



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:13 am BST

PDB ID : 5FGA
Title : Yeast 20S proteasome beta5-K33A mutant (propeptide expressed in trans)
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-12-20
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

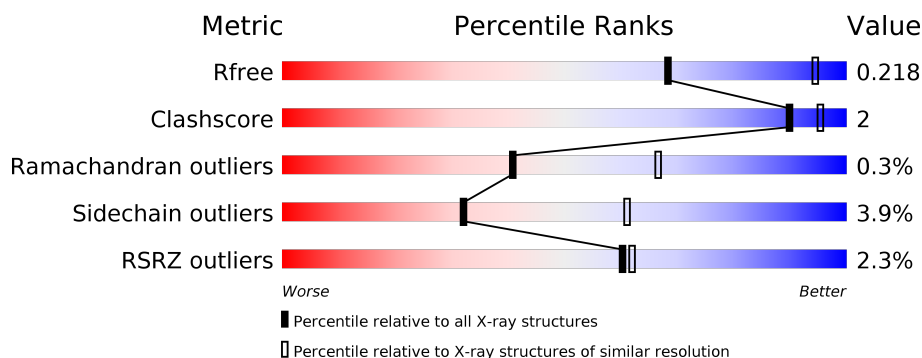
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	<div> <div>2%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>3%</div> <div>97%</div> <div>•</div> </div>
2	B	258	<div> <div>3%</div> <div>86%</div> <div>7% • 5%</div> </div>
2	P	258	<div> <div>3%</div> <div>86%</div> <div>8% • 5%</div> </div>
3	C	254	<div> <div>6%</div> <div>86%</div> <div>7% • 6%</div> </div>
3	Q	254	<div> <div>7%</div> <div>87%</div> <div>7% • 6%</div> </div>

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

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49871 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
			1640	1042	279	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1640	1042	279	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	ALA	LYS	engineered mutation	UNP P30656
Y	33	ALA	LYS	engineered mutation	UNP P30656

- 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	232	Total	C	N	O	S	0	0	0
			1815	1148	311	349	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 (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	20	Total O 20 20	0	0
17	B	14	Total O 14 14	0	0
17	C	20	Total O 20 20	0	0
17	D	16	Total O 16 16	0	0
17	E	10	Total O 10 10	0	0
17	F	18	Total O 18 18	0	0
17	G	23	Total O 23 23	0	0
17	H	25	Total O 25 25	0	0
17	I	16	Total O 16 16	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	16	Total 16	O 16	0	0
17	K	17	Total 17	O 17	0	0
17	L	31	Total 31	O 31	0	0
17	M	24	Total 24	O 24	0	0
17	N	22	Total 22	O 22	0	0
17	O	7	Total 7	O 7	0	0
17	P	13	Total 13	O 13	0	0
17	Q	13	Total 13	O 13	0	0
17	R	17	Total 17	O 17	0	0
17	S	5	Total 5	O 5	0	0
17	T	19	Total 19	O 19	0	0
17	U	23	Total 23	O 23	0	0
17	V	18	Total 18	O 18	0	0
17	W	16	Total 16	O 16	0	0
17	X	15	Total 15	O 15	0	0
17	Y	25	Total 25	O 25	0	0
17	Z	19	Total 19	O 19	0	0
17	a	30	Total 30	O 30	0	0
17	b	20	Total 20	O 20	0	0

3 Residue-property plots [i](#)

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

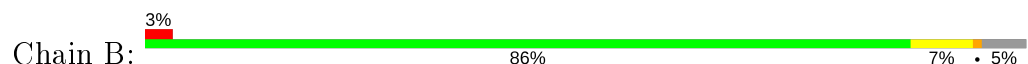
- Molecule 1: Proteasome subunit alpha type-2



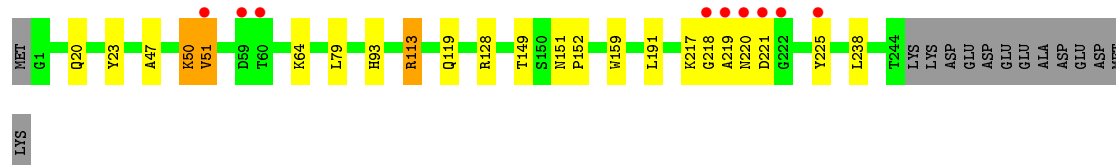
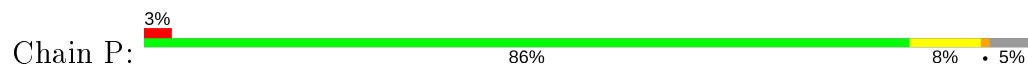
- Molecule 1: Proteasome subunit alpha type-2



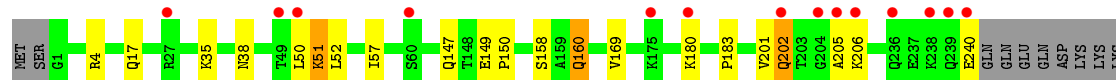
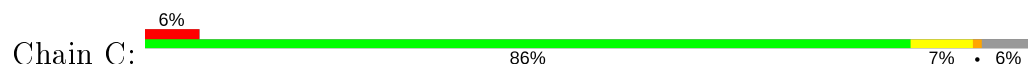
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3




- Molecule 3: Proteasome subunit alpha type-4



LYS
SER
ASN
HIS


• Molecule 3: Proteasome subunit alpha type-4

Chain Q: 

MET SER G1 R4 K35 N38 R46 R47 S48 T49 L50 K51 L52 L55 T55 N77 Q147 T148 E149 P150 S158 A159 Q160 V169 K180 P183 V201 Q202 T203 G204 A205 K206 S223 Q233 Q236 E237 K238 Q239 E240 GLN GLN GLU GLN ASP LYS


LYS
LYS
SER
ASN
HIS

• Molecule 4: Proteasome subunit alpha type-5

Chain D: 

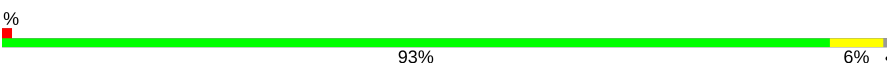
MET PHE LEU ARG THR ARG SER GLU TYR D1 L51 A88 H91 I99 E117 GLY ALA SER GLY GLU GLU ARG L125 D143 N160 L176 N177 E178 W179 L193 I214 Q217 L235 K236 E242 SER PRO GLU GLU ALA ASP VAL GLU MET SER

• Molecule 4: Proteasome subunit alpha type-5

Chain R: 

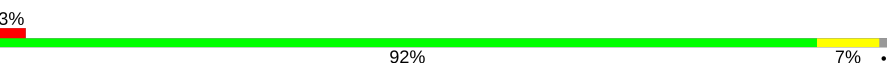
MET PHE LEU ARG THR ARG SER GLU TYR D1 L51 A88 H91 I99 E116 E117 GLY ALA SER GLY GLU GLU ARG L125 D143 N160 L176 W179 L193 E201 I214 Q217 L235 K236 A241 E242 SER PRO GLU GLU ALA ASP VAL GLU MET SER

• Molecule 5: Proteasome subunit alpha type-6

Chain E: 


MET PHE ARG N3 T9 F12 K29 L55 L71 L87 A107 R173 T174 L175 F178 N184 L188 D202 D208 K231 Y232 I233

• Molecule 5: Proteasome subunit alpha type-6

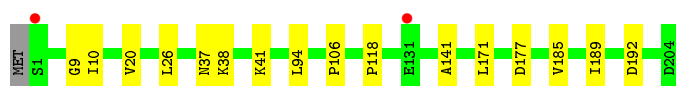
Chain S: 

MET PHE ARG N3 T9 F12 K29 E54 L55 H68 I71 L87 L102 A107 R173 T174 L175 F178 I179 K180 N184 L188 D202 D208 E227 K231 Y232 I233

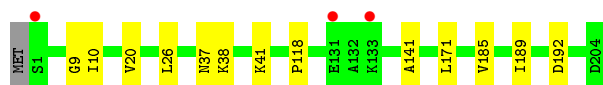
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F: 

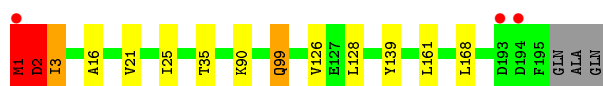
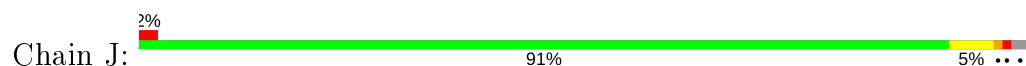
MET THR SER ILE GLY T2 Q19 Q117 Y122 N123 K139 L172 E181 L198 E201 D202 N203 K204 E205 K206 D207 K214 Q240 I243 N244 GLY ASP ASP ASP GLU ASP GLU ASP ASP SER ASP ASN VAL MET SER SER ASP ASP GLU ASN ALA PRO VAL ALA



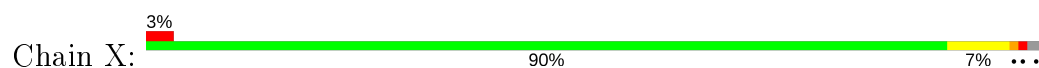
- Molecule 9: Proteasome subunit beta type-3



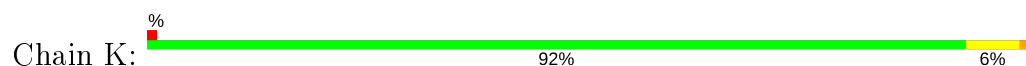
- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



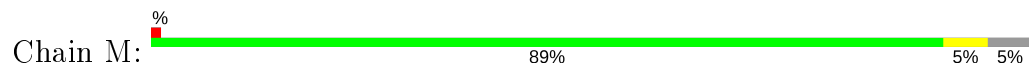
- Molecule 12: Proteasome subunit beta type-6



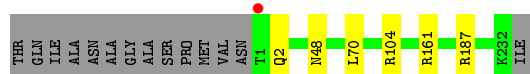
- Molecule 12: Proteasome subunit beta type-6



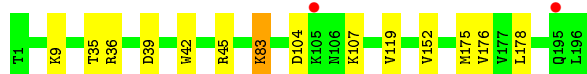
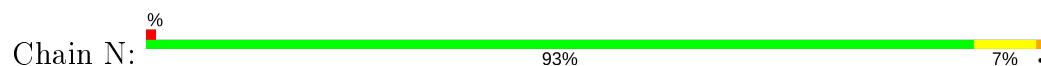
- Molecule 13: Proteasome subunit beta type-7



- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.35Å 300.50Å 144.44Å 90.00° 113.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.70) 98.6 (15.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.188 , 0.214 0.193 , 0.218	Depositor DCC
R_{free} test set	14192 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.2	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	49871	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, CL

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	0.26	0/1952	0.46	0/2642
1	O	0.26	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.50	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.47	0/2475
4	R	0.26	0/1837	0.47	0/2475
5	E	0.26	0/1800	0.47	0/2433
5	S	0.26	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.26	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.26	0/1945	0.47	0/2634
8	H	0.25	0/1750	0.48	0/2373
8	V	0.25	0/1750	0.48	0/2373
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.50	0/2174
10	J	0.39	1/1589 (0.1%)	0.76	5/2142 (0.2%)
10	X	0.36	0/1589	0.73	3/2142 (0.1%)
11	K	0.26	0/1677	0.50	0/2270
11	Y	0.26	0/1677	0.50	0/2270
12	L	0.26	0/1795	0.49	0/2420
12	Z	0.26	0/1795	0.49	0/2420
13	M	0.27	0/1855	0.52	0/2514
13	a	0.27	0/1846	0.51	0/2503
14	N	0.25	0/1541	0.49	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.27	1/50247 (0.0%)	0.51	8/67943 (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
10	J	0	2
10	X	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1	MET	SD-CE	8.51	2.25	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	1	MET	CG-SD-CE	15.16	124.46	100.20
10	X	1	MET	CB-CA-C	-15.09	80.22	110.40
10	X	1	MET	CG-SD-CE	13.91	122.46	100.20
10	J	1	MET	CB-CA-C	-12.72	84.96	110.40
10	J	1	MET	CA-CB-CG	-9.42	97.29	113.30
10	J	1	MET	N-CA-C	8.69	134.47	111.00
10	X	1	MET	CA-CB-CG	-8.21	99.35	113.30
10	J	2	ASP	CB-CG-OD2	5.97	123.67	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	1	MET	Mainchain
10	J	2	ASP	Peptide
10	X	1	MET	Mainchain

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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1915	0	1929	4	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	12	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	6	0
8	H	1719	0	1719	8	0
8	V	1719	0	1719	14	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	6	0
10	J	1561	0	1568	13	0
10	X	1561	0	1569	21	0
11	K	1640	0	1587	8	0
11	Y	1640	0	1587	8	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	3	0
13	M	1824	0	1832	5	0
13	a	1815	0	1821	0	0
14	N	1512	0	1481	7	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	A	20	0	0	0	0
17	B	14	0	0	1	0
17	C	20	0	0	0	0
17	D	16	0	0	0	0
17	E	10	0	0	0	0
17	F	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	23	0	0	0	0
17	H	25	0	0	0	0
17	I	16	0	0	0	0
17	J	16	0	0	1	0
17	K	17	0	0	1	0
17	L	31	0	0	0	0
17	M	24	0	0	1	0
17	N	22	0	0	0	0
17	O	7	0	0	0	0
17	P	13	0	0	2	0
17	Q	13	0	0	0	0
17	R	17	0	0	0	0
17	S	5	0	0	0	0
17	T	19	0	0	0	0
17	U	23	0	0	0	0
17	V	18	0	0	0	0
17	W	16	0	0	0	0
17	X	15	0	0	1	0
17	Y	25	0	0	1	0
17	Z	19	0	0	0	0
17	a	30	0	0	0	0
17	b	20	0	0	0	0
All	All	49871	0	49102	162	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 (162) 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:J:1:MET:CE	10:J:1:MET:SD	2.25	1.25
10:X:1:MET:O	10:X:1:MET:CE	1.68	1.15
10:X:3:ILE:HD11	10:X:168:LEU:HD13	1.15	1.11
8:V:80:LEU:HG	8:V:113:ILE:HD11	1.33	1.11
13:M:2:GLN:NE2	17:M:301:HOH:O	1.88	1.06
10:J:3:ILE:HD11	10:J:168:LEU:HD13	1.14	1.05
10:X:1:MET:SD	10:X:2:ASP:OD1	2.16	1.03
8:V:113:ILE:HG12	8:V:119:THR:CG2	1.92	0.99
8:V:113:ILE:HG12	8:V:119:THR:HG22	0.99	0.97
8:V:113:ILE:CG1	8:V:119:THR:HG22	1.96	0.94
10:X:1:MET:CE	10:X:2:ASP:OD1	2.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:CE	10:X:2:ASP:CG	2.36	0.93
8:V:80:LEU:CG	8:V:113:ILE:HD11	2.02	0.89
11:K:1:THR:OG1	17:K:401:HOH:O	1.91	0.88
10:J:1:MET:SD	10:J:2:ASP:HB2	2.12	0.88
10:J:1:MET:HG2	10:J:2:ASP:O	1.76	0.82
10:X:1:MET:HE3	10:X:2:ASP:OD2	1.80	0.81
10:X:1:MET:HE1	10:X:2:ASP:OD1	1.83	0.77
10:X:1:MET:HE3	10:X:2:ASP:CG	2.06	0.76
10:X:1:MET:HE3	10:X:1:MET:O	1.83	0.75
11:Y:1:THR:OG1	17:Y:401:HOH:O	2.06	0.73
10:J:1:MET:SD	10:J:2:ASP:CB	2.79	0.71
8:V:80:LEU:CD1	8:V:113:ILE:HD11	2.20	0.70
10:X:1:MET:CE	10:X:2:ASP:OD2	2.40	0.68
8:V:52:THR:O	8:V:56:THR:OG1	2.12	0.67
8:H:52:THR:O	8:H:56:THR:OG1	2.12	0.66
10:X:1:MET:SD	10:X:2:ASP:CG	2.74	0.65
10:J:99:GLN:NE2	17:J:201:HOH:O	2.31	0.62
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.53	0.57
10:X:2:ASP:HB3	10:X:18:SER:OG	2.06	0.55
7:G:23:PHE:O	7:G:26:THR:HB	2.07	0.55
8:H:43:CYS:SG	8:H:56:THR:CG2	2.96	0.54
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.90	0.54
8:V:43:CYS:SG	8:V:56:THR:CG2	2.96	0.54
2:P:93:HIS:HB3	17:P:301:HOH:O	2.07	0.53
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.90	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.91	0.52
14:N:35:THR:HG21	14:N:45:ARG:HE	1.74	0.52
2:P:217:LYS:C	2:P:219:ALA:H	2.14	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.51
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.41	0.51
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.92	0.51
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.76	0.51
2:B:12:PHE:H	3:C:17:GLN:HE22	1.59	0.50
2:B:217:LYS:C	2:B:219:ALA:H	2.13	0.50
14:N:152:VAL:HA	14:N:175:MET:HE1	1.93	0.50
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.95	0.48
2:P:149:THR:HG1	2:P:159:TRP:HE1	1.61	0.48
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.77	0.48
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.48	0.48
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.96	0.48
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.13	0.48
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.96	0.48
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.48	0.48
3:C:51:LYS:O	3:C:52:LEU:HB2	2.13	0.47
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.96	0.47
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.96	0.47
13:M:2:GLN:OE1	13:M:109:PRO:O	2.33	0.47
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.96	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.47
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.44	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.50	0.47
5:S:12:PHE:H	6:T:19:GLN:HE22	1.63	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.46
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.96	0.46
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.50	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
10:X:1:MET:HE1	10:X:2:ASP:CG	2.25	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.46
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.50	0.46
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.96	0.46
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.96	0.46
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.51	0.45
11:Y:4:LEU:HB3	11:Y:128:CYS:SG	2.56	0.45
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.16	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.99	0.45
11:K:4:LEU:HB3	11:K:128:CYS:SG	2.57	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.45
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.45
10:X:3:ILE:O	10:X:3:ILE:CG2	2.65	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
14:N:35:THR:CG2	14:N:45:ARG:HE	2.30	0.45
5:E:12:PHE:H	6:F:19:GLN:HE22	1.64	0.44
11:K:46:ALA:HB3	11:K:98:GLY:O	2.17	0.44
10:X:93:ARG:NH1	17:X:201:HOH:O	2.50	0.44
10:J:3:ILE:CG2	10:J:3:ILE:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
12:Z:5:TYR:CE1	12:Z:106:TYR:HB2	2.53	0.44
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.86	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.44
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.47	0.44
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.44
13:M:1:THR:C	13:M:2:GLN:HG3	2.37	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.43
11:K:209:ASN:O	9:W:38:LYS:NZ	2.51	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.43
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.00	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.43
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.00	0.43
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.00	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
4:R:91:HIS:HB3	4:R:99:ILE:HG22	2.02	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.02	0.42
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.02	0.42
8:H:3:ILE:HG21	8:H:44:ALA:HB3	2.02	0.42
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.02	0.42
10:X:3:ILE:O	10:X:3:ILE:HG22	2.19	0.42
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.02	0.42
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.02	0.42
2:B:96:ASN:ND2	17:B:301:HOH:O	2.45	0.42
7:G:73:VAL:HG12	7:G:133:THR:HB	2.01	0.42
12:L:5:TYR:CE1	12:L:106:TYR:HB2	2.55	0.42
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.01	0.42
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.00	0.42
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.54	0.42
2:B:50:LYS:O	2:B:51:VAL:C	2.57	0.42
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.02	0.42
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.41
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.53	0.41
2:B:219:ALA:HB2	2:B:225:TYR:HB2	2.01	0.41
10:J:3:ILE:O	10:J:3:ILE:HG22	2.19	0.41
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.03	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.41
10:J:139:TYR:OH	10:X:25:ILE:O	2.38	0.41
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.02	0.41
10:X:168:LEU:O	10:X:172:MET:HB2	2.20	0.41
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.02	0.41
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.41
2:P:113:ARG:NE	17:P:301:HOH:O	2.41	0.41
2:P:219:ALA:HB2	2:P:225:TYR:HB2	2.01	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.55	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG11	2.03	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.41
8:V:3:ILE:HG21	8:V:44:ALA:HB3	2.01	0.41
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.56	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.51	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.03	0.41
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.04	0.40
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.04	0.40
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.04	0.40
10:J:25:ILE:O	10:X:139:TYR:OH	2.40	0.40
1:O:12:PHE:H	2:P:20:GLN:HE22	1.69	0.40
5:S:68:HIS:HE1	5:S:102:LEU:O	2.04	0.40
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.02	0.40
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.02	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%)	239 (96%)	8 (3%)	1 (0%)	34	60
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	34	60
2	B	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	23
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	23
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	30
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	30
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	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%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	217 (97%)	7 (3%)	0	100	100
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%)	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%)	222 (96%)	9 (4%)	0	100	100
13	a	230/246 (94%)	221 (96%)	9 (4%)	0	100	100
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	6283/6614 (95%)	6132 (98%)	135 (2%)	16 (0%)	41	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	220	ASN
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
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%)	205 (98%)	4 (2%)	57	82
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	82
2	B	203/216 (94%)	197 (97%)	6 (3%)	41	70
2	P	203/216 (94%)	197 (97%)	6 (3%)	41	70
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	54
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	49
4	D	194/215 (90%)	184 (95%)	10 (5%)	23	49
4	R	194/215 (90%)	184 (95%)	10 (5%)	23	49
5	E	190/193 (98%)	181 (95%)	9 (5%)	26	54
5	S	190/193 (98%)	181 (95%)	9 (5%)	26	54
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	51
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	52
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	52
8	H	185/190 (97%)	178 (96%)	7 (4%)	33	62
8	V	185/190 (97%)	178 (96%)	7 (4%)	33	62
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	84
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	84
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	71
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	71
11	K	168/168 (100%)	160 (95%)	8 (5%)	25	53
11	Y	168/168 (100%)	160 (95%)	8 (5%)	25	53
12	L	185/185 (100%)	177 (96%)	8 (4%)	29	57
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	57
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	65
13	a	198/208 (95%)	192 (97%)	6 (3%)	41	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	63
All	All	5317/5538 (96%)	5112 (96%)	205 (4%)	32	61

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	147	GLN

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Mol	Chain	Res	Type
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
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	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU

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Mol	Chain	Res	Type
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	192	ASP
10	J	1	MET
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	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	130	SER
12	L	132	GLU
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	233	ILE
14	N	9	LYS
14	N	39	ASP

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Mol	Chain	Res	Type
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
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	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	208	ASP

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Mol	Chain	Res	Type
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	192	ASP
10	X	1	MET
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	128	CYS

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Mol	Chain	Res	Type
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	130	SER
12	Z	132	GLU
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	36	ARG
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS

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Mol	Chain	Res	Type
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
8	H	22	GLN
8	H	66	HIS
8	H	165	ASN
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	2	GLN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN

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Mol	Chain	Res	Type
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
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
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
8	V	22	GLN
9	W	37	ASN
10	X	55	GLN
10	X	146	HIS
10	X	147	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	70	ASN
12	Z	158	ASN
13	a	2	GLN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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 ⓘ

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%)	-0.38	6 (2%) 59 60	40, 52, 85, 126	0
1	O	250/250 (100%)	-0.30	8 (3%) 47 48	46, 62, 105, 133	0
2	B	244/258 (94%)	-0.22	8 (3%) 46 46	40, 60, 101, 155	0
2	P	244/258 (94%)	-0.18	9 (3%) 41 41	48, 65, 106, 153	0
3	C	240/254 (94%)	-0.11	14 (5%) 23 22	41, 64, 124, 154	0
3	Q	240/254 (94%)	0.06	18 (7%) 14 12	49, 74, 154, 181	0
4	D	235/260 (90%)	-0.38	5 (2%) 63 65	44, 64, 96, 137	0
4	R	235/260 (90%)	-0.29	7 (2%) 50 51	47, 67, 106, 141	0
5	E	231/234 (98%)	-0.28	3 (1%) 77 78	47, 65, 101, 143	0
5	S	231/234 (98%)	-0.20	6 (2%) 56 57	49, 72, 109, 150	0
6	F	243/288 (84%)	-0.40	4 (1%) 72 74	42, 57, 107, 130	0
6	T	243/288 (84%)	-0.31	6 (2%) 57 59	41, 66, 121, 148	0
7	G	241/252 (95%)	-0.48	2 (0%) 86 87	36, 53, 87, 134	0
7	U	241/252 (95%)	-0.33	9 (3%) 41 41	44, 59, 88, 132	0
8	H	226/232 (97%)	-0.32	8 (3%) 44 44	38, 52, 87, 154	0
8	V	226/232 (97%)	-0.26	7 (3%) 49 49	43, 55, 92, 169	0
9	I	204/205 (99%)	-0.56	2 (0%) 82 83	40, 52, 79, 97	0
9	W	204/205 (99%)	-0.51	3 (1%) 73 76	43, 54, 83, 104	0
10	J	195/198 (98%)	-0.37	3 (1%) 73 76	40, 55, 81, 128	0
10	X	195/198 (98%)	-0.28	5 (2%) 56 57	36, 59, 84, 145	0
11	K	212/212 (100%)	-0.38	2 (0%) 84 85	40, 57, 79, 100	0
11	Y	212/212 (100%)	-0.44	0 100 100	45, 57, 80, 100	0
12	L	222/222 (100%)	-0.53	1 (0%) 91 92	40, 53, 86, 123	0
12	Z	222/222 (100%)	-0.51	2 (0%) 84 85	41, 53, 85, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.60	2 (0%) 84 85	36, 52, 74, 91	0
13	a	232/246 (94%)	-0.54	1 (0%) 92 93	37, 52, 72, 90	0
14	N	196/196 (100%)	-0.60	2 (1%) 82 83	36, 47, 74, 103	0
14	b	196/196 (100%)	-0.59	2 (1%) 82 83	37, 49, 76, 108	0
All	All	6343/6614 (95%)	-0.36	145 (2%) 60 62	36, 58, 100, 181	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	7.5
3	Q	50	LEU	7.1
8	V	224	GLN	7.1
10	X	1	MET	6.7
2	B	219	ALA	6.6
2	P	219	ALA	6.3
3	Q	49	THR	6.3
2	P	51	VAL	6.2
2	P	221	ASP	5.8
3	Q	204	GLY	5.4
10	X	194	ASP	5.1
8	H	226	GLU	5.0
8	V	226	GLU	4.9
8	V	222	ASP	4.9
2	B	51	VAL	4.8
8	V	221	CYS	4.8
2	B	218	GLY	4.7
12	L	174	TYR	4.7
2	P	222	GLY	4.7
2	P	59	ASP	4.6
3	C	50	LEU	4.4
3	Q	236	GLN	4.4
8	H	222	ASP	4.4
1	A	1	MET	4.3
1	O	2	THR	4.2
4	R	241	ALA	4.2
2	P	220	ASN	4.2
3	C	206	LYS	4.2
7	U	242	GLN	4.0
8	H	224	GLN	4.0
1	A	2	THR	4.0
5	E	202	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	239	GLN	3.9
8	V	223	ILE	3.9
4	R	125	LEU	3.9
9	W	1	SER	3.9
8	V	225	GLU	3.9
12	Z	174	TYR	3.8
8	H	225	GLU	3.8
3	C	238	LYS	3.7
3	Q	239	GLN	3.7
2	B	220	ASN	3.7
8	H	223	ILE	3.7
3	Q	203	THR	3.7
3	C	205	ALA	3.6
3	Q	206	LYS	3.6
10	J	1	MET	3.5
8	H	221	CYS	3.5
3	C	49	THR	3.5
14	N	195	GLN	3.4
3	Q	202	GLN	3.4
3	Q	48	SER	3.4
6	T	244	ASN	3.3
5	S	202	ASP	3.3
14	b	195	GLN	3.2
3	C	240	GLU	3.2
3	Q	240	GLU	3.2
13	a	1	THR	3.2
1	O	249	ALA	3.2
5	S	173	ARG	3.2
3	Q	205	ALA	3.1
13	M	1	THR	3.1
14	N	105	LYS	3.1
4	R	242	GLU	3.0
3	Q	223	SER	3.0
3	C	236	GLN	2.9
4	R	1	ASP	2.9
14	b	105	LYS	2.9
1	O	1	MET	2.9
10	X	2	ASP	2.9
7	U	206	GLY	2.8
3	Q	237	GLU	2.8
11	K	212	GLY	2.8
5	E	233	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	248	GLU	2.8
13	M	47	ASP	2.7
3	C	175	LYS	2.7
9	W	133	LYS	2.7
7	U	222	ASP	2.7
3	Q	238	LYS	2.7
4	R	116	GLY	2.6
10	X	149	ARG	2.6
6	F	205	GLU	2.6
10	X	193	ASP	2.6
2	B	217	LYS	2.6
8	H	198	GLU	2.6
7	U	181	LYS	2.5
1	A	249	ALA	2.5
2	B	60	THR	2.5
7	G	3	TYR	2.5
3	C	202	GLN	2.5
11	K	147	ASP	2.5
6	F	244	ASN	2.5
3	Q	1	GLY	2.5
4	D	125	LEU	2.5
2	B	59	ASP	2.5
7	U	2	GLY	2.4
5	S	233	ILE	2.4
7	U	51	PRO	2.4
10	J	193	ASP	2.4
3	C	27	ARG	2.4
3	Q	46	ARG	2.4
1	O	231	LYS	2.4
9	I	131	GLU	2.4
5	S	54	GLU	2.4
6	T	243	ILE	2.4
2	P	60	THR	2.4
9	I	1	SER	2.4
12	Z	173	LYS	2.3
1	O	203	GLU	2.3
6	T	181	GLU	2.3
1	O	250	LEU	2.3
4	R	217	GLN	2.3
8	H	217	ILE	2.3
4	D	242	GLU	2.3
4	D	1	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	180	LYS	2.3
7	U	241	GLU	2.3
3	C	204	GLY	2.3
1	O	201	GLU	2.3
7	G	68	ARG	2.2
10	J	194	ASP	2.2
6	T	241	LYS	2.2
9	W	131	GLU	2.2
2	P	225	TYR	2.2
6	T	180	PRO	2.2
1	A	202	GLY	2.1
3	Q	55	THR	2.1
4	D	217	GLN	2.1
7	U	3	TYR	2.1
3	C	60	SER	2.1
1	O	52	SER	2.1
2	P	218	GLY	2.1
1	A	203	GLU	2.1
4	R	201	GLU	2.1
6	F	181	GLU	2.1
7	U	179	LYS	2.1
3	Q	233	GLN	2.1
5	E	173	ARG	2.1
5	S	227	GLU	2.1
6	F	204	LYS	2.0
5	S	180	LYS	2.0
6	T	206	LYS	2.0
8	V	145	ASP	2.0
4	D	177	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
15	MG	I	301	1/1	0.93	0.39	72,72,72,72	0
15	MG	W	301	1/1	0.94	0.48	73,73,73,73	0
15	MG	I	302	1/1	0.95	0.13	57,57,57,57	0
15	MG	Z	301	1/1	0.96	0.40	61,61,61,61	0
15	MG	N	201	1/1	0.97	0.10	49,49,49,49	0
15	MG	K	301	1/1	0.98	0.05	56,56,56,56	0
15	MG	G	301	1/1	0.98	0.09	63,63,63,63	0
16	CL	U	301	1/1	0.99	0.14	46,46,46,46	0
15	MG	L	301	1/1	0.99	0.05	58,58,58,58	0
16	CL	G	302	1/1	1.00	0.12	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.