



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:54 PM UTC

PDB ID : 4X6Z / pdb_00004x6z
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

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>.

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

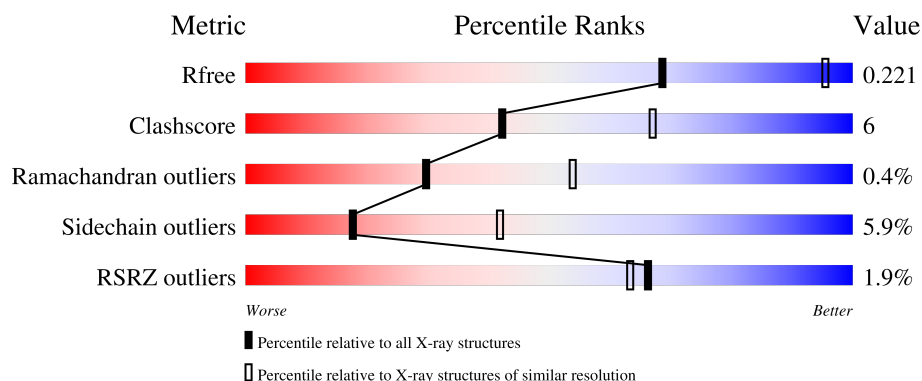
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1	241	2% 78% 13% 8%
1	M	241	2% 75% 17% 8%
2	2	266	68% 18% 12%
2	N	266	2% 72% 15% 12%
3	A	252	0% 83% 12% 5%

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Mol	Chain	Length	Quality of chain
3	O	252	79% 13% • •
4	B	250	83% 13% • •
4	P	250	81% 16% •
5	C	258	71% 21% • 5%
5	Q	258	72% 21% • 5%
6	D	254	71% 20% • 5%
6	R	254	70% 23% • 5%
7	E	260	70% 19% • 7%
7	S	260	73% 18% • 7%
8	F	234	79% 18% • •
8	T	234	82% 16% • •
9	G	288	72% 11% • 15%
9	U	288	71% 13% • 15%
10	H	215	82% 7% • 9%
10	V	215	77% 13% • 9%
11	I	261	69% 14% • 15%
11	W	261	70% 14% • 16%
12	J	205	88% 10% •
12	X	205	85% 12% •
13	K	198	83% 15% • •
13	Y	198	80% 18% • •
14	L	287	63% 11% 26%
14	Z	287	64% 9% • 26%
15	a	13	8% 15% 8% 77%
15	e	13	8% 15% 77%

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	V	201	-	-	X	-
17	GOL	V	203	-	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			

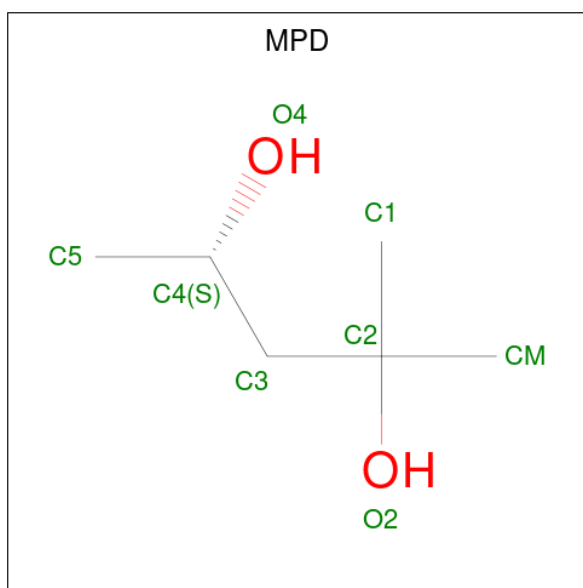
- Molecule 14 is a protein called Proteasome subunit beta type-5.

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 (CCD ID: 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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	1	1	Total	Mg	0	0
			1	1		
18	2	5	Total	Mg	0	0
			5	5		
18	B	1	Total	Mg	0	0
			1	1		
18	C	2	Total	Mg	0	0
			2	2		
18	D	1	Total	Mg	0	0
			1	1		
18	F	1	Total	Mg	0	0
			1	1		
18	H	4	Total	Mg	0	0
			4	4		
18	J	6	Total	Mg	0	0
			6	6		
18	K	2	Total	Mg	0	0
			2	2		
18	L	2	Total	Mg	0	0
			2	2		
18	M	4	Total	Mg	0	0
			4	4		
18	N	4	Total	Mg	0	0
			4	4		
18	O	1	Total	Mg	0	0
			1	1		
18	P	1	Total	Mg	0	0
			1	1		
18	Q	2	Total	Mg	0	0
			2	2		
18	R	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	S	2	Total 2	Mg 2	0	0
18	T	2	Total 2	Mg 2	0	0
18	V	4	Total 4	Mg 4	0	0
18	W	1	Total 1	Mg 1	0	0
18	X	3	Total 3	Mg 3	0	0
18	Y	2	Total 2	Mg 2	0	0
18	Z	2	Total 2	Mg 2	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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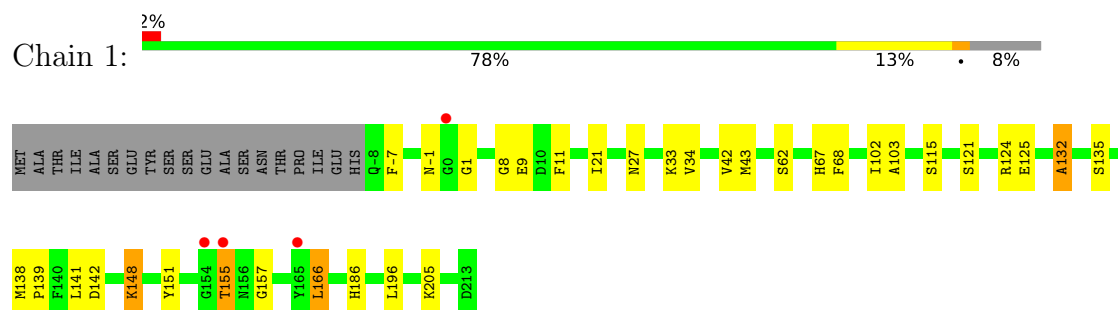
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	K	11	Total 11	O 11	0	0
19	L	14	Total 14	O 14	0	0
19	M	9	Total 9	O 9	0	0
19	N	15	Total 15	O 15	0	0
19	O	14	Total 14	O 14	0	0
19	P	13	Total 13	O 13	0	0
19	Q	13	Total 13	O 13	0	0
19	R	11	Total 11	O 11	0	0
19	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

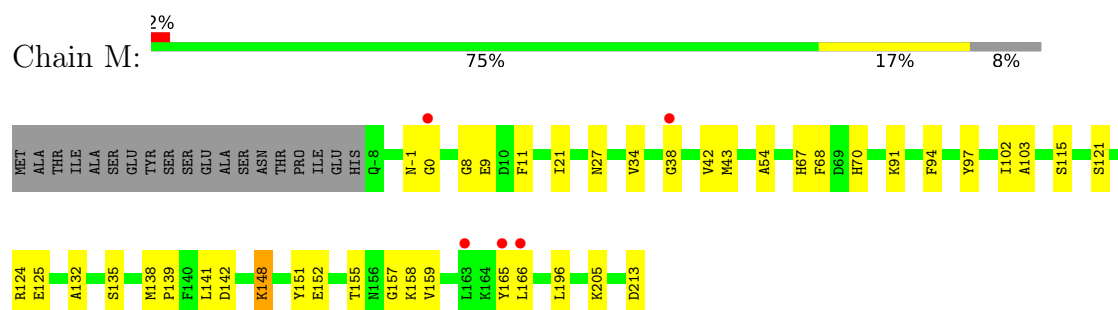
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

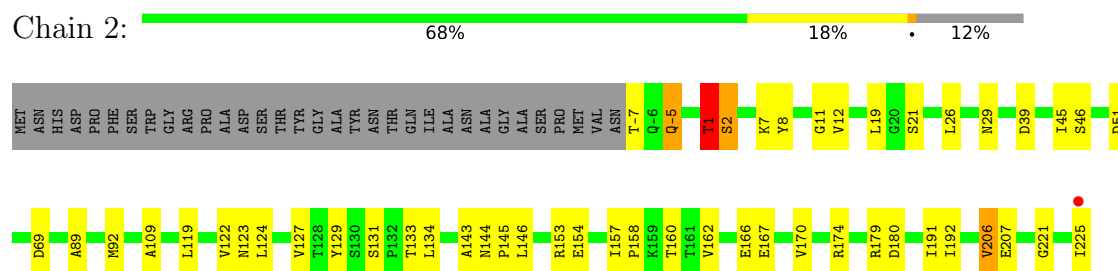
- Molecule 1: Proteasome subunit beta type-6



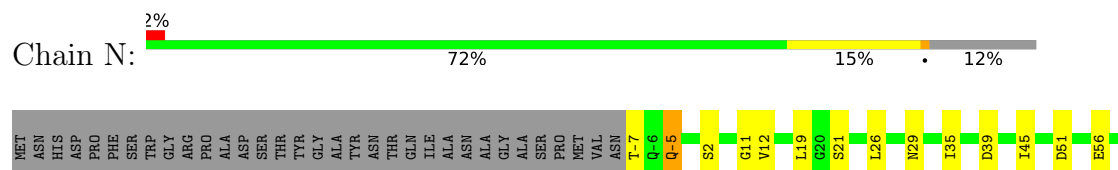
- Molecule 1: Proteasome subunit beta type-6



- Molecule 2: Proteasome subunit beta type-7

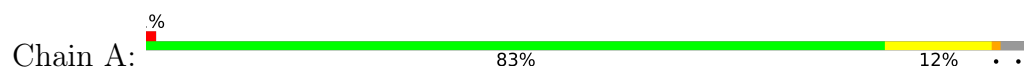


- Molecule 2: Proteasome subunit beta type-7

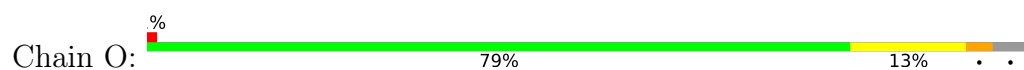




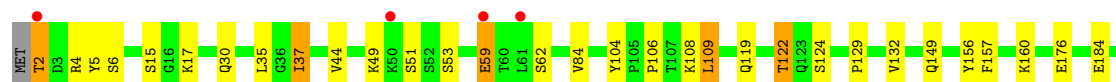
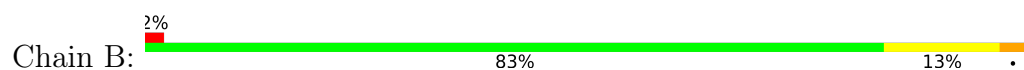
• Molecule 3: Proteasome subunit alpha type-1



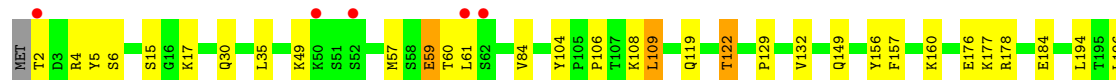
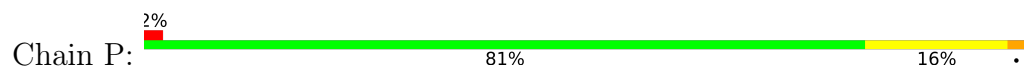
• Molecule 3: Proteasome subunit alpha type-1



• Molecule 4: Proteasome subunit alpha type-2

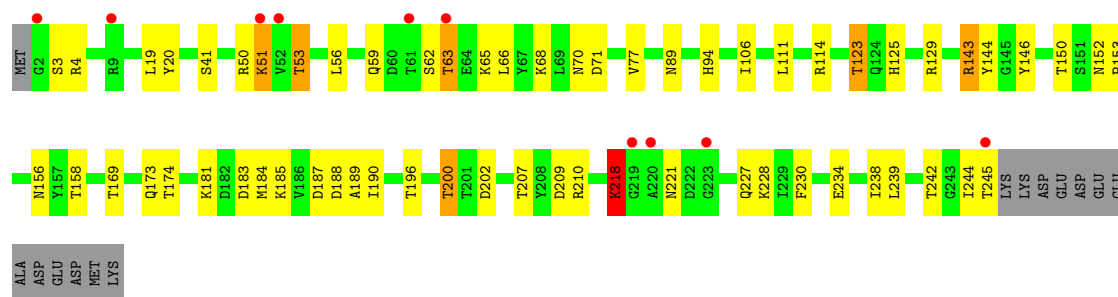


• Molecule 4: Proteasome subunit alpha type-2

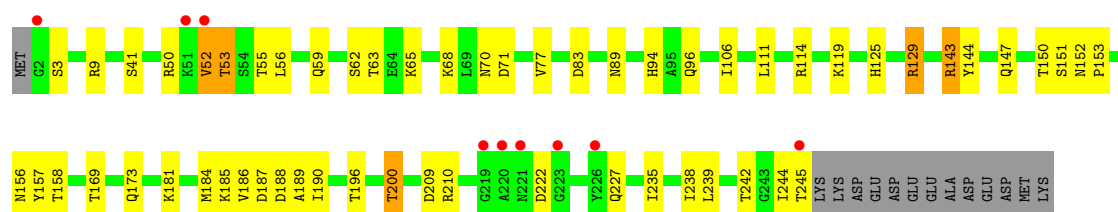
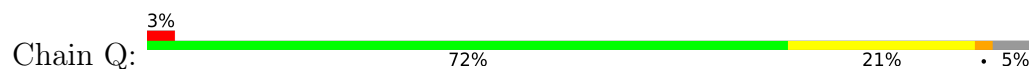


• Molecule 5: Proteasome subunit alpha type-3

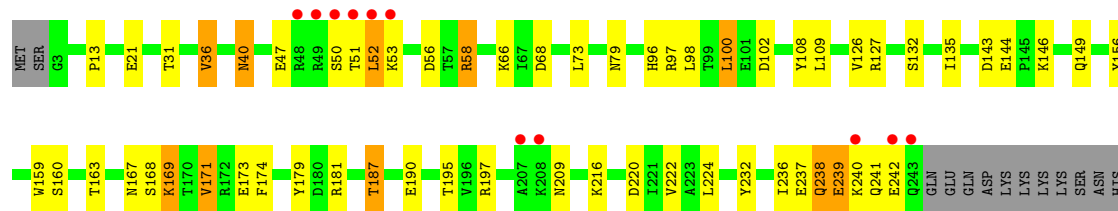




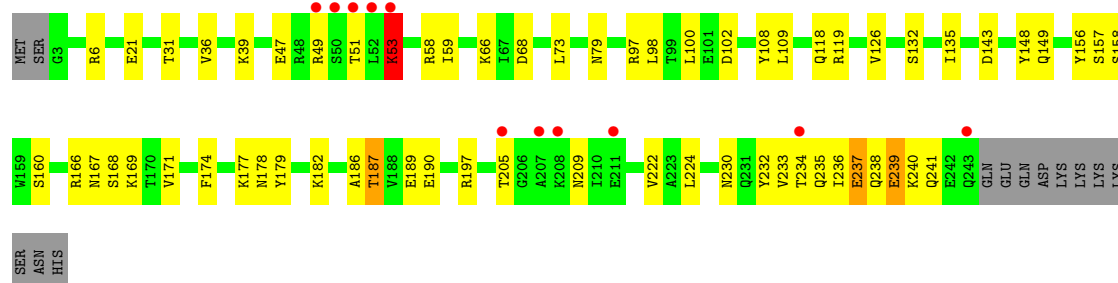
• Molecule 5: Proteasome subunit alpha type-3



• Molecule 6: Proteasome subunit alpha type-4

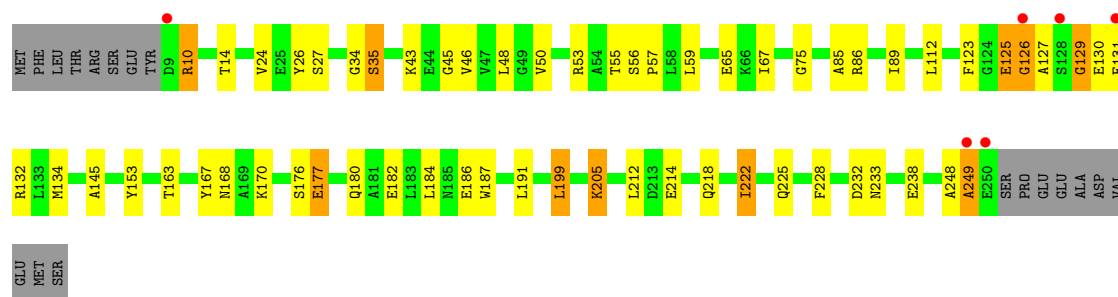


• Molecule 6: Proteasome subunit alpha type-4

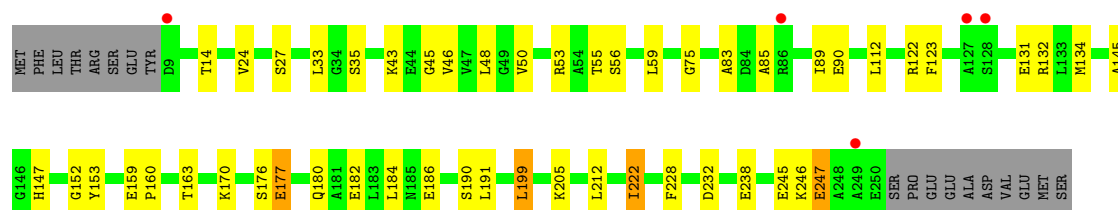


• Molecule 7: Proteasome subunit alpha type-5

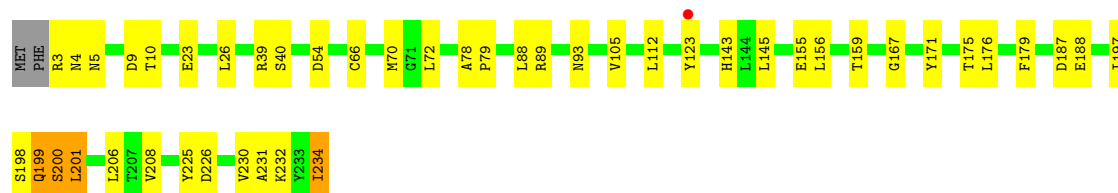
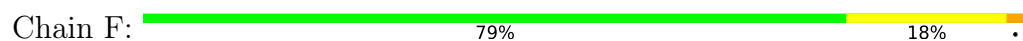




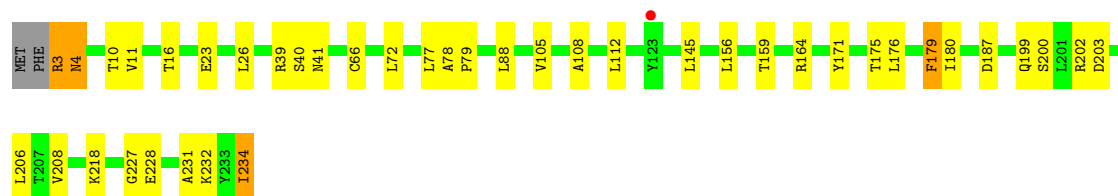
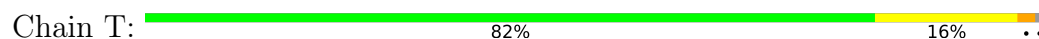
• Molecule 7: Proteasome subunit alpha type-5



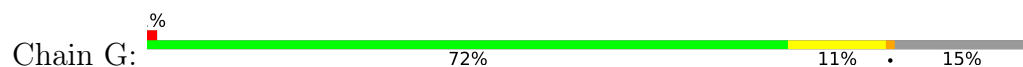
• Molecule 8: Proteasome subunit alpha type-6



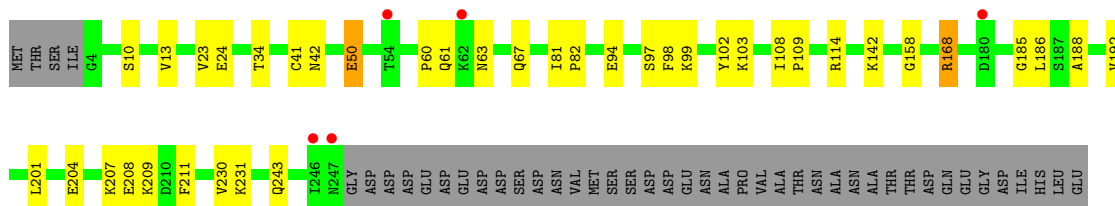
• Molecule 8: Proteasome subunit alpha type-6



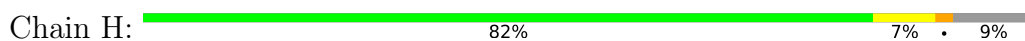
• Molecule 9: Probable proteasome subunit alpha type-7



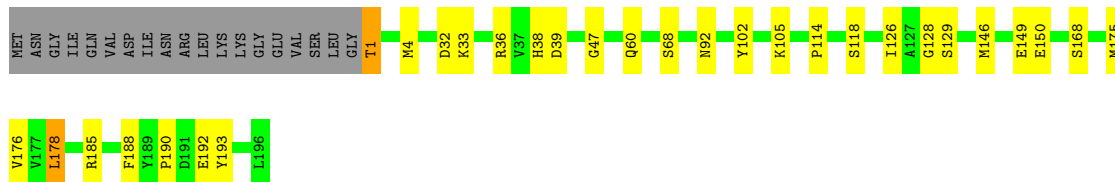
- Molecule 9: Probable proteasome subunit alpha type-7



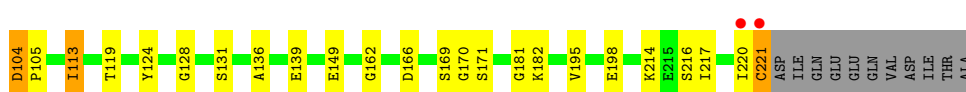
- Molecule 10: Proteasome subunit beta type-1



- Molecule 10: Proteasome subunit beta type-1



- Molecule 11: Proteasome subunit beta type-2

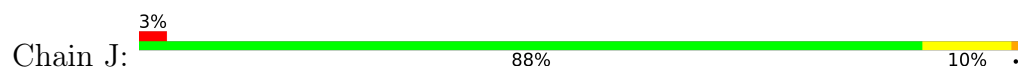


- Molecule 11: Proteasome subunit beta type-2

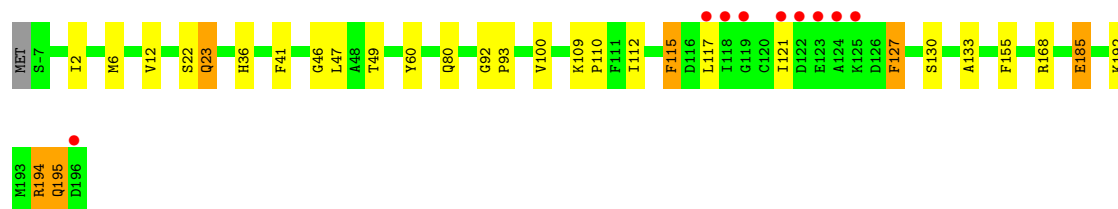
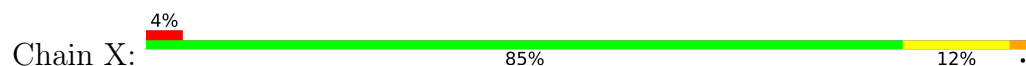




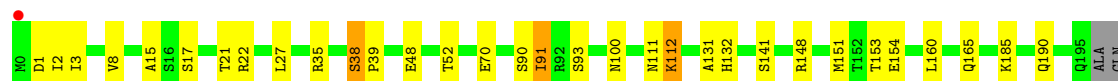
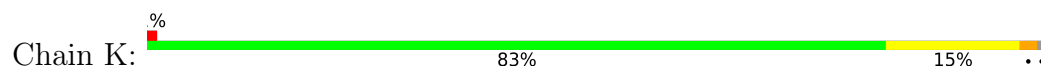
• Molecule 12: Proteasome subunit beta type-3



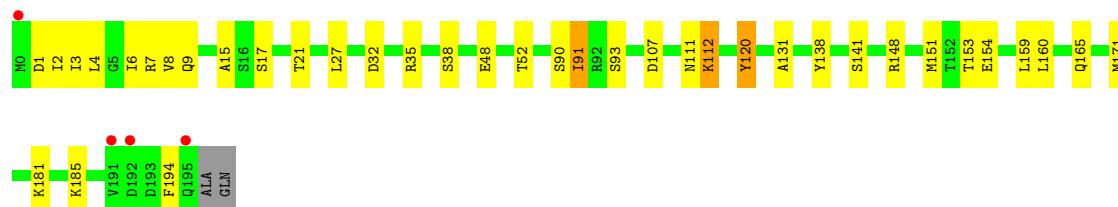
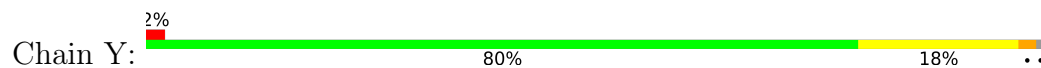
• Molecule 12: Proteasome subunit beta type-3



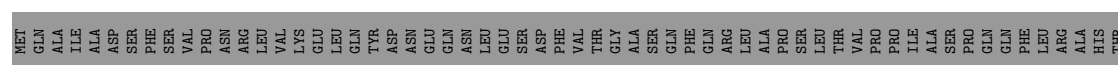
• Molecule 13: Proteasome subunit beta type-4

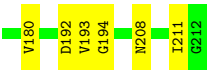


• Molecule 13: Proteasome subunit beta type-4

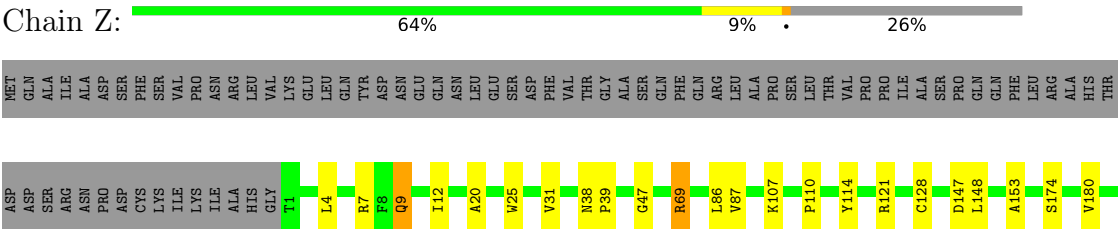


• Molecule 14: Proteasome subunit beta type-5





- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (3.45%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50245	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MPD, MG, GOL

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	0.97	0/1806	1.05	2/2434 (0.1%)
1	M	1.00	2/1795 (0.1%)	1.08	2/2420 (0.1%)
2	2	1.10	1/1864 (0.1%)	1.09	4/2526 (0.2%)
2	N	1.08	0/1855	1.08	1/2514 (0.0%)
3	A	1.07	2/1954 (0.1%)	1.10	3/2645 (0.1%)
3	O	1.05	1/1945 (0.1%)	1.11	5/2634 (0.2%)
4	B	0.99	1/1935 (0.1%)	1.10	4/2621 (0.2%)
4	P	0.93	1/1944 (0.1%)	1.06	1/2632 (0.0%)
5	C	1.02	2/1934 (0.1%)	1.16	3/2618 (0.1%)
5	Q	0.99	3/1934 (0.2%)	1.12	0/2618
6	D	0.90	1/1919 (0.1%)	1.07	3/2598 (0.1%)
6	R	0.89	0/1919	1.06	4/2598 (0.2%)
7	E	0.94	0/1886	1.11	3/2541 (0.1%)
7	S	0.88	0/1886	1.09	4/2541 (0.2%)
8	F	0.91	0/1811	0.98	1/2447 (0.0%)
8	T	0.90	0/1811	1.01	0/2447
9	G	0.94	0/1936	1.04	2/2614 (0.1%)
9	U	0.94	1/1936 (0.1%)	1.07	2/2614 (0.1%)
10	H	1.08	0/1552	1.06	3/2101 (0.1%)
10	V	1.08	1/1541 (0.1%)	1.05	1/2087 (0.0%)
11	I	1.03	0/1720	1.10	3/2333 (0.1%)
11	W	1.00	0/1721	1.10	1/2334 (0.0%)
12	J	1.06	2/1611 (0.1%)	1.09	2/2174 (0.1%)
12	X	1.07	2/1611 (0.1%)	1.09	3/2174 (0.1%)
13	K	1.04	0/1598	1.09	2/2154 (0.1%)
13	Y	0.99	1/1598 (0.1%)	1.07	4/2154 (0.2%)
14	L	1.02	0/1681	1.03	0/2274
14	Z	1.03	0/1690	1.05	1/2286 (0.0%)
15	a	0.76	0/27	1.73	1/32 (3.1%)
15	e	1.11	0/27	1.64	0/32
All	All	1.00	21/50447 (0.0%)	1.08	65/68197 (0.1%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	63	THR	CA-CB	7.46	1.58	1.53
3	A	128	TYR	C-O	6.85	1.32	1.24
12	J	93	PRO	CA-C	-6.82	1.46	1.53
12	X	46	GLY	C-O	-6.50	1.19	1.24
12	X	93	PRO	CA-C	-6.02	1.47	1.53
6	D	52	LEU	CA-C	5.78	1.59	1.52
5	C	89	ASN	N-CA	-5.64	1.39	1.46
9	U	63	ASN	CA-C	-5.63	1.47	1.53
5	C	63	THR	CA-CB	5.53	1.57	1.53
3	A	134	MET	C-O	5.42	1.30	1.24
5	Q	89	ASN	N-CA	-5.37	1.39	1.46
2	2	7	LYS	N-CA	-5.36	1.39	1.45
4	P	129	PRO	CA-C	-5.25	1.46	1.52
1	M	54	ALA	CA-C	-5.21	1.46	1.52
4	B	129	PRO	CA-C	-5.20	1.47	1.52
13	Y	4	LEU	CA-C	-5.19	1.46	1.52
3	O	134	MET	C-O	5.16	1.30	1.24
1	M	97	TYR	CA-C	-5.10	1.48	1.53
12	J	46	GLY	C-O	-5.08	1.20	1.24
5	Q	96	GLN	N-CA	-5.08	1.40	1.46
10	V	68	SER	CA-C	-5.05	1.46	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	237	GLU	N-CA-C	-9.66	98.07	110.53
6	D	102	ASP	CA-C-N	-8.11	112.00	120.03
6	D	102	ASP	C-N-CA	-8.11	112.00	120.03
1	M	38	GLY	N-CA-C	7.87	127.20	115.08
6	R	102	ASP	CA-C-N	-7.46	112.65	120.03
6	R	102	ASP	C-N-CA	-7.46	112.65	120.03
15	a	2	PHE	N-CA-C	-7.38	101.00	110.53
12	X	195	GLN	N-CA-C	7.21	119.62	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	185	GLU	N-CA-C	7.18	119.66	108.96
1	1	155	THR	CB-CA-C	-6.79	98.77	109.70
7	E	129	GLY	N-CA-C	-6.78	100.98	112.77
12	X	185	GLU	N-CA-C	6.74	119.00	108.96
6	D	53	LYS	N-CA-C	6.64	118.91	110.61
3	A	172	GLY	CA-C-N	6.63	125.87	118.97
3	A	172	GLY	C-N-CA	6.63	125.87	118.97
13	Y	38	SER	N-CA-C	-6.51	102.27	108.07
1	M	124	ARG	N-CA-C	-6.14	100.49	110.20
11	I	104	ASP	CA-C-N	-6.14	113.48	119.87
11	I	104	ASP	C-N-CA	-6.14	113.48	119.87
7	E	125	GLU	N-CA-C	-6.10	105.75	113.43
7	S	33	LEU	N-CA-C	-5.96	102.84	110.53
1	1	124	ARG	N-CA-C	-5.93	100.83	110.20
13	K	38	SER	N-CA-C	-5.92	102.80	108.07
4	B	231	LYS	N-CA-C	-5.88	101.30	110.42
3	O	85	GLY	CA-C-N	5.81	125.77	119.78
3	O	85	GLY	C-N-CA	5.81	125.77	119.78
10	H	92	ASN	CB-CA-C	-5.80	102.14	111.18
9	G	11	ASN	CA-C-N	-5.77	112.64	122.56
9	G	11	ASN	C-N-CA	-5.77	112.64	122.56
13	Y	159	LEU	N-CA-C	-5.70	105.15	111.36
5	C	218	LYS	N-CA-C	-5.66	105.87	112.89
10	H	193	TYR	N-CA-C	5.64	118.36	111.82
7	S	247	GLU	CA-C-N	5.63	131.84	121.70
7	S	247	GLU	C-N-CA	5.63	131.84	121.70
2	2	45	ILE	N-CA-C	5.60	116.80	108.46
4	B	53	SER	CA-C-N	-5.60	114.00	120.04
4	B	53	SER	C-N-CA	-5.60	114.00	120.04
8	F	5	ASN	N-CA-C	-5.57	106.45	113.18
3	O	248	ILE	N-CA-CB	5.52	117.01	110.55
3	O	232	LYS	N-CA-C	5.44	116.41	108.14
7	S	50	VAL	N-CA-C	5.37	117.51	108.81
11	W	198	GLU	N-CA-CB	5.37	117.94	109.83
6	R	53	LYS	N-CA-C	5.37	117.32	110.61
3	O	209	HIS	N-CA-C	-5.35	106.45	112.87
14	Z	107	LYS	N-CA-C	5.31	117.82	111.71
12	J	36	HIS	N-CA-C	5.29	117.43	109.23
13	K	91	ILE	N-CA-CB	5.26	118.48	110.58
4	P	178	ARG	N-CA-C	5.26	119.75	113.23
12	X	127	PHE	N-CA-C	5.25	116.83	108.79
13	Y	194	PHE	N-CA-C	5.23	121.93	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	193	TYR	N-CA-C	5.21	117.87	111.82
2	2	29	ASN	N-CA-C	5.20	119.77	113.38
7	E	50	VAL	N-CA-C	5.18	117.21	108.81
9	U	23	VAL	N-CA-C	-5.17	105.50	110.72
4	B	124	SER	N-CA-C	5.14	117.16	110.43
5	C	221	ASN	N-CA-C	5.14	116.57	111.07
11	I	217	ILE	N-CA-C	-5.09	102.53	109.55
2	N	45	ILE	N-CA-C	5.08	116.03	108.46
10	H	122	LEU	N-CA-C	5.07	114.14	108.25
3	A	37	GLN	N-CA-C	5.05	118.91	112.34
5	C	66	LEU	N-CA-C	5.03	116.72	108.52
2	2	179	ARG	N-CA-C	5.03	121.11	114.12
9	U	211	PHE	N-CA-C	5.03	117.02	109.23
13	Y	120	TYR	N-CA-C	5.02	118.51	112.38
2	2	1	THR	CB-CA-C	-5.02	100.44	110.42

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	20	0
1	M	1757	0	1711	25	0
2	2	1833	0	1837	32	0
2	N	1824	0	1832	20	0
3	A	1916	0	1905	13	0
3	O	1907	0	1901	19	0
4	B	1898	0	1906	23	0
4	P	1907	0	1917	28	0
5	C	1904	0	1901	44	0
5	Q	1904	0	1901	39	0
6	D	1890	0	1900	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	1890	0	1900	39	0
7	E	1861	0	1836	39	0
7	S	1861	0	1836	26	0
8	F	1784	0	1788	34	0
8	T	1784	0	1788	26	0
9	G	1896	0	1886	26	0
9	U	1896	0	1886	20	0
10	H	1523	0	1493	11	0
10	V	1512	0	1481	24	0
11	I	1685	0	1693	20	0
11	W	1683	0	1692	21	0
12	J	1581	0	1574	9	0
12	X	1581	0	1574	14	0
13	K	1570	0	1577	11	0
13	Y	1570	0	1577	13	0
14	L	1644	0	1595	17	0
14	Z	1650	0	1603	16	0
15	a	27	0	27	2	0
15	e	27	0	24	1	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	12	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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	623	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 (623) 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
6:D:232:TYR:O	6:D:236:ILE:HG12	1.54	1.06
6:D:238:GLN:OE1	6:D:238:GLN:N	1.97	0.97
10:V:1:THR:H3	16:V:201:MPD:H11	1.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:2:1:THR:HG22	2:2:2:SER:N	2.05	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
5:C:230:PHE:HE2	5:C:238:ILE:CD1	2.04	0.70
8:F:201:LEU:HD23	8:F:201:LEU:N	2.05	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:OE2	4:P:201:GLU:N	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
5:C:111:LEU:HD23	5:C:111:LEU:C	2.23	0.64
2:2:1:THR:HG22	2:2:2:SER:H	1.63	0.64
2:2:1:THR:CG2	2:2:2:SER:H	2.09	0.64
11:I:18:THR:HG22	11:I:31:CYS:O	1.98	0.64
1:M:151:TYR:CD2	1:M:157:GLY:HA2	2.33	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
5:C:230:PHE:CE2	5:C:238:ILE:CD1	2.81	0.63
6:R:197:ARG:CG	6:R:236:ILE:CD1	2.60	0.63
10:V:129:SER:N	16:V:201:MPD:H12	2.10	0.63
5:Q:111:LEU:C	5:Q:111:LEU:HD23	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:232:LYS:HD3	8:T:232:LYS:C	2.24	0.62
10:V:1:THR:CG2	16:V:201:MPD:HM2	2.30	0.61
7:E:129:GLY:CA	7:E:130:GLU:C	2.73	0.61
14:L:25:TRP:CZ3	1:M:135:SER:HA	2.35	0.60
17:D:301:GOL:H2	7:E:86:ARG:HB3	1.84	0.60
6:R:205:THR:HB	6:R:209:ASN:HD22	1.65	0.60
9:U:168:ARG:HD2	19:U:314:HOH:O	2.00	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
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
1:1:151:TYR:CD2	1:1:157:GLY:HA2	2.37	0.58
13:K:2:ILE:HB	13:K:17:SER:HB3	1.85	0.58
7:E:131:GLU:N	7:E:131:GLU:OE1	2.37	0.58
10:V:1:THR:HG23	16:V:201:MPD:H11	1.85	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
1:1:21:ILE:C	1:1:21:ILE:HD12	2.29	0.58
8:F:232:LYS:HD3	8:F:232:LYS:C	2.29	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
15:e:12:PHE:HB3	15:e:13:GLY:HA3	1.87	0.57
4:B:122:THR:CG2	5:C:129:ARG:HH21	2.18	0.57
1:1:138:MET:HE3	12:J:168:ARG:NH2	2.20	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
5:C:123:THR:HG23	6:D:127:ARG:HH21	1.69	0.56
7:E:34:GLY:O	7:E:35:SER:O	2.23	0.56
4:B:35:LEU:C	4:B:35:LEU:HD12	2.30	0.56
9:G:243:GLN:OE1	9:G:243:GLN:HA	2.05	0.56
11:W:10:ASN:HA	19:W:407:HOH:O	2.05	0.56
11:W:163:ILE:HG23	11:W:170:GLY:HA2	1.88	0.56
6:D:96:HIS:CD2	6:D:100:LEU:HD23	2.41	0.56
7:S:112:LEU:C	7:S:112:LEU:HD13	2.31	0.56
10:V:1:THR:HG23	16:V:201:MPD:C1	2.35	0.56
13:Y:2:ILE:HB	13:Y:17:SER:HB3	1.87	0.56
10:H:146:MET:HE2	10:H:150:GLU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:232:LYS:HD3	8:T:232:LYS:O	2.06	0.55
5:C:244:ILE:HG22	5:C:244:ILE:O	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
1:1:34:VAL:HG12	1:1:196:LEU:HD22	1.89	0.55
9:U:94:GLU:HG3	9:U:114:ARG:HD2	1.88	0.55
10:V:1:THR:HB	10:V:33:LYS:HZ3	1.68	0.55
4:B:160:LYS:HG3	5:C:56:LEU:O	2.07	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
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
1:M:21:ILE:C	1:M:21:ILE:HD12	2.31	0.54
19:M:405:HOH:O	16:N:301:MPD:HM3	2.07	0.54
3:O:205:PHE:CD1	3:O:205:PHE:C	2.85	0.54
6:R:157:SER:HB2	7:S:59:LEU:HD11	1.88	0.54
7:E:112:LEU:C	7:E:112:LEU:HD13	2.33	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
17:D:301:GOL:H2	7:E:86:ARG:CB	2.38	0.54
13:K:15:ALA:HB2	13:K:160:LEU:HD21	1.89	0.54
8:T:39:ARG:NH1	8:T:40:SER:O	2.41	0.54
11:W:153:LYS:HE2	11:W:157:ASP:OD1	2.07	0.54
6:D:68:ASP:CG	6:D:97:ARG:HH21	2.14	0.53
7:E:24:VAL:O	7:E:27:SER:HB3	2.09	0.53
10:V:146:MET:HE2	10:V:150:GLU:HB3	1.91	0.53
14:L:148:LEU:HD23	14:L:153:ALA:HA	1.90	0.53
13:Y:15:ALA:HB2	13:Y:160:LEU:HD21	1.91	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
8:F:188:GLU:OE1	8:F:188:GLU:HA	2.08	0.53
8:F:232:LYS:HD3	8:F:232:LYS:O	2.08	0.53
9:G:174:GLU:O	9:G:177:LYS:HB2	2.08	0.53
8:T:164:ARG:HB3	8:T:200:SER:HB2	1.90	0.53
11:I:18:THR:HG21	11:I:30:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:62:ASN:CB	11:I:82:MET:HE1	2.39	0.53
2:N:119:LEU:HG	2:N:134:LEU:HD12	1.90	0.53
8:T:72:LEU:C	8:T:72:LEU:HD12	2.33	0.53
1:M:34:VAL:HG12	1:M:196:LEU:HD22	1.91	0.53
1:M:138:MET:HE3	12:X:168:ARG:NH2	2.24	0.53
3:O:158:ASP:HB2	3:O:159:PRO:CD	2.38	0.53
1:1:1:GLY:HA2	1:1:33:LYS:HZ3	1.74	0.52
6:D:187:THR:HB	6:D:190:GLU:H	1.74	0.52
5:C:210:ARG:HB3	5:C:210:ARG:NH1	2.24	0.52
5:Q:156:ASN:OD1	6:R:79:ASN:HB2	2.09	0.52
6:D:31:THR:HB	6:D:47:GLU:HG3	1.91	0.52
14:L:25:TRP:CH2	1:M:135:SER:HA	2.44	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:D:40:ASN:N	6:D:40:ASN:ND2	2.57	0.52
7:E:34:GLY:C	7:E:35:SER:O	2.53	0.52
6:R:187:THR:HB	6:R:190:GLU:H	1.75	0.52
14:Z:20:ALA:HB2	14:Z:31:VAL:HG21	1.92	0.52
14:Z:148:LEU:HD23	14:Z:153:ALA:HA	1.91	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
9:G:204:GLU:HG2	9:G:207:LYS:HE2	1.90	0.51
10:H:1:THR:HB	10:H:33:LYS:HZ3	1.73	0.51
13:K:148:ARG:O	13:K:151:MET:HG3	2.11	0.51
3:A:205:PHE:CD1	3:A:205:PHE:C	2.89	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
7:E:125:GLU:O	7:E:126:GLY:C	2.53	0.51
5:C:152:ASN:HB2	5:C:153:PRO:CD	2.41	0.51
7:S:122:ARG:HH22	7:S:131:GLU:CG	2.24	0.51
14:Z:38:ASN:HB2	14:Z:39:PRO:HD2	1.92	0.51
15:a:2:PHE:HB3	15:a:3:GLY:HA3	1.92	0.51
7:E:212:LEU:HD23	7:E:212:LEU:C	2.35	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
12:X:80:GLN:OE1	16:X:201:MPD:HM3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:138:MET:N	1:1:139:PRO:CD	2.75	0.50
9:G:34:THR:HB	9:G:50:GLU:HG2	1.93	0.50
10:H:175:MET:HE3	10:H:188:PHE:CE1	2.47	0.50
4:B:205:ASN:OD1	4:B:205:ASN:C	2.54	0.50
3:O:48:LYS:HE2	3:O:195:ASN:OD1	2.12	0.50
7:S:159:GLU:HB3	7:S:160:PRO:CD	2.41	0.50
8:F:72:LEU:C	8:F:72:LEU:HD12	2.36	0.50
12:J:36:HIS:HB3	12:J:41:PHE:CD2	2.47	0.50
14:L:86:LEU:HD13	14:L:86:LEU:C	2.37	0.50
6:R:234:THR:O	6:R:237:GLU:O	2.30	0.50
4:B:62:SER:HA	19:B:411:HOH:O	2.10	0.50
8:F:23:GLU:HA	8:F:26:LEU:HD12	1.94	0.49
14:L:20:ALA:HB2	14:L:31:VAL:HG21	1.92	0.49
14:Z:86:LEU:HD13	14:Z:86:LEU:C	2.37	0.49
8:T:179:PHE:CD1	8:T:180:ILE:N	2.80	0.49
3:A:92:ASN:C	3:A:92:ASN:OD1	2.55	0.49
5:C:68:LYS:HG3	5:C:227:GLN:OE1	2.12	0.49
7:S:53:ARG:HG2	7:S:53:ARG:O	2.12	0.49
7:E:129:GLY:HA3	7:E:130:GLU:C	2.36	0.49
5:Q:210:ARG:NH1	5:Q:210:ARG:HB3	2.27	0.49
10:V:175:MET:HE3	10:V:188:PHE:CE1	2.47	0.49
11:I:1:THR:OG1	11:I:33:LYS:NZ	2.44	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
11:I:3:ILE:HG13	11:I:99:ILE:HD12	1.94	0.49
4:P:15:SER:OG	4:P:17:LYS:HG2	2.12	0.49
4:P:205:ASN:C	4:P:205:ASN:OD1	2.55	0.49
2:2:160:THR:HA	19:2:419:HOH:O	2.13	0.49
6:R:236:ILE:O	6:R:239:GLU:HB3	2.12	0.49
1:1:67:HIS:O	1:1:68:PHE:C	2.56	0.49
4:B:104:TYR:OH	11:I:64:GLU:OE1	2.30	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
6:R:178:ASN:OD1	6:R:197:ARG:NH2	2.46	0.49
1:1:27:ASN:HB3	2:2:129:TYR:CE1	2.48	0.49
10:H:32:ASP:OD2	10:H:185:ARG:NH2	2.46	0.49
7:S:222:ILE:O	7:S:222:ILE:HG13	2.13	0.49
5:C:143:ARG:HD3	5:C:144:TYR:CD2	2.48	0.48
6:D:232:TYR:O	6:D:236:ILE:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:H:114:PRO:HD2	10:H:118:SER:O	2.14	0.48
5:Q:152:ASN:HB2	5:Q:153:PRO:CD	2.43	0.48
7:E:222:ILE:O	7:E:222:ILE:HG13	2.13	0.48
8:F:105:VAL:HG12	8:F:145:LEU:HD22	1.94	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
8:F:156:LEU:HD13	8:F:159:THR:HB	1.95	0.48
14:L:90:TYR:O	14:L:91:LYS:C	2.56	0.48
10:V:176:VAL:HG12	10:V:178:LEU:HD13	1.95	0.48
13:Y:7:ARG:HH11	13:Y:7:ARG:HG2	1.79	0.48
2:2:39:ASP:OD1	2:2:39:ASP:N	2.44	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
11:I:62:ASN:HB2	11:I:82:MET:HE1	1.95	0.48
8:T:175:THR:O	8:T:176:LEU:C	2.57	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:HD13	7:S:112:LEU:O	2.13	0.48
8:T:179:PHE:CD1	8:T:179:PHE:C	2.92	0.48
1:1:142:ASP:O	1:1:148:LYS:HB2	2.14	0.47
6:R:197:ARG:HG3	6:R:236:ILE:HD12	1.92	0.47
7:E:85:ALA:O	7:E:89:ILE:HG12	2.14	0.47
5:Q:59:GLN:OE1	5:Q:209:ASP:HA	2.15	0.47
5:Q:184:MET:HE1	5:Q:189:ALA:HA	1.95	0.47
1:1:8:GLY:HA3	1:1:11:PHE:CE1	2.49	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
7:S:212:LEU:C	7:S:212:LEU:HD23	2.39	0.47
11:W:139:GLU:HA	11:W:139:GLU:OE1	2.14	0.47
11:I:17:ASP:HB2	11:I:170:GLY:HA3	1.96	0.47
7:S:85:ALA:O	7:S:89:ILE:HG12	2.14	0.47
4:B:235:PHE:CD1	4:B:235:PHE:C	2.92	0.47
5:C:152:ASN:HB2	5:C:153:PRO:HD2	1.96	0.47
2:N:122:VAL:HA	2:N:127:VAL:O	2.15	0.47
3:O:92:ASN:OD1	3:O:92:ASN:C	2.57	0.47
4:P:194:LEU:HD21	4:P:250:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:43:LYS:N	7:S:43:LYS:HD2	2.30	0.47
14:Z:12:ILE:HB	14:Z:180:VAL:HB	1.96	0.47
6:D:216:LYS:HE2	6:D:220:ASP:OD2	2.14	0.47
8:T:231:ALA:HA	8:T:234:ILE:HG22	1.96	0.47
4:B:106:PRO:HG2	4:B:109:LEU:HB2	1.95	0.47
7:E:112:LEU:HD13	7:E:112:LEU:O	2.14	0.47
8:F:175:THR:O	8:F:176:LEU:C	2.57	0.47
11:I:17:ASP:OD2	11:I:170:GLY:HA2	2.14	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
5:Q:52:VAL:HG13	5:Q:53:THR:N	2.30	0.47
6:R:238:GLN:O	6:R:238:GLN:HG2	2.15	0.47
6:D:144:GLU:HG3	6:D:146:LYS:HE2	1.97	0.47
5:Q:187:ASP:HA	5:Q:190:ILE:HD12	1.96	0.47
7:S:186:GLU:HB3	7:S:199:LEU:HD21	1.97	0.47
8:T:156:LEU:HD13	8:T:159:THR:HB	1.97	0.47
8:F:66:CYS:SG	8:F:88:LEU:HD23	2.55	0.47
1:M:155:THR:O	1:M:158:LYS:HD2	2.15	0.47
2:N:174:ARG:HA	2:N:206:VAL:HG21	1.97	0.47
5:Q:181:LYS:HG3	5:Q:184:MET:HG3	1.96	0.47
7:S:75:GLY:HA3	7:S:228:PHE:CD2	2.50	0.47
1:M:8:GLY:HA3	1:M:11:PHE:CE1	2.51	0.47
5:Q:169:THR:O	5:Q:173:GLN:HB2	2.14	0.47
6:R:189:GLU:HG2	6:R:232:TYR:OH	2.15	0.47
1:I:1:GLY:HA2	1:I:33:LYS:NZ	2.30	0.46
5:C:187:ASP:HA	5:C:190:ILE:HD12	1.97	0.46
6:D:238:GLN:O	6:D:239:GLU:HG3	2.15	0.46
11:I:128:GLY:O	11:I:131:SER:HB2	2.14	0.46
4:P:106:PRO:HG2	4:P:109:LEU:HB2	1.97	0.46
5:Q:9:ARG:HD3	6:R:6:ARG:NH1	2.31	0.46
5:Q:70:ASN:OD1	5:Q:71:ASP:N	2.47	0.46
10:V:114:PRO:HD2	10:V:118:SER:O	2.15	0.46
11:W:62:ASN:CB	11:W:82:MET:HE1	2.45	0.46
12:X:2:ILE:HG21	12:X:133:ALA:HB3	1.96	0.46
2:2:122:VAL:HA	2:2:127:VAL:O	2.16	0.46
4:B:59:GLU:H	4:B:59:GLU:CD	2.23	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
11:W:3:ILE:HG13	11:W:99:ILE:HD12	1.96	0.46
11:W:104:ASP:HB2	11:W:105:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:219:ASN:HA	19:W:404:HOH:O	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
8:F:225:TYR:C	8:F:226:ASP:OD1	2.59	0.46
12:J:2:ILE:HG21	12:J:133:ALA:HB3	1.98	0.46
1:M:141:LEU:O	1:M:142:ASP:C	2.58	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
7:S:46:VAL:HG11	7:S:145:ALA:HB1	1.98	0.46
8:T:105:VAL:HG12	8:T:145:LEU:HD22	1.96	0.46
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
6:D:174:PHE:C	6:D:174:PHE:CD1	2.94	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
8:F:143:HIS:CD2	8:F:155:GLU:OE2	2.69	0.46
11:I:220:ILE:O	11:I:221:CYS:C	2.57	0.46
3:O:176:GLN:O	3:O:176:GLN:NE2	2.48	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
5:Q:119:LYS:NZ	5:Q:151:SER:OG	2.49	0.45
2:2:157:ILE:HB	2:2:158:PRO:HD3	1.97	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
3:A:68:THR:HG21	9:G:158:GLY:HA3	1.97	0.45
5:C:156:ASN:OD1	6:D:79:ASN:HB2	2.15	0.45
7:E:53:ARG:O	7:E:53:ARG:HG2	2.17	0.45
7:E:75:GLY:HA3	7:E:228:PHE:CD2	2.51	0.45
11:I:19:ARG:HB3	11:I:170:GLY:HA2	1.98	0.45
5:Q:235:ILE:HA	5:Q:238:ILE:CG2	2.46	0.45
2:2:11:GLY:HA3	2:2:192:ILE:O	2.17	0.45
2:2:174:ARG:HA	2:2:206:VAL:HG21	1.99	0.45
8:F:70:MET:HE2	8:F:105:VAL:HG22	1.97	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
6:R:177:LYS:HG3	6:R:178:ASN:HD22	1.82	0.45
4:B:37:ILE:HG23	4:B:44:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:102:TYR:O	9:G:103:LYS:HB3	2.16	0.45
1:M:213:ASP:O	11:W:163:ILE:O	2.35	0.45
3:O:185:HIS:CD2	3:O:209:HIS:CE1	3.04	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
12:J:194:ARG:NH1	12:J:196:ASP:OD2	2.50	0.45
7:S:170:LYS:HA	7:S:180:GLN:OE1	2.17	0.45
4:B:149:GLN:O	4:B:156:TYR:HA	2.17	0.45
4:P:35:LEU:HD12	4:P:35:LEU:C	2.41	0.45
13:Y:32:ASP:OD2	13:Y:181:LYS:NZ	2.48	0.45
7:E:43:LYS:HD2	7:E:43:LYS:N	2.32	0.45
9:G:204:GLU:HA	9:G:207:LYS:HG2	1.98	0.45
14:L:4:LEU:HD12	14:L:4:LEU:C	2.42	0.45
6:R:160:SER:HB3	6:R:179:TYR:CE1	2.52	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
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
9:U:94:GLU:HG3	9:U:114:ARG:HH11	1.82	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
11:W:10:ASN:C	19:W:407:HOH:O	2.60	0.44
2:2:157:ILE:N	2:2:158:PRO:CD	2.80	0.44
5:C:4:ARG:HG2	8:F:123:TYR:OH	2.16	0.44
5:C:146:TYR:OH	5:C:218:LYS:N	2.49	0.44
5:C:184:MET:HE1	5:C:189:ALA:HA	1.98	0.44
3:O:83:VAL:HG22	3:O:141:LEU:HD12	1.99	0.44
19:E:410:HOH:O	1:M:70:HIS:CD2	2.69	0.44
4:P:246:ARG:O	4:P:249:ALA:HB3	2.18	0.44
7:S:83:ALA:HB3	19:S:403:HOH:O	2.17	0.44
1:M:-1:ASN:O	1:M:0:GLY:O	2.36	0.44
1:M:9:GLU:HG3	1:M:165:TYR:CE2	2.53	0.44
4:B:2:THR:O	4:B:2:THR:HG22	2.17	0.44
4:B:49:LYS:HE3	4:B:207:ASP:O	2.18	0.44
8:F:197:ILE:O	8:F:201:LEU:HD21	2.18	0.44
9:G:108:ILE:N	9:G:109:PRO:CD	2.80	0.44
5:Q:244:ILE:O	5:Q:245:THR:HG23	2.17	0.44
5:C:181:LYS:O	5:C:184:MET:HG3	2.17	0.44
6:D:167:ASN:O	6:D:168:SER:C	2.59	0.44
7:E:176:SER:O	7:E:177:GLU:C	2.59	0.44
3:O:245:LEU:O	3:O:248:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:233:VAL:O	6:R:236:ILE:HG22	2.17	0.44
7:S:182:GLU:O	7:S:186:GLU:HG2	2.18	0.44
12:X:36:HIS:HB3	12:X:41:PHE:CD2	2.52	0.44
4:P:59:GLU:H	4:P:59:GLU:CD	2.26	0.44
4:P:61:LEU:HD23	4:P:61:LEU:HA	1.80	0.44
5:C:196:THR:O	5:C:200:THR:HB	2.18	0.44
8:F:112:LEU:HD23	8:F:112:LEU:HA	1.82	0.44
8:F:187:ASP:OD1	8:F:187:ASP:N	2.50	0.44
14:L:174:SER:HA	14:L:193:VAL:HG23	2.00	0.44
1:M:67:HIS:O	1:M:68:PHE:C	2.60	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
6:R:108:TYR:CD1	6:R:108:TYR:C	2.96	0.44
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
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
16:X:201:MPD:HM1	16:X:201:MPD:O4	2.18	0.43
7:E:125:GLU:C	7:E:126:GLY:O	2.56	0.43
9:U:10:SER:HB3	9:U:13:VAL:CG2	2.48	0.43
11:W:62:ASN:HB2	11:W:82:MET:HE1	1.99	0.43
13:Y:111:ASN:O	13:Y:112:LYS:HD2	2.18	0.43
6:D:13:PRO:HA	7:E:26:TYR:CD1	2.53	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
11:I:104:ASP:HB2	11:I:105:PRO:HD2	1.99	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
3:A:83:VAL:HG22	3:A:141:LEU:HD12	1.99	0.43
5:C:65:LYS:HE3	5:C:77:VAL:O	2.19	0.43
5:Q:152:ASN:HB2	5:Q:153:PRO:HD2	2.01	0.43
8:T:72:LEU:HD12	8:T:72:LEU:O	2.18	0.43
1:1:42:VAL:CG2	1:1:103:ALA:HB3	2.49	0.43
1:M:42:VAL:CG2	1:M:103:ALA:HB3	2.48	0.43
4:P:57:MET:HE3	4:P:60:THR:HG21	1.99	0.43
6:R:167:ASN:O	6:R:168:SER:C	2.62	0.43
11:W:213:LEU:HD21	12:X:192:LYS:HD3	1.99	0.43
1:1:141:LEU:O	1:1:142:ASP:C	2.56	0.43
11:I:139:GLU:OE1	11:I:139:GLU:HA	2.18	0.43
12:X:6:MET:HB3	12:X:127:PHE:HB3	2.01	0.43
2:2:166:GLU:O	2:2:170:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:210:ARG:HB3	5:C:210:ARG:HH11	1.82	0.43
6:D:237:GLU:HB3	6:D:238:GLN:OE1	2.18	0.43
8:F:78:ALA:HB3	8:F:79:PRO:HD3	2.00	0.43
13:K:22:ARG:HH21	14:L:120:THR:HG1	1.62	0.43
9:U:98:PHE:CD1	9:U:98:PHE:C	2.97	0.43
15:a:1:ARG:HA	15:a:1:ARG:HD3	1.89	0.43
5:C:244:ILE:O	5:C:245:THR:HG23	2.19	0.43
8:F:72:LEU:HD12	8:F:72:LEU:O	2.19	0.43
9:G:61:GLN:HA	9:G:61:GLN:HE21	1.84	0.43
13:K:111:ASN:O	13:K:112:LYS:HD2	2.18	0.43
1:l:1:ASN:HA	1:l:21:ILE:O	2.19	0.43
8:F:179:PHE:CD2	8:F:179:PHE:C	2.97	0.43
14:L:116:ASP:C	14:L:116:ASP:OD1	2.61	0.43
4:P:227:ILE:HG22	4:P:229:THR:HG23	2.00	0.43
5:Q:106:ILE:O	5:Q:106:ILE:HG23	2.19	0.43
6:R:39:LYS:HG3	6:R:186:ALA:HA	2.01	0.43
2:2:1:THR:O	2:2:46:SER:HB3	2.19	0.43
3:A:245:LEU:O	3:A:248:ILE:HG13	2.18	0.43
5:C:50:ARG:HH12	5:C:62:SER:HB3	1.84	0.43
7:E:182:GLU:O	7:E:186:GLU:HG2	2.19	0.43
9:G:206:ASN:O	9:G:207:LYS:C	2.61	0.43
2:N:61:ASP:O	2:N:65:GLU:HG3	2.19	0.43
4:P:199:SER:O	19:P:403:HOH:O	2.20	0.43
5:Q:181:LYS:O	5:Q:184:MET:HG3	2.19	0.43
5:C:228:LYS:CE	5:C:234:GLU:OE1	2.67	0.42
6:D:169:LYS:O	6:D:173:GLU:HG2	2.19	0.42
11:I:162:GLY:O	11:I:166:ASP:HB3	2.19	0.42
2:N:94:GLN:HG2	2:N:98:LYS:HE3	2.01	0.42
8:T:171:TYR:CD1	8:T:171:TYR:C	2.97	0.42
9:U:41:CYS:HB2	9:U:186:LEU:O	2.18	0.42
6:D:56:ASP:OD1	6:D:58:ARG:HG3	2.19	0.42
6:D:108:TYR:CD1	6:D:108:TYR:C	2.96	0.42
12:J:12:VAL:CG1	12:J:110:PRO:HB3	2.49	0.42
5:Q:185:LYS:CG	5:Q:186:VAL:N	2.82	0.42
9:U:188:ALA:O	9:U:192:VAL:HG23	2.19	0.42
10:V:36:ARG:NH1	10:V:60:GLN:HE21	2.16	0.42
12:J:22:SER:O	12:J:23:GLN:HB2	2.18	0.42
14:L:192:ASP:OD1	14:L:194:GLY:N	2.52	0.42
3:O:100:GLU:HG2	3:O:120:ARG:HG2	2.00	0.42
4:P:235:PHE:CD1	4:P:235:PHE:C	2.96	0.42
8:T:202:ARG:O	8:T:203:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:3:ILE:O	13:Y:131:ALA:HA	2.19	0.42
14:Z:114:TYR:O	14:Z:121:ARG:HA	2.19	0.42
1:1:43:MET:HG3	1:1:102:ILE:HG22	2.02	0.42
6:D:50:SER:C	6:D:52:LEU:N	2.77	0.42
7:E:186:GLU:HB3	7:E:199:LEU:HD21	2.00	0.42
8:F:231:ALA:O	8:F:232:LYS:C	2.62	0.42
2:N:-7:THR:HG21	2:N:51:ASP:OD2	2.19	0.42
3:O:133:TYR:HB3	4:P:5:TYR:CD1	2.55	0.42
7:S:123:PHE:HB3	7:S:134:MET:HE3	2.01	0.42
9:U:102:TYR:O	9:U:103:LYS:HB3	2.19	0.42
5:C:183:ASP:O	5:C:184:MET:C	2.62	0.42
6:D:73:LEU:HD12	6:D:135:ILE:HG12	2.01	0.42
7:E:126:GLY:O	7:E:127:ALA:HB2	2.19	0.42
5:Q:184:MET:HE3	5:Q:188:ASP:HB3	2.02	0.42
6:R:53:LYS:HD3	6:R:53:LYS:HA	1.72	0.42
3:A:96:ARG:O	3:A:100:GLU:HG2	2.20	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
2:2:146:LEU:HD11	11:I:136:ALA:HB1	2.01	0.42
2:2:154:GLU:HB2	16:2:301:MPD:HM1	2.02	0.42
8:F:167:GLY:HA3	8:F:199:GLN:O	2.20	0.42
9:G:61:GLN:NE2	9:G:61:GLN:CA	2.82	0.42
9:G:81:ILE:HB	9:G:82:PRO:HD3	2.00	0.42
14:L:114:TYR:O	14:L:121:ARG:HA	2.20	0.42
14:L:116:ASP:OD1	14:L:120:THR:HB	2.19	0.42
2:N:166:GLU:O	2:N:170:VAL:HG23	2.20	0.42
3:O:68:THR:HG21	9:U:158:GLY:HA3	2.01	0.42
5:Q:50:ARG:HH12	5:Q:62:SER:HB3	1.85	0.42
6:R:178:ASN:HD22	6:R:178:ASN:N	2.17	0.42
2:2:92:MET:HE3	2:2:124:LEU:HA	2.02	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
5:Q:143:ARG:HD3	5:Q:144:TYR:CD2	2.55	0.42
6:R:118:GLN:C	6:R:118:GLN:OE1	2.63	0.42
12:X:194:ARG:C	12:X:195:GLN:HG2	2.45	0.42
2:2:69:ASP:OD2	9:U:67:GLN:HG2	2.20	0.42
2:2:143:ALA:O	2:2:144:ASN:C	2.59	0.42
3:A:189:SER:O	3:A:190:LYS:HB2	2.19	0.42
6:D:240:LYS:HA	6:D:240:LYS:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:115:ASP:HB3	3:O:155:TYR:CE1	2.55	0.42
6:R:174:PHE:CD1	6:R:174:PHE:C	2.97	0.42
13:K:3:ILE:O	13:K:131:ALA:HA	2.20	0.42
2:N:35:ILE:HD13	2:N:56:GLU:HG2	2.02	0.42
2:N:92:MET:HE3	2:N:124:LEU:HA	2.02	0.42
4:P:247:LEU:O	4:P:248:GLU:C	2.62	0.42
10:V:4:MET:HB3	10:V:126:ILE:HG22	2.01	0.42
13:Y:138:TYR:CE2	13:Y:171:MET:HG3	2.55	0.42
14:Z:4:LEU:C	14:Z:4:LEU:HD12	2.45	0.42
12:J:6:MET:HB3	12:J:127:PHE:HB3	2.02	0.41
12:J:115:PHE:CD2	12:J:115:PHE:N	2.88	0.41
8:T:112:LEU:HD23	8:T:112:LEU:HA	1.83	0.41
13:Y:91:ILE:HD13	13:Y:120:TYR:O	2.20	0.41
13:Y:107:ASP:C	13:Y:107:ASP:OD1	2.63	0.41
14:Z:192:ASP:OD1	14:Z:194:GLY:N	2.53	0.41
7:E:34:GLY:O	7:E:35:SER:C	2.62	0.41
9:G:10:SER:HB3	9:G:13:VAL:CG2	2.50	0.41
11:I:62:ASN:HB3	11:I:82:MET:HE1	2.01	0.41
13:K:70:GLU:OE1	13:K:70:GLU:HA	2.21	0.41
3:O:49:ASP:C	3:O:49:ASP:OD1	2.62	0.41
5:Q:196:THR:O	5:Q:200:THR:HB	2.20	0.41
6:R:149:GLN:O	6:R:156:TYR:HA	2.20	0.41
7:S:45:GLY:HA2	7:S:153:TYR:CD1	2.55	0.41
7:S:90:GLU:OE1	14:Z:69:ARG:HD2	2.20	0.41
8:T:78:ALA:HB3	8:T:79:PRO:HD3	2.01	0.41
3:A:54:ILE:HD12	3:A:206:ALA:HB1	2.03	0.41
3:A:87:ILE:N	3:A:88:PRO:CD	2.83	0.41
5:C:106:ILE:O	5:C:106:ILE:HG23	2.20	0.41
7:E:205:LYS:HE2	7:E:205:LYS:HB3	1.83	0.41
6:R:49:ARG:HG3	6:R:166:ARG:HH22	1.85	0.41
7:S:176:SER:O	7:S:177:GLU:C	2.63	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
1:1:132:ALA:HB1	1:1:186:HIS:CE1	2.54	0.41
7:E:123:PHE:HB3	7:E:134:MET:HE3	2.02	0.41
11:I:5:GLY:O	11:I:124:TYR:HA	2.20	0.41
8:T:3:ARG:HA	8:T:4:ASN:HA	1.74	0.41
5:C:19:LEU:O	5:C:20:TYR:C	2.64	0.41
6:D:149:GLN:O	6:D:156:TYR:HA	2.20	0.41
8:F:232:LYS:C	8:F:232:LYS:CD	2.94	0.41
4:P:237:LYS:HE2	4:P:237:LYS:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:38:HIS:O	10:V:39:ASP:C	2.61	0.41
12:X:115:PHE:CD2	12:X:115:PHE:N	2.88	0.41
2:2:-7:THR:HG21	2:2:51:ASP:OD2	2.21	0.41
2:2:89:ALA:HA	2:2:122:VAL:HG21	2.03	0.41
5:C:230:PHE:CE2	5:C:238:ILE:HD11	2.47	0.41
13:K:111:ASN:C	13:K:112:LYS:HD2	2.46	0.41
1:M:43:MET:HG3	1:M:102:ILE:HG22	2.03	0.41
3:O:54:ILE:HD12	3:O:206:ALA:HB1	2.02	0.41
9:U:204:GLU:HA	9:U:207:LYS:HB3	2.02	0.41
9:U:207:LYS:O	9:U:208:GLU:C	2.62	0.41
1:1:166:LEU:HD12	1:1:166:LEU:N	2.35	0.41
3:A:196:GLU:OE2	3:A:201:LYS:HB2	2.19	0.41
6:D:163:THR:HG21	6:D:171:VAL:HG22	2.03	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
2:2:123:ASN:OD1	2:2:123:ASN:C	2.64	0.41
6:D:181:ARG:NH1	7:E:57:PRO:O	2.54	0.41
7:E:67:ILE:HD12	7:E:218:GLN:HG2	2.03	0.41
11:I:113:ILE:HD12	11:I:119:THR:HG22	2.02	0.41
1:M:165:TYR:N	1:M:165:TYR:CD1	2.88	0.41
8:T:187:ASP:OD1	8:T:187:ASP:N	2.53	0.41
8:T:227:GLY:O	8:T:228:GLU:C	2.64	0.41
10:V:102:TYR:CD2	10:V:102:TYR:C	2.98	0.41
11:W:18:THR:OG1	11:W:171:SER:HB2	2.21	0.41
11:W:80:LEU:CD1	11:W:113:ILE:HD11	2.47	0.41
5:C:184:MET:HE3	5:C:188:ASP:HB3	2.02	0.41
6:D:241:GLN:HG3	6:D:242:GLU:N	2.36	0.41
7:E:167:TYR:CZ	7:E:170:LYS:HD3	2.56	0.41
8:F:198:SER:C	8:F:200:SER:N	2.78	0.41
9:G:98:PHE:CD1	9:G:98:PHE:C	2.98	0.41
10:H:102:TYR:CD2	10:H:102:TYR:C	2.99	0.41
5:Q:65:LYS:HE3	5:Q:77:VAL:O	2.21	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
11:W:162:GLY:O	11:W:166:ASP:HB3	2.21	0.41
13:Y:111:ASN:C	13:Y:112:LYS:HD2	2.45	0.41
3:A:115:ASP:HB3	3:A:155:TYR:CE1	2.56	0.41
7:E:168:ASN:HB3	7:E:187:TRP:CE2	2.56	0.41
9:G:106:ILE:HA	9:G:107:PRO:HD3	1.93	0.41
13:K:48:GLU:O	13:K:52:THR:HG23	2.21	0.41
4:P:247:LEU:HD23	4:P:247:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:222:ILE:HG22	7:S:228:PHE:HD2	1.86	0.41
9:U:108:ILE:N	9:U:109:PRO:CD	2.84	0.41
12:X:60:TYR:CD1	12:X:60:TYR:C	2.99	0.41
8:F:171:TYR:CD1	8:F:171:TYR:C	3.00	0.40
8:F:198:SER:HA	8:F:201:LEU:CD2	2.48	0.40
9:G:41:CYS:HB2	9:G:186:LEU:O	2.21	0.40
13:K:100:ASN:HB3	13:K:132:HIS:CD2	2.56	0.40
2:N:157:ILE:N	2:N:158:PRO:CD	2.84	0.40
5:Q:52:VAL:CG1	5:Q:53:THR:N	2.84	0.40
6:R:158:SER:O	7:S:59:LEU:HD12	2.21	0.40
14:Z:193:VAL:O	14:Z:193:VAL:HG12	2.21	0.40
7:E:214:GLU:HG3	7:E:233:ASN:HB3	2.02	0.40
9:G:156:TYR:CD1	9:G:156:TYR:C	3.00	0.40
9:G:177:LYS:HA	9:G:177:LYS:HD3	1.87	0.40
4:P:227:ILE:CG2	4:P:229:THR:HG23	2.51	0.40
12:X:155:PHE:CD1	12:X:155:PHE:C	2.98	0.40
14:Z:9:GLN:OE1	14:Z:148:LEU:O	2.40	0.40
2:2:8:TYR:CE2	2:2:162:VAL:HB	2.57	0.40
6:D:36:VAL:CG1	6:D:195:THR:OG1	2.69	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
8:T:231:ALA:O	8:T:232:LYS:C	2.64	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
13:Y:48:GLU:O	13:Y:52:THR:HG23	2.22	0.40
12:J:42:LEU:HD12	12:J:99:VAL:O	2.22	0.40
13:K:38:SER:HB2	13:K:39:PRO:CD	2.52	0.40
3:O:112:MET:HA	3:O:113:PRO:HD3	1.91	0.40
4:P:248:GLU:OE1	4:P:248:GLU:N	2.54	0.40
5:Q:210:ARG:HB3	5:Q:210:ARG:HH11	1.85	0.40
13:Y:91:ILE:HD12	13:Y:91:ILE:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	221/241 (92%)	205 (93%)	15 (7%)	1 (0%)	24	48
1	M	220/241 (91%)	202 (92%)	17 (8%)	1 (0%)	24	48
2	2	232/266 (87%)	219 (94%)	12 (5%)	1 (0%)	30	54
2	N	231/266 (87%)	217 (94%)	14 (6%)	0	100	100
3	A	240/252 (95%)	235 (98%)	4 (2%)	1 (0%)	30	54
3	O	239/252 (95%)	235 (98%)	3 (1%)	1 (0%)	30	54
4	B	246/250 (98%)	231 (94%)	14 (6%)	1 (0%)	30	54
4	P	247/250 (99%)	233 (94%)	13 (5%)	1 (0%)	30	54
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%)	30	54
6	R	239/254 (94%)	226 (95%)	12 (5%)	1 (0%)	30	54
7	E	240/260 (92%)	228 (95%)	9 (4%)	3 (1%)	9	25
7	S	240/260 (92%)	227 (95%)	11 (5%)	2 (1%)	16	37
8	F	230/234 (98%)	211 (92%)	16 (7%)	3 (1%)	9	25
8	T	230/234 (98%)	214 (93%)	15 (6%)	1 (0%)	30	54
9	G	242/288 (84%)	228 (94%)	13 (5%)	1 (0%)	30	54
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%)	24	48
11	W	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
12	J	202/205 (98%)	186 (92%)	14 (7%)	2 (1%)	12	32
12	X	202/205 (98%)	189 (94%)	11 (5%)	2 (1%)	12	32
13	K	194/198 (98%)	188 (97%)	5 (3%)	1 (0%)	24	48
13	Y	194/198 (98%)	186 (96%)	7 (4%)	1 (0%)	24	48
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6306/6964 (91%)	5985 (95%)	295 (5%)	26 (0%)	30 54

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	239	GLU
7	E	35	SER
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%)	177 (95%)	9 (5%)	23	50
1	M	185/201 (92%)	179 (97%)	6 (3%)	34	64
2	2	200/224 (89%)	191 (96%)	9 (4%)	24	52
2	N	199/224 (89%)	191 (96%)	8 (4%)	28	56
3	A	207/210 (99%)	198 (96%)	9 (4%)	26	54
3	O	206/210 (98%)	195 (95%)	11 (5%)	20	46
4	B	207/209 (99%)	191 (92%)	16 (8%)	12	30
4	P	208/209 (100%)	194 (93%)	14 (7%)	15	36
5	C	203/216 (94%)	187 (92%)	16 (8%)	11	28
5	Q	203/216 (94%)	192 (95%)	11 (5%)	20	45
6	D	213/226 (94%)	196 (92%)	17 (8%)	11	28
6	R	213/226 (94%)	192 (90%)	21 (10%)	7	19
7	E	198/215 (92%)	181 (91%)	17 (9%)	10	25
7	S	198/215 (92%)	181 (91%)	17 (9%)	10	25
8	F	191/193 (99%)	183 (96%)	8 (4%)	26	55
8	T	191/193 (99%)	180 (94%)	11 (6%)	18	42
9	G	201/239 (84%)	195 (97%)	6 (3%)	36	66
9	U	201/239 (84%)	191 (95%)	10 (5%)	22	48
10	H	163/178 (92%)	155 (95%)	8 (5%)	22	49
10	V	162/178 (91%)	154 (95%)	8 (5%)	22	49
11	I	181/214 (85%)	165 (91%)	16 (9%)	9	23
11	W	181/214 (85%)	169 (93%)	12 (7%)	15	36
12	J	172/173 (99%)	167 (97%)	5 (3%)	37	67
12	X	172/173 (99%)	165 (96%)	7 (4%)	27	56
13	K	174/175 (99%)	160 (92%)	14 (8%)	11	28
13	Y	174/175 (99%)	159 (91%)	15 (9%)	10	25
14	L	169/235 (72%)	163 (96%)	6 (4%)	31	60
14	Z	170/235 (72%)	163 (96%)	7 (4%)	27	56
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%)	5018 (94%)	314 (6%)	18	42

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	9	GLU
1	1	62	SER
1	1	115	SER
1	1	121	SER
1	1	125	GLU
1	1	148	LYS
1	1	155	THR
1	1	166	LEU
1	1	205	LYS
2	2	-5	GLN
2	2	1	THR
2	2	2	SER
2	2	21	SER
2	2	145	PRO
2	2	153	ARG
2	2	167	GLU
2	2	191	ILE
2	2	206	VAL
3	A	17	THR
3	A	42	SER
3	A	92	ASN
3	A	131	ARG
3	A	134	MET
3	A	141	LEU
3	A	163	TYR
3	A	188	LYS
3	A	232	LYS
4	B	2	THR
4	B	6	SER
4	B	30	GLN
4	B	37	ILE
4	B	51	SER
4	B	59	GLU
4	B	84	VAL
4	B	108	LYS
4	B	109	LEU
4	B	122	THR
4	B	132	VAL
4	B	157	PHE
4	B	184	GLU
4	B	200	VAL
4	B	229	THR
4	B	231	LYS

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Mol	Chain	Res	Type
5	C	41	SER
5	C	51	LYS
5	C	53	THR
5	C	63	THR
5	C	123	THR
5	C	143	ARG
5	C	150	THR
5	C	158	THR
5	C	174	THR
5	C	185	LYS
5	C	200	THR
5	C	202	ASP
5	C	207	THR
5	C	218	LYS
5	C	239	LEU
5	C	242	THR
6	D	21	GLU
6	D	36	VAL
6	D	40	ASN
6	D	51	THR
6	D	58	ARG
6	D	66	LYS
6	D	98	LEU
6	D	100	LEU
6	D	109	LEU
6	D	132	SER
6	D	143	ASP
6	D	169	LYS
6	D	171	VAL
6	D	187	THR
6	D	222	VAL
6	D	224	LEU
6	D	238	GLN
7	E	10	ARG
7	E	14	THR
7	E	48	LEU
7	E	55	THR
7	E	56	SER
7	E	65	GLU
7	E	132	ARG
7	E	163	THR
7	E	177	GLU

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Mol	Chain	Res	Type
7	E	184	LEU
7	E	191	LEU
7	E	199	LEU
7	E	205	LYS
7	E	222	ILE
7	E	225	GLN
7	E	232	ASP
7	E	238	GLU
8	F	3	ARG
8	F	9	ASP
8	F	10	THR
8	F	93	ASN
8	F	201	LEU
8	F	208	VAL
8	F	230	VAL
8	F	234	ILE
9	G	50	GLU
9	G	97	SER
9	G	99	LYS
9	G	168	ARG
9	G	177	LYS
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
11	I	1	THR
11	I	3	ILE
11	I	13	VAL
11	I	18	THR
11	I	55	VAL
11	I	77	VAL
11	I	100	VAL
11	I	113	ILE
11	I	149	GLU
11	I	169	SER
11	I	182	LYS
11	I	195	VAL

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Mol	Chain	Res	Type
11	I	198	GLU
11	I	214	LYS
11	I	216	SER
11	I	221	CYS
12	J	109	LYS
12	J	115	PHE
12	J	117	LEU
12	J	121	ILE
12	J	130	SER
13	K	1	ASP
13	K	21	THR
13	K	27	LEU
13	K	35	ARG
13	K	90	SER
13	K	91	ILE
13	K	93	SER
13	K	112	LYS
13	K	141	SER
13	K	153	THR
13	K	154	GLU
13	K	165	GLN
13	K	185	LYS
13	K	190	GLN
14	L	69	ARG
14	L	87	VAL
14	L	128	CYS
14	L	147	ASP
14	L	208	ASN
14	L	211	ILE
1	M	115	SER
1	M	121	SER
1	M	125	GLU
1	M	148	LYS
1	M	166	LEU
1	M	205	LYS
2	N	-5	GLN
2	N	2	SER
2	N	21	SER
2	N	29	ASN
2	N	145	PRO
2	N	153	ARG
2	N	191	ILE

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Mol	Chain	Res	Type
2	N	206	VAL
3	O	17	THR
3	O	42	SER
3	O	48	LYS
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	251	GLN
4	P	2	THR
4	P	6	SER
4	P	30	GLN
4	P	59	GLU
4	P	84	VAL
4	P	108	LYS
4	P	109	LEU
4	P	122	THR
4	P	132	VAL
4	P	157	PHE
4	P	177	LYS
4	P	184	GLU
4	P	229	THR
4	P	248	GLU
5	Q	41	SER
5	Q	52	VAL
5	Q	53	THR
5	Q	55	THR
5	Q	129	ARG
5	Q	143	ARG
5	Q	158	THR
5	Q	200	THR
5	Q	222	ASP
5	Q	239	LEU
5	Q	242	THR
6	R	21	GLU
6	R	36	VAL
6	R	51	THR
6	R	53	LYS
6	R	58	ARG

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Mol	Chain	Res	Type
6	R	66	LYS
6	R	98	LEU
6	R	100	LEU
6	R	109	LEU
6	R	119	ARG
6	R	132	SER
6	R	143	ASP
6	R	169	LYS
6	R	171	VAL
6	R	182	LYS
6	R	187	THR
6	R	222	VAL
6	R	224	LEU
6	R	235	GLN
6	R	240	LYS
6	R	241	GLN
7	S	14	THR
7	S	48	LEU
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	191	LEU
7	S	199	LEU
7	S	205	LYS
7	S	222	ILE
7	S	232	ASP
7	S	238	GLU
7	S	245	GLU
7	S	247	GLU
8	T	3	ARG
8	T	4	ASN
8	T	10	THR
8	T	11	VAL
8	T	16	THR
8	T	41	ASN
8	T	77	LEU
8	T	179	PHE
8	T	208	VAL

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Mol	Chain	Res	Type
8	T	218	LYS
8	T	234	ILE
9	U	24	GLU
9	U	50	GLU
9	U	97	SER
9	U	99	LYS
9	U	142	LYS
9	U	168	ARG
9	U	201	LEU
9	U	209	LYS
9	U	230	VAL
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
10	V	192	GLU
11	W	1	THR
11	W	3	ILE
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	109	LYS
12	X	115	PHE
12	X	117	LEU
12	X	121	ILE
12	X	130	SER
12	X	185	GLU
12	X	194	ARG
13	Y	1	ASP
13	Y	6	ILE
13	Y	9	GLN

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Mol	Chain	Res	Type
13	Y	21	THR
13	Y	27	LEU
13	Y	35	ARG
13	Y	90	SER
13	Y	91	ILE
13	Y	93	SER
13	Y	112	LYS
13	Y	141	SER
13	Y	153	THR
13	Y	154	GLU
13	Y	165	GLN
13	Y	185	LYS
14	Z	9	GLN
14	Z	69	ARG
14	Z	87	VAL
14	Z	128	CYS
14	Z	147	ASP
14	Z	208	ASN
14	Z	211	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	27	ASN
1	1	61	ASN
1	1	71	ASN
1	1	126	GLN
1	1	144	GLN
1	1	149	ASN
1	1	150	GLN
1	1	188	GLN
2	2	18	ASN
2	2	186	ASN
4	B	149	GLN
5	C	31	HIS
5	C	125	HIS
6	D	40	ASN
6	D	94	GLN
6	D	209	ASN
7	E	114	GLN
7	E	147	HIS
7	E	154	GLN

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Mol	Chain	Res	Type
7	E	168	ASN
8	F	199	GLN
9	G	42	ASN
9	G	61	GLN
10	H	92	ASN
11	I	35	HIS
11	I	57	GLN
11	I	85	GLN
11	I	114	HIS
11	I	194	ASN
11	I	200	GLN
12	J	80	GLN
12	J	164	ASN
12	J	195	GLN
13	K	36	GLN
13	K	62	ASN
13	K	85	GLN
13	K	111	ASN
14	L	143	ASN
1	M	86	HIS
1	M	126	GLN
1	M	144	GLN
1	M	150	GLN
1	M	156	ASN
1	M	188	GLN
2	N	18	ASN
2	N	54	HIS
2	N	186	ASN
3	O	185	HIS
3	O	209	HIS
4	P	149	GLN
4	P	190	HIS
5	Q	125	HIS
5	Q	173	GLN
6	R	178	ASN
7	S	114	GLN
7	S	147	HIS
7	S	154	GLN
7	S	168	ASN
7	S	188	HIS
8	T	93	ASN
9	U	42	ASN

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Mol	Chain	Res	Type
10	V	60	GLN
11	W	35	HIS
11	W	219	ASN
12	X	23	GLN
12	X	148	ASN
13	Y	36	GLN
13	Y	62	ASN
13	Y	85	GLN
13	Y	111	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
17	GOL	J	202	-	5,5,5	0.62	0	5,5,5	0.42	0
17	GOL	V	203	-	5,5,5	1.27	0	5,5,5	1.56	2 (40%)
17	GOL	A	302	-	5,5,5	0.25	0	5,5,5	0.49	0
17	GOL	F	304	-	5,5,5	0.40	0	5,5,5	0.67	0
17	GOL	K	201	-	5,5,5	0.48	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	GOL	Z	303	-	5,5,5	0.34	0	5,5,5	0.94	0
17	GOL	A	301	-	5,5,5	0.62	0	5,5,5	0.56	0
16	MPD	Z	301	-	7,7,7	0.51	0	9,10,10	0.88	0
17	GOL	L	303	-	5,5,5	0.42	0	5,5,5	0.39	0
17	GOL	G	301	-	5,5,5	0.35	0	5,5,5	0.73	0
16	MPD	L	301	-	7,7,7	0.68	0	9,10,10	0.66	0
17	GOL	N	303	-	5,5,5	0.23	0	5,5,5	0.75	0
17	GOL	V	202	-	5,5,5	0.51	0	5,5,5	0.33	0
16	MPD	V	201	-	7,7,7	0.81	0	9,10,10	1.74	1 (11%)
17	GOL	O	302	-	5,5,5	0.30	0	5,5,5	0.64	0
17	GOL	N	302	-	5,5,5	0.58	0	5,5,5	0.65	0
16	MPD	M	301	-	7,7,7	0.51	0	9,10,10	0.53	0
17	GOL	2	303	-	5,5,5	0.29	0	5,5,5	1.02	0
17	GOL	Z	304	-	5,5,5	0.47	0	5,5,5	0.60	0
16	MPD	T	301	-	7,7,7	1.00	0	9,10,10	0.94	0
17	GOL	A	304	-	5,5,5	0.44	0	5,5,5	0.83	0
17	GOL	X	202	-	5,5,5	0.42	0	5,5,5	0.78	0
17	GOL	M	303	-	5,5,5	0.56	0	5,5,5	0.35	0
16	MPD	2	301	-	7,7,7	0.55	0	9,10,10	0.93	1 (11%)
17	GOL	G	302	-	5,5,5	0.34	0	5,5,5	0.53	0
17	GOL	Z	302	-	5,5,5	0.74	0	5,5,5	1.13	0
17	GOL	1	303	-	5,5,5	0.57	0	5,5,5	0.43	0
17	GOL	H	201	-	5,5,5	0.15	0	5,5,5	0.65	0
16	MPD	1	301	-	7,7,7	0.76	0	9,10,10	0.90	1 (11%)
17	GOL	F	302	-	5,5,5	0.31	0	5,5,5	0.46	0
17	GOL	W	301	-	5,5,5	0.57	0	5,5,5	0.91	0
17	GOL	M	302	-	5,5,5	0.55	0	5,5,5	1.08	0
17	GOL	F	301	-	5,5,5	0.61	0	5,5,5	0.43	0
17	GOL	2	302	-	5,5,5	0.57	0	5,5,5	0.31	0
17	GOL	A	303	-	5,5,5	0.77	0	5,5,5	1.29	0
17	GOL	I	301	-	5,5,5	0.85	0	5,5,5	0.74	0
16	MPD	N	301	-	7,7,7	0.60	0	9,10,10	0.37	0
17	GOL	1	302	-	5,5,5	0.47	0	5,5,5	0.30	0
17	GOL	F	303	-	5,5,5	0.31	0	5,5,5	0.56	0
16	MPD	X	201	-	7,7,7	0.61	0	9,10,10	0.67	0
17	GOL	E	301	-	5,5,5	0.42	0	5,5,5	1.21	0
17	GOL	S	301	-	5,5,5	0.58	0	5,5,5	0.32	0
17	GOL	T	302	-	5,5,5	0.66	0	5,5,5	0.91	0
17	GOL	L	302	-	5,5,5	0.38	0	5,5,5	0.44	0
17	GOL	O	301	-	5,5,5	0.74	0	5,5,5	0.70	0
17	GOL	I	302	-	5,5,5	0.47	0	5,5,5	0.69	0
17	GOL	D	301	-	5,5,5	0.93	0	5,5,5	1.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GOL	J	202	-	-	2/4/4/4	-
17	GOL	V	203	-	-	4/4/4/4	-
17	GOL	A	302	-	-	0/4/4/4	-
17	GOL	F	304	-	-	0/4/4/4	-
17	GOL	K	201	-	-	3/4/4/4	-
17	GOL	Z	303	-	-	2/4/4/4	-
17	GOL	A	301	-	-	1/4/4/4	-
16	MPD	Z	301	-	-	4/5/5/5	-
17	GOL	L	303	-	-	2/4/4/4	-
17	GOL	G	301	-	-	1/4/4/4	-
16	MPD	L	301	-	-	1/5/5/5	-
17	GOL	N	303	-	-	2/4/4/4	-
17	GOL	V	202	-	-	2/4/4/4	-
16	MPD	V	201	-	-	3/5/5/5	-
17	GOL	O	302	-	-	2/4/4/4	-
17	GOL	N	302	-	-	2/4/4/4	-
16	MPD	M	301	-	-	5/5/5/5	-
17	GOL	2	303	-	-	0/4/4/4	-
17	GOL	Z	304	-	-	2/4/4/4	-
16	MPD	T	301	-	-	2/5/5/5	-
17	GOL	A	304	-	-	0/4/4/4	-
17	GOL	X	202	-	-	2/4/4/4	-
17	GOL	M	303	-	-	2/4/4/4	-
16	MPD	2	301	-	-	3/5/5/5	-
17	GOL	G	302	-	-	4/4/4/4	-
17	GOL	Z	302	-	-	0/4/4/4	-
17	GOL	1	303	-	-	4/4/4/4	-
17	GOL	H	201	-	-	0/4/4/4	-
16	MPD	1	301	-	-	2/5/5/5	-
17	GOL	F	302	-	-	0/4/4/4	-
17	GOL	W	301	-	-	3/4/4/4	-
17	GOL	M	302	-	-	2/4/4/4	-
17	GOL	F	301	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GOL	2	302	-	-	4/4/4/4	-
17	GOL	A	303	-	-	4/4/4/4	-
17	GOL	I	301	-	-	4/4/4/4	-
16	MPD	N	301	-	-	2/5/5/5	-
17	GOL	1	302	-	-	0/4/4/4	-
17	GOL	F	303	-	-	2/4/4/4	-
16	MPD	X	201	-	-	0/5/5/5	-
17	GOL	E	301	-	-	2/4/4/4	-
17	GOL	S	301	-	-	2/4/4/4	-
17	GOL	T	302	-	-	4/4/4/4	-
17	GOL	L	302	-	-	2/4/4/4	-
17	GOL	O	301	-	-	0/4/4/4	-
17	GOL	I	302	-	-	2/4/4/4	-
17	GOL	D	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	201	MPD	O2-C2-C1	-4.15	95.05	107.99
17	V	203	GOL	O1-C1-C2	2.23	120.42	110.38
16	2	301	MPD	O2-C2-CM	-2.16	101.26	107.99
17	V	203	GOL	C3-C2-C1	2.09	119.45	111.80
16	1	301	MPD	CM-C2-C1	-2.05	106.04	110.63

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	M	301	MPD	C2-C3-C4-O4
16	M	301	MPD	C2-C3-C4-C5
16	Z	301	MPD	C2-C3-C4-O4
16	Z	301	MPD	C2-C3-C4-C5
17	1	303	GOL	C1-C2-C3-O3
17	2	302	GOL	C1-C2-C3-O3
17	A	303	GOL	O1-C1-C2-C3
17	E	301	GOL	O1-C1-C2-C3
17	F	301	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
17	F	303	GOL	C1-C2-C3-O3
17	G	302	GOL	O1-C1-C2-C3
17	G	302	GOL	C1-C2-C3-O3
17	I	301	GOL	C1-C2-C3-O3
17	J	202	GOL	C1-C2-C3-O3
17	J	202	GOL	O2-C2-C3-O3
17	L	303	GOL	O1-C1-C2-C3
17	M	303	GOL	O1-C1-C2-C3
17	S	301	GOL	O1-C1-C2-C3
17	T	302	GOL	C1-C2-C3-O3
17	V	202	GOL	C1-C2-C3-O3
17	V	202	GOL	O2-C2-C3-O3
17	X	202	GOL	O1-C1-C2-C3
17	Z	303	GOL	O1-C1-C2-C3
17	A	303	GOL	O1-C1-C2-O2
17	A	303	GOL	O2-C2-C3-O3
17	M	303	GOL	O1-C1-C2-O2
17	S	301	GOL	O1-C1-C2-O2
17	X	202	GOL	O1-C1-C2-O2
17	1	303	GOL	O1-C1-C2-C3
17	2	302	GOL	O1-C1-C2-C3
17	A	303	GOL	C1-C2-C3-O3
17	D	301	GOL	C1-C2-C3-O3
17	F	301	GOL	O1-C1-C2-C3
17	I	302	GOL	C1-C2-C3-O3
17	K	201	GOL	C1-C2-C3-O3
17	L	302	GOL	O1-C1-C2-C3
17	M	302	GOL	O1-C1-C2-C3
17	N	303	GOL	O1-C1-C2-C3
17	O	302	GOL	O1-C1-C2-C3
17	T	302	GOL	O1-C1-C2-C3
17	V	203	GOL	O1-C1-C2-C3
17	V	203	GOL	C1-C2-C3-O3
17	W	301	GOL	O1-C1-C2-C3
17	Z	304	GOL	O1-C1-C2-C3
17	1	303	GOL	O2-C2-C3-O3
17	2	302	GOL	O2-C2-C3-O3
17	E	301	GOL	O1-C1-C2-O2
17	F	301	GOL	O2-C2-C3-O3
17	F	303	GOL	O2-C2-C3-O3
17	G	302	GOL	O1-C1-C2-O2
17	G	302	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
17	I	301	GOL	O2-C2-C3-O3
17	I	302	GOL	O2-C2-C3-O3
17	L	303	GOL	O1-C1-C2-O2
17	T	302	GOL	O2-C2-C3-O3
17	V	203	GOL	O1-C1-C2-O2
17	W	301	GOL	O1-C1-C2-O2
17	Z	303	GOL	O1-C1-C2-O2
17	L	302	GOL	O1-C1-C2-O2
17	N	302	GOL	O2-C2-C3-O3
17	N	303	GOL	O1-C1-C2-O2
17	O	302	GOL	O1-C1-C2-O2
17	Z	304	GOL	O1-C1-C2-O2
17	2	302	GOL	O1-C1-C2-O2
17	A	301	GOL	O1-C1-C2-O2
17	K	201	GOL	O1-C1-C2-O2
17	K	201	GOL	O2-C2-C3-O3
17	V	203	GOL	O2-C2-C3-O3
17	G	301	GOL	C1-C2-C3-O3
17	T	302	GOL	O1-C1-C2-O2
16	1	301	MPD	C1-C2-C3-C4
16	M	301	MPD	CM-C2-C3-C4
16	T	301	MPD	CM-C2-C3-C4
16	2	301	MPD	C2-C3-C4-C5
16	N	301	MPD	C2-C3-C4-C5
16	V	201	MPD	C2-C3-C4-C5
17	D	301	GOL	O2-C2-C3-O3
17	M	302	GOL	O1-C1-C2-O2
17	I	301	GOL	O1-C1-C2-C3
17	N	302	GOL	C1-C2-C3-O3
17	F	301	GOL	O1-C1-C2-O2
17	1	303	GOL	O1-C1-C2-O2
17	W	301	GOL	C1-C2-C3-O3
16	2	301	MPD	O2-C2-C3-C4
16	M	301	MPD	O2-C2-C3-C4
16	Z	301	MPD	O2-C2-C3-C4
16	2	301	MPD	C2-C3-C4-O4
16	L	301	MPD	C2-C3-C4-O4
16	N	301	MPD	C2-C3-C4-O4
16	1	301	MPD	CM-C2-C3-C4
16	M	301	MPD	C1-C2-C3-C4
16	T	301	MPD	C1-C2-C3-C4
16	V	201	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
16	V	201	MPD	CM-C2-C3-C4
16	Z	301	MPD	C1-C2-C3-C4
17	I	301	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Z	301	MPD	2	0
16	V	201	MPD	12	0
16	2	301	MPD	1	0
16	N	301	MPD	1	0
16	X	201	MPD	3	0
17	D	301	GOL	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, 95th 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 ²)	Q<0.9
1	1	222/241 (92%)	-0.25	4 (1%) 67 65	22, 39, 65, 98	1 (0%)
1	M	222/241 (92%)	-0.23	5 (2%) 61 58	22, 39, 64, 98	0
2	2	233/266 (87%)	-0.46	1 (0%) 88 87	19, 33, 52, 86	1 (0%)
2	N	233/266 (87%)	-0.42	4 (1%) 69 67	19, 34, 55, 90	0
3	A	242/252 (96%)	-0.33	3 (1%) 76 75	19, 36, 65, 126	0
3	O	241/252 (95%)	-0.27	3 (1%) 76 75	22, 39, 70, 91	0
4	B	248/250 (99%)	-0.23	6 (2%) 59 56	20, 37, 67, 104	0
4	P	249/250 (99%)	-0.13	6 (2%) 59 56	23, 44, 77, 110	0
5	C	244/258 (94%)	0.09	10 (4%) 41 37	23, 44, 86, 129	0
5	Q	244/258 (94%)	0.05	9 (3%) 45 41	26, 46, 88, 141	0
6	D	241/254 (94%)	0.06	11 (4%) 37 34	24, 47, 103, 133	0
6	R	241/254 (94%)	0.21	11 (4%) 37 34	30, 53, 108, 125	0
7	E	242/260 (93%)	0.11	6 (2%) 58 55	26, 47, 86, 160	0
7	S	242/260 (93%)	0.07	5 (2%) 63 61	27, 51, 81, 119	0
8	F	232/234 (99%)	-0.08	1 (0%) 88 87	29, 49, 76, 101	0
8	T	232/234 (99%)	0.03	1 (0%) 88 87	29, 52, 79, 105	0
9	G	244/288 (84%)	-0.16	4 (1%) 70 68	23, 41, 78, 117	0
9	U	244/288 (84%)	-0.10	5 (2%) 65 62	22, 44, 83, 104	0
10	H	196/215 (91%)	-0.55	0 100 100	15, 27, 51, 84	1 (0%)
10	V	196/215 (91%)	-0.57	0 100 100	18, 29, 56, 77	0
11	I	221/261 (84%)	-0.29	2 (0%) 81 80	15, 34, 59, 94	1 (0%)
11	W	220/261 (84%)	-0.34	1 (0%) 87 86	14, 37, 60, 77	2 (0%)
12	J	204/205 (99%)	-0.31	6 (2%) 53 50	23, 35, 72, 91	0
12	X	204/205 (99%)	-0.27	9 (4%) 39 35	22, 36, 71, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	K	196/198 (98%)	-0.30	1 (0%) 87 86	20, 36, 57, 93	0
13	Y	196/198 (98%)	-0.29	4 (2%) 65 62	25, 39, 59, 100	0
14	L	212/287 (73%)	-0.42	0 100 100	21, 37, 56, 66	0
14	Z	212/287 (73%)	-0.30	0 100 100	14, 38, 58, 76	1 (0%)
15	a	3/13 (23%)	1.40	1 (33%) 1 1	63, 63, 78, 96	0
15	e	3/13 (23%)	1.23	0 100 100	45, 45, 56, 83	1 (33%)
All	All	6359/6964 (91%)	-0.19	119 (1%) 66 63	14, 40, 76, 160	8 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	X	121	ILE	5.3
5	C	52	VAL	4.9
6	R	51	THR	4.8
2	N	225	ILE	4.6
6	D	52	LEU	4.5
4	P	250	LEU	4.4
6	D	49	ARG	4.3
4	B	201	GLU	4.3
4	B	249	ALA	4.2
7	S	127	ALA	4.2
5	Q	52	VAL	4.2
6	R	49	ARG	4.2
13	Y	191	VAL	4.2
6	D	51	THR	4.1
6	D	243	GLN	4.0
6	R	53	LYS	3.9
12	J	122	ASP	3.8
5	Q	51	LYS	3.8
7	E	128	SER	3.8
2	2	225	ILE	3.7
5	Q	220	ALA	3.6
12	J	121	ILE	3.5
7	E	250	GLU	3.5
9	G	205	ASP	3.4
4	P	61	LEU	3.4
6	R	52	LEU	3.4
13	Y	0	MET	3.4
11	W	220	ILE	3.3
5	C	2	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
7	E	9	ASP	3.3
2	N	222	THR	3.3
9	G	4	GLY	3.3
9	U	246	ILE	3.3
5	C	220	ALA	3.2
6	D	208	LYS	3.1
7	E	249	ALA	3.1
5	C	245	THR	3.1
5	C	219	GLY	3.0
5	C	223	GLY	3.0
12	J	119	GLY	3.0
4	P	62	SER	3.0
9	U	247	ASN	3.0
7	S	128	SER	2.9
12	J	117	LEU	2.9
12	J	116	ASP	2.9
12	X	122	ASP	2.9
5	Q	226	TYR	2.9
4	P	52	SER	2.8
6	D	53	LYS	2.8
3	A	252	ASP	2.8
5	Q	245	THR	2.8
6	R	208	LYS	2.8
11	I	220	ILE	2.8
7	E	126	GLY	2.8
6	D	207	ALA	2.8
12	X	118	ILE	2.7
5	Q	219	GLY	2.7
1	M	166	LEU	2.7
13	K	0	MET	2.7
9	U	180	ASP	2.7
5	C	61	THR	2.7
6	R	207	ALA	2.7
9	U	62	LYS	2.7
5	Q	223	GLY	2.6
1	1	155	THR	2.6
4	B	2	THR	2.6
6	R	205	THR	2.6
13	Y	195	GLN	2.6
5	C	51	LYS	2.6
5	C	63	THR	2.6
8	F	123	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
9	U	54	THR	2.5
4	P	50	LYS	2.5
12	X	125	LYS	2.5
12	X	117	LEU	2.5
12	X	123	GLU	2.5
1	M	165	TYR	2.5
3	A	12	TYR	2.5
2	N	224	LYS	2.4
3	A	248	ILE	2.4
1	M	38	GLY	2.4
6	R	234	THR	2.4
7	S	9	ASP	2.4
12	X	119	GLY	2.4
6	D	240	LYS	2.4
6	D	48	ARG	2.4
9	G	247	ASN	2.4
2	N	221	GLY	2.3
15	a	1	ARG	2.3
8	T	123	TYR	2.3
5	Q	221	ASN	2.3
1	M	163	LEU	2.3
7	S	249	ALA	2.2
4	B	59	GLU	2.2
12	X	196	ASP	2.2
3	O	212	ASP	2.2
1	1	0	GLY	2.2
13	Y	192	ASP	2.2
4	P	2	THR	2.1
4	B	61	LEU	2.1
6	R	50	SER	2.1
7	E	131	GLU	2.1
11	I	221	CYS	2.1
1	1	154	GLY	2.1
5	Q	2	GLY	2.1
6	D	50	SER	2.1
4	B	50	LYS	2.1
6	R	243	GLN	2.1
1	1	165	TYR	2.1
12	J	115	PHE	2.1
7	S	86	ARG	2.0
9	G	208	GLU	2.0
12	X	124	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	0	GLY	2.0
3	O	11	GLY	2.0
3	O	162	TYR	2.0
6	D	242	GLU	2.0
6	R	211	GLU	2.0
5	C	9	ARG	2.0

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

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

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, 95th 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 ²)	Q<0.9
18	MG	T	303	1/1	0.56	0.13	51,51,51,51	0
17	GOL	F	301	6/6	0.68	0.16	64,75,77,79	0
16	MPD	T	301	8/8	0.68	0.32	52,70,76,77	0
18	MG	S	303	1/1	0.74	0.15	55,55,55,55	0
16	MPD	N	301	8/8	0.74	0.28	60,65,69,69	0
18	MG	P	301	1/1	0.78	0.08	49,49,49,49	0
16	MPD	2	301	8/8	0.78	0.28	61,65,74,74	0
18	MG	J	206	1/1	0.78	0.14	42,42,42,42	0
16	MPD	Z	301	8/8	0.79	0.29	56,65,76,84	0
16	MPD	1	301	8/8	0.80	0.27	58,64,66,70	0
18	MG	M	304	1/1	0.81	0.10	40,40,40,40	0
18	MG	K	202	1/1	0.83	0.14	35,35,35,35	0
17	GOL	A	302	6/6	0.84	0.14	67,70,71,73	0
17	GOL	T	302	6/6	0.84	0.17	53,67,67,68	0
18	MG	Y	202	1/1	0.84	0.16	31,31,31,31	0
18	MG	H	205	1/1	0.85	0.12	29,29,29,29	0
16	MPD	V	201	8/8	0.85	0.21	38,42,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MPD	X	201	8/8	0.85	0.28	67,81,88,90	0
16	MPD	L	301	8/8	0.85	0.26	55,70,75,76	0
18	MG	V	207	1/1	0.86	0.08	39,39,39,39	0
18	MG	F	305	1/1	0.87	0.08	50,50,50,50	0
18	MG	Y	201	1/1	0.87	0.10	40,40,40,40	0
17	GOL	F	303	6/6	0.87	0.18	56,64,73,74	0
17	GOL	V	202	6/6	0.88	0.15	89,93,98,98	0
18	MG	2	304	1/1	0.88	0.14	22,22,22,22	0
18	MG	L	304	1/1	0.88	0.15	30,30,30,30	0
17	GOL	D	301	6/6	0.88	0.18	64,69,72,75	0
16	MPD	M	301	8/8	0.88	0.21	66,83,98,111	0
18	MG	D	302	1/1	0.89	0.06	27,27,27,27	0
17	GOL	S	301	6/6	0.89	0.14	63,65,69,69	0
17	GOL	M	303	6/6	0.89	0.18	62,72,77,77	0
18	MG	X	205	1/1	0.89	0.10	35,35,35,35	0
18	MG	M	305	1/1	0.89	0.09	55,55,55,55	0
18	MG	2	307	1/1	0.89	0.11	53,53,53,53	0
17	GOL	A	304	6/6	0.90	0.12	48,50,51,51	0
17	GOL	G	302	6/6	0.90	0.17	61,63,64,64	0
17	GOL	I	302	6/6	0.90	0.15	53,58,59,60	0
17	GOL	J	202	6/6	0.90	0.17	56,61,71,75	0
18	MG	O	303	1/1	0.90	0.06	34,34,34,34	0
17	GOL	L	302	6/6	0.90	0.14	70,73,75,82	0
17	GOL	1	303	6/6	0.91	0.11	58,61,61,62	0
17	GOL	1	302	6/6	0.91	0.14	54,58,62,64	0
18	MG	H	203	1/1	0.91	0.06	38,38,38,38	0
18	MG	S	302	1/1	0.91	0.10	31,31,31,31	0
17	GOL	V	203	6/6	0.91	0.19	43,55,58,59	0
17	GOL	W	301	6/6	0.91	0.13	51,57,58,64	0
18	MG	J	207	1/1	0.91	0.10	34,34,34,34	0
17	GOL	Z	302	6/6	0.91	0.17	47,56,58,59	0
17	GOL	I	301	6/6	0.91	0.18	64,68,72,72	0
17	GOL	A	303	6/6	0.91	0.14	44,49,55,57	0
17	GOL	N	302	6/6	0.92	0.13	50,57,60,62	0
18	MG	N	307	1/1	0.92	0.14	27,27,27,27	0
17	GOL	2	302	6/6	0.92	0.12	39,43,49,51	0
17	GOL	E	301	6/6	0.92	0.14	50,53,54,56	0
17	GOL	2	303	6/6	0.92	0.13	51,54,56,62	0
17	GOL	F	302	6/6	0.92	0.11	52,59,66,66	0
17	GOL	K	201	6/6	0.92	0.14	57,62,63,63	0
17	GOL	A	301	6/6	0.92	0.11	51,58,60,63	0
17	GOL	Z	303	6/6	0.92	0.11	36,40,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	GOL	G	301	6/6	0.92	0.12	52,55,57,57	0
18	MG	2	305	1/1	0.92	0.13	39,39,39,39	0
17	GOL	X	202	6/6	0.93	0.12	47,48,50,51	0
17	GOL	O	301	6/6	0.93	0.14	53,54,60,60	0
18	MG	V	206	1/1	0.93	0.15	28,28,28,28	0
17	GOL	L	303	6/6	0.93	0.10	49,55,59,60	0
18	MG	X	204	1/1	0.93	0.14	35,35,35,35	0
18	MG	L	305	1/1	0.93	0.16	32,32,32,32	0
18	MG	R	303	1/1	0.93	0.10	39,39,39,39	0
17	GOL	Z	304	6/6	0.93	0.10	49,54,57,60	0
18	MG	V	205	1/1	0.94	0.07	33,33,33,33	0
18	MG	Q	301	1/1	0.94	0.14	25,25,25,25	0
18	MG	R	301	1/1	0.94	0.12	28,28,28,28	0
17	GOL	O	302	6/6	0.94	0.14	63,67,69,70	0
18	MG	B	301	1/1	0.94	0.11	42,42,42,42	0
17	GOL	M	302	6/6	0.94	0.11	33,37,41,41	0
17	GOL	F	304	6/6	0.94	0.11	50,56,60,61	0
18	MG	M	306	1/1	0.95	0.06	37,37,37,37	0
18	MG	N	305	1/1	0.95	0.23	28,28,28,28	0
18	MG	W	302	1/1	0.95	0.07	37,37,37,37	0
18	MG	X	203	1/1	0.95	0.07	26,26,26,26	0
18	MG	J	204	1/1	0.95	0.06	35,35,35,35	0
17	GOL	N	303	6/6	0.95	0.09	44,51,52,52	0
18	MG	1	304	1/1	0.95	0.12	35,35,35,35	0
18	MG	J	201	1/1	0.95	0.08	36,36,36,36	0
18	MG	Z	305	1/1	0.95	0.09	31,31,31,31	0
18	MG	R	302	1/1	0.96	0.12	26,26,26,26	0
18	MG	H	204	1/1	0.96	0.13	18,18,18,18	0
18	MG	J	205	1/1	0.96	0.12	23,23,23,23	0
18	MG	H	202	1/1	0.96	0.12	28,28,28,28	0
17	GOL	H	201	6/6	0.96	0.13	62,68,72,75	0
18	MG	2	306	1/1	0.97	0.15	43,43,43,43	0
18	MG	N	306	1/1	0.97	0.07	39,39,39,39	0
18	MG	J	203	1/1	0.97	0.13	30,30,30,30	0
18	MG	C	301	1/1	0.97	0.16	20,20,20,20	0
18	MG	C	302	1/1	0.97	0.07	28,28,28,28	0
18	MG	T	304	1/1	0.97	0.06	47,47,47,47	0
18	MG	M	307	1/1	0.97	0.06	25,25,25,25	0
18	MG	N	304	1/1	0.97	0.09	34,34,34,34	0
18	MG	K	203	1/1	0.98	0.10	25,25,25,25	0
18	MG	V	204	1/1	0.98	0.11	21,21,21,21	0
18	MG	2	308	1/1	0.98	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	MG	Q	302	1/1	0.99	0.10	30,30,30,30	0
18	MG	Z	306	1/1	0.99	0.11	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.