



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:19 PM UTC

PDB ID : 5L5W / pdb_00005l5w
Title : Yeast 20S proteasome with human beta5c (1-138) and human beta6 (97-111; 118-133)
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
Resolution : 2.80 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

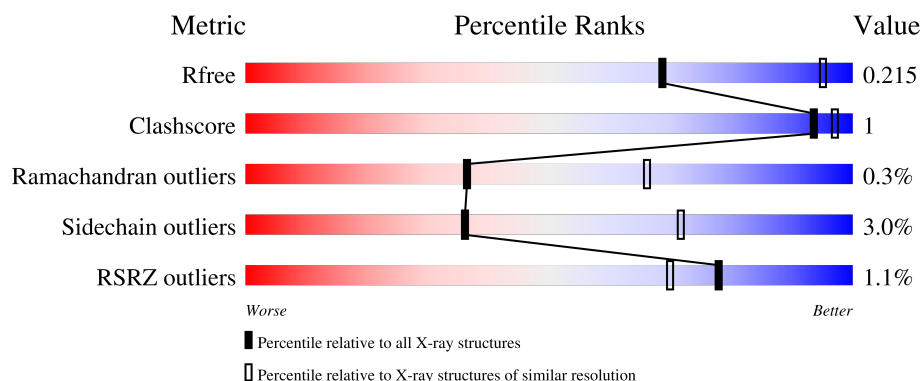
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

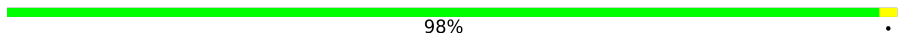
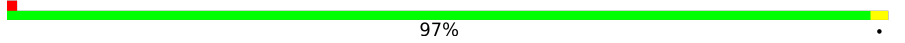
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	 97% .
2	B	258	 88% 6% 5%
2	P	258	 88% 6% . 5%
3	C	254	 87% 6% . 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	 3% 87% 6% • 6%
4	D	260	 2% 87% • • 10%
4	R	260	 87% • 10%
5	E	234	 95% • •
5	S	234	 95% • •
6	F	288	 82% • 16%
6	T	288	 82% • 16%
7	G	252	 91% • •
7	U	252	 90% 5% •
8	H	232	 92% 5% •
8	V	232	 93% • •
9	I	205	 94% 6%
9	W	205	 91% 8%
10	J	198	 92% 6% • •
10	X	198	 92% 6% • •
11	K	211	 84% 13% •
11	Y	211	 83% 14% •
12	L	222	 93% 6% •
12	Z	222	 94% 5% •
13	M	246	 91% • 5%
13	a	246	 91% • 5%
14	N	196	 93% 6% •
14	b	196	 93% 6% •

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49684 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			

Continued on next page...

Continued from previous page...

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,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1632	1036	282	306	8			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	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	1	0
			1832	1159	315	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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	E	1	Total Cl 1 1	0	0
15	G	1	Total Cl 1 1	0	0
15	U	1	Total Cl 1 1	0	0
15	b	1	Total Cl 1 1	0	0

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

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	10	Total O 10 10	0	0
17	B	11	Total O 11 11	0	0
17	C	10	Total O 10 10	0	0
17	D	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	E	5	Total O 5 5	0	0
17	F	9	Total O 9 9	0	0
17	G	13	Total O 13 13	0	0
17	H	11	Total O 11 11	0	0
17	I	10	Total O 10 10	0	0
17	J	7	Total O 7 7	0	0
17	K	16	Total O 16 16	0	0
17	L	14	Total O 14 14	0	0
17	M	16	Total O 16 16	0	0
17	N	12	Total O 12 12	0	0
17	O	6	Total O 6 6	0	0
17	P	9	Total O 9 9	0	0
17	Q	11	Total O 11 11	0	0
17	R	13	Total O 13 13	0	0
17	S	11	Total O 11 11	0	0
17	T	8	Total O 8 8	0	0
17	U	17	Total O 17 17	0	0
17	V	16	Total O 16 16	0	0
17	W	13	Total O 13 13	0	0
17	X	6	Total O 6 6	0	0
17	Y	15	Total O 15 15	0	0

Continued on next page...

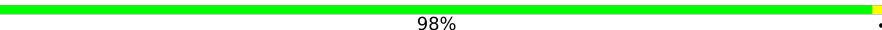
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	Z	4	Total 4	O 4	0	0
17	a	13	Total 13	O 13	0	0
17	b	12	Total 12	O 12	0	0

3 Residue-property plots [i](#)

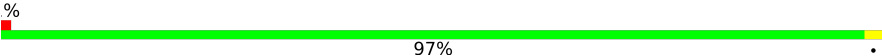
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Proteasome subunit alpha type-2

Chain A:  98% .



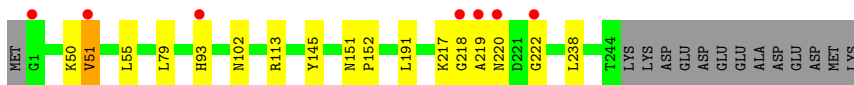
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  97% .



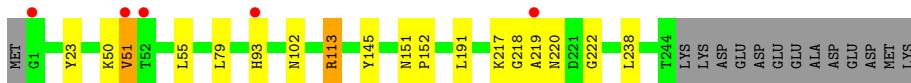
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 6% 5% .



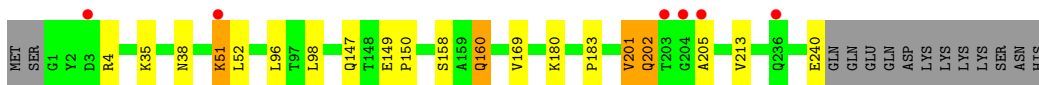
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  88% 6% 5% .

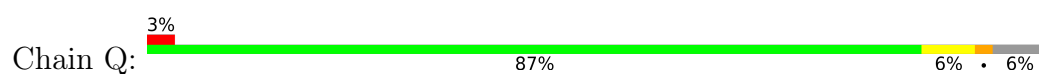


- Molecule 3: Proteasome subunit alpha type-4

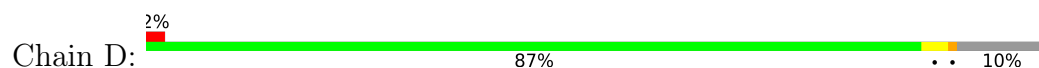
Chain C:  87% 6% 6% .



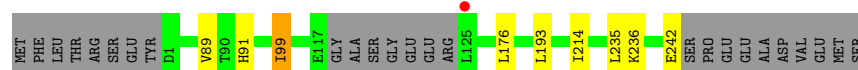
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



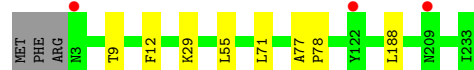
- Molecule 4: Proteasome subunit alpha type-5



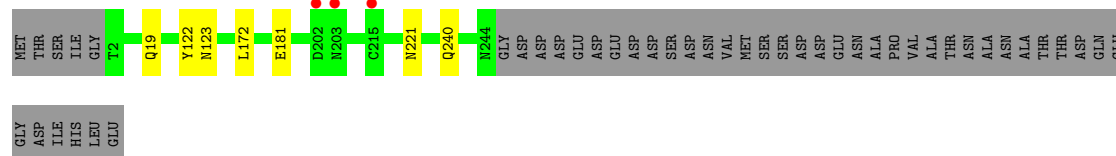
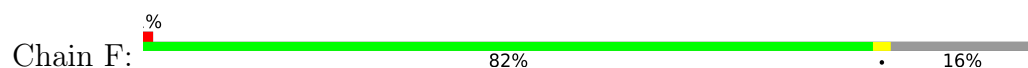
- Molecule 5: Proteasome subunit alpha type-6



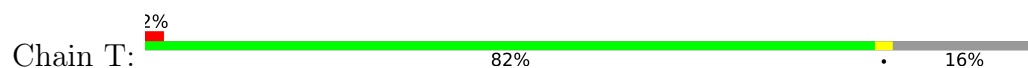
- Molecule 5: Proteasome subunit alpha type-6

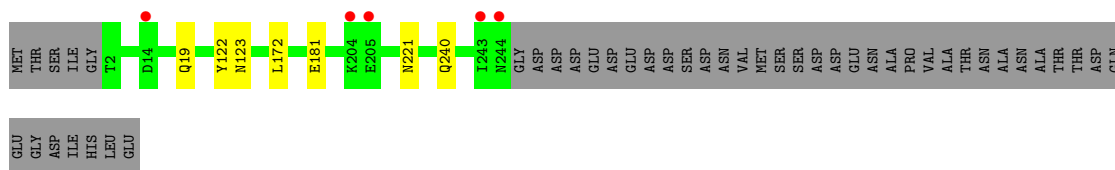


- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 7: Proteasome subunit alpha type-1

Chain G: 91%



- Molecule 7: Proteasome subunit alpha type-1

Chain U: 90%



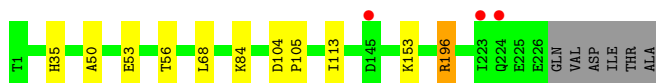
- Molecule 8: Proteasome subunit beta type-2

Chain H: 92%



- Molecule 8: Proteasome subunit beta type-2

Chain V: 93%



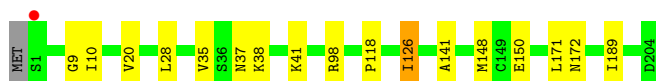
- Molecule 9: Proteasome subunit beta type-3

Chain I: 94%

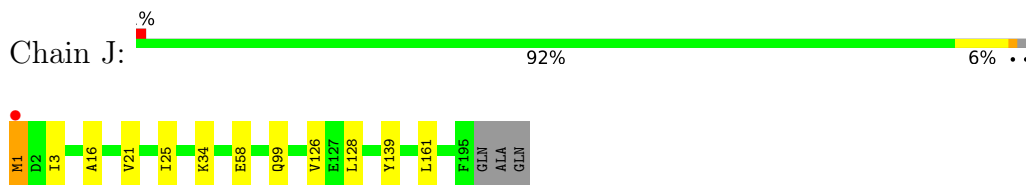


- Molecule 9: Proteasome subunit beta type-3

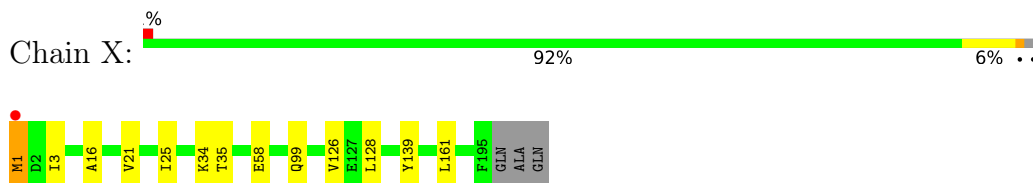
Chain W: 91%



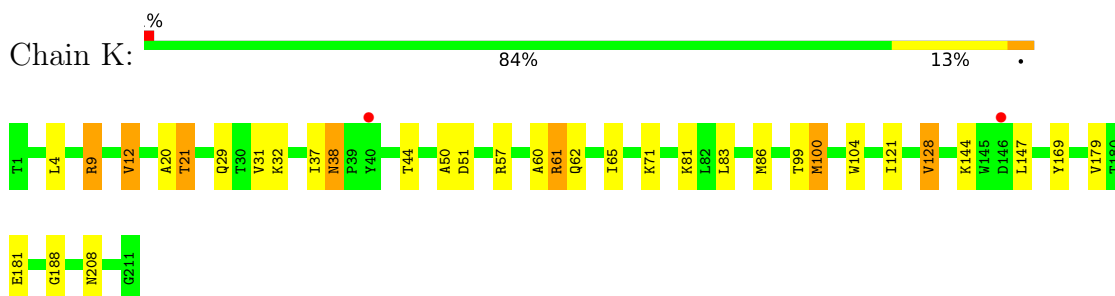
- Molecule 10: Proteasome subunit beta type-4



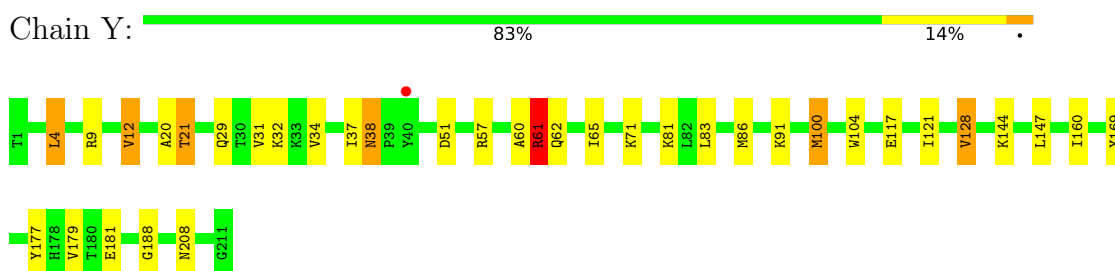
- Molecule 10: Proteasome subunit beta type-4



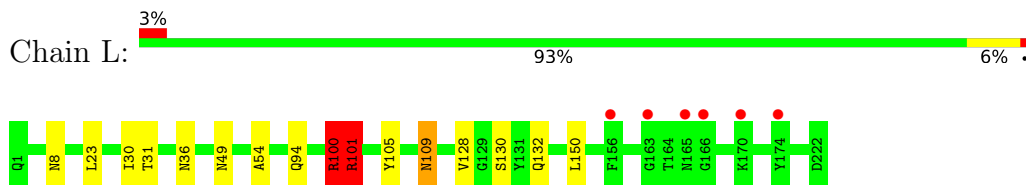
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



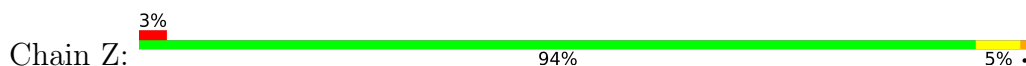
- Molecule 11: Proteasome subunit beta type-5, Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6, Proteasome subunit beta type-1, Proteasome subunit beta type-6





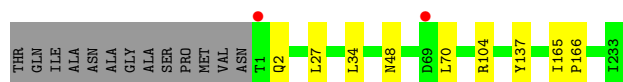
- Molecule 13: Proteasome subunit beta type-7

Chain M: 91% 5%



- Molecule 13: Proteasome subunit beta type-7

Chain a: 91% 5%



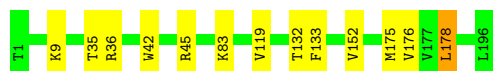
- Molecule 14: Proteasome subunit beta type-1

Chain N: 93% 6%



- Molecule 14: Proteasome subunit beta type-1

Chain b: 93% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.07Å 300.35Å 145.24Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-2.80) 97.3 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.185 , 0.212 0.192 , 0.215	Depositor DCC
R_{free} test set	12718 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49684	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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	0.40	0/1952	0.69	0/2642
1	O	0.40	0/1952	0.68	0/2642
2	B	0.42	0/1934	0.69	0/2618
2	P	0.41	0/1934	0.68	0/2618
3	C	0.40	0/1910	0.70	1/2586 (0.0%)
3	Q	0.40	0/1910	0.70	1/2586 (0.0%)
4	D	0.40	0/1837	0.66	0/2475
4	R	0.39	0/1837	0.66	0/2475
5	E	0.41	0/1800	0.65	0/2433
5	S	0.41	0/1800	0.65	0/2433
6	F	0.41	0/1932	0.69	0/2609
6	T	0.40	0/1932	0.69	0/2609
7	G	0.39	0/1945	0.67	0/2634
7	U	0.39	0/1945	0.67	0/2634
8	H	0.35	0/1750	0.67	0/2373
8	V	0.35	0/1750	0.67	0/2373
9	I	0.35	0/1611	0.69	0/2174
9	W	0.34	0/1611	0.70	0/2174
10	J	0.39	0/1589	0.66	0/2142
10	X	0.39	0/1589	0.66	0/2142
11	K	0.38	0/1668	0.80	4/2253 (0.2%)
11	Y	0.38	0/1668	0.80	3/2253 (0.1%)
12	L	0.48	3/1802 (0.2%)	0.82	5/2430 (0.2%)
12	Z	0.47	2/1802 (0.1%)	0.86	6/2430 (0.2%)
13	M	0.36	0/1855	0.68	0/2514
13	a	0.36	0/1866	0.68	0/2528
14	N	0.35	0/1541	0.69	0/2087
14	b	0.35	0/1541	0.69	0/2087
All	All	0.39	5/50263 (0.0%)	0.70	20/67954 (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
12	L	0	1
12	Z	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	109	ASN	CG-ND2	-6.67	1.19	1.33
12	Z	94	GLN	CD-NE2	-6.54	1.19	1.33
12	L	94	GLN	CD-NE2	-6.41	1.19	1.33
12	Z	109	ASN	CG-ND2	-6.37	1.19	1.33
12	L	94	GLN	CD-OE1	-5.07	1.14	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	100	ARG	NE-CZ-NH1	-12.39	109.11	121.50
12	Z	100	ARG	NE-CZ-NH2	12.36	130.32	119.20
11	Y	61	ARG	CB-CG-CD	11.73	138.28	111.30
11	K	61	ARG	CB-CG-CD	11.59	137.95	111.30
12	L	101	ARG	NE-CZ-NH2	11.50	129.55	119.20
12	L	101	ARG	NE-CZ-NH1	-11.49	110.00	121.50
12	Z	101	ARG	NE-CZ-NH2	-10.43	109.81	119.20
12	L	101	ARG	CD-NE-CZ	8.99	136.99	124.40
12	Z	101	ARG	CD-NE-CZ	8.53	136.34	124.40
12	Z	100	ARG	CD-NE-CZ	8.30	136.02	124.40
12	Z	101	ARG	NE-CZ-NH1	7.70	129.20	121.50
11	K	9	ARG	CG-CD-NE	7.55	128.61	112.00
12	L	100	ARG	NE-CZ-NH2	-7.49	112.46	119.20
11	Y	9	ARG	CG-CD-NE	7.17	127.78	112.00
12	L	100	ARG	CD-NE-CZ	6.83	133.96	124.40
3	Q	201	VAL	N-CA-C	5.97	116.15	110.42
3	C	201	VAL	N-CA-C	5.87	116.05	110.42
11	K	9	ARG	CB-CG-CD	-5.32	99.06	111.30
11	Y	188	GLY	N-CA-C	5.13	118.54	112.33
11	K	188	GLY	N-CA-C	5.06	118.45	112.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	100	ARG	Sidechain
12	Z	100	ARG	Sidechain

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	3	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	3	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	8	0
8	V	1719	0	1719	7	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	7	0
11	K	1632	0	1593	22	0
11	Y	1632	0	1593	18	0
12	L	1764	0	1716	7	0
12	Z	1764	0	1716	5	0
13	M	1824	0	1832	4	0
13	a	1832	0	1845	3	0
14	N	1512	0	1481	7	0
14	b	1512	0	1481	7	0
15	E	1	0	0	0	0
15	G	1	0	0	0	0
15	U	1	0	0	0	0
15	b	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	K	2	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	A	10	0	0	0	0
17	B	11	0	0	1	0
17	C	10	0	0	0	0
17	D	6	0	0	0	0
17	E	5	0	0	0	0
17	F	9	0	0	0	0
17	G	13	0	0	0	0
17	H	11	0	0	0	0
17	I	10	0	0	0	0
17	J	7	0	0	0	0
17	K	16	0	0	0	0
17	L	14	0	0	0	0
17	M	16	0	0	1	0
17	N	12	0	0	0	0
17	O	6	0	0	0	0
17	P	9	0	0	2	0
17	Q	11	0	0	0	0
17	R	13	0	0	0	0
17	S	11	0	0	0	0
17	T	8	0	0	0	0
17	U	17	0	0	0	0
17	V	16	0	0	0	0
17	W	13	0	0	0	0
17	X	6	0	0	0	0
17	Y	15	0	0	0	0
17	Z	4	0	0	0	0
17	a	13	0	0	0	0
17	b	12	0	0	0	0
All	All	49684	0	49149	142	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 (142) 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)
4:R:89:VAL:HG12	11:Y:61:ARG:HD3	1.72	0.72
4:D:89:VAL:CG1	11:K:61:ARG:HG2	2.21	0.71
4:D:89:VAL:HG12	11:K:61:ARG:HG2	1.74	0.70
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.86	0.58
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.85	0.58
14:b:152:VAL:HA	14:b:175:MET:HE1	1.86	0.56
11:K:12:VAL:HG13	11:K:179:VAL:HB	1.88	0.56
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.56
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	1.88	0.55
4:D:89:VAL:HG12	11:K:61:ARG:CG	2.36	0.55
13:M:2:GLN:NE2	17:M:401:HOH:O	2.40	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.52
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.44	0.52
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.52
8:H:196:ARG:NH2	9:I:150:GLU:O	2.42	0.52
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.44	0.52
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.92	0.52
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.74	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.92	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:96:LEU:O	11:Y:81:LYS:HE2	2.10	0.51
3:C:51:LYS:O	3:C:52:LEU:HB2	2.09	0.51
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.40	0.51
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.75	0.51
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.92	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.50
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.93	0.50
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.94	0.50
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.42	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
10:J:25:ILE:O	10:X:139:TYR:OH	2.30	0.49
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.49
10:J:139:TYR:OH	10:X:25:ILE:O	2.30	0.49
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.48
2:P:50:LYS:O	2:P:51:VAL:C	2.56	0.48
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.57	0.48
11:K:208:ASN:O	9:W:38:LYS:NZ	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:HIS:HB3	17:B:301:HOH:O	2.14	0.48
2:P:113:ARG:NE	17:P:301:HOH:O	2.34	0.48
8:H:35:HIS:CB	8:H:56:THR:HG21	2.44	0.47
2:B:217:LYS:C	2:B:219:ALA:H	2.22	0.47
11:Y:37:ILE:HG23	11:Y:60:ALA:HB2	1.96	0.47
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.97	0.47
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.45	0.47
8:V:196:ARG:NH2	9:W:150:GLU:O	2.47	0.47
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.15	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.47
3:C:201:VAL:O	3:C:202:GLN:HB3	2.15	0.47
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.30	0.47
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.96	0.47
11:K:37:ILE:HG23	11:K:60:ALA:HB2	1.96	0.47
11:K:38:ASN:OD1	11:K:38:ASN:C	2.57	0.46
2:P:93:HIS:HB3	17:P:301:HOH:O	2.16	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.96	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
10:J:58:GLU:OE1	11:K:81:LYS:NZ	2.47	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.81	0.46
2:P:217:LYS:C	2:P:219:ALA:H	2.23	0.46
11:Y:100:MET:SD	11:Y:128:VAL:CG1	3.03	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.46
12:L:54:ALA:HB2	12:L:109:ASN:OD1	2.16	0.46
11:K:100:MET:SD	11:K:128:VAL:CG1	3.04	0.45
11:K:51:ASP:OD2	12:L:101:ARG:NH2	2.49	0.45
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.81	0.45
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.97	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.50	0.45
10:X:58:GLU:OE1	11:Y:81:LYS:NZ	2.49	0.45
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.99	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.44
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.52	0.44
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.98	0.44
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.98	0.44
2:B:145:TYR:OH	2:B:217:LYS:N	2.51	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.00	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.18	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
11:Y:61:ARG:O	11:Y:65:ILE:HG13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.99	0.43
11:K:61:ARG:O	11:K:65:ILE:HG13	2.19	0.43
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.49	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.43
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.49	0.43
14:N:35:THR:HG21	14:N:45:ARG:HE	1.84	0.43
2:P:145:TYR:OH	2:P:217:LYS:N	2.51	0.43
14:b:35:THR:HG21	14:b:45:ARG:HE	1.84	0.43
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.49	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.42
11:K:50:ALA:CB	12:L:128:VAL:HG23	2.49	0.42
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.33	0.42
9:W:28:LEU:HD23	9:W:35:VAL:HB	2.02	0.42
11:Y:91:LYS:HE3	11:Y:117:GLU:O	2.20	0.42
12:Z:36:ASN:HB3	13:a:137:TYR:CD1	2.54	0.42
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.54	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
5:S:12:PHE:H	6:T:19:GLN:HE22	1.67	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.42
12:L:100:ARG:HD3	12:L:105:TYR:CZ	2.54	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.42
10:J:21:VAL:HG11	11:K:121:ILE:HD11	2.01	0.42
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.42
4:D:89:VAL:HG11	11:K:61:ARG:HG2	2.02	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.41
9:I:148:MET:HE2	9:I:172:ASN:HB2	2.02	0.41
9:W:98:ARG:O	9:W:126:ILE:HD11	2.20	0.41
11:Y:51:ASP:OD2	12:Z:101:ARG:NH2	2.50	0.41
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.56	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.41
14:N:133:PHE:HA	14:b:132:THR:O	2.20	0.41
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
5:E:12:PHE:H	6:F:19:GLN:HE22	1.69	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
9:W:148:MET:HE2	9:W:172:ASN:HB2	2.03	0.41
10:X:21:VAL:HG11	11:Y:121:ILE:HD11	2.03	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.03	0.41
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.03	0.41
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.03	0.41
11:Y:4:LEU:HD13	11:Y:160:ILE:HD11	2.03	0.41
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.22	0.40
11:K:21:THR:HG21	11:K:169:TYR:CD1	2.56	0.40
11:K:44:THR:O	11:K:99:THR:OG1	2.39	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.03	0.40
11:Y:34:VAL:HG11	11:Y:177:TYR:CD1	2.56	0.40
11:K:9:ARG:HH21	11:K:9:ARG:HD3	1.74	0.40
11:K:51:ASP:CG	12:L:101:ARG:HH21	2.29	0.40
13:M:17:ASP:OD1	13:M:18:ASN:N	2.54	0.40
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.89	0.40
11:Y:21:THR:HG21	11:Y:169:TYR:CD1	2.56	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.84	0.40
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.04	0.40
3:C:96:LEU:O	11:K:81:LYS:HE2	2.22	0.40
14:N:132:THR:O	14:b:133:PHE:HA	2.21	0.40
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	2.04	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%)	30	60
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	60
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	25
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	31
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	31
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
8	V	224/232 (97%)	220 (98%)	4 (2%)	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%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	232/246 (94%)	223 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6283/6612 (95%)	6115 (97%)	152 (2%)	16 (0%)	36	66

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
2	B	220	ASN
2	P	220	ASN
3	Q	183	PRO
3	C	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	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	81
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	72
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	72
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	57
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	57
4	D	194/215 (90%)	187 (96%)	7 (4%)	31	66
4	R	194/215 (90%)	187 (96%)	7 (4%)	31	66
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	75
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	75
6	F	201/239 (84%)	196 (98%)	5 (2%)	42	76
6	T	201/239 (84%)	196 (98%)	5 (2%)	42	76
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	68
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	68
8	H	185/190 (97%)	181 (98%)	4 (2%)	45	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	185/190 (97%)	181 (98%)	4 (2%)	45	78
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	87
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	83
10	J	173/175 (99%)	170 (98%)	3 (2%)	53	83
10	X	173/175 (99%)	169 (98%)	4 (2%)	44	78
11	K	165/165 (100%)	152 (92%)	13 (8%)	11	35
11	Y	165/165 (100%)	151 (92%)	14 (8%)	10	31
12	L	186/186 (100%)	179 (96%)	7 (4%)	29	64
12	Z	186/186 (100%)	182 (98%)	4 (2%)	45	78
13	M	199/208 (96%)	195 (98%)	4 (2%)	48	80
13	a	200/208 (96%)	196 (98%)	4 (2%)	48	80
14	N	162/162 (100%)	160 (99%)	2 (1%)	63	87
14	b	162/162 (100%)	160 (99%)	2 (1%)	63	87
All	All	5315/5534 (96%)	5157 (97%)	158 (3%)	36	72

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	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	98	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	240	GLU
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
6	F	123	ASN
6	F	172	LEU
6	F	181	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	53	GLU
8	H	68	LEU
8	H	153	LYS
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	21	THR
11	K	29	GLN
11	K	32	LYS
11	K	38	ASN
11	K	57	ARG
11	K	62	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	71	LYS
11	K	83	LEU
11	K	86	MET
11	K	100	MET
11	K	128	VAL
12	L	23	LEU
12	L	49	ASN
12	L	100	ARG
12	L	101	ARG
12	L	130	SER
12	L	132	GLN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
14	N	9	LYS
14	N	178	LEU
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	98	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	99	ILE
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
6	T	123	ASN
6	T	172	LEU
6	T	181	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	53	GLU
8	V	68	LEU
8	V	153	LYS
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	35	THR
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	21	THR
11	Y	29	GLN
11	Y	32	LYS
11	Y	38	ASN
11	Y	57	ARG
11	Y	61	ARG
11	Y	62	GLN
11	Y	71	LYS
11	Y	83	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	86	MET
11	Y	100	MET
11	Y	128	VAL
12	Z	23	LEU
12	Z	49	ASN
12	Z	130	SER
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
14	b	9	LYS
14	b	178	LEU

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

Mol	Chain	Res	Type
2	B	123	GLN
2	B	124	HIS
3	C	17	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	180	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	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	123	ASN
7	G	30	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	175	ASN
8	H	35	HIS
8	H	200	GLN
9	I	37	ASN
9	I	63	ASN
9	I	172	ASN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
11	K	10	HIS
11	K	85	ASN
11	K	175	ASN
11	K	187	HIS
11	K	207	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
12	L	197	GLN
13	M	48	ASN
13	M	62	HIS
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
7	U	30	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	175	ASN
8	V	30	ASN
8	V	35	HIS
8	V	189	ASN
8	V	200	GLN
9	W	37	ASN
9	W	63	ASN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
11	Y	85	ASN
11	Y	175	ASN
11	Y	187	HIS
11	Y	207	ASN
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	94	GLN
12	Z	197	GLN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
14	b	38	HIS
14	b	141	ASN

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 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.38	1 (0%) 88 84	33, 50, 89, 127	0
1	O	250/250 (100%)	-0.32	2 (0%) 82 75	37, 54, 100, 136	0
2	B	244/258 (94%)	-0.17	7 (2%) 53 43	38, 55, 99, 156	0
2	P	244/258 (94%)	-0.18	5 (2%) 65 56	41, 58, 101, 154	0
3	C	240/254 (94%)	-0.11	6 (2%) 58 48	36, 64, 130, 167	0
3	Q	240/254 (94%)	0.02	7 (2%) 53 43	37, 68, 138, 181	0
4	D	235/260 (90%)	-0.24	4 (1%) 69 60	42, 60, 90, 129	0
4	R	235/260 (90%)	-0.16	1 (0%) 88 84	49, 67, 106, 134	0
5	E	231/234 (98%)	-0.26	1 (0%) 88 84	41, 60, 99, 139	0
5	S	231/234 (98%)	-0.19	3 (1%) 75 66	45, 64, 101, 134	0
6	F	243/288 (84%)	-0.34	3 (1%) 76 68	36, 56, 102, 128	0
6	T	243/288 (84%)	-0.23	5 (2%) 63 54	37, 62, 114, 143	0
7	G	241/252 (95%)	-0.34	1 (0%) 88 84	35, 53, 93, 149	0
7	U	241/252 (95%)	-0.34	1 (0%) 88 84	37, 53, 87, 125	0
8	H	226/232 (97%)	-0.37	0 100 100	34, 49, 84, 149	0
8	V	226/232 (97%)	-0.35	3 (1%) 75 66	35, 50, 82, 164	0
9	I	204/205 (99%)	-0.53	1 (0%) 87 82	32, 47, 75, 97	0
9	W	204/205 (99%)	-0.52	1 (0%) 87 82	29, 48, 74, 100	0
10	J	195/198 (98%)	-0.27	1 (0%) 87 82	36, 55, 86, 131	0
10	X	195/198 (98%)	-0.27	1 (0%) 87 82	38, 57, 89, 136	0
11	K	211/211 (100%)	-0.19	2 (0%) 81 74	36, 54, 82, 112	0
11	Y	211/211 (100%)	-0.13	1 (0%) 87 82	37, 56, 88, 112	0
12	L	222/222 (100%)	-0.17	6 (2%) 56 46	41, 55, 99, 128	0
12	Z	222/222 (100%)	-0.09	6 (2%) 56 46	38, 57, 99, 130	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.44	1 (0%) 88 84	33, 50, 72, 90	0
13	a	233/246 (94%)	-0.43	2 (0%) 81 74	33, 52, 75, 92	1 (0%)
14	N	196/196 (100%)	-0.47	0 100 100	34, 46, 77, 102	0
14	b	196/196 (100%)	-0.54	0 100 100	33, 46, 76, 106	0
All	All	6342/6612 (95%)	-0.28	72 (1%) 78 70	29, 55, 98, 181	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	5.5
10	J	1	MET	5.4
2	P	51	VAL	3.8
2	B	1	GLY	3.7
8	V	224	GLN	3.6
4	D	241	ALA	3.5
2	P	1	GLY	3.5
9	W	1	SER	3.4
3	Q	204	GLY	3.3
6	F	215	CYS	3.1
2	P	219	ALA	3.1
6	T	204	LYS	3.1
3	C	205	ALA	3.1
13	a	1	THR	3.0
12	Z	174	TYR	2.8
13	a	69	ASP	2.8
6	F	202	ASP	2.8
2	B	218	GLY	2.7
7	G	68	ARG	2.7
12	L	166	GLY	2.7
11	K	146	ASP	2.7
9	I	1	SER	2.7
3	Q	3	ASP	2.6
6	T	244	ASN	2.6
3	Q	205	ALA	2.6
2	B	51	VAL	2.6
3	C	203	THR	2.6
1	O	1	MET	2.5
6	T	243	ILE	2.5
8	V	145	ASP	2.5
12	L	170	LYS	2.5
2	B	219	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	206	LYS	2.5
13	M	1	THR	2.5
3	Q	51	LYS	2.5
1	A	1	MET	2.5
6	T	205	GLU	2.5
2	B	220	ASN	2.4
6	T	14	ASP	2.4
2	P	93	HIS	2.4
8	V	223	ILE	2.4
2	B	93	HIS	2.3
12	L	156	PHE	2.3
3	Q	238	LYS	2.3
4	D	117	GLU	2.3
4	D	240	ALA	2.3
3	C	51	LYS	2.3
11	Y	40	TYR	2.3
12	L	174	TYR	2.3
5	S	3	ASN	2.2
5	S	209	ASN	2.2
6	F	203	ASN	2.2
3	Q	50	LEU	2.2
4	R	125	LEU	2.2
11	K	40	TYR	2.2
4	D	242	GLU	2.2
12	Z	170	LYS	2.2
12	Z	161	GLU	2.2
3	C	236	GLN	2.2
2	P	52	THR	2.2
12	Z	163	GLY	2.2
1	O	53	SER	2.2
3	C	3	ASP	2.1
12	Z	162	PRO	2.1
3	C	204	GLY	2.1
5	S	122	TYR	2.1
2	B	222	GLY	2.1
7	U	24	LYS	2.1
12	L	163	GLY	2.0
12	Z	169	LYS	2.0
5	E	207	VAL	2.0
12	L	165	ASN	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
16	MG	M	301	1/1	0.75	0.35	68,68,68,68	0
16	MG	Z	301	1/1	0.87	0.12	78,78,78,78	0
16	MG	N	201	1/1	0.90	0.11	59,59,59,59	0
16	MG	K	302	1/1	0.92	0.09	59,59,59,59	0
16	MG	J	201	1/1	0.93	0.14	60,60,60,60	0
16	MG	b	201	1/1	0.94	0.06	54,54,54,54	0
16	MG	H	301	1/1	0.95	0.17	56,56,56,56	0
15	CL	b	202	1/1	0.97	0.10	53,53,53,53	0
15	CL	G	302	1/1	0.97	0.08	44,44,44,44	0
16	MG	I	302	1/1	0.97	0.07	53,53,53,53	0
15	CL	E	301	1/1	0.98	0.04	58,58,58,58	0
16	MG	L	301	1/1	0.98	0.09	60,60,60,60	0
16	MG	I	301	1/1	0.98	0.04	45,45,45,45	0
15	CL	U	301	1/1	0.99	0.09	41,41,41,41	0
16	MG	G	301	1/1	0.99	0.05	46,46,46,46	0
16	MG	K	301	1/1	1.00	0.07	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.