



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2016 – 02:20 PM EST

PDB ID : 5LF7
Title : Human 20S proteasome complex with Ixazomib at 2.0 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 : 2.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

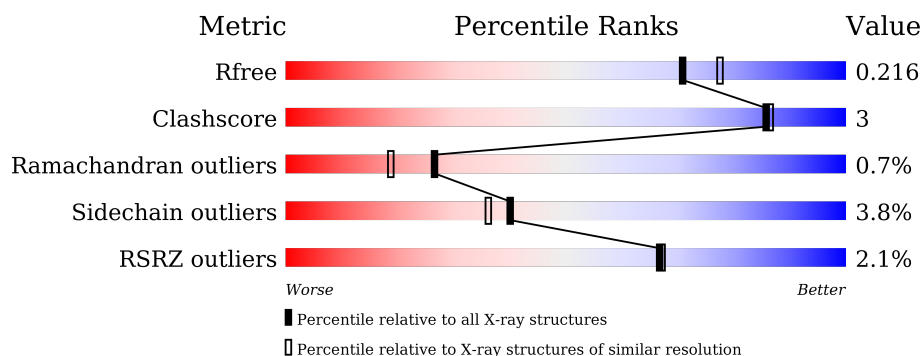
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	234	<div> <div></div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	O	234	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</div> </div> </div>
2	B	261	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>5%</div> </div> </div>
2	P	261	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>..</div> <div>5%</div> </div> </div>
3	C	248	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>..</div> </div> </div>
3	Q	248	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>..</div> </div> </div>

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	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
15	CL	B	302	-	-	-	X
15	CL	D	301	-	-	-	X
15	CL	M	301	-	-	-	X
15	CL	M	302	-	-	-	X
15	CL	N	302	-	-	-	X
15	CL	S	301	-	-	-	X
15	CL	b	301	-	-	-	X
18	1PE	H	304	-	-	-	X
18	1PE	I	303	-	-	-	X
18	1PE	I	304	-	-	-	X
18	1PE	L	301	-	-	-	X
18	1PE	M	305	-	-	-	X
19	6V8	H	305	-	-	-	X
19	6V8	K	305	-	-	-	X
19	6V8	V	303	-	-	-	X
7	6V1	U	47	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 52085 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	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
			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			

- 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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1576	1012	267	287	10			

- 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
			1545	974	269	293	9			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	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			
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
			1516	950	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	P	1	Total	Cl	0	0
			1	1		
15	K	3	Total	Cl	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	2	Total 2	Cl 2	0	0
15	W	1	Total 1	Cl 1	0	0
15	N	2	Total 2	Cl 2	0	0
15	S	3	Total 3	Cl 3	0	0
15	E	3	Total 3	Cl 3	0	0
15	b	1	Total 1	Cl 1	0	0
15	V	1	Total 1	Cl 1	0	0
15	A	4	Total 4	Cl 4	0	0
15	R	2	Total 2	Cl 2	0	0
15	M	4	Total 4	Cl 4	0	0
15	D	2	Total 2	Cl 2	0	0
15	I	1	Total 1	Cl 1	0	0
15	a	4	Total 4	Cl 4	0	0
15	U	1	Total 1	Cl 1	0	0
15	G	2	Total 2	Cl 2	0	0
15	Q	2	Total 2	Cl 2	0	0
15	H	1	Total 1	Cl 1	0	0
15	C	2	Total 2	Cl 2	0	0
15	O	4	Total 4	Cl 4	0	0
15	Y	4	Total 4	Cl 4	0	0
15	F	1	Total 1	Cl 1	0	0

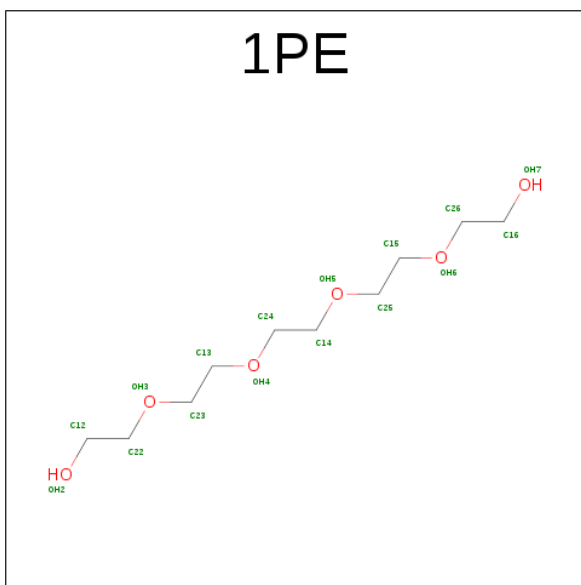
- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

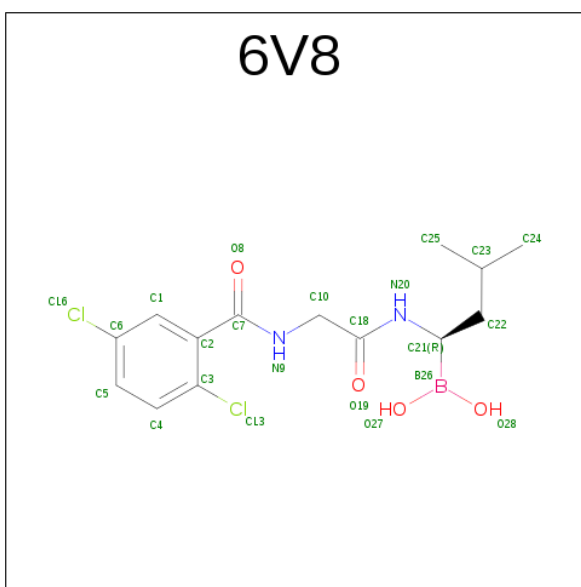
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0
17	H	2	Total Mg 2 2	0	0
17	I	2	Total Mg 2 2	0	0
17	V	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	X	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0

- Molecule 18 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	H	1	Total 16	C 10	O 6	0	0
18	I	1	Total 16	C 10	O 6	0	0
18	I	1	Total 16	C 10	O 6	0	0
18	L	1	Total 16	C 10	O 6	0	0
18	M	1	Total 16	C 10	O 6	0	0
18	N	1	Total 16	C 10	O 6	0	0
18	W	1	Total 16	C 10	O 6	0	0
18	Y	1	Total 16	C 10	O 6	0	0
18	b	1	Total 16	C 10	O 6	0	0

- Molecule 19 is [(1 {R})-1-[2-[[2,5-bis(chloranyl)phenyl]carbonylamino]ethanoylamino]-3-methyl-butyl]boronic acid (three-letter code: 6V8) (formula: C₁₄H₁₉BCl₂N₂O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
19	H	1	Total	B	C	Cl	N	O	0	0
			23	1	14	2	2	4		
19	K	1	Total	B	C	Cl	N	O	0	0
			23	1	14	2	2	4		
19	N	1	Total	B	C	Cl	N	O	0	0
			23	1	14	2	2	4		
19	V	1	Total	B	C	Cl	N	O	0	0
			23	1	14	2	2	4		
19	Y	1	Total	B	C	Cl	N	O	0	0
			23	1	14	2	2	4		
19	b	1	Total	B	C	Cl	N	O	0	0
			23	1	14	2	2	4		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	110	Total	O	0	0
			110	110		
20	B	124	Total	O	0	0
			124	124		
20	C	76	Total	O	0	0
			76	76		
20	D	88	Total	O	0	0
			88	88		
20	E	143	Total	O	0	0
			143	143		
20	F	189	Total	O	0	0
			189	189		

Continued on next page...

Continued from previous page...

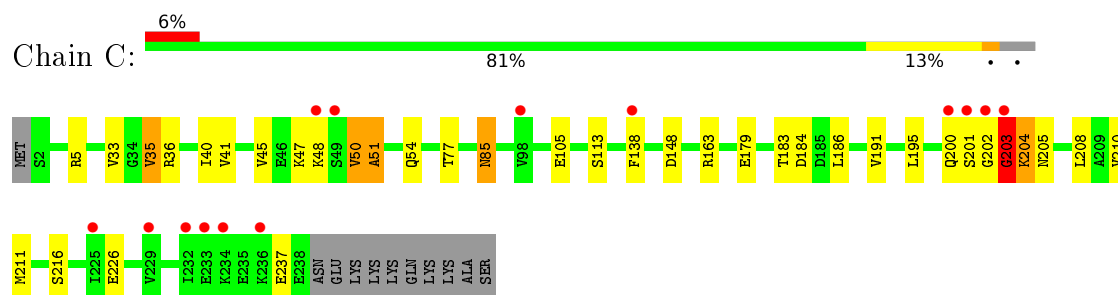
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	G	190	Total 190	O 190	0	0
20	H	158	Total 158	O 158	0	0
20	I	153	Total 153	O 153	0	0
20	J	137	Total 137	O 137	0	0
20	K	100	Total 100	O 100	0	0
20	L	131	Total 131	O 131	0	0
20	M	146	Total 146	O 146	0	0
20	N	158	Total 158	O 158	0	0
20	O	92	Total 92	O 92	0	0
20	P	117	Total 117	O 117	0	0
20	Q	73	Total 73	O 73	0	0
20	R	124	Total 124	O 124	0	0
20	S	122	Total 122	O 122	0	0
20	T	89	Total 89	O 89	0	0
20	U	106	Total 106	O 106	0	0
20	V	114	Total 114	O 114	0	0
20	W	114	Total 114	O 114	0	0
20	X	128	Total 128	O 128	0	0
20	Y	150	Total 150	O 150	0	0
20	Z	169	Total 169	O 169	0	0
20	a	173	Total 173	O 173	0	0

Continued on next page...

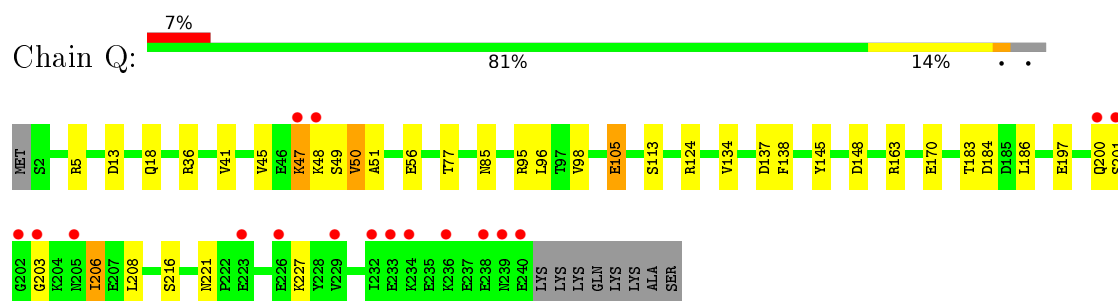
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	b	121	Total	O	0	0
			121	121		

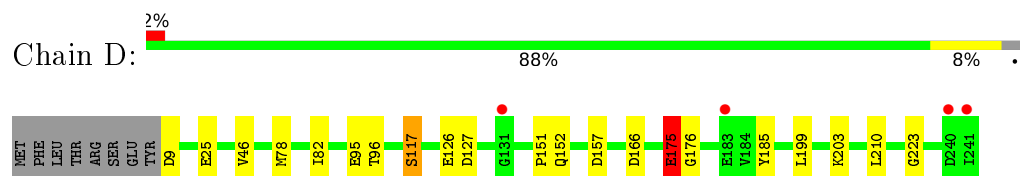
- Molecule 3: Proteasome subunit alpha type-7



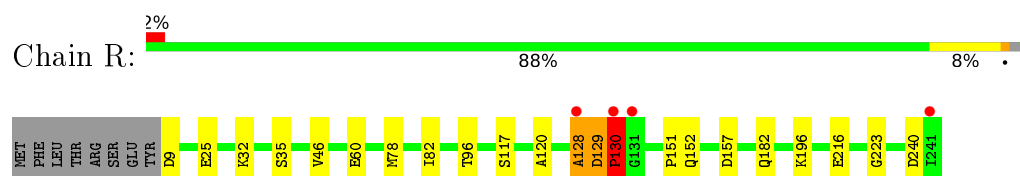
- Molecule 3: Proteasome subunit alpha type-7



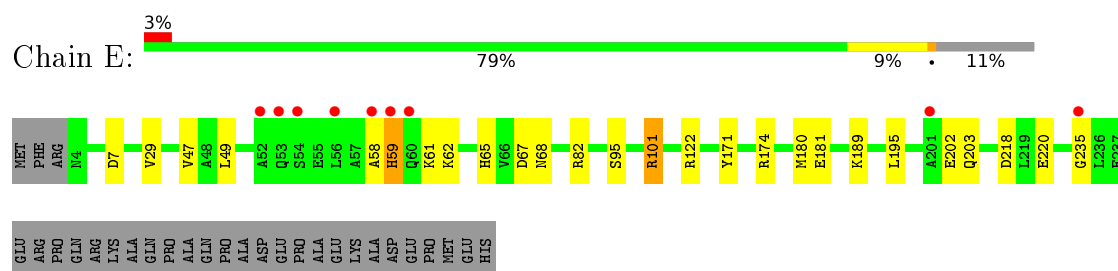
- Molecule 4: Proteasome subunit alpha type-5



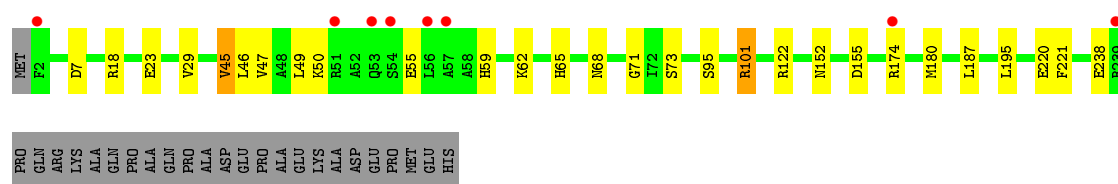
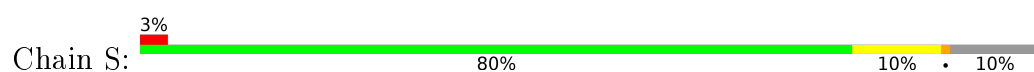
- Molecule 4: Proteasome subunit alpha type-5



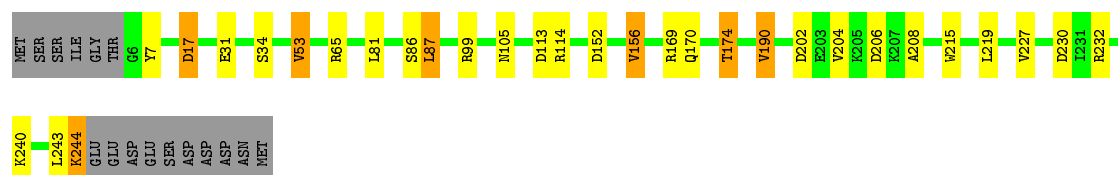
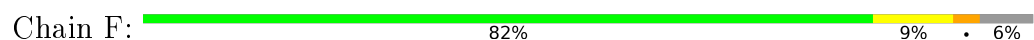
- Molecule 5: Proteasome subunit alpha type-1



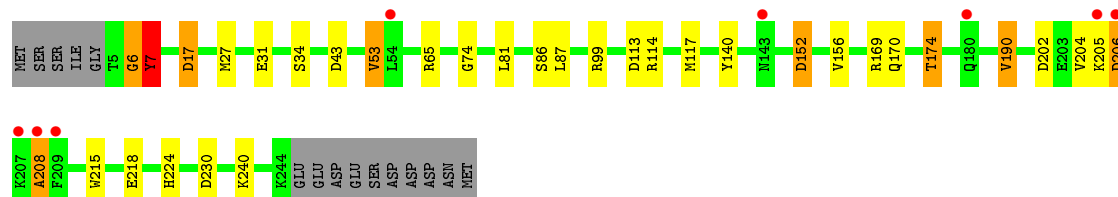
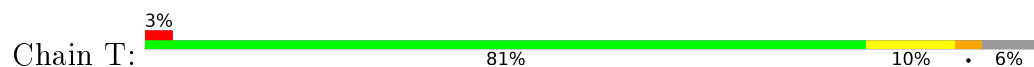
- Molecule 5: Proteasome subunit alpha type-1



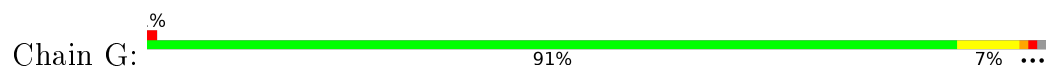
- Molecule 6: Proteasome subunit alpha type-3



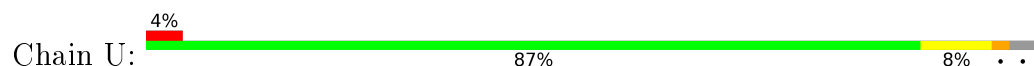
- Molecule 6: Proteasome subunit alpha type-3



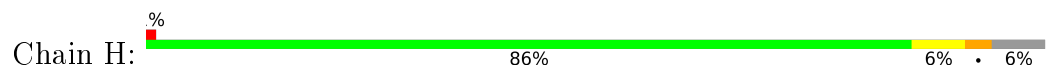
- Molecule 7: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-6

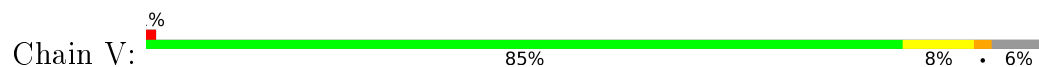


- Molecule 8: Proteasome subunit beta type-7





- Molecule 8: Proteasome subunit beta type-7



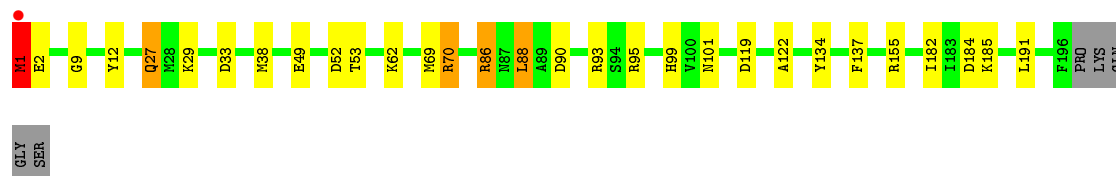
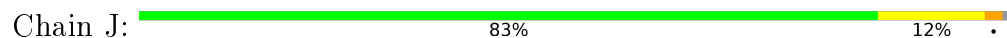
- Molecule 9: Proteasome subunit beta type-3



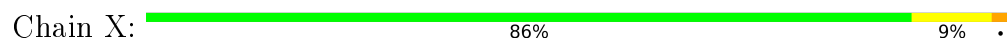
- Molecule 9: Proteasome subunit beta type-3



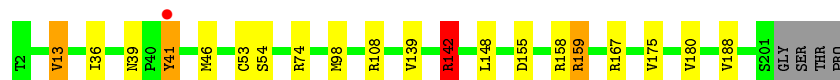
- Molecule 10: Proteasome subunit beta type-2



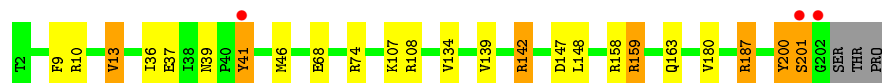
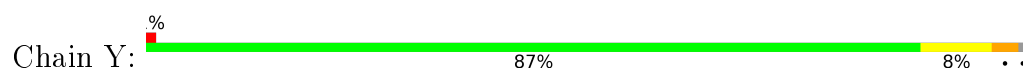
- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-1



- Molecule 12: Proteasome subunit beta type-1



- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.41Å 202.61Å 314.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.33 – 2.00 106.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (170.33-2.00) 99.4 (106.69-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.175 , 0.213 0.181 , 0.216	Depositor DCC
R_{free} test set	24018 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52085	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6V8, K, CL, 6V1, 1PE, 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	0.95	2/1833 (0.1%)	0.94	2/2489 (0.1%)
1	O	0.81	2/1778 (0.1%)	0.87	2/2419 (0.1%)
2	B	0.90	2/1962 (0.1%)	0.94	6/2649 (0.2%)
2	P	0.92	2/1934 (0.1%)	0.96	6/2617 (0.2%)
3	C	0.84	1/1818 (0.1%)	0.98	5/2469 (0.2%)
3	Q	0.87	2/1834 (0.1%)	0.96	5/2490 (0.2%)
4	D	0.87	1/1789 (0.1%)	0.91	3/2424 (0.1%)
4	R	0.98	3/1780 (0.2%)	0.98	5/2408 (0.2%)
5	E	0.94	1/1842 (0.1%)	0.98	2/2493 (0.1%)
5	S	0.85	0/1901	0.93	4/2571 (0.2%)
6	F	1.08	1/1935 (0.1%)	1.09	9/2605 (0.3%)
6	T	0.82	1/1894 (0.1%)	1.02	15/2556 (0.6%)
7	G	1.07	5/1909 (0.3%)	0.96	6/2579 (0.2%)
7	U	0.79	2/1804 (0.1%)	0.88	6/2441 (0.2%)
8	H	1.09	4/1697 (0.2%)	1.14	12/2299 (0.5%)
8	V	0.94	2/1655 (0.1%)	1.02	11/2251 (0.5%)
9	I	1.05	4/1648 (0.2%)	1.16	11/2219 (0.5%)
9	W	0.96	0/1630	1.10	11/2197 (0.5%)
10	J	0.94	1/1613 (0.1%)	1.14	10/2180 (0.5%)
10	X	0.99	2/1599 (0.1%)	1.14	8/2163 (0.4%)
11	K	1.04	3/1576 (0.2%)	1.04	6/2131 (0.3%)
11	Y	1.09	1/1620 (0.1%)	1.08	7/2185 (0.3%)
12	L	1.02	1/1672 (0.1%)	1.04	5/2257 (0.2%)
12	Z	1.11	3/1675 (0.2%)	1.09	7/2257 (0.3%)
13	M	1.01	1/1728 (0.1%)	1.04	7/2339 (0.3%)
13	a	1.01	3/1724 (0.2%)	1.01	3/2336 (0.1%)
14	N	1.06	5/1545 (0.3%)	0.98	4/2091 (0.2%)
14	b	0.92	1/1554 (0.1%)	0.99	4/2104 (0.2%)
All	All	0.96	56/48949 (0.1%)	1.01	182/66219 (0.3%)

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	C	0	2
3	Q	0	2
4	D	0	4
4	R	0	2
5	E	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
11	Y	0	1
13	a	0	1
All	All	1	20

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	10.94	1.37	1.25
8	H	32	CYS	CB-SG	-9.11	1.66	1.82
12	Z	3	SER	CB-OG	9.01	1.53	1.42
2	P	103	GLU	CD-OE2	8.79	1.35	1.25
12	Z	142	SER	CB-OG	-7.82	1.32	1.42
1	O	123	SER	CB-OG	-7.69	1.32	1.42
2	B	103	GLU	CD-OE2	7.33	1.33	1.25
1	A	123	SER	CB-OG	-7.22	1.32	1.42
7	U	108	GLU	CD-OE1	7.06	1.33	1.25
10	X	86	ARG	CD-NE	-7.01	1.34	1.46
12	L	129	SER	CB-OG	-6.86	1.33	1.42
14	N	25	SER	CB-OG	-6.76	1.33	1.42
10	J	86	ARG	CD-NE	-6.75	1.34	1.46
8	V	105[A]	ASP	CB-CG	-6.67	1.37	1.51
8	V	105[B]	ASP	CB-CG	-6.67	1.37	1.51
8	H	132	SER	CB-OG	-6.47	1.33	1.42
9	I	105	GLU	CD-OE2	6.34	1.32	1.25
4	R	35	SER	CB-OG	-6.33	1.34	1.42
3	Q	13	ASP	CB-CG	6.25	1.64	1.51
6	F	17	ASP	CG-OD2	6.21	1.39	1.25
11	K	41	TYR	CG-CD1	6.19	1.47	1.39
3	Q	113	SER	CB-OG	-6.07	1.34	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	7	ASP	CB-CG	-5.87	1.39	1.51
11	K	54	SER	CB-OG	-5.76	1.34	1.42
1	O	115	SER	CB-OG	-5.76	1.34	1.42
13	M	74	GLU	CD-OE1	5.72	1.31	1.25
7	G	78	CYS	CB-SG	-5.68	1.72	1.81
2	B	103	GLU	CD-OE1	5.63	1.31	1.25
13	a	75	GLU	CG-CD	5.61	1.60	1.51
14	N	93	GLU	CD-OE1	5.60	1.31	1.25
8	H	7	VAL	CB-CG1	-5.59	1.41	1.52
14	N	93	GLU	CG-CD	5.58	1.60	1.51
11	Y	41	TYR	CG-CD1	5.50	1.46	1.39
4	R	25	GLU	CD-OE1	5.49	1.31	1.25
7	G	39	SER	CB-OG	5.48	1.49	1.42
13	a	119	GLU	CG-CD	5.47	1.60	1.51
1	A	97	TYR	CE1-CZ	5.46	1.45	1.38
13	a	82	SER	CB-OG	-5.44	1.35	1.42
7	G	108	GLU	CD-OE2	5.42	1.31	1.25
3	C	113	SER	CB-OG	-5.42	1.35	1.42
11	K	159	ARG	CZ-NH2	-5.40	1.26	1.33
12	Z	31	GLU	CD-OE2	5.36	1.31	1.25
14	N	26	TYR	CZ-OH	5.35	1.47	1.37
10	X	154	GLU	CG-CD	5.29	1.59	1.51
6	T	7	TYR	N-CA	5.28	1.56	1.46
4	R	216	GLU	CD-OE2	5.20	1.31	1.25
9	I	102	TYR	CG-CD2	5.18	1.45	1.39
7	G	101	TRP	CG-CD1	-5.14	1.29	1.36
9	I	16[A]	LYS	C-O	5.12	1.33	1.23
9	I	16[B]	LYS	C-O	5.12	1.33	1.23
4	D	25	GLU	CD-OE1	5.12	1.31	1.25
8	H	92	GLN	CG-CD	5.09	1.62	1.51
14	b	30	ARG	CD-NE	-5.07	1.37	1.46
2	P	124	PHE	CG-CD1	5.07	1.46	1.38
14	N	125	SER	CB-OG	-5.07	1.35	1.42
7	U	108	GLU	CD-OE2	5.00	1.31	1.25

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	86	ARG	NE-CZ-NH2	-18.15	111.23	120.30
10	J	86	ARG	NE-CZ-NH2	-17.76	111.42	120.30
9	I	69	ARG	NE-CZ-NH1	15.65	128.12	120.30
9	W	69	ARG	NE-CZ-NH1	13.79	127.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	86	ARG	NE-CZ-NH1	13.19	126.89	120.30
10	X	86	ARG	NE-CZ-NH1	12.78	126.69	120.30
8	H	73	ARG	NE-CZ-NH2	-12.55	114.03	120.30
14	b	30	ARG	NE-CZ-NH1	11.76	126.18	120.30
6	F	17	ASP	CB-CG-OD1	-10.77	108.60	118.30
2	P	124	PHE	CB-CG-CD1	-10.36	113.55	120.80
11	Y	158	ARG	NE-CZ-NH2	-10.11	115.25	120.30
2	P	124	PHE	CB-CG-CD2	9.80	127.66	120.80
12	Z	99	ARG	NE-CZ-NH2	-9.78	115.41	120.30
9	I	69	ARG	NE-CZ-NH2	-9.74	115.43	120.30
11	Y	158	ARG	NE-CZ-NH1	9.61	125.10	120.30
4	R	120[A]	ALA	C-N-CA	9.59	145.67	121.70
4	R	120[B]	ALA	C-N-CA	9.59	145.67	121.70
12	L	99	ARG	NE-CZ-NH1	9.23	124.92	120.30
9	I	25[A]	ARG	NE-CZ-NH1	8.93	124.77	120.30
9	I	25[B]	ARG	NE-CZ-NH1	8.93	124.77	120.30
12	L	99	ARG	NE-CZ-NH2	-8.67	115.97	120.30
7	G	117	ARG	NE-CZ-NH1	8.54	124.57	120.30
12	Z	99	ARG	NE-CZ-NH1	8.44	124.52	120.30
9	W	16[A]	LYS	C-N-CA	8.37	142.63	121.70
9	W	16[B]	LYS	C-N-CA	8.37	142.63	121.70
9	W	69	ARG	NE-CZ-NH2	-8.23	116.19	120.30
12	Z	172	MET	CG-SD-CE	-8.23	87.03	100.20
6	T	27	MET	CG-SD-CE	8.18	113.28	100.20
13	M	151	ARG	NE-CZ-NH1	8.04	124.32	120.30
6	F	206	ASP	CB-CG-OD1	-7.99	111.11	118.30
11	Y	159	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	B	6	ASP	CB-CG-OD1	7.74	125.27	118.30
11	K	158	ARG	NE-CZ-NH1	7.67	124.14	120.30
11	Y	142[A]	ARG	NE-CZ-NH1	7.64	124.12	120.30
11	Y	142[B]	ARG	NE-CZ-NH1	7.64	124.12	120.30
8	H	73	ARG	NE-CZ-NH1	7.60	124.10	120.30
11	K	142	ARG	NE-CZ-NH1	7.56	124.08	120.30
11	K	155	ASP	CB-CG-OD2	7.54	125.08	118.30
11	Y	159	ARG	NE-CZ-NH2	-7.45	116.57	120.30
11	K	158	ARG	NE-CZ-NH2	-7.43	116.58	120.30
2	B	4	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	B	4	ARG	NE-CZ-NH2	-7.39	116.60	120.30
12	L	172	MET	CG-SD-CE	-7.38	88.39	100.20
6	T	17	ASP	CB-CG-OD1	-7.35	111.68	118.30
7	G	86	ASP	CB-CG-OD1	7.29	124.86	118.30
7	U	117	ARG	NE-CZ-NH1	7.23	123.92	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	16[A]	LYS	C-N-CA	7.22	139.76	121.70
9	I	16[B]	LYS	C-N-CA	7.22	139.76	121.70
8	H	82	ARG	NE-CZ-NH2	-7.11	116.75	120.30
6	T	99	ARG	NE-CZ-NH1	7.10	123.85	120.30
13	M	100	ARG	NE-CZ-NH1	-7.00	116.80	120.30
12	Z	71	ARG	NE-CZ-NH2	6.98	123.79	120.30
7	U	88	ARG	NE-CZ-NH1	6.96	123.78	120.30
14	N	46	ARG	NE-CZ-NH2	-6.90	116.85	120.30
6	T	113	ASP	CB-CG-OD2	-6.90	112.09	118.30
3	Q	5	ARG	NE-CZ-NH2	-6.86	116.87	120.30
6	T	43	ASP	CB-CG-OD2	6.70	124.33	118.30
6	T	6	GLY	C-N-CA	6.68	138.41	121.70
10	X	184	ASP	CB-CG-OD1	6.68	124.31	118.30
7	U	80[A]	MET	CG-SD-CE	6.66	110.86	100.20
7	U	80[B]	MET	CG-SD-CE	6.66	110.86	100.20
14	b	30	ARG	NE-CZ-NH2	-6.64	116.98	120.30
10	J	70	ARG	NE-CZ-NH1	6.61	123.60	120.30
5	E	122	ARG	NE-CZ-NH2	-6.57	117.02	120.30
13	M	151	ARG	NE-CZ-NH2	-6.57	117.02	120.30
6	F	190	VAL	CB-CA-C	-6.55	98.96	111.40
6	F	113	ASP	CB-CG-OD2	-6.54	112.41	118.30
8	H	199	ARG	NE-CZ-NH2	-6.48	117.06	120.30
8	H	133	LEU	CB-CG-CD2	6.45	121.97	111.00
8	H	87	MET	CG-SD-CE	-6.44	89.90	100.20
10	X	70	ARG	NE-CZ-NH1	6.42	123.51	120.30
8	V	105[A]	ASP	CB-CG-OD1	-6.38	112.56	118.30
8	V	105[B]	ASP	CB-CG-OD1	-6.38	112.56	118.30
3	Q	5	ARG	NE-CZ-NH1	6.37	123.48	120.30
6	F	99	ARG	NE-CZ-NH1	6.33	123.47	120.30
10	J	184	ASP	CB-CG-OD1	6.33	123.99	118.30
6	F	156	VAL	CG1-CB-CG2	-6.25	100.90	110.90
13	a	151	ARG	NE-CZ-NH1	6.25	123.42	120.30
14	N	46	ARG	NE-CZ-NH1	6.24	123.42	120.30
7	G	183	VAL	CB-CA-C	-6.23	99.56	111.40
6	T	7	TYR	N-CA-CB	6.22	121.80	110.60
11	K	108	ARG	NE-CZ-NH1	6.21	123.41	120.30
6	F	87	LEU	CB-CG-CD1	6.15	121.46	111.00
1	O	181	LEU	CA-CB-CG	6.14	129.43	115.30
2	P	4	ARG	NE-CZ-NH1	6.14	123.37	120.30
10	X	52	ASP	CB-CG-OD2	-6.14	112.78	118.30
3	C	36	ARG	NE-CZ-NH1	6.13	123.36	120.30
9	I	158	ASP	CB-CG-OD1	6.11	123.80	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	88	ARG	NE-CZ-NH2	-6.11	117.25	120.30
4	R	157	ASP	CB-CG-OD1	6.02	123.72	118.30
3	C	5	ARG	NE-CZ-NH2	-6.01	117.29	120.30
11	K	167	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	B	226	ARG	NE-CZ-NH2	-5.97	117.32	120.30
13	a	182	ARG	NE-CZ-NH1	5.96	123.28	120.30
9	W	25[A]	ARG	NE-CZ-NH1	5.96	123.28	120.30
9	W	25[B]	ARG	NE-CZ-NH1	5.96	123.28	120.30
9	I	192	ASP	CB-CG-OD1	5.95	123.66	118.30
4	D	175[A]	GLU	N-CA-C	-5.95	94.94	111.00
4	D	175[B]	GLU	N-CA-C	-5.95	94.94	111.00
13	M	73	ASP	CB-CG-OD2	-5.95	112.95	118.30
13	M	182	ARG	NE-CZ-NH1	5.93	123.27	120.30
6	T	190	VAL	CB-CA-C	-5.93	100.13	111.40
2	P	103	GLU	OE1-CD-OE2	5.90	130.38	123.30
9	W	158	ASP	CB-CG-OD1	5.89	123.61	118.30
8	V	73	ARG	NE-CZ-NH2	-5.89	117.35	120.30
8	V	185	ASP	CB-CG-OD1	-5.87	113.02	118.30
10	J	38	MET	CG-SD-CE	-5.87	90.81	100.20
8	V	87	MET	CG-SD-CE	-5.84	90.85	100.20
6	T	230	ASP	CB-CG-OD2	5.84	123.56	118.30
10	J	86	ARG	CD-NE-CZ	5.83	131.77	123.60
9	W	175	ASP	CB-CG-OD1	5.83	123.55	118.30
1	O	73	LEU	CB-CA-C	-5.82	99.13	110.20
8	V	133	LEU	CB-CG-CD2	5.81	120.88	111.00
5	S	155	ASP	CB-CG-OD2	5.81	123.53	118.30
9	W	77	GLU	C-N-CA	-5.80	110.11	122.30
4	D	157	ASP	CB-CG-OD1	5.80	123.52	118.30
12	Z	125	ASP	CB-CG-OD1	5.80	123.52	118.30
8	V	29	ASP	CB-CG-OD1	5.79	123.52	118.30
5	S	122	ARG	NE-CZ-NH2	-5.79	117.41	120.30
10	J	33	ASP	CB-CG-OD1	5.77	123.49	118.30
13	M	99	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	B	96	ARG	NE-CZ-NH1	5.73	123.17	120.30
6	T	169	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	17	LYS	CD-CE-NZ	5.70	124.82	111.70
3	C	5	ARG	NE-CZ-NH1	5.70	123.15	120.30
7	U	11	ARG	NE-CZ-NH1	5.69	123.15	120.30
9	I	77	GLU	C-N-CA	-5.69	110.36	122.30
6	F	114	ARG	NE-CZ-NH2	-5.68	117.46	120.30
3	Q	137	ASP	CB-CG-OD2	-5.67	113.20	118.30
8	H	199	ARG	NE-CZ-NH1	5.65	123.13	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	73	ARG	NE-CZ-NH1	5.63	123.11	120.30
6	T	117	MET	CG-SD-CE	5.61	109.17	100.20
1	A	73	LEU	CB-CA-C	-5.61	99.55	110.20
9	I	47	ARG	NE-CZ-NH1	5.60	123.10	120.30
10	X	86	ARG	CD-NE-CZ	5.60	131.44	123.60
10	X	70	ARG	NE-CZ-NH2	-5.59	117.50	120.30
5	E	174	ARG	NE-CZ-NH1	5.57	123.09	120.30
8	H	69	LEU	CA-CB-CG	5.57	128.12	115.30
14	N	168	ASP	CB-CG-OD1	-5.56	113.29	118.30
12	Z	173	ARG	NE-CZ-NH1	5.56	123.08	120.30
10	J	70	ARG	NE-CZ-NH2	-5.54	117.53	120.30
7	G	226	LYS	CD-CE-NZ	5.54	124.44	111.70
13	M	166	ARG	NE-CZ-NH2	-5.54	117.53	120.30
8	V	82	ARG	NE-CZ-NH2	-5.50	117.55	120.30
7	U	88	ARG	NE-CZ-NH2	-5.49	117.56	120.30
3	Q	13	ASP	CB-CG-OD2	5.48	123.23	118.30
13	a	43	MET	CG-SD-CE	-5.40	91.56	100.20
9	I	175	ASP	CB-CG-OD2	-5.34	113.49	118.30
8	V	69	LEU	CB-CG-CD1	5.33	120.06	111.00
9	W	47	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	P	116	ASP	CB-CG-OD1	5.29	123.06	118.30
5	S	7	ASP	CB-CG-OD1	-5.25	113.58	118.30
7	G	88	ARG	CG-CD-NE	-5.25	100.78	111.80
8	H	90	ARG	NE-CZ-NH1	5.24	122.92	120.30
6	T	114	ARG	NE-CZ-NH2	-5.23	117.69	120.30
14	b	23	THR	CB-CA-C	-5.22	97.51	111.60
8	H	73	ARG	CD-NE-CZ	5.21	130.89	123.60
6	F	230	ASP	CB-CG-OD1	-5.20	113.62	118.30
8	H	29	ASP	CB-CG-OD1	5.18	122.97	118.30
3	Q	36	ARG	NE-CZ-NH1	5.17	122.88	120.30
12	L	102	PHE	CB-CG-CD1	5.16	124.41	120.80
5	S	174	ARG	NE-CZ-NH1	5.16	122.88	120.30
14	N	23	THR	CB-CA-C	-5.15	97.69	111.60
8	V	13	ILE	CG1-CB-CG2	-5.15	100.07	111.40
14	b	168	ASP	CB-CG-OD1	-5.15	113.67	118.30
10	J	69	MET	CG-SD-CE	-5.14	91.97	100.20
9	W	192	ASP	CB-CG-OD1	5.14	122.92	118.30
6	T	17	ASP	CB-CG-OD2	5.13	122.92	118.30
2	P	96	ARG	NE-CZ-NH1	5.13	122.86	120.30
10	J	52	ASP	CB-CG-OD2	-5.12	113.69	118.30
10	X	69	MET	CG-SD-CE	-5.10	92.04	100.20
8	H	13	ILE	CG1-CB-CG2	-5.09	100.20	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	85[A]	ASN	CB-CA-C	5.07	120.54	110.40
3	C	85[B]	ASN	CB-CA-C	5.07	120.54	110.40
12	L	156	LYS	CD-CE-NZ	-5.06	100.06	111.70
6	T	113	ASP	CB-CG-OD1	5.05	122.85	118.30
6	T	152	ASP	CB-CG-OD1	5.03	122.83	118.30
12	Z	169	ASP	CB-CG-OD2	5.02	122.82	118.30
4	R	120[A]	ALA	N-CA-C	-5.02	97.46	111.00
4	R	120[B]	ALA	N-CA-C	-5.02	97.46	111.00
2	B	3	ARG	NE-CZ-NH2	-5.01	117.80	120.30
11	Y	108	ARG	NE-CZ-NH1	5.01	122.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	203	GLY	Peptide
3	C	237	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
4	D	223	GLY	Peptide
5	E	235	GLY	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	245	ALA	Peptide
2	P	54	LYS	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
11	Y	200	TYR	Peptide
13	a	215	ILE	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	13	0
1	O	1741	0	1683	7	0
2	B	1926	0	1924	10	0
2	P	1898	0	1861	13	0
3	C	1798	0	1718	17	0
3	Q	1820	0	1749	12	0
4	D	1762	0	1709	6	0
4	R	1753	0	1726	9	0
5	E	1822	0	1779	12	0
5	S	1875	0	1818	17	0
6	F	1888	0	1882	12	0
6	T	1856	0	1816	10	0
7	G	1912	0	1882	9	0
7	U	1815	0	1748	14	0
8	H	1664	0	1677	8	0
8	V	1622	0	1591	5	0
9	I	1613	0	1646	10	0
9	W	1599	0	1621	11	0
10	J	1590	0	1581	19	0
10	X	1576	0	1561	14	0
11	K	1545	0	1494	7	0
11	Y	1580	0	1554	15	0
12	L	1636	0	1625	6	0
12	Z	1642	0	1635	4	0
13	M	1692	0	1670	4	0
13	a	1688	0	1658	0	0
14	N	1516	0	1483	5	0
14	b	1524	0	1492	0	0
15	A	4	0	0	1	0
15	B	2	0	0	1	0
15	C	2	0	0	0	0
15	D	2	0	0	0	0
15	E	3	0	0	0	0
15	F	1	0	0	1	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K	3	0	0	0	0
15	M	4	0	0	1	0
15	N	2	0	0	0	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	1	0
15	R	2	0	0	0	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	4	0	0	0	0
15	a	4	0	0	0	0
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	16	0	22	0	0
18	I	32	0	44	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0
18	N	16	0	22	1	0
18	W	16	0	22	0	0
18	Y	16	0	22	0	0
18	b	16	0	22	0	0
19	H	23	0	0	0	0
19	K	23	0	0	0	0
19	N	23	0	0	0	0
19	V	23	0	0	0	0
19	Y	23	0	0	0	0
19	b	23	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	110	0	0	2	0
20	B	124	0	0	1	0
20	C	76	0	0	0	0
20	D	88	0	0	1	0
20	E	143	0	0	2	0
20	F	189	0	0	5	0
20	G	190	0	0	3	0
20	H	158	0	0	5	0
20	I	153	0	0	1	0
20	J	137	0	0	3	0
20	K	100	0	0	0	0
20	L	131	0	0	0	0
20	M	146	0	0	1	0
20	N	158	0	0	1	0
20	O	92	0	0	2	0
20	P	117	0	0	1	0
20	Q	73	0	0	1	0
20	R	124	0	0	2	0
20	S	122	0	0	3	0
20	T	89	0	0	0	0
20	U	106	0	0	2	0
20	V	114	0	0	0	0
20	W	114	0	0	1	0
20	X	128	0	0	1	0
20	Y	150	0	0	2	0
20	Z	169	0	0	1	0
20	a	173	0	0	0	0
20	b	121	0	0	0	0
All	All	52085	0	47542	254	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 3.

All (254) 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)
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.32	0.95
11:Y:36:ILE:HD11	11:Y:46:MET:SD	2.12	0.90
8:H:78:VAL:HB	20:H:540:HOH:O	1.72	0.88
11:K:36:ILE:HD11	11:K:46:MET:SD	2.15	0.85
2:P:155:ASN:OD1	3:Q:77:THR:OG1	1.98	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:HE1	10:X:134:TYR:H	1.46	0.81
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.26	0.80
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.65	0.78
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.66	0.78
11:Y:200:TYR:HA	11:Y:201:SER:HB2	1.68	0.76
14:N:36:THR:CG2	14:N:46:ARG:HE	2.00	0.75
5:S:152[B]:ASN:OD1	20:S:401:HOH:O	2.06	0.73
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.03	0.72
1:O:10:THR:HG23	20:O:403:HOH:O	1.89	0.72
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.71	0.70
15:F:301:CL:CL	20:F:401:HOH:O	2.47	0.69
10:J:185:LYS:NZ	20:J:401:HOH:O	2.25	0.69
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.74	0.69
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.10	0.69
4:D:96:THR:OG1	20:D:401:HOH:O	2.10	0.69
6:F:169[A]:ARG:NH1	20:F:401:HOH:O	2.26	0.68
9:I:13[A]:MET:HE1	9:I:166:ILE:CA	2.25	0.67
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.77	0.67
3:C:47:LYS:CB	3:C:48:LYS:HA	2.25	0.67
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.43	0.66
10:J:99[A]:HIS:CD2	20:J:414:HOH:O	2.49	0.66
1:A:88[B]:ARG:NH2	20:A:401:HOH:O	2.28	0.65
5:E:68:ASN:ND2	5:E:220:GLU:OE1	2.28	0.65
10:X:1:MET:HE1	10:X:134:TYR:N	2.12	0.64
5:E:58:ALA:O	5:E:59:HIS:CB	2.45	0.64
7:U:195:VAL:O	7:U:199:ILE:HG23	1.98	0.63
5:E:101[A]:ARG:NH1	20:E:401:HOH:O	2.32	0.62
9:W:13:MET:HE1	9:W:166:ILE:N	2.14	0.62
1:A:108:GLN:NE2	1:A:112:ARG:HH12	1.96	0.62
11:Y:41:TYR:HB3	11:Y:74:ARG:NH1	2.14	0.62
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.81	0.62
9:I:13[A]:MET:CE	9:I:166:ILE:HB	2.30	0.61
4:R:129:ASP:CB	4:R:130:PRO:CD	2.79	0.61
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.33	0.61
15:M:302:CL:CL	15:M:303:CL:CL	2.92	0.61
3:C:47:LYS:CB	3:C:48:LYS:CA	2.79	0.60
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.16	0.60
15:A:302:CL:CL	15:A:303:CL:CL	13.36	0.60
5:S:68:ASN:ND2	5:S:220:GLU:OE1	2.35	0.59
9:W:13:MET:CE	9:W:166:ILE:HB	2.33	0.59
11:Y:159:ARG:HE	11:Y:163:GLN:HE21	1.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:CE	10:X:134:TYR:H	2.14	0.59
5:S:65[A]:HIS:CE1	20:Z:414:HOH:O	2.55	0.59
8:H:78:VAL:HG13	20:H:428:HOH:O	2.02	0.59
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.83	0.59
7:U:58:ASP:O	7:U:59:LYS:CB	2.51	0.59
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.85	0.58
11:Y:41:TYR:CZ	11:Y:74:ARG:HB3	2.38	0.58
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	2.04	0.58
9:W:13:MET:HE1	9:W:166:ILE:CA	2.32	0.58
11:K:41:TYR:HB3	11:K:74:ARG:NH1	2.19	0.58
8:H:154:ASN:ND2	20:H:404:HOH:O	2.37	0.58
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.69	0.57
10:J:27[A]:GLN:HE21	10:J:29:LYS:N	2.02	0.57
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.86	0.57
9:I:35:THR:HG21	20:I:487:HOH:O	2.04	0.57
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.35	0.57
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.86	0.57
6:T:6:GLY:HA3	6:T:7:TYR:CD2	2.39	0.57
10:J:1[A]:MET:CE	10:J:134:TYR:H	2.11	0.57
7:G:116:LYS:NZ	20:G:402:HOH:O	2.38	0.56
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.35	0.56
9:I:13[A]:MET:HE1	9:I:166:ILE:HB	1.88	0.56
7:U:118:ILE:HG21	7:U:138:MET:HE2	1.88	0.56
11:K:41:TYR:CZ	11:K:74:ARG:HB3	2.42	0.55
12:L:144:MET:CE	12:L:185:ARG:HB2	2.34	0.55
14:N:15:LEU:HD23	14:N:45:CYS:SG	2.46	0.55
2:B:92[B]:LEU:HG	2:B:96:ARG:NH1	2.22	0.55
10:J:182:ILE:CD1	10:J:191:LEU:HD11	2.37	0.55
4:R:129:ASP:CB	4:R:130:PRO:HD3	2.37	0.55
2:P:246:LYS:HE3	2:P:246:LYS:N	2.22	0.55
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.47	0.54
7:U:185:LYS:HD3	20:U:402:HOH:O	2.07	0.54
7:U:43:ARG:HB3	7:U:151:VAL:HG13	1.89	0.54
11:Y:39:ASN:ND2	11:Y:41:TYR:CZ	2.76	0.54
2:B:243:GLU:OE2	2:B:246:LYS:HD3	2.08	0.54
20:S:461:HOH:O	12:Z:66:LYS:HE3	2.07	0.54
6:T:53:VAL:HG12	6:T:208:ALA:HB1	1.90	0.54
9:W:13:MET:HE2	9:W:166:ILE:HB	1.89	0.54
15:B:301:CL:CL	15:B:302:CL:CL	2.99	0.54
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.90	0.54
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.90	0.53
8:H:78:VAL:CB	20:H:540:HOH:O	2.41	0.53
7:U:196:GLU:HG2	7:U:242:LEU:HD21	1.90	0.53
7:G:11:ARG:HH11	7:G:11:ARG:HG2	1.74	0.53
12:L:148:LEU:HD23	12:L:178:VAL:HG12	1.91	0.53
9:W:16[B]:LYS:NZ	20:W:401:HOH:O	2.25	0.52
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.58	0.52
3:Q:95:ARG:HG2	15:Q:301:CL:CL	2.46	0.52
4:R:96:THR:OG1	20:R:401:HOH:O	2.19	0.52
20:G:504:HOH:O	8:H:73:ARG:HD3	2.10	0.52
8:V:203:TYR:O	8:V:205:CYS:N	2.42	0.52
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.91	0.51
13:M:47:ASN:ND2	20:M:404:HOH:O	2.43	0.51
1:O:227:ASP:HB2	20:O:468:HOH:O	2.09	0.51
3:Q:96:LEU:HD13	10:X:62:LYS:HG2	1.92	0.51
1:A:158:LYS:HB3	1:A:177:TYR:CZ	2.45	0.51
13:M:112:ILE:HD12	13:M:112:ILE:N	2.25	0.51
1:O:10:THR:HB	1:O:20:GLN:HB2	1.92	0.51
11:Y:200:TYR:HA	11:Y:201:SER:CB	2.39	0.51
3:C:35:VAL:HG13	3:C:191:VAL:HG22	1.93	0.51
11:Y:41:TYR:HD1	20:Y:413:HOH:O	1.93	0.51
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.40	0.50
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.93	0.50
4:R:182:GLN:OE1	5:S:55:GLU:HB3	2.11	0.50
5:S:49:LEU:O	5:S:62:LYS:HD2	2.11	0.50
11:Y:10:ARG:NH2	11:Y:147:ASP:OD1	2.42	0.50
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.60	0.49
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.44	0.49
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.94	0.49
5:E:202:GLU:HG2	5:E:203:GLN:N	2.27	0.49
5:E:49:LEU:O	5:E:62:LYS:HD2	2.11	0.49
6:F:105:ASN:ND2	20:F:402:HOH:O	2.44	0.49
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	1.95	0.49
5:S:18[B]:ARG:CG	5:S:23:GLU:OE2	2.60	0.49
8:V:214:THR:HB	9:W:198:THR:OG1	2.12	0.49
11:Y:37:GLU:OE2	11:Y:187[A]:ARG:NH2	2.46	0.49
9:I:13[A]:MET:HE1	9:I:166:ILE:CB	2.43	0.49
3:C:183:THR:OG1	3:C:184:ASP:N	2.46	0.49
9:W:25[A]:ARG:HH11	9:W:25[A]:ARG:HG2	1.78	0.48
6:F:219:LEU:HD22	20:F:447:HOH:O	2.13	0.48
13:M:92:LEU:HD23	13:M:112:ILE:HD11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:202:ASP:OD1	6:T:204:VAL:HG12	2.13	0.48
3:C:183:THR:HG23	3:C:186:LEU:H	1.78	0.48
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.13	0.48
2:P:25[B]:MET:HE2	20:P:458:HOH:O	2.13	0.48
2:B:44:LEU:HD12	2:B:44:LEU:C	2.34	0.48
14:N:191:LEU:H	14:N:194:GLN:HE21	1.62	0.48
10:X:132:HIS:HD2	20:X:481:HOH:O	1.97	0.47
13:M:92:LEU:CD2	13:M:112:ILE:HD11	2.45	0.47
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.97	0.47
1:A:214:GLU:HB3	20:A:499:HOH:O	2.14	0.47
1:A:58[B]:GLU:H	1:A:58[B]:GLU:CD	2.18	0.47
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.97	0.47
2:P:53:HIS:O	2:P:54:LYS:HB2	2.14	0.47
9:I:27:PHE:HB3	9:I:35:THR:HG22	1.97	0.47
7:G:192:GLU:HG2	7:G:193:GLN:OE1	2.14	0.47
11:K:39:ASN:ND2	11:K:41:TYR:CZ	2.82	0.47
10:J:182:ILE:HD12	10:J:191:LEU:HD11	1.98	0.46
3:Q:183:THR:HG23	3:Q:186:LEU:H	1.80	0.46
6:F:34:SER:OG	6:F:65:ARG:NH1	2.48	0.46
5:S:50:LYS:CB	5:S:59:HIS:HB3	2.45	0.46
7:G:192:GLU:HG3	20:G:407:HOH:O	2.15	0.46
10:J:86:ARG:HD3	10:J:90:ASP:OD1	2.15	0.46
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.98	0.46
6:F:170:GLN:O	6:F:174:THR:HG23	2.16	0.46
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.98	0.46
18:N:303:1PE:H222	20:N:480:HOH:O	2.16	0.46
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.97	0.46
10:X:49:GLU:O	10:X:53:THR:HG23	2.16	0.46
2:P:44:LEU:HD12	2:P:44:LEU:C	2.36	0.46
6:T:170:GLN:O	6:T:174:THR:HG23	2.16	0.46
8:V:98:ALA:HB1	8:V:128[B]:MET:SD	2.56	0.45
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.41	0.45
10:X:86:ARG:HD3	10:X:90:ASP:OD1	2.16	0.45
5:E:65:HIS:HB2	20:E:435:HOH:O	2.16	0.45
6:F:7:TYR:OH	7:G:11:ARG:HD3	2.16	0.45
2:P:171:ALA:HB2	2:P:200:THR:HG21	1.99	0.45
7:G:42:VAL:HG13	7:G:198:ALA:HB2	1.99	0.45
1:A:94:GLN:HG3	8:H:66:LEU:HD13	1.99	0.45
8:H:133:LEU:HD22	14:N:26:TYR:CZ	2.51	0.45
2:P:124:PHE:CD1	3:Q:124:ARG:HG2	2.52	0.45
10:J:49:GLU:O	10:J:53:THR:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25[A]:ARG:HG2	9:I:25[A]:ARG:HH11	1.80	0.45
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	2.17	0.45
9:W:13:MET:HE1	9:W:166:ILE:HB	1.98	0.45
3:Q:183:THR:OG1	3:Q:184:ASP:N	2.50	0.45
4:D:166:ASP:HB3	4:D:185:TYR:CZ	2.52	0.44
7:U:80[A]:MET:HE3	7:U:91:VAL:HG23	1.99	0.44
6:F:243:LEU:O	6:F:244:LYS:C	2.55	0.44
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.46	0.44
3:C:41:VAL:CG2	3:C:211:MET:HB3	2.47	0.44
2:P:76:VAL:HG12	2:P:134:LEU:HG	1.98	0.44
9:W:27:PHE:HB3	9:W:35:THR:HG22	1.99	0.44
2:P:190:LEU:HG	2:P:236:LEU:HD21	1.99	0.44
4:R:151:PRO:O	4:R:152:GLN:HG3	2.18	0.44
6:T:206:ASP:O	6:T:206:ASP:OD1	2.35	0.44
5:E:218:ASP:OD1	5:E:218:ASP:N	2.47	0.44
6:T:34:SER:OG	6:T:65:ARG:NH1	2.49	0.44
3:C:50:VAL:O	3:C:51:ALA:HB3	2.17	0.44
20:Q:463:HOH:O	4:R:60:GLU:HG3	2.17	0.44
6:T:152:ASP:OD1	6:T:156:VAL:HG12	2.18	0.44
7:U:51:VAL:HG12	7:U:198:ALA:HB1	2.00	0.44
10:X:1:MET:HG2	10:X:2:GLU:H	1.83	0.44
11:Y:68:GLU:HB2	20:Y:401:HOH:O	2.18	0.43
12:Z:148:LEU:HD23	12:Z:178:VAL:HG12	1.99	0.43
2:P:194:ILE:CD1	2:P:236:LEU:HB3	2.48	0.43
11:Y:13:VAL:HG13	11:Y:180:VAL:HB	1.99	0.43
1:A:158:LYS:HB3	1:A:177:TYR:CE1	2.53	0.43
12:L:184:GLU:OE2	12:L:211:ARG:HD2	2.18	0.43
2:B:33:THR:HB	2:B:166:ASN:O	2.17	0.43
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.18	0.43
1:A:74:VAL:HG22	1:A:75:TYR:H	1.84	0.43
6:F:202:ASP:OD1	6:F:204:VAL:HG22	2.19	0.43
8:H:78:VAL:CG1	20:H:540:HOH:O	2.67	0.43
7:G:188:ASP:O	7:G:190:THR:HG22	2.17	0.43
2:P:33:THR:HB	2:P:166:ASN:O	2.17	0.43
5:E:202:GLU:CG	5:E:203:GLN:N	2.82	0.43
5:S:71:GLY:HA3	5:S:221:PHE:CZ	2.54	0.43
4:R:196:LYS:HE3	4:R:240:ASP:HB3	2.00	0.43
6:T:205:LYS:O	6:T:206:ASP:CG	2.57	0.43
2:B:76:VAL:HG12	2:B:134:LEU:HG	2.00	0.42
3:C:40:ILE:HD11	3:C:210:VAL:CG1	2.48	0.42
5:E:67:ASP:OD1	12:L:73:LYS:HE2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:PRO:O	4:D:152:GLN:HG3	2.19	0.42
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.19	0.42
14:N:36:THR:HG21	14:N:46:ARG:HE	1.77	0.42
7:U:195:VAL:HG13	7:U:196:GLU:OE1	2.20	0.42
3:C:35:VAL:CG1	3:C:191:VAL:HG22	2.50	0.42
8:V:140:GLU:HA	8:V:140:GLU:OE2	2.20	0.42
11:K:142:ARG:NH1	10:X:166:GLU:OE2	2.53	0.42
4:R:128:ALA:HB1	20:R:435:HOH:O	2.19	0.42
3:C:33:VAL:HG21	3:C:195:LEU:HD12	2.02	0.42
1:O:230:ALA:O	1:O:231:ALA:CB	2.68	0.42
1:A:142:ARG:NH1	1:A:143:PRO:O	2.49	0.42
2:B:176:LYS:NZ	20:B:403:HOH:O	2.47	0.42
4:D:203:LYS:HE2	4:D:210:LEU:HB3	2.00	0.42
6:F:53:VAL:HG12	6:F:208:ALA:HB3	2.01	0.42
5:S:101:ARG:NH1	20:S:405:HOH:O	2.52	0.42
7:U:199:ILE:HD11	7:U:239:LEU:CD2	2.46	0.42
7:U:42:VAL:HG13	7:U:198:ALA:HB2	2.01	0.42
10:J:1[A]:MET:HG2	10:J:2:GLU:H	1.84	0.41
5:S:46:LEU:HD13	5:S:73:SER:HB2	2.01	0.41
2:B:171:ALA:HB2	2:B:200:THR:HG21	2.02	0.41
10:X:46[B]:CYS:SG	10:X:102:LEU:CD2	3.09	0.41
5:S:45:VAL:CG1	5:S:187:LEU:HD23	2.50	0.41
3:C:203:GLY:CA	3:C:204:LYS:CB	2.99	0.41
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.55	0.41
7:U:186:LYS:HA	20:U:432:HOH:O	2.21	0.41
11:Y:200:TYR:CA	11:Y:201:SER:CB	2.99	0.41
10:J:9:GLY:HA3	10:J:12:TYR:CE2	2.55	0.41
3:C:201:SER:O	3:C:202:GLY:C	2.59	0.41
7:G:183:VAL:HG13	7:G:191:PHE:CZ	2.56	0.41
11:K:13:VAL:HG13	11:K:180:VAL:HB	2.02	0.41
10:J:93:ARG:HD2	20:J:485:HOH:O	2.21	0.41
11:Y:36:ILE:CD1	11:Y:46:MET:SD	2.98	0.41
4:D:117:SER:OG	5:E:82:ARG:NH2	2.54	0.40
6:F:169[A]:ARG:NH1	20:F:409:HOH:O	2.54	0.40
5:E:171:TYR:CD2	5:E:171:TYR:C	2.95	0.40
10:J:137:PHE:HB3	11:Y:134:VAL:HG21	2.03	0.40
11:K:53:CYS:SG	11:K:98:MET:HG3	2.61	0.40
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.21	0.40
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.53	0.40
3:Q:105:GLU:HG3	3:Q:145:TYR:OH	2.22	0.40
6:T:140:TYR:CE2	6:T:218:GLU:HG2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:50:ALA:HB1	9:W:128:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/234 (99%)	220 (95%)	7 (3%)	4 (2%)	11	4
1	O	228/234 (97%)	215 (94%)	8 (4%)	5 (2%)	8	3
2	B	248/261 (95%)	239 (96%)	8 (3%)	1 (0%)	39	33
2	P	247/261 (95%)	233 (94%)	10 (4%)	4 (2%)	12	5
3	C	236/248 (95%)	222 (94%)	7 (3%)	7 (3%)	5	1
3	Q	236/248 (95%)	219 (93%)	7 (3%)	10 (4%)	3	1
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	15	7
4	R	232/241 (96%)	225 (97%)	4 (2%)	3 (1%)	15	7
5	E	232/263 (88%)	228 (98%)	3 (1%)	1 (0%)	39	33
5	S	238/263 (90%)	232 (98%)	5 (2%)	1 (0%)	39	33
6	F	241/255 (94%)	237 (98%)	4 (2%)	0	100	100
6	T	239/255 (94%)	234 (98%)	2 (1%)	3 (1%)	15	7
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%)	217 (99%)	2 (1%)	1 (0%)	34	26
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	34	26
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100	100
9	W	204/205 (100%)	200 (98%)	4 (2%)	0	100	100
10	J	195/201 (97%)	193 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	198/204 (97%)	195 (98%)	3 (2%)	0	100	100
11	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	34	26
12	L	213/213 (100%)	210 (99%)	3 (1%)	0	100	100
12	Z	212/213 (100%)	209 (99%)	3 (1%)	0	100	100
13	M	215/219 (98%)	210 (98%)	5 (2%)	0	100	100
13	a	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	201 (100%)	1 (0%)	0	100	100
All	All	6211/6458 (96%)	6043 (97%)	123 (2%)	45 (1%)	26	19

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
5	E	59	HIS
1	O	52	LYS
1	O	53	SER
2	P	54	LYS
3	Q	47	LYS
3	Q	201	SER
3	Q	206	ILE
3	Q	221	ASN
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
6	T	7	TYR
8	V	204	ARG
11	Y	201	SER
1	A	50	LYS
3	C	200	GLN
4	D	176	GLY
1	O	176	ARG
1	O	231	ALA
2	P	204	SER
2	P	247	ALA
3	Q	138	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	200	GLN
6	T	206	ASP
1	A	176	ARG
2	B	203	VAL
3	C	50	VAL
3	C	138	PHE
8	H	204	ARG
1	O	50	LYS
3	Q	50	VAL
6	T	208	ALA
3	C	51	ALA
3	C	204	LYS
3	Q	48	LYS
3	C	203	GLY
3	C	216	SER
4	D	175[A]	GLU
4	D	175[B]	GLU
2	P	52	ILE
3	Q	216	SER
3	Q	203	GLY

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%)	175 (95%)	10 (5%)	27	21
1	O	176/191 (92%)	165 (94%)	11 (6%)	22	16
2	B	200/221 (90%)	195 (98%)	5 (2%)	55	55
2	P	196/221 (89%)	184 (94%)	12 (6%)	23	17
3	C	179/210 (85%)	169 (94%)	10 (6%)	26	20
3	Q	184/210 (88%)	173 (94%)	11 (6%)	24	17
4	D	189/203 (93%)	183 (97%)	6 (3%)	46	44
4	R	187/203 (92%)	183 (98%)	4 (2%)	61	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	192/223 (86%)	184 (96%)	8 (4%)	36	31
5	S	197/223 (88%)	192 (98%)	5 (2%)	55	55
6	F	199/212 (94%)	188 (94%)	11 (6%)	27	21
6	T	192/212 (91%)	182 (95%)	10 (5%)	29	23
7	G	202/207 (98%)	195 (96%)	7 (4%)	43	40
7	U	186/207 (90%)	181 (97%)	5 (3%)	52	52
8	H	181/195 (93%)	175 (97%)	6 (3%)	45	43
8	V	172/195 (88%)	162 (94%)	10 (6%)	25	19
9	I	176/174 (101%)	174 (99%)	2 (1%)	80	83
9	W	173/174 (99%)	171 (99%)	2 (1%)	78	81
10	J	166/170 (98%)	158 (95%)	8 (5%)	31	26
10	X	165/170 (97%)	158 (96%)	7 (4%)	36	31
11	K	154/159 (97%)	147 (96%)	7 (4%)	34	29
11	Y	159/159 (100%)	150 (94%)	9 (6%)	25	19
12	L	175/178 (98%)	167 (95%)	8 (5%)	33	28
12	Z	175/178 (98%)	169 (97%)	6 (3%)	44	41
13	M	180/181 (99%)	175 (97%)	5 (3%)	51	50
13	a	178/181 (98%)	174 (98%)	4 (2%)	60	62
14	N	157/159 (99%)	153 (98%)	4 (2%)	55	55
14	b	158/159 (99%)	153 (97%)	5 (3%)	46	44
All	All	5033/5366 (94%)	4835 (96%)	198 (4%)	40	35

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	53	SER
1	A	54	ILE
1	A	142	ARG
1	A	176	ARG
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	33	THR
2	B	59	VAL
2	B	190	LEU
2	B	229	LYS
2	B	249	ARG
3	C	35	VAL
3	C	45	VAL
3	C	54	GLN
3	C	105	GLU
3	C	148	ASP
3	C	163	ARG
3	C	179	GLU
3	C	205	ASN
3	C	208	LEU
3	C	226	GLU
4	D	9	ASP
4	D	46	VAL
4	D	95	GLU
4	D	117	SER
4	D	126	GLU
4	D	199	LEU
5	E	29	VAL
5	E	61	LYS
5	E	95	SER
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	180	MET
5	E	181	GLU
5	E	189	LYS
6	F	17	ASP
6	F	31	GLU
6	F	53	VAL
6	F	81	LEU
6	F	86	SER
6	F	87	LEU
6	F	174	THR
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	88	ARG
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
7	G	209	ASP
8	H	7	VAL
8	H	13	ILE
8	H	66	LEU
8	H	69	LEU
8	H	74	LEU
8	H	184	LEU
9	I	35	THR
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	27[A]	GLN
10	J	27[B]	GLN
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	155	ARG
11	K	13	VAL
11	K	139	VAL
11	K	142	ARG
11	K	148	LEU
11	K	159	ARG
11	K	175	VAL
11	K	188	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	102	PHE
12	L	163	HIS
12	L	169	ASP
12	L	172	MET
12	L	174	LEU
12	L	207	THR
13	M	100	ARG
13	M	154	LEU
13	M	155	GLU
13	M	198	GLU
13	M	216	SER
14	N	23	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	36	THR
14	N	85	LYS
14	N	197	LYS
1	O	10	THR
1	O	53	SER
1	O	118	GLN
1	O	142	ARG
1	O	176	ARG
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	221	THR
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	59	VAL
2	P	124	PHE
2	P	183	GLU
2	P	190	LEU
2	P	204	SER
2	P	230	GLN
2	P	235	GLN
2	P	236	LEU
2	P	246	LYS
3	Q	45	VAL
3	Q	56	GLU
3	Q	98	VAL
3	Q	105	GLU
3	Q	148	ASP
3	Q	163	ARG
3	Q	170	GLU
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	227	LYS
4	R	9	ASP
4	R	32	LYS
4	R	46	VAL
4	R	117	SER
5	S	29	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	45	VAL
5	S	95	SER
5	S	101	ARG
5	S	180	MET
6	T	17	ASP
6	T	31	GLU
6	T	53	VAL
6	T	81	LEU
6	T	86	SER
6	T	87	LEU
6	T	174	THR
6	T	190	VAL
6	T	215	TRP
6	T	240	LYS
7	U	42	VAL
7	U	78	CYS
7	U	196	GLU
7	U	199	ILE
7	U	206	LEU
8	V	7	VAL
8	V	13	ILE
8	V	66	LEU
8	V	69	LEU
8	V	74	LEU
8	V	105[A]	ASP
8	V	105[B]	ASP
8	V	184	LEU
8	V	200	LEU
8	V	214	THR
9	W	35	THR
9	W	193	LYS
10	X	1	MET
10	X	27	GLN
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	158	GLU
10	X	174	ASN
11	Y	9	PHE
11	Y	13	VAL
11	Y	107	LYS
11	Y	139	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	142[A]	ARG
11	Y	142[B]	ARG
11	Y	148	LEU
11	Y	187[A]	ARG
11	Y	187[B]	ARG
12	Z	102	PHE
12	Z	169	ASP
12	Z	172	MET
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
13	a	100	ARG
13	a	154	LEU
13	a	198	GLU
13	a	216	SER
14	b	23	THR
14	b	30	ARG
14	b	36	THR
14	b	85	LYS
14	b	197	LYS

Some 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
2	B	109	GLN
3	C	175	ASN
5	E	65	HIS
6	F	143	ASN
8	H	117	HIS
8	H	154	ASN
9	I	161	HIS
10	J	101	ASN
10	J	132	HIS
11	K	163	GLN
12	L	157	ASN
13	M	162	GLN
14	N	194	GLN
1	O	62	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	146	GLN
3	Q	18	GLN
3	Q	175	ASN
4	R	186	HIS
5	S	86	ASN
6	T	68	ASN
6	T	143	ASN
8	V	117	HIS
9	W	172	ASN
10	X	24	ASN
10	X	132	HIS
10	X	174	ASN
11	Y	163	GLN
12	Z	79	ASN
12	Z	157	ASN
13	a	89	HIS
13	a	162	GLN
14	b	194	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	$\# Z > 2$
3	YCM	C	63	3	7,9,10	1.25	2 (28%)	5,10,12	1.79	2 (40%)
5	6V1	E	148	5	11,15,16	1.33	2 (18%)	11,20,22	2.14	6 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	YCM	G	137	7	7,9,10	3.32	4 (57%)	5,10,12	6.90	4 (80%)
7	6V1	G	161	7	11,15,16	1.39	2 (18%)	11,20,22	3.59	8 (72%)
7	6V1	G	47	7	11,15,16	1.72	3 (27%)	11,20,22	2.99	3 (27%)
10	6V1	J	91	10	11,15,16	1.53	3 (27%)	11,20,22	5.68	7 (63%)
3	YCM	Q	63	3	7,9,10	1.45	2 (28%)	5,10,12	3.06	3 (60%)
5	6V1	S	148	5	11,15,16	1.39	3 (27%)	11,20,22	1.84	4 (36%)
7	YCM	U	137	7	7,9,10	1.74	2 (28%)	5,10,12	1.80	3 (60%)
7	6V1	U	161	7	11,15,16	1.35	2 (18%)	11,20,22	2.81	4 (36%)
7	6V1	U	47	7	11,15,16	1.14	1 (9%)	11,20,22	3.61	3 (27%)
10	6V1	X	91	10	11,15,16	1.57	3 (27%)	11,20,22	5.71	7 (63%)

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

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CB-SG	-4.91	1.71	1.81
7	U	137	YCM	CB-SG	-3.61	1.74	1.81
7	G	47	6V1	C4-N3	-3.34	1.32	1.38
7	U	161	6V1	C4-N3	-2.98	1.33	1.38
7	G	161	6V1	C2-N3	-2.95	1.34	1.38
10	J	91	6V1	C1-SG	-2.85	1.79	1.83
7	G	47	6V1	C2-N3	-2.62	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	148	6V1	C2-N3	-2.58	1.35	1.38
3	Q	63	YCM	CD-SG	-2.56	1.76	1.81
10	J	91	6V1	C4-N3	-2.52	1.34	1.38
5	E	148	6V1	C4-N3	-2.50	1.34	1.38
7	U	161	6V1	C2-N3	-2.43	1.35	1.38
7	G	161	6V1	C4-N3	-2.40	1.34	1.38
7	U	47	6V1	C4-N3	-2.30	1.34	1.38
3	C	63	YCM	CB-SG	-2.26	1.76	1.81
3	C	63	YCM	CD-SG	-2.23	1.76	1.81
5	S	148	6V1	C4-N3	-2.20	1.34	1.38
10	X	91	6V1	C4-N3	-2.19	1.34	1.38
3	Q	63	YCM	CB-SG	-2.18	1.77	1.81
5	S	148	6V1	C2-N3	-2.12	1.35	1.38
10	X	91	6V1	C5-C4	2.08	1.54	1.50
10	J	91	6V1	O7-C2	2.23	1.26	1.22
5	S	148	6V1	C1-C2	2.27	1.54	1.52
7	U	137	YCM	CD-CE	2.32	1.58	1.51
7	G	47	6V1	C1-SG	2.91	1.86	1.83
10	X	91	6V1	C1-C2	3.28	1.55	1.52
7	G	137	YCM	CE-NZ2	3.34	1.43	1.32
7	G	137	YCM	CD-CE	4.40	1.63	1.51
7	G	137	YCM	CD-SG	4.50	1.91	1.81

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	47	6V1	C5-C1-C2	-6.29	99.20	103.98
10	X	91	6V1	O7-C2-C1	-5.89	114.55	125.18
7	G	161	6V1	C5-C1-C2	-5.81	99.56	103.98
7	U	161	6V1	C5-C1-C2	-5.51	99.79	103.98
10	J	91	6V1	C6-N3-C4	-5.48	117.41	123.24
10	X	91	6V1	C6-N3-C4	-5.38	117.52	123.24
7	U	47	6V1	C5-C1-C2	-5.26	99.98	103.98
10	J	91	6V1	O7-C2-C1	-5.10	115.98	125.18
10	X	91	6V1	O8-C4-C5	-4.98	120.71	127.38
7	G	161	6V1	O8-C4-C5	-4.56	121.27	127.38
10	J	91	6V1	O8-C4-C5	-4.28	121.64	127.38
5	E	148	6V1	C5-C1-C2	-4.27	100.73	103.98
3	Q	63	YCM	CA-CB-SG	-4.02	103.33	112.84
5	S	148	6V1	C5-C1-C2	-3.71	101.16	103.98
7	G	161	6V1	O7-C2-C1	-3.49	118.88	125.18
7	G	137	YCM	OZ1-CE-CD	-3.46	113.19	120.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	161	6V1	O8-C4-C5	-3.27	122.99	127.38
5	S	148	6V1	O8-C4-C5	-2.90	123.49	127.38
3	C	63	YCM	CD-CE-NZ2	-2.74	112.47	115.48
5	E	148	6V1	CA-CB-SG	-2.65	106.74	112.87
7	G	137	YCM	OZ1-CE-NZ2	-2.54	115.30	122.52
7	G	137	YCM	CA-CB-SG	-2.52	106.88	112.84
7	G	161	6V1	CA-CB-SG	-2.49	107.12	112.87
10	J	91	6V1	CA-CB-SG	-2.46	107.18	112.87
3	Q	63	YCM	O-C-CA	-2.36	119.39	125.72
5	E	148	6V1	O8-C4-C5	-2.32	124.27	127.38
5	E	148	6V1	O-C-CA	-2.31	119.53	125.72
10	X	91	6V1	CA-CB-SG	-2.24	107.68	112.87
5	S	148	6V1	O-C-CA	-2.20	119.82	125.72
7	U	137	YCM	CA-CB-SG	-2.15	107.76	112.84
3	C	63	YCM	O-C-CA	-2.13	120.01	125.72
7	U	137	YCM	O-C-CA	-2.03	120.28	125.72
7	G	161	6V1	O7-C2-N3	2.06	127.04	124.19
5	E	148	6V1	C6-N3-C2	2.07	125.02	123.42
7	U	137	YCM	OZ1-CE-CD	2.27	126.10	120.98
5	S	148	6V1	C6-N3-C2	2.44	125.31	123.42
5	E	148	6V1	C6-N3-C4	2.69	126.11	123.24
7	G	161	6V1	CB-SG-C1	3.13	107.81	101.58
7	G	47	6V1	C6-N3-C2	3.18	125.89	123.42
7	U	161	6V1	C6-N3-C2	3.93	126.47	123.42
7	G	161	6V1	O8-C4-N3	4.09	128.99	123.91
7	U	161	6V1	CB-SG-C1	4.14	109.81	101.58
7	U	47	6V1	C6-N3-C2	4.54	126.95	123.42
3	Q	63	YCM	CD-CE-NZ2	4.85	120.83	115.48
7	G	161	6V1	C6-N3-C2	5.63	127.80	123.42
7	G	47	6V1	CB-SG-C1	6.60	114.70	101.58
10	J	91	6V1	O7-C2-N3	6.92	133.75	124.19
10	X	91	6V1	O7-C2-N3	7.17	134.10	124.19
10	X	91	6V1	CB-SG-C1	8.07	117.63	101.58
10	J	91	6V1	CB-SG-C1	8.60	118.69	101.58
7	U	47	6V1	CB-SG-C1	9.36	120.20	101.58
10	X	91	6V1	C6-N3-C2	11.81	132.60	123.42
10	J	91	6V1	C6-N3-C2	12.03	132.78	123.42
7	G	137	YCM	CD-CE-NZ2	14.51	131.46	115.48

All (1) chirality outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
-----	-------	-----	------	------

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 67 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
18	1PE	H	304	-	15,15,15	0.45	0	14,14,14	0.48	0
19	6V8	H	305	8	22,23,23	2.35	3 (13%)	26,31,31	2.80	9 (34%)
18	1PE	I	303	-	15,15,15	0.58	0	14,14,14	0.91	0
18	1PE	I	304	-	15,15,15	0.52	0	14,14,14	0.80	0
19	6V8	K	305	11	22,23,23	1.60	3 (13%)	26,31,31	2.09	6 (23%)
18	1PE	L	301	-	15,15,15	0.62	0	14,14,14	0.76	0
18	1PE	M	305	-	15,15,15	0.52	0	14,14,14	0.44	0
18	1PE	N	303	-	15,15,15	0.52	0	14,14,14	0.79	0
19	6V8	N	305	14	22,23,23	1.31	2 (9%)	26,31,31	1.92	7 (26%)
19	6V8	V	303	8	22,23,23	2.67	3 (13%)	26,31,31	2.89	10 (38%)
18	1PE	W	303	-	15,15,15	0.59	0	14,14,14	0.48	0
18	1PE	Y	305	-	15,15,15	0.58	0	14,14,14	0.56	0
19	6V8	Y	306	11	22,23,23	1.61	4 (18%)	26,31,31	2.64	9 (34%)
18	1PE	b	302	-	15,15,15	0.65	0	14,14,14	1.08	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	6V8	b	304	14	22,23,23	1.69	1 (4%)	26,31,31	1.47	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	H	304	-	-	0/13/13/13	0/0/0/0
19	6V8	H	305	8	-	0/15/21/21	0/1/1/1
18	1PE	I	303	-	-	0/13/13/13	0/0/0/0
18	1PE	I	304	-	-	0/13/13/13	0/0/0/0
19	6V8	K	305	11	-	0/15/21/21	0/1/1/1
18	1PE	L	301	-	-	0/13/13/13	0/0/0/0
18	1PE	M	305	-	-	0/13/13/13	0/0/0/0
18	1PE	N	303	-	-	0/13/13/13	0/0/0/0
19	6V8	N	305	14	-	0/15/21/21	0/1/1/1
19	6V8	V	303	8	-	0/15/21/21	0/1/1/1
18	1PE	W	303	-	-	0/13/13/13	0/0/0/0
18	1PE	Y	305	-	-	0/13/13/13	0/0/0/0
19	6V8	Y	306	11	-	0/15/21/21	0/1/1/1
18	1PE	b	302	-	-	0/13/13/13	0/0/0/0
19	6V8	b	304	14	-	0/15/21/21	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	306	6V8	C1-C2	-4.74	1.32	1.39
19	Y	306	6V8	C4-C5	-2.73	1.33	1.38
19	K	305	6V8	C1-C2	-2.56	1.35	1.39
19	Y	306	6V8	O8-C7	-2.12	1.19	1.23
19	Y	306	6V8	C2-C3	2.29	1.42	1.39
19	K	305	6V8	C6-CL6	2.44	1.80	1.74
19	V	303	6V8	C6-CL6	2.57	1.80	1.74
19	H	305	6V8	C3-CL3	2.80	1.80	1.73
19	N	305	6V8	C3-CL3	2.82	1.80	1.73
19	H	305	6V8	C6-CL6	2.98	1.81	1.74
19	V	303	6V8	C3-CL3	3.36	1.82	1.73
19	N	305	6V8	C2-C3	3.99	1.44	1.39
19	K	305	6V8	C2-C3	5.47	1.46	1.39
19	b	304	6V8	C2-C3	6.94	1.48	1.39
19	H	305	6V8	C2-C3	9.28	1.52	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	V	303	6V8	C2-C3	11.01	1.54	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	306	6V8	C2-C3-CL3	-6.51	111.06	121.03
19	K	305	6V8	C2-C3-CL3	-5.69	112.31	121.03
19	Y	306	6V8	C1-C6-CL6	-5.53	111.77	119.13
19	H	305	6V8	O8-C7-C2	-4.68	111.77	120.94
19	H	305	6V8	C4-C3-C2	-4.31	116.20	121.32
19	V	303	6V8	C4-C3-C2	-3.91	116.68	121.32
19	V	303	6V8	C1-C2-C7	-3.81	105.85	117.47
19	V	303	6V8	C4-C3-CL3	-3.61	110.88	118.40
19	K	305	6V8	C5-C4-C3	-3.60	114.70	119.96
19	N	305	6V8	C1-C6-CL6	-3.51	114.47	119.13
19	Y	306	6V8	C5-C4-C3	-3.44	114.93	119.96
19	Y	306	6V8	C1-C2-C3	-3.36	113.44	117.90
19	N	305	6V8	O8-C7-C2	-3.33	114.41	120.94
19	K	305	6V8	C1-C6-CL6	-2.95	115.20	119.13
19	N	305	6V8	C2-C1-C6	-2.94	114.65	119.78
19	H	305	6V8	C4-C3-CL3	-2.90	112.36	118.40
19	H	305	6V8	C1-C2-C7	-2.88	108.68	117.47
19	b	304	6V8	O8-C7-C2	-2.64	115.77	120.94
19	V	303	6V8	C1-C6-CL6	-2.46	115.86	119.13
19	N	305	6V8	C4-C5-C6	-2.43	116.59	119.22
19	Y	306	6V8	O8-C7-C2	-2.40	116.24	120.94
19	b	304	6V8	C1-C6-CL6	-2.39	115.96	119.13
19	V	303	6V8	O8-C7-C2	-2.05	116.91	120.94
19	N	305	6V8	C10-N9-C7	2.10	126.12	121.33
19	N	305	6V8	C4-C3-C2	2.19	123.93	121.32
19	V	303	6V8	C5-C6-CL6	2.38	123.37	119.35
19	Y	306	6V8	C10-N9-C7	2.47	126.98	121.33
19	K	305	6V8	C5-C6-C1	2.66	125.17	121.53
19	K	305	6V8	C10-N9-C7	2.91	127.99	121.33
19	H	305	6V8	O8-C7-N9	3.01	128.81	122.52
18	b	302	1PE	C26-OH6-C15	3.12	126.63	113.31
19	V	303	6V8	C4-C5-C6	3.13	122.62	119.22
19	Y	306	6V8	C3-C2-C7	3.27	127.37	122.74
19	H	305	6V8	C4-C5-C6	3.27	122.78	119.22
19	Y	306	6V8	C5-C6-C1	3.54	126.38	121.53
19	b	304	6V8	C5-C6-C1	3.63	126.50	121.53
19	V	303	6V8	C10-N9-C7	3.84	130.11	121.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	H	305	6V8	C10-N9-C7	4.18	130.88	121.33
19	K	305	6V8	C4-C3-C2	4.62	126.82	121.32
19	N	305	6V8	C5-C6-C1	5.24	128.69	121.53
19	Y	306	6V8	C4-C3-C2	5.92	128.36	121.32
19	H	305	6V8	C2-C3-CL3	6.80	131.44	121.03
19	H	305	6V8	C3-C2-C7	6.85	132.45	122.74
19	V	303	6V8	C2-C3-CL3	7.46	132.44	121.03
19	V	303	6V8	C3-C2-C7	8.00	134.08	122.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	303	1PE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/234 (98%)	-0.15	2 (0%) 85 86	31, 45, 86, 98	0
1	O	230/234 (98%)	0.29	14 (6%) 25 26	43, 67, 110, 149	0
2	B	248/261 (95%)	-0.01	4 (1%) 74 75	34, 54, 98, 137	0
2	P	247/261 (94%)	0.21	14 (5%) 27 29	39, 60, 107, 154	0
3	C	236/248 (95%)	0.23	14 (5%) 26 27	37, 65, 106, 136	0
3	Q	238/248 (95%)	0.32	17 (7%) 19 20	37, 66, 126, 160	0
4	D	233/241 (96%)	0.05	4 (1%) 73 73	38, 61, 91, 135	0
4	R	233/241 (96%)	-0.11	4 (1%) 73 73	32, 48, 76, 116	0
5	E	233/263 (88%)	-0.04	9 (3%) 43 45	27, 43, 91, 112	0
5	S	237/263 (90%)	0.02	8 (3%) 49 50	37, 53, 88, 113	0
6	F	239/255 (93%)	-0.19	0 100 100	26, 36, 60, 82	0
6	T	240/255 (94%)	0.17	8 (3%) 50 51	41, 61, 96, 135	0
7	G	241/246 (97%)	-0.15	3 (1%) 81 81	28, 40, 72, 110	0
7	U	235/246 (95%)	0.21	11 (4%) 35 37	48, 70, 106, 140	0
8	H	220/234 (94%)	-0.12	3 (1%) 78 78	27, 38, 75, 126	0
8	V	220/234 (94%)	-0.10	3 (1%) 78 78	39, 52, 83, 120	0
9	I	204/205 (99%)	-0.22	0 100 100	29, 38, 60, 77	0
9	W	204/205 (99%)	-0.13	0 100 100	33, 50, 78, 88	0
10	J	195/201 (97%)	-0.22	1 (0%) 91 92	33, 44, 62, 78	0
10	X	195/201 (97%)	-0.26	0 100 100	33, 44, 60, 81	0
11	K	200/204 (98%)	-0.21	1 (0%) 91 92	33, 47, 76, 88	0
11	Y	201/204 (98%)	-0.23	3 (1%) 76 77	29, 39, 64, 84	0
12	L	213/213 (100%)	-0.13	0 100 100	32, 48, 71, 91	0
12	Z	213/213 (100%)	-0.21	0 100 100	28, 39, 65, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.16	0 100 100	28, 42, 67, 96	0
13	a	216/219 (98%)	-0.19	1 (0%) 91 92	31, 44, 64, 86	0
14	N	202/205 (98%)	-0.16	3 (1%) 76 77	28, 38, 60, 101	0
14	b	203/205 (99%)	-0.14	2 (0%) 84 84	36, 47, 72, 111	0
All	All	6222/6458 (96%)	-0.05	129 (2%) 67 67	26, 49, 91, 160	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	232	ILE	12.9
2	P	204	SER	12.3
4	D	241	ILE	8.5
3	Q	234	LYS	6.7
13	a	216	SER	6.5
2	P	203	VAL	6.1
11	K	41	TYR	5.9
3	C	49	SER	5.9
8	V	204	ARG	5.5
1	O	225	VAL	5.2
3	Q	202	GLY	5.1
8	H	205	CYS	5.1
6	T	208	ALA	5.1
3	Q	232	ILE	5.0
7	U	2	SER	5.0
5	E	54	SER	5.0
2	P	61	PHE	4.8
5	S	57	ALA	4.7
8	V	200	LEU	4.6
2	B	61	PHE	4.4
5	E	52	ALA	4.3
3	C	138	PHE	4.2
3	Q	238	GLU	4.2
7	U	206	LEU	4.1
8	H	204	ARG	4.1
1	O	201	GLN	3.9
3	Q	233	GLU	3.9
4	R	241	ILE	3.9
7	U	3	ARG	3.8
6	T	206	ASP	3.8
5	E	58	ALA	3.7
2	P	234	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	203	GLY	3.6
4	R	130	PRO	3.5
5	S	2	PHE	3.4
2	P	205	LYS	3.4
3	Q	200	GLN	3.4
11	Y	41	TYR	3.4
5	E	201	ALA	3.3
2	P	202	ASP	3.2
5	E	53	GLN	3.2
3	Q	236	LYS	3.2
2	P	247	ALA	3.2
3	Q	229	VAL	3.2
2	P	51	ASN	3.1
2	B	203	VAL	3.1
5	S	174	ARG	3.1
1	O	200	GLY	3.0
14	N	201	ALA	3.0
5	S	56	LEU	3.0
1	O	186	ALA	2.9
3	C	225	ILE	2.8
7	G	187	PHE	2.8
3	C	236	LYS	2.8
7	U	178	PHE	2.8
3	Q	240	GLU	2.8
7	U	186	LYS	2.7
5	S	54	SER	2.7
3	C	232	ILE	2.7
3	C	48	LYS	2.7
7	U	58	ASP	2.7
1	A	232	ILE	2.7
7	G	188	ASP	2.7
1	O	181	LEU	2.6
11	Y	202	GLY	2.6
1	O	229	LEU	2.6
6	T	205	LYS	2.6
6	T	54	LEU	2.6
7	G	189	TRP	2.5
3	Q	201	SER	2.5
3	Q	48	LYS	2.5
2	B	204	SER	2.5
4	R	131	GLY	2.5
14	b	204	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	184	GLU	2.4
3	Q	223	GLU	2.4
5	S	239	ARG	2.4
1	A	231	ALA	2.4
3	C	203	GLY	2.4
3	Q	226	GLU	2.4
7	U	7	ALA	2.4
3	C	200	GLN	2.4
3	C	98	VAL	2.4
1	O	157	TRP	2.4
3	C	202	GLY	2.4
4	D	131	GLY	2.4
5	S	51	ARG	2.4
4	R	128	ALA	2.4
5	E	56	LEU	2.3
3	C	234	LYS	2.3
2	B	205	LYS	2.3
14	N	203	LEU	2.3
3	C	201	SER	2.3
7	U	50	ILE	2.3
2	P	233	VAL	2.3
3	C	229	VAL	2.3
2	P	230	GLN	2.3
1	O	198	PHE	2.3
3	C	233	GLU	2.3
2	P	244	GLU	2.3
14	b	201	ALA	2.2
6	T	180	GLN	2.2
11	Y	201	SER	2.2
3	Q	47	LYS	2.2
1	O	199	GLU	2.2
3	Q	239	ASN	2.2
5	E	60	GLN	2.2
3	Q	205	ASN	2.2
1	O	192	LEU	2.2
1	O	194	LEU	2.2
6	T	209	PHE	2.2
2	P	52	ILE	2.2
6	T	207	LYS	2.2
8	H	202	ARG	2.2
8	V	205	CYS	2.2
10	J	1[A]	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	U	204	THR	2.2
7	U	208	ILE	2.1
7	U	240	VAL	2.1
4	D	240	ASP	2.1
14	N	202	THR	2.1
2	P	58	GLU	2.0
5	S	53	GLN	2.0
2	P	56	LEU	2.0
5	E	235	GLY	2.0
6	T	143	ASN	2.0
4	D	183	GLU	2.0
5	E	59	HIS	2.0
1	O	59	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	YCM	Q	63	10/11	0.92	0.12	-	56,59,73,73	0
7	6V1	G	47	15/16	0.94	0.18	-	37,63,69,70	0
5	6V1	E	148	15/16	0.94	0.13	-	32,66,78,78	0
10	6V1	J	91	15/16	0.93	0.17	-	35,59,70,71	0
3	YCM	C	63	10/11	0.90	0.11	-	58,60,68,69	0
7	6V1	G	161	15/16	0.94	0.15	-	33,53,59,61	0
7	6V1	U	47	15/16	0.80	0.29	-	85,120,126,126	0
7	YCM	U	137	10/11	0.86	0.19	-	59,67,78,79	0
7	YCM	G	137	10/11	0.89	0.15	-	32,40,55,61	0
5	6V1	S	148	15/16	0.91	0.19	-	45,78,85,86	0
7	6V1	U	161	15/16	0.93	0.13	-	66,88,97,97	0
10	6V1	X	91	15/16	0.91	0.19	-	37,67,74,80	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	CL	M	301	1/1	0.98	0.27	20.73	70,70,70,70	0
18	1PE	L	301	16/16	0.85	0.20	11.62	59,76,84,85	0
15	CL	M	302	1/1	0.94	0.21	11.18	62,62,62,62	0
18	1PE	I	304	16/16	0.84	0.23	11.02	60,79,98,99	0
19	6V8	V	303	23/23	0.83	0.25	6.83	60,69,96,114	0
15	CL	S	301	1/1	0.94	0.29	6.09	77,77,77,77	0
18	1PE	M	305	16/16	0.86	0.19	5.82	68,77,95,97	0
19	6V8	H	305	23/23	0.82	0.22	5.22	47,57,91,103	0
15	CL	B	302	1/1	0.96	0.20	4.39	64,64,64,64	0
15	CL	b	301	1/1	0.97	0.17	3.42	61,61,61,61	0
18	1PE	H	304	16/16	0.88	0.17	3.12	59,66,97,97	0
15	CL	N	302	1/1	0.96	0.14	3.08	58,58,58,58	0
19	6V8	K	305	23/23	0.92	0.14	2.98	41,45,60,77	0
15	CL	D	301	1/1	0.95	0.24	2.90	84,84,84,84	0
18	1PE	I	303	16/16	0.89	0.14	2.04	54,61,77,87	0
18	1PE	Y	305	16/16	0.88	0.14	1.74	56,74,81,83	0
19	6V8	Y	306	23/23	0.93	0.12	1.47	35,37,53,63	0
18	1PE	b	302	16/16	0.89	0.15	1.27	50,59,91,96	0
18	1PE	W	303	16/16	0.89	0.13	0.86	62,71,82,82	0
19	6V8	b	304	23/23	0.94	0.12	0.82	39,41,48,54	0
15	CL	Q	302	1/1	0.91	0.16	0.78	72,72,72,72	0
15	CL	a	302	1/1	0.91	0.11	0.48	67,67,67,67	0
17	MG	L	303	1/1	0.94	0.12	0.13	42,42,42,42	0
15	CL	a	301	1/1	0.96	0.11	0.06	73,73,73,73	0
18	1PE	N	303	16/16	0.92	0.13	0.03	43,48,66,68	0
15	CL	Y	302	1/1	0.97	0.12	-0.00	76,76,76,76	0
15	CL	S	302	1/1	0.97	0.14	-0.04	75,75,75,75	0
15	CL	C	301	1/1	0.93	0.12	-0.15	72,72,72,72	0
15	CL	G	301	1/1	0.97	0.11	-0.26	58,58,58,58	0
15	CL	F	301	1/1	0.97	0.12	-0.39	58,58,58,58	0
19	6V8	N	305	23/23	0.94	0.10	-0.50	32,34,37,43	0
15	CL	K	302	1/1	0.97	0.10	-0.51	80,80,80,80	0
15	CL	E	301	1/1	0.96	0.10	-0.56	69,69,69,69	0
15	CL	A	301	1/1	0.96	0.09	-0.74	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	CL	E	303	1/1	0.97	0.09	-0.84	62,62,62,62	0
17	MG	H	302	1/1	0.96	0.10	-0.97	34,34,34,34	0
15	CL	S	303	1/1	0.95	0.08	-1.28	63,63,63,63	0
15	CL	G	302	1/1	0.99	0.06	-1.46	64,64,64,64	0
15	CL	A	304	1/1	0.94	0.09	-1.55	68,68,68,68	0
16	K	b	303	1/1	0.88	0.08	-1.66	54,54,54,54	0
15	CL	U	301	1/1	0.93	0.08	-1.70	68,68,68,68	0
15	CL	O	301	1/1	0.95	0.06	-1.74	64,64,64,64	0
16	K	U	302	1/1	0.96	0.09	-1.92	53,53,53,53	0
17	MG	K	301	1/1	0.93	0.07	-1.96	37,37,37,37	0
15	CL	N	301	1/1	0.98	0.09	-2.00	40,40,40,40	0
16	K	L	302	1/1	0.93	0.08	-2.39	57,57,57,57	0
17	MG	I	301	1/1	0.96	0.07	-2.51	34,34,34,34	0
16	K	N	304	1/1	0.96	0.05	-2.73	49,49,49,49	0
17	MG	W	301	1/1	0.94	0.07	-2.83	38,38,38,38	0
16	K	Z	301	1/1	0.97	0.06	-2.91	48,48,48,48	0
17	MG	I	305	1/1	0.97	0.08	-3.58	33,33,33,33	0
16	K	G	303	1/1	0.98	0.06	-6.88	41,41,41,41	0
17	MG	V	301	1/1	0.75	0.18	-	75,75,75,75	0
15	CL	A	302	1/1	0.84	0.10	-	72,72,72,72	0
15	CL	O	302	1/1	0.94	0.11	-	67,67,67,67	0
15	CL	K	303	1/1	0.87	0.17	-	78,78,78,78	0
15	CL	Y	303	1/1	0.95	0.08	-	60,60,60,60	0
15	CL	C	302	1/1	0.90	0.17	-	76,76,76,76	0
17	MG	H	301	1/1	0.96	0.12	-	69,69,69,69	0
15	CL	W	302	1/1	0.97	0.07	-	55,55,55,55	0
15	CL	Y	301	1/1	0.98	0.16	-	65,65,65,65	0
15	CL	D	302	1/1	0.92	0.12	-	71,71,71,71	0
15	CL	Q	301	1/1	0.80	0.19	-	92,92,92,92	0
15	CL	O	304	1/1	0.88	0.18	-	77,77,77,77	0
15	CL	R	301	1/1	0.96	0.10	-	64,64,64,64	0
15	CL	A	303	1/1	0.99	0.08	-	56,56,56,56	0
15	CL	a	303	1/1	0.96	0.09	-	49,49,49,49	0
15	CL	K	304	1/1	0.94	0.22	-	70,70,70,70	0
15	CL	V	302	1/1	0.93	0.09	-	66,66,66,66	0
15	CL	H	303	1/1	0.99	0.09	-	50,50,50,50	0
15	CL	R	302	1/1	0.93	0.27	-	69,69,69,69	0
17	MG	X	301	1/1	0.98	0.07	-	49,49,49,49	0
15	CL	B	301	1/1	0.98	0.07	-	44,44,44,44	0
15	CL	O	303	1/1	0.70	0.16	-	103,103,103,103	0
15	CL	M	304	1/1	0.94	0.08	-	59,59,59,59	0
15	CL	I	302	1/1	0.98	0.10	-	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	CL	Y	304	1/1	0.94	0.19	-	77,77,77,77	0
17	MG	J	301	1/1	0.96	0.08	-	48,48,48,48	0
15	CL	M	303	1/1	0.98	0.06	-	45,45,45,45	0
15	CL	a	304	1/1	0.96	0.09	-	68,68,68,68	0
15	CL	P	301	1/1	0.97	0.10	-	57,57,57,57	0
15	CL	E	302	1/1	0.97	0.07	-	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.