



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 10:37 AM UTC

PDB ID : 4R18 / pdb_00004r18
Title : Ligand-induced Lys33-Thr1 crosslinking at subunit beta5 of the yeast 20S proteasome
Authors : Dubiella, C.; Cui, H.; Gersch, M.; Brouwer, A.J.; Sieber, S.A.; Krueger, A.; Liskamp, R.; Groll, M.
Deposited on : 2014-08-04
Resolution : 2.40 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

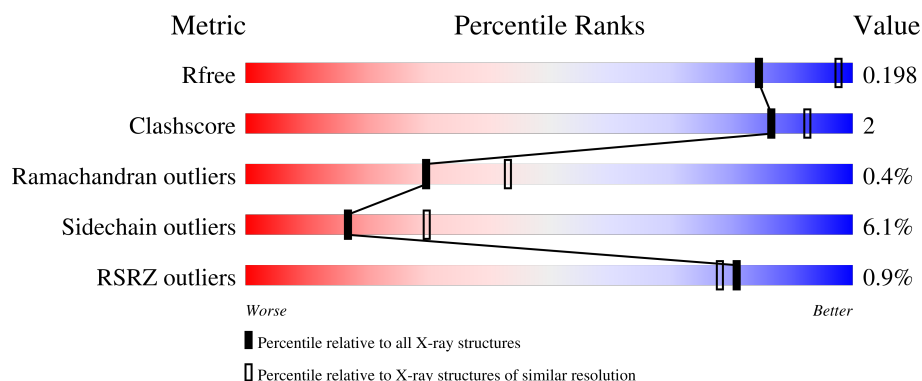
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	250	0% (Poor fit) 94% (Green) 5% (Yellow) 5% (Orange)
1	O	250	2% (Poor fit) 95% (Green) 5% (Yellow)
2	B	258	3% (Poor fit) 84% (Green) 9% (Yellow) 5% (Orange) 5% (Grey)
2	P	258	2% (Poor fit) 84% (Green) 9% (Yellow) 5% (Orange) 5% (Grey)
3	C	254	0% (Poor fit) 80% (Green) 13% (Yellow) 6% (Orange)

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51115 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-2.

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

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-3.

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

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-4.

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

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-5.

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

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-6.

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

- Molecule 6 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-7.

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

- Molecule 7 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-1.

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

- Molecule 8 is a protein called PROTEASOME SUBUNIT BETA TYPE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE-3.

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

- Molecule 10 is a protein called PROTEASOME SUBUNIT BETA TYPE-4.

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

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

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

- Molecule 12 is a protein called PROTEASOME SUBUNIT BETA TYPE-6.

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

- Molecule 13 is a protein called PROTEASOME SUBUNIT BETA TYPE-7.

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

- Molecule 14 is a protein called PROTEASOME SUBUNIT BETA TYPE-1.

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

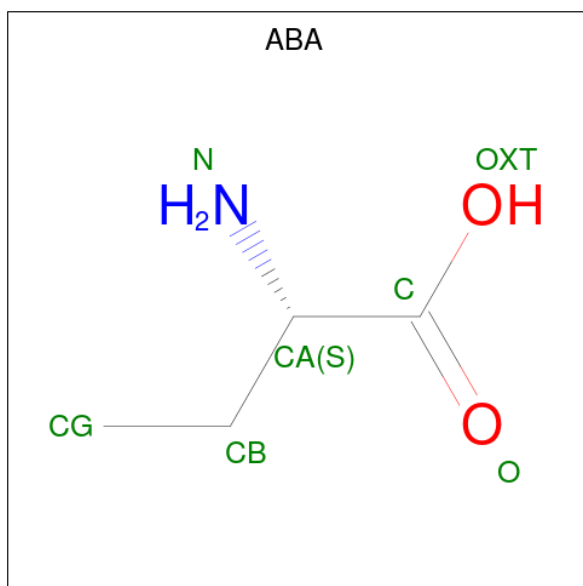
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	2	Total	Mg	0	0
			2	2		
15	J	1	Total	Mg	0	0
			1	1		
15	K	2	Total	Mg	0	0
			2	2		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

- Molecule 16 is ALPHA-AMINOBUTYRIC ACID (CCD ID: ABA) (formula: $C_4H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			6	4	1	1		
16	Y	1	Total	C	N	O	0	0
			6	4	1	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	79	Total O 79 79	0	0
17	B	62	Total O 62 62	0	0
17	C	48	Total O 48 48	0	0
17	D	56	Total O 56 56	0	0
17	E	18	Total O 18 18	0	0
17	F	67	Total O 67 67	0	0
17	G	83	Total O 83 83	0	0
17	H	66	Total O 66 66	0	0
17	I	73	Total O 73 73	0	0
17	J	85	Total O 85 85	0	0
17	K	77	Total O 77 77	0	0
17	L	69	Total O 69 69	0	0
17	M	81	Total O 81 81	0	0
17	N	61	Total O 61 61	0	0
17	O	42	Total O 42 42	0	0
17	P	52	Total O 52 52	0	0
17	Q	31	Total O 31 31	0	0
17	R	50	Total O 50 50	0	0
17	S	24	Total O 24 24	0	0
17	T	62	Total O 62 62	0	0
17	U	62	Total O 62 62	0	0
17	V	58	Total O 58 58	0	0

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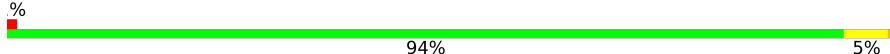
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	68	Total 68	O 68	0	0
17	X	66	Total 66	O 66	0	0
17	Y	69	Total 69	O 69	0	0
17	Z	81	Total 81	O 81	0	0
17	a	84	Total 84	O 84	0	0
17	b	66	Total 66	O 66	0	0

3 Residue-property plots [i](#)

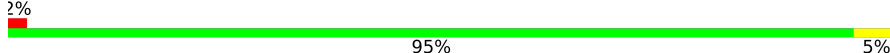
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-2

Chain A: 



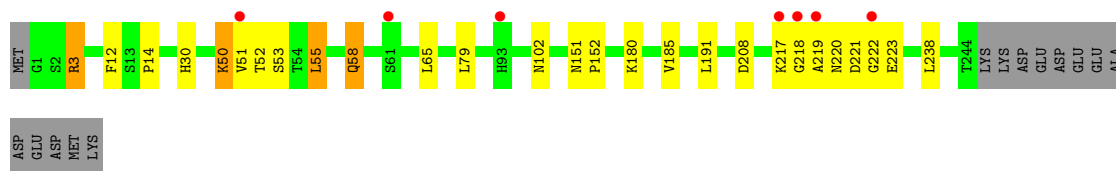
- Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-2

Chain O: 



- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-3

Chain B: 



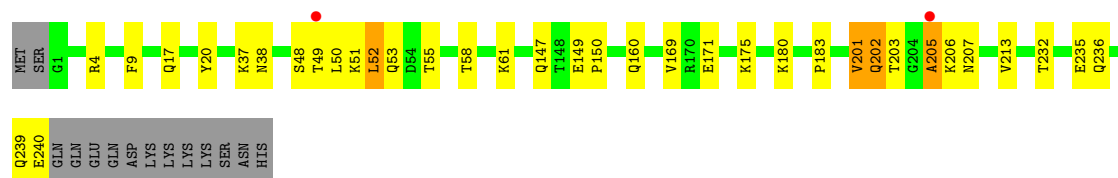
- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-3

Chain P: 

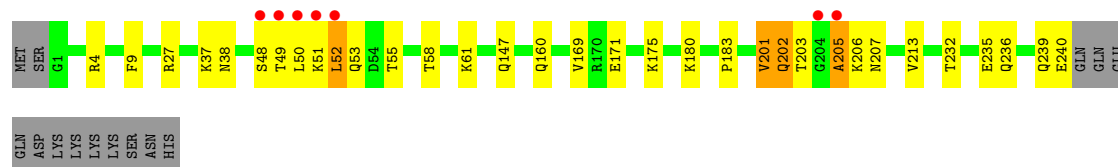
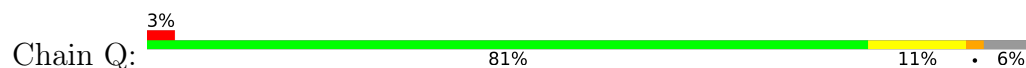


- Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

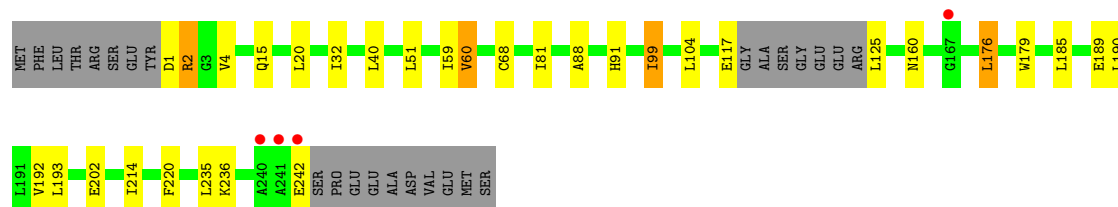
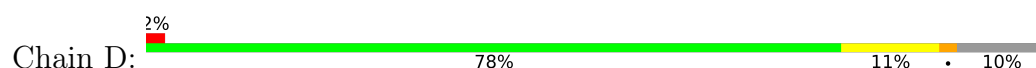
Chain C: 



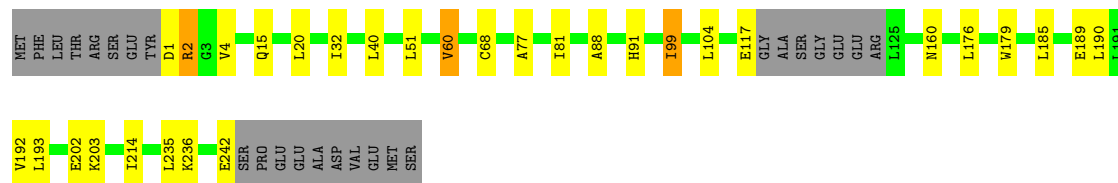
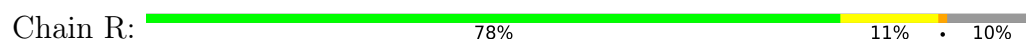
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4



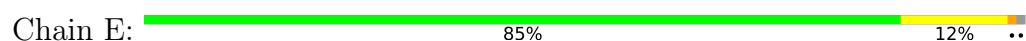
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5



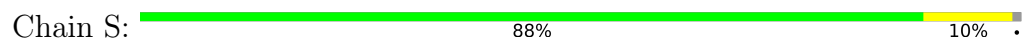
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5



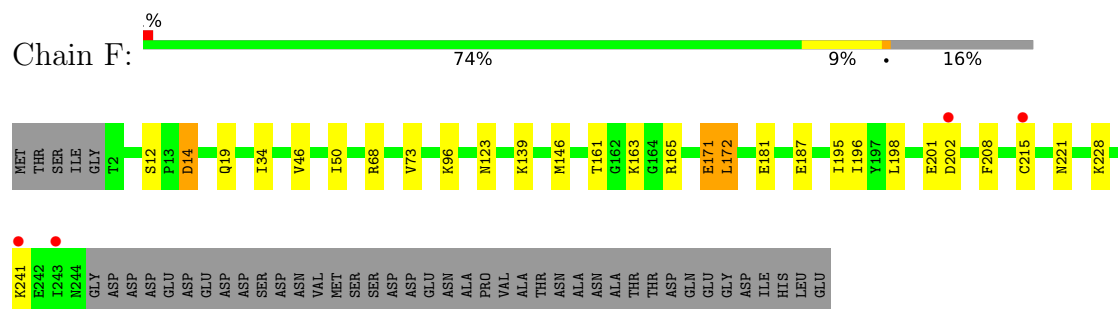
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6



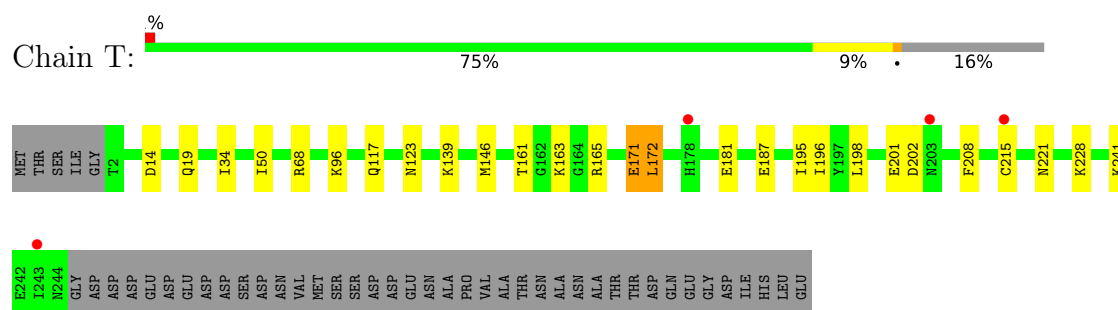
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6



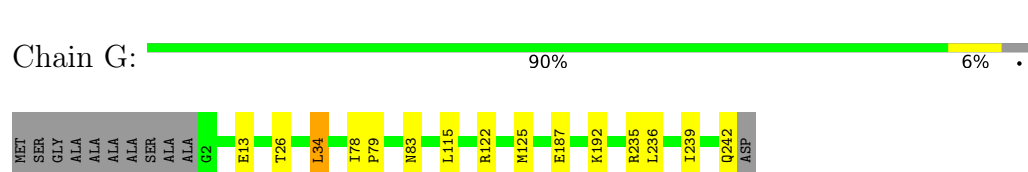
- Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-7



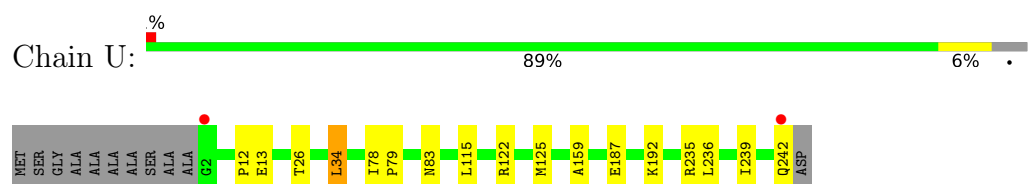
- Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-7



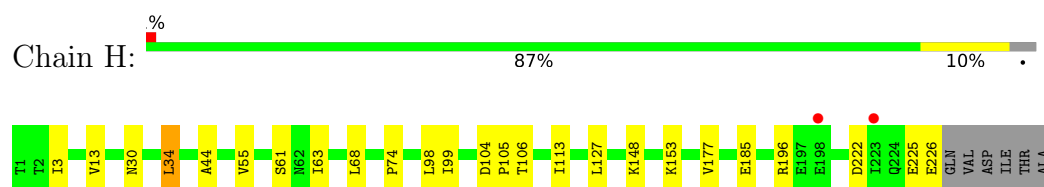
- Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1



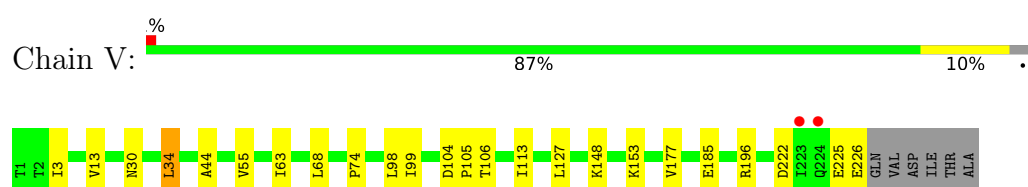
- Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1



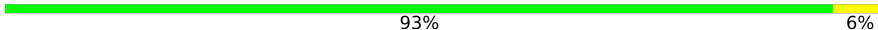
- Molecule 8: PROTEASOME SUBUNIT BETA TYPE-2



- Molecule 8: PROTEASOME SUBUNIT BETA TYPE-2

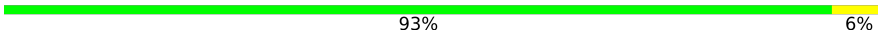


- Molecule 9: PROTEASOME SUBUNIT BETA TYPE-3

Chain I:  93% 6%



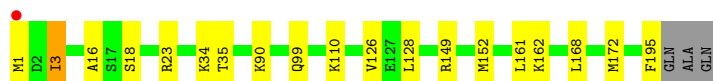
- Molecule 9: PROTEASOME SUBUNIT BETA TYPE-3

Chain W:  93% 6%



- Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4

Chain J:  89% 9% ..



- Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4

Chain X:  88% 10% ..



- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain K:  90% 8% .

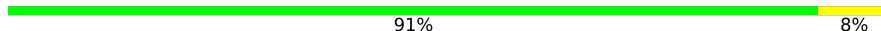


- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain Y:  90% 8% .

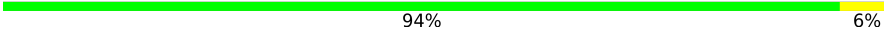


- Molecule 12: PROTEASOME SUBUNIT BETA TYPE-6

Chain L:  91% 8%



- Molecule 12: PROTEASOME SUBUNIT BETA TYPE-6

Chain Z:  94% 6%



- Molecule 13: PROTEASOME SUBUNIT BETA TYPE-7

Chain M:  87% 7% • 5%

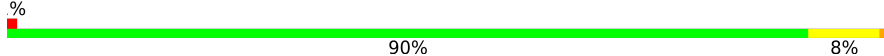


- Molecule 13: PROTEASOME SUBUNIT BETA TYPE-7

Chain a:  88% 6% • 5%

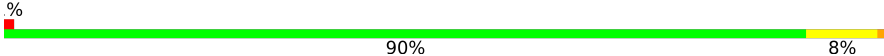


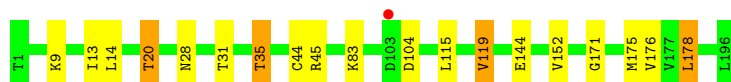
- Molecule 14: PROTEASOME SUBUNIT BETA TYPE-1

Chain N:  90% 8% •



- Molecule 14: PROTEASOME SUBUNIT BETA TYPE-1

Chain b:  90% 8% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.58Å 300.82Å 146.29Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.40) 96.6 (15.00-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.195 0.181 , 0.198	Depositor DCC
R_{free} test set	20336 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51115	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: MG, ABA

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	0.39	0/1952	0.71	0/2642
1	O	0.39	0/1952	0.71	0/2642
2	B	0.43	0/1934	0.71	0/2618
2	P	0.42	0/1934	0.71	0/2618
3	C	0.41	0/1910	0.73	1/2586 (0.0%)
3	Q	0.41	0/1910	0.73	1/2586 (0.0%)
4	D	0.39	0/1837	0.70	0/2475
4	R	0.39	0/1837	0.70	0/2475
5	E	0.40	0/1800	0.69	0/2433
5	S	0.40	0/1800	0.69	0/2433
6	F	0.41	0/1932	0.72	0/2609
6	T	0.40	0/1932	0.72	0/2609
7	G	0.39	0/1945	0.69	0/2634
7	U	0.39	0/1945	0.69	0/2634
8	H	0.45	0/1750	0.68	0/2373
8	V	0.39	0/1750	0.68	0/2373
9	I	0.38	0/1611	0.70	0/2174
9	W	0.38	0/1611	0.70	0/2174
10	J	0.40	0/1589	0.68	0/2142
10	X	0.40	0/1589	0.68	0/2142
11	K	0.37	0/1674	0.69	0/2264
11	Y	0.37	0/1674	0.68	0/2264
12	L	0.44	0/1795	0.68	0/2420
12	Z	0.38	0/1795	0.68	0/2420
13	M	0.47	0/1855	0.72	0/2514
13	a	0.48	0/1855	0.72	0/2514
14	N	0.38	0/1541	0.67	0/2087
14	b	0.38	0/1541	0.67	0/2087
All	All	0.41	0/50250	0.70	2/67942 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.14	116.30	110.53
3	C	201	VAL	N-CA-C	6.13	116.29	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	4	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	16	0
2	P	1904	0	1904	18	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	12	0
4	R	1813	0	1797	11	0
5	E	1773	0	1775	12	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	9	0
6	T	1892	0	1883	7	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	5	0
8	H	1719	0	1719	9	0
8	V	1719	0	1719	8	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	7	0
11	K	1637	0	1583	7	0
11	Y	1637	0	1583	7	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	3	0
13	M	1824	0	1832	7	0
13	a	1824	0	1832	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	12	0
14	b	1512	0	1481	12	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	K	6	0	7	0	0
16	Y	6	0	7	0	0
17	A	79	0	0	0	0
17	B	62	0	0	0	0
17	C	48	0	0	0	0
17	D	56	0	0	0	0
17	E	18	0	0	0	0
17	F	67	0	0	0	0
17	G	83	0	0	0	0
17	H	66	0	0	0	0
17	I	73	0	0	0	0
17	J	85	0	0	0	0
17	K	77	0	0	0	0
17	L	69	0	0	1	0
17	M	81	0	0	1	0
17	N	61	0	0	0	0
17	O	42	0	0	0	0
17	P	52	0	0	1	0
17	Q	31	0	0	0	0
17	R	50	0	0	0	0
17	S	24	0	0	0	0
17	T	62	0	0	0	0
17	U	62	0	0	0	0
17	V	58	0	0	0	0
17	W	68	0	0	0	0
17	X	66	0	0	0	0
17	Y	69	0	0	0	0
17	Z	81	0	0	0	0
17	a	84	0	0	0	0
17	b	66	0	0	1	0
All	All	51115	0	49120	206	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 2.

All (206) 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)
2:P:50:LYS:HE3	2:P:50:LYS:HA	1.28	1.13
2:P:52:THR:HG22	2:P:53:SER:N	1.82	0.94
2:B:52:THR:HG22	2:B:53:SER:N	1.89	0.88
2:P:52:THR:CG2	2:P:53:SER:N	2.38	0.86
2:P:50:LYS:HA	2:P:50:LYS:CE	2.01	0.85
2:B:30:HIS:O	2:B:50:LYS:HE3	1.86	0.74
2:B:52:THR:CG2	2:B:53:SER:N	2.53	0.72
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.75	0.68
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.76	0.67
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.77	0.67
2:P:52:THR:CG2	2:P:53:SER:H	2.05	0.67
11:K:53:GLN:O	11:K:57:THR:HG23	1.95	0.66
3:C:51:LYS:O	3:C:52:LEU:HB2	1.95	0.66
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.77	0.66
2:B:12:PHE:H	3:C:17:GLN:HE22	1.44	0.65
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.96	0.65
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.96	0.65
6:F:146:MET:HE3	6:F:161:THR:HB	1.80	0.64
2:B:52:THR:HG22	2:B:53:SER:O	1.97	0.63
6:T:146:MET:HE3	6:T:161:THR:HB	1.81	0.63
2:P:52:THR:HG22	2:P:53:SER:C	2.25	0.62
2:P:217:LYS:O	2:P:219:ALA:N	2.33	0.62
7:U:187:GLU:HG2	7:U:192:LYS:HB3	1.82	0.61
2:B:217:LYS:O	2:B:219:ALA:N	2.33	0.61
7:G:187:GLU:HG2	7:G:192:LYS:HB3	1.82	0.60
5:E:12:PHE:H	6:F:19:GLN:HE22	1.50	0.59
1:A:176:GLU:HG2	2:B:55:LEU:HD22	1.83	0.59
14:b:20:THR:HG22	14:b:31:THR:OG1	2.03	0.58
5:S:12:PHE:H	6:T:19:GLN:HE22	1.52	0.58
14:N:20:THR:HG22	14:N:31:THR:OG1	2.04	0.58
3:C:201:VAL:O	3:C:202:GLN:CB	2.53	0.57
6:T:146:MET:CE	6:T:161:THR:HB	2.35	0.56
6:F:146:MET:CE	6:F:161:THR:HB	2.35	0.56
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.53	0.56
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.88	0.56
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.88	0.56
14:b:35:THR:HG21	14:b:45:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.88	0.55
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.87	0.54
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.37	0.54
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.37	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.54
14:N:35:THR:HG21	14:N:45:ARG:HE	1.71	0.54
2:P:52:THR:HG22	2:P:53:SER:CA	2.38	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.53
2:B:52:THR:CG2	2:B:53:SER:H	2.20	0.53
5:S:9:THR:HG21	5:S:119:THR:HA	1.91	0.53
14:b:20:THR:CG2	14:b:31:THR:OG1	2.57	0.53
14:N:20:THR:CG2	14:N:31:THR:OG1	2.57	0.53
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.92	0.52
5:E:9:THR:HG21	5:E:119:THR:HA	1.90	0.52
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.92	0.52
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.92	0.50
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.92	0.49
2:B:52:THR:HG22	2:B:53:SER:C	2.37	0.49
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.94	0.49
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.95	0.49
14:N:35:THR:CG2	14:N:45:ARG:HE	2.26	0.49
2:P:93:HIS:HB3	17:P:302:HOH:O	2.13	0.49
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.95	0.49
6:T:34:ILE:HG12	6:T:196:ILE:HD11	1.95	0.49
13:a:2:GLN:HB3	17:b:221:HOH:O	2.13	0.49
10:J:149:ARG:O	10:J:152:MET:HG3	2.13	0.49
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.47	0.49
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.48	0.49
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.95	0.49
3:C:205:ALA:C	3:C:207:ASN:H	2.21	0.48
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.62	0.48
10:X:149:ARG:O	10:X:152:MET:HG3	2.12	0.48
6:F:34:ILE:HG12	6:F:196:ILE:HD11	1.95	0.48
14:N:13:ILE:HG21	14:N:175:MET:CE	2.43	0.48
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.96	0.48
14:b:35:THR:CG2	14:b:45:ARG:HE	2.26	0.48
14:b:13:ILE:HG21	14:b:175:MET:CE	2.44	0.48
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.96	0.48
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.48	0.48
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.14	0.48
3:Q:205:ALA:C	3:Q:207:ASN:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:150:MET:HE1	13:M:187:ARG:HG2	1.96	0.47
13:M:159:VAL:HG23	13:M:159:VAL:O	2.14	0.47
5:E:176:ASP:O	5:E:180:LYS:HD3	2.15	0.47
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.49	0.47
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.97	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.50	0.47
6:F:12:SER:OG	6:F:14:ASP:OD2	2.32	0.47
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.96	0.47
5:S:176:ASP:O	5:S:180:LYS:HD3	2.15	0.47
9:W:98:ARG:HD2	9:W:126:ILE:HG12	1.97	0.47
2:P:52:THR:HG22	2:P:53:SER:O	2.15	0.46
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.97	0.46
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.96	0.46
9:I:98:ARG:HD2	9:I:126:ILE:HG12	1.97	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.98	0.46
13:a:96:LEU:O	13:a:100:MET:HG2	2.15	0.46
13:a:159:VAL:O	13:a:159:VAL:HG23	2.15	0.46
13:M:96:LEU:O	13:M:100:MET:HG2	2.15	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.46	0.46
2:B:52:THR:HG22	2:B:53:SER:H	1.72	0.46
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.46
14:b:152:VAL:HA	14:b:175:MET:HE1	1.97	0.46
7:G:34:LEU:C	7:G:34:LEU:HD23	2.40	0.45
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.45
4:D:176:LEU:HD22	5:E:55:LEU:HD22	1.98	0.45
14:N:152:VAL:HA	14:N:175:MET:HE1	1.97	0.45
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.46	0.45
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.97	0.45
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.46	0.45
2:P:52:THR:CG2	2:P:53:SER:O	2.64	0.45
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.47	0.45
8:H:225:GLU:O	8:H:226:GLU:HB2	2.16	0.44
3:Q:232:THR:O	3:Q:236:GLN:HG3	2.18	0.44
7:U:34:LEU:HD23	7:U:34:LEU:C	2.41	0.44
8:V:225:GLU:O	8:V:226:GLU:HB2	2.16	0.44
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.00	0.44
10:J:1:MET:CB	10:J:34:LYS:HE3	2.48	0.44
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.52	0.44
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.44
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.00	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:213:ARG:NH1	17:L:331:HOH:O	2.51	0.44
3:C:232:THR:O	3:C:236:GLN:HG3	2.17	0.44
10:X:1:MET:CB	10:X:34:LYS:HE3	2.48	0.44
11:K:12:ILE:HB	11:K:180:VAL:HB	2.00	0.44
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	2.00	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.43
2:P:52:THR:HG23	2:P:53:SER:H	1.79	0.43
2:P:58:GLN:NE2	2:P:208:ASP:HA	2.33	0.43
6:T:171:GLU:HB3	6:T:195:ILE:HG12	2.00	0.43
8:V:3:ILE:HG22	8:V:99:ILE:HD12	2.00	0.43
3:C:201:VAL:O	3:C:202:GLN:HB2	2.18	0.43
5:E:178:PHE:C	5:E:178:PHE:CD1	2.97	0.43
8:H:3:ILE:HG22	8:H:99:ILE:HD12	2.00	0.43
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.43
8:V:148:LYS:HE3	8:V:177:VAL:HG11	2.00	0.43
2:B:30:HIS:O	2:B:50:LYS:CE	2.60	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.43
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.01	0.43
8:H:148:LYS:HE3	8:H:177:VAL:HG11	2.00	0.43
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.18	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.43
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.42
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.54	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.19	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
4:D:1:ASP:O	4:D:2:ARG:HB2	2.19	0.42
6:F:171:GLU:HB3	6:F:195:ILE:HG12	2.00	0.42
10:J:168:LEU:O	10:J:172:MET:HB2	2.19	0.42
5:S:178:PHE:CD1	5:S:178:PHE:C	2.97	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.42
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.59	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.54	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.42
2:P:50:LYS:CE	2:P:50:LYS:CA	2.85	0.42
10:X:162:LYS:HG3	10:X:195:PHE:CZ	2.55	0.42
4:D:185:LEU:O	4:D:189:GLU:HG3	2.20	0.42
2:B:58:GLN:NE2	2:B:208:ASP:HA	2.34	0.42
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:170:TYR:CD1	5:E:170:TYR:C	2.98	0.42
6:F:50:ILE:HG13	6:F:208:PHE:HA	2.01	0.42
4:R:185:LEU:O	4:R:189:GLU:HG3	2.20	0.42
5:S:170:TYR:CD1	5:S:170:TYR:C	2.98	0.42
12:L:147:MET:N	12:L:148:PRO:CD	2.82	0.42
1:A:99:ARG:HE	8:H:61:SER:HG	1.68	0.42
13:M:2:GLN:NE2	17:M:377:HOH:O	2.53	0.42
4:D:60:VAL:HG11	4:D:81:ILE:HG21	2.03	0.41
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.60	0.41
6:T:50:ILE:HG13	6:T:208:PHE:HA	2.01	0.41
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.41
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.02	0.41
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.50	0.41
14:N:20:THR:HG23	14:N:28:ASN:HB3	2.02	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
8:V:34:LEU:HD12	8:V:44:ALA:HB2	2.02	0.41
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.86	0.41
8:H:34:LEU:HD12	8:H:44:ALA:HB2	2.02	0.41
10:J:162:LYS:HG3	10:J:195:PHE:CZ	2.55	0.41
4:R:60:VAL:HG11	4:R:81:ILE:HG21	2.02	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.34	0.41
12:L:164:THR:O	12:L:167:LYS:HE3	2.21	0.41
4:R:4:VAL:HG13	4:R:15:GLN:HG3	2.03	0.41
4:R:77:ALA:O	4:R:81:ILE:HG12	2.21	0.41
4:D:4:VAL:HG13	4:D:15:GLN:HG3	2.03	0.41
5:E:35:VAL:HG22	5:E:159:ALA:HB2	2.03	0.41
5:E:68:HIS:HE1	5:E:102:LEU:O	2.04	0.41
4:R:1:ASP:O	4:R:2:ARG:HB2	2.19	0.41
11:Y:13:ILE:HG13	11:Y:153:ALA:HB1	2.03	0.41
14:b:20:THR:HG23	14:b:28:ASN:HB3	2.02	0.41
8:V:98:LEU:HB2	8:V:113:ILE:CG2	2.50	0.41
5:E:155:LEU:HD13	5:E:158:THR:HB	2.03	0.40
5:E:206:THR:OG1	5:E:209:ASN:HB2	2.21	0.40
6:F:46:VAL:HB	6:F:73:VAL:HG21	2.03	0.40
5:S:35:VAL:HG22	5:S:159:ALA:HB2	2.03	0.40
1:A:1:MET:CG	1:A:2:THR:N	2.85	0.40
3:C:9:PHE:H	4:D:15:GLN:HE22	1.69	0.40
1:O:55:LEU:HB3	7:U:159:ALA:O	2.21	0.40
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.57	0.40
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.57	0.40
1:A:115:ALA:HB1	1:A:154:GLY:O	2.21	0.40
11:K:33:LYS:HG2	11:K:45:MET:HE2	2.04	0.40
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.87	0.40
12:Z:164:THR:O	12:Z:167:LYS:HE3	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	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	25
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	25
2	B	242/258 (94%)	233 (96%)	4 (2%)	5 (2%)	5	7
2	P	242/258 (94%)	232 (96%)	4 (2%)	6 (2%)	4	5
3	C	238/254 (94%)	231 (97%)	3 (1%)	4 (2%)	7	10
3	Q	238/254 (94%)	230 (97%)	4 (2%)	4 (2%)	7	10
4	D	231/260 (89%)	227 (98%)	3 (1%)	1 (0%)	30	43
4	R	231/260 (89%)	227 (98%)	3 (1%)	1 (0%)	30	43
5	E	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
5	S	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
6	F	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
6	T	241/288 (84%)	235 (98%)	6 (2%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
10	X	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
11	K	209/212 (99%)	201 (96%)	8 (4%)	0	100	100
11	Y	209/212 (99%)	201 (96%)	8 (4%)	0	100	100
12	L	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	24	37
12	Z	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	24	37
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6282/6614 (95%)	6102 (97%)	153 (2%)	27 (0%)	30	43

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
3	C	202	GLN
3	C	205	ALA
1	O	2	THR
2	P	51	VAL
2	P	218	GLY
2	P	222	GLY
3	Q	202	GLN
3	Q	205	ALA
1	A	166	LYS
2	B	51	VAL
1	O	166	LYS
2	B	220	ASN
12	L	165	ASN
2	P	220	ASN
12	Z	165	ASN
4	D	2	ARG
4	R	2	ARG
2	B	221	ASP

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Mol	Chain	Res	Type
3	C	183	PRO
3	C	239	GLN
2	P	52	THR
2	P	221	ASP
3	Q	183	PRO
3	Q	239	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	200 (96%)	9 (4%)	26	44
1	O	209/209 (100%)	200 (96%)	9 (4%)	26	44
2	B	203/216 (94%)	191 (94%)	12 (6%)	18	31
2	P	203/216 (94%)	189 (93%)	14 (7%)	14	24
3	C	212/226 (94%)	190 (90%)	22 (10%)	7	10
3	Q	212/226 (94%)	190 (90%)	22 (10%)	7	10
4	D	194/215 (90%)	178 (92%)	16 (8%)	10	18
4	R	194/215 (90%)	178 (92%)	16 (8%)	10	18
5	E	190/193 (98%)	176 (93%)	14 (7%)	13	22
5	S	190/193 (98%)	176 (93%)	14 (7%)	13	22
6	F	201/239 (84%)	183 (91%)	18 (9%)	9	15
6	T	201/239 (84%)	182 (90%)	19 (10%)	8	13
7	G	206/210 (98%)	195 (95%)	11 (5%)	20	36
7	U	206/210 (98%)	195 (95%)	11 (5%)	20	36
8	H	185/190 (97%)	174 (94%)	11 (6%)	18	31
8	V	185/190 (97%)	174 (94%)	11 (6%)	18	31
9	I	172/173 (99%)	165 (96%)	7 (4%)	27	46
9	W	172/173 (99%)	165 (96%)	7 (4%)	27	46
10	J	173/175 (99%)	167 (96%)	6 (4%)	32	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	X	173/175 (99%)	166 (96%)	7 (4%)	28	47
11	K	168/169 (99%)	160 (95%)	8 (5%)	23	40
11	Y	168/169 (99%)	160 (95%)	8 (5%)	23	40
12	L	185/185 (100%)	177 (96%)	8 (4%)	26	44
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	44
13	M	199/208 (96%)	188 (94%)	11 (6%)	19	34
13	a	199/208 (96%)	189 (95%)	10 (5%)	22	38
14	N	162/162 (100%)	154 (95%)	8 (5%)	22	39
14	b	162/162 (100%)	154 (95%)	8 (5%)	22	39
All	All	5318/5540 (96%)	4993 (94%)	325 (6%)	17	30

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	29	LYS
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	201	GLU
1	A	231	LYS
1	A	250	LEU
2	B	3	ARG
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN
2	B	180	LYS
2	B	185	VAL
2	B	191	LEU
2	B	223	GLU
2	B	238	LEU
3	C	4	ARG
3	C	37	LYS
3	C	38	ASN
3	C	48	SER

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Mol	Chain	Res	Type
3	C	49	THR
3	C	50	LEU
3	C	52	LEU
3	C	53	GLN
3	C	55	THR
3	C	58	THR
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	175	LYS
3	C	180	LYS
3	C	203	THR
3	C	206	LYS
3	C	213	VAL
3	C	235	GLU
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	68	CYS
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU

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Mol	Chain	Res	Type
5	E	174	THR
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	217	LYS
5	E	231	LYS
6	F	14	ASP
6	F	68	ARG
6	F	96	LYS
6	F	123	ASN
6	F	139	LYS
6	F	163	LYS
6	F	165	ARG
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	187	GLU
6	F	198	LEU
6	F	201	GLU
6	F	202	ASP
6	F	215	CYS
6	F	221	ASN
6	F	228	LYS
6	F	241	LYS
7	G	13	GLU
7	G	26	THR
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
7	G	239	ILE
7	G	242	GLN
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	106	THR
8	H	127	LEU

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Mol	Chain	Res	Type
8	H	153	LYS
8	H	185	GLU
8	H	196	ARG
8	H	222	ASP
9	I	37	ASN
9	I	96	GLU
9	I	117	LYS
9	I	126	ILE
9	I	171	LEU
9	I	192	ASP
9	I	195	VAL
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	57	THR
11	K	67	GLU
11	K	97	MET
11	K	128	CYS
11	K	148	LEU
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	108	HIS
12	L	136	CYS
12	L	150	LEU
12	L	172	LEU
13	M	2	GLN
13	M	43	ILE
13	M	48	ASN
13	M	73	GLU
13	M	104	ARG
13	M	106	LYS
13	M	146	PHE
13	M	161	ARG
13	M	187	ARG

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Mol	Chain	Res	Type
13	M	206	LEU
13	M	212	LEU
14	N	9	LYS
14	N	20	THR
14	N	35	THR
14	N	104	ASP
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	1	MET
1	O	29	LYS
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	201	GLU
1	O	231	LYS
1	O	250	LEU
2	P	3	ARG
2	P	38	MET
2	P	50	LYS
2	P	51	VAL
2	P	55	LEU
2	P	58	GLN
2	P	65	LEU
2	P	79	LEU
2	P	102	ASN
2	P	180	LYS
2	P	185	VAL
2	P	191	LEU
2	P	223	GLU
2	P	238	LEU
3	Q	4	ARG
3	Q	37	LYS
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	50	LEU
3	Q	52	LEU
3	Q	53	GLN
3	Q	55	THR

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Mol	Chain	Res	Type
3	Q	58	THR
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
3	Q	175	LYS
3	Q	180	LYS
3	Q	203	THR
3	Q	206	LYS
3	Q	213	VAL
3	Q	235	GLU
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	68	CYS
4	R	99	ILE
4	R	117	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	203	LYS
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	174	THR
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	217	LYS

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Mol	Chain	Res	Type
5	S	231	LYS
6	T	14	ASP
6	T	68	ARG
6	T	96	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	163	LYS
6	T	165	ARG
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	187	GLU
6	T	198	LEU
6	T	201	GLU
6	T	202	ASP
6	T	215	CYS
6	T	221	ASN
6	T	228	LYS
6	T	241	LYS
7	U	13	GLU
7	U	26	THR
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
7	U	239	ILE
7	U	242	GLN
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	106	THR
8	V	127	LEU
8	V	153	LYS
8	V	185	GLU
8	V	196	ARG
8	V	222	ASP

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Mol	Chain	Res	Type
9	W	37	ASN
9	W	96	GLU
9	W	117	LYS
9	W	126	ILE
9	W	171	LEU
9	W	192	ASP
9	W	195	VAL
10	X	2	ASP
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	67	GLU
11	Y	97	MET
11	Y	128	CYS
11	Y	148	LEU
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	108	HIS
12	Z	136	CYS
12	Z	150	LEU
12	Z	172	LEU
13	a	2	GLN
13	a	43	ILE
13	a	48	ASN
13	a	73	GLU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	187	ARG
13	a	206	LEU
13	a	212	LEU
14	b	9	LYS
14	b	20	THR

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Mol	Chain	Res	Type
14	b	35	THR
14	b	104	ASP
14	b	115	LEU
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	149	HIS
4	D	225	ASN
5	E	68	HIS
5	E	85	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN

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Mol	Chain	Res	Type
6	F	240	GLN
6	F	244	ASN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
8	H	66	HIS
8	H	86	HIS
8	H	194	ASN
9	I	37	ASN
9	I	63	ASN
9	I	88	GLN
10	J	10	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	76	HIS
12	L	79	HIS
12	L	80	ASN
12	L	197	GLN
13	M	48	ASN
13	M	62	HIS
13	M	102	GLN
13	M	194	ASN
13	M	203	ASN
13	M	213	GLN
14	N	141	ASN
1	O	94	HIS
2	P	58	GLN
2	P	119	GLN

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Mol	Chain	Res	Type
2	P	123	GLN
2	P	167	ASN
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	149	HIS
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
6	T	244	ASN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS

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Mol	Chain	Res	Type
8	V	189	ASN
8	V	194	ASN
9	W	37	ASN
9	W	63	ASN
9	W	88	GLN
10	X	10	GLN
10	X	55	GLN
10	X	63	ASN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	79	HIS
12	Z	197	GLN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	194	ASN
13	a	203	ASN
13	a	213	GLN
14	b	141	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	ABA	Y	301	11	4,5,6	0.91	0	1,5,7	0.22	0
16	ABA	K	301	11	4,5,6	0.92	0	1,5,7	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	ABA	Y	301	11	-	2/3/4/6	-
16	ABA	K	301	11	-	2/3/4/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	301	ABA	N-CA-CB-CG
16	K	301	ABA	C-CA-CB-CG
16	Y	301	ABA	N-CA-CB-CG
16	Y	301	ABA	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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	250/250 (100%)	-0.36	3 (1%) 76 73	33, 46, 82, 120	0
1	O	250/250 (100%)	-0.24	4 (1%) 70 66	39, 55, 102, 134	0
2	B	244/258 (94%)	-0.23	7 (2%) 53 50	33, 51, 95, 158	0
2	P	244/258 (94%)	-0.10	6 (2%) 58 54	37, 54, 105, 160	0
3	C	240/254 (94%)	-0.17	2 (0%) 82 80	33, 56, 123, 146	0
3	Q	240/254 (94%)	0.05	7 (2%) 53 50	36, 65, 146, 163	0
4	D	235/260 (90%)	-0.22	4 (1%) 69 65	37, 57, 94, 141	0
4	R	235/260 (90%)	-0.22	0 100 100	39, 60, 97, 131	0
5	E	231/234 (98%)	-0.22	1 (0%) 88 86	41, 60, 96, 135	0
5	S	231/234 (98%)	-0.10	0 100 100	42, 66, 107, 152	0
6	F	243/288 (84%)	-0.31	4 (1%) 70 66	33, 53, 98, 141	0
6	T	243/288 (84%)	-0.17	4 (1%) 70 66	36, 60, 116, 150	0
7	G	241/252 (95%)	-0.38	0 100 100	32, 48, 84, 129	0
7	U	241/252 (95%)	-0.28	2 (0%) 82 80	37, 53, 89, 126	0
8	H	226/232 (97%)	-0.40	2 (0%) 81 78	34, 45, 81, 154	0
8	V	226/232 (97%)	-0.36	2 (0%) 81 78	36, 51, 88, 161	0
9	I	204/205 (99%)	-0.58	1 (0%) 87 85	31, 43, 70, 105	0
9	W	204/205 (99%)	-0.54	0 100 100	31, 45, 77, 102	0
10	J	195/198 (98%)	-0.44	1 (0%) 87 85	31, 46, 74, 138	0
10	X	195/198 (98%)	-0.38	2 (1%) 79 76	35, 48, 77, 143	0
11	K	211/212 (99%)	-0.49	0 100 100	33, 46, 72, 86	0
11	Y	211/212 (99%)	-0.46	0 100 100	34, 46, 72, 93	0
12	L	222/222 (100%)	-0.48	1 (0%) 87 85	33, 49, 78, 133	0
12	Z	222/222 (100%)	-0.50	0 100 100	28, 47, 76, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.46	2 (0%) 81 78	31, 48, 76, 144	0
13	a	233/246 (94%)	-0.46	2 (0%) 81 78	31, 46, 75, 142	0
14	N	196/196 (100%)	-0.51	1 (0%) 87 85	31, 44, 73, 114	0
14	b	196/196 (100%)	-0.49	1 (0%) 87 85	33, 45, 73, 109	0
All	All	6342/6614 (95%)	-0.33	59 (0%) 81 78	28, 51, 95, 163	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	7.0
13	a	233	ILE	6.8
10	J	1	MET	5.6
13	M	233	ILE	5.4
3	Q	50	LEU	5.1
8	V	223	ILE	5.1
3	Q	49	THR	4.8
2	B	219	ALA	4.6
2	P	219	ALA	4.5
8	H	223	ILE	4.4
2	B	218	GLY	4.1
2	P	218	GLY	3.8
6	T	243	ILE	3.4
6	F	202	ASP	3.3
3	C	205	ALA	3.3
3	Q	205	ALA	3.3
5	E	122	TYR	3.1
3	Q	204	GLY	3.0
6	T	178	HIS	2.8
9	I	1	SER	2.8
2	P	51	VAL	2.8
6	T	203	ASN	2.8
14	b	103	ASP	2.7
13	M	1	THR	2.6
1	O	53	SER	2.6
6	F	215	CYS	2.6
1	O	1	MET	2.6
2	B	51	VAL	2.5
2	P	220	ASN	2.5
3	Q	48	SER	2.5
4	D	242	GLU	2.4
2	B	222	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
7	U	242	GLN	2.4
12	L	174	TYR	2.4
13	a	1	THR	2.3
1	A	62	SER	2.3
1	A	249	ALA	2.3
2	B	93	HIS	2.3
4	D	240	ALA	2.3
2	P	1	GLY	2.3
8	V	224	GLN	2.2
3	Q	51	LYS	2.2
3	C	49	THR	2.2
6	T	215	CYS	2.2
6	F	241	LYS	2.2
2	B	217	LYS	2.1
10	X	174	MET	2.1
4	D	241	ALA	2.1
3	Q	52	LEU	2.1
14	N	116	GLY	2.1
6	F	243	ILE	2.1
8	H	198	GLU	2.1
1	O	231	LYS	2.1
4	D	167	GLY	2.1
2	B	61	SER	2.1
1	A	1	MET	2.1
2	P	58	GLN	2.0
7	U	2	GLY	2.0
1	O	62	SER	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
15	MG	H	301	1/1	0.85	0.33	83,83,83,83	0
16	ABA	K	301	6/7	0.89	0.14	43,45,46,48	0
15	MG	I	302	1/1	0.92	0.21	79,79,79,79	0
16	ABA	Y	301	6/7	0.93	0.11	44,45,47,49	0
15	MG	K	302	1/1	0.96	0.09	42,42,42,42	0
15	MG	K	303	1/1	0.96	0.19	48,48,48,48	0
15	MG	Y	302	1/1	0.97	0.11	37,37,37,37	0
15	MG	J	201	1/1	0.98	0.12	56,56,56,56	0
15	MG	Z	301	1/1	0.98	0.04	57,57,57,57	0
15	MG	N	201	1/1	0.98	0.03	43,43,43,43	0
15	MG	V	301	1/1	0.98	0.09	52,52,52,52	0
15	MG	G	301	1/1	0.99	0.05	43,43,43,43	0
15	MG	I	301	1/1	0.99	0.06	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.