Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 06:16 am GMT

PDB ID	:	5LF6
Title	:	Human 20S proteasome complex with Z-LLY-ketoaldehyde at 2.1 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	:	2.07 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:

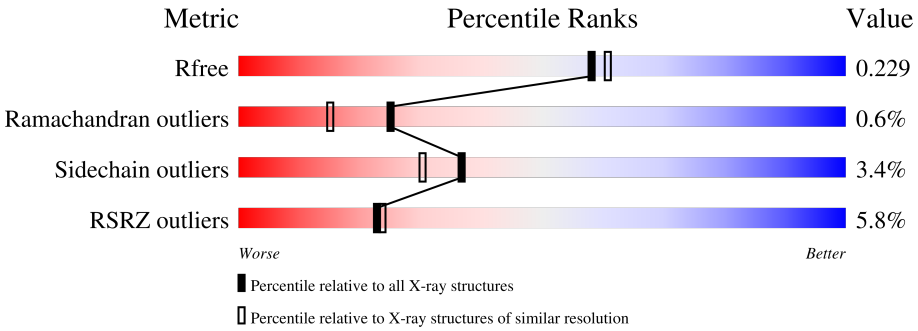
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 Å.

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



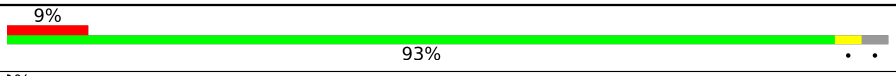
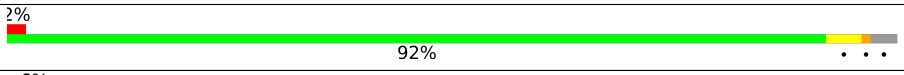
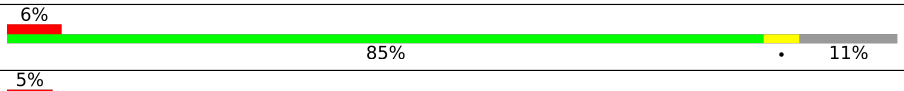
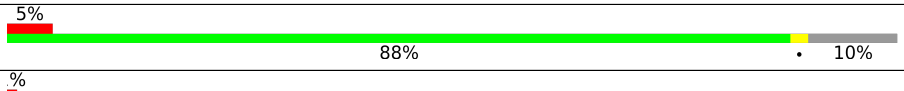
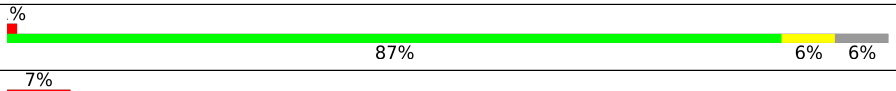
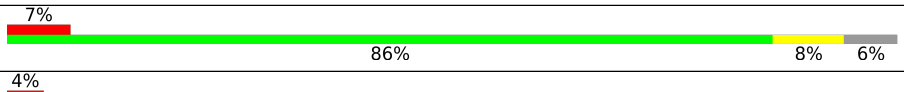
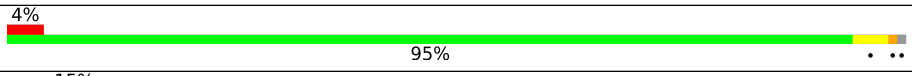
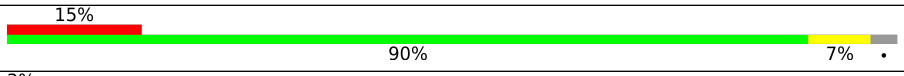
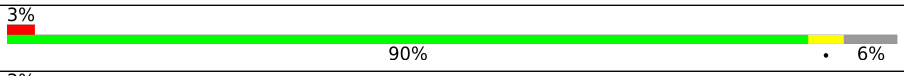
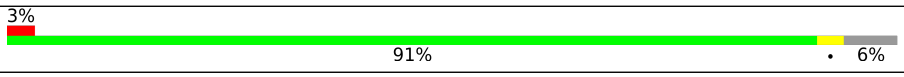
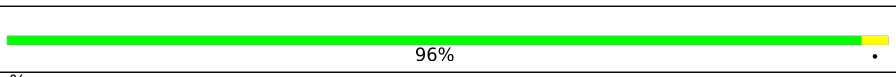
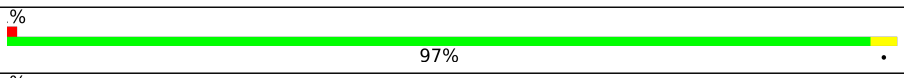
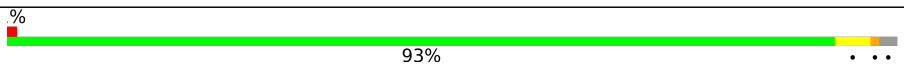
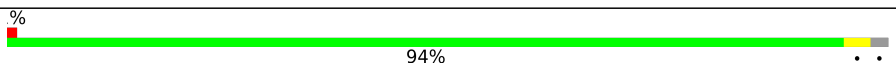
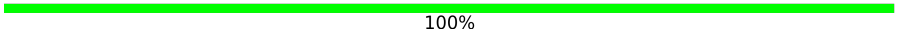
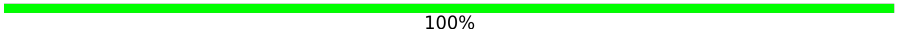
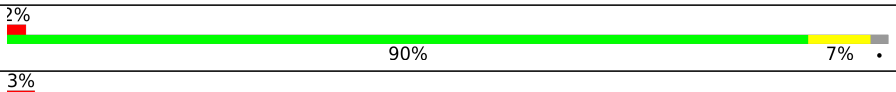
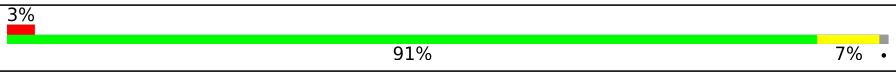
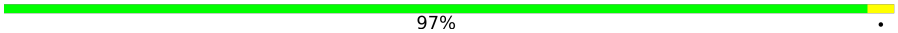
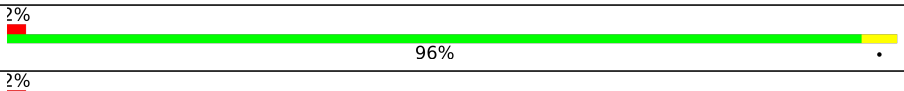
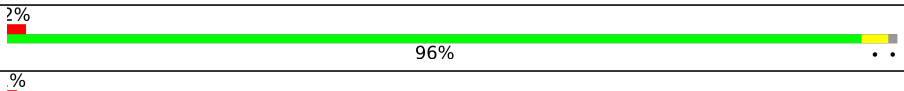
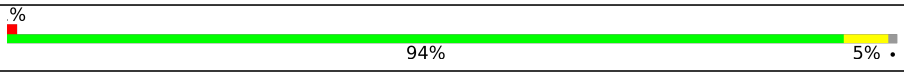
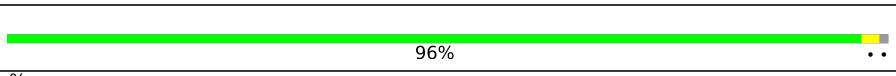
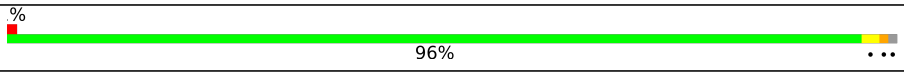
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	6% 91% 6% ·
1	O	234	18% 92% 6% ··
2	B	261	6% 91% · 5%
2	P	261	15% 87% 8% 5%
3	C	248	13% 89% 6% ·
3	Q	248	19% 89% 7% · ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	c	3	
11	d	3	
12	K	204	
12	Y	204	
13	L	213	
13	Z	213	
14	M	219	
14	a	219	
15	N	205	
15	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	6V1	U	47	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 51953 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
			1926	1220	332	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	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
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	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	238	Total	C	N	O	S	0	3	0
			1875	1175	340	349	11			

There are 2 discrepancies between the modelled and reference sequences:

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

- 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			

- Molecule 11 is a protein called LLY-ketoaldehyde peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	c	3	Total	C	N	O	0	0	0
			30	22	3	5			
11	d	3	Total	C	N	O	0	0	0
			30	22	3	5			

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	200	Total	C	N	O	S	0	1	0
			1550	978	269	293	10			
12	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

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

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
14	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 15 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	202	Total 1516	C 950	N 258	O 295	S 13	0	1	0
15	b	203	Total 1524	C 956	N 259	O 296	S 13	0	1	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	4	Total 4	Cl 4	0	0
16	B	2	Total 2	Cl 2	0	0
16	C	2	Total 2	Cl 2	0	0
16	D	2	Total 2	Cl 2	0	0
16	E	3	Total 3	Cl 3	0	0
16	F	1	Total 1	Cl 1	0	0
16	G	2	Total 2	Cl 2	0	0
16	H	2	Total 2	Cl 2	0	0
16	I	1	Total 1	Cl 1	0	0
16	K	3	Total 3	Cl 3	0	0
16	M	3	Total 3	Cl 3	0	0
16	N	4	Total 4	Cl 4	0	0
16	O	4	Total 4	Cl 4	0	0
16	P	1	Total 1	Cl 1	0	0
16	Q	2	Total 2	Cl 2	0	0
16	R	2	Total 2	Cl 2	0	0
16	S	3	Total 3	Cl 3	0	0
16	U	1	Total 1	Cl 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	V	2	Total Cl 2 2	0	0
16	W	1	Total Cl 1 1	0	0
16	Y	4	Total Cl 4 4	0	0
16	a	3	Total Cl 3 3	0	0
16	b	3	Total Cl 3 3	0	0

- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

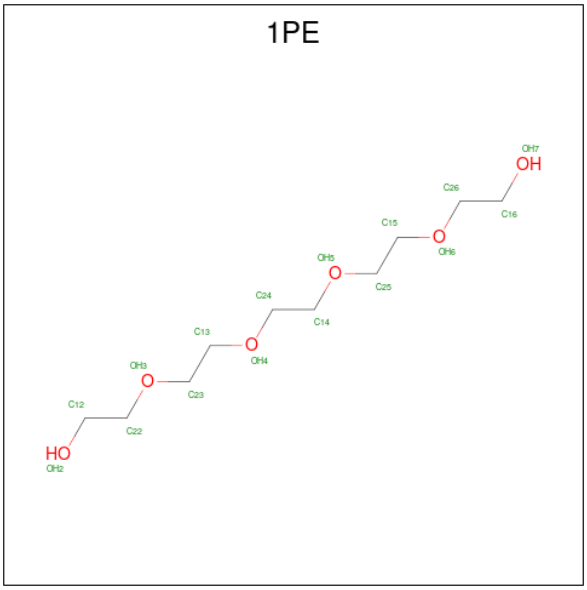
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	H	2	Total Mg 2 2	0	0
18	I	2	Total Mg 2 2	0	0
18	J	1	Total Mg 1 1	0	0
18	K	1	Total Mg 1 1	0	0
18	L	1	Total Mg 1 1	0	0
18	V	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

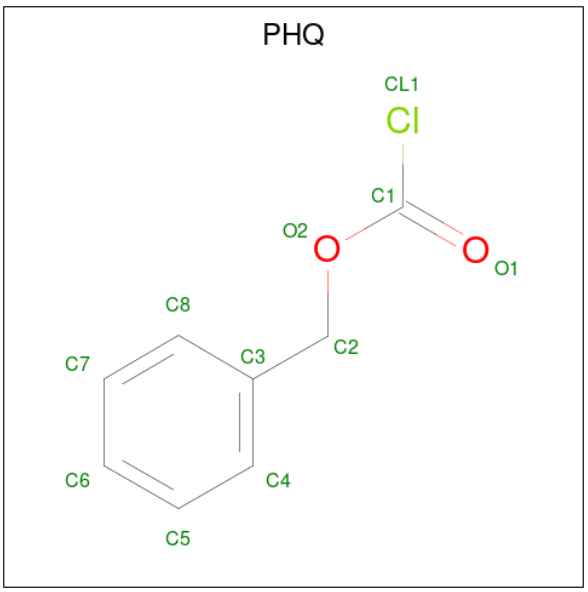
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	W	1	Total Mg 1 1	0	0
18	X	1	Total Mg 1 1	0	0

- Molecule 19 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 20 is benzyl chlorocarbonate (three-letter code: PHQ) (formula: $C_8H_7ClO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	c	1	Total C O 10 8 2	0	0
20	d	1	Total C O 10 8 2	0	0

- Molecule 21 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	108	Total O 108 108	0	0
21	B	119	Total O 119 119	0	0
21	C	75	Total O 75 75	0	0
21	D	86	Total O 86 86	0	0
21	E	137	Total O 137 137	0	0
21	F	179	Total O 179 179	0	0
21	G	190	Total O 190 190	0	0
21	H	150	Total O 150 150	0	0
21	I	157	Total O 157 157	0	0

Continued on next page...

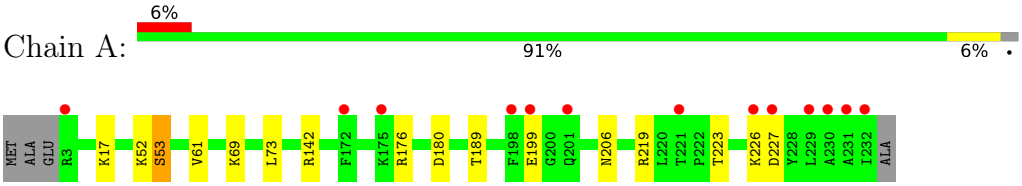
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	J	133	Total O 133 133	0	0
21	c	3	Total O 3 3	0	0
21	K	92	Total O 92 92	0	0
21	L	121	Total O 121 121	0	0
21	M	145	Total O 145 145	0	0
21	N	156	Total O 156 156	0	0
21	O	89	Total O 89 89	0	0
21	P	109	Total O 109 109	0	0
21	Q	71	Total O 71 71	0	0
21	R	119	Total O 119 119	0	0
21	S	124	Total O 124 124	0	0
21	T	91	Total O 91 91	0	0
21	U	103	Total O 103 103	0	0
21	V	109	Total O 109 109	0	0
21	W	108	Total O 108 108	0	0
21	X	124	Total O 124 124	0	0
21	d	2	Total O 2 2	0	0
21	Y	141	Total O 141 141	0	0
21	Z	167	Total O 167 167	0	0
21	a	172	Total O 172 172	0	0
21	b	121	Total O 121 121	0	0

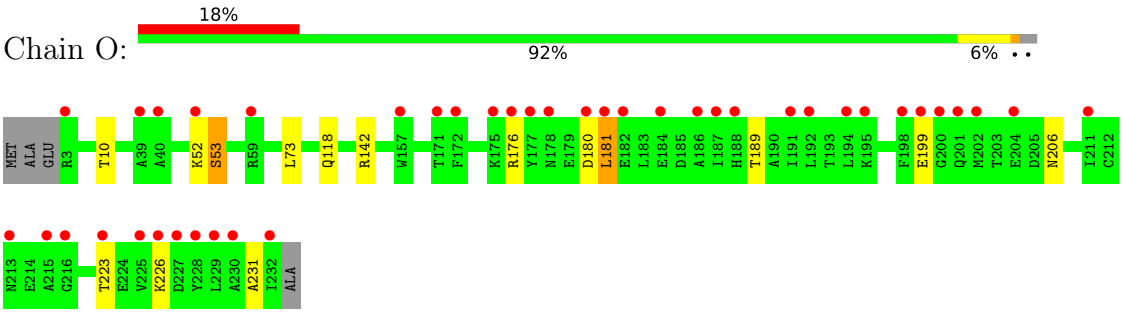
3 Residue-property plots (i)

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

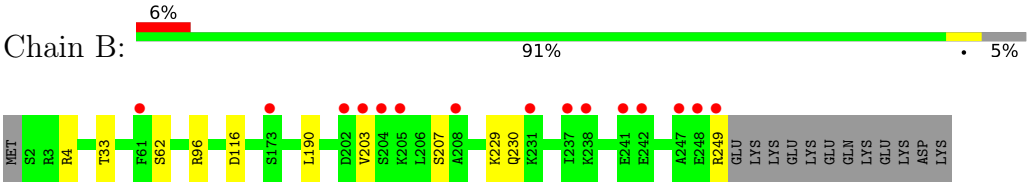
• Molecule 1: Proteasome subunit alpha type-2



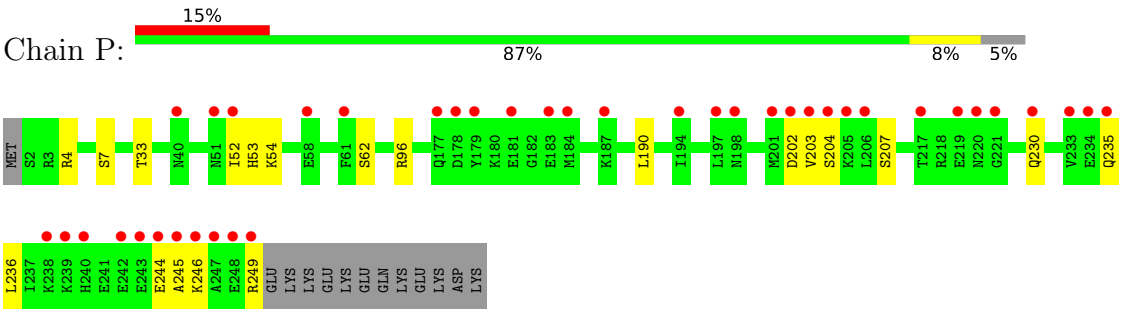
• Molecule 1: Proteasome subunit alpha type-2



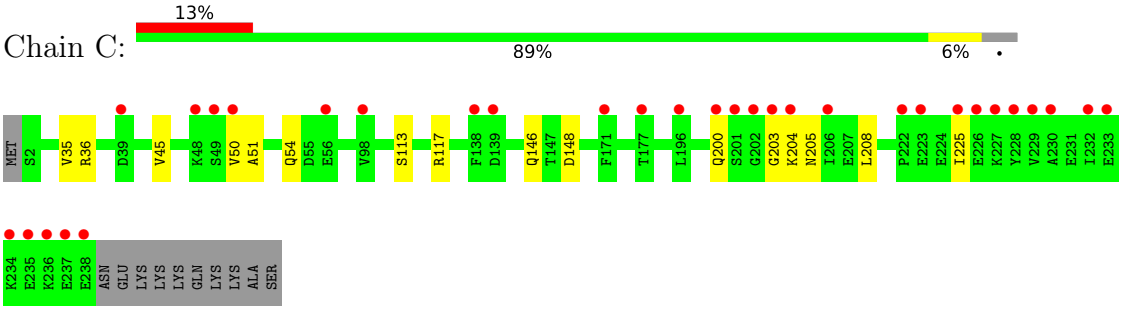
• Molecule 2: Proteasome subunit alpha type-4



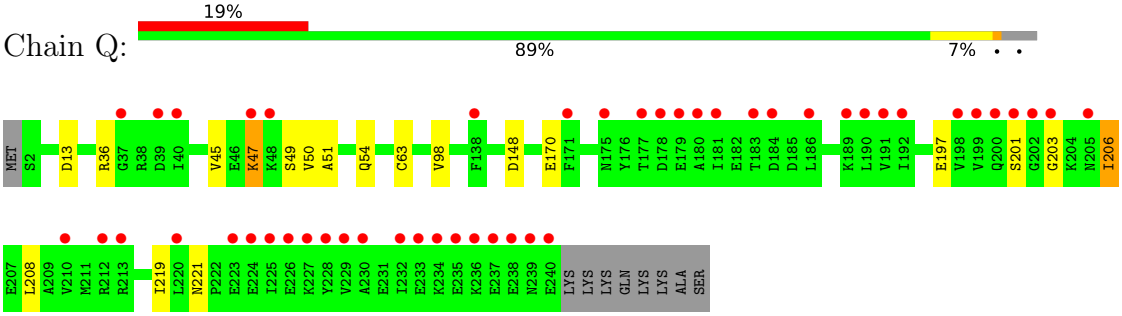
• Molecule 2: Proteasome subunit alpha type-4



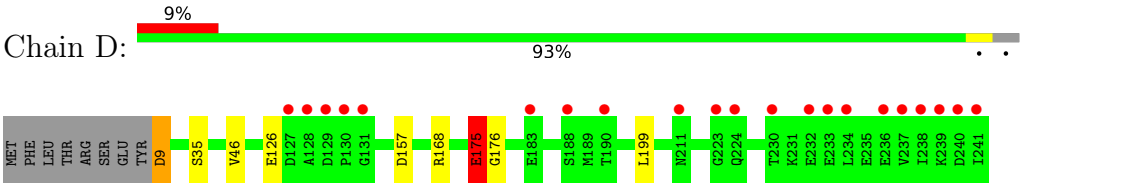
• Molecule 3: Proteasome subunit alpha type-7



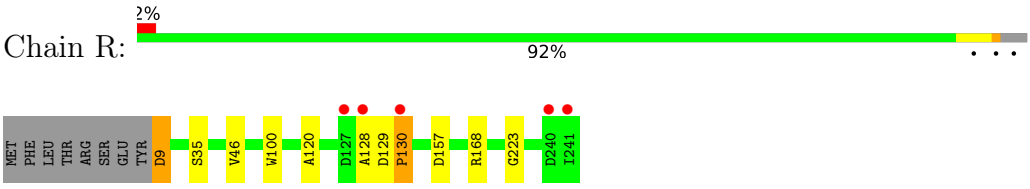
• Molecule 3: Proteasome subunit alpha type-7



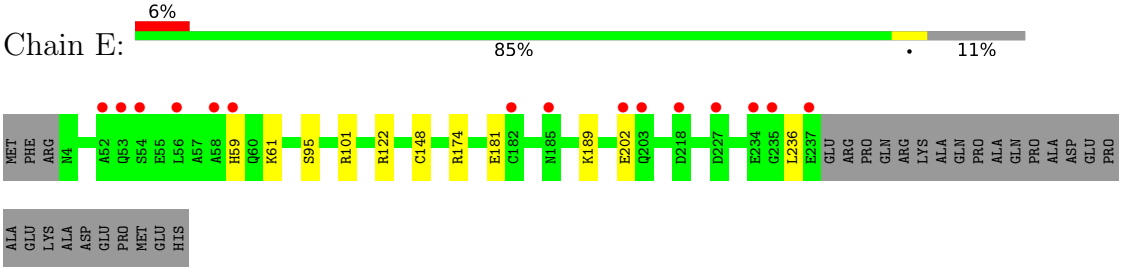
• Molecule 4: Proteasome subunit alpha type-5



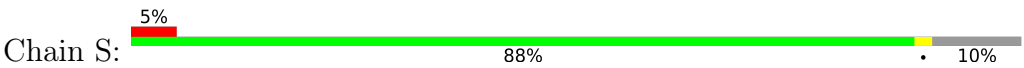
• Molecule 4: Proteasome subunit alpha type-5

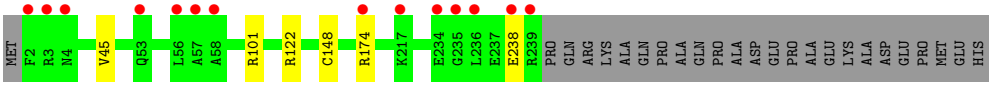


• Molecule 5: Proteasome subunit alpha type-1

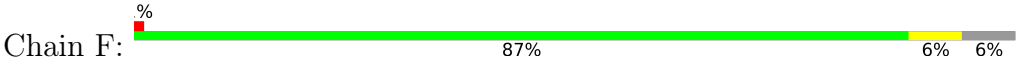


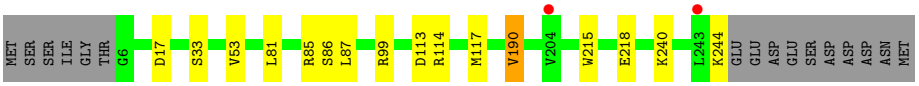
• Molecule 5: Proteasome subunit alpha type-1



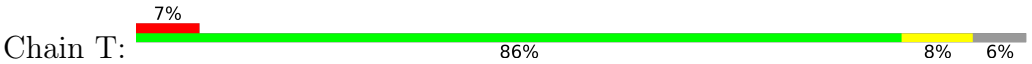


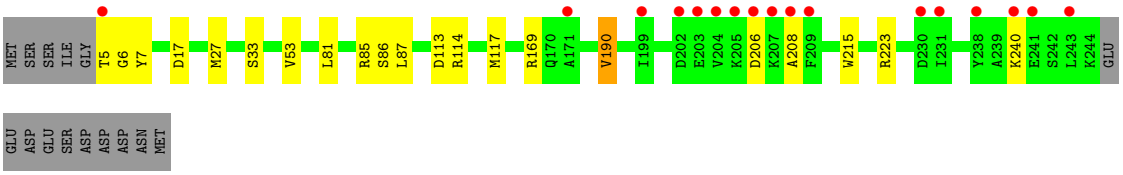
• Molecule 6: Proteasome subunit alpha type-3



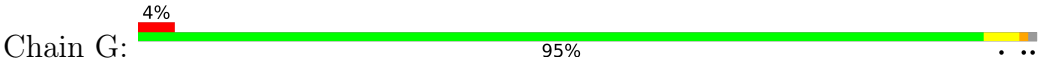


• Molecule 6: Proteasome subunit alpha type-3

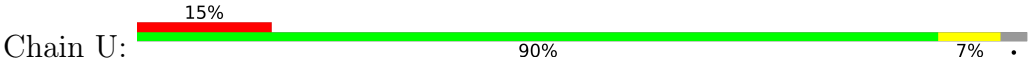


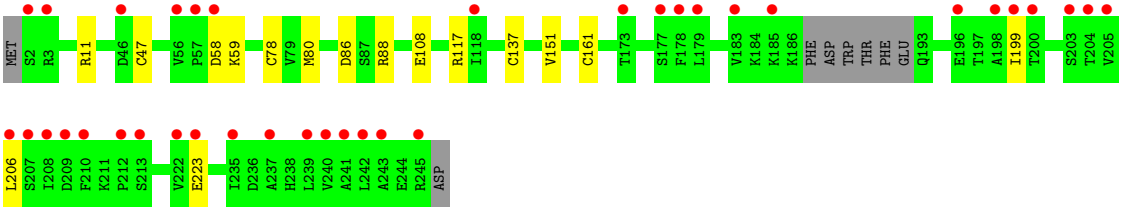


• Molecule 7: Proteasome subunit alpha type-6

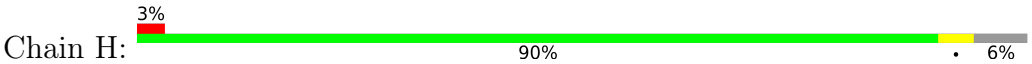


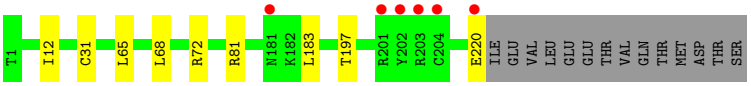
• Molecule 7: Proteasome subunit alpha type-6



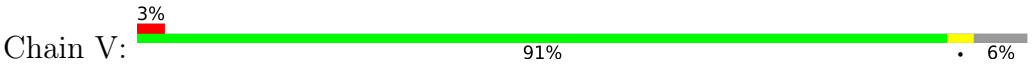


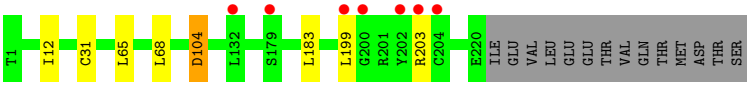
• Molecule 8: Proteasome subunit beta type-7



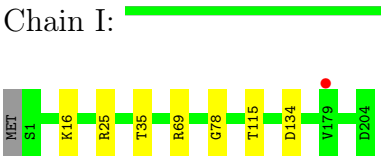


• Molecule 8: Proteasome subunit beta type-7

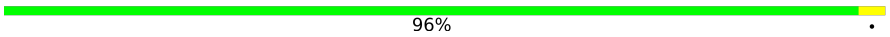




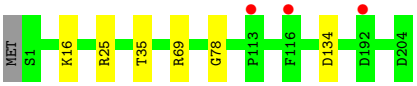
• Molecule 9: Proteasome subunit beta type-3



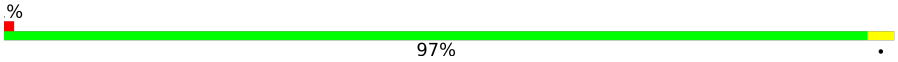
Chain I:



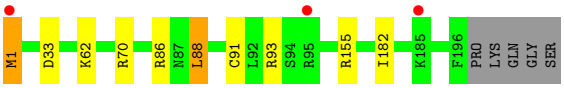
• Molecule 9: Proteasome subunit beta type-3



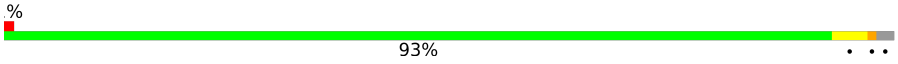
Chain W:



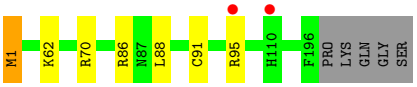
• Molecule 10: Proteasome subunit beta type-2



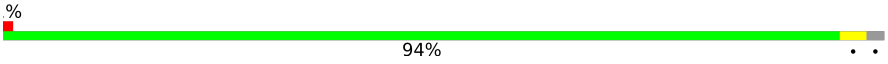
Chain J:



• Molecule 10: Proteasome subunit beta type-2

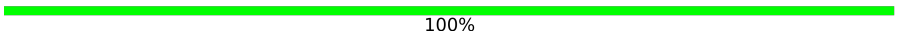


Chain X:



• Molecule 11: LLY-ketoaldehyde peptide

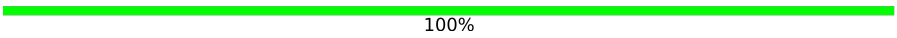
Chain c:



There are no outlier residues recorded for this chain.

• Molecule 11: LLY-ketoaldehyde peptide

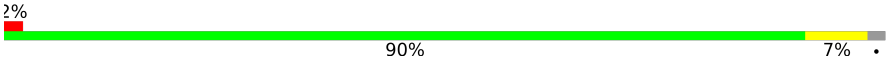
Chain d:

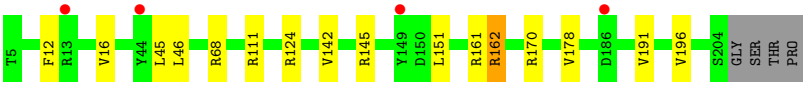


There are no outlier residues recorded for this chain.

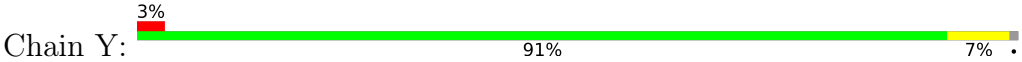
• Molecule 12: Proteasome subunit beta type-5

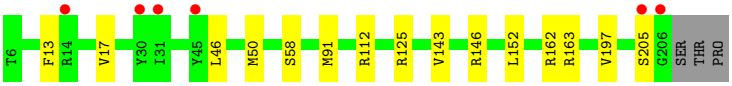
Chain K:





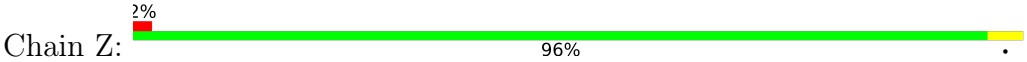
• Molecule 12: Proteasome subunit beta type-5

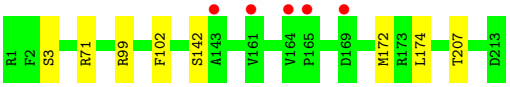




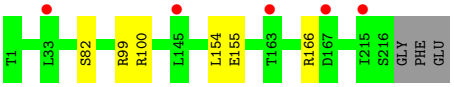
• Molecule 13: Proteasome subunit beta type-1

• Molecule 13: Proteasome subunit beta type-1

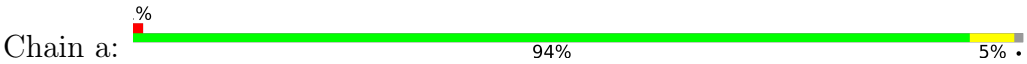




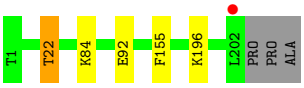
• Molecule 14: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-4

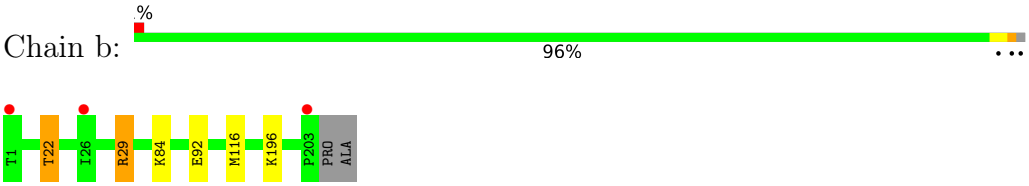


• Molecule 15: Proteasome subunit beta type-6



• Molecule 15: Proteasome subunit beta type-6

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.87Å 203.48Å 315.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.02 – 2.07 49.08 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.4 (171.02-2.07) 96.4 (49.08-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.186 , 0.227 0.193 , 0.229	Depositor DCC
R_{free} test set	21152 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	51953	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PHQ, K, CL, 6V1, MG, 1PE, 6VF, YCM

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	0.71	0/1833	0.81	2/2489 (0.1%)
1	O	0.61	0/1778	0.79	2/2419 (0.1%)
2	B	0.78	0/1962	0.86	4/2649 (0.2%)
2	P	0.65	0/1945	0.84	2/2631 (0.1%)
3	C	0.73	1/1818 (0.1%)	0.91	2/2469 (0.1%)
3	Q	0.70	1/1834 (0.1%)	0.89	2/2490 (0.1%)
4	D	0.69	0/1789	0.85	5/2424 (0.2%)
4	R	0.81	1/1780 (0.1%)	0.93	5/2408 (0.2%)
5	E	0.74	0/1842	0.85	2/2493 (0.1%)
5	S	0.75	0/1901	0.86	2/2571 (0.1%)
6	F	0.87	1/1935 (0.1%)	0.95	8/2605 (0.3%)
6	T	0.78	0/1894	0.96	11/2556 (0.4%)
7	G	0.84	3/1909 (0.2%)	0.86	5/2579 (0.2%)
7	U	0.69	1/1804 (0.1%)	0.85	6/2441 (0.2%)
8	H	0.84	0/1697	0.93	4/2299 (0.2%)
8	V	0.69	0/1655	0.87	3/2251 (0.1%)
9	I	0.82	0/1648	1.05	9/2219 (0.4%)
9	W	0.65	0/1630	0.96	7/2197 (0.3%)
10	J	0.84	0/1613	0.99	7/2180 (0.3%)
10	X	0.73	0/1599	0.96	4/2163 (0.2%)
11	c	0.69	0/15	1.15	0/19
11	d	0.85	0/15	1.08	0/19
12	K	0.77	0/1584	0.96	10/2141 (0.5%)
12	Y	0.88	0/1620	1.08	11/2185 (0.5%)
13	L	0.71	0/1672	0.86	3/2257 (0.1%)
13	Z	0.87	2/1675 (0.1%)	0.91	4/2257 (0.2%)
14	M	0.81	0/1728	0.93	3/2339 (0.1%)
14	a	0.87	1/1724 (0.1%)	0.95	3/2336 (0.1%)
15	N	0.90	0/1545	0.89	3/2091 (0.1%)
15	b	0.88	1/1554 (0.1%)	0.90	4/2104 (0.2%)
All	All	0.77	12/48998 (0.0%)	0.91	133/66281 (0.2%)

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	4
3	Q	0	2
4	D	0	2
4	R	0	2
6	T	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
14	a	0	1
All	All	1	17

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	9.58	1.36	1.25
15	b	92	GLU	CD-OE2	7.86	1.34	1.25
3	Q	13	ASP	CB-CG	6.72	1.65	1.51
14	a	75	GLU	CD-OE1	5.71	1.31	1.25
7	G	108	GLU	CD-OE2	5.66	1.31	1.25
13	Z	3	SER	CB-OG	5.61	1.49	1.42
7	G	78	CYS	CB-SG	-5.40	1.73	1.81
3	C	113	SER	CB-OG	-5.32	1.35	1.42
13	Z	142	SER	CB-OG	-5.25	1.35	1.42
7	U	108	GLU	CD-OE1	5.15	1.31	1.25
4	R	100	TRP	CE3-CZ3	5.09	1.47	1.38
6	F	218	GLU	CD-OE2	5.05	1.31	1.25

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	69	ARG	NE-CZ-NH1	14.57	127.58	120.30
9	W	69	ARG	NE-CZ-NH1	13.28	126.94	120.30
9	I	69	ARG	NE-CZ-NH2	-11.86	114.37	120.30
10	J	86	ARG	NE-CZ-NH2	-11.17	114.72	120.30
9	W	69	ARG	NE-CZ-NH2	-11.02	114.79	120.30
4	R	120[A]	ALA	C-N-CA	10.88	148.91	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	120[B]	ALA	C-N-CA	10.88	148.91	121.70
12	Y	50	MET	CG-SD-CE	-10.87	82.81	100.20
10	X	86	ARG	NE-CZ-NH2	-10.55	115.03	120.30
10	J	86	ARG	NE-CZ-NH1	10.50	125.55	120.30
10	X	86	ARG	NE-CZ-NH1	10.08	125.34	120.30
9	I	16[A]	LYS	C-N-CA	8.84	143.80	121.70
9	I	16[B]	LYS	C-N-CA	8.84	143.80	121.70
9	W	16[A]	LYS	C-N-CA	8.59	143.18	121.70
9	W	16[B]	LYS	C-N-CA	8.59	143.18	121.70
12	Y	162	ARG	NE-CZ-NH1	8.59	124.60	120.30
9	I	25[A]	ARG	NE-CZ-NH1	8.38	124.49	120.30
9	I	25[B]	ARG	NE-CZ-NH1	8.38	124.49	120.30
8	H	72	ARG	NE-CZ-NH2	-7.90	116.35	120.30
12	Y	162	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	O	181	LEU	CA-CB-CG	7.40	132.32	115.30
7	U	88	ARG	NE-CZ-NH1	7.31	123.95	120.30
13	Z	99	ARG	NE-CZ-NH2	-7.19	116.70	120.30
12	Y	163	ARG	NE-CZ-NH2	-7.16	116.72	120.30
6	T	113	ASP	CB-CG-OD2	-7.16	111.86	118.30
2	P	96	ARG	NE-CZ-NH1	7.13	123.86	120.30
13	Z	172	MET	CG-SD-CE	-7.11	88.83	100.20
12	Y	125	ARG	NE-CZ-NH1	7.10	123.85	120.30
7	G	117	ARG	NE-CZ-NH1	7.05	123.83	120.30
12	K	124	ARG	NE-CZ-NH1	7.03	123.81	120.30
3	C	117	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	B	96	ARG	NE-CZ-NH1	7.03	123.81	120.30
13	L	99	ARG	NE-CZ-NH1	7.02	123.81	120.30
4	D	9	ASP	CB-CG-OD1	7.00	124.60	118.30
7	U	11	ARG	NE-CZ-NH1	6.99	123.79	120.30
7	U	86	ASP	CB-CG-OD2	6.92	124.53	118.30
13	Z	99	ARG	NE-CZ-NH1	6.79	123.69	120.30
12	K	162	ARG	NE-CZ-NH2	-6.78	116.91	120.30
9	W	25[A]	ARG	NE-CZ-NH1	6.71	123.66	120.30
9	W	25[B]	ARG	NE-CZ-NH1	6.71	123.66	120.30
6	F	190	VAL	CB-CA-C	-6.67	98.73	111.40
13	L	99	ARG	NE-CZ-NH2	-6.60	117.00	120.30
6	F	85	ARG	NE-CZ-NH1	6.59	123.59	120.30
6	F	85	ARG	NE-CZ-NH2	-6.59	117.01	120.30
6	F	117	MET	CG-SD-CE	6.55	110.67	100.20
13	L	172	MET	CG-SD-CE	-6.52	89.77	100.20
12	Y	146[A]	ARG	NE-CZ-NH1	6.47	123.53	120.30
12	Y	146[B]	ARG	NE-CZ-NH1	6.47	123.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	9	ASP	CB-CG-OD1	6.46	124.12	118.30
6	T	27	MET	CG-SD-CE	6.37	110.39	100.20
15	b	29	ARG	NE-CZ-NH1	6.35	123.48	120.30
8	V	104[A]	ASP	CB-CG-OD1	-6.30	112.63	118.30
8	V	104[B]	ASP	CB-CG-OD1	-6.30	112.63	118.30
12	K	161	ARG	NE-CZ-NH1	6.27	123.44	120.30
3	C	36	ARG	NE-CZ-NH1	6.21	123.40	120.30
6	T	117	MET	CG-SD-CE	6.20	110.12	100.20
3	Q	36	ARG	NE-CZ-NH1	6.19	123.40	120.30
8	H	81	ARG	NE-CZ-NH2	-6.18	117.21	120.30
6	T	6	GLY	N-CA-C	6.11	128.38	113.10
6	T	114	ARG	NE-CZ-NH2	-6.07	117.26	120.30
7	U	117	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	219	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	Q	13	ASP	CB-CA-C	5.93	122.25	110.40
7	G	117	ARG	NE-CZ-NH2	-5.87	117.36	120.30
9	I	134	ASP	CB-CG-OD1	5.87	123.58	118.30
2	B	4	ARG	NE-CZ-NH1	5.86	123.23	120.30
14	a	166	ARG	NE-CZ-NH2	-5.81	117.39	120.30
8	H	72	ARG	NE-CZ-NH1	5.81	123.21	120.30
12	K	162	ARG	NE-CZ-NH1	5.81	123.20	120.30
12	K	170	ARG	NE-CZ-NH1	5.79	123.20	120.30
6	T	85	ARG	NE-CZ-NH2	-5.78	117.41	120.30
4	D	168	ARG	NE-CZ-NH1	5.78	123.19	120.30
6	T	190	VAL	CB-CA-C	-5.76	100.45	111.40
12	K	145	ARG	NE-CZ-NH1	5.76	123.18	120.30
6	F	113	ASP	CB-CG-OD2	-5.70	113.17	118.30
4	R	168	ARG	NE-CZ-NH1	5.70	123.15	120.30
6	T	169	ARG	NE-CZ-NH1	5.68	123.14	120.30
15	b	116	MET	CG-SD-CE	-5.66	91.14	100.20
5	E	174	ARG	NE-CZ-NH1	5.63	123.12	120.30
12	Y	163	ARG	NE-CZ-NH1	5.62	123.11	120.30
15	N	22	THR	CB-CA-C	-5.62	96.44	111.60
9	W	134	ASP	CB-CG-OD1	5.58	123.32	118.30
6	F	114	ARG	NE-CZ-NH2	-5.58	117.51	120.30
10	X	70	ARG	NE-CZ-NH1	5.57	123.08	120.30
10	J	88	LEU	CB-CG-CD2	5.56	120.46	111.00
10	J	93	ARG	NE-CZ-NH1	5.54	123.07	120.30
6	F	113	ASP	CB-CG-OD1	5.53	123.28	118.30
5	S	174	ARG	NE-CZ-NH1	5.52	123.06	120.30
5	E	122	ARG	NE-CZ-NH1	5.52	123.06	120.30
13	Z	71	ARG	NE-CZ-NH2	5.51	123.06	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Y	125	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	P	4	ARG	NE-CZ-NH1	5.48	123.04	120.30
10	J	93	ARG	NE-CZ-NH2	-5.47	117.57	120.30
15	b	29	ARG	CB-CA-C	-5.43	99.53	110.40
10	J	70	ARG	NE-CZ-NH2	-5.43	117.58	120.30
10	X	70	ARG	NE-CZ-NH2	-5.41	117.60	120.30
2	B	96	ARG	NE-CZ-NH2	-5.38	117.61	120.30
6	F	99	ARG	NE-CZ-NH1	5.37	122.99	120.30
12	K	111	ARG	NE-CZ-NH1	5.36	122.98	120.30
4	D	157	ASP	CB-CG-OD1	5.34	123.10	118.30
8	H	12	ILE	CG1-CB-CG2	-5.33	99.68	111.40
14	M	166	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	73	LEU	CA-CB-CG	5.28	127.44	115.30
12	K	161	ARG	NE-CZ-NH2	-5.28	117.66	120.30
5	S	122	ARG	NE-CZ-NH1	5.27	122.94	120.30
15	N	92	GLU	OE1-CD-OE2	-5.24	117.01	123.30
15	b	22	THR	CB-CA-C	-5.22	97.49	111.60
4	D	175[A]	GLU	N-CA-C	-5.22	96.90	111.00
4	D	175[B]	GLU	N-CA-C	-5.22	96.90	111.00
4	R	157	ASP	CB-CG-OD1	5.21	122.99	118.30
7	U	80[A]	MET	CG-SD-CE	5.21	108.53	100.20
7	U	80[B]	MET	CG-SD-CE	5.21	108.53	100.20
12	Y	112	ARG	NE-CZ-NH1	5.21	122.90	120.30
15	N	155	PHE	CB-CG-CD2	5.20	124.44	120.80
10	J	33	ASP	CB-CG-OD1	5.20	122.98	118.30
12	Y	91	MET	CG-SD-CE	5.18	108.50	100.20
6	T	6	GLY	C-N-CA	5.18	134.65	121.70
14	M	99	ARG	NE-CZ-NH1	5.15	122.87	120.30
12	K	46	LEU	CA-CB-CG	5.13	127.10	115.30
7	G	88	ARG	NE-CZ-NH1	5.12	122.86	120.30
6	T	114	ARG	NE-CZ-NH1	5.12	122.86	120.30
14	a	151	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	O	73	LEU	CB-CA-C	-5.11	100.49	110.20
6	T	113	ASP	CB-CG-OD1	5.10	122.89	118.30
14	a	94	ARG	NE-CZ-NH1	5.09	122.85	120.30
12	K	68	ARG	NE-CZ-NH1	5.07	122.84	120.30
7	G	78	CYS	CA-CB-SG	5.07	123.12	114.00
8	V	12	ILE	CG1-CB-CG2	-5.05	100.29	111.40
2	B	116	ASP	CB-CG-OD1	5.04	122.83	118.30
14	M	166	ARG	NE-CZ-NH1	5.04	122.82	120.30
7	G	120	ASP	CB-CG-OD1	5.03	122.83	118.30
9	I	25[A]	ARG	NE-CZ-NH2	-5.02	117.79	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	25[B]	ARG	NE-CZ-NH2	-5.02	117.79	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	202	ASP	Peptide
2	P	203	VAL	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
6	T	5	THR	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
14	a	215	ILE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	218 (94%)	9 (4%)	4 (2%)	9 2
1	O	228/234 (97%)	214 (94%)	9 (4%)	5 (2%)	6 1
2	B	248/261 (95%)	234 (94%)	13 (5%)	1 (0%)	34 25
2	P	248/261 (95%)	234 (94%)	12 (5%)	2 (1%)	19 9
3	C	236/248 (95%)	217 (92%)	14 (6%)	5 (2%)	7 1
3	Q	236/248 (95%)	217 (92%)	12 (5%)	7 (3%)	4 0
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	12 4
4	R	232/241 (96%)	221 (95%)	8 (3%)	3 (1%)	12 4
5	E	232/263 (88%)	226 (97%)	4 (2%)	2 (1%)	17 8
5	S	238/263 (90%)	231 (97%)	6 (2%)	1 (0%)	34 25
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100 100
6	T	239/255 (94%)	230 (96%)	6 (2%)	3 (1%)	12 4
7	G	241/246 (98%)	235 (98%)	6 (2%)	0	100 100
7	U	232/246 (94%)	227 (98%)	3 (1%)	2 (1%)	17 8
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	29 19
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100 100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100 100
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	c	1/3 (33%)	1 (100%)	0	0	100 100
11	d	1/3 (33%)	1 (100%)	0	0	100 100
12	K	199/204 (98%)	196 (98%)	3 (2%)	0	100 100
12	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	29 19
13	L	213/213 (100%)	211 (99%)	2 (1%)	0	100 100
13	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100 100
14	M	215/219 (98%)	208 (97%)	7 (3%)	0	100 100
14	a	216/219 (99%)	207 (96%)	9 (4%)	0	100 100
15	N	201/205 (98%)	200 (100%)	1 (0%)	0	100 100
15	b	202/205 (98%)	201 (100%)	1 (0%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6215/6464 (96%)	6012 (97%)	163 (3%)	40 (1%)	25 15

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
4	D	176	GLY
5	E	59	HIS
1	O	52	LYS
1	O	53	SER
3	Q	47	LYS
3	Q	206	ILE
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
12	Y	205	SER
1	A	176	ARG
2	B	203	VAL
3	C	50	VAL
3	C	51	ALA
3	C	200	GLN
3	C	204	LYS
5	E	236	LEU
1	O	176	ARG
1	O	231	ALA
2	P	54	LYS
3	Q	50	VAL
3	Q	201	SER
6	T	7	TYR
7	U	58	ASP
7	U	59	LYS
4	D	175[A]	GLU
4	D	175[B]	GLU
2	P	52	ILE
3	Q	51	ALA
3	Q	221	ASN
6	T	206	ASP
8	V	203	ARG
6	T	208	ALA
3	C	203	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	199	GLU
1	O	199	GLU
3	Q	203	GLY

5.3.2 Protein sidechains (i)

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%)	174 (94%)	11 (6%)	19	11
1	O	176/191 (92%)	166 (94%)	10 (6%)	20	12
2	B	200/221 (90%)	193 (96%)	7 (4%)	36	29
2	P	197/221 (89%)	184 (93%)	13 (7%)	16	9
3	C	179/210 (85%)	171 (96%)	8 (4%)	27	20
3	Q	184/210 (88%)	175 (95%)	9 (5%)	25	17
4	D	189/203 (93%)	184 (97%)	5 (3%)	46	40
4	R	187/203 (92%)	184 (98%)	3 (2%)	62	59
5	E	192/223 (86%)	185 (96%)	7 (4%)	35	28
5	S	197/223 (88%)	195 (99%)	2 (1%)	76	75
6	F	199/212 (94%)	189 (95%)	10 (5%)	24	16
6	T	192/212 (91%)	182 (95%)	10 (5%)	23	14
7	G	202/207 (98%)	197 (98%)	5 (2%)	47	41
7	U	186/207 (90%)	181 (97%)	5 (3%)	44	39
8	H	181/195 (93%)	175 (97%)	6 (3%)	38	31
8	V	172/195 (88%)	165 (96%)	7 (4%)	30	23
9	I	176/174 (101%)	174 (99%)	2 (1%)	73	72
9	W	173/174 (99%)	172 (99%)	1 (1%)	86	86
10	J	166/170 (98%)	160 (96%)	6 (4%)	35	28
10	X	165/170 (97%)	161 (98%)	4 (2%)	49	43
11	c	2/2 (100%)	2 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	d	2/2 (100%)	2 (100%)	0	100	100
12	K	155/159 (98%)	146 (94%)	9 (6%)	20	11
12	Y	159/159 (100%)	152 (96%)	7 (4%)	28	21
13	L	175/178 (98%)	169 (97%)	6 (3%)	37	30
13	Z	175/178 (98%)	172 (98%)	3 (2%)	60	57
14	M	180/181 (99%)	176 (98%)	4 (2%)	52	46
14	a	178/181 (98%)	172 (97%)	6 (3%)	37	30
15	N	157/159 (99%)	154 (98%)	3 (2%)	57	53
15	b	158/159 (99%)	154 (98%)	4 (2%)	47	41
All	All	5039/5370 (94%)	4866 (97%)	173 (3%)	37	30

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	53	SER
1	A	61	VAL
1	A	69	LYS
1	A	142	ARG
1	A	180	ASP
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP
2	B	33	THR
2	B	62	SER
2	B	190	LEU
2	B	207	SER
2	B	229	LYS
2	B	230	GLN
2	B	249	ARG
3	C	35	VAL
3	C	45	VAL
3	C	54	GLN
3	C	146	GLN
3	C	148	ASP
3	C	205	ASN
3	C	208	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	225	ILE
4	D	9	ASP
4	D	35	SER
4	D	46	VAL
4	D	126	GLU
4	D	199	LEU
5	E	61	LYS
5	E	95	SER
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	181	GLU
5	E	189	LYS
5	E	202	GLU
6	F	17	ASP
6	F	33	SER
6	F	53	VAL
6	F	81	LEU
6	F	86	SER
6	F	87	LEU
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	244	LYS
7	G	78	CYS
7	G	88	ARG
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
8	H	31	CYS
8	H	65	LEU
8	H	68	LEU
8	H	183	LEU
8	H	197	THR
8	H	220	GLU
9	I	35	THR
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	62	LYS
10	J	88	LEU
10	J	155	ARG
10	J	182	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	K	12	PHE
12	K	16	VAL
12	K	45	LEU
12	K	142	VAL
12	K	151	LEU
12	K	162	ARG
12	K	178	VAL
12	K	191	VAL
12	K	196	VAL
13	L	3[A]	SER
13	L	3[B]	SER
13	L	102	PHE
13	L	163	HIS
13	L	174	LEU
13	L	207	THR
14	M	82	SER
14	M	100	ARG
14	M	154	LEU
14	M	155	GLU
15	N	22	THR
15	N	84	LYS
15	N	196	LYS
1	O	10	THR
1	O	53	SER
1	O	118	GLN
1	O	142	ARG
1	O	180	ASP
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	53	HIS
2	P	62	SER
2	P	190	LEU
2	P	204	SER
2	P	207	SER
2	P	230	GLN
2	P	235	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	236	LEU
2	P	246	LYS
2	P	249	ARG
3	Q	45	VAL
3	Q	54	GLN
3	Q	98	VAL
3	Q	148	ASP
3	Q	170	GLU
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	219	ILE
4	R	9	ASP
4	R	35	SER
4	R	46	VAL
5	S	45	VAL
5	S	101	ARG
6	T	17	ASP
6	T	33	SER
6	T	53	VAL
6	T	81	LEU
6	T	86	SER
6	T	87	LEU
6	T	190	VAL
6	T	215	TRP
6	T	223	ARG
6	T	240	LYS
7	U	78	CYS
7	U	151	VAL
7	U	199	ILE
7	U	206	LEU
7	U	223	GLU
8	V	31	CYS
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	183	LEU
8	V	199	LEU
9	W	35	THR
10	X	1	MET
10	X	62	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	X	88	LEU
10	X	95	ARG
12	Y	13	PHE
12	Y	17	VAL
12	Y	46	LEU
12	Y	58	SER
12	Y	143	VAL
12	Y	152	LEU
12	Y	197	VAL
13	Z	102	PHE
13	Z	174	LEU
13	Z	207	THR
14	a	71	VAL
14	a	82	SER
14	a	92	LEU
14	a	100	ARG
14	a	154	LEU
14	a	216	SER
15	b	22	THR
15	b	29	ARG
15	b	84	LYS
15	b	196	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
3	C	54	GLN
4	D	227	HIS
5	E	65	HIS
6	F	143	ASN
8	H	116	HIS
8	H	153	ASN
8	H	193	ASN
9	I	161	HIS
10	J	87	ASN
10	J	101	ASN
10	J	132	HIS
12	K	166	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	L	157	ASN
14	M	162	GLN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	109	GLN
2	P	142	HIS
2	P	146	GLN
3	Q	18	GLN
4	R	186	HIS
4	R	227	HIS
5	S	86	ASN
6	T	63	ASN
6	T	68	ASN
6	T	143	ASN
8	V	116	HIS
8	V	193	ASN
9	W	172	ASN
10	X	174	ASN
12	Y	167	GLN
13	Z	157	ASN
14	a	89	HIS
14	a	162	GLN

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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	6V1	J	91	10	12,15,16	1.69	2 (16%)	9,20,22	4.60	6 (66%)
7	6V1	U	161	7	12,15,16	1.58	3 (25%)	9,20,22	3.78	5 (55%)
5	6V1	E	148	5	12,15,16	2.12	3 (25%)	9,20,22	2.76	4 (44%)
5	6V1	S	148	5	12,15,16	1.93	3 (25%)	9,20,22	2.61	4 (44%)
3	YCM	Q	63	3	7,9,10	1.25	1 (14%)	4,10,12	3.61	3 (75%)
7	YCM	G	137	7	7,9,10	1.71	2 (28%)	4,10,12	2.38	1 (25%)
3	YCM	C	63	3	7,9,10	0.99	0	4,10,12	0.84	0
7	YCM	U	137	7	7,9,10	0.94	0	4,10,12	1.65	1 (25%)
10	6V1	X	91	10	12,15,16	2.00	3 (25%)	9,20,22	4.84	6 (66%)
7	6V1	G	47	7	12,15,16	2.18	3 (25%)	9,20,22	1.35	2 (22%)
7	6V1	G	161	7	12,15,16	1.64	3 (25%)	9,20,22	2.63	4 (44%)
7	6V1	U	47	7	12,15,16	1.78	3 (25%)	9,20,22	2.16	3 (33%)

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	148	6V1	CB-SG	-5.78	1.75	1.82
10	X	91	6V1	C1-SG	-4.95	1.77	1.83
5	S	148	6V1	CB-SG	-4.76	1.76	1.82
7	G	47	6V1	CB-SG	-4.69	1.77	1.82
10	J	91	6V1	C1-SG	-4.65	1.78	1.83
7	G	47	6V1	C4-N3	-4.14	1.31	1.38
7	U	47	6V1	CB-SG	-3.96	1.77	1.82
7	G	47	6V1	C2-N3	-3.61	1.33	1.38
7	G	161	6V1	C4-N3	-3.55	1.32	1.38
10	X	91	6V1	C4-N3	-3.45	1.33	1.38
7	U	47	6V1	C4-N3	-3.12	1.33	1.38
7	U	161	6V1	C4-N3	-2.95	1.33	1.38
7	G	137	YCM	CE-NZ2	2.87	1.42	1.32
5	E	148	6V1	C4-N3	-2.84	1.34	1.38
7	U	161	6V1	CB-SG	-2.84	1.79	1.82
5	S	148	6V1	C2-N3	-2.81	1.34	1.38
7	G	161	6V1	C2-N3	-2.80	1.34	1.38
7	G	161	6V1	CB-SG	-2.77	1.79	1.82
5	S	148	6V1	C5-C4	2.64	1.54	1.50
3	Q	63	YCM	CD-SG	-2.52	1.75	1.81
7	U	47	6V1	C2-N3	-2.52	1.35	1.38
7	U	161	6V1	C2-N3	-2.42	1.35	1.38
10	X	91	6V1	O7-C2	2.40	1.26	1.22
7	G	137	YCM	CD-SG	2.14	1.87	1.81
5	E	148	6V1	C2-N3	-2.13	1.35	1.38
10	J	91	6V1	C4-N3	-2.10	1.35	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	X	91	6V1	C5-C4-N3	8.45	113.11	108.13
10	J	91	6V1	C5-C4-N3	8.14	112.93	108.13
7	U	161	6V1	C2-N3-C4	-8.05	108.26	113.04
10	J	91	6V1	C6-N3-C2	6.34	131.40	123.36
10	X	91	6V1	O7-C2-N3	6.33	131.88	124.14
10	X	91	6V1	C2-N3-C4	-6.20	109.36	113.04
10	X	91	6V1	C6-N3-C2	6.13	131.13	123.36
10	J	91	6V1	O7-C2-N3	5.92	131.38	124.14
7	U	161	6V1	C5-C4-N3	5.81	111.55	108.13
5	E	148	6V1	C2-N3-C4	-5.73	109.64	113.04
10	J	91	6V1	C2-N3-C4	-5.42	109.83	113.04
5	S	148	6V1	C5-C4-N3	5.27	111.24	108.13
3	Q	63	YCM	CE-CD-SG	-5.16	98.41	113.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	47	6V1	C5-C4-N3	4.25	110.64	108.13
7	G	137	YCM	CE-CD-SG	4.23	126.04	113.59
5	S	148	6V1	C2-N3-C4	-4.12	110.59	113.04
7	U	47	6V1	C2-N3-C4	-4.09	110.61	113.04
5	E	148	6V1	C5-C4-N3	4.01	110.49	108.13
7	G	161	6V1	O8-C4-N3	4.00	128.35	123.92
7	G	161	6V1	O8-C4-C5	-3.89	121.58	127.24
7	U	161	6V1	O8-C4-C5	-3.68	121.88	127.24
7	G	161	6V1	C2-N3-C4	-3.65	110.88	113.04
3	Q	63	YCM	CA-CB-SG	-3.63	100.45	113.74
10	X	91	6V1	O8-C4-C5	-3.57	122.03	127.24
7	G	47	6V1	C2-N3-C4	-3.40	111.02	113.04
7	G	161	6V1	C5-C4-N3	3.23	110.04	108.13
10	J	91	6V1	C6-N3-C4	-3.20	118.42	122.59
3	Q	63	YCM	CB-SG-CD	3.17	133.92	104.44
5	E	148	6V1	C6-N3-C2	3.15	127.36	123.36
7	U	137	YCM	CE-CD-SG	2.91	122.14	113.59
7	U	161	6V1	C6-N3-C2	2.83	126.95	123.36
10	X	91	6V1	C6-N3-C4	-2.79	118.96	122.59
5	S	148	6V1	C6-N3-C4	2.74	126.16	122.59
10	J	91	6V1	O8-C4-C5	-2.59	123.47	127.24
5	S	148	6V1	O8-C4-C5	-2.47	123.65	127.24
7	U	161	6V1	O8-C4-N3	2.38	126.56	123.92
7	U	47	6V1	C6-N3-C2	2.22	126.17	123.36
5	E	148	6V1	O7-C2-N3	2.16	126.78	124.14
7	G	47	6V1	C6-N3-C2	2.12	126.04	123.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	CE-CD-SG-CB
7	G	137	YCM	SG-CD-CE-NZ2
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	U	137	YCM	CE-CD-SG-CB
10	X	91	6V1	C3-C6-N3-C2
10	X	91	6V1	C3-C6-N3-C4
5	E	148	6V1	C3-C6-N3-C2
5	E	148	6V1	C3-C6-N3-C4
7	G	161	6V1	C3-C6-N3-C4
7	U	161	6V1	C3-C6-N3-C4
7	G	137	YCM	SG-CD-CE-OZ1
7	G	161	6V1	C3-C6-N3-C2
7	U	161	6V1	C3-C6-N3-C2
7	G	161	6V1	N-CA-CB-SG
7	U	161	6V1	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 82 ligands modelled in this entry, 71 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
19	1PE	I	303	-	15,15,15	0.57	0	14,14,14	1.10	2 (14%)
19	1PE	M	304	-	15,15,15	0.53	0	14,14,14	0.38	0
19	1PE	N	305	-	15,15,15	0.57	0	14,14,14	0.58	0
20	PHQ	c	101	11	9,10,11	1.75	3 (33%)	10,11,13	2.48	1 (10%)
20	PHQ	d	101	11	9,10,11	1.93	4 (44%)	10,11,13	2.53	1 (10%)
19	1PE	I	304	-	15,15,15	0.51	0	14,14,14	0.52	0
19	1PE	b	304	-	15,15,15	0.67	0	14,14,14	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	1PE	a	304	-	15,15,15	0.52	0	14,14,14	0.41	0
19	1PE	W	303	-	15,15,15	0.52	0	14,14,14	0.43	0
19	1PE	L	301	-	15,15,15	0.59	0	14,14,14	0.72	0
19	1PE	Z	301	-	15,15,15	0.54	0	14,14,14	0.40	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
19	1PE	I	303	-	-	8/13/13/13	-
19	1PE	M	304	-	-	7/13/13/13	-
19	1PE	N	305	-	-	6/13/13/13	-
20	PHQ	c	101	11	-	0/4/4/5	0/1/1/1
20	PHQ	d	101	11	-	0/4/4/5	0/1/1/1
19	1PE	I	304	-	-	8/13/13/13	-
19	1PE	b	304	-	-	8/13/13/13	-
19	1PE	a	304	-	-	5/13/13/13	-
19	1PE	W	303	-	-	6/13/13/13	-
19	1PE	L	301	-	-	6/13/13/13	-
19	1PE	Z	301	-	-	6/13/13/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	101	PHQ	C2-C3	3.18	1.58	1.50
20	d	101	PHQ	C2-C3	3.07	1.57	1.50
20	d	101	PHQ	O2-C1	3.02	1.45	1.33
20	d	101	PHQ	C4-C3	2.22	1.43	1.38
20	c	101	PHQ	O2-C1	2.18	1.41	1.33
20	c	101	PHQ	C4-C3	2.11	1.43	1.38
20	d	101	PHQ	C8-C3	2.09	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	d	101	PHQ	O2-C2-C3	7.73	127.96	109.40
20	c	101	PHQ	O2-C2-C3	7.57	127.59	109.40
19	I	303	1PE	C25-OH5-C14	2.73	125.12	113.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	I	303	1PE	OH5-C25-C15	2.32	120.85	110.39

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	I	303	1PE	C15-C25-OH5-C14
19	I	304	1PE	C24-C14-OH5-C25
19	I	304	1PE	OH7-C16-C26-OH6
19	M	304	1PE	OH4-C13-C23-OH3
19	I	304	1PE	OH4-C13-C23-OH3
19	Z	301	1PE	OH6-C15-C25-OH5
19	b	304	1PE	OH4-C13-C23-OH3
19	W	303	1PE	OH6-C15-C25-OH5
19	L	301	1PE	OH5-C14-C24-OH4
19	b	304	1PE	OH6-C15-C25-OH5
19	M	304	1PE	OH5-C14-C24-OH4
19	a	304	1PE	OH5-C14-C24-OH4
19	L	301	1PE	OH6-C15-C25-OH5
19	a	304	1PE	OH4-C13-C23-OH3
19	N	305	1PE	OH4-C13-C23-OH3
19	L	301	1PE	OH2-C12-C22-OH3
19	N	305	1PE	OH2-C12-C22-OH3
19	I	304	1PE	OH5-C14-C24-OH4
19	L	301	1PE	C16-C26-OH6-C15
19	Z	301	1PE	C16-C26-OH6-C15
19	N	305	1PE	OH7-C16-C26-OH6
19	M	304	1PE	OH6-C15-C25-OH5
19	M	304	1PE	OH2-C12-C22-OH3
19	b	304	1PE	OH5-C14-C24-OH4
19	b	304	1PE	C25-C15-OH6-C26
19	I	303	1PE	OH5-C14-C24-OH4
19	I	303	1PE	OH6-C15-C25-OH5
19	I	303	1PE	OH4-C13-C23-OH3
19	L	301	1PE	C25-C15-OH6-C26
19	Z	301	1PE	C12-C22-OH3-C23
19	Z	301	1PE	C15-C25-OH5-C14
19	I	304	1PE	C12-C22-OH3-C23
19	L	301	1PE	C13-C23-OH3-C22
19	W	303	1PE	C13-C23-OH3-C22
19	I	304	1PE	C16-C26-OH6-C15
19	b	304	1PE	C12-C22-OH3-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	Z	301	1PE	OH7-C16-C26-OH6
19	I	303	1PE	C24-C14-OH5-C25
19	M	304	1PE	C23-C13-OH4-C24
19	W	303	1PE	C14-C24-OH4-C13
19	M	304	1PE	C15-C25-OH5-C14
19	W	303	1PE	C24-C14-OH5-C25
19	b	304	1PE	C24-C14-OH5-C25
19	N	305	1PE	C12-C22-OH3-C23
19	M	304	1PE	C14-C24-OH4-C13
19	I	304	1PE	C15-C25-OH5-C14
19	W	303	1PE	OH7-C16-C26-OH6
19	a	304	1PE	OH2-C12-C22-OH3
19	a	304	1PE	OH6-C15-C25-OH5
19	I	303	1PE	C23-C13-OH4-C24
19	N	305	1PE	C25-C15-OH6-C26
19	b	304	1PE	C14-C24-OH4-C13
19	I	303	1PE	OH2-C12-C22-OH3
19	b	304	1PE	C23-C13-OH4-C24
19	W	303	1PE	C23-C13-OH4-C24
19	a	304	1PE	C25-C15-OH6-C26
19	I	303	1PE	C13-C23-OH3-C22
19	N	305	1PE	C13-C23-OH3-C22
19	I	304	1PE	OH6-C15-C25-OH5
19	Z	301	1PE	OH4-C13-C23-OH3

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, 95^{th} 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%)	0.07	13 (5%) 23 24	34, 52, 90, 106	0
1	O	230/234 (98%)	0.71	41 (17%) 1 1	43, 70, 110, 140	0
2	B	248/261 (95%)	0.29	15 (6%) 21 22	36, 56, 99, 133	0
2	P	248/261 (95%)	0.84	40 (16%) 1 1	45, 66, 117, 153	0
3	C	236/248 (95%)	0.69	32 (13%) 3 2	41, 67, 112, 136	0
3	Q	238/248 (95%)	1.02	48 (20%) 1 0	36, 68, 128, 154	0
4	D	233/241 (96%)	0.28	21 (9%) 9 9	41, 67, 99, 141	0
4	R	233/241 (96%)	-0.02	5 (2%) 63 65	32, 47, 75, 115	0
5	E	233/263 (88%)	0.17	15 (6%) 19 19	32, 47, 98, 121	0
5	S	237/263 (90%)	0.13	14 (5%) 22 23	36, 50, 89, 110	0
6	F	239/255 (93%)	-0.11	2 (0%) 86 87	30, 39, 64, 80	0
6	T	240/255 (94%)	0.27	17 (7%) 16 16	36, 55, 92, 134	0
7	G	241/246 (97%)	0.22	10 (4%) 37 39	30, 43, 80, 113	0
7	U	235/246 (95%)	0.72	37 (15%) 2 1	46, 64, 98, 116	0
8	H	220/234 (94%)	-0.09	6 (2%) 54 57	30, 39, 70, 117	0
8	V	220/234 (94%)	0.15	7 (3%) 47 50	38, 54, 85, 123	0
9	I	204/205 (99%)	0.02	1 (0%) 91 91	31, 40, 61, 73	0
9	W	204/205 (99%)	0.08	3 (1%) 73 75	40, 55, 81, 92	0
10	J	195/201 (97%)	-0.14	3 (1%) 73 75	33, 43, 61, 85	0
10	X	195/201 (97%)	-0.03	2 (1%) 82 83	34, 47, 62, 86	0
11	c	2/3 (66%)	0.47	0 100 100	40, 40, 40, 43	0
11	d	2/3 (66%)	0.31	0 100 100	32, 32, 32, 36	0
12	K	200/204 (98%)	0.15	4 (2%) 65 67	38, 51, 78, 95	0
12	Y	201/204 (98%)	0.07	6 (2%) 50 53	30, 40, 61, 78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	L	213/213 (100%)	-0.08	0 100 100	36, 54, 77, 91	0
13	Z	213/213 (100%)	0.11	5 (2%) 60 63	30, 40, 64, 78	0
14	M	216/219 (98%)	0.15	5 (2%) 60 63	30, 43, 68, 103	0
14	a	216/219 (98%)	0.00	3 (1%) 75 76	30, 42, 64, 97	0
15	N	202/205 (98%)	-0.08	1 (0%) 91 91	29, 37, 59, 94	0
15	b	203/205 (99%)	0.13	3 (1%) 73 75	33, 42, 71, 99	0
All	All	6227/6464 (96%)	0.22	359 (5%) 23 24	29, 50, 93, 154	0

All (359) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	204	SER	19.2
1	O	232	ILE	11.2
3	Q	232	ILE	10.0
2	P	203	VAL	9.8
3	Q	238	GLU	9.6
5	E	54	SER	9.1
4	D	241	ILE	8.9
3	Q	229	VAL	8.3
3	Q	48	LYS	8.2
5	E	237	GLU	8.2
3	Q	236	LYS	8.1
3	C	225	ILE	7.9
7	G	187	PHE	7.8
7	U	2	SER	7.5
2	B	61	PHE	7.4
3	Q	202	GLY	7.3
3	Q	239	ASN	7.3
3	C	49	SER	7.2
3	Q	201	SER	7.1
8	H	204	CYS	7.0
3	Q	233	GLU	6.7
3	Q	234	LYS	6.6
7	U	242	LEU	6.4
2	P	234	GLU	6.3
12	K	44	TYR	6.3
3	C	232	ILE	6.3
3	C	229	VAL	6.2
3	C	202	GLY	6.2
1	O	181	LEU	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	202	ASP	6.0
2	P	246	LYS	6.0
5	S	2	PHE	5.9
7	U	206	LEU	5.8
14	a	216	SER	5.7
2	P	205	LYS	5.7
2	P	247	ALA	5.6
3	Q	203	GLY	5.6
4	D	230	THR	5.6
2	P	220	ASN	5.6
2	P	61	PHE	5.6
1	O	3	ARG	5.5
1	O	177	TYR	5.5
2	P	243	GLU	5.5
2	B	203	VAL	5.5
4	R	241	ILE	5.5
8	V	203	ARG	5.5
3	Q	240	GLU	5.4
7	G	188	ASP	5.3
3	Q	200	GLN	5.3
5	E	56	LEU	5.2
3	C	138	PHE	5.2
3	C	234	LYS	5.2
3	C	201	SER	5.1
1	O	223	THR	5.1
3	Q	230	ALA	5.1
6	T	206	ASP	5.0
7	U	243	ALA	5.0
3	Q	179	GLU	4.9
7	G	189	TRP	4.9
2	P	249	ARG	4.9
1	A	231	ALA	4.8
3	C	236	LYS	4.8
3	C	230	ALA	4.7
3	C	222	PRO	4.7
6	T	207	LYS	4.7
7	U	212	PRO	4.7
2	P	201	MET	4.6
1	O	184	GLU	4.6
2	B	204	SER	4.5
2	P	52	ILE	4.5
3	Q	225	ILE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	Z	161	VAL	4.5
4	R	128	ALA	4.5
3	C	200	GLN	4.5
7	U	208	ILE	4.5
7	U	240	VAL	4.5
3	Q	223	GLU	4.5
6	T	209	PHE	4.5
4	D	237	VAL	4.5
3	Q	237	GLU	4.5
1	A	232	ILE	4.4
2	B	248	GLU	4.3
15	b	203	PRO	4.3
1	A	230	ALA	4.3
7	U	207	SER	4.3
2	B	202	ASP	4.3
2	P	244	GLU	4.3
7	U	200	THR	4.3
1	O	176	ARG	4.2
3	C	237	GLU	4.2
7	U	204	THR	4.2
6	T	205	LYS	4.2
3	C	203	GLY	4.1
5	E	218	ASP	4.1
7	U	177	SER	4.1
7	U	3	ARG	4.1
4	D	188	SER	4.0
5	S	3	ARG	4.0
2	B	237	ILE	4.0
3	C	233	GLU	4.0
2	B	205	LYS	4.0
1	O	198	PHE	4.0
1	O	201	GLN	4.0
7	U	205	VAL	3.9
3	Q	138	PHE	3.9
4	D	239	LYS	3.9
4	R	127	ASP	3.9
5	E	52	ALA	3.9
7	U	57	PRO	3.8
1	O	182	GLU	3.8
1	O	40	ALA	3.8
7	G	3	ARG	3.8
7	U	183	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	235	GLY	3.8
3	C	238	GLU	3.8
3	Q	192	ILE	3.7
7	U	223	GLU	3.7
3	Q	199	VAL	3.6
3	Q	178	ASP	3.6
1	A	198	PHE	3.6
3	C	228	TYR	3.6
3	Q	177	THR	3.6
1	O	157	TRP	3.6
1	A	229	LEU	3.6
4	D	130	PRO	3.6
4	R	130	PRO	3.6
10	X	95	ARG	3.6
6	T	208	ALA	3.5
3	Q	181	ILE	3.5
5	E	53	GLN	3.5
1	O	200	GLY	3.5
6	T	202	ASP	3.5
10	J	1[A]	MET	3.5
12	Y	45	TYR	3.5
8	H	201	ARG	3.5
8	V	200	GLY	3.5
4	D	129	ASP	3.4
4	D	234	LEU	3.4
3	C	48	LYS	3.4
7	U	178	PHE	3.4
2	P	233	VAL	3.4
1	O	171	THR	3.4
2	P	206	LEU	3.4
6	T	203	GLU	3.4
5	S	239	ARG	3.3
1	O	226	LYS	3.3
10	X	110	HIS	3.3
3	Q	183	THR	3.3
1	O	192	LEU	3.3
13	Z	164	VAL	3.3
1	O	191	ILE	3.3
5	S	236	LEU	3.3
3	Q	205	ASN	3.3
3	C	171	PHE	3.3
4	D	232	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	180	ALA	3.3
1	O	59	ARG	3.2
12	K	149	TYR	3.2
2	P	51	ASN	3.2
3	C	223	GLU	3.2
5	S	174	ARG	3.2
3	Q	47	LYS	3.2
2	P	235	GLN	3.2
3	C	50	VAL	3.2
1	O	172	PHE	3.2
7	U	245	ARG	3.2
2	B	247	ALA	3.2
3	Q	213	ARG	3.2
7	G	2	SER	3.1
7	U	235	ILE	3.1
5	E	58	ALA	3.1
1	A	175	LYS	3.1
2	P	178	ASP	3.1
8	H	203	ARG	3.1
1	O	227	ASP	3.0
1	O	199	GLU	3.0
6	T	241	GLU	3.0
3	Q	226	GLU	3.0
2	B	242	GLU	3.0
3	Q	186	LEU	3.0
15	b	26	ILE	3.0
2	P	183	GLU	3.0
5	S	234	GLU	3.0
2	B	173	SER	3.0
6	T	243	LEU	3.0
3	Q	210	VAL	2.9
7	U	199	ILE	2.9
2	P	248	GLU	2.9
3	C	235	GLU	2.9
12	Y	206	GLY	2.9
4	D	238	ILE	2.9
6	F	204	VAL	2.9
3	C	56	GLU	2.9
7	G	57	PRO	2.9
3	Q	37	GLY	2.9
2	P	177	GLN	2.9
2	P	219	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	98	VAL	2.9
5	S	57	ALA	2.9
7	U	196	GLU	2.9
2	B	249	ARG	2.8
1	O	229	LEU	2.8
4	D	224	GLN	2.8
15	N	202	LEU	2.8
6	T	199	ILE	2.8
4	D	223	GLY	2.8
5	E	182	CYS	2.8
5	S	238	GLU	2.8
4	D	240	ASP	2.8
3	Q	39	ASP	2.8
2	P	230	GLN	2.8
3	Q	227	LYS	2.8
7	U	239	LEU	2.8
1	A	227	ASP	2.7
2	P	238	LYS	2.7
8	V	202	TYR	2.7
4	D	211	ASN	2.7
7	U	198	ALA	2.7
3	Q	40	ILE	2.7
4	D	127	ASP	2.7
1	O	175	LYS	2.7
6	F	243	LEU	2.7
8	V	132	LEU	2.7
7	U	203	SER	2.7
1	O	228	TYR	2.7
12	Y	31	ILE	2.7
7	U	58	ASP	2.7
5	E	185	ASN	2.7
3	C	226	GLU	2.6
1	O	186	ALA	2.6
5	E	203	GLN	2.6
1	O	216	GLY	2.6
3	Q	198	VAL	2.6
5	S	217	LYS	2.6
7	U	210	PHE	2.6
14	a	194	GLU	2.6
3	C	196	LEU	2.6
14	M	33	LEU	2.6
3	Q	235	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	T	240	LYS	2.6
6	T	204	VAL	2.6
1	O	195	LYS	2.6
2	P	245	ALA	2.6
4	D	131	GLY	2.6
2	P	194	ILE	2.5
5	E	234	GLU	2.5
1	A	201	GLN	2.5
2	P	187	LYS	2.5
4	D	236	GLU	2.5
14	a	215	ILE	2.5
5	S	4	ASN	2.5
5	S	235	GLY	2.5
1	A	221	THR	2.5
1	O	202	MET	2.5
13	Z	165	PRO	2.5
1	O	230	ALA	2.5
15	b	1	THR	2.4
7	U	241	ALA	2.4
1	A	3	ARG	2.4
3	Q	171	PHE	2.4
9	W	113	PRO	2.4
2	P	221	GLY	2.4
3	Q	184	ASP	2.4
7	U	209	ASP	2.4
3	Q	212	ARG	2.4
2	P	240	HIS	2.4
1	O	178	ASN	2.4
2	P	181	GLU	2.4
3	C	204	LYS	2.4
12	K	186	ASP	2.4
1	O	213	ASN	2.4
2	B	241	GLU	2.4
2	P	184	MET	2.4
3	C	227	LYS	2.4
6	T	5	THR	2.4
4	R	240	ASP	2.4
8	V	199	LEU	2.3
14	M	145	LEU	2.3
2	P	239	LYS	2.3
4	D	190	THR	2.3
7	G	8	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	187	ILE	2.3
3	Q	175	ASN	2.3
7	U	179	LEU	2.3
8	V	204	CYS	2.3
3	C	139	ASP	2.3
3	Q	220	LEU	2.3
9	I	179	VAL	2.3
13	Z	143	ALA	2.3
1	O	188	HIS	2.3
1	A	226	LYS	2.3
2	P	179	TYR	2.3
8	H	202	TYR	2.3
2	P	217	THR	2.3
14	M	215	ILE	2.3
4	D	128	ALA	2.3
7	G	209	ASP	2.3
12	Y	14	ARG	2.3
5	E	202	GLU	2.3
3	Q	189	LYS	2.2
10	J	185	LYS	2.2
3	Q	228	TYR	2.2
1	O	225	VAL	2.2
2	B	231	LYS	2.2
12	Y	205	SER	2.2
3	C	39	ASP	2.2
5	E	59	HIS	2.2
12	Y	30	TYR	2.2
3	Q	191	VAL	2.2
13	Z	169	ASP	2.2
4	D	233	GLU	2.2
5	S	53	GLN	2.2
2	P	198	ASN	2.2
3	C	206	ILE	2.2
7	U	56	VAL	2.2
9	W	116	PHE	2.2
6	T	230	ASP	2.2
1	O	180	ASP	2.2
7	U	46	ASP	2.2
7	U	237	ALA	2.2
4	D	183	GLU	2.1
5	E	227	ASP	2.1
2	B	208	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	242	GLU	2.1
8	H	220	GLU	2.1
3	Q	190	LEU	2.1
2	B	238	LYS	2.1
6	T	238	TYR	2.1
1	O	211	ILE	2.1
1	O	52	LYS	2.1
2	P	58	GLU	2.1
2	P	40	ASN	2.1
14	M	163	THR	2.1
1	A	199	GLU	2.1
5	S	56	LEU	2.1
8	V	179	SER	2.1
1	O	204	GLU	2.1
3	C	177	THR	2.1
5	S	58	ALA	2.1
7	U	173	THR	2.1
7	U	118	ILE	2.0
8	H	181	ASN	2.0
10	J	95	ARG	2.0
14	M	167[A]	ASP	2.0
6	T	171	ALA	2.0
1	A	172	PHE	2.0
7	G	245	ARG	2.0
9	W	192	ASP	2.0
1	O	194	LEU	2.0
2	P	197	LEU	2.0
6	T	231	ILE	2.0
1	O	39	ALA	2.0
3	Q	224	GLU	2.0
7	U	222	VAL	2.0
12	K	13	ARG	2.0
7	U	185	LYS	2.0
7	U	213	SER	2.0
1	O	215	ALA	2.0
7	G	72	ILE	2.0

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, 95^{th} 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	0.85	0.33	79,115,121,123	0
7	YCM	U	137	10/11	0.85	0.18	55,65,80,83	0
7	YCM	G	137	10/11	0.89	0.14	37,44,55,55	0
3	YCM	C	63	10/11	0.90	0.12	63,66,76,78	0
3	YCM	Q	63	10/11	0.91	0.14	57,61,67,67	0
7	6V1	U	161	15/16	0.91	0.11	60,86,92,92	0
5	6V1	E	148	15/16	0.92	0.14	39,64,73,74	0
5	6V1	S	148	15/16	0.92	0.15	40,71,78,81	0
10	6V1	X	91	15/16	0.93	0.18	41,58,63,71	0
7	6V1	G	161	15/16	0.94	0.12	40,59,63,63	0
10	6V1	J	91	15/16	0.94	0.17	37,57,65,66	0
7	6V1	G	47	15/16	0.94	0.13	42,67,70,75	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
20	PHQ	c	101	10/11	0.65	0.24	49,78,81,83	0
16	CL	Q	301	1/1	0.66	0.20	98,98,98,98	0
20	PHQ	d	101	10/11	0.69	0.28	46,72,78,79	0
19	1PE	L	301	16/16	0.70	0.17	65,79,84,90	0
16	CL	O	303	1/1	0.77	0.25	103,103,103,103	0
19	1PE	Z	301	16/16	0.78	0.17	59,72,80,84	0
19	1PE	M	304	16/16	0.79	0.32	69,80,114,115	0
19	1PE	I	304	16/16	0.79	0.29	69,85,101,102	0
19	1PE	W	303	16/16	0.81	0.18	68,73,84,87	0
16	CL	D	301	1/1	0.82	0.11	83,83,83,83	0
19	1PE	I	303	16/16	0.83	0.16	59,68,77,84	0
16	CL	a	303	1/1	0.84	0.08	69,69,69,69	0
19	1PE	b	304	16/16	0.84	0.16	50,58,92,98	0
19	1PE	N	305	16/16	0.84	0.16	44,57,68,68	0
16	CL	C	301	1/1	0.84	0.10	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	1PE	a	304	16/16	0.86	0.26	62,70,101,101	0
16	CL	O	304	1/1	0.87	0.14	80,80,80,80	0
16	CL	K	302	1/1	0.87	0.27	92,92,92,92	0
16	CL	Y	302	1/1	0.87	0.30	90,90,90,90	0
16	CL	D	302	1/1	0.88	0.11	77,77,77,77	0
16	CL	K	304	1/1	0.88	0.15	79,79,79,79	0
16	CL	C	302	1/1	0.89	0.10	79,79,79,79	0
16	CL	H	303	1/1	0.89	0.08	63,63,63,63	0
16	CL	V	302	1/1	0.91	0.14	73,73,73,73	0
16	CL	K	303	1/1	0.91	0.20	73,73,73,73	0
16	CL	A	302	1/1	0.92	0.11	76,76,76,76	0
16	CL	I	302	1/1	0.92	0.12	57,57,57,57	0
16	CL	M	303	1/1	0.92	0.09	61,61,61,61	0
16	CL	V	303	1/1	0.92	0.10	66,66,66,66	0
16	CL	B	302	1/1	0.92	0.12	69,69,69,69	0
16	CL	Y	304	1/1	0.92	0.16	73,73,73,73	0
16	CL	R	302	1/1	0.93	0.12	62,62,62,62	0
16	CL	S	301	1/1	0.93	0.24	76,76,76,76	0
16	CL	O	302	1/1	0.93	0.08	71,71,71,71	0
16	CL	A	304	1/1	0.93	0.06	63,63,63,63	0
16	CL	Y	301	1/1	0.93	0.09	71,71,71,71	0
16	CL	N	301	1/1	0.93	0.19	55,55,55,55	0
16	CL	P	301	1/1	0.93	0.13	65,65,65,65	0
16	CL	a	301	1/1	0.93	0.10	69,69,69,69	0
16	CL	N	303	1/1	0.93	0.10	70,70,70,70	0
18	MG	I	301	1/1	0.93	0.08	34,34,34,34	0
18	MG	V	301	1/1	0.93	0.21	58,58,58,58	0
16	CL	Y	303	1/1	0.94	0.07	66,66,66,66	0
16	CL	W	302	1/1	0.94	0.07	61,61,61,61	0
18	MG	W	301	1/1	0.94	0.06	43,43,43,43	0
16	CL	R	301	1/1	0.94	0.18	63,63,63,63	0
16	CL	S	302	1/1	0.94	0.09	76,76,76,76	0
16	CL	b	301	1/1	0.94	0.16	66,66,66,66	0
18	MG	H	301	1/1	0.94	0.09	48,48,48,48	0
16	CL	M	301	1/1	0.95	0.13	67,67,67,67	0
18	MG	J	301	1/1	0.95	0.06	55,55,55,55	0
16	CL	E	303	1/1	0.95	0.13	75,75,75,75	0
17	K	U	302	1/1	0.95	0.06	46,46,46,46	0
16	CL	E	301	1/1	0.95	0.13	69,69,69,69	0
16	CL	O	301	1/1	0.96	0.07	63,63,63,63	0
16	CL	G	301	1/1	0.96	0.09	52,52,52,52	0
16	CL	G	302	1/1	0.96	0.06	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	CL	a	302	1/1	0.96	0.11	48,48,48,48	0
16	CL	U	301	1/1	0.96	0.06	67,67,67,67	0
16	CL	E	302	1/1	0.96	0.14	61,61,61,61	0
16	CL	b	303	1/1	0.96	0.15	64,64,64,64	0
17	K	L	302	1/1	0.96	0.05	58,58,58,58	0
16	CL	N	302	1/1	0.96	0.16	66,66,66,66	0
17	K	b	305	1/1	0.96	0.09	49,49,49,49	0
16	CL	H	304	1/1	0.96	0.08	57,57,57,57	0
16	CL	Q	302	1/1	0.96	0.11	77,77,77,77	0
16	CL	N	304	1/1	0.96	0.10	50,50,50,50	0
16	CL	B	301	1/1	0.97	0.12	46,46,46,46	0
16	CL	A	303	1/1	0.97	0.15	58,58,58,58	0
17	K	G	303	1/1	0.97	0.05	38,38,38,38	0
18	MG	I	305	1/1	0.97	0.09	29,29,29,29	0
16	CL	A	301	1/1	0.97	0.06	64,64,64,64	0
18	MG	K	301	1/1	0.97	0.08	40,40,40,40	0
17	K	N	306	1/1	0.97	0.07	44,44,44,44	0
16	CL	F	301	1/1	0.97	0.05	60,60,60,60	0
18	MG	X	301	1/1	0.97	0.09	54,54,54,54	0
17	K	Z	302	1/1	0.97	0.11	44,44,44,44	0
16	CL	b	302	1/1	0.98	0.12	68,68,68,68	0
16	CL	M	302	1/1	0.98	0.12	44,44,44,44	0
16	CL	S	303	1/1	0.98	0.14	60,60,60,60	0
18	MG	H	302	1/1	0.99	0.05	34,34,34,34	0
18	MG	L	303	1/1	0.99	0.04	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.