



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:19 PM UTC

PDB ID : 5LAJ / pdb_00005la.j
Title : Ligand-induced Lys33-Thr1 crosslinking at the yeast proteasomal subunit beta5 by sulfonate esters
Authors : Groll, M.; Dubiella, C.; Cui, H.
Deposited on : 2016-06-14
Resolution : 2.90 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
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

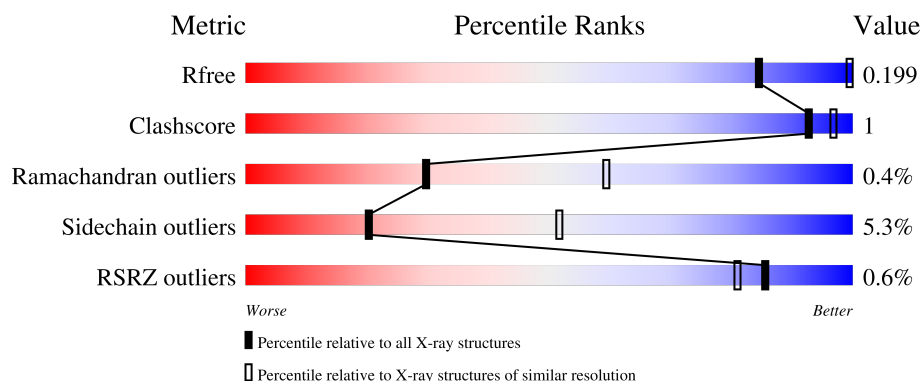
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

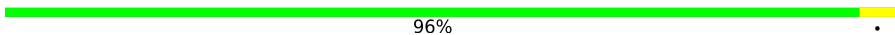
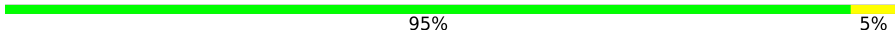
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	 96%
1	O	250	 95% 5%
2	B	258	 2% 86% 8% 5%
2	P	258	 2% 87% 7% 5%
3	C	254	 0% 83% 9% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 2% 83% 9% 6%
4	D	260	 1% 83% 7% 10%
4	R	260	 83% 7% 10%
5	E	234	 88% 10%
5	S	234	 88% 10%
6	F	288	 1% 77% 7% 16%
6	T	288	 1% 77% 7% 16%
7	G	252	 89% 6%
7	U	252	 89% 7%
8	H	232	 1% 91% 7%
8	V	232	 1% 91% 7%
9	I	205	 92% 7%
9	W	205	 93% 6%
10	J	198	 1% 89% 9%
10	X	198	 2% 88% 10%
11	K	212	 90% 9%
11	Y	212	 91% 8%
12	L	222	 95% 5%
12	Z	222	 95% 5%
13	M	246	 85% 7% 7%
13	a	246	 86% 7% 6%
14	N	196	 1% 91% 7%
14	b	196	 1% 91% 7%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 49524 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	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	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	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			
13	a	231	Total	C	N	O	S	0	0	0
			1806	1142	309	348	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	I	3	Total	Mg	0	0
			3	3		

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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	8	Total 8	O 8	0	0
16	B	7	Total 7	O 7	0	0
16	C	7	Total 7	O 7	0	0
16	D	7	Total 7	O 7	0	0
16	E	6	Total 6	O 6	0	0
16	F	6	Total 6	O 6	0	0
16	G	7	Total 7	O 7	0	0
16	H	14	Total 14	O 14	0	0
16	I	5	Total 5	O 5	0	0
16	J	10	Total 10	O 10	0	0
16	K	9	Total 9	O 9	0	0
16	L	11	Total 11	O 11	0	0
16	M	8	Total 8	O 8	0	0
16	N	6	Total 6	O 6	0	0

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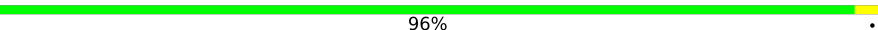
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	O	2	Total O 2 2	0	0
16	P	9	Total O 9 9	0	0
16	Q	5	Total O 5 5	0	0
16	R	3	Total O 3 3	0	0
16	S	4	Total O 4 4	0	0
16	T	3	Total O 3 3	0	0
16	U	10	Total O 10 10	0	0
16	V	9	Total O 9 9	0	0
16	W	6	Total O 6 6	0	0
16	X	5	Total O 5 5	0	0
16	Y	9	Total O 9 9	0	0
16	Z	10	Total O 10 10	0	0
16	a	14	Total O 14 14	0	0
16	b	5	Total O 5 5	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:  96%



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  95%



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  86%



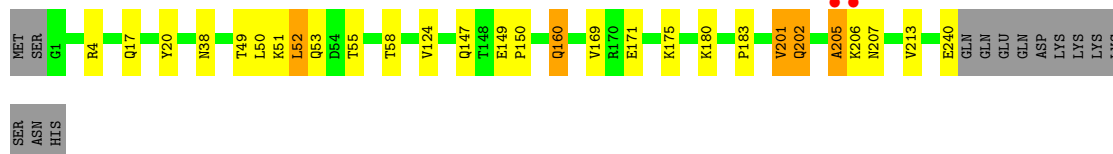
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  87%

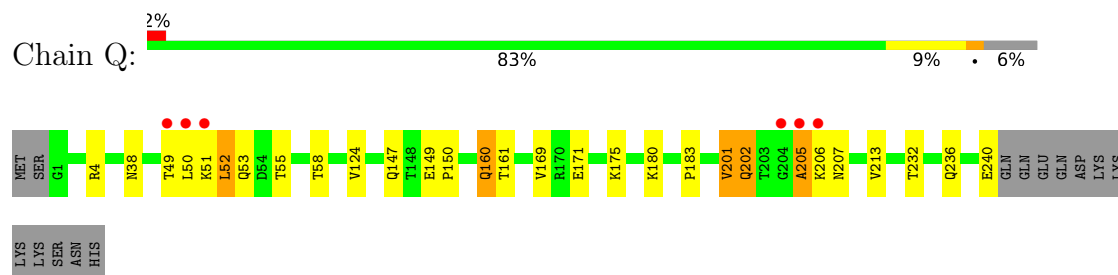


- Molecule 3: Proteasome subunit alpha type-4

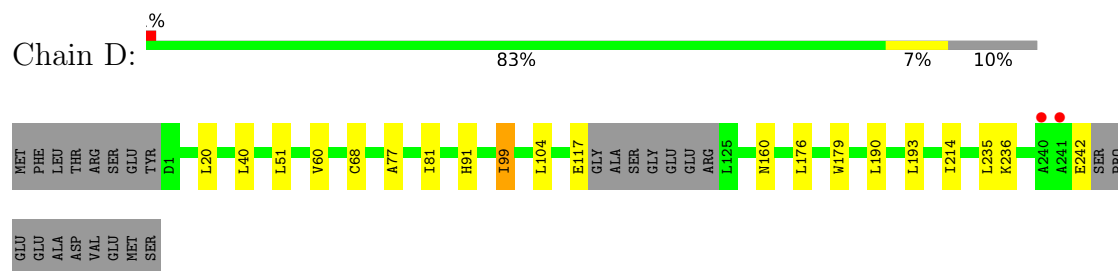
Chain C:  83%



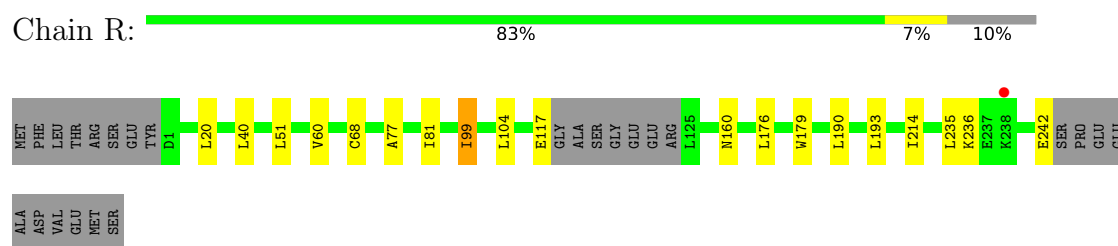
- Molecule 3: Proteasome subunit alpha type-4



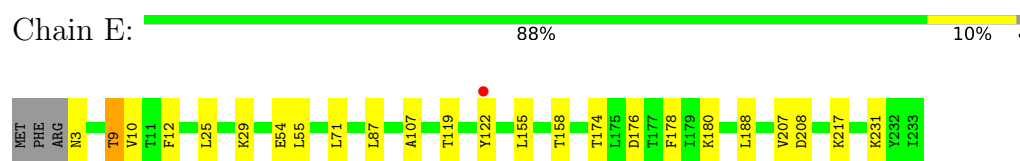
- Molecule 4: Proteasome subunit alpha type-5



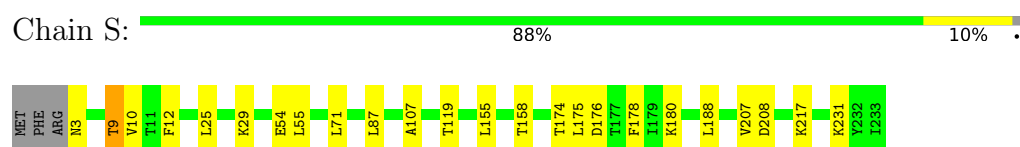
- Molecule 4: Proteasome subunit alpha type-5



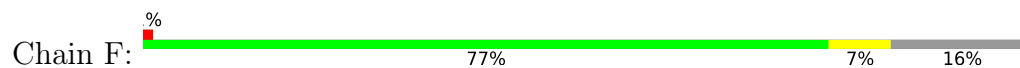
- Molecule 5: Proteasome subunit alpha type-6

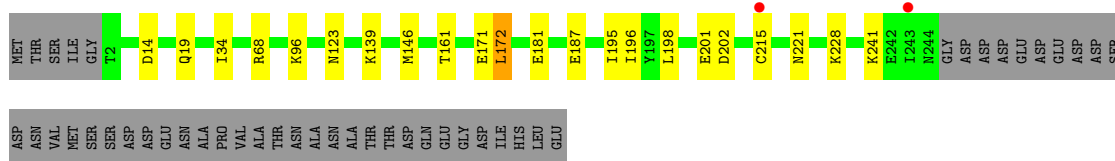


- Molecule 5: Proteasome subunit alpha type-6

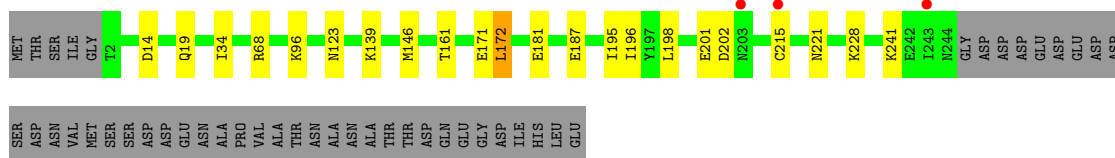
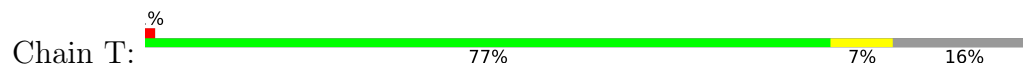


- Molecule 6: Probable proteasome subunit alpha type-7

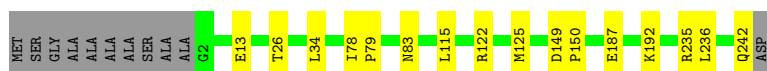




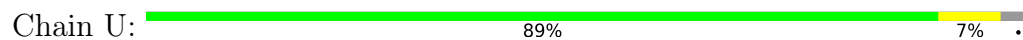
- Molecule 6: Probable proteasome subunit alpha type-7



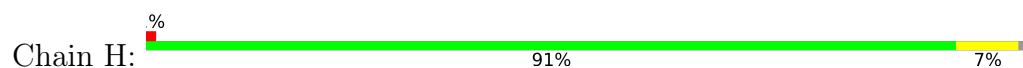
- Molecule 7: Proteasome subunit alpha type-1



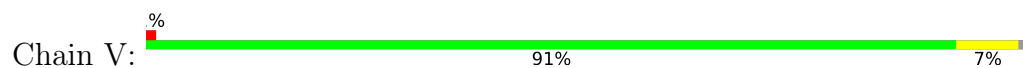
- Molecule 7: Proteasome subunit alpha type-1



- 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

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% 9% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 91% 8% .



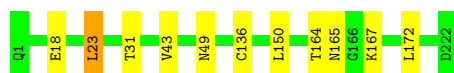
- Molecule 12: Proteasome subunit beta type-6

Chain L: 95% 5%



- Molecule 12: Proteasome subunit beta type-6

Chain Z: 95% 5%



- Molecule 13: Proteasome subunit beta type-7

Chain M: 85% 7% 7%



- Molecule 13: Proteasome subunit beta type-7

Chain a: 86% 7% 6%



- Molecule 14: Proteasome subunit beta type-1

Chain N: 91% 7% .



- Molecule 14: Proteasome subunit beta type-1

Chain b: 91% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.25Å 300.53Å 146.42Å 90.00° 113.73° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (15.00-2.90) 96.1 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.180 , 0.201 (Not available) , 0.199	Depositor DCC
R_{free} test set	11489 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49524	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/1952	0.70	0/2642
1	O	0.40	0/1952	0.70	0/2642
2	B	0.41	0/1934	0.69	0/2618
2	P	0.41	0/1934	0.69	0/2618
3	C	0.41	0/1910	0.71	1/2586 (0.0%)
3	Q	0.41	0/1910	0.71	1/2586 (0.0%)
4	D	0.39	0/1837	0.69	0/2475
4	R	0.39	0/1837	0.69	0/2475
5	E	0.40	0/1800	0.68	0/2433
5	S	0.40	0/1800	0.68	0/2433
6	F	0.40	0/1932	0.70	0/2609
6	T	0.40	0/1932	0.70	0/2609
7	G	0.39	0/1945	0.68	0/2634
7	U	0.40	0/1945	0.68	0/2634
8	H	0.36	0/1750	0.67	0/2373
8	V	0.36	0/1750	0.67	0/2373
9	I	0.36	0/1611	0.69	0/2174
9	W	0.36	0/1611	0.69	0/2174
10	J	0.39	0/1589	0.66	0/2142
10	X	0.39	0/1589	0.66	0/2142
11	K	0.34	0/1680	0.67	0/2272
11	Y	0.35	0/1680	0.67	0/2272
12	L	0.35	0/1795	0.67	0/2420
12	Z	0.36	0/1795	0.67	0/2420
13	M	0.37	0/1817	0.69	0/2465
13	a	0.38	0/1837	0.69	0/2492
14	N	0.35	0/1541	0.67	0/2087
14	b	0.35	0/1541	0.67	0/2087
All	All	0.38	0/50206	0.68	2/67887 (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
2	B	0	1
2	P	0	1
All	All	0	2

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	5.97	116.75	110.72
3	C	201	VAL	N-CA-C	5.96	116.74	110.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	50	LYS	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	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	7	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1892	0	1883	5	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	5	0
8	H	1719	0	1719	3	0
8	V	1719	0	1719	3	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	8	0
11	K	1643	0	1591	9	0
11	Y	1643	0	1591	8	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	2	0
13	M	1786	0	1790	6	0
13	a	1806	0	1808	7	0
14	N	1512	0	1481	10	0
14	b	1512	0	1481	10	0
15	G	1	0	0	0	0
15	I	3	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	2	0	0	0	0
15	Z	1	0	0	0	0
16	A	8	0	0	0	0
16	B	7	0	0	0	0
16	C	7	0	0	0	0
16	D	7	0	0	0	0
16	E	6	0	0	0	0
16	F	6	0	0	0	0
16	G	7	0	0	0	0
16	H	14	0	0	0	0
16	I	5	0	0	0	0
16	J	10	0	0	0	0
16	K	9	0	0	0	0
16	L	11	0	0	0	0
16	M	8	0	0	0	0
16	N	6	0	0	0	0
16	O	2	0	0	0	0
16	P	9	0	0	0	0
16	Q	5	0	0	0	0
16	R	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	S	4	0	0	0	0
16	T	3	0	0	0	0
16	U	10	0	0	0	0
16	V	9	0	0	0	0
16	W	6	0	0	0	0
16	X	5	0	0	0	0
16	Y	9	0	0	0	0
16	Z	10	0	0	0	0
16	a	14	0	0	1	0
16	b	5	0	0	0	0
All	All	49524	0	49056	144	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 1.

All (144) 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)
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.82	0.61
3:C:51:LYS:O	3:C:52:LEU:HB2	1.99	0.61
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.82	0.61
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.99	0.61
2:B:12:PHE:H	3:C:17:GLN:HE22	1.49	0.61
11:K:53:GLN:O	11:K:57:THR:HG23	2.02	0.59
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.02	0.59
2:B:217:LYS:O	2:B:219:ALA:N	2.39	0.56
13:a:2:GLN:NE2	16:a:301:HOH:O	2.37	0.56
2:P:217:LYS:O	2:P:219:ALA:N	2.40	0.55
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.90	0.54
6:F:146:MET:HE3	6:F:161:THR:HB	1.89	0.54
6:T:146:MET:HE3	6:T:161:THR:HB	1.90	0.54
3:C:201:VAL:O	3:C:202:GLN:CB	2.56	0.53
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.90	0.53
14:b:20:THR:HG22	14:b:31:THR:OG1	2.09	0.53
14:N:20:THR:HG22	14:N:31:THR:OG1	2.09	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.53
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.56	0.52
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.90	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.52
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.90	0.52
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.92	0.52
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.91	0.52
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.40	0.51
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.92	0.51
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.51
5:S:12:PHE:H	6:T:19:GLN:HE22	1.58	0.51
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.40	0.51
14:b:152:VAL:HA	14:b:175:MET:HE1	1.93	0.51
7:G:187:GLU:HG2	7:G:192:LYS:HB3	1.93	0.50
7:U:187:GLU:HG2	7:U:192:LYS:HB3	1.94	0.50
5:E:12:PHE:H	6:F:19:GLN:HE22	1.59	0.50
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.47	0.50
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.93	0.49
14:N:152:VAL:HA	14:N:175:MET:HE1	1.94	0.49
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.95	0.48
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.95	0.48
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.48	0.48
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.48	0.48
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.95	0.48
13:M:159:VAL:HG23	13:M:159:VAL:O	2.13	0.48
12:Z:164:THR:O	12:Z:167:LYS:HE3	2.14	0.47
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.95	0.47
12:L:164:THR:O	12:L:167:LYS:HE3	2.15	0.47
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.47
14:b:35:THR:CG2	14:b:45:ARG:HE	2.27	0.47
14:N:35:THR:CG2	14:N:45:ARG:HE	2.28	0.47
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.98	0.46
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.97	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.97	0.46
13:a:159:VAL:O	13:a:159:VAL:HG23	2.14	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.98	0.46
14:N:20:THR:CG2	14:N:31:THR:OG1	2.64	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.98	0.45
14:b:20:THR:CG2	14:b:31:THR:OG1	2.64	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.98	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.45
10:J:162:LYS:HG3	10:J:195:PHE:CZ	2.52	0.45
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.98	0.44
13:M:150:MET:HE1	13:M:187:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:ARG:HD2	9:I:126:ILE:HG12	1.99	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
1:A:176:GLU:HG2	2:B:55:LEU:HD22	1.98	0.44
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.44
5:E:9:THR:HG21	5:E:119:THR:HA	1.99	0.44
14:b:35:THR:HG21	14:b:45:ARG:HE	1.83	0.44
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.99	0.44
5:S:9:THR:HG21	5:S:119:THR:HA	1.99	0.44
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.00	0.44
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.97	0.44
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.53	0.44
14:N:35:THR:HG21	14:N:45:ARG:HE	1.83	0.44
1:O:55:LEU:HB3	7:U:159:ALA:O	2.17	0.44
10:X:162:LYS:HG3	10:X:195:PHE:CZ	2.53	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.47	0.43
2:P:58:GLN:NE2	2:P:208:ASP:HA	2.34	0.43
6:T:172:LEU:HD13	6:T:195:ILE:HD13	2.01	0.43
6:F:172:LEU:HD13	6:F:195:ILE:HD13	2.01	0.43
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.00	0.43
9:W:98:ARG:HD2	9:W:126:ILE:HG12	2.00	0.43
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.99	0.43
11:K:17:ASP:OD1	11:K:33:LYS:NZ	2.52	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.01	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.42
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.00	0.42
10:J:132:ALA:HB1	10:J:136:SER:HB2	2.01	0.42
11:Y:17:ASP:OD1	11:Y:33:LYS:NZ	2.52	0.42
5:E:178:PHE:CD1	5:E:178:PHE:C	2.98	0.42
10:X:132:ALA:HB1	10:X:136:SER:HB2	2.02	0.42
10:J:168:LEU:O	10:J:172:MET:HB2	2.20	0.42
5:S:155:LEU:HD13	5:S:158:THR:HB	2.02	0.42
5:E:155:LEU:HD13	5:E:158:THR:HB	2.02	0.42
14:N:133:PHE:HA	14:b:132:THR:O	2.19	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.20	0.42
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.19	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.42
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.47	0.42
2:B:58:GLN:NE2	2:B:208:ASP:HA	2.34	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:77:ALA:O	4:D:81:ILE:HG12	2.20	0.41
6:F:34:ILE:HG12	6:F:196:ILE:HD11	2.03	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.03	0.41
6:T:34:ILE:HG12	6:T:196:ILE:HD11	2.02	0.41
3:C:205:ALA:C	3:C:207:ASN:H	2.28	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
5:S:178:PHE:CD1	5:S:178:PHE:C	2.98	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.03	0.41
3:Q:205:ALA:C	3:Q:207:ASN:H	2.28	0.41
5:S:176:ASP:O	5:S:180:LYS:HD3	2.20	0.41
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.86	0.41
4:R:77:ALA:O	4:R:81:ILE:HG12	2.21	0.41
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.86	0.41
11:K:45:MET:HG3	11:K:52:CYS:HB2	2.03	0.41
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.03	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.41
6:T:146:MET:CE	6:T:161:THR:HB	2.50	0.41
10:X:149:ARG:O	10:X:152:MET:HG3	2.21	0.41
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.03	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
3:Q:232:THR:O	3:Q:236:GLN:HG3	2.21	0.41
5:E:176:ASP:O	5:E:180:LYS:HD3	2.20	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.46	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.03	0.41
11:K:12:ILE:HB	11:K:180:VAL:HB	2.03	0.40
6:F:146:MET:CE	6:F:161:THR:HB	2.51	0.40
3:Q:160:GLN:HG3	3:Q:161:THR:N	2.36	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.40
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.56	0.40
13:a:96:LEU:O	13:a:100:MET:HG2	2.20	0.40
14:b:163:ILE:HG23	14:b:170:GLY:HA2	2.03	0.40
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.52	0.40
7:G:34:LEU:C	7:G:34:LEU:HD23	2.46	0.40
14:N:132:THR:O	14:b:133:PHE:HA	2.21	0.40
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.04	0.40
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	44
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	44
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	26
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	26
3	C	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	9	32
3	Q	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	9	32
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	217 (97%)	6 (3%)	1 (0%)	30	59
8	V	224/232 (97%)	217 (97%)	6 (3%)	1 (0%)	30	59
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	24	54
12	Z	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	24	54
13	M	226/246 (92%)	219 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	229/246 (93%)	222 (97%)	5 (2%)	2 (1%)	14	41
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6277/6614 (95%)	6118 (98%)	135 (2%)	24 (0%)	30	59

All (24) 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
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	Q	202	GLN
1	A	166	LYS
3	C	205	ALA
1	O	166	LYS
3	Q	205	ALA
2	B	220	ASN
2	P	220	ASN
8	H	9	ASN
8	V	9	ASN
12	L	165	ASN
12	Z	165	ASN
2	B	221	ASP
3	C	183	PRO
2	P	221	ASP
3	Q	183	PRO
13	a	83	ALA
13	a	229	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	64
1	O	209/209 (100%)	201 (96%)	8 (4%)	29	64
2	B	203/216 (94%)	193 (95%)	10 (5%)	22	54
2	P	185/216 (86%)	176 (95%)	9 (5%)	22	54
3	C	212/226 (94%)	195 (92%)	17 (8%)	11	34
3	Q	212/226 (94%)	195 (92%)	17 (8%)	11	34
4	D	194/215 (90%)	180 (93%)	14 (7%)	13	39
4	R	194/215 (90%)	180 (93%)	14 (7%)	13	39
5	E	190/193 (98%)	176 (93%)	14 (7%)	13	38
5	S	190/193 (98%)	176 (93%)	14 (7%)	13	38
6	F	201/239 (84%)	185 (92%)	16 (8%)	11	34
6	T	201/239 (84%)	185 (92%)	16 (8%)	11	34
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	59
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	59
8	H	185/190 (97%)	175 (95%)	10 (5%)	20	51
8	V	185/190 (97%)	175 (95%)	10 (5%)	20	51
9	I	172/173 (99%)	167 (97%)	5 (3%)	37	71
9	W	172/173 (99%)	167 (97%)	5 (3%)	37	71
10	J	173/175 (99%)	167 (96%)	6 (4%)	32	66
10	X	173/175 (99%)	167 (96%)	6 (4%)	32	66
11	K	168/169 (99%)	162 (96%)	6 (4%)	31	65
11	Y	168/169 (99%)	162 (96%)	6 (4%)	31	65
12	L	185/185 (100%)	178 (96%)	7 (4%)	29	64
12	Z	185/185 (100%)	178 (96%)	7 (4%)	29	64
13	M	195/208 (94%)	185 (95%)	10 (5%)	21	53
13	a	197/208 (95%)	187 (95%)	10 (5%)	21	53
14	N	162/162 (100%)	154 (95%)	8 (5%)	22	54
14	b	162/162 (100%)	154 (95%)	8 (5%)	22	54
All	All	5294/5540 (96%)	5015 (95%)	279 (5%)	20	52

All (279) 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	231	LYS
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
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	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
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	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	175	LYS
3	C	180	LYS
3	C	206	LYS
3	C	213	VAL
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	176	LEU

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Mol	Chain	Res	Type
4	D	190	LEU
4	D	193	LEU
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
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	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	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET

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Mol	Chain	Res	Type
7	G	235	ARG
7	G	236	LEU
7	G	242	GLN
8	H	13	VAL
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	106	THR
8	H	127	LEU
8	H	153	LYS
8	H	195	VAL
8	H	196	ARG
8	H	222	ASP
9	I	37	ASN
9	I	96	GLU
9	I	126	ILE
9	I	171	LEU
9	I	192	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
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	97	MET
11	K	107	LYS
11	K	148	LEU
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
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

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Mol	Chain	Res	Type
13	M	146	PHE
13	M	161	ARG
13	M	187	ARG
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	231	LYS
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	65	LEU
2	P	79	LEU
2	P	180	LYS
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	50	LEU
3	Q	52	LEU
3	Q	53	GLN
3	Q	55	THR
3	Q	58	THR
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU

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Mol	Chain	Res	Type
3	Q	175	LYS
3	Q	180	LYS
3	Q	206	LYS
3	Q	213	VAL
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	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
5	S	231	LYS
6	T	14	ASP
6	T	68	ARG
6	T	96	LYS
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	187	GLU

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Mol	Chain	Res	Type
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	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
7	U	242	GLN
8	V	13	VAL
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	195	VAL
8	V	196	ARG
8	V	222	ASP
9	W	37	ASN
9	W	96	GLU
9	W	126	ILE
9	W	171	LEU
9	W	192	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	97	MET
11	Y	107	LYS

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Mol	Chain	Res	Type
11	Y	148	LEU
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
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
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 (129) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	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	38	ASN
3	C	115	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN

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Mol	Chain	Res	Type
3	C	160	GLN
4	D	91	HIS
4	D	100	ASN
4	D	149	HIS
4	D	225	ASN
5	E	68	HIS
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	123	ASN
6	F	191	GLN
6	F	244	ASN
7	G	30	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
7	G	186	ASN
8	H	30	ASN
8	H	189	ASN
9	I	37	ASN
9	I	44	HIS
9	I	63	ASN
9	I	88	GLN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	80	ASN
12	L	197	GLN

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Mol	Chain	Res	Type
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
1	O	94	HIS
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	115	GLN
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	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	244	ASN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN

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Mol	Chain	Res	Type
7	U	121	GLN
7	U	166	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	66	HIS
8	V	189	ASN
9	W	37	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	146	HIS
11	Y	9	GLN
11	Y	62	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	79	HIS
12	Z	197	GLN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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%)	-0.42	0 100 100	38, 54, 92, 131	0
1	O	250/250 (100%)	-0.37	1 (0%) 88 85	46, 64, 109, 144	0
2	B	244/258 (94%)	-0.28	4 (1%) 70 62	40, 61, 109, 177	0
2	P	244/258 (94%)	-0.19	4 (1%) 70 62	47, 65, 115, 178	0
3	C	240/254 (94%)	-0.24	2 (0%) 82 77	41, 66, 134, 164	0
3	Q	240/254 (94%)	-0.08	6 (2%) 58 48	46, 76, 156, 178	0
4	D	235/260 (90%)	-0.27	2 (0%) 81 75	48, 68, 104, 145	0
4	R	235/260 (90%)	-0.20	1 (0%) 88 85	50, 72, 112, 144	0
5	E	231/234 (98%)	-0.27	1 (0%) 88 85	52, 72, 109, 149	0
5	S	231/234 (98%)	-0.15	0 100 100	53, 78, 122, 168	0
6	F	243/288 (84%)	-0.39	2 (0%) 82 77	42, 60, 107, 146	0
6	T	243/288 (84%)	-0.23	3 (1%) 76 69	44, 69, 128, 164	0
7	G	241/252 (95%)	-0.41	0 100 100	41, 56, 93, 134	0
7	U	241/252 (95%)	-0.44	0 100 100	43, 59, 97, 130	0
8	H	226/232 (97%)	-0.34	2 (0%) 81 75	43, 55, 94, 170	0
8	V	226/232 (97%)	-0.32	2 (0%) 81 75	45, 60, 99, 185	0
9	I	204/205 (99%)	-0.55	1 (0%) 87 83	38, 52, 82, 111	0
9	W	204/205 (99%)	-0.51	0 100 100	40, 56, 91, 114	0
10	J	195/198 (98%)	-0.47	1 (0%) 87 83	39, 58, 86, 144	0
10	X	195/198 (98%)	-0.36	3 (1%) 72 64	39, 61, 90, 150	0
11	K	212/212 (100%)	-0.47	0 100 100	42, 58, 83, 100	0
11	Y	212/212 (100%)	-0.49	0 100 100	41, 56, 81, 104	0
12	L	222/222 (100%)	-0.44	0 100 100	42, 58, 92, 141	0
12	Z	222/222 (100%)	-0.44	0 100 100	34, 57, 90, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	228/246 (92%)	-0.50	0 100 100	37, 56, 85, 102	0
13	a	231/246 (93%)	-0.49	1 (0%) 88 85	38, 57, 86, 109	0
14	N	196/196 (100%)	-0.49	1 (0%) 87 83	38, 52, 85, 121	0
14	b	196/196 (100%)	-0.47	1 (0%) 87 83	40, 53, 85, 119	0
All	All	6337/6614 (95%)	-0.36	38 (0%) 85 81	34, 61, 106, 185	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	7.4
8	H	223	ILE	6.2
3	Q	50	LEU	5.1
8	V	223	ILE	4.9
3	Q	49	THR	4.7
10	J	1	MET	3.8
2	P	219	ALA	3.7
3	Q	205	ALA	3.5
6	F	215	CYS	3.3
4	D	241	ALA	3.2
2	B	218	GLY	3.1
8	V	224	GLN	3.0
2	B	219	ALA	2.8
14	N	1	THR	2.7
6	T	215	CYS	2.7
2	P	218	GLY	2.6
8	H	224	GLN	2.6
4	D	240	ALA	2.6
6	T	243	ILE	2.6
3	Q	206	LYS	2.4
13	a	1	THR	2.4
5	E	122	TYR	2.4
4	R	238	LYS	2.3
14	b	103	ASP	2.3
3	Q	204	GLY	2.3
2	B	220	ASN	2.3
3	C	205	ALA	2.3
2	P	93	HIS	2.3
3	C	206	LYS	2.2
10	X	2	ASP	2.2
1	O	53	SER	2.2
9	I	1	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	52	THR	2.1
6	T	203	ASN	2.1
6	F	243	ILE	2.1
10	X	174	MET	2.0
2	B	51	VAL	2.0
3	Q	51	LYS	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	I	302	1/1	0.57	0.37	110,110,110,110	0
15	MG	I	301	1/1	0.93	0.16	71,71,71,71	0
15	MG	K	302	1/1	0.93	0.09	70,70,70,70	0
15	MG	N	202	1/1	0.95	0.07	69,69,69,69	0
15	MG	L	301	1/1	0.97	0.11	67,67,67,67	0
15	MG	K	301	1/1	0.97	0.11	57,57,57,57	0
15	MG	Z	301	1/1	0.97	0.07	64,64,64,64	0
15	MG	G	301	1/1	0.98	0.03	55,55,55,55	0
15	MG	N	201	1/1	0.98	0.04	50,50,50,50	0
15	MG	I	303	1/1	0.99	0.08	46,46,46,46	0
15	MG	J	201	1/1	0.99	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.