



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:10 PM UTC

PDB ID : 5LF6 / pdb_00005lf6
Title : Human 20S proteasome complex with Z-LLY-ketoaldehyde at 2.1 Angstrom
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on : 2016-06-30
Resolution : 2.07 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

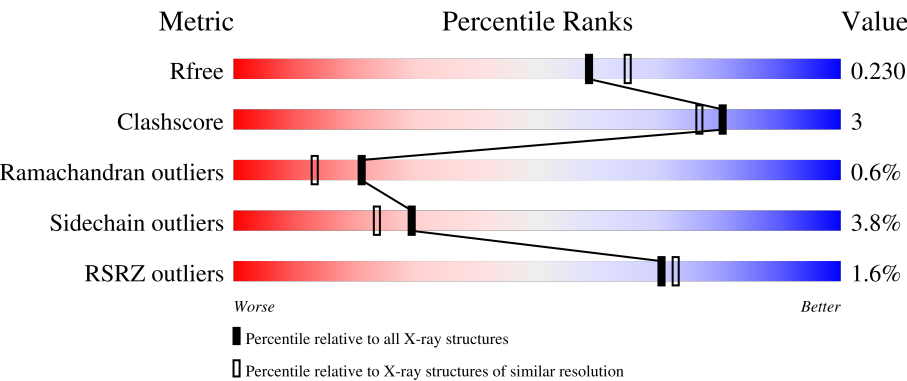
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	A	234	2% 88% 9% ..
1	O	234	2% 90% 7% ..
2	B	261	% 85% 9% 5%
2	P	261	3% 83% 11% 5%
3	C	248	3% 85% 7% . .

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Mol	Chain	Length	Quality of chain
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	c	4	
11	d	4	
12	K	204	
12	Y	204	
13	L	213	
13	Z	213	
14	M	219	
14	a	219	
15	N	205	
15	b	205	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51953 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	1	0
			1813	1138	324	340	11			
5	S	238	Total	C	N	O	S	0	3	0
			1866	1169	339	347	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	239	Total	C	N	O	S	0	4	0
			1888	1198	325	353	12			
6	T	240	Total	C	N	O	S	0	1	0
			1856	1178	315	351	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	2	0
			1894	1202	319	360	13			
7	U	238	Total	C	N	O	S	0	1	0
			1797	1135	302	346	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	2	0
			1664	1047	284	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1622	1023	269	318	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1581	1015	270	286	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1567	1006	266	285	10			

- Molecule 11 is a protein called Z-LLY-ketoaldehyde peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	c	4	Total	C	N	O	0	0	0
			40	30	3	7			
11	d	4	Total	C	N	O	0	0	0
			40	30	3	7			

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	200	Total	C	N	O	S	0	1	0
			1550	978	269	293	10			
12	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	213	Total	C	N	O	S	0	2	0
			1636	1038	277	310	11			
13	Z	213	Total	C	N	O	S	0	1	0
			1642	1041	280	310	11			

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
14	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 15 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	202	Total	C	N	O	S	0	1	0
			1516	950	258	295	13			
15	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

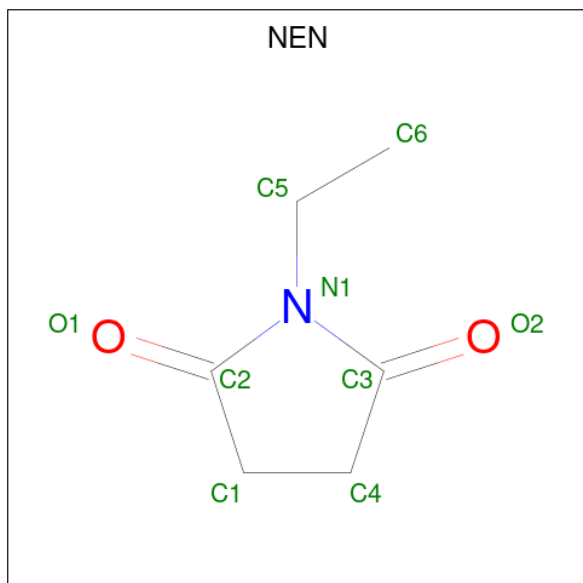
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	4	Total 4	Cl 4	0	0
16	B	2	Total 2	Cl 2	0	0
16	C	2	Total 2	Cl 2	0	0
16	D	2	Total 2	Cl 2	0	0
16	E	3	Total 3	Cl 3	0	0
16	F	1	Total 1	Cl 1	0	0
16	G	2	Total 2	Cl 2	0	0
16	H	2	Total 2	Cl 2	0	0
16	I	1	Total 1	Cl 1	0	0
16	K	3	Total 3	Cl 3	0	0
16	M	3	Total 3	Cl 3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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	a	3	Total	Cl	0	0
			3	3		
16	b	3	Total	Cl	0	0
			3	3		

- Molecule 17 is 1-ETHYL-PYRROLIDINE-2,5-DIONE (CCD ID: NEN) (formula: $C_6H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	E	1	Total	C	N	O	0	0
			9	6	1	2		
17	G	1	Total	C	N	O	0	0
			9	6	1	2		
17	G	1	Total	C	N	O	0	0
			9	6	1	2		
17	J	1	Total	C	N	O	0	0
			9	6	1	2		
17	S	1	Total	C	N	O	0	0
			9	6	1	2		
17	U	1	Total	C	N	O	0	0
			9	6	1	2		
17	U	1	Total	C	N	O	0	0
			9	6	1	2		
17	X	1	Total	C	N	O	0	0
			9	6	1	2		

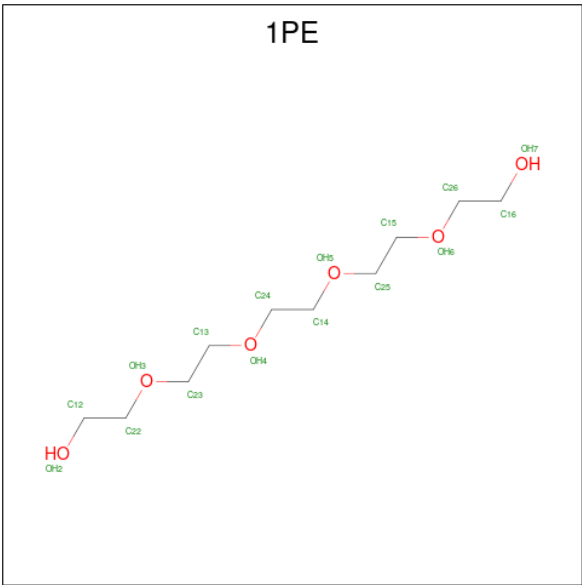
- Molecule 18 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 20 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	108	Total	O	0	0
			108	108		
21	B	119	Total	O	0	0
			119	119		
21	C	75	Total	O	0	0
			75	75		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	D	86	Total O 86 86	0	0
21	E	137	Total O 137 137	0	0
21	F	179	Total O 179 179	0	0
21	G	190	Total O 190 190	0	0
21	H	150	Total O 150 150	0	0
21	I	157	Total O 157 157	0	0
21	J	133	Total O 133 133	0	0
21	c	3	Total O 3 3	0	0
21	K	92	Total O 92 92	0	0
21	L	121	Total O 121 121	0	0
21	M	145	Total O 145 145	0	0
21	N	156	Total O 156 156	0	0
21	O	89	Total O 89 89	0	0
21	P	109	Total O 109 109	0	0
21	Q	71	Total O 71 71	0	0
21	R	119	Total O 119 119	0	0
21	S	124	Total O 124 124	0	0
21	T	91	Total O 91 91	0	0
21	U	103	Total O 103 103	0	0
21	V	109	Total O 109 109	0	0
21	W	108	Total O 108 108	0	0

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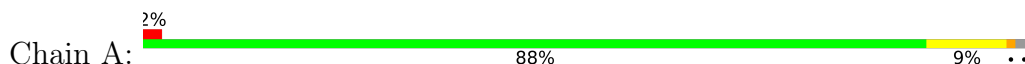
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	X	124	Total 124	O 124	0	0
21	d	2	Total 2	O 2	0	0
21	Y	141	Total 141	O 141	0	0
21	Z	167	Total 167	O 167	0	0
21	a	172	Total 172	O 172	0	0
21	b	121	Total 121	O 121	0	0

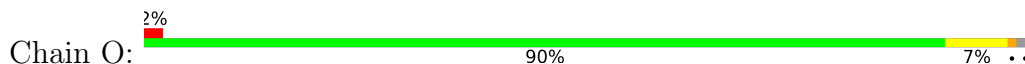
3 Residue-property plots

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

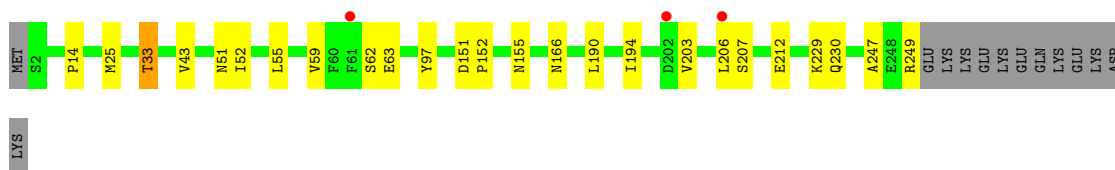
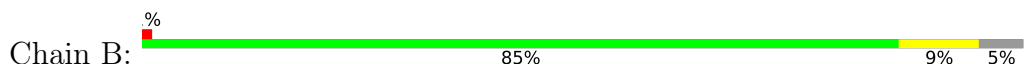
- Molecule 1: Proteasome subunit alpha type-2



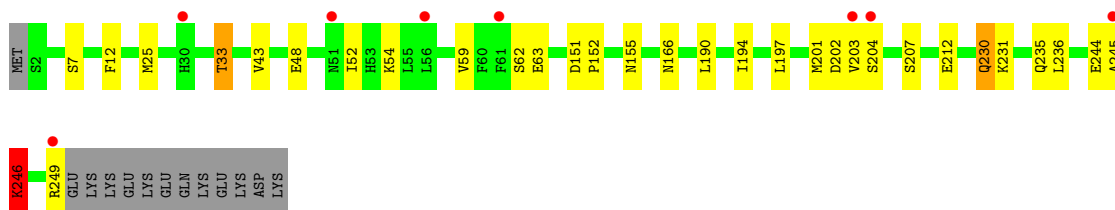
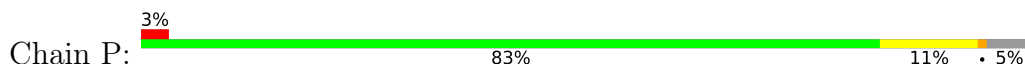
- Molecule 1: Proteasome subunit alpha type-2



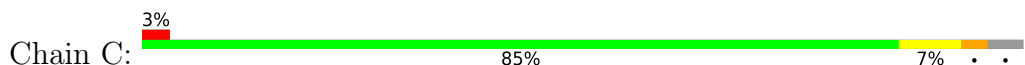
- Molecule 2: Proteasome subunit alpha type-4

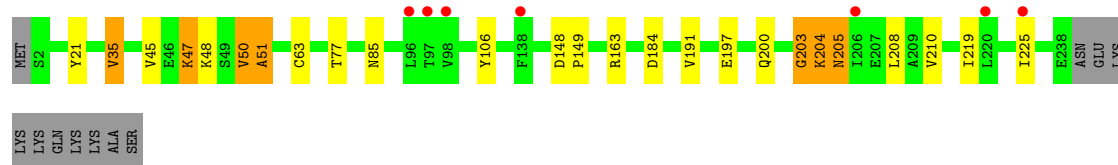


- Molecule 2: Proteasome subunit alpha type-4

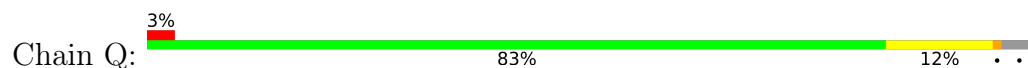


- Molecule 3: Proteasome subunit alpha type-7

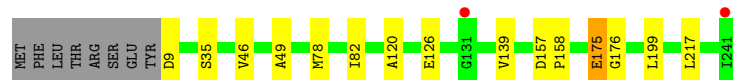
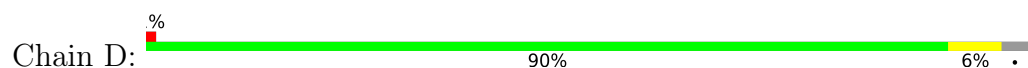




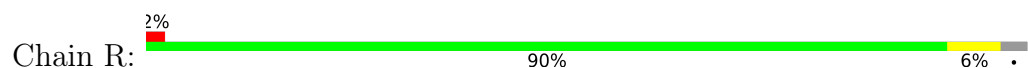
• Molecule 3: Proteasome subunit alpha type-7



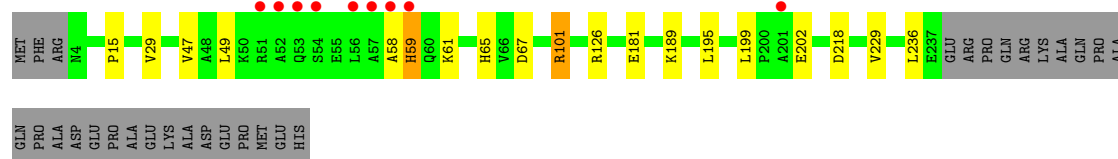
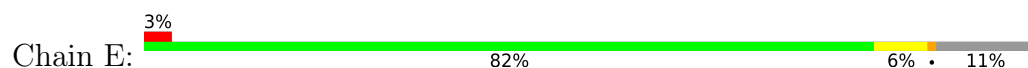
• Molecule 4: Proteasome subunit alpha type-5



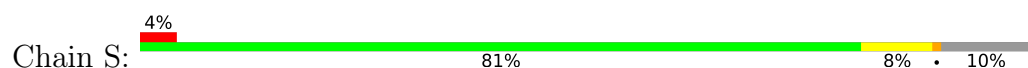
• Molecule 4: Proteasome subunit alpha type-5

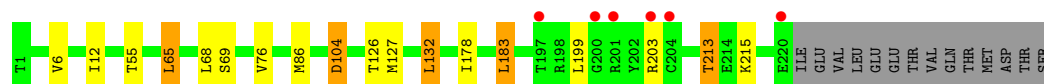


• Molecule 5: Proteasome subunit alpha type-1

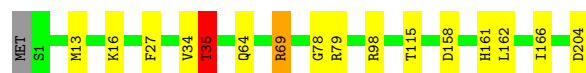


• Molecule 5: Proteasome subunit alpha type-1





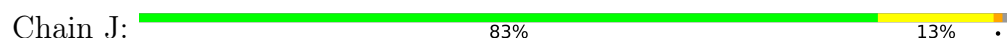
- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Z-LLY-ketoaldehyde peptide



There are no outlier residues recorded for this chain.

- Molecule 11: Z-LLY-ketoaldehyde peptide

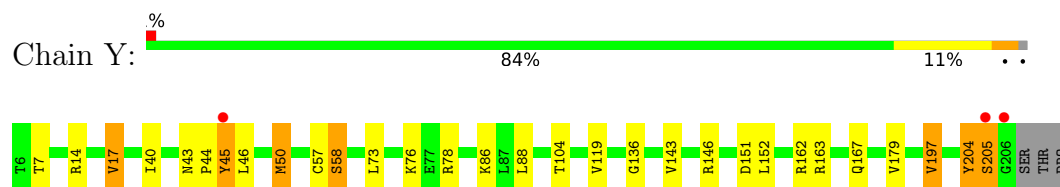


There are no outlier residues recorded for this chain.

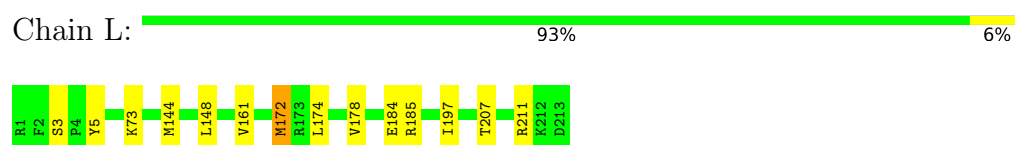
- Molecule 12: Proteasome subunit beta type-5



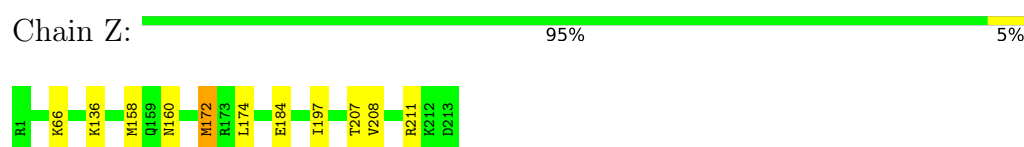
- Molecule 12: Proteasome subunit beta type-5



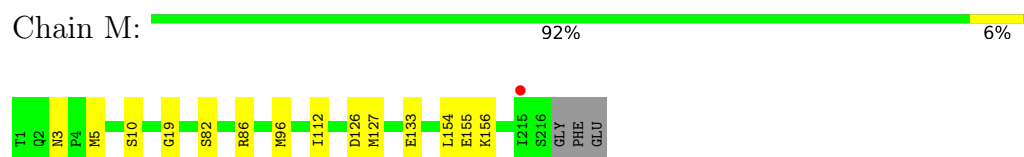
- Molecule 13: Proteasome subunit beta type-1



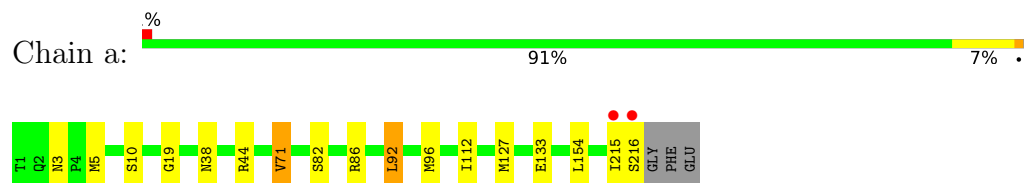
- Molecule 13: Proteasome subunit beta type-1



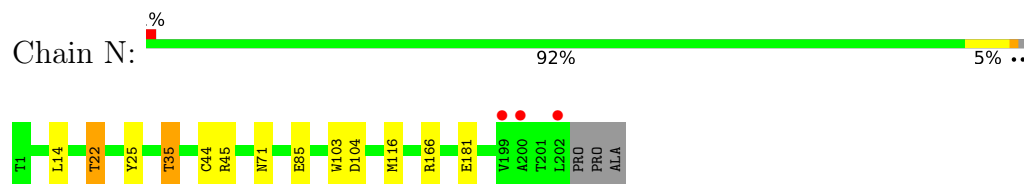
- Molecule 14: Proteasome subunit beta type-4



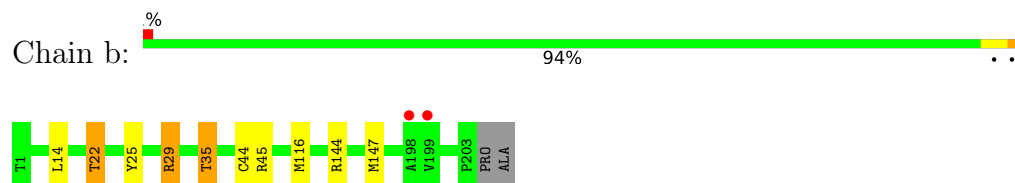
- Molecule 14: Proteasome subunit beta type-4



- Molecule 15: Proteasome subunit beta type-6



- Molecule 15: Proteasome subunit beta type-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.87Å 203.48Å 315.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.02 – 2.07 171.02 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.4 (171.02-2.07) 96.4 (171.02-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.186 , 0.227 0.193 , 0.230	Depositor DCC
R_{free} test set	21152 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51953	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: YCM, PHQ, CL, 1PE, NEN, MG, 6VF, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	0/1833	0.95	0/2489
1	O	0.82	0/1778	0.94	0/2419
2	B	1.00	1/1962 (0.1%)	1.02	5/2649 (0.2%)
2	P	0.84	0/1945	0.98	1/2631 (0.0%)
3	C	0.98	0/1818	1.09	3/2469 (0.1%)
3	Q	0.96	2/1834 (0.1%)	1.09	8/2490 (0.3%)
4	D	0.91	0/1789	0.99	1/2424 (0.0%)
4	R	1.06	1/1780 (0.1%)	1.04	2/2408 (0.1%)
5	E	1.02	1/1849 (0.1%)	1.03	1/2505 (0.0%)
5	S	1.01	1/1908 (0.1%)	1.05	3/2583 (0.1%)
6	F	1.12	1/1935 (0.1%)	1.08	4/2605 (0.2%)
6	T	1.02	1/1894 (0.1%)	1.10	6/2556 (0.2%)
7	G	1.07	3/1923 (0.2%)	1.04	4/2601 (0.2%)
7	U	0.92	1/1818 (0.1%)	0.98	1/2463 (0.0%)
8	H	1.13	0/1697	1.01	1/2299 (0.0%)
8	V	0.93	0/1655	0.96	0/2251
9	I	1.07	2/1648 (0.1%)	1.12	8/2219 (0.4%)
9	W	0.84	0/1630	1.01	7/2197 (0.3%)
10	J	1.14	2/1620 (0.1%)	1.02	0/2191
10	X	0.99	0/1606	0.98	0/2174
11	c	0.72	0/15	1.44	0/19
11	d	1.17	0/15	1.24	0/19
12	K	0.99	0/1584	1.02	0/2141
12	Y	1.11	1/1620 (0.1%)	1.10	4/2185 (0.2%)
13	L	0.93	1/1672 (0.1%)	0.98	1/2257 (0.0%)
13	Z	1.11	0/1675	1.03	1/2257 (0.0%)
14	M	1.06	1/1728 (0.1%)	1.01	2/2339 (0.1%)
14	a	1.12	1/1724 (0.1%)	1.05	3/2336 (0.1%)
15	N	1.18	2/1545 (0.1%)	1.10	2/2091 (0.1%)
15	b	1.11	0/1554	1.10	2/2104 (0.1%)
All	All	1.02	22/49054 (0.0%)	1.03	70/66371 (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
2	P	0	4
3	Q	0	2
4	D	0	2
4	R	0	2
6	T	0	1
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
14	a	0	1
All	All	0	17

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	3	ASN	C-O	-7.96	1.18	1.25
9	I	34	VAL	N-CA	6.83	1.53	1.45
5	S	3	ARG	N-CA	6.50	1.54	1.46
9	I	98	ARG	C-O	-6.12	1.16	1.24
3	Q	206	ILE	CA-C	5.83	1.60	1.52
2	B	97	TYR	N-CA	-5.72	1.39	1.46
7	G	108	GLU	CD-OE1	5.70	1.36	1.25
12	Y	45	TYR	CA-C	5.63	1.59	1.52
6	F	44	GLY	N-CA	5.61	1.51	1.45
14	a	3	ASN	C-O	-5.56	1.20	1.25
10	J	127	ALA	C-O	-5.55	1.19	1.24
7	G	82	GLY	C-O	-5.54	1.20	1.24
3	Q	13	ASP	CB-CG	5.52	1.65	1.52
5	E	126	ARG	N-CA	-5.47	1.40	1.45
15	N	104	ASP	N-CA	5.27	1.50	1.45
7	G	121	ILE	CA-C	5.23	1.59	1.52
13	L	5	TYR	C-O	-5.16	1.17	1.23
4	R	39	GLY	N-CA	-5.12	1.40	1.45
10	J	23	SER	N-CA	-5.07	1.40	1.46
15	N	85	GLU	C-O	-5.05	1.18	1.24
7	U	115	CYS	C-O	-5.04	1.18	1.24
6	T	38	GLY	N-CA	-5.02	1.41	1.45

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-10.16	98.73	112.04
6	T	190	VAL	CB-CA-C	-8.85	100.45	112.04
9	I	16[A]	LYS	CA-C-N	8.65	134.80	122.08
9	I	16[A]	LYS	C-N-CA	8.65	134.80	122.08
9	I	16[B]	LYS	CA-C-N	8.65	134.80	122.08
9	I	16[B]	LYS	C-N-CA	8.65	134.80	122.08
15	N	22	THR	CB-CA-C	-8.27	96.44	110.16
12	Y	50	MET	CG-SD-CE	-8.22	82.81	100.90
4	D	120	ALA	N-CA-C	7.84	120.52	111.11
15	b	22	THR	CB-CA-C	-7.63	97.49	110.16
2	P	246	LYS	N-CA-C	7.62	121.83	112.54
14	M	10	SER	N-CA-C	7.48	119.97	110.24
6	T	6	GLY	CA-C-N	7.19	134.65	121.70
6	T	6	GLY	C-N-CA	7.19	134.65	121.70
7	U	208	ILE	N-CA-C	7.01	117.16	111.62
3	Q	13	ASP	CB-CA-C	6.91	122.25	111.13
3	C	197	GLU	N-CA-C	6.81	119.28	111.11
12	Y	204	TYR	CA-C-N	6.78	133.91	121.70
12	Y	204	TYR	C-N-CA	6.78	133.91	121.70
7	G	244	GLU	N-CA-C	6.70	119.66	109.62
14	a	71	VAL	N-CA-CB	6.68	120.61	110.58
4	R	120[A]	ALA	N-CA-C	6.62	118.16	111.07
4	R	120[B]	ALA	N-CA-C	6.62	118.16	111.07
6	F	143	ASN	N-CA-C	6.50	118.37	111.28
3	Q	12	PRO	CA-C-N	-6.49	112.92	122.86
3	Q	12	PRO	C-N-CA	-6.49	112.92	122.86
6	T	6	GLY	N-CA-C	6.41	128.38	113.18
14	a	10	SER	N-CA-C	6.41	118.57	110.24
2	B	55	LEU	N-CA-C	6.33	120.72	113.19
6	F	190	VAL	N-CA-CB	6.27	118.30	110.47
6	T	143	ASN	N-CA-C	6.27	118.11	111.28
2	B	247	ALA	N-CA-C	6.23	118.87	111.33
9	W	16[A]	LYS	CA-C-N	6.19	134.83	123.13
9	W	16[A]	LYS	C-N-CA	6.19	134.83	123.13
9	W	16[B]	LYS	CA-C-N	6.19	134.83	123.13
9	W	16[B]	LYS	C-N-CA	6.19	134.83	123.13
9	I	79	ARG	N-CA-C	6.19	117.64	108.60
9	W	79	ARG	N-CA-C	6.12	117.53	108.60
9	I	69	ARG	NE-CZ-NH1	6.08	127.58	121.50
9	I	35	THR	N-CA-CB	-6.07	101.53	111.66
6	T	190	VAL	N-CA-CB	5.99	117.95	110.47
7	G	208	ILE	N-CA-C	5.94	116.32	111.62
7	G	183	VAL	CB-CA-C	-5.92	102.66	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	12	PRO	N-CA-C	5.80	122.22	113.81
3	Q	220	LEU	CA-C-N	5.78	132.10	121.70
3	Q	220	LEU	C-N-CA	5.78	132.10	121.70
5	S	118	ILE	CA-C-N	-5.77	113.86	119.87
5	S	118	ILE	C-N-CA	-5.77	113.86	119.87
3	C	47	LYS	N-CA-C	5.75	118.27	108.67
2	B	206	LEU	N-CA-C	5.69	118.09	110.35
5	E	199	LEU	N-CA-C	5.60	117.81	110.08
7	G	183	VAL	N-CA-CB	5.50	120.73	110.77
13	Z	172	MET	CG-SD-CE	-5.49	88.83	100.90
6	F	204	VAL	N-CA-CB	5.45	116.81	110.65
9	W	69	ARG	NE-CZ-NH1	5.44	126.94	121.50
15	N	166	ARG	N-CA-C	5.37	119.94	112.90
9	I	69	ARG	NE-CZ-NH2	-5.37	114.37	119.20
14	M	19	GLY	N-CA-C	5.35	118.07	110.74
15	b	29	ARG	CB-CA-C	-5.31	99.53	109.72
3	Q	220	LEU	N-CA-C	-5.29	101.07	109.96
12	Y	17	VAL	CB-CA-C	5.27	117.29	110.12
2	B	52	ILE	N-CA-C	5.21	118.73	113.47
2	B	97	TYR	N-CA-C	-5.19	105.52	111.07
14	a	19	GLY	N-CA-C	5.14	118.05	110.80
3	C	184	ASP	N-CA-C	5.10	116.52	111.07
3	Q	206	ILE	N-CA-C	5.07	119.89	109.34
13	L	172	MET	CG-SD-CE	-5.06	89.77	100.90
5	S	58	ALA	N-CA-C	-5.05	103.87	110.53
8	H	77	VAL	CB-CA-C	-5.02	104.38	112.16
9	W	35	THR	N-CA-CB	-5.01	103.29	111.66

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	202	ASP	Peptide
2	P	203	VAL	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
3	Q	47	LYS	Peptide

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Mol	Chain	Res	Type	Group
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
6	T	5	THR	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
14	a	215	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1761	9	0
1	O	1741	0	1683	6	0
2	B	1926	0	1924	7	0
2	P	1909	0	1874	10	0
3	C	1798	0	1718	16	0
3	Q	1820	0	1749	8	0
4	D	1762	0	1709	3	0
4	R	1753	0	1726	6	0
5	E	1813	0	1783	9	0
5	S	1866	0	1822	23	0
6	F	1888	0	1882	14	0
6	T	1856	0	1816	9	0
7	G	1894	0	1890	6	0
7	U	1797	0	1756	14	0
8	H	1664	0	1681	11	0
8	V	1622	0	1595	8	0
9	I	1613	0	1646	8	0
9	W	1599	0	1621	8	0
10	J	1581	0	1585	20	0
10	X	1567	0	1565	16	0
11	c	40	0	28	0	0
11	d	40	0	28	0	0
12	K	1550	0	1503	8	0
12	Y	1580	0	1554	20	0
13	L	1636	0	1625	6	0
13	Z	1642	0	1635	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	1692	0	1670	7	0
14	a	1688	0	1658	9	0
15	N	1516	0	1487	9	0
15	b	1524	0	1496	8	0
16	A	4	0	0	0	0
16	B	2	0	0	0	0
16	C	2	0	0	0	0
16	D	2	0	0	0	0
16	E	3	0	0	0	0
16	F	1	0	0	0	0
16	G	2	0	0	1	0
16	H	2	0	0	0	0
16	I	1	0	0	0	0
16	K	3	0	0	0	0
16	M	3	0	0	0	0
16	N	4	0	0	0	0
16	O	4	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	0	0
16	R	2	0	0	0	0
16	S	3	0	0	0	0
16	U	1	0	0	0	0
16	V	2	0	0	0	0
16	W	1	0	0	0	0
16	Y	4	0	0	0	0
16	a	3	0	0	2	0
16	b	3	0	0	1	0
17	E	9	0	8	0	0
17	G	18	0	16	1	0
17	J	9	0	8	1	0
17	S	9	0	8	0	0
17	U	18	0	16	0	0
17	X	9	0	8	1	0
18	G	1	0	0	0	0
18	L	1	0	0	0	0
18	N	1	0	0	0	0
18	U	1	0	0	0	0
18	Z	1	0	0	0	0
18	b	1	0	0	0	0
19	H	2	0	0	0	0
19	I	1	0	0	0	0
19	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	1	0	0	0	0
19	V	2	0	0	0	0
19	W	1	0	0	0	0
19	X	1	0	0	0	0
19	Y	1	0	0	0	0
20	I	32	0	44	0	0
20	L	16	0	22	0	0
20	M	16	0	22	0	0
20	N	16	0	22	0	0
20	W	16	0	22	0	0
20	Z	16	0	22	0	0
20	a	16	0	22	0	0
20	b	16	0	22	0	0
21	A	108	0	0	0	0
21	B	119	0	0	0	0
21	C	75	0	0	0	0
21	D	86	0	0	0	0
21	E	137	0	0	2	0
21	F	179	0	0	6	0
21	G	190	0	0	0	0
21	H	150	0	0	2	0
21	I	157	0	0	1	0
21	J	133	0	0	3	0
21	K	92	0	0	0	0
21	L	121	0	0	0	0
21	M	145	0	0	0	0
21	N	156	0	0	1	0
21	O	89	0	0	1	0
21	P	109	0	0	0	0
21	Q	71	0	0	1	0
21	R	119	0	0	0	0
21	S	124	0	0	5	0
21	T	91	0	0	1	0
21	U	103	0	0	0	0
21	V	109	0	0	0	0
21	W	108	0	0	1	0
21	X	124	0	0	1	0
21	Y	141	0	0	0	0
21	Z	167	0	0	2	0
21	a	172	0	0	1	0
21	b	121	0	0	0	0
21	c	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	d	2	0	0	0	0
All	All	51953	0	47732	252	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 3.

All (252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:50:MET:HE1	12:Y:58:SER:HA	1.46	0.97
5:S:152[B]:ASN:ND2	21:S:401:HOH:O	2.07	0.87
5:S:65[A]:HIS:CE1	21:S:402:HOH:O	2.29	0.84
13:L:144:MET:HE1	13:L:185:ARG:HB2	1.66	0.78
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.32	0.74
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.06	0.74
7:U:118:ILE:HG13	7:U:138:MET:HE1	1.69	0.73
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.52	0.73
12:Y:204:TYR:HA	12:Y:205:SER:HB2	1.72	0.72
12:Y:50:MET:HE2	12:Y:57:CYS:HB3	1.72	0.70
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.24	0.69
1:A:17:LYS:HE2	1:A:22:GLU:OE2	1.93	0.69
6:F:169[A]:ARG:NH1	21:F:401:HOH:O	2.25	0.68
1:O:10:THR:HG23	21:O:401:HOH:O	1.93	0.67
5:S:65[A]:HIS:ND1	21:S:402:HOH:O	2.25	0.67
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.77	0.66
10:X:1:MET:HE1	10:X:134:TYR:H	1.60	0.66
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.41	0.66
9:I:35:THR:HG21	21:I:446:HOH:O	1.96	0.66
7:U:138:MET:HE3	7:U:140:LEU:HD11	1.78	0.65
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	1.95	0.65
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.78	0.65
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.31	0.64
12:Y:163:ARG:HE	12:Y:167:GLN:HE21	1.44	0.63
7:U:58:ASP:O	7:U:59:LYS:CB	2.46	0.63
10:J:185:LYS:NZ	21:J:401:HOH:O	2.10	0.63
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.81	0.63
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.81	0.62
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.66	0.61
3:C:47:LYS:CB	3:C:48:LYS:CA	2.79	0.60
15:N:35:THR:CG2	15:N:45:ARG:HE	2.14	0.60
3:C:47:LYS:CB	3:C:48:LYS:HA	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:40:ILE:HD12	12:Y:50:MET:HE3	1.82	0.60
8:H:220:GLU:N	8:H:220:GLU:OE1	2.35	0.60
7:U:195:VAL:O	7:U:199:ILE:HG23	2.03	0.59
2:B:33:THR:HB	2:B:166:ASN:O	2.03	0.59
12:Y:50:MET:HE1	12:Y:58:SER:CA	2.29	0.59
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.84	0.59
15:b:35:THR:CG2	15:b:45:ARG:HE	2.15	0.59
8:V:126:THR:O	8:V:127[B]:MET:HG2	2.02	0.59
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.50	0.59
5:E:58:ALA:O	5:E:59:HIS:CB	2.51	0.59
4:R:129:ASP:CB	4:R:130:PRO:CD	2.80	0.59
2:P:246:LYS:HE3	2:P:246:LYS:N	2.18	0.59
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	2.03	0.58
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.85	0.58
12:K:145:ARG:NH1	10:X:166:GLU:OE2	2.37	0.58
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.01	0.58
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.84	0.58
12:Y:45:TYR:CD2	12:Y:78:ARG:CZ	2.87	0.58
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.85	0.57
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.22	0.57
15:b:14:LEU:HD23	15:b:44:CYS:SG	2.45	0.57
6:F:64:LYS:NZ	21:F:402:HOH:O	2.32	0.57
2:P:33:THR:HB	2:P:166:ASN:O	2.04	0.56
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.88	0.56
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.87	0.56
15:N:14:LEU:HD23	15:N:44:CYS:SG	2.47	0.55
10:J:166:GLU:OE2	12:Y:146[A]:ARG:NH1	2.40	0.55
13:Z:172:MET:HE1	13:Z:197:ILE:HD11	1.87	0.55
10:X:1:MET:HE3	10:X:1:MET:C	2.32	0.55
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.88	0.54
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.88	0.54
5:S:154:PHE:HD2	6:T:63:ASN:HD21	1.56	0.54
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	1.89	0.54
5:E:47:VAL:CG1	5:E:195:LEU:HD22	2.38	0.53
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.41	0.53
2:P:197:LEU:HD22	2:P:201:MET:HE3	1.91	0.53
13:L:144:MET:CE	13:L:185:ARG:HB2	2.38	0.53
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.91	0.52
10:X:1:MET:HE1	10:X:134:TYR:N	2.25	0.52
13:L:172:MET:HE1	13:L:197:ILE:HD11	1.90	0.52
12:Y:204:TYR:HA	12:Y:205:SER:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:144:ARG:O	15:b:147[B]:MET:SD	2.68	0.52
2:P:230:GLN:OE1	2:P:231:LYS:N	2.43	0.51
5:S:47:VAL:CG1	5:S:195:LEU:HD22	2.40	0.51
1:A:58[B]:GLU:CD	1:A:58[B]:GLU:H	2.19	0.51
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.92	0.51
9:I:27:PHE:HB3	9:I:35:THR:HG22	1.93	0.51
12:K:44:TYR:CD2	12:K:77:ARG:CZ	2.94	0.50
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.21	0.50
14:a:92:LEU:HD12	14:a:112:ILE:HD11	1.93	0.50
5:E:65:HIS:HB2	21:E:463:HOH:O	2.10	0.50
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.44	0.50
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.42	0.50
9:W:13:MET:HE2	9:W:166:ILE:HB	1.94	0.50
9:W:27:PHE:HB3	9:W:35:THR:HG22	1.94	0.50
3:C:203:GLY:CA	3:C:204:LYS:CB	2.90	0.49
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.94	0.49
3:C:35:VAL:CG1	3:C:191:VAL:CG2	2.91	0.49
10:X:38:MET:HE1	10:X:61:GLN:HB2	1.95	0.49
10:J:12:TYR:HB2	10:J:182:ILE:HD11	1.95	0.48
3:C:35:VAL:CG1	3:C:191:VAL:HG22	2.43	0.48
6:T:173:LYS:HB3	6:T:173:LYS:HE2	1.59	0.48
14:a:5:MET:HE3	15:b:116:MET:CB	2.43	0.48
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.54	0.48
7:U:244:GLU:O	7:U:245:ARG:C	2.56	0.48
7:U:113:MET:HE1	8:V:69:SER:OG	2.13	0.48
9:W:13:MET:HE3	9:W:162:LEU:HD12	1.95	0.48
6:F:105:ASN:ND2	21:F:404:HOH:O	2.47	0.48
16:a:302:CL:CL	16:b:302:CL:CL	3.06	0.48
12:Y:14:ARG:NH2	12:Y:151:ASP:OD1	2.42	0.47
21:H:531:HOH:O	13:Z:160:ASN:CB	2.62	0.47
9:W:13:MET:HE1	9:W:166:ILE:N	2.30	0.47
14:a:5:MET:HE3	15:b:116:MET:HB2	1.97	0.47
3:C:50:VAL:O	3:C:51:ALA:HB3	2.15	0.47
5:E:218:ASP:OD1	5:E:218:ASP:N	2.46	0.47
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.63	0.47
10:X:87:ASN:O	17:X:302:NEN:H11	2.15	0.47
12:K:6:THR:OG1	12:K:135:GLY:HA3	2.14	0.47
10:X:95:ARG:HH11	10:X:95:ARG:HB2	1.80	0.47
3:C:35:VAL:HG12	3:C:191:VAL:HG22	1.97	0.46
5:E:101[A]:ARG:NH1	21:E:402:HOH:O	2.48	0.46
10:J:87:ASN:O	17:J:302:NEN:H11	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:184:GLU:OE2	13:Z:211:ARG:HD2	2.15	0.46
8:H:132:LEU:HD22	15:N:25:TYR:CE2	2.50	0.46
21:Q:461:HOH:O	4:R:60:GLU:HG3	2.14	0.46
7:G:186:LYS:NZ	16:G:302:CL:CL	2.84	0.46
8:V:213:THR:HB	9:W:198:THR:OG1	2.15	0.46
14:a:86:ARG:NH1	14:a:133:GLU:OE1	2.41	0.46
10:J:27[A]:GLN:NE2	21:J:405:HOH:O	2.49	0.46
14:a:5:MET:CE	15:b:116:MET:HB3	2.46	0.46
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.98	0.46
12:Y:7:THR:OG1	12:Y:136:GLY:HA3	2.16	0.46
14:a:96:MET:HE3	14:a:127:MET:HA	1.96	0.46
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.15	0.46
10:J:182:ILE:HG13	10:J:183:ILE:N	2.31	0.46
12:K:162:ARG:HD2	12:K:166:GLN:HE21	1.81	0.46
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.94	0.46
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.97	0.46
14:M:5:MET:HE3	15:N:116:MET:HB2	1.97	0.46
7:G:113:MET:HE1	8:H:69:SER:OG	2.15	0.45
3:C:106:TYR:CD1	3:C:106:TYR:C	2.93	0.45
5:S:238:GLU:CB	5:S:239:ARG:C	2.89	0.45
14:M:5:MET:HE3	15:N:116:MET:CB	2.46	0.45
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.17	0.45
14:M:96:MET:HE3	14:M:127:MET:HA	1.99	0.45
2:B:63:GLU:N	2:B:212:GLU:OE2	2.49	0.45
3:C:47:LYS:HA	3:C:205:ASN:HB2	1.97	0.45
7:G:188:ASP:O	7:G:190:THR:HG22	2.16	0.45
5:S:18[B]:ARG:CG	5:S:23:GLU:OE2	2.65	0.45
5:S:176:MET:HA	5:S:179:PHE:CD2	2.52	0.45
8:H:204:CYS:SG	13:Z:158:MET:HE2	2.57	0.45
2:P:48:GLU:HB2	2:P:201:MET:HE2	1.99	0.45
9:I:158:ASP:OD1	9:I:161:HIS:CD2	2.70	0.45
14:a:112:ILE:HD12	14:a:112:ILE:N	2.32	0.45
8:V:132:LEU:HD22	15:b:25:TYR:CZ	2.52	0.45
7:G:72:ILE:HG21	7:G:114:LEU:HD21	1.99	0.45
10:X:49:GLU:O	10:X:53:THR:HG23	2.17	0.45
6:F:34:SER:OG	6:F:65:ARG:NH1	2.49	0.44
10:J:27[A]:GLN:HE21	10:J:29:LYS:N	2.15	0.44
6:T:152:ASP:OD1	6:T:156:VAL:HG12	2.17	0.44
1:A:56:TYR:CE1	17:G:304:NEN:H62	2.53	0.44
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.47	0.44
6:F:169[B]:ARG:NH2	21:F:406:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLN:HE22	1:A:58[B]:GLU:HB3	1.83	0.44
1:A:94:GLN:HG3	8:H:65:LEU:HD13	2.00	0.44
7:U:80[A]:MET:HE2	7:U:91:VAL:HG22	1.99	0.44
9:W:35:THR:HG21	21:W:447:HOH:O	2.17	0.44
8:H:77:VAL:HG12	8:H:111:TYR:OH	2.17	0.44
10:J:118:MET:HE2	10:J:124:LEU:HD13	1.99	0.44
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.17	0.44
13:Z:66:LYS:NZ	21:Z:405:HOH:O	2.50	0.44
5:S:50:LYS:CB	5:S:59:HIS:HB3	2.47	0.44
8:V:178:ILE:HG12	8:V:183:LEU:HD12	1.99	0.44
10:J:38:MET:HE1	10:J:61:GLN:HB2	1.99	0.44
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.99	0.44
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.33	0.44
12:K:196:VAL:HG11	9:W:204:ASP:HB3	1.99	0.44
14:a:38:ASN:N	16:a:301:CL:CL	2.76	0.44
1:O:55:LEU:HD12	7:U:176:THR:HG23	2.00	0.44
7:U:80[A]:MET:HE2	7:U:91:VAL:CG2	2.48	0.44
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.48	0.43
12:Y:73:LEU:O	12:Y:76:LYS:CE	2.66	0.43
3:C:47:LYS:CB	3:C:48:LYS:C	2.91	0.43
6:F:87:LEU:CD2	6:F:133[A]:CYS:SG	3.06	0.43
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	2.17	0.43
12:Y:162:ARG:HA	12:Y:179:VAL:HG11	1.99	0.43
2:B:25[B]:MET:HE3	2:B:25[B]:MET:HB3	1.79	0.43
12:K:87:LEU:HD21	12:K:103:THR:HG21	1.99	0.43
13:L:184:GLU:OE2	13:L:211:ARG:HD2	2.18	0.43
1:A:147:GLN:HG3	1:A:162:MET:HE1	2.00	0.43
7:U:62:ASP:OD2	7:U:62:ASP:C	2.60	0.43
5:E:67:ASP:OD1	13:L:73:LYS:HE2	2.19	0.43
10:J:10:PRO:HG3	10:J:150:THR:HA	2.00	0.43
12:Y:104:THR:HG22	12:Y:119:VAL:O	2.18	0.43
5:S:49:LEU:HG	5:S:195:LEU:HD21	2.00	0.43
8:H:132:LEU:HD22	15:N:25:TYR:CZ	2.54	0.43
15:b:35:THR:HG23	15:b:45:ARG:HE	1.83	0.43
15:N:103:TRP:CH2	15:N:181:GLU:HG3	2.54	0.43
4:R:157:ASP:HB2	4:R:158:PRO:CD	2.49	0.43
10:X:118:MET:HE2	10:X:124:LEU:HD13	2.01	0.42
14:a:44:ARG:HD2	21:a:530:HOH:O	2.19	0.42
6:F:151:ILE:N	6:F:151:ILE:HD12	2.33	0.42
12:K:103:THR:HG22	12:K:118:VAL:O	2.19	0.42
5:S:176:MET:HA	5:S:179:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:43:ASN:HB2	12:Y:44:PRO:CD	2.49	0.42
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.49	0.42
14:M:126:ASP:OD2	14:M:126:ASP:C	2.61	0.42
6:T:87:LEU:CD2	6:T:133[A]:CYS:SG	3.07	0.42
14:M:86:ARG:NH1	14:M:133:GLU:OE2	2.48	0.42
6:T:205:LYS:O	6:T:206:ASP:CG	2.63	0.42
2:B:151:ASP:HB2	2:B:152:PRO:CD	2.50	0.42
5:E:15:PRO:O	6:F:28:LYS:HD2	2.19	0.42
5:S:202:GLU:CD	5:S:202:GLU:H	2.27	0.42
5:S:237:GLU:O	5:S:238:GLU:CB	2.68	0.42
6:T:169:ARG:NH2	21:T:302:HOH:O	2.52	0.42
10:J:49:GLU:O	10:J:53:THR:HG23	2.19	0.42
8:V:55:THR:HG23	8:V:86:MET:HE1	2.00	0.42
13:L:148:LEU:HD23	13:L:178:VAL:CG1	2.50	0.42
4:D:157:ASP:HB2	4:D:158:PRO:CD	2.50	0.41
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.50	0.41
14:M:112:ILE:HD12	14:M:112:ILE:N	2.36	0.41
10:X:132:HIS:HD2	21:X:468:HOH:O	2.03	0.41
8:H:178:ILE:HG12	8:H:183:LEU:HD12	2.01	0.41
2:B:14:PRO:HA	3:C:21:TYR:CD1	2.55	0.41
6:F:87:LEU:HD22	6:F:133[A]:CYS:SG	2.60	0.41
6:T:191:LYS:HB3	6:T:238:TYR:CD1	2.56	0.41
13:Z:136:LYS:NZ	21:Z:406:HOH:O	2.52	0.41
5:E:49:LEU:HG	5:E:195:LEU:HD21	2.02	0.41
6:F:150:MET:C	6:F:151:ILE:HD12	2.46	0.41
1:O:94:GLN:HG3	8:V:65:LEU:HD13	2.02	0.41
1:O:230:ALA:O	1:O:231:ALA:CB	2.68	0.41
3:Q:204:LYS:HA	3:Q:205:ASN:C	2.46	0.41
12:Y:146[B]:ARG:HD2	12:Y:146[B]:ARG:HA	1.70	0.41
8:H:55:THR:HG23	8:H:86:MET:HE1	2.02	0.41
12:Y:88:LEU:HD21	12:Y:104:THR:HG21	2.02	0.41
6:F:219:LEU:HD22	21:F:439:HOH:O	2.20	0.41
4:R:129:ASP:CB	4:R:130:PRO:HD2	2.50	0.41
5:S:101:ARG:NH1	21:S:406:HOH:O	2.53	0.41
9:I:204:ASP:HB3	12:Y:197:VAL:HG11	2.02	0.41
6:T:34:SER:OG	6:T:65:ARG:NH1	2.51	0.41
6:F:221:ASN:HB2	21:F:564:HOH:O	2.21	0.41
8:H:153:ASN:ND2	21:H:402:HOH:O	2.49	0.41
12:K:101[B]:MET:HB3	12:K:101[B]:MET:HE2	1.89	0.41
15:N:71:ASN:HB2	21:N:518:HOH:O	2.21	0.41
7:U:43:ARG:HB3	7:U:151:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:63:GLU:N	2:P:212:GLU:OE2	2.51	0.41
12:Y:40:ILE:CD1	12:Y:50:MET:HE3	2.47	0.41
12:Y:204:TYR:CA	12:Y:205:SER:CB	2.99	0.41
10:J:161:ARG:HD3	21:J:437:HOH:O	2.19	0.40
10:X:182:ILE:HD13	10:X:182:ILE:HG21	1.77	0.40
5:S:171:TYR:CD1	5:S:171:TYR:C	2.98	0.40
14:M:5:MET:CE	15:N:116:MET:HB3	2.52	0.40
10:X:154:GLU:H	10:X:154:GLU:CD	2.29	0.40
7:G:49[A]:VAL:HG23	7:G:219:VAL:HG12	2.04	0.40
5:S:152[B]:ASN:ND2	21:S:407:HOH:O	2.54	0.40
5:S:158:ALA:O	6:T:57:LEU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/234 (99%)	218 (94%)	9 (4%)	4 (2%)	7	2
1	O	228/234 (97%)	214 (94%)	9 (4%)	5 (2%)	5	1
2	B	248/261 (95%)	234 (94%)	13 (5%)	1 (0%)	30	23
2	P	248/261 (95%)	234 (94%)	12 (5%)	2 (1%)	16	8
3	C	236/248 (95%)	217 (92%)	14 (6%)	5 (2%)	5	1
3	Q	236/248 (95%)	217 (92%)	12 (5%)	7 (3%)	3	0
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	9	3
4	R	232/241 (96%)	221 (95%)	8 (3%)	3 (1%)	9	3
5	E	233/263 (89%)	227 (97%)	4 (2%)	2 (1%)	14	7
5	S	239/263 (91%)	232 (97%)	6 (2%)	1 (0%)	30	23
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	239/255 (94%)	230 (96%)	6 (2%)	3 (1%)	9	3
7	G	243/246 (99%)	237 (98%)	6 (2%)	0	100	100
7	U	234/246 (95%)	229 (98%)	3 (1%)	2 (1%)	14	7
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	24	17
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100	100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100	100
10	J	196/201 (98%)	192 (98%)	4 (2%)	0	100	100
10	X	196/201 (98%)	193 (98%)	3 (2%)	0	100	100
11	c	1/4 (25%)	1 (100%)	0	0	100	100
11	d	1/4 (25%)	1 (100%)	0	0	100	100
12	K	199/204 (98%)	196 (98%)	3 (2%)	0	100	100
12	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	24	17
13	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
13	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
14	M	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
14	a	216/219 (99%)	207 (96%)	9 (4%)	0	100	100
15	N	201/205 (98%)	200 (100%)	1 (0%)	0	100	100
15	b	202/205 (98%)	201 (100%)	1 (0%)	0	100	100
All	All	6223/6466 (96%)	6020 (97%)	163 (3%)	40 (1%)	21	13

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
4	D	176	GLY
5	E	59	HIS
1	O	52	LYS
1	O	53	SER
3	Q	47	LYS
3	Q	206	ILE
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO

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Mol	Chain	Res	Type
5	S	238	GLU
12	Y	205	SER
1	A	176	ARG
2	B	203	VAL
3	C	50	VAL
3	C	51	ALA
3	C	200	GLN
3	C	204	LYS
5	E	236	LEU
1	O	176	ARG
1	O	231	ALA
2	P	54	LYS
3	Q	50	VAL
3	Q	201	SER
6	T	7	TYR
7	U	58	ASP
7	U	59	LYS
4	D	175[A]	GLU
4	D	175[B]	GLU
2	P	52	ILE
3	Q	51	ALA
3	Q	221	ASN
6	T	206	ASP
8	V	203	ARG
6	T	208	ALA
3	C	203	GLY
1	A	199	GLU
1	O	199	GLU
3	Q	203	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	174 (94%)	11 (6%)	18	10
1	O	176/191 (92%)	167 (95%)	9 (5%)	21	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	200/221 (90%)	190 (95%)	10 (5%)	22	14
2	P	197/221 (89%)	182 (92%)	15 (8%)	12	6
3	C	179/210 (85%)	171 (96%)	8 (4%)	24	18
3	Q	184/210 (88%)	172 (94%)	12 (6%)	15	8
4	D	189/203 (93%)	183 (97%)	6 (3%)	34	29
4	R	187/203 (92%)	183 (98%)	4 (2%)	47	45
5	E	193/224 (86%)	185 (96%)	8 (4%)	27	21
5	S	198/224 (88%)	193 (98%)	5 (2%)	42	38
6	F	199/212 (94%)	190 (96%)	9 (4%)	24	18
6	T	192/212 (91%)	183 (95%)	9 (5%)	23	16
7	G	204/209 (98%)	197 (97%)	7 (3%)	32	27
7	U	188/209 (90%)	182 (97%)	6 (3%)	34	29
8	H	181/195 (93%)	172 (95%)	9 (5%)	22	14
8	V	172/195 (88%)	161 (94%)	11 (6%)	16	9
9	I	176/174 (101%)	173 (98%)	3 (2%)	53	53
9	W	173/174 (99%)	171 (99%)	2 (1%)	63	65
10	J	167/171 (98%)	161 (96%)	6 (4%)	31	25
10	X	166/171 (97%)	162 (98%)	4 (2%)	43	40
11	c	2/2 (100%)	2 (100%)	0	100	100
11	d	2/2 (100%)	2 (100%)	0	100	100
12	K	155/159 (98%)	145 (94%)	10 (6%)	15	8
12	Y	159/159 (100%)	152 (96%)	7 (4%)	25	19
13	L	175/178 (98%)	170 (97%)	5 (3%)	37	33
13	Z	175/178 (98%)	172 (98%)	3 (2%)	53	53
14	M	180/181 (99%)	176 (98%)	4 (2%)	45	43
14	a	178/181 (98%)	173 (97%)	5 (3%)	38	34
15	N	157/159 (99%)	155 (99%)	2 (1%)	61	62
15	b	158/159 (99%)	155 (98%)	3 (2%)	50	49
All	All	5047/5378 (94%)	4854 (96%)	193 (4%)	29	23

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	53	SER
1	A	61	VAL
1	A	69	LYS
1	A	73	LEU
1	A	180	ASP
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP
2	B	33	THR
2	B	43	VAL
2	B	59	VAL
2	B	62	SER
2	B	190	LEU
2	B	194	ILE
2	B	207	SER
2	B	229	LYS
2	B	230	GLN
2	B	249	ARG
3	C	35	VAL
3	C	45	VAL
3	C	163	ARG
3	C	205	ASN
3	C	208	LEU
3	C	210	VAL
3	C	219	ILE
3	C	225	ILE
4	D	9	ASP
4	D	35	SER
4	D	46	VAL
4	D	126	GLU
4	D	139	VAL
4	D	199	LEU
5	E	29	VAL
5	E	61	LYS
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	181	GLU
5	E	189	LYS
5	E	202	GLU
5	E	229	VAL

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Mol	Chain	Res	Type
6	F	17	ASP
6	F	53	VAL
6	F	81	LEU
6	F	86	SER
6	F	87	LEU
6	F	187	ARG
6	F	190	VAL
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
7	G	226	LYS
8	H	6	VAL
8	H	12	ILE
8	H	65	LEU
8	H	68	LEU
8	H	132	LEU
8	H	183	LEU
8	H	197	THR
8	H	215	LYS
8	H	220	GLU
9	I	35	THR
9	I	69	ARG
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	62	LYS
10	J	88	LEU
10	J	155	ARG
10	J	182	ILE
12	K	16	VAL
12	K	45	LEU
12	K	46	LEU
12	K	85	LYS
12	K	142	VAL
12	K	151	LEU
12	K	162	ARG
12	K	178	VAL

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Mol	Chain	Res	Type
12	K	191	VAL
12	K	196	VAL
13	L	3[A]	SER
13	L	3[B]	SER
13	L	161	VAL
13	L	174	LEU
13	L	207	THR
14	M	82	SER
14	M	154	LEU
14	M	155	GLU
14	M	156	LYS
15	N	22	THR
15	N	35	THR
1	O	10	THR
1	O	53	SER
1	O	167	VAL
1	O	180	ASP
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	43	VAL
2	P	59	VAL
2	P	62	SER
2	P	190	LEU
2	P	194	ILE
2	P	204	SER
2	P	207	SER
2	P	230	GLN
2	P	235	GLN
2	P	236	LEU
2	P	246	LYS
2	P	249	ARG
3	Q	45	VAL
3	Q	54	GLN
3	Q	98	VAL
3	Q	163	ARG
3	Q	170	GLU

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Mol	Chain	Res	Type
3	Q	206	ILE
3	Q	208	LEU
3	Q	219	ILE
3	Q	223	GLU
3	Q	225	ILE
3	Q	226	GLU
3	Q	227	LYS
4	R	9	ASP
4	R	35	SER
4	R	46	VAL
4	R	139	VAL
5	S	29	VAL
5	S	45	VAL
5	S	101	ARG
5	S	202	GLU
5	S	229	VAL
6	T	17	ASP
6	T	33	SER
6	T	53	VAL
6	T	81	LEU
6	T	86	SER
6	T	87	LEU
6	T	190	VAL
6	T	223	ARG
6	T	240	LYS
7	U	42	VAL
7	U	78	CYS
7	U	151	VAL
7	U	199	ILE
7	U	206	LEU
7	U	223	GLU
8	V	6	VAL
8	V	12	ILE
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	132	LEU
8	V	183	LEU
8	V	199	LEU
8	V	213	THR
8	V	215	LYS

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Mol	Chain	Res	Type
9	W	35	THR
9	W	69	ARG
10	X	1	MET
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
12	Y	17	VAL
12	Y	46	LEU
12	Y	58	SER
12	Y	86	LYS
12	Y	143	VAL
12	Y	152	LEU
12	Y	197	VAL
13	Z	174	LEU
13	Z	207	THR
13	Z	208	VAL
14	a	71	VAL
14	a	82	SER
14	a	92	LEU
14	a	154	LEU
14	a	216	SER
15	b	22	THR
15	b	29	ARG
15	b	35	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	62	HIS
1	A	94	GLN
1	A	108	GLN
1	A	111	GLN
1	A	206	ASN
2	B	40	ASN
2	B	88	ASN
2	B	100	GLN
2	B	102	GLN
3	C	94	HIS
4	D	122	GLN
4	D	152	GLN
4	D	227	HIS

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Mol	Chain	Res	Type
5	E	65	HIS
6	F	143	ASN
7	G	68	HIS
7	G	100	ASN
8	H	80	ASN
8	H	172	ASN
9	I	161	HIS
10	J	61	GLN
10	J	63	ASN
10	J	101	ASN
10	J	132	HIS
10	J	186	ASN
12	K	66	GLN
12	K	123	ASN
12	K	166	GLN
13	L	152	GLN
13	L	157	ASN
14	M	65	GLN
14	M	162	GLN
14	M	188	GLN
1	O	111	GLN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	88	ASN
2	P	102	GLN
2	P	142	HIS
2	P	146	GLN
2	P	166	ASN
3	Q	18	GLN
3	Q	94	HIS
3	Q	221	ASN
4	R	97	GLN
4	R	152	GLN
4	R	186	HIS
4	R	227	HIS
5	S	8	ASN
5	S	60	GLN
6	T	63	ASN
6	T	68	ASN
6	T	110	HIS
6	T	143	ASN

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Mol	Chain	Res	Type
7	U	68	HIS
7	U	100	ASN
8	V	80	ASN
8	V	116	HIS
8	V	172	ASN
9	W	32	GLN
9	W	172	ASN
10	X	24	ASN
10	X	61	GLN
10	X	63	ASN
10	X	174	ASN
12	Y	67	GLN
12	Y	124	ASN
12	Y	167	GLN
13	Z	77	HIS
13	Z	79	ASN
14	a	47	ASN
14	a	65	GLN
14	a	89	HIS
14	a	162	GLN
14	a	188	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	YCM	U	137	7	7,9,10	0.96	0	5,10,12	1.36	1 (20%)
3	YCM	C	63	3	7,9,10	1.04	1 (14%)	5,10,12	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	YCM	Q	63	3	7,9,10	1.30	1 (14%)	5,10,12	3.38	4 (80%)
7	YCM	G	137	7	7,9,10	1.73	2 (28%)	5,10,12	2.05	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	YCM	U	137	7	-	2/6/8/10	-
3	YCM	C	63	3	-	0/6/8/10	-
3	YCM	Q	63	3	-	3/6/8/10	-
7	YCM	G	137	7	-	3/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CE-NZ2	2.88	1.42	1.32
3	Q	63	YCM	CD-SG	-2.60	1.75	1.81
7	G	137	YCM	CD-SG	2.23	1.87	1.81
3	C	63	YCM	CD-SG	-2.04	1.76	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	63	YCM	CE-CD-SG	-4.88	98.41	113.81
7	G	137	YCM	CE-CD-SG	3.87	126.04	113.81
3	Q	63	YCM	CA-CB-SG	-3.54	100.45	113.51
3	Q	63	YCM	CB-SG-CD	3.33	133.92	104.24
3	Q	63	YCM	CB-CA-C	-2.69	103.48	110.80
7	U	137	YCM	CE-CD-SG	2.64	122.14	113.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	CE-CD-SG-CB
7	G	137	YCM	SG-CD-CE-NZ2
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1

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Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-OZ1
7	U	137	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-NZ2
7	U	137	YCM	SG-CD-CE-NZ2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 71 are monoatomic - leaving 17 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	NEN	G	304	7	9,9,9	1.57	2 (22%)	12,12,12	3.17	9 (75%)
17	NEN	S	304	5	9,9,9	1.25	2 (22%)	12,12,12	2.86	6 (50%)
20	1PE	I	303	-	15,15,15	0.58	0	14,14,14	1.09	2 (14%)
17	NEN	J	302	10	9,9,9	0.94	1 (11%)	12,12,12	4.34	7 (58%)
20	1PE	M	304	-	15,15,15	0.53	0	14,14,14	0.38	0
20	1PE	b	304	-	15,15,15	0.68	0	14,14,14	0.78	0
20	1PE	L	301	-	15,15,15	0.59	0	14,14,14	0.72	0
17	NEN	X	302	10	9,9,9	1.43	1 (11%)	12,12,12	4.69	9 (75%)
20	1PE	W	303	-	15,15,15	0.52	0	14,14,14	0.42	0
20	1PE	Z	301	-	15,15,15	0.55	0	14,14,14	0.40	0
20	1PE	a	304	-	15,15,15	0.53	0	14,14,14	0.41	0
17	NEN	E	304	5	9,9,9	1.27	1 (11%)	12,12,12	3.04	7 (58%)
20	1PE	N	305	-	15,15,15	0.57	0	14,14,14	0.57	0
20	1PE	I	304	-	15,15,15	0.51	0	14,14,14	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NEN	U	304	7	9,9,9	1.44	2 (22%)	12,12,12	2.92	5 (41%)
17	NEN	G	305	7	9,9,9	1.89	2 (22%)	12,12,12	3.02	4 (33%)
17	NEN	U	303	7	9,9,9	1.38	2 (22%)	12,12,12	4.41	7 (58%)

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	NEN	G	304	7	-	2/2/15/15	0/1/1/1
17	NEN	S	304	5	-	0/2/15/15	0/1/1/1
20	1PE	I	303	-	-	8/13/13/13	-
17	NEN	J	302	10	-	2/2/15/15	0/1/1/1
20	1PE	M	304	-	-	7/13/13/13	-
20	1PE	b	304	-	-	8/13/13/13	-
20	1PE	L	301	-	-	6/13/13/13	-
17	NEN	X	302	10	-	2/2/15/15	0/1/1/1
20	1PE	W	303	-	-	6/13/13/13	-
20	1PE	Z	301	-	-	5/13/13/13	-
20	1PE	a	304	-	-	5/13/13/13	-
17	NEN	E	304	5	-	2/2/15/15	0/1/1/1
20	1PE	N	305	-	-	6/13/13/13	-
20	1PE	I	304	-	-	7/13/13/13	-
17	NEN	U	304	7	-	0/2/15/15	0/1/1/1
17	NEN	G	305	7	-	0/2/15/15	0/1/1/1
17	NEN	U	303	7	-	2/2/15/15	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	305	NEN	C3-N1	-4.45	1.31	1.38
17	G	304	NEN	C3-N1	-3.81	1.32	1.38
17	X	302	NEN	C3-N1	-3.70	1.33	1.38
17	G	305	NEN	C2-N1	-3.36	1.33	1.38
17	U	304	NEN	C3-N1	-3.35	1.33	1.38
17	U	303	NEN	C3-N1	-3.16	1.33	1.38
17	E	304	NEN	C3-N1	-3.05	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	S	304	NEN	C2-N1	-2.60	1.34	1.38
17	G	304	NEN	C2-N1	-2.59	1.34	1.38
17	U	304	NEN	C2-N1	-2.33	1.35	1.38
17	J	302	NEN	C3-N1	-2.25	1.35	1.38
17	U	303	NEN	C2-N1	-2.24	1.35	1.38
17	S	304	NEN	C3-N1	-2.02	1.35	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	U	303	NEN	C3-N1-C2	-10.71	108.26	112.94
17	X	302	NEN	C3-N1-C2	-8.19	109.36	112.94
17	E	304	NEN	C3-N1-C2	-7.55	109.64	112.94
17	J	302	NEN	C5-N1-C2	7.51	131.40	122.52
17	X	302	NEN	O1-C2-N1	7.41	131.88	123.94
17	X	302	NEN	C5-N1-C2	7.28	131.13	122.52
17	J	302	NEN	C3-N1-C2	-7.13	109.83	112.94
17	J	302	NEN	O1-C2-N1	6.93	131.38	123.94
17	U	303	NEN	C1-C2-N1	6.73	113.87	108.03
17	G	305	NEN	C4-C1-C2	-6.41	98.67	105.24
17	G	305	NEN	C1-C2-N1	6.04	113.27	108.03
17	X	302	NEN	C4-C3-N1	5.85	113.11	108.03
17	J	302	NEN	C4-C3-N1	5.64	112.93	108.03
17	G	304	NEN	C1-C2-N1	5.50	112.81	108.03
17	S	304	NEN	C3-N1-C2	-5.37	110.59	112.94
17	U	304	NEN	C3-N1-C2	-5.32	110.61	112.94
17	S	304	NEN	C1-C2-N1	5.25	112.59	108.03
17	U	304	NEN	C1-C2-N1	5.02	112.38	108.03
17	U	303	NEN	C4-C1-C2	-5.01	100.10	105.24
17	U	304	NEN	C4-C1-C2	-4.86	100.26	105.24
17	G	304	NEN	C3-N1-C2	-4.72	110.88	112.94
17	G	304	NEN	C4-C1-C2	-4.70	100.42	105.24
17	G	305	NEN	C3-N1-C2	-4.38	111.02	112.94
17	G	304	NEN	O2-C3-N1	4.11	128.35	123.94
17	E	304	NEN	C5-N1-C2	4.09	127.36	122.52
17	U	303	NEN	C4-C3-N1	4.06	111.55	108.03
17	X	302	NEN	O1-C2-C1	-3.90	117.05	127.12
17	U	303	NEN	C5-N1-C2	3.75	126.95	122.52
17	S	304	NEN	C4-C3-N1	3.70	111.24	108.03
17	X	302	NEN	C1-C2-N1	3.47	111.04	108.03
17	J	302	NEN	C5-N1-C3	-3.47	118.42	122.52
17	J	302	NEN	O1-C2-C1	-3.16	118.96	127.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	U	304	NEN	C5-N1-C2	3.09	126.17	122.52
17	S	304	NEN	C5-N1-C3	3.08	126.16	122.52
17	X	302	NEN	C5-N1-C3	-3.01	118.96	122.52
17	U	304	NEN	C4-C3-N1	3.00	110.64	108.03
17	G	305	NEN	C5-N1-C2	2.98	126.04	122.52
17	J	302	NEN	C1-C4-C3	-2.94	102.22	105.24
17	E	304	NEN	C4-C3-N1	2.84	110.49	108.03
17	E	304	NEN	C4-C1-C2	-2.78	102.40	105.24
20	I	303	1PE	C25-OH5-C14	2.71	125.12	113.26
17	E	304	NEN	O1-C2-N1	2.65	126.78	123.94
17	S	304	NEN	C4-C1-C2	-2.57	102.61	105.24
17	E	304	NEN	C1-C4-C3	-2.57	102.61	105.24
17	X	302	NEN	C4-C1-C2	-2.52	102.66	105.24
17	X	302	NEN	C1-C4-C3	-2.49	102.69	105.24
17	G	304	NEN	O1-C2-C1	-2.47	120.73	127.12
17	U	303	NEN	O2-C3-N1	2.44	126.56	123.94
17	S	304	NEN	C1-C4-C3	-2.42	102.76	105.24
17	G	304	NEN	C4-C3-N1	2.31	110.04	108.03
17	G	304	NEN	O1-C2-N1	2.31	126.42	123.94
20	I	303	1PE	OH5-C25-C15	2.30	120.85	110.35
17	G	304	NEN	C5-N1-C2	2.26	125.19	122.52
17	G	304	NEN	O2-C3-C4	-2.14	121.58	127.12
17	E	304	NEN	C1-C2-N1	2.09	109.85	108.03
17	U	303	NEN	O2-C3-C4	-2.03	121.88	127.12

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	E	304	NEN	C6-C5-N1-C2
17	E	304	NEN	C6-C5-N1-C3
17	J	302	NEN	C6-C5-N1-C2
17	J	302	NEN	C6-C5-N1-C3
17	X	302	NEN	C6-C5-N1-C2
17	X	302	NEN	C6-C5-N1-C3
20	I	303	1PE	C15-C25-OH5-C14
20	I	304	1PE	C24-C14-OH5-C25
20	I	304	1PE	OH4-C13-C23-OH3
20	M	304	1PE	OH4-C13-C23-OH3
20	Z	301	1PE	OH6-C15-C25-OH5
20	b	304	1PE	OH4-C13-C23-OH3
20	b	304	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
20	W	303	1PE	OH6-C15-C25-OH5
20	L	301	1PE	OH5-C14-C24-OH4
20	I	304	1PE	OH7-C16-C26-OH6
20	M	304	1PE	OH5-C14-C24-OH4
20	a	304	1PE	OH5-C14-C24-OH4
20	L	301	1PE	OH6-C15-C25-OH5
20	a	304	1PE	OH4-C13-C23-OH3
20	N	305	1PE	OH4-C13-C23-OH3
20	L	301	1PE	OH2-C12-C22-OH3
20	N	305	1PE	OH2-C12-C22-OH3
20	I	304	1PE	OH5-C14-C24-OH4
20	L	301	1PE	C16-C26-OH6-C15
20	N	305	1PE	OH7-C16-C26-OH6
20	M	304	1PE	OH2-C12-C22-OH3
20	M	304	1PE	OH6-C15-C25-OH5
20	Z	301	1PE	C16-C26-OH6-C15
20	I	303	1PE	OH6-C15-C25-OH5
20	b	304	1PE	C25-C15-OH6-C26
20	b	304	1PE	OH5-C14-C24-OH4
20	I	303	1PE	OH5-C14-C24-OH4
20	I	303	1PE	OH4-C13-C23-OH3
20	L	301	1PE	C25-C15-OH6-C26
20	Z	301	1PE	C12-C22-OH3-C23
20	I	304	1PE	C12-C22-OH3-C23
20	Z	301	1PE	C15-C25-OH5-C14
20	L	301	1PE	C13-C23-OH3-C22
20	W	303	1PE	C13-C23-OH3-C22
20	I	304	1PE	C16-C26-OH6-C15
20	b	304	1PE	C12-C22-OH3-C23
17	G	304	NEN	C6-C5-N1-C3
20	Z	301	1PE	OH7-C16-C26-OH6
20	I	303	1PE	C24-C14-OH5-C25
20	M	304	1PE	C23-C13-OH4-C24
20	W	303	1PE	C14-C24-OH4-C13
17	U	303	NEN	C6-C5-N1-C3
20	M	304	1PE	C15-C25-OH5-C14
20	W	303	1PE	C24-C14-OH5-C25
20	b	304	1PE	C24-C14-OH5-C25
20	N	305	1PE	C12-C22-OH3-C23
20	a	304	1PE	OH2-C12-C22-OH3
20	M	304	1PE	C14-C24-OH4-C13
20	I	304	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
20	a	304	1PE	OH6-C15-C25-OH5
20	W	303	1PE	OH7-C16-C26-OH6
20	I	303	1PE	C23-C13-OH4-C24
20	N	305	1PE	C25-C15-OH6-C26
20	b	304	1PE	C14-C24-OH4-C13
20	b	304	1PE	C23-C13-OH4-C24
17	G	304	NEN	C6-C5-N1-C2
17	U	303	NEN	C6-C5-N1-C2
20	a	304	1PE	C25-C15-OH6-C26
20	I	303	1PE	OH2-C12-C22-OH3
20	I	303	1PE	C13-C23-OH3-C22
20	W	303	1PE	C23-C13-OH4-C24
20	N	305	1PE	C13-C23-OH3-C22

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	304	NEN	1	0
17	J	302	NEN	1	0
17	X	302	NEN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	A	230/234 (98%)	-0.03	4 (1%) 69 71	27, 52, 90, 106	3 (1%)
1	O	230/234 (98%)	0.33	5 (2%) 62 64	43, 70, 110, 140	0
2	B	248/261 (95%)	0.05	3 (1%) 76 78	23, 56, 99, 133	2 (0%)
2	P	248/261 (95%)	0.27	8 (3%) 50 50	34, 66, 117, 153	2 (0%)
3	C	236/248 (95%)	0.36	7 (2%) 52 53	31, 67, 112, 136	2 (0%)
3	Q	238/248 (95%)	0.41	7 (2%) 53 55	36, 68, 128, 154	0
4	D	233/241 (96%)	0.21	2 (0%) 81 83	34, 66, 99, 141	1 (0%)
4	R	233/241 (96%)	-0.07	6 (2%) 57 59	22, 47, 75, 115	1 (0%)
5	E	234/263 (88%)	0.01	9 (3%) 44 44	27, 47, 98, 121	1 (0%)
5	S	238/263 (90%)	-0.01	10 (4%) 40 41	22, 50, 89, 110	3 (1%)
6	F	239/255 (93%)	-0.30	3 (1%) 75 77	23, 39, 64, 80	4 (1%)
6	T	240/255 (94%)	0.14	5 (2%) 63 66	30, 55, 92, 134	1 (0%)
7	G	243/246 (98%)	-0.20	4 (1%) 70 73	23, 43, 80, 113	2 (0%)
7	U	237/246 (96%)	0.20	4 (1%) 69 71	32, 64, 98, 116	1 (0%)
8	H	220/234 (94%)	-0.25	1 (0%) 87 89	21, 39, 70, 117	2 (0%)
8	V	220/234 (94%)	0.05	6 (2%) 56 58	27, 54, 85, 123	2 (0%)
9	I	204/205 (99%)	-0.40	0 100 100	23, 39, 60, 73	3 (1%)
9	W	204/205 (99%)	0.02	1 (0%) 87 89	32, 55, 80, 92	2 (0%)
10	J	196/201 (97%)	-0.30	1 (0%) 87 89	18, 43, 61, 85	3 (1%)
10	X	196/201 (97%)	-0.17	0 100 100	20, 47, 62, 86	2 (1%)
11	c	2/4 (50%)	-0.27	0 100 100	40, 40, 40, 43	0
11	d	2/4 (50%)	-0.68	0 100 100	32, 32, 32, 36	0
12	K	200/204 (98%)	-0.08	1 (0%) 87 89	28, 51, 78, 95	1 (0%)
12	Y	201/204 (98%)	-0.34	3 (1%) 72 74	23, 40, 61, 78	3 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	L	213/213 (100%)	-0.04	0 100 100	27, 54, 77, 91	2 (0%)
13	Z	213/213 (100%)	-0.33	0 100 100	29, 40, 64, 78	1 (0%)
14	M	216/219 (98%)	-0.27	1 (0%) 87 89	30, 43, 68, 103	1 (0%)
14	a	216/219 (98%)	-0.33	2 (0%) 81 83	26, 41, 64, 97	2 (0%)
15	N	202/205 (98%)	-0.37	3 (1%) 72 74	23, 37, 59, 94	1 (0%)
15	b	203/205 (99%)	-0.21	2 (0%) 79 82	32, 42, 71, 99	1 (0%)
All	All	6235/6466 (96%)	-0.05	98 (1%) 70 73	18, 50, 93, 154	49 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	5	THR	5.0
15	N	202	LEU	4.7
12	K	44	TYR	4.3
12	Y	45	TYR	4.2
12	Y	206	GLY	4.0
8	V	204	CYS	4.0
5	E	58	ALA	3.9
5	E	52	ALA	3.7
14	M	215	ILE	3.7
5	E	57	ALA	3.6
14	a	215	ILE	3.5
5	E	59	HIS	3.5
4	D	241	ILE	3.5
5	E	54	SER	3.4
5	S	2	PHE	3.4
2	P	51	ASN	3.3
4	R	241	ILE	3.3
15	b	199	VAL	3.3
5	S	57	ALA	3.2
3	C	138	PHE	3.2
14	a	216	SER	3.1
2	B	202	ASP	3.1
3	Q	50	VAL	3.1
5	E	56	LEU	3.1
7	U	186	LYS	3.1
3	C	98	VAL	3.0
1	O	3	ARG	3.0
2	P	203	VAL	3.0
2	B	61	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	3	ARG	2.9
5	S	3	ARG	2.9
3	C	206	ILE	2.8
1	A	230	ALA	2.8
7	G	189	TRP	2.8
2	P	61	PHE	2.7
7	U	183	VAL	2.7
1	O	232	ILE	2.7
3	C	225	ILE	2.7
6	T	53	VAL	2.7
4	R	128	ALA	2.6
1	A	181	LEU	2.6
5	S	239	ARG	2.6
3	Q	98	VAL	2.6
5	E	53	GLN	2.6
1	O	231	ALA	2.6
5	S	58	ALA	2.6
3	Q	138	PHE	2.6
5	S	53	GLN	2.5
8	V	201	ARG	2.5
1	A	231	ALA	2.5
3	Q	217	LEU	2.5
4	R	130	PRO	2.4
7	G	208	ILE	2.4
8	V	220	GLU	2.4
2	P	245	ALA	2.4
4	D	131	GLY	2.4
6	T	6	GLY	2.4
3	C	97	THR	2.4
4	R	120[A]	ALA	2.4
6	T	208	ALA	2.4
15	N	200	ALA	2.4
6	T	209	PHE	2.4
15	N	199	VAL	2.4
3	Q	49	SER	2.4
3	Q	48	LYS	2.3
5	S	18[A]	ARG	2.3
3	Q	225	ILE	2.3
1	O	230	ALA	2.3
15	b	198	ALA	2.3
7	G	187	PHE	2.3
2	P	56	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	249	ARG	2.3
7	U	2	SER	2.3
12	Y	205	SER	2.3
6	F	53	VAL	2.3
8	H	204	CYS	2.3
8	V	200	GLY	2.3
2	B	206	LEU	2.3
3	C	96	LEU	2.3
5	E	51	ARG	2.2
2	P	30	HIS	2.2
8	V	197	THR	2.2
6	F	204	VAL	2.2
4	R	9	ASP	2.2
10	J	1[A]	MET	2.2
6	F	6	GLY	2.2
5	S	54	SER	2.2
2	P	204	SER	2.1
7	G	245	ARG	2.1
1	O	177	TYR	2.1
4	R	131	GLY	2.1
5	S	51	ARG	2.0
8	V	203	ARG	2.0
5	E	201	ALA	2.0
3	C	220	LEU	2.0
5	S	56	LEU	2.0
7	U	185	LYS	2.0
9	W	84	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	YCM	G	137	10/11	0.88	0.13	37,44,55,55	0
7	YCM	U	137	10/11	0.90	0.12	55,65,80,83	0
3	YCM	C	63	10/11	0.93	0.10	63,66,76,78	0
3	YCM	Q	63	10/11	0.95	0.08	57,61,67,67	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. 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
17	NEN	U	304	9/9	0.82	0.16	115,118,121,123	0
17	NEN	E	304	9/9	0.83	0.16	64,68,73,74	0
16	CL	Q	301	1/1	0.83	0.11	98,98,98,98	0
17	NEN	S	304	9/9	0.84	0.17	71,76,78,81	0
16	CL	D	301	1/1	0.84	0.21	83,83,83,83	0
20	1PE	I	304	16/16	0.84	0.15	69,85,101,102	0
16	CL	S	301	1/1	0.85	0.23	76,76,76,76	0
16	CL	D	302	1/1	0.86	0.20	77,77,77,77	0
16	CL	O	304	1/1	0.87	0.19	80,80,80,80	0
17	NEN	X	302	9/9	0.87	0.13	58,60,63,71	0
17	NEN	U	303	9/9	0.87	0.14	86,89,92,92	0
20	1PE	M	304	16/16	0.87	0.17	69,80,114,115	0
20	1PE	W	303	16/16	0.87	0.13	68,73,84,87	0
17	NEN	J	302	9/9	0.88	0.12	57,62,65,66	0
20	1PE	I	303	16/16	0.88	0.13	59,68,77,84	0
16	CL	E	303	1/1	0.88	0.16	75,75,75,75	0
16	CL	Y	305	1/1	0.88	0.28	73,73,73,73	0
16	CL	O	303	1/1	0.88	0.10	103,103,103,103	0
16	CL	S	302	1/1	0.89	0.14	76,76,76,76	0
16	CL	K	304	1/1	0.89	0.22	79,79,79,79	0
20	1PE	Z	301	16/16	0.89	0.12	59,72,80,84	0
20	1PE	b	304	16/16	0.89	0.14	50,58,92,98	0
20	1PE	L	301	16/16	0.90	0.12	65,79,84,90	0
17	NEN	G	305	9/9	0.90	0.12	65,68,70,75	0
16	CL	V	303	1/1	0.90	0.16	73,73,73,73	0
16	CL	K	303	1/1	0.90	0.17	73,73,73,73	0
20	1PE	a	304	16/16	0.90	0.15	62,70,101,101	0
16	CL	Q	302	1/1	0.90	0.19	77,77,77,77	0
16	CL	K	302	1/1	0.91	0.14	92,92,92,92	0
20	1PE	N	305	16/16	0.91	0.11	44,57,68,68	0
16	CL	C	302	1/1	0.91	0.21	79,79,79,79	0
16	CL	C	301	1/1	0.91	0.12	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	CL	O	302	1/1	0.91	0.14	71,71,71,71	0
16	CL	a	303	1/1	0.91	0.11	69,69,69,69	0
16	CL	H	303	1/1	0.92	0.20	63,63,63,63	0
16	CL	I	302	1/1	0.92	0.11	57,57,57,57	0
16	CL	M	303	1/1	0.92	0.11	61,61,61,61	0
16	CL	N	301	1/1	0.92	0.11	55,55,55,55	0
16	CL	G	302	1/1	0.92	0.09	76,76,76,76	0
16	CL	N	302	1/1	0.93	0.14	66,66,66,66	0
17	NEN	G	304	9/9	0.93	0.09	59,60,63,63	0
16	CL	R	301	1/1	0.93	0.11	63,63,63,63	0
16	CL	N	303	1/1	0.93	0.22	70,70,70,70	0
16	CL	B	302	1/1	0.93	0.15	69,69,69,69	0
16	CL	E	302	1/1	0.93	0.14	61,61,61,61	0
16	CL	A	302	1/1	0.93	0.09	76,76,76,76	0
16	CL	F	301	1/1	0.93	0.12	60,60,60,60	0
18	K	b	305	1/1	0.93	0.14	49,49,49,49	0
16	CL	A	304	1/1	0.94	0.13	63,63,63,63	0
16	CL	V	304	1/1	0.94	0.15	66,66,66,66	0
16	CL	Y	303	1/1	0.94	0.12	90,90,90,90	0
18	K	U	302	1/1	0.94	0.11	46,46,46,46	0
16	CL	A	301	1/1	0.94	0.12	64,64,64,64	0
16	CL	a	301	1/1	0.94	0.15	69,69,69,69	0
16	CL	H	304	1/1	0.94	0.12	57,57,57,57	0
16	CL	b	301	1/1	0.94	0.18	66,66,66,66	0
16	CL	b	302	1/1	0.94	0.17	68,68,68,68	0
16	CL	N	304	1/1	0.94	0.17	50,50,50,50	0
16	CL	R	302	1/1	0.94	0.21	62,62,62,62	0
16	CL	M	301	1/1	0.94	0.29	67,67,67,67	0
16	CL	E	301	1/1	0.94	0.14	69,69,69,69	0
16	CL	S	303	1/1	0.94	0.15	60,60,60,60	0
16	CL	Y	302	1/1	0.95	0.22	71,71,71,71	0
16	CL	O	301	1/1	0.95	0.12	63,63,63,63	0
16	CL	b	303	1/1	0.95	0.14	64,64,64,64	0
16	CL	B	301	1/1	0.95	0.10	46,46,46,46	0
16	CL	P	301	1/1	0.95	0.09	65,65,65,65	0
16	CL	a	302	1/1	0.95	0.09	48,48,48,48	0
19	MG	I	301	1/1	0.95	0.09	34,34,34,34	0
16	CL	W	302	1/1	0.95	0.07	61,61,61,61	0
16	CL	Y	304	1/1	0.96	0.09	66,66,66,66	0
16	CL	G	301	1/1	0.96	0.24	52,52,52,52	0
18	K	G	303	1/1	0.96	0.10	38,38,38,38	0
18	K	N	306	1/1	0.96	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	CL	A	303	1/1	0.97	0.08	58,58,58,58	0
19	MG	W	301	1/1	0.97	0.08	43,43,43,43	0
19	MG	Y	301	1/1	0.97	0.10	29,29,29,29	0
16	CL	M	302	1/1	0.97	0.10	44,44,44,44	0
19	MG	V	302	1/1	0.98	0.05	58,58,58,58	0
18	K	Z	302	1/1	0.98	0.09	44,44,44,44	0
16	CL	U	301	1/1	0.98	0.13	67,67,67,67	0
19	MG	H	302	1/1	0.98	0.11	34,34,34,34	0
18	K	L	302	1/1	0.98	0.09	58,58,58,58	0
19	MG	K	301	1/1	0.98	0.11	40,40,40,40	0
19	MG	H	301	1/1	0.99	0.04	48,48,48,48	0
19	MG	X	301	1/1	0.99	0.02	54,54,54,54	0
19	MG	V	301	1/1	0.99	0.09	43,43,43,43	0
19	MG	J	301	1/1	0.99	0.04	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.