



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:49 PM UTC

PDB ID : 5LAI / pdb_00005lai
Title : Ligand-induced aziridine-formation at the yeast proteasomal subunit beta5 by sulfonate esters
Authors : Groll, M.; Dubiella, C.; Cui, H.
Deposited on : 2016-06-14
Resolution : 2.50 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:

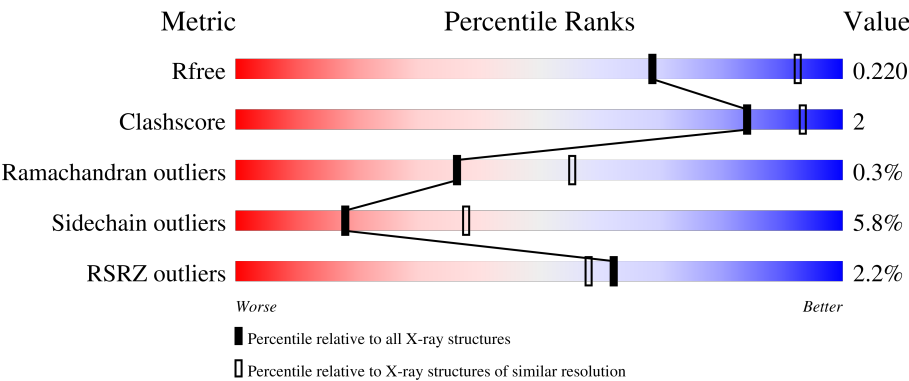
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	2% 95% • •
1	O	250	2% 94% • •
2	B	258	3% 83% 10% • 5%
2	P	258	5% 83% 10% • 5%
3	C	254	5% 82% 10% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 6% 84% 9% • 6%
4	D	260	 2% 80% 9% • 10%
4	R	260	 % 80% 9% • 10%
5	E	234	 2% 89% 9% ••
5	S	234	 3% 88% 10% ••
6	F	288	 2% 76% 7% • 16%
6	T	288	 4% 76% 7% • 16%
7	G	252	 % 87% 8% ••
7	U	252	 2% 87% 9% •
8	H	232	 2% 89% 7% ••
8	V	232	 3% 90% 6% ••
9	I	205	 % 90% 9%
9	W	205	 % 90% 9%
10	J	198	 % 88% 9% ••
10	X	198	 2% 89% 8% ••
11	K	212	 % 91% 8% •
11	Y	212	 % 91% 8% •
12	L	222	 % 91% 7% •
12	Z	222	 % 91% 7% •
13	M	246	 % 87% 7% 5%
13	a	246	 % 88% 7% 5%
14	N	196	 % 91% 8% •
14	b	196	 % 90% 9% •

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	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).

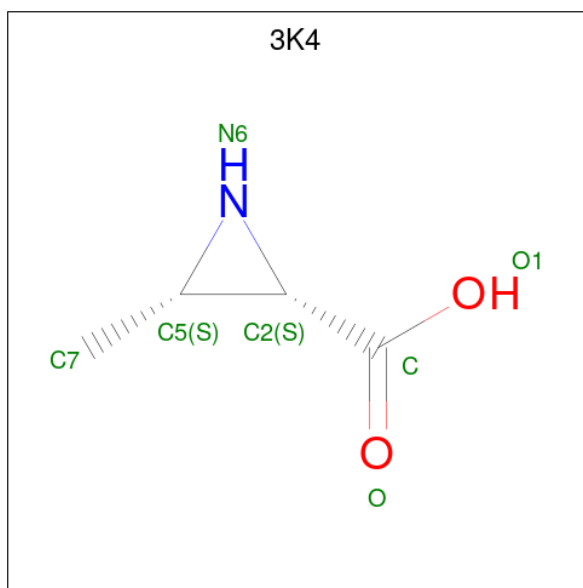
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		

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

- Molecule 16 is (2S,3S)-3-methylaziridine-2-carboxylic acid (CCD ID: 3K4) (formula: $C_4H_7NO_2$).



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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	51	Total O 51 51	0	0
17	B	31	Total O 31 31	0	0
17	C	25	Total O 25 25	0	0
17	D	21	Total O 21 21	0	0
17	E	24	Total O 24 24	0	0
17	F	28	Total O 28 28	0	0
17	G	42	Total O 42 42	0	0
17	H	41	Total O 41 41	0	0
17	I	34	Total O 34 34	0	0
17	J	39	Total O 39 39	0	0
17	K	40	Total O 40 40	0	0
17	L	47	Total O 47 47	0	0
17	M	46	Total O 46 46	0	0
17	N	33	Total O 33 33	0	0
17	O	23	Total O 23 23	0	0
17	P	28	Total O 28 28	0	0
17	Q	23	Total O 23 23	0	0
17	R	24	Total O 24 24	0	0
17	S	8	Total O 8 8	0	0
17	T	35	Total O 35 35	0	0
17	U	38	Total O 38 38	0	0
17	V	23	Total O 23 23	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	39	Total 39	O 39	0	0
17	X	34	Total 34	O 34	0	0
17	Y	30	Total 30	O 30	0	0
17	Z	35	Total 35	O 35	0	0
17	a	55	Total 55	O 55	0	0
17	b	40	Total 40	O 40	0	0

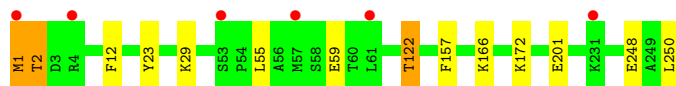
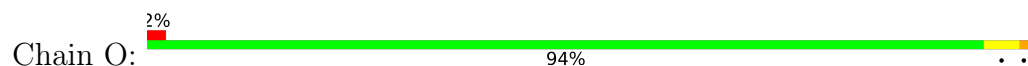
3 Residue-property plots [i](#)

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.

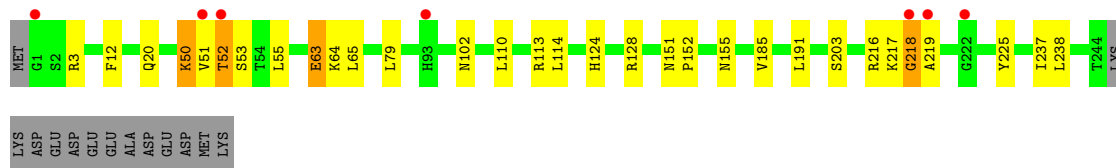
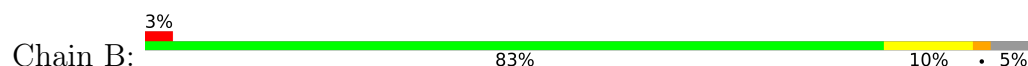
- Molecule 1: Proteasome subunit alpha type-2



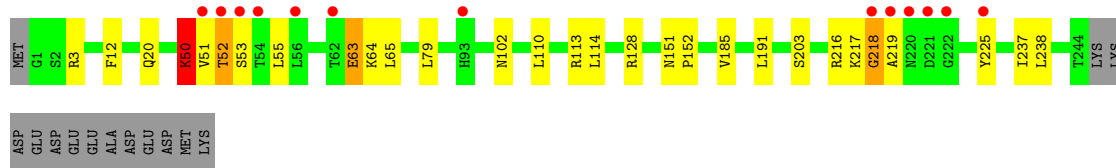
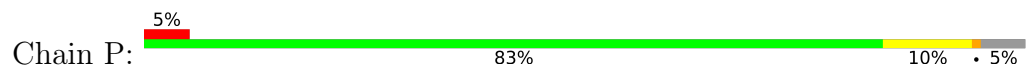
- Molecule 1: Proteasome subunit alpha type-2



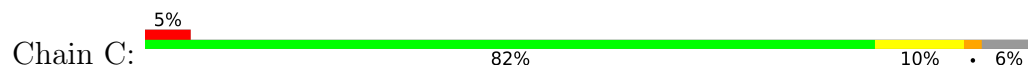
- Molecule 2: Proteasome subunit alpha type-3

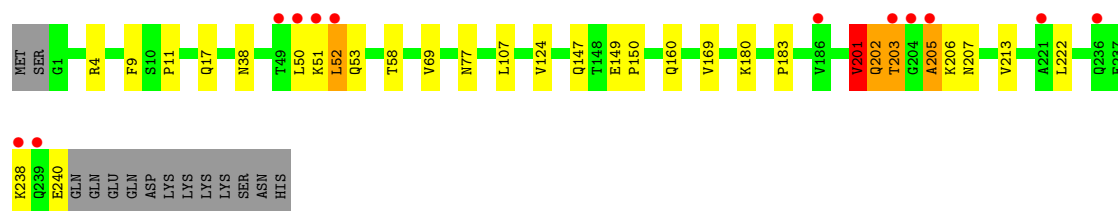


- Molecule 2: Proteasome subunit alpha type-3

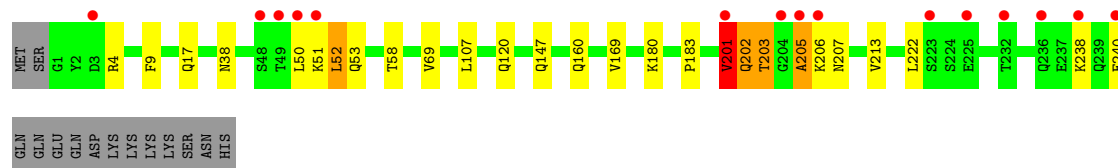
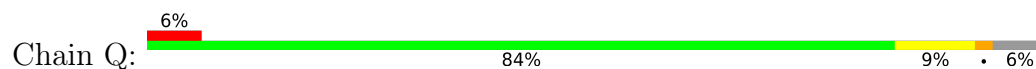


- Molecule 3: Proteasome subunit alpha type-4

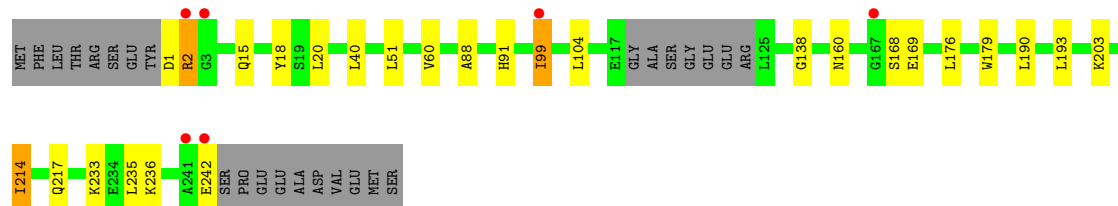
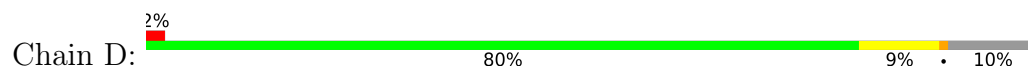




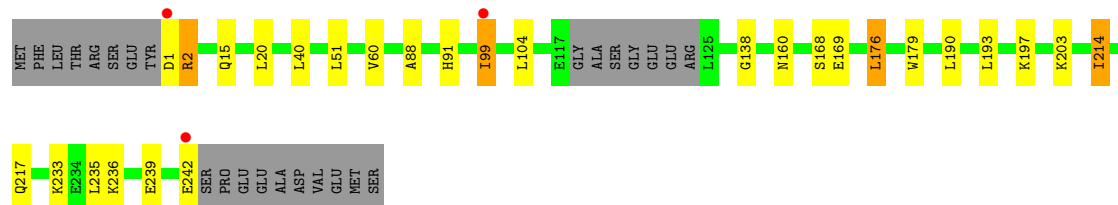
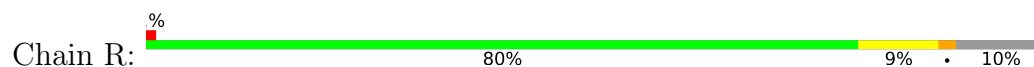
- Molecule 3: Proteasome subunit alpha type-4



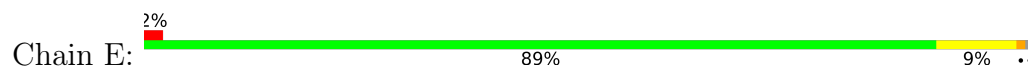
- Molecule 4: Proteasome subunit alpha type-5



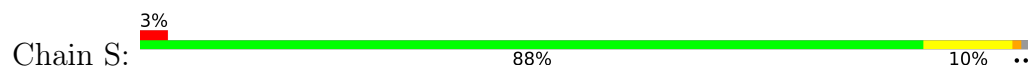
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 5: Proteasome subunit alpha type-6

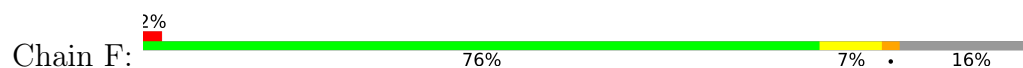


- Molecule 5: Proteasome subunit alpha type-6

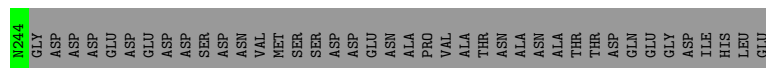
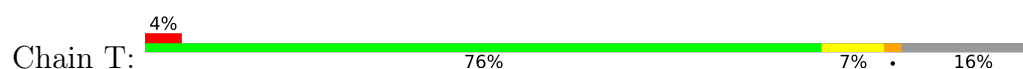




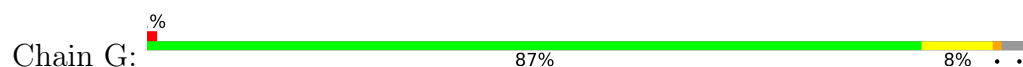
- Molecule 6: Probable proteasome subunit alpha type-7



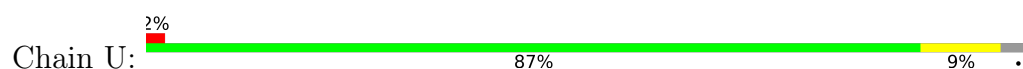
- Molecule 6: Probable proteasome subunit alpha type-7



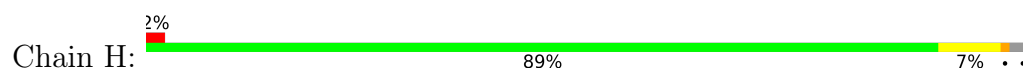
- Molecule 7: Proteasome subunit alpha type-1



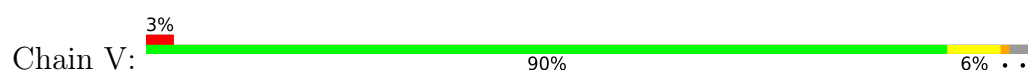
- Molecule 7: Proteasome subunit alpha type-1



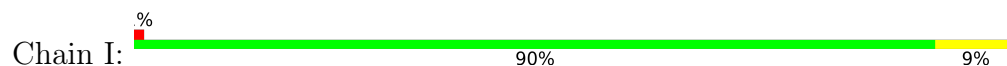
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



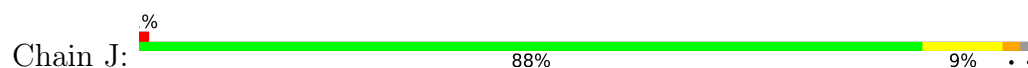
• Molecule 9: Proteasome subunit beta type-3



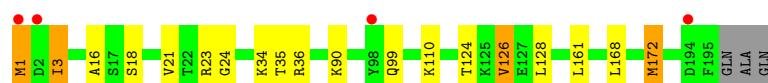
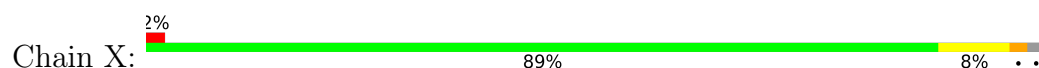
• Molecule 9: Proteasome subunit beta type-3



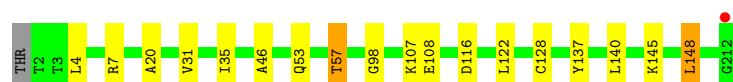
• Molecule 10: Proteasome subunit beta type-4



• Molecule 10: Proteasome subunit beta type-4



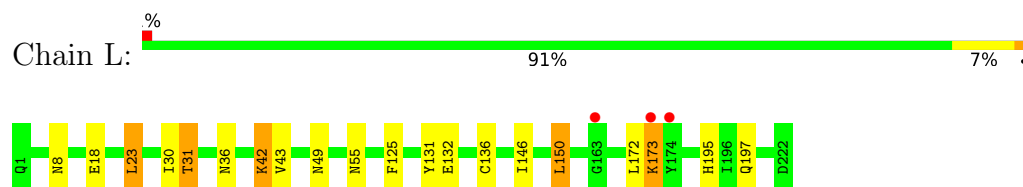
• Molecule 11: Proteasome subunit beta type-5



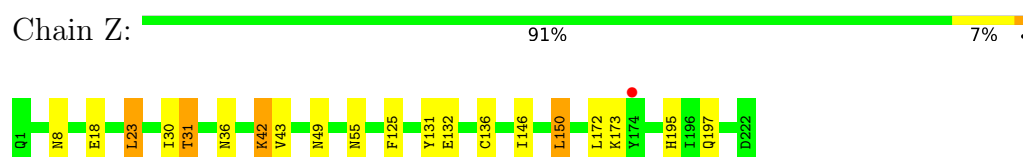
• Molecule 11: Proteasome subunit beta type-5



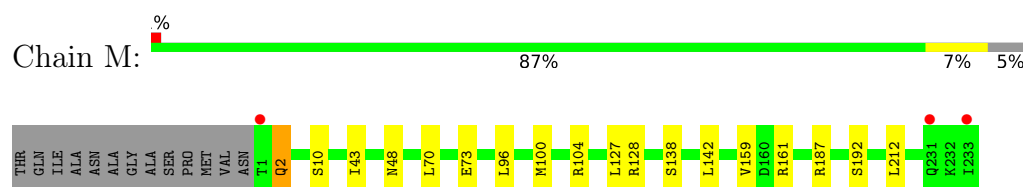
- Molecule 12: Proteasome subunit beta type-6



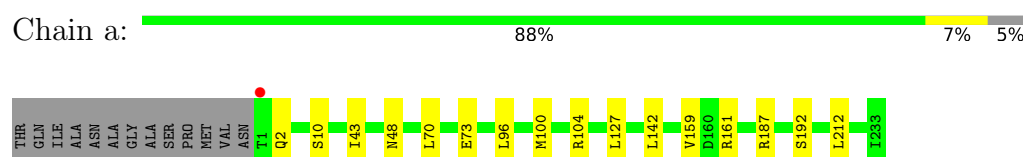
- Molecule 12: Proteasome subunit beta type-6



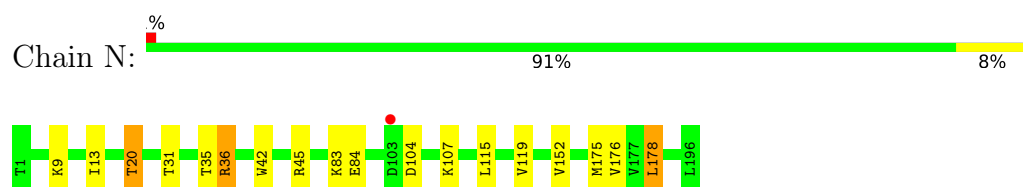
- Molecule 13: Proteasome subunit beta type-7



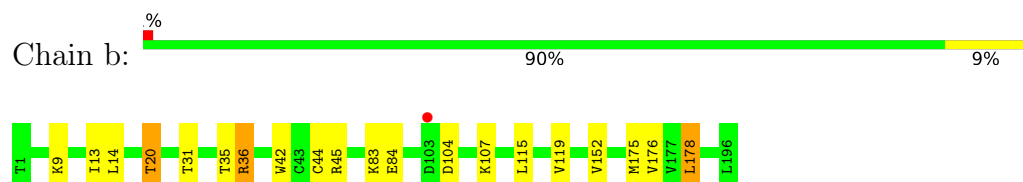
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.15Å 300.75Å 145.66Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-2.50) 97.0 (15.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.219 0.204 , 0.220	Depositor DCC
R_{free} test set	17995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50312	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: 3K4, MG

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	0.43	0/1952	0.71	0/2642
1	O	0.43	0/1952	0.71	0/2642
2	B	0.43	0/1934	0.71	0/2618
2	P	0.43	0/1934	0.71	0/2618
3	C	0.44	0/1910	0.73	1/2586 (0.0%)
3	Q	0.44	0/1910	0.74	1/2586 (0.0%)
4	D	0.42	0/1837	0.70	1/2475 (0.0%)
4	R	0.42	0/1837	0.71	1/2475 (0.0%)
5	E	0.43	0/1800	0.68	0/2433
5	S	0.42	0/1800	0.69	0/2433
6	F	0.42	0/1932	0.71	0/2609
6	T	0.42	0/1932	0.71	0/2609
7	G	0.41	0/1945	0.70	1/2634 (0.0%)
7	U	0.41	0/1945	0.70	1/2634 (0.0%)
8	H	0.35	0/1750	0.70	0/2373
8	V	0.35	0/1750	0.70	0/2373
9	I	0.35	0/1611	0.72	0/2174
9	W	0.35	0/1611	0.72	0/2174
10	J	0.43	0/1589	0.67	0/2142
10	X	0.43	0/1589	0.67	0/2142
11	K	0.35	0/1674	0.70	0/2264
11	Y	0.35	0/1674	0.70	0/2264
12	L	0.34	0/1795	0.70	0/2420
12	Z	0.34	0/1795	0.70	0/2420
13	M	0.36	0/1855	0.70	1/2514 (0.0%)
13	a	0.36	0/1855	0.70	1/2514 (0.0%)
14	N	0.34	0/1541	0.67	0/2087
14	b	0.34	0/1541	0.68	0/2087
All	All	0.40	0/50250	0.70	8/67942 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	O	0	1
2	B	0	1
2	P	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.35	116.98	110.82
3	C	201	VAL	N-CA-C	6.21	116.84	110.82
13	a	10	SER	N-CA-C	5.81	117.79	110.24
13	M	10	SER	N-CA-C	5.66	117.60	110.24
7	U	223	LYS	N-CA-C	5.56	117.55	108.76
7	G	223	LYS	N-CA-C	5.55	117.54	108.76
4	D	168	SER	N-CA-C	5.44	117.01	111.14
4	R	168	SER	N-CA-C	5.39	116.96	111.14

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
2	B	50	LYS	Peptide
1	O	1	MET	Peptide
2	P	50	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1915	0	1929	6	0
2	B	1904	0	1904	17	0
2	P	1904	0	1904	13	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	9	0
4	R	1813	0	1797	10	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	11	0
6	F	1892	0	1883	12	0
6	T	1892	0	1883	15	0
7	G	1907	0	1901	7	1
7	U	1907	0	1901	9	1
8	H	1719	0	1719	9	0
8	V	1719	0	1719	7	0
9	I	1581	0	1574	12	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	11	0
10	X	1561	0	1569	10	0
11	K	1637	0	1585	9	0
11	Y	1637	0	1585	9	0
12	L	1757	0	1711	9	0
12	Z	1757	0	1711	8	0
13	M	1824	0	1832	5	0
13	a	1824	0	1832	3	0
14	N	1512	0	1481	9	0
14	b	1512	0	1481	11	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	5	0	0
16	Y	6	0	5	0	0
17	A	51	0	0	0	0
17	B	31	0	0	0	0
17	C	25	0	0	0	0
17	D	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	E	24	0	0	0	0
17	F	28	0	0	0	0
17	G	42	0	0	0	0
17	H	41	0	0	0	0
17	I	34	0	0	0	0
17	J	39	0	0	0	0
17	K	40	0	0	0	0
17	L	47	0	0	0	0
17	M	46	0	0	1	0
17	N	33	0	0	0	0
17	O	23	0	0	0	0
17	P	28	0	0	0	0
17	Q	23	0	0	0	0
17	R	24	0	0	1	0
17	S	8	0	0	0	0
17	T	35	0	0	0	0
17	U	38	0	0	0	0
17	V	23	0	0	0	0
17	W	39	0	0	0	0
17	X	34	0	0	0	0
17	Y	30	0	0	0	0
17	Z	35	0	0	0	0
17	a	55	0	0	0	0
17	b	40	0	0	0	0
All	All	50312	0	49120	227	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:146:MET:CE	6:F:161:THR:HB	2.22	0.70
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.91	0.70
11:K:53:GLN:O	11:K:57:THR:HG23	1.92	0.69
6:T:146:MET:CE	6:T:161:THR:HB	2.22	0.69
14:b:35:THR:HG21	14:b:45:ARG:HE	1.58	0.68
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.77	0.67
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.77	0.67
14:N:35:THR:HG21	14:N:45:ARG:HE	1.59	0.66
2:B:12:PHE:H	3:C:17:GLN:HE22	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ARG:HB3	5:E:122:TYR:OH	1.98	0.63
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.83	0.60
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.84	0.60
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.83	0.59
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.84	0.58
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.83	0.58
2:P:3:ARG:HB3	5:S:122:TYR:OH	2.03	0.58
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.34	0.57
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.85	0.57
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.84	0.57
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.34	0.57
2:P:217:LYS:C	2:P:219:ALA:H	2.12	0.57
7:G:34:LEU:C	7:G:34:LEU:HD23	2.30	0.56
2:B:217:LYS:C	2:B:219:ALA:H	2.12	0.56
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.86	0.56
6:F:202:ASP:OD1	6:F:202:ASP:N	2.38	0.56
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.88	0.56
5:S:12:PHE:H	6:T:19:GLN:HE22	1.53	0.55
6:T:146:MET:HE1	6:T:161:THR:HB	1.88	0.55
6:T:202:ASP:OD1	6:T:202:ASP:N	2.39	0.55
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.88	0.55
7:U:34:LEU:C	7:U:34:LEU:HD23	2.31	0.55
6:F:146:MET:HE1	6:F:161:THR:HB	1.88	0.55
1:O:12:PHE:H	2:P:20:GLN:HE22	1.54	0.55
14:b:35:THR:CG2	14:b:45:ARG:HE	2.20	0.55
14:N:35:THR:CG2	14:N:45:ARG:HE	2.20	0.55
3:C:9:PHE:H	4:D:15:GLN:HE22	1.54	0.54
3:C:201:VAL:O	3:C:202:GLN:CB	2.56	0.54
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.91	0.53
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.56	0.53
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.90	0.53
14:b:152:VAL:HA	14:b:175:MET:HE1	1.91	0.52
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.52
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.45	0.51
8:H:114:HIS:HD2	8:H:116:HIS:H	1.59	0.51
14:N:20:THR:CG2	14:N:31:THR:OG1	2.60	0.50
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.93	0.50
14:b:20:THR:CG2	14:b:31:THR:OG1	2.60	0.50
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.60	0.50
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:152:VAL:HA	14:N:175:MET:HE1	1.92	0.50
3:C:203:THR:C	3:C:205:ALA:H	2.19	0.50
3:Q:203:THR:C	3:Q:205:ALA:H	2.19	0.50
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.94	0.50
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.94	0.50
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.93	0.49
8:V:114:HIS:HD2	8:V:116:HIS:H	1.60	0.49
7:G:165:LYS:HD2	7:G:205:LEU:HD22	1.94	0.49
7:U:165:LYS:HD2	7:U:205:LEU:HD22	1.94	0.49
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.26	0.49
13:M:159:VAL:HG23	13:M:159:VAL:O	2.13	0.49
2:B:63:GLU:HG2	2:B:64:LYS:HG2	1.95	0.48
13:a:96:LEU:O	13:a:100:MET:HG2	2.13	0.48
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.95	0.48
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.43	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.93	0.48
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.95	0.48
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.43	0.48
13:M:96:LEU:O	13:M:100:MET:HG2	2.13	0.48
2:P:63:GLU:HG2	2:P:64:LYS:HG2	1.95	0.48
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.96	0.48
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.96	0.47
13:a:159:VAL:HG23	13:a:159:VAL:O	2.14	0.47
1:A:12:PHE:H	2:B:20:GLN:HE22	1.61	0.47
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.96	0.47
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.49	0.47
2:B:216:ARG:HB3	2:B:218:GLY:H	1.80	0.47
10:J:91:SER:HG	10:J:98:TYR:H	1.63	0.47
2:P:216:ARG:HB3	2:P:218:GLY:H	1.80	0.47
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.80	0.47
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.95	0.47
11:K:46:ALA:HB3	11:K:98:GLY:O	2.15	0.47
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.95	0.47
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.63	0.47
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.45	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.47
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.96	0.47
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.44	0.47
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.80	0.47
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.96	0.47
9:I:98:ARG:HD2	9:I:126:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.80	0.47
8:H:196:ARG:NH2	9:I:150:GLU:O	2.48	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.47
9:W:98:ARG:HD2	9:W:126:ILE:HG12	1.97	0.46
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.97	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.97	0.46
12:L:8:ASN:HA	12:L:30:ILE:O	2.16	0.46
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.15	0.46
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.97	0.46
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.80	0.46
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.97	0.46
13:M:2:GLN:NE2	17:M:301:HOH:O	2.49	0.46
4:R:176:LEU:HD11	5:S:54:GLU:HB2	1.98	0.46
5:E:9:THR:HG21	5:E:119:THR:HA	1.98	0.46
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.46
9:W:187:TYR:OH	9:W:196:LYS:HE3	2.15	0.46
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.50	0.46
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.97	0.45
9:W:56:ALA:HB3	10:X:124:THR:HG23	1.99	0.45
9:W:170:LEU:C	9:W:170:LEU:HD23	2.41	0.45
9:I:170:LEU:C	9:I:170:LEU:HD23	2.41	0.45
6:T:146:MET:HE3	6:T:161:THR:HB	1.98	0.45
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.99	0.45
1:O:55:LEU:HB3	7:U:159:ALA:O	2.17	0.45
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.45
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.16	0.45
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.99	0.45
5:S:9:THR:HG21	5:S:119:THR:HA	1.98	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.45
14:b:35:THR:HG21	14:b:45:ARG:NE	2.31	0.45
9:I:187:TYR:OH	9:I:196:LYS:HE3	2.16	0.45
10:X:1:MET:CB	10:X:34:LYS:HE3	2.47	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
8:V:99:ILE:HG13	8:V:127:LEU:HD22	1.99	0.45
8:V:196:ARG:NH2	9:W:150:GLU:O	2.51	0.44
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.29	0.44
5:S:12:PHE:N	6:T:19:GLN:HE22	2.16	0.44
10:X:168:LEU:O	10:X:172:MET:HB2	2.17	0.44
8:H:99:ILE:HG13	8:H:127:LEU:HD22	1.99	0.44
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:LEU:HD23	2:B:110:LEU:C	2.43	0.44
2:B:155:ASN:ND2	3:C:77:ASN:HB2	2.32	0.44
2:B:3:ARG:CB	5:E:122:TYR:OH	2.65	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.44
11:K:31:VAL:HA	12:L:132:GLU:OE1	2.18	0.44
10:J:1:MET:CB	10:J:34:LYS:HE3	2.47	0.43
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.00	0.43
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.53	0.43
3:C:201:VAL:O	3:C:202:GLN:HB2	2.18	0.43
2:P:110:LEU:C	2:P:110:LEU:HD23	2.43	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.99	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.47	0.43
9:I:56:ALA:HB3	10:J:124:THR:HG23	2.00	0.43
10:J:168:LEU:O	10:J:172:MET:HB2	2.17	0.43
12:L:195:HIS:HD2	12:L:197:GLN:H	1.66	0.43
5:E:12:PHE:H	6:F:19:GLN:HE22	1.65	0.43
1:A:1:MET:CG	1:A:2:THR:N	2.82	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.43
7:G:61:SER:OG	7:G:215:GLU:OE2	2.34	0.43
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.00	0.43
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.00	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.43
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.33	0.42
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.01	0.42
6:T:123:ASN:C	6:T:123:ASN:HD22	2.26	0.42
6:F:123:ASN:C	6:F:123:ASN:HD22	2.26	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.42
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.66	0.42
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.00	0.42
1:O:1:MET:CG	1:O:2:THR:N	2.82	0.42
4:R:1:ASP:O	4:R:2:ARG:HB2	2.20	0.42
5:S:206:THR:C	5:S:233:ILE:HD11	2.45	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.42
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.01	0.42
14:b:13:ILE:HG21	14:b:175:MET:HE2	2.01	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.42
6:F:14:ASP:OD2	6:F:14:ASP:N	2.52	0.42
2:P:50:LYS:HA	2:P:50:LYS:HD2	1.48	0.42
3:Q:120:GLN:NE2	17:R:301:HOH:O	2.53	0.42
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:206:THR:C	5:E:233:ILE:HD11	2.45	0.41
1:A:1:MET:SD	1:A:2:THR:N	2.92	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.41
12:L:173:LYS:HA	12:L:173:LYS:HD3	1.88	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.01	0.41
2:B:217:LYS:C	2:B:219:ALA:N	2.78	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
6:F:172:LEU:HD13	6:F:195:ILE:CD1	2.50	0.41
10:J:1:MET:CG	10:J:34:LYS:HE3	2.50	0.41
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.85	0.41
2:P:52:THR:CG2	2:P:53:SER:N	2.83	0.41
6:T:172:LEU:HB3	7:U:54:LEU:CD2	2.49	0.41
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.33	0.41
4:D:1:ASP:O	4:D:2:ARG:HB2	2.20	0.41
6:F:122:TYR:CE1	7:G:125:MET:HE3	2.55	0.41
6:T:172:LEU:HD13	6:T:195:ILE:CD1	2.50	0.41
5:E:170:TYR:CD1	5:E:170:TYR:C	2.99	0.41
2:P:114:LEU:HD23	2:P:114:LEU:HA	1.97	0.41
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.02	0.41
2:B:114:LEU:HD23	2:B:114:LEU:HA	1.96	0.41
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.33	0.41
4:R:138:GLY:HA2	4:R:214:ILE:HG12	2.03	0.41
10:X:1:MET:CG	10:X:34:LYS:HE3	2.49	0.41
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.51	0.41
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.50	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.41
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.56	0.41
1:O:1:MET:SD	1:O:2:THR:N	2.93	0.41
5:S:170:TYR:CD1	5:S:170:TYR:C	2.99	0.41
2:B:52:THR:CG2	2:B:53:SER:N	2.83	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
3:C:205:ALA:C	3:C:207:ASN:H	2.29	0.41
6:F:97:LYS:NZ	14:N:84:GLU:OE1	2.50	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.84	0.41
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.36	0.41
5:S:174:THR:O	5:S:175:LEU:C	2.64	0.41
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.50	0.41
10:X:36:ARG:HA	10:X:36:ARG:HD3	1.96	0.41
1:A:122:THR:HG23	2:B:128:ARG:HH21	1.86	0.41
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.50	0.40
10:J:3:ILE:HD12	10:J:168:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.56	0.40
6:T:97:LYS:NZ	14:b:84:GLU:OE1	2.48	0.40
9:W:101:PRO:HB3	9:W:126:ILE:CD1	2.51	0.40
5:E:71:LEU:CD2	5:E:71:LEU:C	2.94	0.40
3:Q:205:ALA:C	3:Q:207:ASN:H	2.29	0.40
5:S:71:LEU:C	5:S:71:LEU:CD2	2.94	0.40
11:Y:31:VAL:HA	12:Z:132:GLU:OE1	2.22	0.40
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.61	0.40
4:D:138:GLY:HA2	4:D:214:ILE:HG12	2.03	0.40
4:R:197:LYS:NZ	4:R:239:GLU:OE2	2.52	0.40
7:U:78:ILE:N	7:U:79:PRO:CD	2.84	0.40
7:U:72:MET:HE3	7:U:74:VAL:CG2	2.51	0.40
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:167:GLN:OE1	7:U:165:LYS:NZ[2_656]	2.14	0.06

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	31
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	31
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	31
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	16	31
3	C	238/254 (94%)	228 (96%)	7 (3%)	3 (1%)	9	18
3	Q	238/254 (94%)	227 (95%)	8 (3%)	3 (1%)	9	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	231/260 (89%)	229 (99%)	1 (0%)	1 (0%)	30	49
4	R	231/260 (89%)	229 (99%)	1 (0%)	1 (0%)	30	49
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%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	24	43
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	43
11	K	209/212 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/212 (99%)	205 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (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%)	6117 (97%)	147 (2%)	18 (0%)	36	55

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
3	C	202	GLN
3	C	205	ALA
1	O	2	THR
3	Q	202	GLN
3	Q	205	ALA
4	D	2	ARG

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Mol	Chain	Res	Type
4	R	2	ARG
1	A	166	LYS
1	O	166	LYS
2	B	51	VAL
2	P	51	VAL
3	C	183	PRO
10	J	24	GLY
3	Q	183	PRO
10	X	24	GLY
2	B	218	GLY
2	P	218	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	209/209 (100%)	201 (96%)	8 (4%)	29	56
1	O	209/209 (100%)	201 (96%)	8 (4%)	29	56
2	B	203/216 (94%)	190 (94%)	13 (6%)	16	33
2	P	203/216 (94%)	190 (94%)	13 (6%)	16	33
3	C	212/226 (94%)	193 (91%)	19 (9%)	9	19
3	Q	212/226 (94%)	193 (91%)	19 (9%)	9	19
4	D	194/215 (90%)	178 (92%)	16 (8%)	10	23
4	R	194/215 (90%)	178 (92%)	16 (8%)	10	23
5	E	190/193 (98%)	175 (92%)	15 (8%)	11	24
5	S	190/193 (98%)	175 (92%)	15 (8%)	11	24
6	F	201/239 (84%)	184 (92%)	17 (8%)	10	22
6	T	201/239 (84%)	184 (92%)	17 (8%)	10	22
7	G	206/210 (98%)	196 (95%)	10 (5%)	22	45
7	U	206/210 (98%)	196 (95%)	10 (5%)	22	45
8	H	185/190 (97%)	175 (95%)	10 (5%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	185/190 (97%)	176 (95%)	9 (5%)	22	45
9	I	172/173 (99%)	167 (97%)	5 (3%)	37	65
9	W	172/173 (99%)	167 (97%)	5 (3%)	37	65
10	J	173/175 (99%)	163 (94%)	10 (6%)	18	38
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	42
11	K	168/169 (99%)	161 (96%)	7 (4%)	26	52
11	Y	168/169 (99%)	161 (96%)	7 (4%)	26	52
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	45
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	45
13	M	199/208 (96%)	189 (95%)	10 (5%)	22	44
13	a	199/208 (96%)	189 (95%)	10 (5%)	22	44
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	51
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	51
All	All	5318/5540 (96%)	5008 (94%)	310 (6%)	18	38

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	59	GLU
1	A	122	THR
1	A	157	PHE
1	A	172	LYS
1	A	201	GLU
1	A	248	GLU
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	63	GLU
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG
2	B	185	VAL
2	B	191	LEU
2	B	203	SER

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Mol	Chain	Res	Type
2	B	237	ILE
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	52	LEU
3	C	53	GLN
3	C	58	THR
3	C	69	VAL
3	C	107	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	201	VAL
3	C	203	THR
3	C	206	LYS
3	C	213	VAL
3	C	222	LEU
3	C	238	LYS
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	169	GLU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	203	LYS
4	D	214	ILE
4	D	217	GLN
4	D	233	LYS
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	4	ASN
5	E	9	THR
5	E	25	LEU
5	E	29	LYS

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Mol	Chain	Res	Type
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU
5	E	106	ARG
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	217	LYS
5	E	222	THR
5	E	231	LYS
6	F	68	ARG
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	165	ARG
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	206	LYS
6	F	207	ASP
6	F	215	CYS
6	F	221	ASN
6	F	240	GLN
6	F	241	LYS
6	F	243	ILE
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	166	GLN
7	G	235	ARG
7	G	236	LEU
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	63	ILE

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Mol	Chain	Res	Type
8	H	68	LEU
8	H	106	THR
8	H	127	LEU
8	H	153	LYS
8	H	196	ARG
9	I	37	ASN
9	I	96	GLU
9	I	126	ILE
9	I	133	LYS
9	I	171	LEU
10	J	1	MET
10	J	2	ASP
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
10	J	126	VAL
10	J	172	MET
11	K	4	LEU
11	K	7	ARG
11	K	35	ILE
11	K	57	THR
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	42	LYS
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
12	L	172	LEU
12	L	173	LYS
13	M	2	GLN
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	73	GLU
13	M	104	ARG

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Mol	Chain	Res	Type
13	M	161	ARG
13	M	187	ARG
13	M	192	SER
13	M	212	LEU
14	N	9	LYS
14	N	20	THR
14	N	36	ARG
14	N	104	ASP
14	N	107	LYS
14	N	115	LEU
14	N	178	LEU
1	O	29	LYS
1	O	59	GLU
1	O	122	THR
1	O	157	PHE
1	O	172	LYS
1	O	201	GLU
1	O	248	GLU
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	63	GLU
2	P	65	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	185	VAL
2	P	191	LEU
2	P	203	SER
2	P	237	ILE
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	52	LEU
3	Q	53	GLN
3	Q	58	THR
3	Q	69	VAL
3	Q	107	LEU
3	Q	147	GLN
3	Q	160	GLN

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Mol	Chain	Res	Type
3	Q	169	VAL
3	Q	180	LYS
3	Q	201	VAL
3	Q	203	THR
3	Q	206	LYS
3	Q	213	VAL
3	Q	222	LEU
3	Q	238	LYS
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	169	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	203	LYS
4	R	214	ILE
4	R	217	GLN
4	R	233	LYS
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	4	ASN
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	106	ARG
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	217	LYS
5	S	222	THR
5	S	231	LYS
6	T	68	ARG
6	T	117	GLN

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Mol	Chain	Res	Type
6	T	123	ASN
6	T	139	LYS
6	T	165	ARG
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	206	LYS
6	T	207	ASP
6	T	215	CYS
6	T	221	ASN
6	T	240	GLN
6	T	241	LYS
6	T	243	ILE
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	166	GLN
7	U	235	ARG
7	U	236	LEU
8	V	13	VAL
8	V	34	LEU
8	V	55	VAL
8	V	63	ILE
8	V	68	LEU
8	V	106	THR
8	V	127	LEU
8	V	153	LYS
8	V	196	ARG
9	W	37	ASN
9	W	96	GLU
9	W	126	ILE
9	W	133	LYS
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	23	ARG

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Mol	Chain	Res	Type
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
10	X	126	VAL
10	X	172	MET
11	Y	4	LEU
11	Y	7	ARG
11	Y	35	ILE
11	Y	57	THR
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	42	LYS
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
13	a	2	GLN
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	73	GLU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	192	SER
13	a	212	LEU
14	b	9	LYS
14	b	20	THR
14	b	36	ARG
14	b	104	ASP
14	b	107	LYS
14	b	115	LEU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	20	GLN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	53	GLN
3	C	77	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	106	GLN
4	D	207	ASN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	165	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	203	ASN
6	F	240	GLN
7	G	6	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN

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Mol	Chain	Res	Type
7	G	175	ASN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	114	HIS
8	H	165	ASN
8	H	189	ASN
8	H	194	ASN
9	I	37	ASN
9	I	63	ASN
9	I	168	GLN
10	J	55	GLN
10	J	63	ASN
10	J	112	ASN
10	J	146	HIS
10	J	147	HIS
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
12	L	197	GLN
13	M	48	ASN
13	M	62	HIS
13	M	102	GLN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN

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Mol	Chain	Res	Type
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	53	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	106	GLN
4	R	146	GLN
4	R	207	ASN
4	R	210	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	165	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	172	ASN
7	U	175	ASN
8	V	66	HIS
8	V	86	HIS
8	V	114	HIS

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Mol	Chain	Res	Type
8	V	116	HIS
8	V	165	ASN
8	V	194	ASN
9	W	37	ASN
9	W	63	ASN
9	W	168	GLN
9	W	203	GLN
10	X	10	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	146	HIS
11	Y	85	ASN
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	79	HIS
12	Z	80	ASN
12	Z	152	ASN
12	Z	153	GLN
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	149	HIS
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	3K4	K	301	-	5,6,7	3.93	3 (60%)	4,8,10	5.15	3 (75%)
16	3K4	Y	302	-	5,6,7	4.22	3 (60%)	4,8,10	4.97	3 (75%)

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	3K4	K	301	-	-	1/1/7/9	0/1/1/1
16	3K4	Y	302	-	-	1/1/7/9	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	302	3K4	C5-N6	-7.79	1.42	1.48
16	K	301	3K4	C5-N6	-6.94	1.43	1.48
16	K	301	3K4	C2-C5	-4.33	1.39	1.48
16	Y	302	3K4	C2-C5	-4.24	1.39	1.48
16	K	301	3K4	C7-C5	-2.61	1.47	1.52
16	Y	302	3K4	C7-C5	-2.44	1.47	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	301	3K4	C7-C5-C2	6.60	133.85	122.56
16	Y	302	3K4	C7-C5-N6	6.32	136.13	117.83
16	K	301	3K4	C7-C5-N6	6.21	135.82	117.83
16	Y	302	3K4	C7-C5-C2	6.20	133.16	122.56
16	K	301	3K4	C2-C5-N6	4.69	61.64	59.83
16	Y	302	3K4	C2-C5-N6	4.31	61.49	59.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	301	3K4	O-C-C2-C5
16	Y	302	3K4	O-C-C2-C5

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%)	-0.08	5 (2%) 65 61	34, 46, 78, 120	0
1	O	250/250 (100%)	0.07	6 (2%) 59 55	38, 52, 94, 128	0
2	B	244/258 (94%)	0.12	7 (2%) 53 49	34, 51, 90, 149	0
2	P	244/258 (94%)	0.20	13 (5%) 32 28	38, 54, 95, 143	0
3	C	240/254 (94%)	0.11	12 (5%) 34 30	33, 54, 117, 137	0
3	Q	240/254 (94%)	0.39	15 (6%) 26 23	39, 62, 132, 163	0
4	D	235/260 (90%)	0.03	6 (2%) 57 52	39, 54, 84, 125	0
4	R	235/260 (90%)	0.13	3 (1%) 75 71	42, 59, 90, 123	0
5	E	231/234 (98%)	0.17	5 (2%) 62 58	41, 57, 94, 140	0
5	S	231/234 (98%)	0.36	7 (3%) 52 48	45, 65, 98, 146	0
6	F	243/288 (84%)	0.06	7 (2%) 53 49	36, 53, 99, 126	0
6	T	243/288 (84%)	0.21	11 (4%) 38 33	37, 59, 108, 131	0
7	G	241/252 (95%)	-0.07	3 (1%) 76 73	32, 47, 79, 129	0
7	U	241/252 (95%)	-0.00	4 (1%) 69 65	37, 50, 78, 112	0
8	H	226/232 (97%)	-0.01	5 (2%) 62 58	33, 46, 76, 136	0
8	V	226/232 (97%)	0.08	8 (3%) 47 42	37, 50, 80, 146	0
9	I	204/205 (99%)	-0.31	3 (1%) 72 68	32, 44, 71, 90	0
9	W	204/205 (99%)	-0.27	3 (1%) 72 68	34, 46, 71, 98	0
10	J	195/198 (98%)	-0.12	1 (0%) 87 85	33, 47, 73, 134	0
10	X	195/198 (98%)	-0.09	4 (2%) 63 59	34, 48, 73, 132	0
11	K	211/212 (99%)	-0.30	1 (0%) 87 85	35, 46, 66, 84	0
11	Y	211/212 (99%)	-0.24	2 (0%) 81 78	37, 46, 69, 85	0
12	L	222/222 (100%)	-0.22	3 (1%) 73 70	34, 47, 74, 106	0
12	Z	222/222 (100%)	-0.16	1 (0%) 87 85	35, 48, 74, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.22	3 (1%) 75 71	31, 47, 70, 87	0
13	a	233/246 (94%)	-0.23	1 (0%) 88 86	32, 46, 66, 83	0
14	N	196/196 (100%)	-0.29	1 (0%) 87 85	33, 43, 70, 97	0
14	b	196/196 (100%)	-0.27	1 (0%) 87 85	34, 44, 69, 103	0
All	All	6342/6614 (95%)	-0.02	141 (2%) 62 58	31, 50, 88, 163	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	7.8
8	V	223	ILE	7.4
10	X	1	MET	7.3
2	B	219	ALA	6.5
10	J	1	MET	6.2
2	B	218	GLY	5.6
6	T	243	ILE	5.0
8	V	224	GLN	4.6
2	B	51	VAL	4.3
2	P	222	GLY	4.3
8	H	223	ILE	3.9
6	T	201	GLU	3.7
6	T	204	LYS	3.7
2	P	218	GLY	3.7
9	W	133	LYS	3.6
13	a	1	THR	3.5
6	F	202	ASP	3.5
13	M	233	ILE	3.5
3	Q	205	ALA	3.4
8	H	224	GLN	3.4
13	M	1	THR	3.4
3	Q	49	THR	3.3
3	Q	50	LEU	3.3
2	P	51	VAL	3.3
3	Q	204	GLY	3.3
7	U	203	ASP	3.2
2	P	220	ASN	3.2
6	F	215	CYS	3.2
3	C	203	THR	3.2
3	C	49	THR	3.1
3	Q	240	GLU	3.1
5	E	122	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	52	THR	3.0
3	C	205	ALA	2.9
5	S	209	ASN	2.9
7	U	40	ASP	2.9
12	L	174	TYR	2.9
7	U	242	GLN	2.8
6	T	206	LYS	2.8
5	E	209	ASN	2.8
14	b	103	ASP	2.8
4	D	167	GLY	2.8
6	T	215	CYS	2.8
6	T	178	HIS	2.8
12	Z	174	TYR	2.7
2	B	93	HIS	2.7
4	D	99	ILE	2.7
9	W	1	SER	2.7
4	D	241	ALA	2.7
9	I	131	GLU	2.7
13	M	231	GLN	2.7
1	O	231	LYS	2.7
3	C	50	LEU	2.7
3	Q	236	GLN	2.7
2	B	222	GLY	2.7
1	O	61	LEU	2.7
14	N	103	ASP	2.6
3	Q	51	LYS	2.6
5	S	122	TYR	2.6
5	S	233	ILE	2.6
1	O	1	MET	2.6
1	O	53	SER	2.6
3	C	204	GLY	2.6
5	S	121	SER	2.6
6	T	2	THR	2.6
2	P	225	TYR	2.6
6	T	203	ASN	2.5
6	F	2	THR	2.5
8	V	114	HIS	2.5
5	S	173	ARG	2.5
6	T	202	ASP	2.5
1	A	231	LYS	2.5
3	C	51	LYS	2.5
1	A	62	SER	2.5

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Mol	Chain	Res	Type	RSRZ
4	R	99	ILE	2.4
1	A	1	MET	2.4
2	B	1	GLY	2.4
3	C	236	GLN	2.4
2	P	52	THR	2.4
2	P	54	THR	2.3
12	L	163	GLY	2.3
7	G	68	ARG	2.3
2	P	93	HIS	2.3
3	C	186	VAL	2.3
8	V	226	GLU	2.3
4	D	3	GLY	2.3
6	T	53	LYS	2.3
6	F	243	ILE	2.3
6	T	226	PHE	2.3
9	I	132	ALA	2.3
2	P	53	SER	2.3
11	Y	18	SER	2.3
3	Q	206	LYS	2.3
7	U	24	LYS	2.3
1	O	4	ARG	2.3
3	Q	48	SER	2.2
3	Q	3	ASP	2.2
3	Q	225	GLU	2.2
8	H	221	CYS	2.2
3	C	52	LEU	2.2
3	Q	223	SER	2.2
1	A	201	GLU	2.2
1	A	249	ALA	2.2
5	S	228	ALA	2.2
4	D	2	ARG	2.2
5	E	173	ARG	2.2
3	Q	201	VAL	2.2
3	C	221	ALA	2.2
2	P	62	THR	2.2
10	X	2	ASP	2.2
6	F	204	LYS	2.2
12	L	173	LYS	2.2
3	C	239	GLN	2.1
2	P	56	LEU	2.1
7	G	3	TYR	2.1
4	D	242	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
4	R	1	ASP	2.1
9	I	1	SER	2.1
3	Q	238	LYS	2.1
8	H	27	ALA	2.1
8	V	9	ASN	2.1
3	Q	232	THR	2.1
10	X	98	TYR	2.1
1	O	57	MET	2.1
11	Y	209	ASN	2.1
6	F	242	GLU	2.1
7	G	177	PHE	2.1
5	E	123	GLY	2.1
4	R	242	GLU	2.1
5	E	233	ILE	2.1
3	C	238	LYS	2.1
2	P	221	ASP	2.1
10	X	194	ASP	2.1
9	W	151	SER	2.1
8	V	31	CYS	2.1
11	K	212	GLY	2.0
6	F	206	LYS	2.0
5	S	52	ALA	2.0
8	H	32	ALA	2.0
8	V	32	ALA	2.0
8	V	120	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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($\text{\AA}^2$)	Q<0.9
15	MG	H	301	1/1	0.69	0.14	74,74,74,74	0
15	MG	I	302	1/1	0.69	0.35	81,81,81,81	0
16	3K4	Y	302	6/7	0.87	0.14	48,54,57,58	0
16	3K4	K	301	6/7	0.89	0.12	45,50,53,55	0
15	MG	N	201	1/1	0.92	0.07	48,48,48,48	0
15	MG	I	301	1/1	0.92	0.08	53,53,53,53	0
15	MG	J	201	1/1	0.92	0.19	55,55,55,55	0
15	MG	Z	301	1/1	0.94	0.08	46,46,46,46	0
15	MG	Y	301	1/1	0.95	0.10	47,47,47,47	0
15	MG	V	301	1/1	0.96	0.07	44,44,44,44	0
15	MG	G	301	1/1	0.97	0.08	41,41,41,41	0
15	MG	K	302	1/1	0.98	0.13	51,51,51,51	0
15	MG	K	303	1/1	0.98	0.14	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.