



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 08:42 PM UTC

PDB ID : 4Y8N / pdb_00004y8n
Title : Yeast 20S proteasome beta7-delta7_Cter mutant in complex with Ac-PAE-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

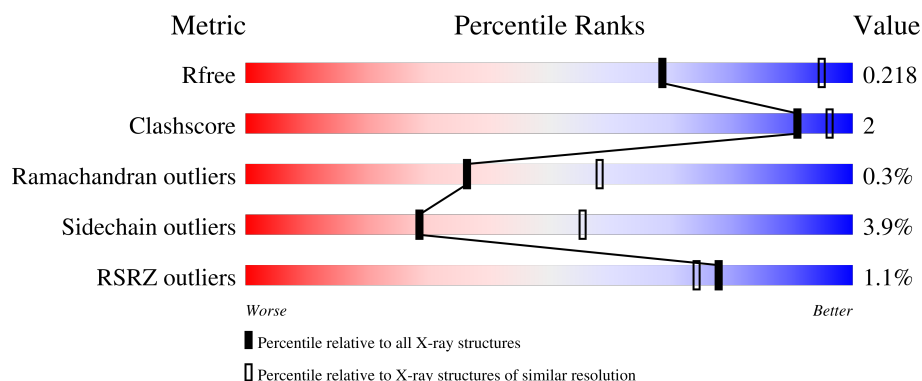
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	0% 97% 0%
1	O	250	0% 96% 0%
2	B	258	2% 85% 9% • 5%
2	P	258	3% 86% 8% • 5%
3	C	254	2% 84% 8% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 2% 85% 7% • 6%
4	D	260	 % 85% 5% • 10%
4	R	260	 % 84% 6% 10%
5	E	234	 93% 6% •
5	S	234	 2% 93% 6% •
6	F	288	 % 81% • 16%
6	T	288	 3% 82% • 16%
7	G	252	 % 88% 8% •
7	U	252	 88% 7% •
8	H	232	 90% 7% •
8	V	232	 % 91% 6% •
9	I	205	 94% 5%
9	W	205	 93% 6%
10	J	198	 % 88% 10% ••
10	X	198	 % 90% 8% ••
11	K	212	 92% 7% •
11	Y	212	 93% 6% •
12	L	222	 97% •
12	Z	222	 96% •
13	M	239	 % 88% 5% • 6%
13	a	239	 2% 87% 5% • 7%
14	N	196	 92% 7% •
14	b	196	 % 90% 9% •
15	c	5	 20% 60% 20%
15	d	5	 60% 20% 20%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49891 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
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	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	224	Total	C	N	O	S	0	0	0
			1753	1108	300	338	7			
13	a	223	Total	C	N	O	S	0	0	0
			1745	1104	299	335	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 a protein called Ac-PAE-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			28	18	3	7			
15	d	5	Total	C	N	O	0	0	0
			28	18	3	7			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	I	2	Total 2	Mg 2	0	0
16	K	1	Total 1	Mg 1	0	0
16	L	1	Total 1	Mg 1	0	0
16	N	1	Total 1	Mg 1	0	0
16	Z	1	Total 1	Mg 1	0	0

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total 1	Cl 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	28	Total 28	O 28	0	0
18	B	23	Total 23	O 23	0	0
18	C	19	Total 19	O 19	0	0
18	D	16	Total 16	O 16	0	0
18	E	9	Total 9	O 9	0	0
18	F	26	Total 26	O 26	0	0
18	G	30	Total 30	O 30	0	0
18	H	25	Total 25	O 25	0	0
18	I	24	Total 24	O 24	0	0
18	J	22	Total 22	O 22	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	20	Total 20	O 20	0	0
18	L	31	Total 31	O 31	0	0
18	M	27	Total 27	O 27	0	0
18	N	19	Total 19	O 19	0	0
18	O	15	Total 15	O 15	0	0
18	P	18	Total 18	O 18	0	0
18	Q	15	Total 15	O 15	0	0
18	R	21	Total 21	O 21	0	0
18	S	9	Total 9	O 9	0	0
18	T	19	Total 19	O 19	0	0
18	U	26	Total 26	O 26	0	0
18	V	20	Total 20	O 20	0	0
18	W	16	Total 16	O 16	0	0
18	X	19	Total 19	O 19	0	0
18	Y	31	Total 31	O 31	0	0
18	Z	27	Total 27	O 27	0	0
18	a	27	Total 27	O 27	0	0
18	b	24	Total 24	O 24	0	0
18	c	3	Total 3	O 3	0	0
18	d	2	Total 2	O 2	0	0

SER
ASN
HIS

• Molecule 3: Proteasome subunit alpha type-4

Chain Q: 2% 85% 7% • 6%

MET SER G1 R4 T29 K35 N38 T49 L80 K51 L52 S60 K61 V124 Q147 T148 E149 P150 S158 A159 Q160 V169 K180 P183 V201 Q202 T203 G204 A205 V213 E240 GLN GLN ASP LYS LYS LYS SER ASN HIS

• Molecule 4: Proteasome subunit alpha type-5

Chain D: 0% 85% 5% • 10%

MET PHE LEU THR ARG SER GLU TYR D1 Q15 L20 L40 L51 V60 H91 I99 E117 GLY ALA SER GLY GLU ARG L125 G167 L176 L190 L193 E202 I214 L235 K236 A240 A241 E242 SER PRO GLU ALA ASP VAL GLU

MET
SER

• Molecule 4: Proteasome subunit alpha type-5

Chain R: 0% 84% 6% • 10%

MET PHE LEU THR ARG SER GLU TYR D1 L20 L40 L51 V60 H91 I99 A112 L113 E117 GLY ALA SER GLY GLU ARG L125 M160 L176 L179 L190 L193 E202 I214 L235 K236 A241 E242 SER PRO GLU ALA ASP

VAL
GLU
MET
SER

• Molecule 5: Proteasome subunit alpha type-6

Chain E: 0% 93% 6% •

MET PHE ARG N3 T9 F12 K29 L55 L71 L87 A107 Y122 L175 F178 L188 V207 D208 K231 Y232 I233

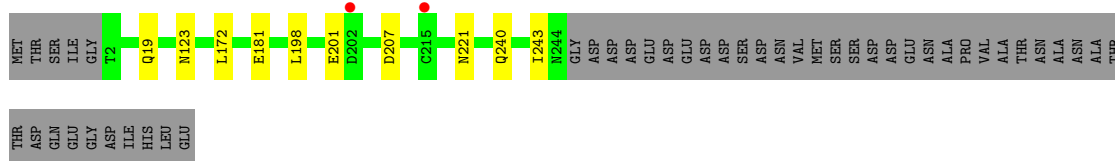
• Molecule 5: Proteasome subunit alpha type-6

Chain S: 2% 93% 6% •

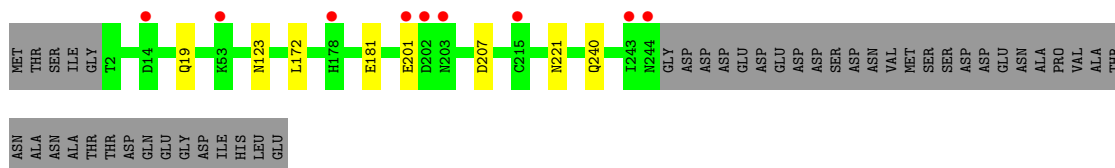
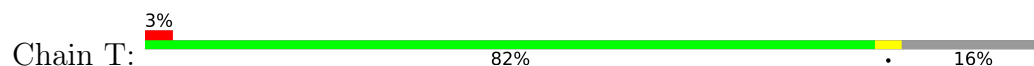
MET PHE ARG N3 T9 F12 K29 A52 L55 L71 L87 A107 Y122 R173 T174 L175 F178 L188 V207 D208 K231 Y232 I233

• Molecule 6: Probable proteasome subunit alpha type-7

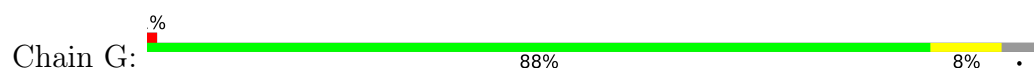
Chain F: 0% 81% • 16%



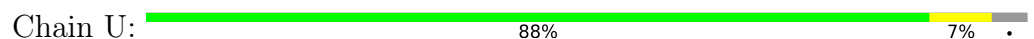
- Molecule 6: Probable proteasome subunit alpha type-7



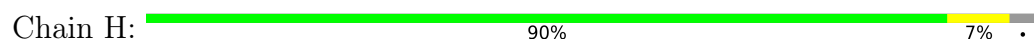
- Molecule 7: Proteasome subunit alpha type-1



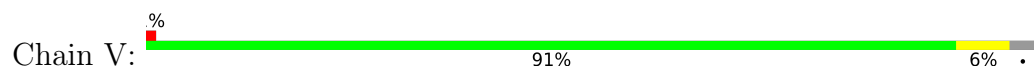
- Molecule 7: Proteasome subunit alpha type-1



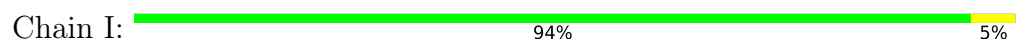
- Molecule 8: Proteasome subunit beta type-2



- 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: 88% 10% ..



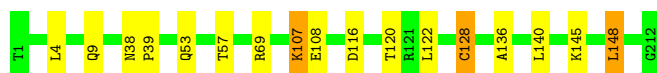
- Molecule 10: Proteasome subunit beta type-4

Chain X: 90% 8% ..



- Molecule 11: Proteasome subunit beta type-5

Chain K: 92% 7% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 93% 6% .

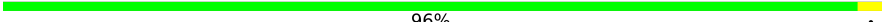


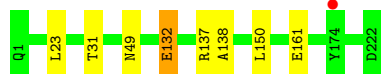
- Molecule 12: Proteasome subunit beta type-6

Chain L: 97% .



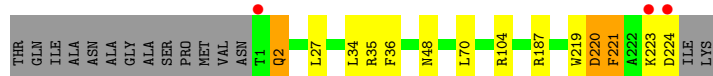
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  96% .



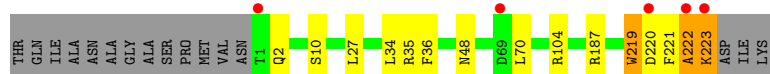
- Molecule 13: Proteasome subunit beta type-7

Chain M:  88% 5% • 6%



- Molecule 13: Proteasome subunit beta type-7

Chain a:  87% 5% • 7%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  92% 7% .

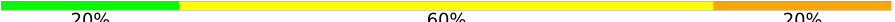


- Molecule 14: Proteasome subunit beta type-1

Chain b:  90% 9% .

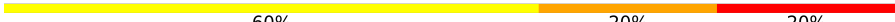


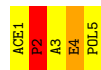
- Molecule 15: Ac-PAE-ep

Chain c:  20% 60% 20%



- Molecule 15: Ac-PAE-ep

Chain d:  60% 20% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.41Å 301.59Å 145.62Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.60) 95.0 (15.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.197 , 0.215 0.199 , 0.218	Depositor DCC
R_{free} test set	15717 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49891	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: ACE, CL, POL, GAU, 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	0.42	0/1952	0.69	0/2642
1	O	0.42	0/1952	0.69	0/2642
2	B	0.43	0/1934	0.68	0/2618
2	P	0.42	0/1934	0.68	0/2618
3	C	0.42	0/1910	0.70	1/2586 (0.0%)
3	Q	0.42	0/1910	0.70	1/2586 (0.0%)
4	D	0.41	0/1837	0.67	0/2475
4	R	0.41	0/1837	0.67	0/2475
5	E	0.42	0/1800	0.65	0/2433
5	S	0.42	0/1800	0.65	0/2433
6	F	0.41	0/1932	0.68	0/2609
6	T	0.42	0/1932	0.69	0/2609
7	G	0.41	0/1945	0.68	0/2634
7	U	0.41	0/1945	0.68	0/2634
8	H	0.45	0/1750	0.66	0/2373
8	V	0.40	0/1750	0.67	0/2373
9	I	0.47	0/1611	0.69	0/2174
9	W	0.41	0/1611	0.67	0/2174
10	J	0.45	1/1589 (0.1%)	0.67	0/2142
10	X	0.43	1/1589 (0.1%)	0.65	0/2142
11	K	0.41	0/1681	0.68	0/2274
11	Y	0.39	0/1681	0.66	0/2274
12	L	0.40	0/1795	0.68	1/2420 (0.0%)
12	Z	0.41	0/1795	0.68	1/2420 (0.0%)
13	M	0.46	0/1783	0.69	0/2420
13	a	0.46	0/1775	0.70	2/2409 (0.1%)
14	N	0.53	0/1541	0.71	1/2087 (0.0%)
14	b	0.51	0/1541	0.70	0/2087
15	c	3.88	2/13 (15.4%)	1.25	0/18
15	d	3.94	2/13 (15.4%)	1.37	0/18
All	All	0.44	6/50138 (0.0%)	0.68	7/67799 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	1	ACE	C-N	-11.15	1.32	1.43
15	d	1	ACE	C-N	-10.71	1.32	1.43
15	d	2	PRO	CA-C	-7.30	1.37	1.52
15	c	2	PRO	CA-C	-6.94	1.38	1.52
10	J	2	ASP	CA-C	5.37	1.55	1.52
10	X	2	ASP	CA-C	5.08	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.55	116.69	110.53
3	C	201	VAL	N-CA-C	6.49	116.63	110.53
13	a	219	TRP	N-CA-C	-5.39	108.48	114.62
12	L	132	GLU	CA-CB-CG	5.38	124.87	114.10
14	N	19	ARG	N-CA-C	5.14	117.62	109.24
12	Z	132	GLU	CA-CB-CG	5.05	124.21	114.10
13	a	10	SER	N-CA-C	5.05	117.37	110.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	12	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1892	0	1883	1	0
7	G	1907	0	1901	7	0
7	U	1907	0	1901	7	0
8	H	1719	0	1719	10	0
8	V	1719	0	1719	10	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	13	0
10	X	1561	0	1569	9	0
11	K	1644	0	1595	7	0
11	Y	1644	0	1595	6	0
12	L	1757	0	1711	0	0
12	Z	1757	0	1711	1	0
13	M	1753	0	1754	13	0
13	a	1745	0	1750	15	0
14	N	1512	0	1478	9	0
14	b	1512	0	1478	12	0
15	c	28	0	26	3	0
15	d	28	0	26	3	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
18	A	28	0	0	0	0
18	B	23	0	0	0	0
18	C	19	0	0	0	0
18	D	16	0	0	0	0
18	E	9	0	0	0	0
18	F	26	0	0	1	0
18	G	30	0	0	0	0
18	H	25	0	0	0	0
18	I	24	0	0	0	0
18	J	22	0	0	0	0
18	K	20	0	0	0	0
18	L	31	0	0	0	0
18	M	27	0	0	1	0
18	N	19	0	0	0	0
18	O	15	0	0	0	0
18	P	18	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Q	15	0	0	0	0
18	R	21	0	0	0	0
18	S	9	0	0	0	0
18	T	19	0	0	0	0
18	U	26	0	0	0	0
18	V	20	0	0	0	0
18	W	16	0	0	0	0
18	X	19	0	0	0	0
18	Y	31	0	0	0	0
18	Z	27	0	0	0	0
18	a	27	0	0	0	0
18	b	24	0	0	0	0
18	c	3	0	0	1	0
18	d	2	0	0	0	0
All	All	49891	0	49016	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (170) 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)
13:a:221:PHE:O	13:a:223:LYS:N	1.71	1.21
13:a:221:PHE:C	13:a:223:LYS:H	1.85	0.84
15:c:4:GAU:OE2	18:c:101:HOH:O	2.04	0.76
8:V:53:GLU:OE1	8:V:57:GLN:NE2	2.21	0.73
13:a:221:PHE:C	13:a:223:LYS:N	2.41	0.73
8:H:53:GLU:OE1	8:H:57:GLN:NE2	2.21	0.72
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.26	0.71
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.46	0.63
13:M:220:ASP:O	13:M:223:LYS:HG2	2.00	0.61
13:M:224:ASP:OD2	8:V:123:TYR:OH	2.17	0.61
14:N:13:ILE:HG21	14:N:175:MET:CE	2.31	0.61
13:M:35:ARG:HH12	14:N:114:PRO:HB3	1.67	0.60
5:S:12:PHE:H	6:T:19:GLN:HE22	1.50	0.59
13:a:219:TRP:O	13:a:222:ALA:N	2.34	0.59
2:B:12:PHE:H	3:C:17:GLN:HE22	1.51	0.59
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.85	0.58
14:b:152:VAL:HA	14:b:175:MET:HE1	1.85	0.58
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.86	0.58
8:V:113:ILE:HG13	8:V:119:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:93:HIS:HB3	18:P:301:HOH:O	2.04	0.57
13:a:35:ARG:HH12	14:b:114:PRO:HB3	1.70	0.57
2:B:221:ASP:O	2:B:223:GLU:N	2.38	0.56
2:P:221:ASP:O	2:P:223:GLU:N	2.39	0.56
13:M:223:LYS:O	13:M:224:ASP:HB3	2.06	0.56
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.05	0.55
2:P:217:LYS:C	2:P:219:ALA:H	2.15	0.55
13:a:221:PHE:C	13:a:221:PHE:CD2	2.85	0.54
14:N:168:SER:HB3	15:c:5:POL:H33	1.89	0.54
5:E:12:PHE:H	6:F:19:GLN:HE22	1.56	0.54
2:B:217:LYS:C	2:B:219:ALA:H	2.14	0.54
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.91	0.53
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.53
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.91	0.53
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
11:K:53:GLN:O	11:K:57:THR:HG23	2.11	0.51
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.76	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.50
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.77	0.50
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.11	0.50
8:H:113:ILE:CG1	8:H:119:THR:HG22	2.41	0.50
13:M:224:ASP:O	13:M:224:ASP:OD1	2.28	0.50
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.46	0.50
8:H:35:HIS:CE1	8:H:53:GLU:OE2	2.65	0.50
13:M:35:ARG:NH1	14:N:114:PRO:HB3	2.26	0.50
8:V:113:ILE:CG1	8:V:119:THR:HG22	2.41	0.50
13:a:35:ARG:HD3	13:a:36:PHE:CZ	2.47	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.77	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.95	0.49
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.95	0.49
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.95	0.49
1:O:12:PHE:H	2:P:20:GLN:HE22	1.61	0.49
8:H:123:TYR:OH	13:a:223:LYS:HB3	2.13	0.48
13:M:35:ARG:HD3	13:M:36:PHE:CZ	2.48	0.48
13:a:220:ASP:C	13:a:222:ALA:H	2.21	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.48
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.95	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.48
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.96	0.48
7:U:68:ARG:HH12	14:b:36:ARG:HH22	1.62	0.48
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.96	0.48
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.95	0.48
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.49	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.95	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.47
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.44	0.47
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.44	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.97	0.46
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.97	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.81	0.46
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.97	0.46
13:a:35:ARG:NH1	14:b:114:PRO:HB3	2.30	0.46
13:M:219:TRP:CZ3	14:b:171:GLY:HA2	2.50	0.46
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.98	0.46
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.46	0.46
10:J:91:SER:HG	10:J:98:TYR:H	1.62	0.45
3:C:9:PHE:H	4:D:15:GLN:HE22	1.64	0.45
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.45
11:K:116:ASP:HB2	11:K:120:THR:HB	1.99	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
14:b:22:THR:HG22	15:d:2:PRO:HA	1.99	0.45
13:M:221:PHE:O	13:M:224:ASP:OD1	2.35	0.45
1:O:55:LEU:HB3	7:U:159:ALA:O	2.17	0.45
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.99	0.45
8:H:22:GLN:NE2	8:H:27:ALA:HB2	2.32	0.45
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.99	0.44
13:a:221:PHE:O	13:a:221:PHE:CD2	2.70	0.44
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.00	0.44
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.99	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.52	0.44
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:ARG:HA	10:J:23:ARG:HD3	1.76	0.44
13:M:224:ASP:CG	8:V:123:TYR:OH	2.61	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.47	0.44
13:a:221:PHE:O	13:a:221:PHE:HD2	2.01	0.44
13:a:223:LYS:HD3	13:a:223:LYS:HA	1.65	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.60	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.44
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.54	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.00	0.43
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.00	0.43
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.00	0.43
2:B:217:LYS:C	2:B:219:ALA:N	2.77	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.43
9:W:98:ARG:O	9:W:126:ILE:HD11	2.19	0.43
12:Z:137:ARG:HD3	12:Z:138:ALA:O	2.19	0.43
9:I:98:ARG:O	9:I:126:ILE:HD11	2.18	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.43
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.43
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.01	0.43
14:b:19:ARG:NH1	14:b:167:GLY:O	2.50	0.43
2:B:50:LYS:O	2:B:51:VAL:C	2.61	0.43
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.43
6:F:19:GLN:NE2	18:F:301:HOH:O	2.49	0.42
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.99	0.42
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.54	0.42
2:P:113:ARG:NE	18:P:301:HOH:O	2.45	0.42
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.01	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.42
15:c:4:GAU:HA	15:c:5:POL:H31	1.87	0.42
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.42
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.02	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.02	0.42
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.50	0.42
2:B:3:ARG:CB	5:E:122:TYR:OH	2.68	0.42
2:P:217:LYS:C	2:P:219:ALA:N	2.77	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.02	0.41
14:b:168:SER:HB3	15:d:5:POL:H33	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:29:THR:HG1	3:Q:61:LYS:HZ2	1.68	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
10:X:1:MET:CB	10:X:34:LYS:HE3	2.50	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.50	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
10:J:1:MET:HB3	10:J:34:LYS:HE3	2.02	0.41
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.61	0.41
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.51	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
10:J:25:ILE:O	10:X:139:TYR:OH	2.39	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.41
7:G:34:LEU:C	7:G:34:LEU:HD23	2.46	0.41
10:J:1:MET:CB	10:J:34:LYS:HE3	2.51	0.41
7:G:73:VAL:HG12	7:G:133:THR:HB	2.01	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.41
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.61	0.41
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.03	0.40
13:M:2:GLN:NE2	18:M:301:HOH:O	2.54	0.40
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.03	0.40
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.04	0.40
15:d:3:ALA:C	15:d:4:GAU:HG2	2.46	0.40
10:J:139:TYR:OH	10:X:25:ILE:O	2.40	0.40
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.04	0.40
10:J:168:LEU:O	10:J:172:MET:HB2	2.21	0.40
7:U:34:LEU:C	7:U:34:LEU:HD23	2.46	0.40
7:U:73:VAL:HG12	7:U:133:THR:HB	2.02	0.40
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.04	0.40
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	51
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	51
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	15
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	15
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	21
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	21
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	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%)	217 (97%)	7 (3%)	0	100	100
8	V	224/232 (97%)	217 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	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%)	189 (98%)	3 (2%)	1 (0%)	24	46
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	222/239 (93%)	212 (96%)	9 (4%)	1 (0%)	24	46
13	a	221/239 (92%)	211 (96%)	9 (4%)	1 (0%)	24	46
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
15	c	2/5 (40%)	2 (100%)	0	0	100	100
15	d	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6269/6610 (95%)	6116 (98%)	134 (2%)	19 (0%)	36	58

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
13	a	222	ALA
1	A	2	THR
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
13	M	221	PHE
2	P	220	ASN
3	Q	205	ALA
10	X	24	GLY
3	C	183	PRO
3	Q	183	PRO

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%)	203 (97%)	6 (3%)	37	65
1	O	209/209 (100%)	203 (97%)	6 (3%)	37	65
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	60
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	60
3	C	212/226 (94%)	199 (94%)	13 (6%)	17	37
3	Q	212/226 (94%)	199 (94%)	13 (6%)	17	37
4	D	194/215 (90%)	181 (93%)	13 (7%)	15	33
4	R	194/215 (90%)	180 (93%)	14 (7%)	13	30
5	E	190/193 (98%)	182 (96%)	8 (4%)	26	52
5	S	190/193 (98%)	182 (96%)	8 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	201/239 (84%)	194 (96%)	7 (4%)	32	59
6	T	201/239 (84%)	194 (96%)	7 (4%)	32	59
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	50
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	50
8	H	185/190 (97%)	180 (97%)	5 (3%)	39	67
8	V	185/190 (97%)	180 (97%)	5 (3%)	39	67
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	78
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	78
10	J	173/175 (99%)	169 (98%)	4 (2%)	44	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	65
11	K	169/169 (100%)	162 (96%)	7 (4%)	27	54
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	54
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	62
12	Z	185/185 (100%)	179 (97%)	6 (3%)	34	62
13	M	192/203 (95%)	186 (97%)	6 (3%)	35	63
13	a	191/203 (94%)	185 (97%)	6 (3%)	35	63
14	N	162/162 (100%)	154 (95%)	8 (5%)	22	47
14	b	162/162 (100%)	154 (95%)	8 (5%)	22	47
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	0	1 (100%)	0	0
All	All	5307/5532 (96%)	5100 (96%)	207 (4%)	28	55

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	59	GLU
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN

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Mol	Chain	Res	Type
2	B	113	ARG
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	51	LYS
3	C	52	LEU
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	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	99	ILE
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	207	ASP

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Mol	Chain	Res	Type
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	34	LEU
8	H	68	LEU
8	H	113	ILE
8	H	144	GLN
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	69	ARG
11	K	107	LYS
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	132	GLU
12	L	150	LEU
12	L	161	GLU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
13	M	220	ASP

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Mol	Chain	Res	Type
14	N	9	LYS
14	N	21	THR
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	59	GLU
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
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	51	LYS
3	Q	52	LEU
3	Q	60	SER
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	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	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU

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Mol	Chain	Res	Type
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	231	LYS
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	207	ASP
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	34	LEU
8	V	68	LEU
8	V	113	ILE
8	V	144	GLN
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS

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Mol	Chain	Res	Type
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	69	ARG
11	Y	107	LYS
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	132	GLU
12	Z	150	LEU
12	Z	161	GLU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
13	a	223	LYS
14	b	9	LYS
14	b	21	THR
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS
14	b	115	LEU
14	b	119	VAL
14	b	178	LEU
15	d	2	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	116	GLN

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Mol	Chain	Res	Type
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	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
7	G	175	ASN
8	H	22	GLN
8	H	35	HIS
8	H	66	HIS
8	H	194	ASN
9	I	37	ASN
9	I	203	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN
11	K	85	ASN

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Mol	Chain	Res	Type
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN
12	L	155	ASN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
2	P	20	GLN
2	P	93	HIS
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	115	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN

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Mol	Chain	Res	Type
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
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	175	ASN
8	V	35	HIS
8	V	66	HIS
8	V	86	HIS
8	V	194	ASN
9	W	37	ASN
9	W	88	GLN
9	W	203	GLN
10	X	10	GLN
10	X	55	GLN
10	X	63	ASN
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN

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Mol	Chain	Res	Type
13	a	149	HIS
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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	GAU	c	4	14,15	8,8,8	1.62	2 (25%)	8,9,9	1.30	0
15	GAU	d	4	14,15	8,8,8	1.50	2 (25%)	8,9,9	1.30	1 (12%)

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
15	GAU	c	4	14,15	-	1/7/7/7	-
15	GAU	d	4	14,15	-	0/7/7/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	GAU	C-CA	3.80	1.58	1.52
15	d	4	GAU	C-CA	2.85	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	d	4	GAU	OE2-CD	-2.39	1.22	1.30
15	c	4	GAU	OE2-CD	-2.09	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	4	GAU	CB-CA-N	-2.26	102.29	109.16

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	GAU	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c	4	GAU	2	0
15	d	4	GAU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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%)	-0.34	3 (1%) 76 73	41, 53, 85, 125	0
1	O	250/250 (100%)	-0.16	2 (0%) 82 80	46, 63, 105, 133	0
2	B	244/258 (94%)	-0.14	5 (2%) 65 60	42, 60, 101, 150	0
2	P	244/258 (94%)	-0.04	7 (2%) 53 48	47, 64, 110, 155	0
3	C	240/254 (94%)	-0.12	5 (2%) 63 58	42, 65, 125, 150	0
3	Q	240/254 (94%)	0.13	6 (2%) 58 52	47, 75, 151, 175	0
4	D	235/260 (90%)	-0.15	3 (1%) 75 71	47, 66, 99, 138	0
4	R	235/260 (90%)	-0.07	3 (1%) 75 71	48, 69, 109, 144	0
5	E	231/234 (98%)	-0.06	1 (0%) 88 86	50, 69, 106, 150	0
5	S	231/234 (98%)	0.13	4 (1%) 69 64	52, 75, 118, 164	0
6	F	243/288 (84%)	-0.20	2 (0%) 82 80	44, 61, 109, 139	0
6	T	243/288 (84%)	0.02	9 (3%) 45 39	46, 72, 126, 156	0
7	G	241/252 (95%)	-0.34	2 (0%) 82 80	37, 55, 89, 136	0
7	U	241/252 (95%)	-0.23	1 (0%) 88 86	45, 60, 91, 135	0
8	H	226/232 (97%)	-0.23	1 (0%) 88 86	38, 54, 87, 148	0
8	V	226/232 (97%)	-0.18	2 (0%) 81 78	45, 58, 90, 163	0
9	I	204/205 (99%)	-0.49	1 (0%) 87 85	39, 51, 78, 100	0
9	W	204/205 (99%)	-0.48	1 (0%) 87 85	42, 54, 84, 107	0
10	J	195/198 (98%)	-0.37	1 (0%) 87 85	40, 55, 81, 134	0
10	X	195/198 (98%)	-0.34	1 (0%) 87 85	41, 56, 80, 143	0
11	K	212/212 (100%)	-0.42	0 100 100	38, 56, 78, 99	0
11	Y	212/212 (100%)	-0.41	1 (0%) 87 85	42, 56, 79, 100	0
12	L	222/222 (100%)	-0.37	1 (0%) 87 85	40, 56, 87, 121	0
12	Z	222/222 (100%)	-0.38	1 (0%) 87 85	38, 55, 86, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	224/239 (93%)	-0.35	3 (1%) 75 71	25, 55, 79, 98	0
13	a	223/239 (93%)	-0.35	5 (2%) 62 57	24, 53, 75, 93	0
14	N	196/196 (100%)	-0.38	0 100 100	40, 51, 79, 107	0
14	b	196/196 (100%)	-0.34	1 (0%) 87 85	40, 53, 79, 113	0
15	c	2/5 (40%)	-0.38	0 100 100	66, 66, 66, 67	0
15	d	2/5 (40%)	-0.76	0 100 100	57, 57, 57, 63	0
All	All	6329/6610 (95%)	-0.23	72 (1%) 78 74	24, 59, 103, 175	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	224	ASP	8.0
10	J	1	MET	5.6
2	B	218	GLY	5.5
3	Q	50	LEU	5.5
10	X	1	MET	4.7
13	a	223	LYS	4.5
2	B	51	VAL	4.0
2	B	219	ALA	3.9
3	C	205	ALA	3.8
3	Q	205	ALA	3.8
8	H	223	ILE	3.7
8	V	223	ILE	3.5
2	P	219	ALA	3.4
14	b	103	ASP	3.4
3	Q	49	THR	3.4
6	T	215	CYS	3.3
4	D	167	GLY	3.2
6	T	243	ILE	3.2
13	M	1	THR	3.1
1	O	53	SER	3.0
6	F	215	CYS	2.8
5	E	122	TYR	2.8
3	C	50	LEU	2.8
4	D	241	ALA	2.7
13	M	223	LYS	2.7
5	S	55	LEU	2.7
7	G	68	ARG	2.7
4	D	240	ALA	2.7
13	a	1	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	P	218	GLY	2.6
2	P	53	SER	2.6
2	P	52	THR	2.6
6	F	202	ASP	2.6
1	A	1	MET	2.6
6	T	178	HIS	2.6
12	Z	174	TYR	2.5
3	Q	204	GLY	2.5
13	a	222	ALA	2.5
9	I	1	SER	2.5
3	C	204	GLY	2.5
12	L	174	TYR	2.5
13	a	220	ASP	2.4
2	P	1	GLY	2.4
2	B	93	HIS	2.4
3	Q	240	GLU	2.4
2	B	222	GLY	2.4
5	S	122	TYR	2.4
3	C	51	LYS	2.4
7	U	242	GLN	2.4
4	R	113	LEU	2.3
8	V	224	GLN	2.3
1	O	2	THR	2.3
6	T	201	GLU	2.3
13	a	69	ASP	2.3
3	Q	52	LEU	2.3
5	S	52	ALA	2.3
6	T	203	ASN	2.3
7	G	242	GLN	2.3
6	T	202	ASP	2.2
2	P	220	ASN	2.2
1	A	231	LYS	2.2
6	T	53	LYS	2.2
4	R	112	ALA	2.1
4	R	241	ALA	2.1
1	A	2	THR	2.1
11	Y	18	SER	2.1
6	T	244	ASN	2.1
6	T	14	ASP	2.1
2	P	222	GLY	2.1
3	C	203	THR	2.0
9	W	133	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
5	S	173	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	GAU	c	4	9/9	0.91	0.12	68,72,75,76	0
15	GAU	d	4	9/9	0.92	0.10	61,66,66,72	0

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
16	MG	N	201	1/1	0.92	0.07	52,52,52,52	0
16	MG	Z	301	1/1	0.92	0.08	62,62,62,62	0
16	MG	I	301	1/1	0.93	0.19	64,64,64,64	0
17	CL	G	302	1/1	0.95	0.19	30,30,30,30	0
16	MG	G	301	1/1	0.97	0.08	48,48,48,48	0
16	MG	L	301	1/1	0.98	0.06	56,56,56,56	0
16	MG	K	301	1/1	0.98	0.06	54,54,54,54	0
16	MG	I	302	1/1	0.99	0.12	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.