



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 10:21 AM UTC

PDB ID : 5LEX / pdb_00005lex
Title : Native human 20S proteasome in Mg-Acetate at 2.2 Angstrom
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on : 2016-06-30
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

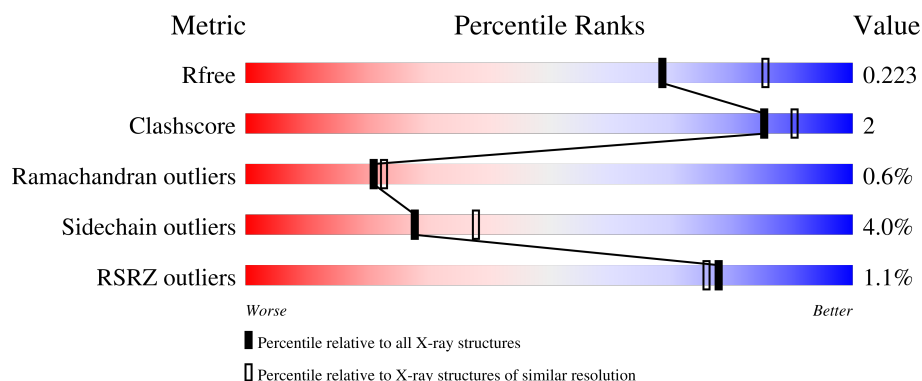
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	234	87% 9% ..
1	O	234	3% 88% 8% ..
2	B	261	% 89% 6% 5%
2	P	261	2% 85% 8% .. 5%
3	C	248	% 84% 10% ..

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Mol	Chain	Length	Quality of chain
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	205	
14	b	205	

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
7	6V1	U	47	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 51579 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	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1922	1217	331	363	11			
2	P	247	Total	C	N	O	S	0	2	0
			1898	1200	321	366	11			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	2	0
			1797	1120	320	352	5			
3	Q	234	Total	C	N	O	S	0	0	0
			1796	1123	315	353	5			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	1	0
			1822	1144	325	342	11			
5	S	236	Total	C	N	O	S	0	3	0
			1853	1160	335	347	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	148	6V1	CYS	conflict	UNP P25786
S	148	6V1	CYS	conflict	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	239	Total	C	N	O	S	0	4	0
			1888	1198	325	353	12			
6	T	240	Total	C	N	O	S	0	1	0
			1856	1178	315	351	12			

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	2	0
			1912	1214	321	364	13			
7	U	238	Total	C	N	O	S	0	1	0
			1815	1147	304	350	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	47	6V1	CYS	conflict	UNP P60900
G	161	6V1	CYS	conflict	UNP P60900
U	47	6V1	CYS	conflict	UNP P60900
U	161	6V1	CYS	conflict	UNP P60900

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	2	0
			1664	1047	284	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1622	1023	269	318	12			

- 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	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			
10	X	196	Total	C	N	O	S	0	2	0
			1576	1012	267	287	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	91	6V1	CYS	conflict	UNP P49721
X	91	6V1	CYS	conflict	UNP P49721

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	0	0
			1551	977	272	293	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1570	991	278	291	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1636	1038	277	310	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1642	1041	280	310	11			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- Molecule 15 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	K	0	0
			1	1		
15	L	1	Total	K	0	0
			1	1		
15	N	1	Total	K	0	0
			1	1		
15	U	1	Total	K	0	0
			1	1		
15	Z	1	Total	K	0	0
			1	1		
15	b	1	Total	K	0	0
			1	1		

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

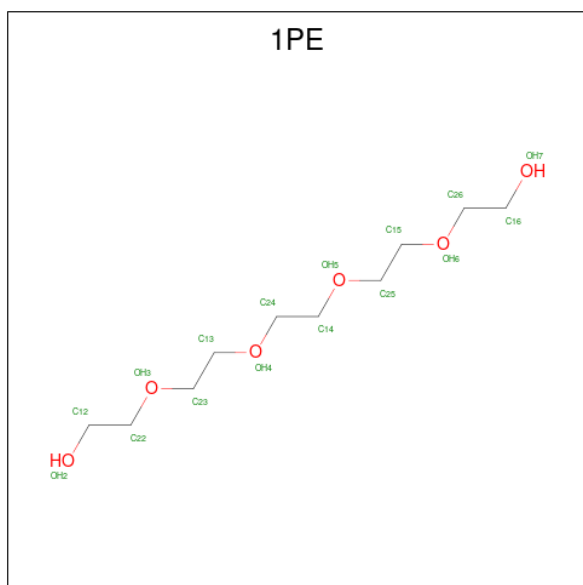
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	1	Total	Mg	0	0
			1	1		
16	I	2	Total	Mg	0	0
			2	2		
16	J	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	L	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	W	1	Total	Mg	0	0
			1	1		
16	X	1	Total	Mg	0	0
			1	1		

- Molecule 17 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	H	1	Total	C	O	0	0
			16	10	6		
17	I	1	Total	C	O	0	0
			16	10	6		
17	K	1	Total	C	O	0	0
			16	10	6		
17	L	1	Total	C	O	0	0
			16	10	6		
17	N	1	Total	C	O	0	0
			16	10	6		
17	W	1	Total	C	O	0	0
			16	10	6		
17	Z	1	Total	C	O	0	0
			16	10	6		
17	a	1	Total	C	O	0	0
			16	10	6		
17	b	1	Total	C	O	0	0
			16	10	6		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	106	Total O 106 106	0	0
18	B	126	Total O 126 126	0	0
18	C	59	Total O 59 59	0	0
18	D	80	Total O 80 80	0	0
18	E	128	Total O 128 128	0	0
18	F	175	Total O 175 175	0	0
18	G	165	Total O 165 165	0	0
18	H	151	Total O 151 151	0	0
18	I	145	Total O 145 145	0	0
18	J	122	Total O 122 122	0	0
18	K	96	Total O 96 96	0	0
18	L	115	Total O 115 115	0	0
18	M	143	Total O 143 143	0	0
18	N	160	Total O 160 160	0	0
18	O	78	Total O 78 78	0	0
18	P	104	Total O 104 104	0	0
18	Q	62	Total O 62 62	0	0
18	R	112	Total O 112 112	0	0
18	S	114	Total O 114 114	0	0
18	T	83	Total O 83 83	0	0
18	U	90	Total O 90 90	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	V	102	Total 102	O 102	0	0
18	W	101	Total 101	O 101	0	0
18	X	110	Total 110	O 110	0	0
18	Y	140	Total 140	O 140	0	0
18	Z	169	Total 169	O 169	0	0
18	a	173	Total 173	O 173	0	0
18	b	122	Total 122	O 122	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: 



- Molecule 1: Proteasome subunit alpha type-2

Chain O: 



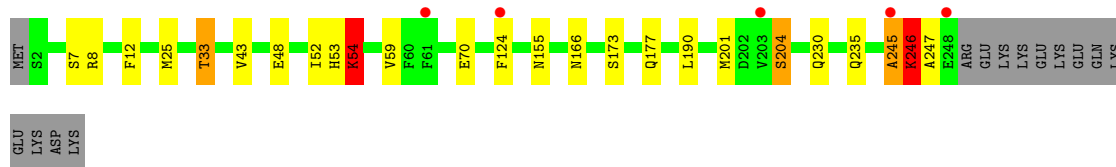
- Molecule 2: Proteasome subunit alpha type-4

Chain B: 



- Molecule 2: Proteasome subunit alpha type-4

Chain P: 

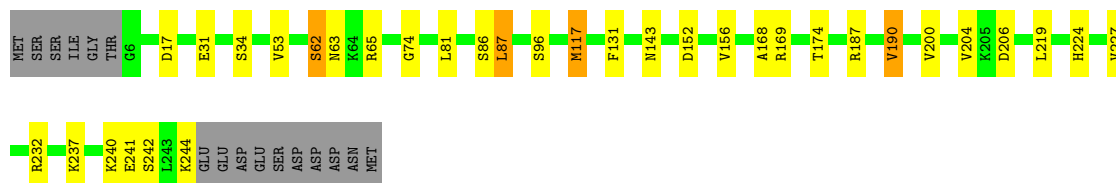


- Molecule 3: Proteasome subunit alpha type-7

Chain C: 

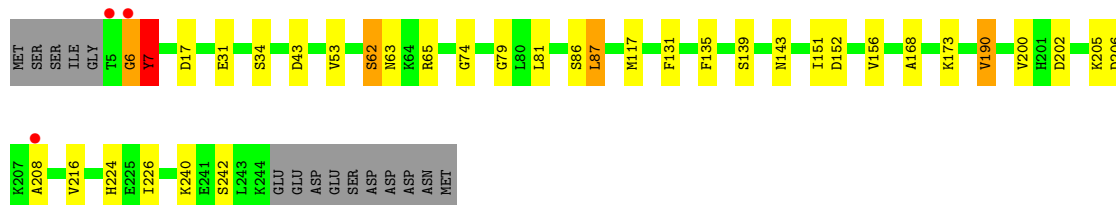


Chain F:  80% 12% • 6%



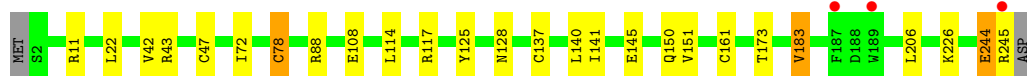
• Molecule 6: Proteasome subunit alpha type-3

Chain T:  80% 12% • 6%



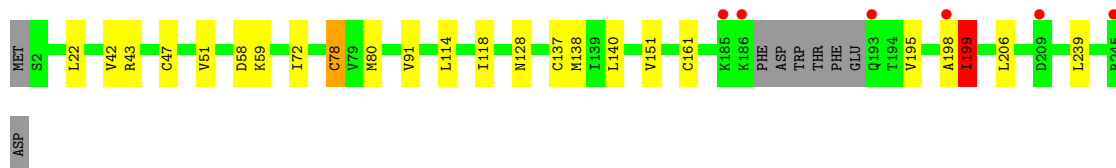
• Molecule 7: Proteasome subunit alpha type-6

Chain G:  89% 9% ••



• Molecule 7: Proteasome subunit alpha type-6

Chain U:  87% 9% •



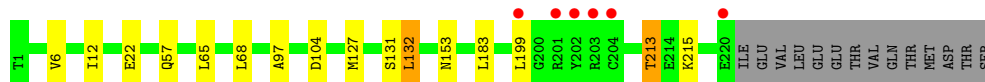
• Molecule 8: Proteasome subunit beta type-7

Chain H:  86% 7% • 6%



• Molecule 8: Proteasome subunit beta type-7

Chain V:  87% 6% • 3%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  91% 7%



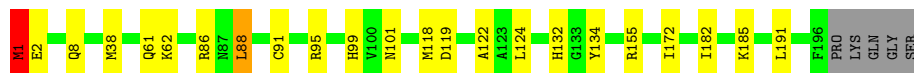
- Molecule 9: Proteasome subunit beta type-3

Chain W:  92% 7%



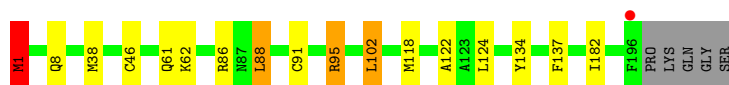
- Molecule 10: Proteasome subunit beta type-2

Chain J:  86% 10%



- Molecule 10: Proteasome subunit beta type-2

Chain X:  89% 6%



- Molecule 11: Proteasome subunit beta type-5

Chain K:  88% 9%



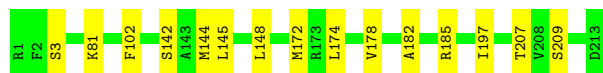
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  91% 5%

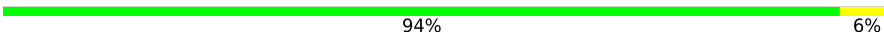


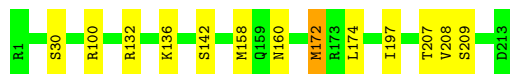
- Molecule 12: Proteasome subunit beta type-1

Chain L:  93% 7%

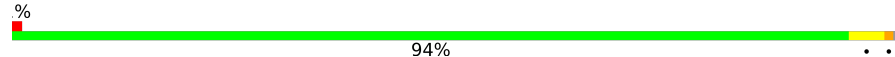


- Molecule 12: Proteasome subunit beta type-1

Chain Z:  94% 6%



- Molecule 13: Proteasome subunit beta type-4

Chain M:  94% . .

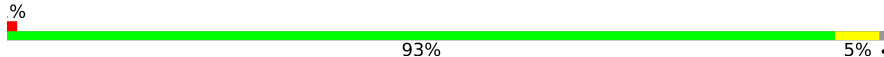


- Molecule 13: Proteasome subunit beta type-4

Chain a:  90% 8% ..

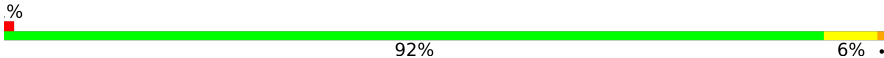


- Molecule 14: Proteasome subunit beta type-6

Chain N:  93% 5% .



- Molecule 14: Proteasome subunit beta type-6

Chain b:  92% 6% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.86Å 203.15Å 316.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.89 – 2.20 170.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (170.89-2.20) 98.8 (170.89-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.177 , 0.221 0.181 , 0.223	Depositor DCC
R_{free} test set	18235 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.3	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	0.97	EDS
Total number of atoms	51579	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: 6V1, YCM, MG, K, 1PE

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	0.97	0/1833	1.01	1/2489 (0.0%)
1	O	0.86	0/1778	0.98	0/2419
2	B	0.99	1/1958 (0.1%)	1.05	2/2645 (0.1%)
2	P	0.92	0/1934	1.03	1/2617 (0.0%)
3	C	1.03	0/1817	1.12	5/2467 (0.2%)
3	Q	1.03	0/1809	1.09	6/2455 (0.2%)
4	D	1.01	1/1789 (0.1%)	1.05	1/2424 (0.0%)
4	R	1.14	2/1780 (0.1%)	1.11	4/2408 (0.2%)
5	E	1.07	0/1842	1.04	1/2493 (0.0%)
5	S	1.06	3/1878 (0.2%)	1.08	3/2541 (0.1%)
6	F	1.10	1/1935 (0.1%)	1.10	5/2605 (0.2%)
6	T	1.07	2/1894 (0.1%)	1.15	11/2556 (0.4%)
7	G	1.10	3/1909 (0.2%)	1.09	3/2579 (0.1%)
7	U	0.99	1/1804 (0.1%)	1.02	1/2441 (0.0%)
8	H	1.18	2/1697 (0.1%)	1.09	3/2299 (0.1%)
8	V	0.96	0/1655	1.00	0/2251
9	I	1.07	0/1648	1.16	7/2219 (0.3%)
9	W	0.85	0/1630	1.02	5/2197 (0.2%)
10	J	1.07	1/1613 (0.1%)	0.99	0/2180
10	X	0.95	0/1599	0.96	0/2163
11	K	0.95	1/1582 (0.1%)	1.05	1/2138 (0.0%)
11	Y	1.11	0/1610	1.04	1/2172 (0.0%)
12	L	0.98	1/1672 (0.1%)	0.98	0/2257
12	Z	1.18	3/1675 (0.2%)	1.03	2/2257 (0.1%)
13	M	1.09	0/1728	1.07	4/2339 (0.2%)
13	a	1.23	1/1724 (0.1%)	1.10	4/2336 (0.2%)
14	N	1.22	2/1548 (0.1%)	1.10	3/2095 (0.1%)
14	b	1.11	2/1554 (0.1%)	1.08	2/2104 (0.1%)
All	All	1.05	27/48895 (0.1%)	1.06	76/66146 (0.1%)

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
2	P	0	2
3	Q	0	2
4	D	0	2
4	R	0	1
5	E	0	1
6	F	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
13	a	0	1
All	All	1	16

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	7	TYR	N-CA	6.65	1.58	1.46
2	B	151	ASP	CA-C	6.21	1.58	1.52
12	L	102	PHE	N-CA	6.03	1.52	1.46
4	D	128	ALA	N-CA	5.99	1.52	1.46
7	G	108	GLU	CD-OE1	5.92	1.36	1.25

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	16[A]	LYS	CA-C-N	9.58	135.96	122.36
9	I	16[A]	LYS	C-N-CA	9.58	135.96	122.36
9	I	16[B]	LYS	CA-C-N	9.58	135.96	122.36
9	I	16[B]	LYS	C-N-CA	9.58	135.96	122.36
6	F	190	VAL	CB-CA-C	-9.37	99.77	112.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
5	E	235	GLY	Peptide
6	F	206	ASP	Peptide
9	I	78	GLY	Peptide

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	1788	0	1761	9	0
1	O	1741	0	1683	9	0
2	B	1922	0	1913	4	0
2	P	1898	0	1861	11	0
3	C	1797	0	1714	12	0
3	Q	1796	0	1733	7	0
4	D	1762	0	1709	3	0
4	R	1753	0	1726	5	0
5	E	1822	0	1779	11	0
5	S	1853	0	1796	14	0
6	F	1888	0	1882	13	0
6	T	1856	0	1816	15	0
7	G	1912	0	1882	8	0
7	U	1815	0	1748	13	0
8	H	1664	0	1681	7	0
8	V	1622	0	1595	6	0
9	I	1613	0	1646	9	0
9	W	1599	0	1621	7	0
10	J	1590	0	1581	12	0
10	X	1576	0	1561	10	0
11	K	1551	0	1509	7	0
11	Y	1570	0	1550	6	0
12	L	1636	0	1625	7	0
12	Z	1642	0	1635	4	0
13	M	1692	0	1670	5	0
13	a	1688	0	1658	9	0
14	N	1519	0	1496	10	0
14	b	1524	0	1496	9	0
15	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	U	1	0	0	0	0
15	Z	1	0	0	0	0
15	b	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	1	0	0	0	0
16	L	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	X	1	0	0	0	0
17	H	16	0	22	0	0
17	I	16	0	22	0	0
17	K	16	0	22	0	0
17	L	16	0	22	0	0
17	N	16	0	22	0	0
17	W	16	0	22	0	0
17	Z	16	0	22	0	0
17	a	16	0	22	0	0
17	b	16	0	22	0	0
18	A	106	0	0	0	0
18	B	126	0	0	0	0
18	C	59	0	0	0	0
18	D	80	0	0	0	0
18	E	128	0	0	2	0
18	F	175	0	0	4	0
18	G	165	0	0	3	0
18	H	151	0	0	2	0
18	I	145	0	0	1	0
18	J	122	0	0	2	0
18	K	96	0	0	0	0
18	L	115	0	0	0	0
18	M	143	0	0	0	0
18	N	160	0	0	0	0
18	O	78	0	0	1	0
18	P	104	0	0	1	0
18	Q	62	0	0	0	0
18	R	112	0	0	0	0
18	S	114	0	0	6	0
18	T	83	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	U	90	0	0	0	0
18	V	102	0	0	2	0
18	W	101	0	0	0	0
18	X	110	0	0	0	0
18	Y	140	0	0	0	0
18	Z	169	0	0	1	0
18	a	173	0	0	0	0
18	b	122	0	0	0	0
All	All	51579	0	47525	214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 214 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)
11:K:9:ARG:NH2	11:K:146:ASP:OD1	1.96	0.98
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.35	0.90
5:S:204:ASP:OD1	18:S:301:HOH:O	1.91	0.86
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.57	0.85
10:X:1:MET:HE1	10:X:134:TYR:H	1.41	0.83

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	231/234 (99%)	222 (96%)	5 (2%)	4 (2%)	7 5
1	O	228/234 (97%)	217 (95%)	6 (3%)	5 (2%)	5 3
2	B	248/261 (95%)	240 (97%)	7 (3%)	1 (0%)	30 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	247/261 (95%)	234 (95%)	8 (3%)	5 (2%)	6	4
3	C	236/248 (95%)	224 (95%)	7 (3%)	5 (2%)	5	3
3	Q	229/248 (92%)	217 (95%)	8 (4%)	4 (2%)	7	5
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	9	8
4	R	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	7	5
5	E	232/263 (88%)	225 (97%)	6 (3%)	1 (0%)	30	34
5	S	236/263 (90%)	229 (97%)	5 (2%)	2 (1%)	16	16
6	F	241/255 (94%)	232 (96%)	8 (3%)	1 (0%)	30	34
6	T	239/255 (94%)	227 (95%)	9 (4%)	3 (1%)	9	8
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
8	H	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
8	V	220/234 (94%)	214 (97%)	6 (3%)	0	100	100
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	3 (2%)	2 (1%)	12	11
10	J	195/201 (97%)	191 (98%)	4 (2%)	0	100	100
10	X	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
11	K	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
11	Y	200/204 (98%)	197 (98%)	3 (2%)	0	100	100
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
13	a	216/219 (99%)	207 (96%)	9 (4%)	0	100	100
14	N	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
14	b	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	6200/6458 (96%)	6021 (97%)	139 (2%)	40 (1%)	21	23

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	53	SER
3	C	47	LYS

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Mol	Chain	Res	Type
5	E	59	HIS
1	O	50	LYS

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	185/191 (97%)	173 (94%)	12 (6%)	15	18
1	O	176/191 (92%)	165 (94%)	11 (6%)	16	19
2	B	199/221 (90%)	191 (96%)	8 (4%)	28	38
2	P	196/221 (89%)	182 (93%)	14 (7%)	13	16
3	C	179/210 (85%)	169 (94%)	10 (6%)	19	24
3	Q	183/210 (87%)	170 (93%)	13 (7%)	13	16
4	D	189/203 (93%)	184 (97%)	5 (3%)	40	55
4	R	187/203 (92%)	184 (98%)	3 (2%)	55	71
5	E	192/223 (86%)	183 (95%)	9 (5%)	23	31
5	S	195/223 (87%)	188 (96%)	7 (4%)	31	42
6	F	199/212 (94%)	187 (94%)	12 (6%)	17	21
6	T	192/212 (91%)	183 (95%)	9 (5%)	23	31
7	G	202/207 (98%)	192 (95%)	10 (5%)	22	28
7	U	186/207 (90%)	180 (97%)	6 (3%)	34	47
8	H	181/195 (93%)	171 (94%)	10 (6%)	19	24
8	V	172/195 (88%)	160 (93%)	12 (7%)	14	16
9	I	176/174 (101%)	173 (98%)	3 (2%)	53	69
9	W	173/174 (99%)	171 (99%)	2 (1%)	63	78
10	J	166/170 (98%)	158 (95%)	8 (5%)	23	30
10	X	165/170 (97%)	159 (96%)	6 (4%)	31	42
11	K	155/159 (98%)	146 (94%)	9 (6%)	18	22
11	Y	158/159 (99%)	154 (98%)	4 (2%)	42	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	175/178 (98%)	168 (96%)	7 (4%)	28	38
12	Z	175/178 (98%)	170 (97%)	5 (3%)	37	51
13	M	180/181 (99%)	177 (98%)	3 (2%)	53	69
13	a	178/181 (98%)	174 (98%)	4 (2%)	45	61
14	N	158/159 (99%)	157 (99%)	1 (1%)	78	89
14	b	158/159 (99%)	155 (98%)	3 (2%)	50	66
All	All	5030/5366 (94%)	4824 (96%)	206 (4%)	28	37

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	206	ASN
3	Q	225	ILE
13	a	92	LEU
2	P	7[B]	SER
2	P	235	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	86	ASN
10	X	174	ASN
6	T	68	ASN
9	W	32	GLN
12	Z	157	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	6V1	X	91	10	13,15,16	1.72	3 (23%)	10,20,22	4.22	7 (70%)
7	YCM	G	137	7	7,9,10	1.18	0	5,10,12	2.23	2 (40%)
7	6V1	G	161	7	13,15,16	1.57	2 (15%)	10,20,22	3.19	6 (60%)
5	6V1	S	148	5	13,15,16	2.22	4 (30%)	10,20,22	3.16	5 (50%)
7	6V1	U	47	7	13,15,16	1.58	4 (30%)	10,20,22	1.49	3 (30%)
10	6V1	J	91	10	13,15,16	1.85	3 (23%)	10,20,22	4.21	7 (70%)
7	6V1	G	47	7	13,15,16	1.85	3 (23%)	10,20,22	1.91	2 (20%)
3	YCM	C	63	3	7,9,10	0.98	0	5,10,12	1.43	1 (20%)
7	YCM	U	137	7	7,9,10	0.92	0	5,10,12	1.97	2 (40%)
3	YCM	Q	63	3	7,9,10	0.82	0	5,10,12	2.19	3 (60%)
7	6V1	U	161	7	13,15,16	2.32	4 (30%)	10,20,22	3.16	5 (50%)
5	6V1	E	148	5	13,15,16	1.87	3 (23%)	10,20,22	2.58	4 (40%)

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
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
7	YCM	G	137	7	-	2/6/8/10	-
7	6V1	G	161	7	-	3/6/25/27	0/1/1/1
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	0/6/25/27	0/1/1/1
10	6V1	J	91	10	-	2/6/25/27	0/1/1/1
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
3	YCM	C	63	3	-	1/6/8/10	-
7	YCM	U	137	7	-	2/6/8/10	-
3	YCM	Q	63	3	-	3/6/8/10	-
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1
5	6V1	E	148	5	-	1/6/25/27	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	148	6V1	CB-SG	-5.94	1.76	1.82
7	U	161	6V1	CB-SG	-5.19	1.76	1.82
10	J	91	6V1	C1-SG	-5.04	1.77	1.83
5	E	148	6V1	CB-SG	-4.92	1.77	1.82
7	G	47	6V1	CB-SG	-4.82	1.77	1.82

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	91	6V1	C5-C4-N3	6.88	112.40	108.07
10	X	91	6V1	C6-N3-C2	6.53	131.02	123.37
10	X	91	6V1	C5-C4-N3	6.29	112.03	108.07
7	U	161	6V1	C5-C4-N3	6.14	111.94	108.07
10	J	91	6V1	C6-N3-C2	5.95	130.34	123.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-NZ2
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2
7	U	137	YCM	SG-CD-CE-NZ2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 15 are monoatomic - leaving 9 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	$\# Z > 2$
17	1PE	a	301	-	15,15,15	0.54	0	14,14,14	0.54	0
17	1PE	Z	301	-	15,15,15	0.64	0	14,14,14	0.46	0
17	1PE	H	302	-	15,15,15	0.64	0	14,14,14	0.73	0
17	1PE	I	302	-	15,15,15	0.71	0	14,14,14	0.85	0
17	1PE	N	301	-	15,15,15	0.58	0	14,14,14	0.54	0
17	1PE	L	301	-	15,15,15	0.65	0	14,14,14	0.43	0
17	1PE	K	302	-	15,15,15	0.79	0	14,14,14	0.78	0
17	1PE	b	301	-	15,15,15	0.73	0	14,14,14	0.76	0
17	1PE	W	302	-	15,15,15	0.75	0	14,14,14	0.44	0

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
17	1PE	a	301	-	-	5/13/13/13	-
17	1PE	Z	301	-	-	7/13/13/13	-
17	1PE	H	302	-	-	10/13/13/13	-
17	1PE	I	302	-	-	9/13/13/13	-
17	1PE	N	301	-	-	6/13/13/13	-
17	1PE	L	301	-	-	8/13/13/13	-
17	1PE	K	302	-	-	7/13/13/13	-
17	1PE	b	301	-	-	8/13/13/13	-
17	1PE	W	302	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	302	1PE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
17	L	301	1PE	OH5-C14-C24-OH4
17	W	302	1PE	OH6-C15-C25-OH5
17	b	301	1PE	OH6-C15-C25-OH5
17	K	302	1PE	OH6-C15-C25-OH5

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	230/234 (98%)	-0.23	1 (0%) 88 87	34, 64, 103, 119	3 (1%)
1	O	230/234 (98%)	0.08	6 (2%) 57 54	57, 83, 127, 149	0
2	B	248/261 (95%)	-0.09	3 (1%) 76 74	31, 71, 121, 170	2 (0%)
2	P	247/261 (94%)	0.03	5 (2%) 65 62	41, 82, 143, 180	2 (0%)
3	C	236/248 (95%)	0.26	3 (1%) 75 73	37, 84, 136, 178	2 (0%)
3	Q	233/248 (93%)	0.15	9 (3%) 43 40	48, 79, 144, 195	0
4	D	233/241 (96%)	0.15	3 (1%) 75 73	41, 80, 113, 148	1 (0%)
4	R	233/241 (96%)	-0.22	5 (2%) 63 60	24, 58, 91, 128	1 (0%)
5	E	233/263 (88%)	-0.21	5 (2%) 63 60	32, 59, 107, 130	1 (0%)
5	S	235/263 (89%)	-0.32	2 (0%) 81 79	28, 58, 92, 139	3 (1%)
6	F	239/255 (93%)	-0.31	0 100 100	30, 52, 79, 98	4 (1%)
6	T	240/255 (94%)	-0.06	3 (1%) 75 73	36, 66, 107, 139	1 (0%)
7	G	241/246 (97%)	-0.28	3 (1%) 76 74	30, 58, 106, 158	2 (0%)
7	U	235/246 (95%)	0.03	6 (2%) 57 54	38, 78, 116, 155	1 (0%)
8	H	220/234 (94%)	-0.50	0 100 100	27, 48, 81, 110	2 (0%)
8	V	220/234 (94%)	-0.11	6 (2%) 56 53	34, 65, 105, 130	2 (0%)
9	I	204/205 (99%)	-0.49	0 100 100	30, 50, 76, 97	3 (1%)
9	W	204/205 (99%)	-0.16	0 100 100	40, 68, 101, 115	2 (0%)
10	J	195/201 (97%)	-0.43	0 100 100	24, 56, 77, 96	3 (1%)
10	X	195/201 (97%)	-0.30	1 (0%) 87 85	27, 59, 80, 97	2 (1%)
11	K	200/204 (98%)	-0.21	2 (1%) 79 77	51, 64, 93, 107	0
11	Y	199/204 (97%)	-0.51	1 (0%) 87 85	26, 49, 73, 83	3 (1%)
12	L	213/213 (100%)	-0.15	0 100 100	32, 67, 95, 112	2 (0%)
12	Z	213/213 (100%)	-0.51	0 100 100	33, 48, 75, 96	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.42	2 (0%) 81 79	37, 52, 81, 124	1 (0%)
13	a	216/219 (98%)	-0.51	1 (0%) 87 85	31, 48, 75, 105	2 (0%)
14	N	202/205 (98%)	-0.56	2 (0%) 79 77	29, 45, 70, 120	1 (0%)
14	b	203/205 (99%)	-0.41	2 (0%) 79 77	39, 52, 82, 126	1 (0%)
All	All	6213/6458 (96%)	-0.21	71 (1%) 78 76	24, 62, 110, 195	48 (0%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	131	GLY	5.2
13	a	215	ILE	4.8
8	V	220	GLU	4.5
13	M	215	ILE	3.8
3	Q	50	VAL	3.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	6V1	U	47	15/16	0.84	0.13	97,136,140,141	0
5	6V1	E	148	15/16	0.88	0.12	47,66,73,74	0
3	YCM	C	63	10/11	0.90	0.11	74,78,93,96	0
7	YCM	G	137	10/11	0.90	0.13	48,54,74,76	0
7	6V1	U	161	15/16	0.90	0.10	70,91,97,99	0
7	6V1	G	47	15/16	0.91	0.14	55,85,90,94	0
5	6V1	S	148	15/16	0.92	0.12	45,73,78,79	0
7	YCM	U	137	10/11	0.93	0.12	65,76,92,93	0
3	YCM	Q	63	10/11	0.94	0.09	71,74,78,80	0
10	6V1	J	91	15/16	0.94	0.10	45,65,72,74	0
10	6V1	X	91	15/16	0.94	0.10	48,69,75,77	0
7	6V1	G	161	15/16	0.95	0.11	47,69,76,77	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	1PE	W	302	16/16	0.80	0.13	79,90,95,97	0
17	1PE	H	302	16/16	0.81	0.14	65,87,100,103	0
17	1PE	I	302	16/16	0.84	0.14	76,85,93,93	0
17	1PE	L	301	16/16	0.85	0.17	93,97,105,106	0
17	1PE	K	302	16/16	0.86	0.14	72,86,101,101	0
17	1PE	Z	301	16/16	0.88	0.13	64,87,93,98	0
17	1PE	a	301	16/16	0.88	0.14	75,87,106,107	0
15	K	U	301	1/1	0.90	0.17	64,64,64,64	0
17	1PE	b	301	16/16	0.90	0.12	58,68,96,96	0
15	K	Z	302	1/1	0.91	0.17	70,70,70,70	0
17	1PE	N	301	16/16	0.92	0.11	54,62,75,78	0
15	K	L	302	1/1	0.93	0.17	74,74,74,74	0
15	K	G	301	1/1	0.94	0.14	64,64,64,64	0
15	K	b	302	1/1	0.95	0.15	63,63,63,63	0
16	MG	W	301	1/1	0.97	0.12	52,52,52,52	0
15	K	N	302	1/1	0.97	0.13	58,58,58,58	0
16	MG	H	301	1/1	0.97	0.18	47,47,47,47	0
16	MG	I	303	1/1	0.97	0.09	45,45,45,45	0
16	MG	K	301	1/1	0.97	0.13	53,53,53,53	0
16	MG	I	301	1/1	0.98	0.07	46,46,46,46	0
16	MG	L	303	1/1	0.98	0.16	53,53,53,53	0
16	MG	V	301	1/1	0.99	0.04	63,63,63,63	0
16	MG	J	301	1/1	0.99	0.03	65,65,65,65	0
16	MG	X	301	1/1	0.99	0.04	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.