



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:58 PM GMT

PDB ID : 4Y82
Title : Yeast 20S proteasome in complex with Ac-LAY-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

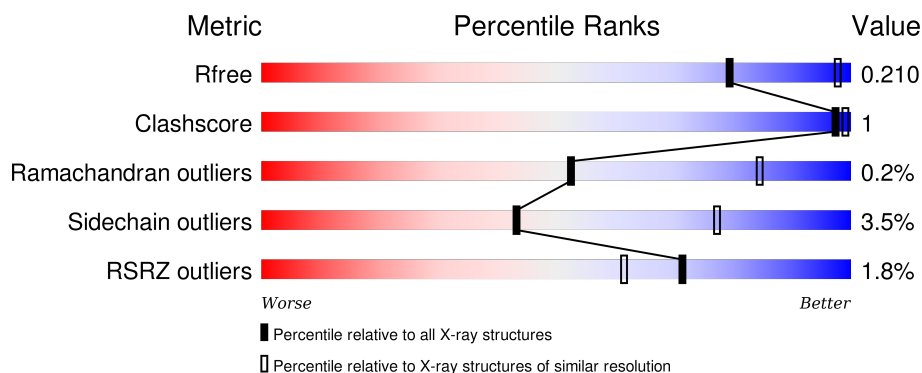
1 Overall quality at a glance ⓘ

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>97%</div> <div>.</div> </div>
1	O	250	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
2	B	258	<div> <div>4%</div> <div>88%</div> <div>6% 5%</div> </div>
2	P	258	<div> <div>4%</div> <div>89%</div> <div>5% 5%</div> </div>
3	C	254	<div> <div>5%</div> <div>88%</div> <div>6% . 6%</div> </div>

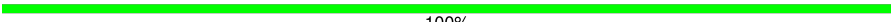
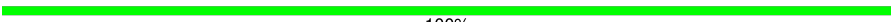

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	e	5	 100%
15	f	5	 100%
15	g	5	 100%
15	h	5	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MG	I	301	-	-	-	X
16	MG	Z	301	-	-	-	X
18	MES	d	101	-	-	-	X
18	MES	g	101	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49969 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	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	1	0
			1764	1120	305	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	230	Total	C	N	O	S	0	0	0
			1797	1137	307	346	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 a protein called Ac-LAY-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			32	23	3	6			
15	d	5	Total	C	N	O	0	0	0
			32	23	3	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	5	Total	C	N	O	0	0	0
			32	23	3	6			
15	f	5	Total	C	N	O	0	0	0
			32	23	3	6			
15	g	5	Total	C	N	O	0	0	0
			32	23	3	6			
15	h	5	Total	C	N	O	0	0	0
			32	23	3	6			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	d	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	g	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	20	Total	O	0	0
			20	20		
19	B	17	Total	O	0	0
			17	17		
19	C	20	Total	O	0	0
			20	20		
19	D	5	Total	O	0	0
			5	5		
19	E	8	Total	O	0	0
			8	8		
19	F	19	Total	O	0	0
			19	19		
19	G	18	Total	O	0	0
			18	18		
19	H	17	Total	O	0	0
			17	17		
19	I	20	Total	O	0	0
			20	20		
19	J	21	Total	O	0	0
			21	21		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	21	Total O 21 21	0	0
19	L	24	Total O 24 24	0	0
19	M	21	Total O 21 21	0	0
19	N	10	Total O 10 10	0	0
19	O	17	Total O 17 17	0	0
19	P	11	Total O 11 11	0	0
19	Q	14	Total O 14 14	0	0
19	R	10	Total O 10 10	0	0
19	S	7	Total O 7 7	0	0
19	T	14	Total O 14 14	0	0
19	U	11	Total O 11 11	0	0
19	V	14	Total O 14 14	0	0
19	W	14	Total O 14 14	0	0
19	X	22	Total O 22 22	0	0
19	Y	20	Total O 20 20	0	0
19	Z	25	Total O 25 25	0	0
19	a	28	Total O 28 28	0	0
19	b	19	Total O 19 19	0	0
19	c	1	Total O 1 1	0	0
19	d	2	Total O 2 2	0	0
19	e	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	f	1	Total 1	O 1	0	0
19	g	2	Total 2	O 2	0	0
19	h	2	Total 2	O 2	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 errors 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.

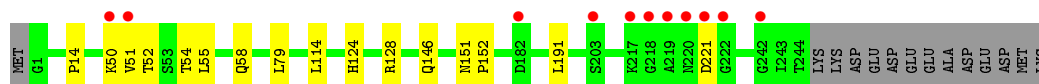
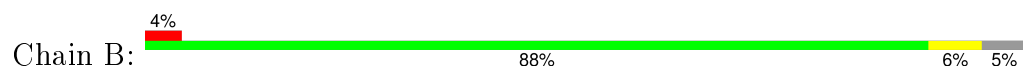
- Molecule 1: Proteasome subunit alpha type-2



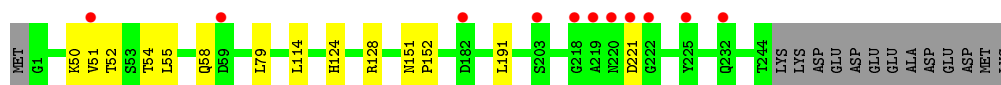
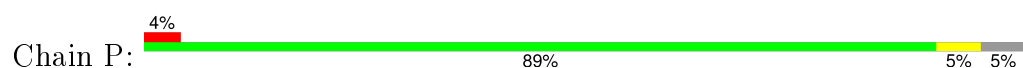
- Molecule 1: Proteasome subunit alpha type-2



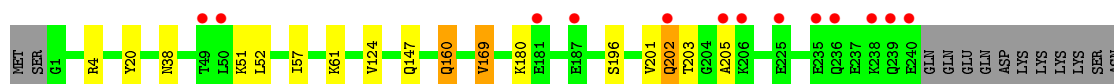
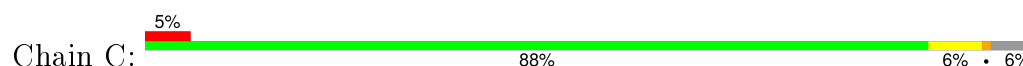
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

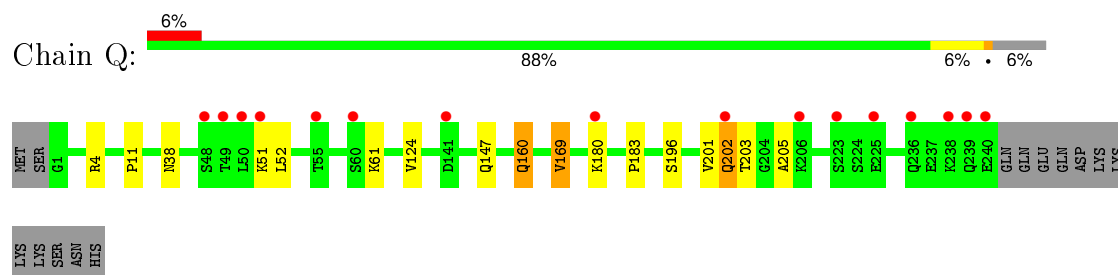


- Molecule 3: Proteasome subunit alpha type-4

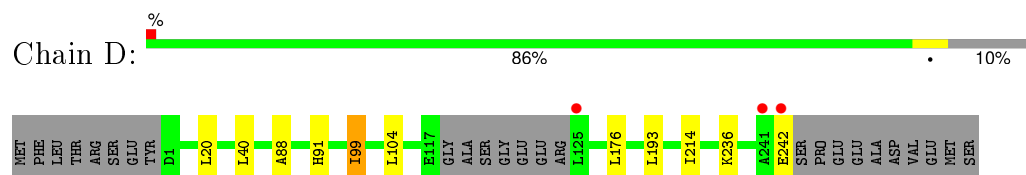


HIS

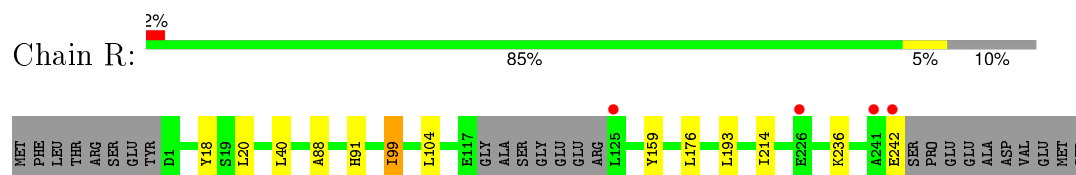
- Molecule 3: Proteasome subunit alpha type-4



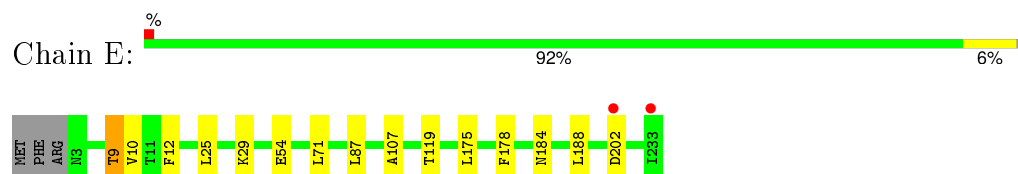
- Molecule 4: Proteasome subunit alpha type-5



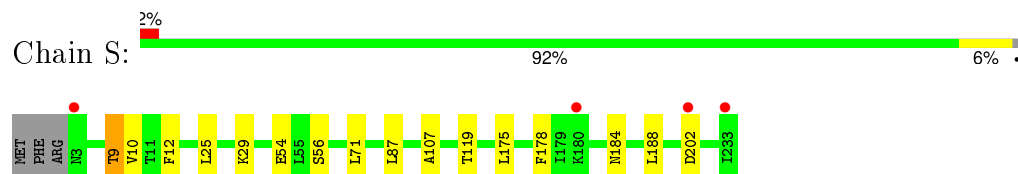
- Molecule 4: Proteasome subunit alpha type-5



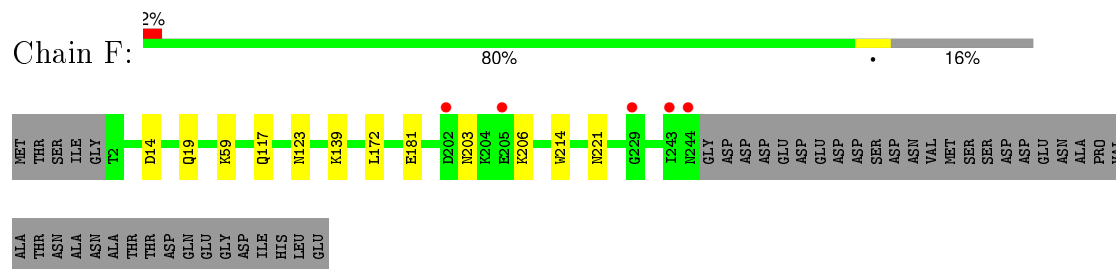
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6

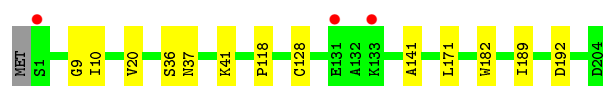


- Molecule 6: Probable proteasome subunit alpha type-7

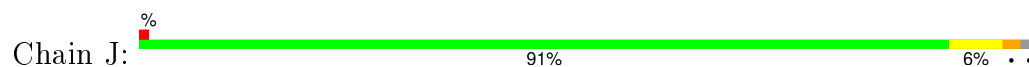


- Molecule 6: Probable proteasome subunit alpha type-7

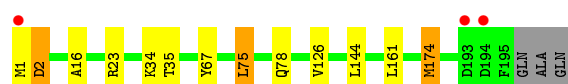




- Molecule 10: Proteasome subunit beta type-4



- Molecule 10: Proteasome subunit beta type-4



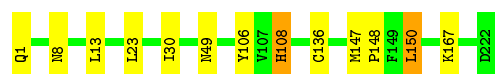
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



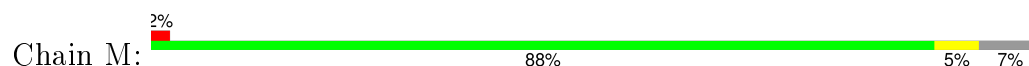
- Molecule 12: Proteasome subunit beta type-6

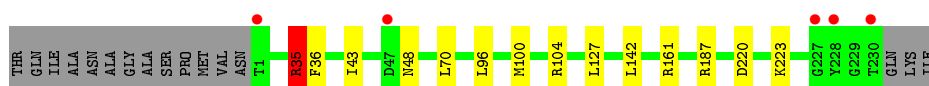


- Molecule 12: Proteasome subunit beta type-6

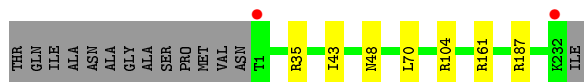


- Molecule 13: Proteasome subunit beta type-7

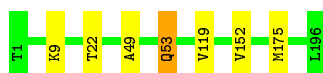




- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



- Molecule 15: Ac-LAY-ep



There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAY-ep



There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAY-ep



There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAY-ep



There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAY-ep



There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAY-ep

Chain h:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.24Å 300.91Å 145.47Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.80) 98.3 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.189 , 0.207 0.193 , 0.210	Depositor DCC
R_{free} test set	12861 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 257214 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49969	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 2.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACE, CL, TYE, POL, MES

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	0.28	0/1952	0.48	0/2642
1	O	0.28	0/1952	0.47	0/2642
2	B	0.29	0/1934	0.49	0/2618
2	P	0.28	0/1934	0.49	0/2618
3	C	0.29	0/1910	0.51	0/2586
3	Q	0.29	0/1910	0.51	0/2586
4	D	0.28	0/1837	0.48	0/2475
4	R	0.28	0/1837	0.48	0/2475
5	E	0.28	0/1800	0.48	0/2433
5	S	0.28	0/1800	0.48	0/2433
6	F	0.29	0/1932	0.46	0/2609
6	T	0.28	0/1932	0.46	0/2609
7	G	0.29	0/1945	0.47	0/2634
7	U	0.29	0/1945	0.47	0/2634
8	H	0.34	0/1715	0.50	0/2326
8	V	0.31	0/1715	0.50	1/2326 (0.0%)
9	I	0.29	0/1611	0.48	0/2174
9	W	0.29	0/1611	0.49	0/2174
10	J	0.28	0/1589	0.49	0/2142
10	X	0.27	0/1589	0.49	0/2142
11	K	0.31	0/1681	0.50	0/2274
11	Y	0.31	0/1681	0.51	0/2274
12	L	0.37	2/1806 (0.1%)	0.57	4/2435 (0.2%)
12	Z	0.32	0/1795	0.48	0/2420
13	M	0.31	0/1828	0.56	2/2480 (0.1%)
13	a	0.31	0/1846	0.56	2/2503 (0.1%)
14	N	0.36	0/1541	0.49	0/2087
14	b	0.37	0/1541	0.49	0/2087
15	c	1.04	0/13	1.38	0/17
15	d	1.46	0/13	1.70	0/17
15	e	1.24	0/13	1.41	0/17
15	f	0.65	0/13	1.05	0/17

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	1.35	0/13	1.50	0/17
15	h	1.04	0/13	1.41	0/17
All	All	0.30	2/50247 (0.0%)	0.50	9/67940 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	108[A]	HIS	CA-C	6.47	1.69	1.52
12	L	108[B]	HIS	CA-C	6.47	1.69	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	35	ARG	NE-CZ-NH2	9.30	124.95	120.30
13	M	35	ARG	NE-CZ-NH2	8.84	124.72	120.30
12	L	108[A]	HIS	CA-C-O	6.80	134.39	120.10
12	L	108[B]	HIS	CA-C-O	6.80	134.39	120.10
13	M	35	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
12	L	108[A]	HIS	CA-C-N	-5.60	104.88	117.20
12	L	108[B]	HIS	CA-C-N	-5.60	104.88	117.20
8	V	1	THR	N-CA-C	5.17	124.96	111.00
13	a	35	ARG	NH1-CZ-NH2	-5.11	113.78	119.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	4	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1813	0	1797	3	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1684	0	1685	5	0
8	V	1684	0	1685	3	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	8	0
10	X	1561	0	1569	6	0
11	K	1644	0	1592	4	0
11	Y	1644	0	1592	3	0
12	L	1764	0	1718	6	0
12	Z	1757	0	1711	4	0
13	M	1797	0	1800	4	0
13	a	1815	0	1821	0	0
14	N	1512	0	1478	3	0
14	b	1512	0	1478	0	0
15	c	32	0	32	0	0
15	d	32	0	32	0	0
15	e	32	0	32	0	0
15	f	32	0	33	0	0
15	g	32	0	32	0	0
15	h	32	0	32	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	d	12	0	13	0	0
18	g	12	0	13	0	0
19	A	20	0	0	0	0
19	B	17	0	0	0	0
19	C	20	0	0	0	0
19	D	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	E	8	0	0	0	0
19	F	19	0	0	0	0
19	G	18	0	0	0	0
19	H	17	0	0	0	0
19	I	20	0	0	0	0
19	J	21	0	0	0	0
19	K	21	0	0	0	0
19	L	24	0	0	3	0
19	M	21	0	0	0	0
19	N	10	0	0	0	0
19	O	17	0	0	0	0
19	P	11	0	0	0	0
19	Q	14	0	0	0	0
19	R	10	0	0	0	0
19	S	7	0	0	0	0
19	T	14	0	0	0	0
19	U	11	0	0	0	0
19	V	14	0	0	0	0
19	W	14	0	0	0	0
19	X	22	0	0	0	0
19	Y	20	0	0	0	0
19	Z	25	0	0	1	0
19	a	28	0	0	0	0
19	b	19	0	0	0	0
19	c	1	0	0	0	0
19	d	2	0	0	0	0
19	e	2	0	0	0	0
19	f	1	0	0	0	0
19	g	2	0	0	0	0
19	h	2	0	0	0	0
All	All	49969	0	49233	100	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 (100) 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)
12:L:108[A]:HIS:ND1	19:L:404:HOH:O	1.64	1.22
12:L:108[A]:HIS:CE1	19:L:404:HOH:O	2.07	1.01
12:Z:106:TYR:OH	19:Z:413:HOH:O	1.97	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:O	10:J:2:ASP:HB2	1.84	0.76
10:X:1:MET:O	10:X:2:ASP:HB2	1.85	0.75
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.79	0.65
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.78	0.65
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.81	0.62
14:N:22:THR:O	14:N:22:THR:HG23	2.01	0.59
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.86	0.57
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.87	0.56
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.88	0.55
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.89	0.55
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
10:J:174:MET:HA	10:X:174:MET:HA	1.91	0.51
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.75	0.51
8:H:28:ASP:OD2	8:H:29:LYS:N	2.44	0.51
8:H:52:THR:O	8:H:56:THR:HB	2.11	0.51
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.10	0.50
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.94	0.50
3:C:51:LYS:O	3:C:52:LEU:HB2	2.10	0.50
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.76	0.50
8:V:52:THR:O	8:V:56:THR:HB	2.13	0.49
3:C:201:VAL:O	3:C:202:GLN:CB	2.61	0.49
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.94	0.49
11:K:100:MET:CE	11:K:127:PHE:HB2	2.42	0.48
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.42	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.96	0.48
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.61	0.48
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.96	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.95	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.96	0.47
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.79	0.47
13:M:35:ARG:HD3	13:M:36:PHE:CZ	2.49	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.47
3:C:201:VAL:HG13	3:C:202:GLN:N	2.29	0.47
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.29	0.47
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.96	0.47
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.50	0.47
14:N:152:VAL:HA	14:N:175:MET:HE1	1.96	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.46
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.97	0.46
9:I:98:ARG:O	9:I:126:ILE:HD11	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.98	0.46
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.51	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.97	0.46
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.16	0.45
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.45
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.99	0.45
12:L:108[B]:HIS:CD2	19:L:404:HOH:O	2.70	0.45
8:H:1:THR:CG2	8:H:3:ILE:HG23	2.47	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.98	0.45
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.82	0.44
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.98	0.44
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.99	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.99	0.44
3:C:201:VAL:O	3:C:202:GLN:HB2	2.16	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.44
5:S:12:PHE:H	6:T:19:GLN:HE22	1.66	0.44
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.44
14:N:49:ALA:O	14:N:53:GLN:HB2	2.18	0.44
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.53	0.44
10:J:1:MET:O	10:J:2:ASP:CB	2.59	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.53	0.43
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.43
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.33	0.43
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.00	0.43
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.19	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.42
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.01	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.42
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.02	0.42
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.01	0.42
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.42
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.41
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.41
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.03	0.41
5:S:9:THR:HG21	5:S:119:THR:HA	2.02	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
13:M:220:ASP:O	13:M:223:LYS:HG2	2.21	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.56	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.50	0.41
1:A:149:GLN:O	1:A:156:TYR:HA	2.21	0.41
10:J:1:MET:HA	10:J:34:LYS:CE	2.51	0.40
5:E:12:PHE:H	6:F:19:GLN:HE22	1.69	0.40
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	24	58
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	24	58
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	24	58
3	Q	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	15	44
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	34	69
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	34	69
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	228/246 (93%)	221 (97%)	7 (3%)	0	100	100
13	a	230/246 (94%)	223 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	c	2/5 (40%)	2 (100%)	0	0	100	100
15	d	2/5 (40%)	2 (100%)	0	0	100	100
15	e	2/5 (40%)	2 (100%)	0	0	100	100
15	f	2/5 (40%)	2 (100%)	0	0	100	100
15	g	2/5 (40%)	2 (100%)	0	0	100	100
15	h	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6285/6644 (95%)	6130 (98%)	144 (2%)	11 (0%)	52	84

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP
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%)	206 (99%)	3 (1%)	74	94
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	94
2	B	203/216 (94%)	195 (96%)	8 (4%)	39	74
2	P	203/216 (94%)	195 (96%)	8 (4%)	39	74
3	C	212/226 (94%)	204 (96%)	8 (4%)	40	74
3	Q	212/226 (94%)	204 (96%)	8 (4%)	40	74
4	D	194/215 (90%)	186 (96%)	8 (4%)	37	72
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	72
5	E	190/193 (98%)	181 (95%)	9 (5%)	32	67
5	S	190/193 (98%)	181 (95%)	9 (5%)	32	67
6	F	201/239 (84%)	190 (94%)	11 (6%)	27	59
6	T	201/239 (84%)	190 (94%)	11 (6%)	27	59
7	G	206/210 (98%)	199 (97%)	7 (3%)	44	78
7	U	206/210 (98%)	198 (96%)	8 (4%)	39	74
8	H	181/190 (95%)	174 (96%)	7 (4%)	39	74
8	V	181/190 (95%)	173 (96%)	8 (4%)	35	69
9	I	172/173 (99%)	168 (98%)	4 (2%)	58	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	168 (98%)	4 (2%)	58	88
10	J	173/175 (99%)	167 (96%)	6 (4%)	43	77
10	X	173/175 (99%)	167 (96%)	6 (4%)	43	77
11	K	169/169 (100%)	164 (97%)	5 (3%)	48	82
11	Y	169/169 (100%)	164 (97%)	5 (3%)	48	82
12	L	186/185 (100%)	179 (96%)	7 (4%)	40	74
12	Z	185/185 (100%)	179 (97%)	6 (3%)	46	80
13	M	196/208 (94%)	189 (96%)	7 (4%)	42	76
13	a	198/208 (95%)	192 (97%)	6 (3%)	48	82
14	N	162/162 (100%)	159 (98%)	3 (2%)	65	91
14	b	162/162 (100%)	160 (99%)	2 (1%)	78	95
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
All	All	5315/5546 (96%)	5130 (96%)	185 (4%)	43	77

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	61	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	40	LEU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	43	CYS
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	182	TRP
9	I	192	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	35	ARG
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	53	GLN
14	N	119	VAL
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	40	LEU
4	R	99	ILE
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	59	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	154	TYR
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	20	SER
8	V	22	GLN
8	V	30	ASN
8	V	43	CYS
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	182	TRP
9	W	192	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	a	187	ARG
14	b	9	LYS
14	b	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
8	H	22	GLN
8	H	57	GLN
10	J	55	GLN
11	K	85	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
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	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
8	V	22	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	35	HIS
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	95	HIS
12	Z	158	ASN
13	a	18	ASN
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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	MES	d	101	-	12,12,12	2.15	1 (8%)	15,16,16	1.51	3 (20%)
18	MES	g	101	-	12,12,12	2.15	1 (8%)	15,16,16	1.62	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	d	101	-	-	0/6/14/14	0/1/1/1
18	MES	g	101	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	d	101	MES	C8-S	-7.18	1.66	1.77
18	g	101	MES	C8-S	-7.16	1.66	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	d	101	MES	O1S-S-C8	2.15	108.39	106.87
18	g	101	MES	O3S-S-C8	2.46	110.11	104.99
18	d	101	MES	O3S-S-C8	2.56	110.31	104.99
18	d	101	MES	O2S-S-C8	3.76	109.52	106.87
18	g	101	MES	O2S-S-C8	4.72	110.20	106.87

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 ⓘ

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%)	-0.41	5 (2%) 68 58	39, 53, 91, 132	0
1	O	250/250 (100%)	-0.33	6 (2%) 62 50	43, 61, 105, 135	0
2	B	244/258 (94%)	-0.28	11 (4%) 37 26	39, 58, 110, 168	0
2	P	244/258 (94%)	-0.19	11 (4%) 37 26	44, 62, 113, 169	0
3	C	240/254 (94%)	-0.19	13 (5%) 29 19	38, 62, 127, 163	0
3	Q	240/254 (94%)	0.09	16 (6%) 21 12	49, 79, 162, 213	0
4	D	235/260 (90%)	-0.35	3 (1%) 79 71	43, 65, 98, 147	0
4	R	235/260 (90%)	-0.25	4 (1%) 73 63	52, 70, 107, 155	0
5	E	231/234 (98%)	-0.26	2 (0%) 85 79	47, 67, 102, 145	0
5	S	231/234 (98%)	-0.17	4 (1%) 73 63	48, 75, 119, 157	0
6	F	243/288 (84%)	-0.39	5 (2%) 67 56	41, 61, 111, 142	0
6	T	243/288 (84%)	-0.20	4 (1%) 74 66	39, 73, 128, 166	0
7	G	241/252 (95%)	-0.42	4 (1%) 73 63	39, 55, 98, 150	0
7	U	241/252 (95%)	-0.42	3 (1%) 81 73	42, 58, 92, 140	0
8	H	222/232 (95%)	-0.33	2 (0%) 85 79	39, 53, 83, 127	0
8	V	222/232 (95%)	-0.34	3 (1%) 78 69	42, 56, 83, 138	0
9	I	204/205 (99%)	-0.64	3 (1%) 76 68	35, 48, 80, 99	0
9	W	204/205 (99%)	-0.58	3 (1%) 76 68	36, 51, 81, 105	0
10	J	195/198 (98%)	-0.59	2 (1%) 84 77	36, 49, 74, 122	0
10	X	195/198 (98%)	-0.57	3 (1%) 76 68	37, 51, 78, 129	0
11	K	212/212 (100%)	-0.60	1 (0%) 91 88	36, 49, 75, 97	0
11	Y	212/212 (100%)	-0.56	1 (0%) 91 88	37, 50, 78, 103	0
12	L	222/222 (100%)	-0.55	0 100 100	36, 53, 81, 107	0
12	Z	222/222 (100%)	-0.49	0 100 100	37, 52, 83, 110	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	230/246 (93%)	-0.52	5 (2%) 65 54	32, 52, 76, 101	0
13	a	232/246 (94%)	-0.54	2 (0%) 85 79	34, 51, 77, 101	0
14	N	196/196 (100%)	-0.59	0 100 100	36, 48, 78, 105	0
14	b	196/196 (100%)	-0.54	1 (0%) 91 88	36, 49, 80, 101	0
15	c	2/5 (40%)	-1.03	0 100 100	56, 56, 56, 63	0
15	d	2/5 (40%)	-1.29	0 100 100	43, 43, 43, 50	0
15	e	2/5 (40%)	-0.88	0 100 100	42, 42, 42, 52	0
15	f	2/5 (40%)	0.04	0 100 100	60, 60, 60, 70	0
15	g	2/5 (40%)	-0.89	0 100 100	42, 42, 42, 53	0
15	h	2/5 (40%)	-1.03	0 100 100	42, 42, 42, 57	0
All	All	6344/6644 (95%)	-0.39	117 (1%) 71 61	32, 57, 105, 213	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	8.0
3	Q	49	THR	7.1
2	P	219	ALA	7.0
8	V	222	ASP	6.8
3	C	206	LYS	6.2
8	H	221	CYS	6.0
2	P	220	ASN	5.5
1	A	1	MET	5.4
2	P	222	GLY	5.4
8	H	222	ASP	5.2
5	S	202	ASP	5.1
8	V	221	CYS	5.0
3	Q	50	LEU	5.0
2	P	51	VAL	4.9
3	Q	48	SER	4.8
3	Q	206	LYS	4.8
10	X	1	MET	4.7
2	P	221	ASP	4.6
1	O	1	MET	4.4
11	Y	212	GLY	4.4
2	B	219	ALA	4.1
2	B	221	ASP	4.1
4	D	242	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	1	THR	3.9
3	Q	240	GLU	3.9
3	Q	239	GLN	3.8
1	O	249	ALA	3.7
10	J	1	MET	3.6
3	C	49	THR	3.6
10	J	194	ASP	3.6
4	D	241	ALA	3.6
11	K	212	GLY	3.4
2	P	59	ASP	3.3
9	I	1	SER	3.3
5	E	202	ASP	3.3
7	U	222	ASP	3.3
3	Q	236	GLN	3.3
9	W	1	SER	3.2
3	C	239	GLN	3.2
5	E	233	ILE	3.1
2	B	51	VAL	3.1
6	T	244	ASN	3.1
1	O	52	SER	3.0
3	Q	238	LYS	3.0
9	I	133	LYS	3.0
2	P	203	SER	3.0
3	C	225	GLU	2.9
13	a	1	THR	2.9
1	A	249	ALA	2.9
3	C	236	GLN	2.9
7	G	3	TYR	2.9
4	R	242	GLU	2.9
10	X	194	ASP	2.9
4	R	241	ALA	2.8
9	I	131	GLU	2.8
3	C	238	LYS	2.8
3	Q	225	GLU	2.8
3	C	202	GLN	2.8
13	M	227	GLY	2.7
3	C	235	GLU	2.7
13	M	230	THR	2.7
10	X	193	ASP	2.6
2	B	218	GLY	2.6
2	B	182	ASP	2.6
5	S	180	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	W	133	LYS	2.5
3	Q	55	THR	2.5
7	G	179	LYS	2.5
2	B	222	GLY	2.5
2	P	232	GLN	2.5
5	S	233	ILE	2.5
6	F	244	ASN	2.5
7	G	222	ASP	2.5
4	R	125	LEU	2.5
9	W	131	GLU	2.4
3	C	205	ALA	2.4
1	O	229	THR	2.4
1	A	250	LEU	2.4
1	A	248	GLU	2.4
2	P	218	GLY	2.4
6	T	181	GLU	2.4
13	M	47	ASP	2.4
3	C	240	GLU	2.3
6	F	202	ASP	2.3
3	Q	202	GLN	2.3
6	T	215	CYS	2.3
3	C	187	GLU	2.3
6	F	229	GLY	2.3
1	O	201	GLU	2.3
7	U	241	GLU	2.3
2	P	182	ASP	2.2
7	U	2	GLY	2.2
6	T	205	GLU	2.2
2	P	225	TYR	2.2
3	Q	60	SER	2.2
1	A	229	THR	2.2
13	M	228	TYR	2.2
8	V	145	ASP	2.1
4	R	226	GLU	2.1
7	G	208	GLU	2.1
3	Q	141	ASP	2.1
2	B	50	LYS	2.1
3	C	181	GLU	2.1
2	B	217	LYS	2.1
3	C	50	LEU	2.1
3	Q	180	LYS	2.1
13	a	232	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	248	GLU	2.1
4	D	125	LEU	2.1
5	S	3	ASN	2.1
3	Q	223	SER	2.1
6	F	205	GLU	2.1
2	B	242	GLY	2.1
6	F	243	ILE	2.0
3	Q	51	LYS	2.0
2	B	203	SER	2.0
14	b	105	LYS	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
16	MG	Z	301	1/1	0.99	0.31	5.01	59,59,59,59	0
18	MES	d	101	12/12	0.92	0.21	3.00	51,76,84,86	0
18	MES	g	101	12/12	0.94	0.21	2.81	51,74,82,83	0
16	MG	I	301	1/1	0.97	0.18	2.12	61,61,61,61	0
16	MG	N	201	1/1	0.94	0.13	0.07	50,50,50,50	0
16	MG	K	301	1/1	0.98	0.07	-1.26	51,51,51,51	0
16	MG	G	301	1/1	0.94	0.07	-1.39	47,47,47,47	0
16	MG	I	302	1/1	0.99	0.05	-1.73	43,43,43,43	0
16	MG	L	301	1/1	0.99	0.06	-3.01	51,51,51,51	0
17	CL	U	301	1/1	0.98	0.22	-	30,30,30,30	0
17	CL	G	302	1/1	0.97	0.23	-	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.