



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:14 PM UTC

PDB ID : 4Y8U / pdb_00004y8u
Title : Yeast 20S proteasome beta2-H116D mutant in complex with Ac-PAD-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
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
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

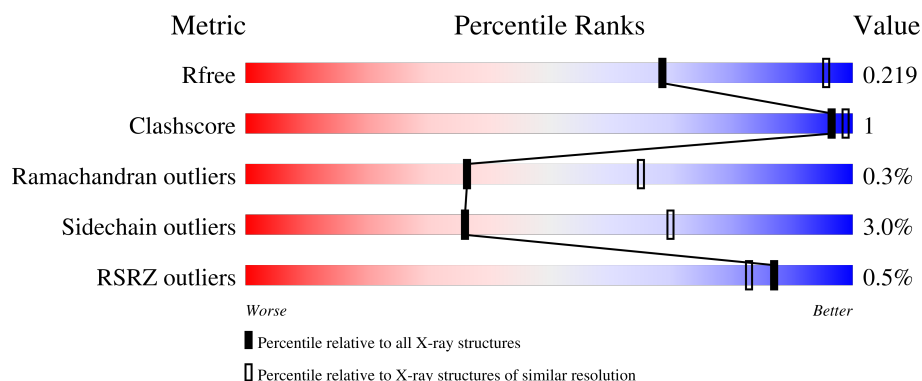
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



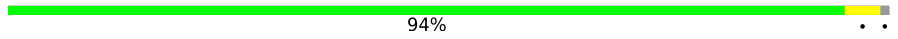
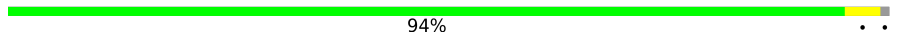
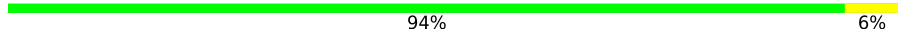
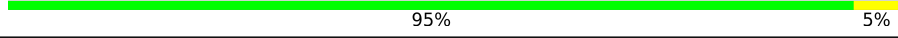
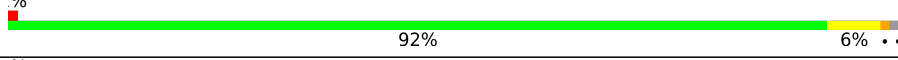
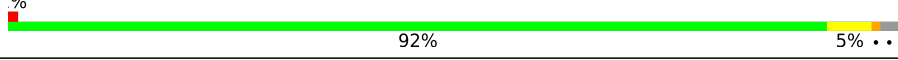
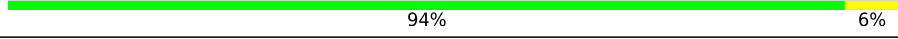
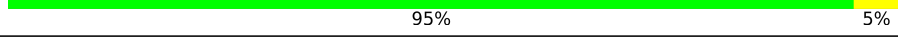
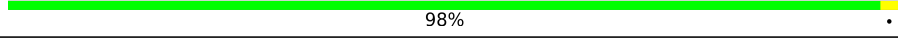
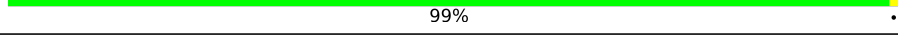
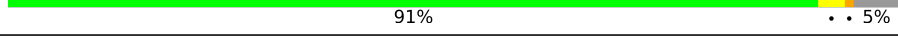
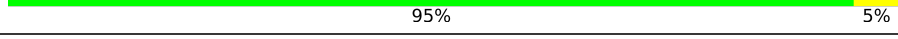
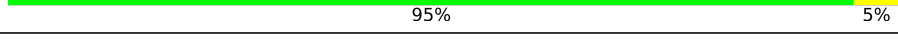
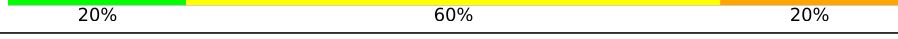
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	98%
1	O	250	98%
2	B	258	88% 6% • 5%
2	P	258	87% 7% • 5%
3	C	254	88% 5% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	1	5	
15	2	5	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49607 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
			1717	1080	296	334	7			
8	V	226	Total	C	N	O	S	0	0	0
			1717	1080	296	334	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	116	ASP	HIS	engineered mutation	UNP P25043
V	116	ASP	HIS	engineered mutation	UNP P25043

- 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			
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	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 a protein called Ac-PAD-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	1	5	Total	C	N	O	0	0	0
			27	17	3	7			
15	2	5	Total	C	N	O	0	0	0
			27	17	3	7			

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

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

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

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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	5	Total	O	0	0
			5	5		
18	B	6	Total	O	0	0
			6	6		
18	C	5	Total	O	0	0
			5	5		
18	D	3	Total	O	0	0
			3	3		
18	E	3	Total	O	0	0
			3	3		
18	F	3	Total	O	0	0
			3	3		

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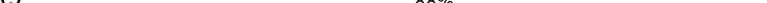
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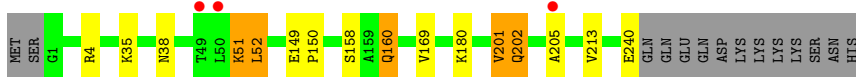
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	5	Total O 5 5	0	0
18	H	11	Total O 11 11	0	0
18	I	2	Total O 2 2	0	0
18	J	9	Total O 9 9	0	0
18	K	8	Total O 8 8	0	0
18	L	8	Total O 8 8	0	0
18	M	9	Total O 9 9	0	0
18	N	8	Total O 8 8	0	0
18	O	1	Total O 1 1	0	0
18	P	5	Total O 5 5	0	0
18	Q	10	Total O 10 10	0	0
18	R	2	Total O 2 2	0	0
18	S	2	Total O 2 2	0	0
18	T	5	Total O 5 5	0	0
18	U	10	Total O 10 10	0	0
18	V	10	Total O 10 10	0	0
18	W	2	Total O 2 2	0	0
18	X	10	Total O 10 10	0	0
18	Y	13	Total O 13 13	0	0
18	Z	11	Total O 11 11	0	0
18	a	10	Total O 10 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	6	Total 6	O 6	0	0
18	1	1	Total 1	O 1	0	0
18	2	1	Total 1	O 1	0	0

Chain Q:  88% 6% 6%

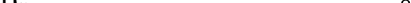


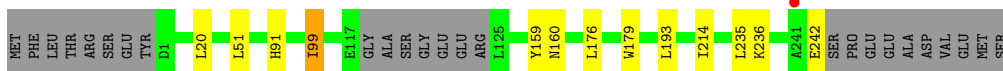
- Molecule 4: Proteasome subunit alpha type-5

Chain D:  86% 10%

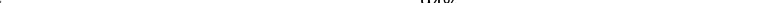


- Molecule 4: Proteasome subunit alpha type-5

Chain R:  85% 5% 10%



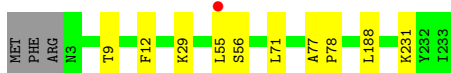
- Molecule 5: Proteasome subunit alpha type-6

Chain E:  94% . .



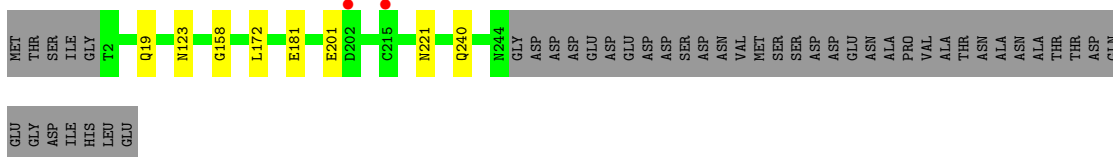
- Molecule 5: Proteasome subunit alpha type-6

Chain S: 94%



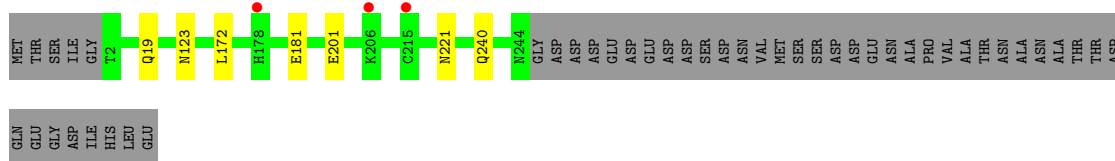
- Molecule 6: Probable proteasome subunit alpha type-7

Chain F:  82% 16% 2%



- Molecule 6: Probable proteasome subunit alpha type-7

Chain T:  82% 16% 2%



- Molecule 7: Proteasome subunit alpha type-1

Chain G: 90% 6% .



- Molecule 7: Proteasome subunit alpha type-1

Chain U: 90% 5% .



- Molecule 8: Proteasome subunit beta type-2

Chain H: 91% 6% . .



- Molecule 8: Proteasome subunit beta type-2

Chain V: 91% 6% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I: 94% 6%

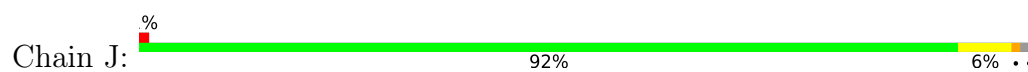


- Molecule 9: Proteasome subunit beta type-3

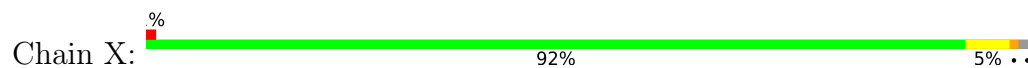
Chain W: 95% 5%



- 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



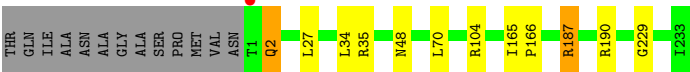
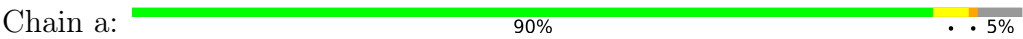
- Molecule 12: Proteasome subunit beta type-6



- 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



• Molecule 15: Ac-PAD-ep



• Molecule 15: Ac-PAD-ep



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.12Å 302.00Å 145.44Å 90.00° 113.16° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (15.00-2.90) 95.2 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.214 0.192 , 0.219	Depositor DCC
R_{free} test set	11407 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.0	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	49607	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, MG, CL, ASJ, POL

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	0.41	0/1952	0.68	0/2642
1	O	0.40	0/1952	0.68	0/2642
2	B	0.42	0/1934	0.66	0/2618
2	P	0.41	0/1934	0.67	0/2618
3	C	0.40	0/1910	0.69	1/2586 (0.0%)
3	Q	0.40	0/1910	0.69	1/2586 (0.0%)
4	D	0.40	0/1837	0.66	0/2475
4	R	0.40	0/1837	0.66	0/2475
5	E	0.39	0/1800	0.64	0/2433
5	S	0.39	0/1800	0.64	0/2433
6	F	0.41	0/1932	0.69	0/2609
6	T	0.41	0/1932	0.69	0/2609
7	G	0.40	0/1945	0.67	0/2634
7	U	0.40	0/1945	0.68	0/2634
8	H	0.93	2/1747 (0.1%)	0.82	4/2369 (0.2%)
8	V	0.41	0/1747	0.65	0/2369
9	I	0.39	0/1611	0.68	0/2174
9	W	0.40	0/1611	0.70	0/2174
10	J	0.41	0/1589	0.66	0/2142
10	X	0.41	0/1589	0.66	0/2142
11	K	0.40	0/1681	0.66	0/2274
11	Y	0.39	0/1681	0.66	0/2274
12	L	0.39	0/1795	0.67	0/2420
12	Z	0.39	0/1795	0.67	0/2420
13	M	0.41	0/1855	0.68	0/2514
13	a	0.40	0/1855	0.68	0/2514
14	N	0.45	0/1541	0.70	0/2087
14	b	0.46	0/1541	0.69	0/2087
15	1	2.79	2/13 (15.4%)	1.54	0/18
15	2	2.83	2/13 (15.4%)	1.56	0/18
All	All	0.44	6/50284 (0.0%)	0.68	6/67990 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	113	ILE	C-N	-32.06	0.87	1.33
8	H	112	SER	C-N	13.63	1.51	1.33
15	2	1	ACE	C-N	-8.00	1.35	1.43
15	1	1	ACE	C-N	-7.72	1.35	1.43
15	1	2	PRO	CA-C	-6.12	1.40	1.52
15	2	2	PRO	CA-C	-5.96	1.40	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	113	ILE	O-C-N	-20.46	101.10	123.20
8	H	113	ILE	CA-C-N	7.58	136.54	122.74
8	H	113	ILE	C-N-CA	7.58	136.54	122.74
8	H	112	SER	O-C-N	-6.74	114.08	123.11
3	C	201	VAL	N-CA-C	6.57	116.70	110.53
3	Q	201	VAL	N-CA-C	6.55	116.69	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1907	0	1901	5	0
7	U	1907	0	1901	4	0
8	H	1717	0	1715	9	0
8	V	1717	0	1716	9	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	4	0
11	K	1644	0	1595	5	0
11	Y	1644	0	1595	3	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	0	0
13	M	1824	0	1832	4	0
13	a	1824	0	1832	6	0
14	N	1512	0	1478	4	0
14	b	1512	0	1478	3	0
15	1	27	0	25	1	0
15	2	27	0	25	0	0
16	G	1	0	0	0	0
16	I	1	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	1	0
18	1	1	0	0	0	0
18	2	1	0	0	0	0
18	A	5	0	0	0	0
18	B	6	0	0	0	0
18	C	5	0	0	0	0
18	D	3	0	0	0	0
18	E	3	0	0	0	0
18	F	3	0	0	0	0
18	G	5	0	0	0	0
18	H	11	0	0	1	0
18	I	2	0	0	0	0
18	J	9	0	0	0	0
18	K	8	0	0	0	0
18	L	8	0	0	0	0
18	M	9	0	0	1	0
18	N	8	0	0	0	0
18	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	5	0	0	1	0
18	Q	10	0	0	0	0
18	R	2	0	0	0	0
18	S	2	0	0	0	0
18	T	5	0	0	0	0
18	U	10	0	0	0	0
18	V	10	0	0	0	0
18	W	2	0	0	0	0
18	X	10	0	0	0	0
18	Y	13	0	0	0	0
18	Z	11	0	0	0	0
18	a	10	0	0	2	0
18	b	6	0	0	0	0
All	All	49607	0	49167	101	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 (101) 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)
8:H:91:GLN:NE2	18:H:301:HOH:O	2.11	0.79
8:V:53:GLU:OE2	8:V:57:GLN:NE2	2.26	0.68
2:P:93:HIS:HB3	18:P:301:HOH:O	1.97	0.64
8:V:114:HIS:ND1	8:V:116:ASP:OD2	2.30	0.64
8:H:91:GLN:HA	8:H:91:GLN:OE1	2.04	0.57
8:V:35:HIS:CE1	8:V:53:GLU:HG2	2.39	0.57
15:1:4:ASJ:O	15:1:5:POL:O	2.08	0.56
14:b:152:VAL:HA	14:b:175:MET:HE1	1.88	0.55
7:G:23:PHE:O	7:G:26:THR:HB	2.07	0.54
7:U:23:PHE:O	7:U:26:THR:HB	2.07	0.54
14:N:152:VAL:HA	14:N:175:MET:HE1	1.90	0.54
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.92	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.48
11:K:25:TRP:CZ3	12:L:144:SER:HA	2.47	0.48
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.42	0.47
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:53:GLU:O	8:H:57:GLN:HG3	2.15	0.47
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.47
8:V:116:ASP:OD2	8:V:116:ASP:N	2.42	0.47
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.47
2:B:50:LYS:O	2:B:51:VAL:C	2.57	0.47
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.97	0.47
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.50	0.46
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.50	0.46
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.79	0.46
8:V:53:GLU:O	8:V:57:GLN:HG3	2.16	0.46
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.46
13:M:2:GLN:NE2	18:M:301:HOH:O	2.48	0.46
2:B:217:LYS:C	2:B:219:ALA:H	2.25	0.45
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.98	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.45
17:G:302:CL:CL	8:H:69:TYR:OH	2.71	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.47	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.98	0.44
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.44
2:P:217:LYS:C	2:P:219:ALA:H	2.25	0.44
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.48	0.44
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.44
2:P:221:ASP:O	2:P:223:GLU:N	2.51	0.44
2:B:221:ASP:O	2:B:223:GLU:N	2.51	0.43
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.43
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.43
5:E:12:PHE:H	6:F:19:GLN:HE22	1.67	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.48	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.01	0.43
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.01	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.43
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.43
3:C:51:LYS:O	3:C:52:LEU:HB2	2.19	0.42
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.42
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.01	0.42
11:K:25:TRP:CH2	12:L:144:SER:HA	2.54	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.42
9:I:98:ARG:O	9:I:126:ILE:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
9:I:131:GLU:O	9:I:131:GLU:CG	2.68	0.42
14:N:13:ILE:HG21	14:N:175:MET:HE2	2.02	0.42
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.19	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.02	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.42
13:a:2:GLN:NE2	18:a:302:HOH:O	2.52	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.67	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.41
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.50	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
9:W:131:GLU:O	9:W:131:GLU:CG	2.68	0.41
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.03	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.41
6:F:158:GLY:O	7:G:54:LEU:HB3	2.21	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.50	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.56	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.02	0.41
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.51	0.41
3:C:201:VAL:O	3:C:202:GLN:HB3	2.20	0.40
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.40
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.02	0.40
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.20	0.40
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.56	0.40
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.40
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.03	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.03	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.40
13:a:35:ARG:NH1	14:b:114:PRO:HB3	2.36	0.40
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.03	0.40
13:a:190:ARG:NH2	18:a:303:HOH:O	2.54	0.40
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.03	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.52	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%)	7 (3%)	1 (0%)	30	59
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	59
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	26
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	26
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
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%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (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%)	218 (97%)	6 (3%)	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	54
10	X	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	24	54
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	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	30	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	224 (97%)	6 (3%)	1 (0%)	30	59
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	1	2/5 (40%)	2 (100%)	0	0	100	100
15	2	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6288/6624 (95%)	6132 (98%)	138 (2%)	18 (0%)	36	65

All (18) 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
1	A	2	THR
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA
13	M	229	GLY
13	a	229	GLY
10	X	24	GLY
10	J	24	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%)	205 (98%)	4 (2%)	50	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	79
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	70
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	70
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	56
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	60
4	D	194/215 (90%)	185 (95%)	9 (5%)	24	57
4	R	194/215 (90%)	185 (95%)	9 (5%)	24	57
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	68
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	68
6	F	201/239 (84%)	195 (97%)	6 (3%)	36	70
6	T	201/239 (84%)	195 (97%)	6 (3%)	36	70
7	G	206/210 (98%)	198 (96%)	8 (4%)	28	63
7	U	206/210 (98%)	198 (96%)	8 (4%)	28	63
8	H	185/190 (97%)	182 (98%)	3 (2%)	55	83
8	V	185/190 (97%)	179 (97%)	6 (3%)	34	68
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	86
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	86
10	J	173/175 (99%)	167 (96%)	6 (4%)	32	66
10	X	173/175 (99%)	167 (96%)	6 (4%)	32	66
11	K	169/169 (100%)	163 (96%)	6 (4%)	31	65
11	Y	169/169 (100%)	163 (96%)	6 (4%)	31	65
12	L	185/185 (100%)	183 (99%)	2 (1%)	65	88
12	Z	185/185 (100%)	183 (99%)	2 (1%)	65	88
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	74
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	74
14	N	162/162 (100%)	157 (97%)	5 (3%)	35	69
14	b	162/162 (100%)	157 (97%)	5 (3%)	35	69
15	1	1/1 (100%)	1 (100%)	0	100	100
15	2	1/1 (100%)	1 (100%)	0	100	100
All	All	5322/5542 (96%)	5164 (97%)	158 (3%)	36	70

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
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	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	52	LEU
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	51	LEU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
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	231	LYS
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR

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Mol	Chain	Res	Type
7	G	75	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	55	VAL
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	35	ILE
11	K	107	LYS
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	9	LYS
14	N	21	THR
14	N	104	ASP
14	N	107	LYS
14	N	119	VAL
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU

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Mol	Chain	Res	Type
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
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	51	LEU
4	R	99	ILE
4	R	176	LEU
4	R	193	LEU
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	231	LYS
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	75	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	53	GLU

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Mol	Chain	Res	Type
8	V	55	VAL
8	V	68	LEU
8	V	113	ILE
8	V	116	ASP
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	35	ILE
11	Y	107	LYS
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	9	LYS
14	b	21	THR
14	b	104	ASP
14	b	107	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	176	GLN
3	C	17	GLN

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Mol	Chain	Res	Type
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	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	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	35	HIS
8	H	66	HIS
8	H	194	ASN
9	I	37	ASN
9	I	44	HIS
9	I	63	ASN
9	I	88	GLN
9	I	168	GLN
9	I	203	GLN
10	J	55	GLN
10	J	61	GLN
10	J	63	ASN
10	J	146	HIS
10	J	147	HIS
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	85	ASN
11	K	143	ASN
11	K	208	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	153	GLN
12	L	155	ASN
12	L	158	ASN
12	L	197	GLN
13	M	102	GLN
13	M	149	HIS
14	N	141	ASN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	106	GLN
4	R	146	GLN
4	R	160	ASN
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	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN

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Mol	Chain	Res	Type
8	V	35	HIS
8	V	66	HIS
8	V	194	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
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	102	GLN
13	a	149	HIS
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	ASJ	2	4	15,14	7,7,7	1.28	1 (14%)	5,8,8	1.57	1 (20%)
15	ASJ	1	4	15,14	7,7,7	1.29	1 (14%)	5,8,8	1.55	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ASJ	2	4	15,14	-	1/6/6/6	-
15	ASJ	1	4	15,14	-	1/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	4	ASJ	C-CA	2.36	1.56	1.52
15	2	4	ASJ	C-CA	2.27	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	4	ASJ	CB-CA-C	-2.51	107.67	112.21
15	1	4	ASJ	CB-CA-C	-2.46	107.76	112.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	1	4	ASJ	O-C-CA-CB
15	2	4	ASJ	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	1	4	ASJ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	113:ILE	C	114:HIS	N	0.87

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%)	-0.39	2 (0%) 82 77	46, 64, 103, 140	0
1	O	250/250 (100%)	-0.34	2 (0%) 82 77	49, 71, 118, 147	0
2	B	244/258 (94%)	-0.30	2 (0%) 82 77	47, 68, 117, 168	0
2	P	244/258 (94%)	-0.25	5 (2%) 65 56	56, 74, 120, 169	0
3	C	240/254 (94%)	-0.27	3 (1%) 75 67	48, 73, 140, 165	0
3	Q	240/254 (94%)	-0.13	3 (1%) 75 67	58, 84, 160, 185	0
4	D	235/260 (90%)	-0.30	3 (1%) 75 67	56, 78, 113, 152	0
4	R	235/260 (90%)	-0.17	1 (0%) 88 85	63, 83, 121, 148	0
5	E	231/234 (98%)	-0.16	0 100 100	60, 83, 122, 164	0
5	S	231/234 (98%)	-0.08	1 (0%) 88 85	60, 86, 135, 172	0
6	F	243/288 (84%)	-0.31	2 (0%) 82 77	47, 72, 124, 154	0
6	T	243/288 (84%)	-0.25	3 (1%) 76 69	52, 78, 134, 165	0
7	G	241/252 (95%)	-0.42	1 (0%) 88 85	46, 66, 103, 149	0
7	U	241/252 (95%)	-0.33	0 100 100	52, 70, 106, 152	0
8	H	226/232 (97%)	-0.34	0 100 100	46, 62, 98, 158	0
8	V	226/232 (97%)	-0.33	1 (0%) 88 85	52, 67, 102, 184	0
9	I	204/205 (99%)	-0.53	0 100 100	45, 59, 89, 118	0
9	W	204/205 (99%)	-0.51	0 100 100	48, 63, 97, 124	0
10	J	195/198 (98%)	-0.49	1 (0%) 87 83	44, 63, 88, 141	0
10	X	195/198 (98%)	-0.43	1 (0%) 87 83	46, 64, 91, 151	0
11	K	212/212 (100%)	-0.46	0 100 100	42, 64, 89, 112	0
11	Y	212/212 (100%)	-0.50	0 100 100	46, 64, 90, 113	0
12	L	222/222 (100%)	-0.39	1 (0%) 87 83	46, 66, 104, 139	0
12	Z	222/222 (100%)	-0.43	0 100 100	47, 65, 98, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.44	1 (0%) 88 85	44, 64, 89, 109	0
13	a	233/246 (94%)	-0.47	1 (0%) 88 85	44, 63, 87, 104	0
14	N	196/196 (100%)	-0.54	0 100 100	42, 58, 88, 122	0
14	b	196/196 (100%)	-0.52	0 100 100	43, 58, 90, 127	0
15	1	2/5 (40%)	-0.63	0 100 100	64, 64, 64, 65	0
15	2	2/5 (40%)	-0.65	0 100 100	59, 59, 59, 61	0
All	All	6348/6624 (95%)	-0.36	34 (0%) 87 83	42, 69, 116, 185	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	4.8
8	V	223	ILE	4.0
10	J	1	MET	3.7
2	P	218	GLY	3.4
4	D	241	ALA	3.4
3	Q	50	LEU	3.3
2	B	218	GLY	3.2
3	Q	49	THR	3.0
2	P	219	ALA	3.0
13	a	1	THR	2.9
6	T	178	HIS	2.9
4	R	241	ALA	2.8
6	F	215	CYS	2.8
2	P	1	GLY	2.8
4	D	240	ALA	2.7
5	S	55	LEU	2.7
3	C	205	ALA	2.7
3	Q	205	ALA	2.6
1	O	2	THR	2.5
6	T	206	LYS	2.5
7	G	176	HIS	2.4
3	C	3	ASP	2.4
2	P	52	THR	2.4
12	L	166	GLY	2.3
1	O	1	MET	2.3
1	A	2	THR	2.3
3	C	50	LEU	2.2
2	B	51	VAL	2.2
4	D	167	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	ALA	2.2
6	T	215	CYS	2.2
2	P	60	THR	2.0
13	M	233	ILE	2.0
6	F	202	ASP	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	ASJ	2	4	8/8	0.95	0.08	62,66,67,67	0
15	ASJ	1	4	8/8	0.97	0.08	66,70,73,74	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
17	CL	G	302	1/1	0.87	0.24	30,30,30,30	0
16	MG	Z	301	1/1	0.95	0.04	70,70,70,70	0
16	MG	N	201	1/1	0.97	0.04	47,47,47,47	0
16	MG	L	301	1/1	0.98	0.07	69,69,69,69	0
16	MG	G	301	1/1	0.98	0.07	61,61,61,61	0
16	MG	I	301	1/1	0.98	0.13	56,56,56,56	0
16	MG	K	301	1/1	0.98	0.11	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.