



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:14 PM UTC

PDB ID : 4QV1 / pdb_00004qv1
Title : yCP beta5-M45A mutant
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2014-07-14
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

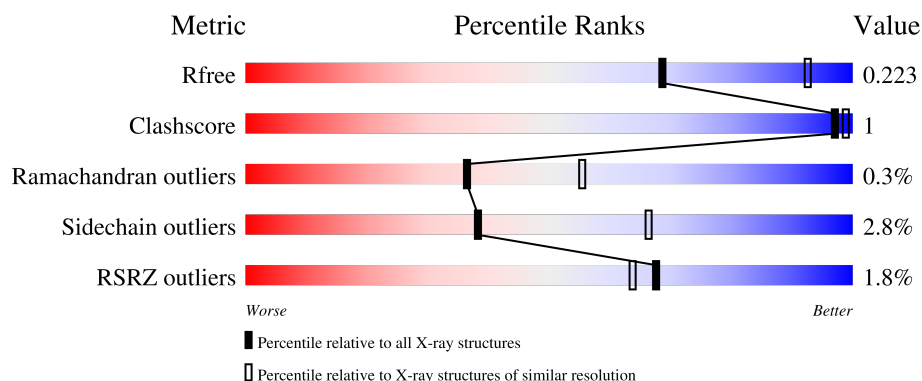
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	250	0% (red) 98% (green) 2% (yellow) 0% (orange) 0% (red)
1	O	250	4% (red) 98% (green) 2% (yellow) 0% (orange) 0% (red)
2	B	258	3% (red) 86% (green) 7% (yellow) 5% (orange) 0% (red)
2	P	258	3% (red) 87% (green) 7% (yellow) 5% (orange) 0% (red)
3	C	254	3% (red) 87% (green) 6% (yellow) 6% (orange) 0% (red)

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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	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50296 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
			1641	1043	280	312	6			
11	Y	212	Total	C	N	O	S	0	0	0
			1641	1043	280	312	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	45	ALA	MET	engineered mutation	UNP P30656
Y	45	ALA	MET	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	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (CCD ID: 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	36	Total O 36 36	0	0
17	B	25	Total O 25 25	0	0
17	C	23	Total O 23 23	0	0
17	D	32	Total O 32 32	0	0
17	E	19	Total O 19 19	0	0
17	F	29	Total O 29 29	0	0
17	G	42	Total O 42 42	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	34	Total 34	O 34	0	0
17	I	39	Total 39	O 39	0	0
17	J	38	Total 38	O 38	0	0
17	K	44	Total 44	O 44	0	0
17	L	42	Total 42	O 42	0	0
17	M	53	Total 53	O 53	0	0
17	N	38	Total 38	O 38	0	0
17	O	25	Total 25	O 25	0	0
17	P	21	Total 21	O 21	0	0
17	Q	20	Total 20	O 20	0	0
17	R	14	Total 14	O 14	0	0
17	S	16	Total 16	O 16	0	0
17	T	25	Total 25	O 25	0	0
17	U	42	Total 42	O 42	0	0
17	V	24	Total 24	O 24	0	0
17	W	39	Total 39	O 39	0	0
17	X	30	Total 30	O 30	0	0
17	Y	36	Total 36	O 36	0	0
17	Z	29	Total 29	O 29	0	0
17	a	60	Total 60	O 60	0	0
17	b	49	Total 49	O 49	0	0

3 Residue-property plots [i](#)

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

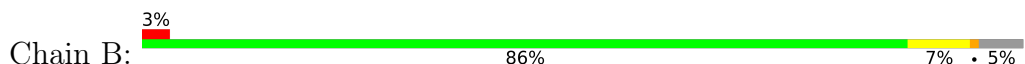
- Molecule 1: Proteasome subunit alpha type-2



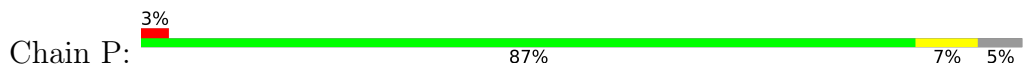
- Molecule 1: Proteasome subunit alpha type-2



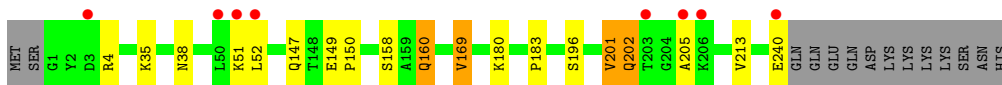
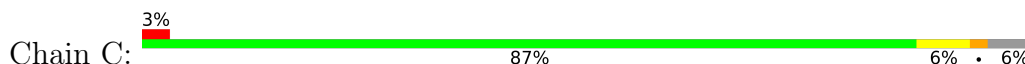
- Molecule 2: Proteasome subunit alpha type-3



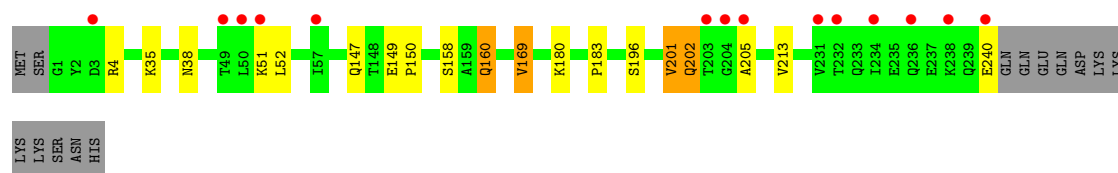
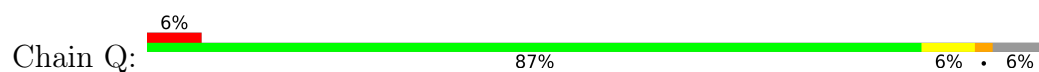
- Molecule 2: Proteasome subunit alpha type-3



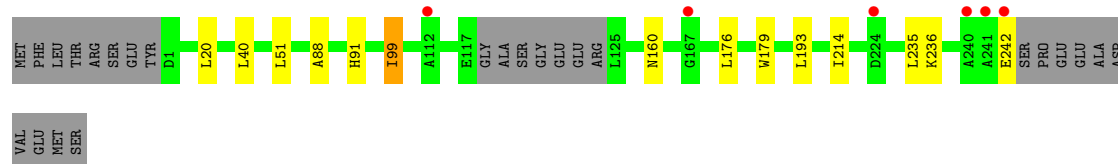
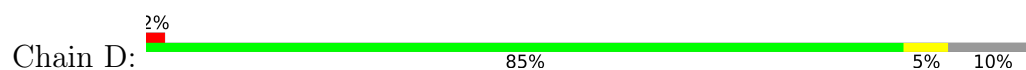
- Molecule 3: Proteasome subunit alpha type-4



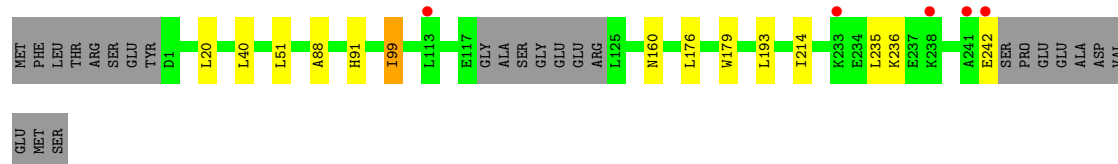
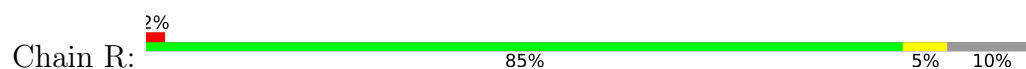
- Molecule 3: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-5



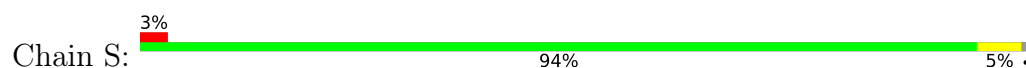
• Molecule 4: Proteasome subunit alpha type-5



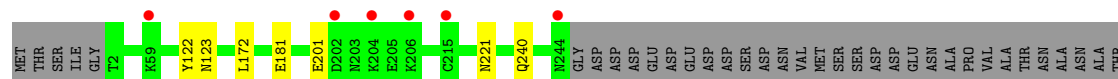
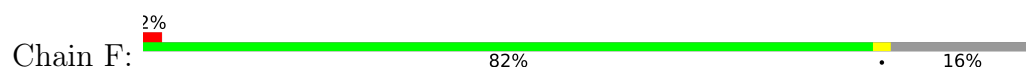
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 5: Proteasome subunit alpha type-6



• Molecule 6: Probable proteasome subunit alpha type-7



THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

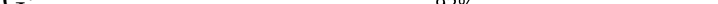
- Molecule 6: Probable proteasome subunit alpha type-7

Chain T:  2% 82% 16%

MET
 THR
 SER
 ILE
 GLY
 T2
 D14
 Q19
 Y122
 N123
 L172
 H178
 E181
 E201
 K204
 N221
 Q240
 K241
 E242
 T243
 T244
 GLY
 ASP
 ASP
 ASP
 ASP
 GLU
 ASP
 GLU
 ASP
 ASP
 ASP
 SER
 ASP
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 GLU
 ASP
 ALA
 PRO
 VAL
 THR
 ASN
 ALA
 ASN
 ASN

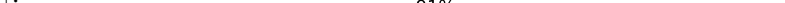
THR
THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

- Molecule 7: Proteasome subunit alpha type-1

Chain G:  92%

MET	SER	GLY	ALA	ALA	ALA	ALA	SER	ALA	ALA	ALA	G2	F23	T26	R68	N75	I78	P79	L115	R122	M125	R235	L236	A240	E241	Q242	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	-----

- Molecule 7: Proteasome subunit alpha type-1

Chain U:  4% 91% . .

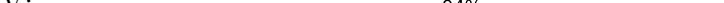
Metabolite	Log ₂ fold change	P-value
MET		
SER		
GLY		
ALA		
ALA		
ALA		
ALA		
ALA		
SER		
ALA		
ALA		
G2		
P12		
F23		
A24		
T26		
D40		
R68		
N75		
I78		
P79		
L115		
R122		
M125		
E168		
T171		
K179		
E188		
D222		
R235		
L236		
Q242		
GSP		

- Molecule 8: Proteasome subunit beta type-2

Chain H: 93% . .

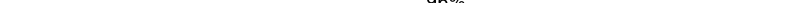
T1	Q22	A27	A50	D51	T52	T56	L68	D104	P105	L127	R196	T223	E226	GLN	VAL	ASP	ILE	THR	ALA
----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----

- Molecule 8: Proteasome subunit beta type-2

Chain V:  94% 2% . .

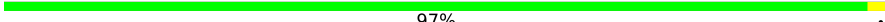
T1 M9 Q22 A27 T52 T56 L68 D104 P105 L127 R196 T223 Q224 E225 E226 GLN VAL ASP ILE THR ALA

- Molecule 9: Proteasome subunit beta type-3

Chain I:  96%

Sequence logo for the 1000bp upstream region of the human HNF1A gene. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows positions from -1000 to +1000. The sequence logo shows a strong enrichment of the TATA box (TATAAT) around position -25, with a peak of approximately 1.4 bits. Other notable features include a GC-rich region around position +100 and a T-rich region around position +200.

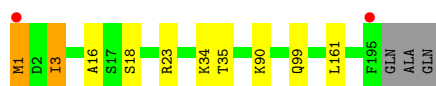
- Molecule 9: Proteasome subunit beta type-3

Chain W:  97%



- Molecule 10: Proteasome subunit beta type-4

Chain J:  93%

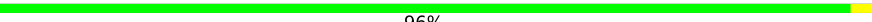


- Molecule 10: Proteasome subunit beta type-4

Chain X:  93%

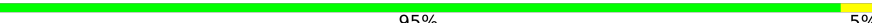


- Molecule 11: Proteasome subunit beta type-5

Chain K:  96%



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  95%

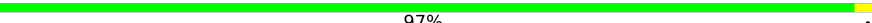


- Molecule 12: Proteasome subunit beta type-6

Chain L:  97%

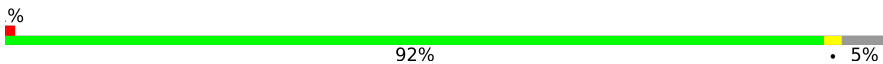


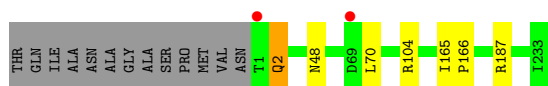
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  97%

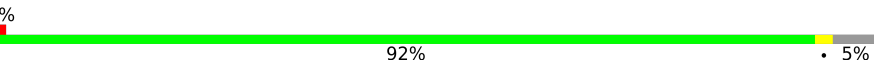


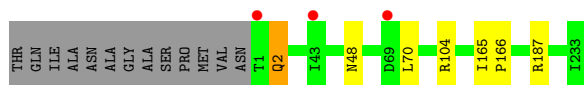
• Molecule 13: Proteasome subunit beta type-7

Chain M:  92% 5%

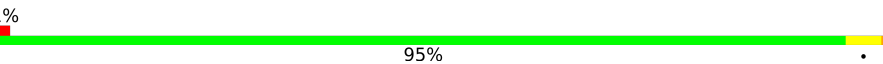


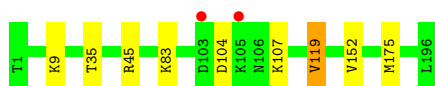
• Molecule 13: Proteasome subunit beta type-7

Chain a:  92% 5%

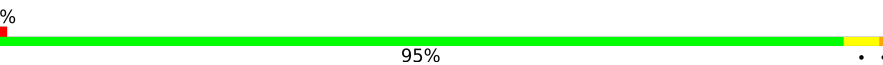


• Molecule 14: Proteasome subunit beta type-1

Chain N:  95%



• Molecule 14: Proteasome subunit beta type-1

Chain b:  95%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.54Å 300.51Å 144.28Å 90.00° 112.67° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.50) 98.4 (15.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.216 0.202 , 0.223	Depositor DCC
R_{free} test set	17852 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50296	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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	0.39	0/1952	0.68	0/2642
1	O	0.39	0/1952	0.68	0/2642
2	B	0.40	0/1934	0.67	0/2618
2	P	0.40	0/1934	0.67	0/2618
3	C	0.39	0/1910	0.69	1/2586 (0.0%)
3	Q	0.39	0/1910	0.69	1/2586 (0.0%)
4	D	0.38	0/1837	0.66	0/2475
4	R	0.38	0/1837	0.66	0/2475
5	E	0.39	0/1800	0.64	0/2433
5	S	0.39	0/1800	0.65	0/2433
6	F	0.40	0/1932	0.70	0/2609
6	T	0.40	0/1932	0.70	0/2609
7	G	0.39	0/1945	0.67	0/2634
7	U	0.38	0/1945	0.66	0/2634
8	H	0.38	0/1750	0.64	0/2373
8	V	0.38	0/1750	0.64	0/2373
9	I	0.38	0/1611	0.66	0/2174
9	W	0.38	0/1611	0.66	0/2174
10	J	0.40	0/1589	0.67	0/2142
10	X	0.40	0/1589	0.67	0/2142
11	K	0.37	0/1678	0.66	0/2271
11	Y	0.36	0/1678	0.66	0/2271
12	L	0.38	0/1795	0.65	0/2420
12	Z	0.37	0/1795	0.65	0/2420
13	M	0.40	0/1855	0.67	0/2514
13	a	0.39	0/1855	0.66	0/2514
14	N	0.37	0/1541	0.66	0/2087
14	b	0.37	0/1541	0.66	0/2087
All	All	0.39	0/50258	0.67	2/67956 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	5.47	116.20	110.62
3	C	201	VAL	N-CA-C	5.45	116.18	110.62

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	2	0
2	B	1904	0	1904	9	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	3	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	2	0
7	U	1907	0	1901	3	0
8	H	1719	0	1719	5	0
8	V	1719	0	1719	4	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	2	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	4	0
11	K	1641	0	1591	3	0
11	Y	1641	0	1591	4	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	2	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	4	0
14	b	1512	0	1481	3	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	A	36	0	0	0	0
17	B	25	0	0	2	0
17	C	23	0	0	0	0
17	D	32	0	0	0	0
17	E	19	0	0	0	0
17	F	29	0	0	0	0
17	G	42	0	0	0	0
17	H	34	0	0	0	0
17	I	39	0	0	0	0
17	J	38	0	0	0	0
17	K	44	0	0	0	0
17	L	42	0	0	0	0
17	M	53	0	0	1	0
17	N	38	0	0	1	0
17	O	25	0	0	0	0
17	P	21	0	0	0	0
17	Q	20	0	0	0	0
17	R	14	0	0	0	0
17	S	16	0	0	1	0
17	T	25	0	0	0	0
17	U	42	0	0	0	0
17	V	24	0	0	0	0
17	W	39	0	0	0	0
17	X	30	0	0	0	0
17	Y	36	0	0	0	0
17	Z	29	0	0	0	0
17	a	60	0	0	1	0
17	b	49	0	0	0	0
All	All	50296	0	49122	92	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 (92) 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)
14:N:35:THR:HG22	17:N:302:HOH:O	1.98	0.64
2:B:93:HIS:HB3	17:B:304:HOH:O	2.00	0.60
14:b:152:VAL:HA	14:b:175:MET:HE1	1.85	0.59
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.58
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.53
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.52
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.92	0.52
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.51
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.45	0.51
2:B:217:LYS:C	2:B:219:ALA:H	2.18	0.51
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.46	0.51
2:P:217:LYS:C	2:P:219:ALA:H	2.18	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.93	0.51
2:B:113:ARG:NE	17:B:304:HOH:O	2.35	0.50
13:a:2:GLN:NE2	17:a:357:HOH:O	2.44	0.50
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.47	0.50
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.49
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.48
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.43	0.48
2:P:50:LYS:O	2:P:51:VAL:C	2.56	0.48
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.43	0.48
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.48
13:M:2:GLN:NE2	17:M:347:HOH:O	2.47	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.95	0.47
8:V:52:THR:O	8:V:56:THR:HG23	2.14	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.14	0.47
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.49	0.47
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.97	0.47
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.97	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.15	0.46
3:C:201:VAL:O	3:C:202:GLN:HB3	2.16	0.46
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.98	0.46
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.51	0.46
8:H:52:THR:O	8:H:56:THR:HG23	2.15	0.46
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:ARG:HA	10:J:23:ARG:HD3	1.74	0.46
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.51	0.45
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.16	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.44
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.44
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.44
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.82	0.44
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.82	0.43
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.86	0.43
2:P:145:TYR:OH	2:P:217:LYS:N	2.51	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.43
2:B:145:TYR:OH	2:B:217:LYS:N	2.51	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.43
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.48	0.42
11:Y:44:THR:HG1	11:Y:100:MET:H	1.67	0.42
2:B:221:ASP:O	2:B:223:GLU:N	2.53	0.42
17:S:301:HOH:O	6:T:19:GLN:NE2	2.50	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.48	0.42
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.84	0.42
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.50	0.42
2:P:221:ASP:O	2:P:223:GLU:N	2.53	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.42
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.42
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.85	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.02	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
10:X:23:ARG:HD3	10:X:23:ARG:HA	1.74	0.41
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.02	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.51	0.40
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.57	0.40
2:B:217:LYS:C	2:B:219:ALA:N	2.79	0.40
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.03	0.40
14:b:35:THR:HG21	14:b:45:ARG:HE	1.86	0.40
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.02	0.40
9:I:98:ARG:O	9:I:126:ILE:HD11	2.22	0.40
14:N:35:THR:HG21	14:N:45:ARG:HE	1.86	0.40
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.40
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.04	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%)	239 (96%)	8 (3%)	1 (0%)	30	49
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	49
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	7	13
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	7	13
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	18
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	18
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%)	220 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	229/234 (98%)	220 (96%)	9 (4%)	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%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	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%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	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%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (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	6284/6614 (95%)	6122 (97%)	146 (2%)	16 (0%)	36	55

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
2	B	220	ASN

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Mol	Chain	Res	Type
3	C	205	ALA
2	P	220	ASN
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%)	50	76
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	76
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	64
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	64
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	47
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	47
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	42
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	42
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	62
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	62
6	F	201/239 (84%)	195 (97%)	6 (3%)	36	64
6	T	201/239 (84%)	195 (97%)	6 (3%)	36	64
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	60
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	60
8	H	185/190 (97%)	182 (98%)	3 (2%)	55	79
8	V	185/190 (97%)	182 (98%)	3 (2%)	55	79
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	83
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	83
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	65
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	168/168 (100%)	164 (98%)	4 (2%)	43	70
11	Y	168/168 (100%)	164 (98%)	4 (2%)	43	70
12	L	185/185 (100%)	183 (99%)	2 (1%)	65	84
12	Z	185/185 (100%)	183 (99%)	2 (1%)	65	84
13	M	199/208 (96%)	194 (98%)	5 (2%)	42	69
13	a	199/208 (96%)	194 (98%)	5 (2%)	42	69
14	N	162/162 (100%)	158 (98%)	4 (2%)	42	69
14	b	162/162 (100%)	158 (98%)	4 (2%)	42	69
All	All	5318/5538 (96%)	5170 (97%)	148 (3%)	38	66

All (148) 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	55	LEU
2	B	79	LEU
2	B	102	ASN
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	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU

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Mol	Chain	Res	Type
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	26	THR
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	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
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	107	LYS
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

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Mol	Chain	Res	Type
13	M	104	ARG
13	M	187	ARG
14	N	9	LYS
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	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	51	LYS
3	Q	52	LEU
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	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

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Mol	Chain	Res	Type
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	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	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
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	107	LYS
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	104	ASP
14	b	107	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	115	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	66	HIS
8	H	194	ASN
9	I	44	HIS
9	I	88	GLN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	208	ASN
12	L	49	ASN
12	L	70	ASN

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Mol	Chain	Res	Type
12	L	79	HIS
12	L	155	ASN
12	L	197	GLN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
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	100	ASN
4	R	106	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	123	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	66	HIS
8	V	194	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN

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Mol	Chain	Res	Type
12	Z	49	ASN
12	Z	79	HIS
12	Z	155	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	149	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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%)	-0.19	3 (1%) 76 73	34, 48, 88, 125	0
1	O	250/250 (100%)	-0.09	9 (3%) 46 41	38, 55, 103, 131	0
2	B	244/258 (94%)	0.00	9 (3%) 45 40	34, 54, 99, 155	0
2	P	244/258 (94%)	-0.03	8 (3%) 49 45	40, 57, 98, 152	0
3	C	240/254 (94%)	0.02	8 (3%) 49 45	35, 57, 117, 146	0
3	Q	240/254 (94%)	0.28	14 (5%) 29 25	43, 71, 150, 182	0
4	D	235/260 (90%)	-0.05	6 (2%) 57 52	40, 59, 92, 132	0
4	R	235/260 (90%)	0.09	5 (2%) 63 59	43, 64, 107, 141	0
5	E	231/234 (98%)	-0.04	2 (0%) 81 78	39, 61, 98, 139	0
5	S	231/234 (98%)	0.26	6 (2%) 57 52	43, 70, 114, 156	0
6	F	243/288 (84%)	-0.19	6 (2%) 58 54	34, 55, 104, 127	0
6	T	243/288 (84%)	0.10	7 (2%) 53 49	39, 67, 119, 155	0
7	G	241/252 (95%)	-0.21	2 (0%) 82 80	31, 51, 86, 137	0
7	U	241/252 (95%)	-0.07	9 (3%) 45 40	39, 55, 87, 129	0
8	H	226/232 (97%)	-0.19	1 (0%) 88 86	31, 48, 78, 145	0
8	V	226/232 (97%)	-0.16	4 (1%) 67 64	33, 50, 79, 166	0
9	I	204/205 (99%)	-0.48	0 100 100	28, 42, 70, 99	0
9	W	204/205 (99%)	-0.41	1 (0%) 87 85	31, 45, 74, 100	0
10	J	195/198 (98%)	-0.33	2 (1%) 79 76	31, 47, 73, 117	0
10	X	195/198 (98%)	-0.29	1 (0%) 87 85	32, 48, 74, 128	0
11	K	212/212 (100%)	-0.28	0 100 100	29, 47, 73, 87	0
11	Y	212/212 (100%)	-0.30	1 (0%) 87 85	34, 48, 75, 93	0
12	L	222/222 (100%)	-0.26	2 (0%) 81 78	31, 48, 86, 123	0
12	Z	222/222 (100%)	-0.27	1 (0%) 87 85	28, 49, 84, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.32	2 (0%)	81 78	28, 47, 71, 92	0
13	a	233/246 (94%)	-0.31	3 (1%)	75 71	28, 49, 71, 92	0
14	N	196/196 (100%)	-0.44	2 (1%)	79 76	31, 42, 71, 99	0
14	b	196/196 (100%)	-0.40	1 (0%)	87 85	30, 43, 72, 104	0
All	All	6344/6614 (95%)	-0.15	115 (1%)	67 64	28, 52, 99, 182	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	6.7
3	Q	50	LEU	5.9
8	V	223	ILE	5.6
2	B	51	VAL	5.0
10	J	1	MET	4.6
8	H	223	ILE	4.2
12	L	174	TYR	4.2
2	P	219	ALA	4.0
2	P	51	VAL	3.9
3	Q	205	ALA	3.9
13	a	1	THR	3.8
6	T	243	ILE	3.7
2	B	218	GLY	3.6
3	C	50	LEU	3.5
3	Q	49	THR	3.5
13	a	69	ASP	3.4
2	B	220	ASN	3.3
4	D	224	ASP	3.2
5	S	209	ASN	3.2
13	M	1	THR	3.2
4	D	240	ALA	3.2
12	Z	174	TYR	3.2
3	Q	234	ILE	3.2
1	O	53	SER	3.1
7	U	68	ARG	3.1
4	D	241	ALA	3.1
1	A	1	MET	3.1
3	Q	3	ASP	3.0
2	P	218	GLY	3.0
2	P	52	THR	2.9
6	T	204	LYS	2.9
1	O	1	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	2.8
3	C	203	THR	2.8
6	T	178	HIS	2.8
12	L	166	GLY	2.8
3	C	205	ALA	2.8
4	R	113	LEU	2.8
1	O	231	LYS	2.8
7	U	24	LYS	2.8
13	M	69	ASP	2.8
14	b	103	ASP	2.8
2	B	1	GLY	2.7
1	A	2	THR	2.7
2	P	1	GLY	2.7
3	Q	204	GLY	2.7
7	U	242	GLN	2.7
4	R	238	LYS	2.6
6	T	14	ASP	2.6
5	S	122	TYR	2.6
5	S	207	VAL	2.5
14	N	105	LYS	2.5
1	O	2	THR	2.5
3	Q	236	GLN	2.5
3	C	51	LYS	2.4
3	C	206	LYS	2.4
3	Q	51	LYS	2.4
2	P	220	ASN	2.4
2	P	222	GLY	2.4
6	F	215	CYS	2.4
6	F	244	ASN	2.4
6	T	244	ASN	2.4
1	O	62	SER	2.4
2	B	50	LYS	2.4
7	G	68	ARG	2.4
11	Y	208	ASN	2.4
3	C	3	ASP	2.4
13	a	43	ILE	2.3
4	R	233	LYS	2.3
3	C	240	GLU	2.3
5	S	55	LEU	2.3
3	Q	232	THR	2.3
6	F	202	ASP	2.3
3	Q	231	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	2.3
5	S	56	SER	2.3
1	O	3	ASP	2.3
6	T	241	LYS	2.3
4	D	112	ALA	2.2
3	Q	203	THR	2.2
9	W	1	SER	2.2
7	U	188	GLU	2.2
4	D	167	GLY	2.2
5	E	123	GLY	2.2
1	O	61	LEU	2.2
3	C	52	LEU	2.2
1	A	62	SER	2.2
7	G	240	ALA	2.2
5	E	122	TYR	2.2
5	S	52	ALA	2.2
6	F	204	LYS	2.2
4	R	242	GLU	2.2
8	V	9	ASN	2.1
14	N	103	ASP	2.1
3	Q	238	LYS	2.1
2	B	93	HIS	2.1
1	O	249	ALA	2.1
2	B	222	GLY	2.1
2	B	243	ILE	2.1
2	P	221	ASP	2.1
7	U	40	ASP	2.1
1	O	4	ARG	2.1
4	R	241	ALA	2.1
6	T	2	THR	2.1
7	U	168	GLU	2.1
7	U	179	LYS	2.1
7	U	222	ASP	2.1
3	Q	57	ILE	2.0
6	F	59	LYS	2.0
6	F	206	LYS	2.0
10	J	195	PHE	2.0
3	Q	240	GLU	2.0
4	D	242	GLU	2.0
8	V	226	GLU	2.0
7	U	171	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	I	301	1/1	0.87	0.10	61,61,61,61	0
15	MG	H	301	1/1	0.88	0.16	58,58,58,58	0
15	MG	J	201	1/1	0.92	0.09	59,59,59,59	0
15	MG	Z	301	1/1	0.92	0.08	63,63,63,63	0
15	MG	G	301	1/1	0.96	0.05	49,49,49,49	0
15	MG	Y	301	1/1	0.97	0.06	48,48,48,48	0
15	MG	K	302	1/1	0.97	0.18	51,51,51,51	0
15	MG	N	201	1/1	0.98	0.04	50,50,50,50	0
15	MG	V	301	1/1	0.98	0.10	48,48,48,48	0
15	MG	K	301	1/1	0.99	0.10	39,39,39,39	0
16	CL	G	302	1/1	0.99	0.04	36,36,36,36	0
16	CL	U	301	1/1	1.00	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.