	E	14	THR
7	E	55	THR
7	E	56	SER
7	E	132	ARG
7	E	150	ASP
7	E	163	THR
7	E	184	LEU
7	E	199	LEU
7	E	205	LYS
7	E	222	ILE
7	E	225	GLN
7	E	232	ASP
8	F	3	ARG
8	F	9	ASP
8	F	164	ARG
8	F	179	PHE
8	F	187	ASP
8	F	201	LEU
8	F	208	VAL
8	F	226	ASP
8	F	230	VAL
8	F	234	ILE
9	G	50	GLU
9	G	97	SER
9	G	142	LYS
9	G	168	ARG
9	G	177	LYS
9	G	217	TRP

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Mol	Chain	Res	Type
9	G	231	LYS
10	H	1	THR
10	H	36[A]	ARG
10	H	36[B]	ARG
10	H	92	ASN
10	H	105	LYS
10	H	168	SER
10	H	178	LEU
10	H	190	PRO
10	H	191	ASP
11	I	13	VAL
11	I	18	THR
11	I	55	VAL
11	I	77	VAL
11	I	100	VAL
11	I	169	SER
11	I	182	LYS
11	I	195	VAL
11	I	198	GLU
11	I	214	LYS
11	I	216	SER
11	I	221	CYS
12	J	115	PHE
12	J	117	LEU
12	J	130	SER
12	J	174	TRP
13	K	1	ASP
13	K	21	THR
13	K	90	SER
13	K	93	SER
13	K	141	SER
13	K	153	THR
13	K	154	GLU
13	K	190	GLN
14	L	87	VAL
14	L	104	TYR
14	L	128	CYS
14	L	147	ASP
1	M	99	HIS
1	M	115	SER
1	M	121	SER
1	M	158	LYS

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Mol	Chain	Res	Type
1	M	165	TYR
1	M	166	LEU
1	M	212	ARG
2	N	-5	GLN
2	N	2	SER
2	N	29	ASN
2	N	96	ARG
2	N	131	SER
2	N	145	PRO
2	N	153	ARG
2	N	206	VAL
3	O	17	THR
3	O	42	SER
3	O	92	ASN
3	O	134	MET
3	O	141	LEU
3	O	163	TYR
3	O	171	THR
3	O	175	GLN
3	O	188	LYS
3	O	198	SER
4	P	2	THR
4	P	6	SER
4	P	30	GLN
4	P	108	LYS
4	P	109	LEU
4	P	122	THR
4	P	157	PHE
4	P	177	LYS
4	P	184	GLU
4	P	229	THR
4	P	240	SER
4	P	248	GLU
5	Q	41	SER
5	Q	53	THR
5	Q	55	THR
5	Q	129	ARG
5	Q	143	ARG
5	Q	200	THR
5	Q	242	THR
6	R	36	VAL
6	R	51	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	R	58	ARG
6	R	98	LEU
6	R	100	LEU
6	R	132	SER
6	R	143	ASP
6	R	171	VAL
6	R	182	LYS
6	R	187	THR
6	R	224	LEU
6	R	230	ASN
6	R	240	LYS
6	R	241	GLN
7	S	14	THR
7	S	55	THR
7	S	56	SER
7	S	132	ARG
7	S	163	THR
7	S	177	GLU
7	S	184	LEU
7	S	190	SER
7	S	199	LEU
7	S	205	LYS
7	S	222	ILE
7	S	232	ASP
7	S	238	GLU
7	S	245	GLU
8	T	4	ASN
8	T	10	THR
8	T	11	VAL
8	T	16	THR
8	T	41	ASN
8	T	54	ASP
8	T	77	LEU
8	T	179	PHE
8	T	187	ASP
8	T	208	VAL
8	T	234	ILE
9	U	50	GLU
9	U	97	SER
9	U	142	LYS
9	U	168	ARG
9	U	207	LYS

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Mol	Chain	Res	Type
9	U	217	TRP
9	U	231	LYS
10	V	1	THR
10	V	92	ASN
10	V	105	LYS
10	V	149	GLU
10	V	168	SER
10	V	178	LEU
10	V	190	PRO
11	W	13	VAL
11	W	55	VAL
11	W	77	VAL
11	W	100	VAL
11	W	153	LYS
11	W	169	SER
11	W	182	LYS
11	W	195	VAL
11	W	214	LYS
11	W	216	SER
12	X	115	PHE
12	X	117	LEU
12	X	130	SER
12	X	174	TRP
12	X	185	GLU
12	X	194	ARG
12	X	196	ASP
13	Y	1	ASP
13	Y	9	GLN
13	Y	21	THR
13	Y	90	SER
13	Y	93	SER
13	Y	141	SER
13	Y	153	THR
13	Y	154	GLU
14	Z	9	GLN
14	Z	87	VAL
14	Z	104	TYR
14	Z	128	CYS
14	Z	147	ASP
14	Z	211	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	86	HIS
2	2	18	ASN
2	2	186	ASN
3	A	175	GLN
5	C	173	GLN
6	D	40	ASN
6	D	94	GLN
6	D	209	ASN
7	E	147	HIS
7	E	154	GLN
7	E	168	ASN
8	F	199	GLN
9	G	61	GLN
9	G	126	ASN
9	G	194	GLN
10	H	92	ASN
10	H	157	HIS
11	I	57	GLN
11	I	91	GLN
13	K	36	GLN
1	M	70	HIS
1	M	86	HIS
1	M	156	ASN
2	N	18	ASN
2	N	94	GLN
2	N	186	ASN
3	O	185	HIS
3	O	209	HIS
7	S	147	HIS
7	S	154	GLN
7	S	188	HIS
8	T	93	ASN
9	U	42	ASN
9	U	194	GLN
9	U	206	ASN
10	V	60	GLN
11	W	35	HIS
12	X	63	ASN
13	Y	36	GLN
13	Y	195	GLN
14	Z	66	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 103 ligands modelled in this entry, 56 are monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	MPD	1	301	-	6,7,7	0.63	0	6,10,10	0.88	0
17	GOL	1	302	-	5,5,5	0.40	0	5,5,5	0.29	0
17	GOL	1	303	-	5,5,5	0.50	0	5,5,5	0.45	0
16	MPD	2	301	-	6,7,7	0.51	0	6,10,10	0.96	0
17	GOL	2	302	-	5,5,5	0.51	0	5,5,5	0.28	0
17	GOL	2	303	-	5,5,5	0.32	0	5,5,5	0.82	0
17	GOL	A	301	-	5,5,5	0.56	0	5,5,5	0.54	0
17	GOL	A	302	-	5,5,5	0.19	0	5,5,5	0.40	0
17	GOL	A	303	-	5,5,5	0.72	0	5,5,5	1.14	0
17	GOL	A	304	-	5,5,5	0.37	0	5,5,5	0.74	0
17	GOL	D	301	-	5,5,5	0.84	0	5,5,5	1.17	0
17	GOL	E	301	-	5,5,5	0.38	0	5,5,5	1.04	0
17	GOL	F	301	-	5,5,5	0.54	0	5,5,5	0.45	0
17	GOL	F	302	-	5,5,5	0.25	0	5,5,5	0.35	0
17	GOL	F	303	-	5,5,5	0.25	0	5,5,5	0.49	0
17	GOL	F	304	-	5,5,5	0.37	0	5,5,5	0.57	0
17	GOL	G	301	-	5,5,5	0.33	0	5,5,5	0.61	0
17	GOL	G	302	-	5,5,5	0.29	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	GOL	H	201	-	5,5,5	0.18	0	5,5,5	0.50	0
17	GOL	I	301	-	5,5,5	0.77	0	5,5,5	0.74	0
17	GOL	I	302	-	5,5,5	0.42	0	5,5,5	0.61	0
17	GOL	J	202	-	5,5,5	0.55	0	5,5,5	0.43	0
17	GOL	K	201	-	5,5,5	0.41	0	5,5,5	0.84	0
16	MPD	L	301	-	6,7,7	0.59	0	6,10,10	0.65	0
17	GOL	L	302	-	5,5,5	0.32	0	5,5,5	0.44	0
17	GOL	L	303	-	5,5,5	0.35	0	5,5,5	0.36	0
16	MPD	M	301	-	6,7,7	0.49	0	6,10,10	0.44	0
17	GOL	M	302	-	5,5,5	0.50	0	5,5,5	0.94	0
17	GOL	M	303	-	5,5,5	0.50	0	5,5,5	0.39	0
16	MPD	N	301	-	6,7,7	0.55	0	6,10,10	0.36	0
17	GOL	N	302	-	5,5,5	0.51	0	5,5,5	0.60	0
17	GOL	N	303	-	5,5,5	0.21	0	5,5,5	0.59	0
17	GOL	O	301	-	5,5,5	0.66	0	5,5,5	0.68	0
17	GOL	O	302	-	5,5,5	0.28	0	5,5,5	0.54	0
17	GOL	S	301	-	5,5,5	0.51	0	5,5,5	0.39	0
16	MPD	T	301	-	6,7,7	0.70	0	6,10,10	0.93	0
17	GOL	T	302	-	5,5,5	0.60	0	5,5,5	0.84	0
16	MPD	V	201	-	6,7,7	0.77	0	6,10,10	1.76	1 (16%)
17	GOL	V	202	-	5,5,5	0.44	0	5,5,5	0.34	0
17	GOL	V	203	-	5,5,5	1.17	0	5,5,5	1.47	1 (20%)
17	GOL	W	301	-	5,5,5	0.51	0	5,5,5	0.83	0
16	MPD	X	201	-	6,7,7	0.60	0	6,10,10	0.54	0
17	GOL	X	202	-	5,5,5	0.38	0	5,5,5	0.67	0
16	MPD	Z	301	-	6,7,7	0.54	0	6,10,10	0.57	0
17	GOL	Z	302	-	5,5,5	0.66	0	5,5,5	1.05	0
17	GOL	Z	303	-	5,5,5	0.29	0	5,5,5	0.79	0
17	GOL	Z	304	-	5,5,5	0.40	0	5,5,5	0.59	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
16	MPD	1	301	-	-	0/5/5/5	0/0/0/0
17	GOL	1	302	-	-	0/4/4/4	0/0/0/0
17	GOL	1	303	-	-	0/4/4/4	0/0/0/0
16	MPD	2	301	-	-	0/5/5/5	0/0/0/0
17	GOL	2	302	-	-	0/4/4/4	0/0/0/0
17	GOL	2	303	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GOL	A	301	-	-	0/4/4/4	0/0/0/0
17	GOL	A	302	-	-	0/4/4/4	0/0/0/0
17	GOL	A	303	-	-	0/4/4/4	0/0/0/0
17	GOL	A	304	-	-	0/4/4/4	0/0/0/0
17	GOL	D	301	-	-	0/4/4/4	0/0/0/0
17	GOL	E	301	-	-	0/4/4/4	0/0/0/0
17	GOL	F	301	-	-	0/4/4/4	0/0/0/0
17	GOL	F	302	-	-	0/4/4/4	0/0/0/0
17	GOL	F	303	-	-	0/4/4/4	0/0/0/0
17	GOL	F	304	-	-	0/4/4/4	0/0/0/0
17	GOL	G	301	-	-	0/4/4/4	0/0/0/0
17	GOL	G	302	-	-	0/4/4/4	0/0/0/0
17	GOL	H	201	-	-	0/4/4/4	0/0/0/0
17	GOL	I	301	-	-	0/4/4/4	0/0/0/0
17	GOL	I	302	-	-	0/4/4/4	0/0/0/0
17	GOL	J	202	-	-	0/4/4/4	0/0/0/0
17	GOL	K	201	-	-	0/4/4/4	0/0/0/0
16	MPD	L	301	-	-	0/5/5/5	0/0/0/0
17	GOL	L	302	-	-	0/4/4/4	0/0/0/0
17	GOL	L	303	-	-	0/4/4/4	0/0/0/0
16	MPD	M	301	-	-	0/5/5/5	0/0/0/0
17	GOL	M	302	-	-	0/4/4/4	0/0/0/0
17	GOL	M	303	-	-	0/4/4/4	0/0/0/0
16	MPD	N	301	-	-	0/5/5/5	0/0/0/0
17	GOL	N	302	-	-	0/4/4/4	0/0/0/0
17	GOL	N	303	-	-	0/4/4/4	0/0/0/0
17	GOL	O	301	-	-	0/4/4/4	0/0/0/0
17	GOL	O	302	-	-	0/4/4/4	0/0/0/0
17	GOL	S	301	-	-	0/4/4/4	0/0/0/0
16	MPD	T	301	-	-	0/5/5/5	0/0/0/0
17	GOL	T	302	-	-	0/4/4/4	0/0/0/0
16	MPD	V	201	-	-	0/5/5/5	0/0/0/0
17	GOL	V	202	-	-	0/4/4/4	0/0/0/0
17	GOL	V	203	-	-	0/4/4/4	0/0/0/0
17	GOL	W	301	-	-	0/4/4/4	0/0/0/0
16	MPD	X	201	-	-	0/5/5/5	0/0/0/0
17	GOL	X	202	-	-	0/4/4/4	0/0/0/0
16	MPD	Z	301	-	-	0/5/5/5	0/0/0/0
17	GOL	Z	302	-	-	0/4/4/4	0/0/0/0
17	GOL	Z	303	-	-	0/4/4/4	0/0/0/0
17	GOL	Z	304	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	201	MPD	O2-C2-C1	-3.52	95.05	108.01
17	V	203	GOL	O1-C1-C2	2.06	120.42	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	301	MPD	1	0
17	D	301	GOL	2	0
16	N	301	MPD	1	0
16	V	201	MPD	13	0
16	X	201	MPD	3	0
16	Z	301	MPD	2	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 ⓘ

### 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	1	222/241 (92%)	-0.53	1 (0%) 91 93	22, 40, 65, 98	0
1	M	222/241 (92%)	-0.57	2 (0%) 85 86	22, 39, 64, 98	0
2	2	233/266 (87%)	-0.74	1 (0%) 93 94	19, 33, 52, 86	0
2	N	233/266 (87%)	-0.68	1 (0%) 93 94	19, 34, 55, 90	0
3	A	242/252 (96%)	-0.62	2 (0%) 87 88	19, 36, 65, 126	0
3	O	241/252 (95%)	-0.58	0 100 100	22, 39, 70, 91	0
4	B	248/250 (99%)	-0.56	1 (0%) 93 94	20, 37, 67, 104	0
4	P	249/250 (99%)	-0.40	3 (1%) 81 81	23, 44, 77, 110	0
5	C	244/258 (94%)	-0.35	5 (2%) 68 69	23, 44, 86, 129	0
5	Q	244/258 (94%)	-0.35	3 (1%) 81 81	26, 46, 88, 141	0
6	D	241/254 (94%)	-0.28	8 (3%) 50 50	24, 47, 103, 133	0
6	R	241/254 (94%)	-0.13	11 (4%) 36 35	30, 53, 108, 125	0
7	E	242/260 (93%)	-0.35	5 (2%) 67 68	26, 47, 86, 160	0
7	S	242/260 (93%)	-0.43	2 (0%) 87 88	27, 51, 81, 119	0
8	F	232/234 (99%)	-0.35	4 (1%) 73 74	29, 49, 76, 101	0
8	T	232/234 (99%)	-0.25	4 (1%) 73 74	29, 52, 79, 105	0
9	G	244/288 (84%)	-0.50	2 (0%) 87 88	23, 41, 78, 117	0
9	U	244/288 (84%)	-0.45	4 (1%) 74 75	22, 44, 83, 104	0
10	H	196/215 (91%)	-0.76	0 100 100	17, 27, 51, 84	0
10	V	196/215 (91%)	-0.71	0 100 100	18, 29, 56, 77	0
11	I	221/261 (84%)	-0.56	1 (0%) 91 93	20, 34, 59, 94	0
11	W	220/261 (84%)	-0.66	0 100 100	23, 37, 60, 77	0
12	J	204/205 (99%)	-0.57	1 (0%) 91 93	23, 35, 72, 91	0
12	X	204/205 (99%)	-0.56	0 100 100	22, 36, 71, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	K	196/198 (98%)	-0.66	1 (0%) 91 93	20, 36, 57, 93	0
13	Y	196/198 (98%)	-0.61	2 (1%) 84 85	25, 39, 59, 99	0
14	L	212/287 (73%)	-0.62	0 100 100	21, 37, 56, 66	0
14	Z	212/287 (73%)	-0.63	0 100 100	22, 38, 58, 76	0
15	a	3/13 (23%)	0.54	0 100 100	63, 63, 78, 96	0
15	e	3/13 (23%)	-0.04	0 100 100	54, 54, 60, 83	1 (33%)
All	All	6359/6964 (91%)	-0.51	64 (1%) 84 85	17, 40, 76, 160	1 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Q	220	ALA	5.8
3	A	252	ASP	5.5
11	I	221	CYS	5.4
4	P	250	LEU	4.7
5	Q	221	ASN	4.7
8	T	234	ILE	4.6
8	F	234	ILE	3.7
4	B	249	ALA	3.7
7	E	128	SER	3.6
6	D	241	GLN	3.6
5	C	221	ASN	3.6
6	R	207	ALA	3.6
7	E	129	GLY	3.5
6	D	52	LEU	3.5
6	R	243	GLN	3.5
5	C	220	ALA	3.4
6	D	51	THR	3.4
1	M	165	TYR	3.4
7	E	130	GLU	3.2
6	R	238	GLN	3.2
13	K	195	GLN	3.2
6	D	240	LYS	3.1
4	P	249	ALA	3.1
8	F	203	ASP	3.0
9	U	181	HIS	2.9
8	F	3	ARG	2.8
8	T	203	ASP	2.8
7	S	130	GLU	2.7
6	R	51	THR	2.7

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Mol	Chain	Res	Type	RSRZ
6	D	49	ARG	2.7
6	R	208	LYS	2.7
6	R	206	GLY	2.6
2	N	225	ILE	2.5
6	R	205	THR	2.5
13	Y	192	ASP	2.5
9	G	205	ASP	2.4
1	1	165	TYR	2.4
6	R	50	SER	2.4
13	Y	195	GLN	2.4
9	U	4	GLY	2.4
7	S	127	ALA	2.3
5	C	241	LYS	2.3
5	C	219	GLY	2.3
9	U	180	ASP	2.3
9	G	208	GLU	2.3
6	D	207	ALA	2.3
9	U	5	THR	2.2
1	M	-8	GLN	2.2
8	T	4	ASN	2.2
2	2	225	ILE	2.2
8	T	174	ARG	2.2
6	D	242	GLU	2.2
5	C	226	TYR	2.2
3	A	251	GLN	2.2
12	J	119	GLY	2.2
7	E	127	ALA	2.1
8	F	204	GLU	2.1
6	R	237	GLU	2.1
6	R	202	VAL	2.1
6	R	189	GLU	2.1
7	E	9	ASP	2.1
4	P	52	SER	2.1
5	Q	51	LYS	2.0
6	D	227	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
17	GOL	X	202	6/6	0.90	0.32	14.67	47,48,50,51	0
17	GOL	1	303	6/6	0.93	0.27	9.21	58,61,61,62	0
17	GOL	A	304	6/6	0.94	0.22	8.64	48,50,51,51	0
17	GOL	D	301	6/6	0.77	0.37	7.92	64,69,72,75	0
17	GOL	L	303	6/6	0.89	0.26	6.63	49,55,59,60	0
16	MPD	V	201	8/8	0.86	0.29	6.30	38,42,55,56	0
17	GOL	O	302	6/6	0.95	0.20	5.71	63,67,69,70	0
16	MPD	Z	301	8/8	0.86	0.28	5.67	56,65,76,84	0
17	GOL	H	201	6/6	0.93	0.21	5.45	62,68,72,75	0
16	MPD	L	301	8/8	0.89	0.26	4.85	55,70,75,76	0
16	MPD	M	301	8/8	0.85	0.33	4.73	66,83,98,111	0
17	GOL	2	303	6/6	0.90	0.24	4.66	51,54,56,62	0
17	GOL	V	203	6/6	0.83	0.23	4.62	43,55,58,59	0
17	GOL	O	301	6/6	0.91	0.15	4.58	53,54,60,60	0
17	GOL	L	302	6/6	0.92	0.21	4.39	70,73,75,82	0
17	GOL	M	303	6/6	0.92	0.25	4.21	62,72,77,77	0
16	MPD	1	301	8/8	0.89	0.29	4.18	58,64,66,70	0
17	GOL	K	201	6/6	0.93	0.35	3.74	57,62,63,63	0
17	GOL	I	302	6/6	0.89	0.19	3.65	53,58,59,60	0
17	GOL	F	304	6/6	0.93	0.23	3.47	50,56,60,61	0
18	MG	V	206	1/1	0.94	0.17	3.36	28,28,28,28	0
17	GOL	E	301	6/6	0.91	0.31	3.35	50,53,54,56	0
17	GOL	W	301	6/6	0.90	0.21	3.23	51,57,58,64	0
17	GOL	S	301	6/6	0.80	0.25	3.12	63,65,69,69	0
17	GOL	T	302	6/6	0.77	0.29	2.93	53,67,67,68	0
17	GOL	I	301	6/6	0.88	0.20	2.75	64,68,72,72	0
17	GOL	N	303	6/6	0.94	0.18	2.71	44,51,52,52	0
17	GOL	Z	304	6/6	0.91	0.23	2.68	49,54,57,60	0
17	GOL	M	302	6/6	0.92	0.22	2.51	33,37,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	GOL	Z	303	6/6	0.96	0.21	2.31	36,40,41,42	0
17	GOL	A	302	6/6	0.86	0.30	2.18	67,70,71,73	0
17	GOL	1	302	6/6	0.94	0.19	1.80	54,58,62,64	0
16	MPD	X	201	8/8	0.89	0.25	1.76	67,81,88,90	0
18	MG	V	205	1/1	0.97	0.15	1.25	33,33,33,33	0
16	MPD	2	301	8/8	0.92	0.19	1.23	61,65,74,74	0
17	GOL	F	303	6/6	0.86	0.25	1.11	56,64,73,74	0
18	MG	2	307	1/1	0.89	0.14	0.75	53,53,53,53	0
16	MPD	N	301	8/8	0.87	0.17	0.72	60,65,69,69	0
17	GOL	2	302	6/6	0.93	0.15	0.72	39,43,49,51	0
17	GOL	J	202	6/6	0.92	0.18	0.40	56,61,71,75	0
17	GOL	Z	302	6/6	0.93	0.14	0.35	47,56,58,59	0
18	MG	X	203	1/1	0.97	0.13	-0.48	26,26,26,26	0
17	GOL	N	302	6/6	0.96	0.10	-0.97	50,57,60,62	0
18	MG	2	308	1/1	0.97	0.07	-2.07	32,32,32,32	0
18	MG	M	305	1/1	0.92	0.34	-	55,55,55,55	0
18	MG	N	307	1/1	0.94	0.09	-	27,27,27,27	0
18	MG	J	205	1/1	0.99	0.04	-	23,23,23,23	0
18	MG	Q	301	1/1	0.97	0.13	-	25,25,25,25	0
18	MG	J	206	1/1	0.95	0.11	-	42,42,42,42	0
18	MG	B	301	1/1	0.93	0.12	-	42,42,42,42	0
18	MG	N	305	1/1	0.98	0.19	-	28,28,28,28	0
18	MG	C	302	1/1	0.99	0.07	-	28,28,28,28	0
17	GOL	V	202	6/6	0.57	0.59	-	89,93,98,98	0
18	MG	O	303	1/1	0.94	0.16	-	34,34,34,34	0
17	GOL	A	303	6/6	0.90	0.21	-	44,49,55,57	0
18	MG	N	306	1/1	0.93	0.16	-	39,39,39,39	0
18	MG	T	304	1/1	0.95	0.12	-	47,47,47,47	0
18	MG	2	304	1/1	0.94	0.15	-	22,22,22,22	0
18	MG	2	305	1/1	0.93	0.16	-	39,39,39,39	0
18	MG	1	304	1/1	0.93	0.06	-	35,35,35,35	0
17	GOL	F	301	6/6	0.62	0.52	-	64,75,77,79	0
18	MG	K	202	1/1	0.89	0.20	-	35,35,35,35	0
18	MG	V	207	1/1	0.91	0.14	-	39,39,39,39	0
18	MG	L	304	1/1	0.97	0.17	-	30,30,30,30	0
18	MG	X	204	1/1	0.96	0.11	-	35,35,35,35	0
18	MG	H	205	1/1	0.96	0.11	-	29,29,29,29	0
18	MG	S	302	1/1	0.98	0.05	-	31,31,31,31	0
18	MG	2	306	1/1	0.95	0.09	-	43,43,43,43	0
18	MG	Z	305	1/1	0.98	0.05	-	31,31,31,31	0
18	MG	Z	306	1/1	0.98	0.12	-	35,35,35,35	0
18	MG	J	201	1/1	0.94	0.11	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
18	MG	R	302	1/1	0.99	0.06	-	26,26,26,26	0
17	GOL	G	301	6/6	0.91	0.22	-	52,55,57,57	0
18	MG	W	302	1/1	0.90	0.14	-	37,37,37,37	0
18	MG	Y	201	1/1	0.93	0.18	-	40,40,40,40	0
18	MG	Y	202	1/1	0.96	0.21	-	31,31,31,31	0
18	MG	H	203	1/1	0.97	0.25	-	38,38,38,38	0
18	MG	F	305	1/1	0.90	0.27	-	50,50,50,50	0
18	MG	P	301	1/1	0.91	0.34	-	49,49,49,49	0
18	MG	K	203	1/1	0.98	0.11	-	25,25,25,25	0
18	MG	D	302	1/1	0.95	0.10	-	27,27,27,27	0
18	MG	V	204	1/1	0.97	0.06	-	21,21,21,21	0
18	MG	X	205	1/1	0.94	0.13	-	35,35,35,35	0
18	MG	M	304	1/1	0.93	0.19	-	40,40,40,40	0
18	MG	M	307	1/1	0.99	0.06	-	25,25,25,25	0
18	MG	S	303	1/1	0.74	0.40	-	55,55,55,55	0
17	GOL	F	302	6/6	0.89	0.17	-	52,59,66,66	0
18	MG	M	306	1/1	0.94	0.20	-	37,37,37,37	0
18	MG	L	305	1/1	0.98	0.09	-	32,32,32,32	0
18	MG	T	303	1/1	0.82	0.23	-	51,51,51,51	0
18	MG	C	301	1/1	0.99	0.20	-	20,20,20,20	0
18	MG	N	304	1/1	0.98	0.07	-	34,34,34,34	0
18	MG	H	204	1/1	0.99	0.24	-	18,18,18,18	0
18	MG	H	202	1/1	0.97	0.07	-	28,28,28,28	0
18	MG	R	301	1/1	0.94	0.07	-	28,28,28,28	0
18	MG	J	204	1/1	0.97	0.13	-	35,35,35,35	0
18	MG	J	203	1/1	0.97	0.10	-	30,30,30,30	0
16	MPD	T	301	8/8	0.69	0.30	-	52,70,76,77	0
18	MG	R	303	1/1	0.96	0.12	-	39,39,39,39	0
17	GOL	G	302	6/6	0.91	0.29	-	61,63,64,64	0
18	MG	Q	302	1/1	0.99	0.05	-	30,30,30,30	0
18	MG	J	207	1/1	0.95	0.16	-	34,34,34,34	0
17	GOL	A	301	6/6	0.79	0.26	-	51,58,60,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.