Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2016 – 02:33 PM EDT

PDB ID	:	5LF3
Title	:	Human 20S proteasome complex with Bortezomib 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	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

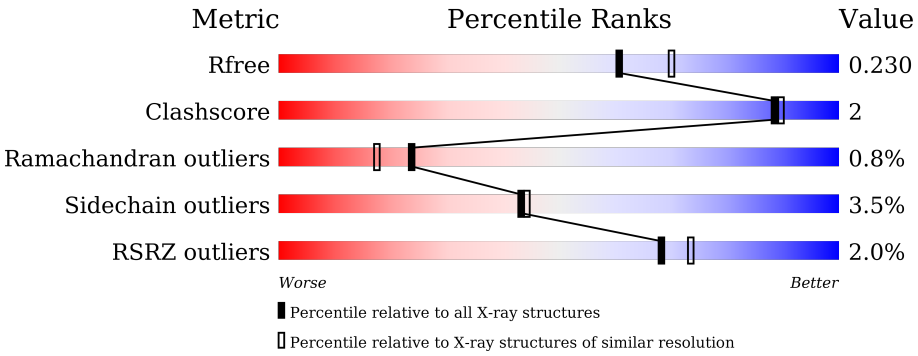
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	86% 9% • •
1	O	234	4% 89% 8% ••
2	B	261	2% 88% 7% • 5%
2	P	261	5% 84% 9% • 5%
3	C	248	3% 85% 8% • •
3	Q	248	10% 80% 13% • •

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Mol	Chain	Length	Quality of chain
4	D	241	2% 89% 6%
4	R	241	% 91%
5	E	263	4% 81% 6% 11%
5	S	263	3% 81% 8% 10%
6	F	255	83% 10% 6%
6	T	255	3% 80% 12% 6%
7	G	246	% 94% 5%
7	U	246	5% 87% 9%
8	H	234	2% 87% 7% 6%
8	V	234	2% 87% 7% 6%
9	I	205	93% 5%
9	W	205	94%
10	J	201	87% 8%
10	X	201	91% 5%
11	K	204	87% 10%
11	Y	204	% 85% 12%
12	L	213	92% 7%
12	Z	213	95% 5%
13	M	219	95%
13	a	219	94%
14	N	205	93%
14	b	205	97%

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	301	-	-	X	-
15	CL	M	301	-	-	-	X
15	CL	M	302	-	-	-	X
15	CL	S	301	-	-	-	X
15	CL	b	301	-	-	-	X
15	CL	b	302	-	-	-	X
17	MG	H	302	-	-	-	X
18	1PE	H	305	-	-	-	X
18	1PE	I	303	-	-	-	X
18	1PE	I	304	-	-	-	X
18	1PE	L	301	-	-	-	X
18	1PE	M	305	-	-	-	X
18	1PE	Z	301	-	-	-	X
18	1PE	b	303	-	-	-	X
19	BO2	b	305	-	-	-	X
7	6V1	U	47	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 52211 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	engineered mutation	UNP P25786
S	148	6V1	CYS	engineered mutation	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
			1574	1012	267	285	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	1	0
			1550	978	269	293	10			
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
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	1	THR	-	expression tag	UNP P28072

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Chain	Residue	Modelled	Actual	Comment	Reference
b	1	THR	-	expression tag	UNP P28072

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	2	Total Cl 2 2	0	0
15	O	4	Total Cl 4 4	0	0
15	Y	4	Total Cl 4 4	0	0
15	F	1	Total Cl 1 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

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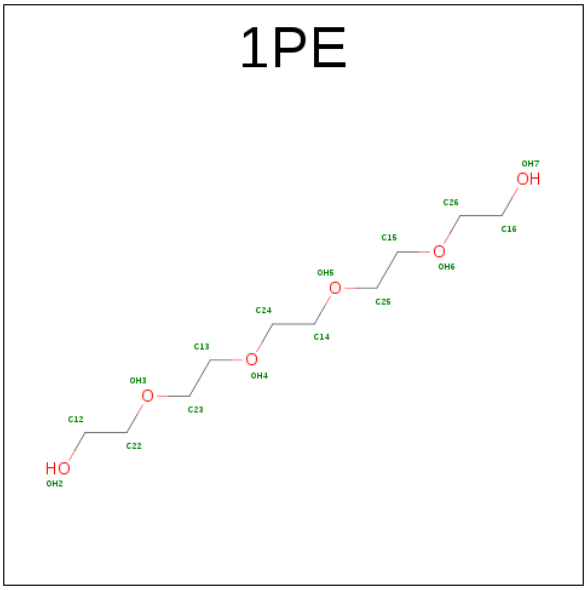
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	L	1	Total Mg 1 1	0	0

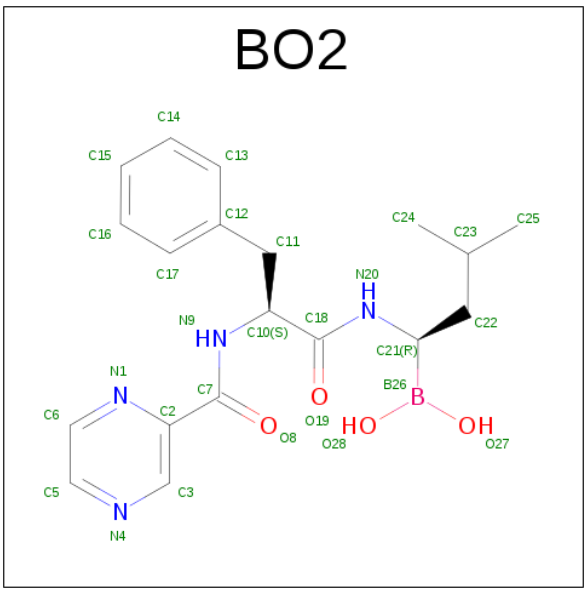
- Molecule 18 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 19 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula:

$C_{19}H_{25}BN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	H	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	K	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	N	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	V	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	Y	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	b	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	115	Total	O	0	0
			115	115		
20	B	131	Total	O	0	0
			131	131		
20	C	75	Total	O	0	0
			75	75		
20	D	95	Total	O	0	0
			95	95		
20	E	147	Total	O	0	0
			147	147		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	F	186	Total O 186 186	0	0
20	G	196	Total O 196 196	0	0
20	H	159	Total O 159 159	0	0
20	I	157	Total O 157 157	0	0
20	J	138	Total O 138 138	0	0
20	K	105	Total O 105 105	0	0
20	L	125	Total O 125 125	0	0
20	M	147	Total O 147 147	0	0
20	N	162	Total O 162 162	0	0
20	O	95	Total O 95 95	0	0
20	P	125	Total O 125 125	0	0
20	Q	75	Total O 75 75	0	0
20	R	132	Total O 132 132	0	0
20	S	130	Total O 130 130	0	0
20	T	100	Total O 100 100	0	0
20	U	107	Total O 107 107	0	0
20	V	120	Total O 120 120	0	0
20	W	118	Total O 118 118	0	0
20	X	125	Total O 125 125	0	0
20	Y	142	Total O 142 142	0	0
20	Z	169	Total O 169 169	0	0

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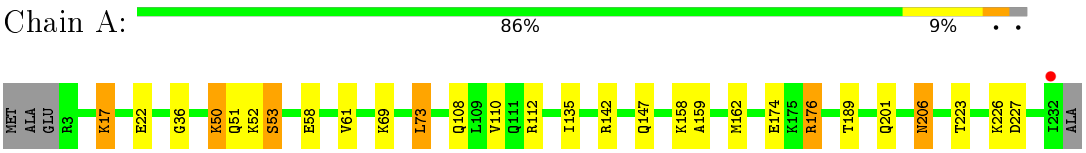
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	a	174	Total O 174 174	0	0
20	b	124	Total O 124 124	0	0

3 Residue-property plots (i)

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

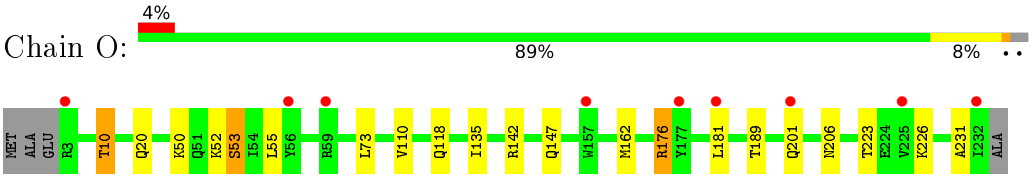
- Molecule 1: Proteasome subunit alpha type-2

Chain A:



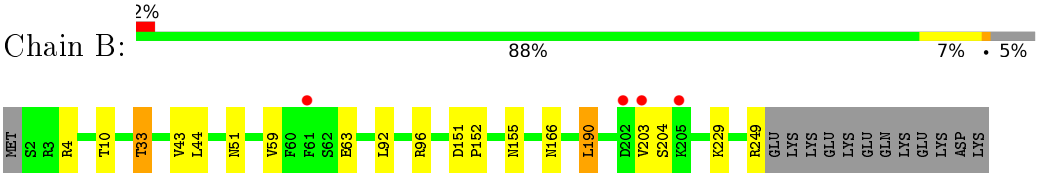
- Molecule 1: Proteasome subunit alpha type-2

Chain O:



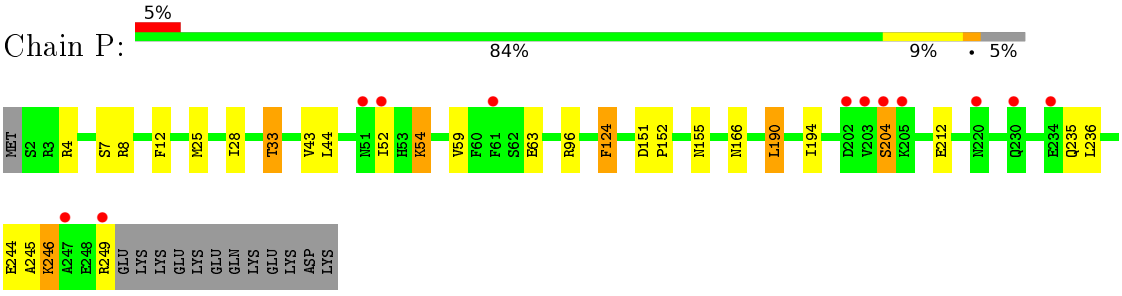
- Molecule 2: Proteasome subunit alpha type-4

Chain B:



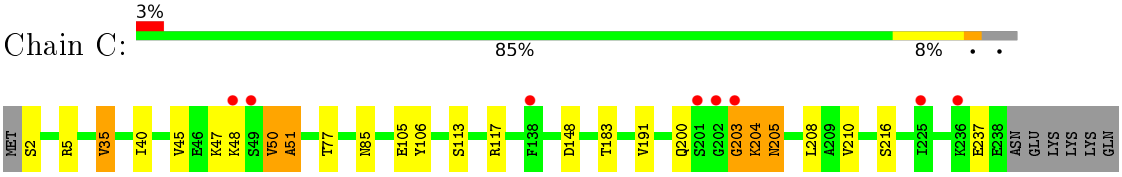
- Molecule 2: Proteasome subunit alpha type-4

Chain P:

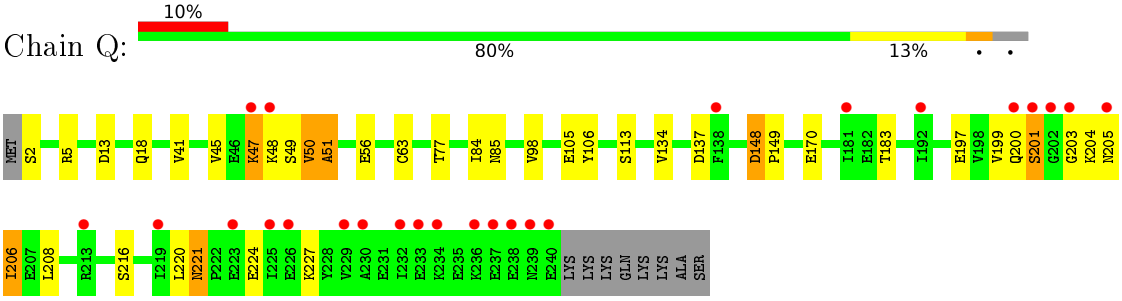


- Molecule 3: Proteasome subunit alpha type-7

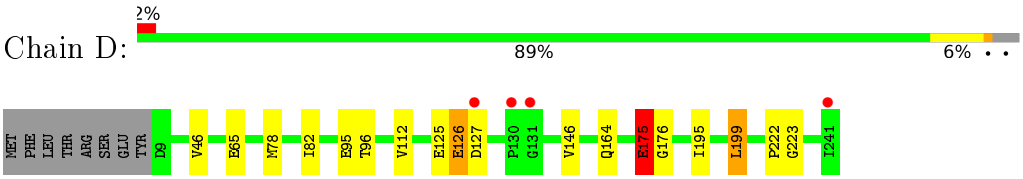
Chain C:



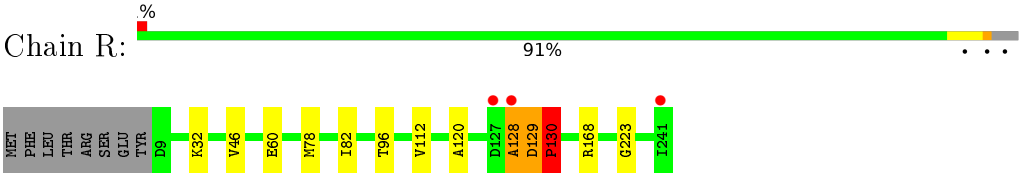
• Molecule 3: Proteasome subunit alpha type-7



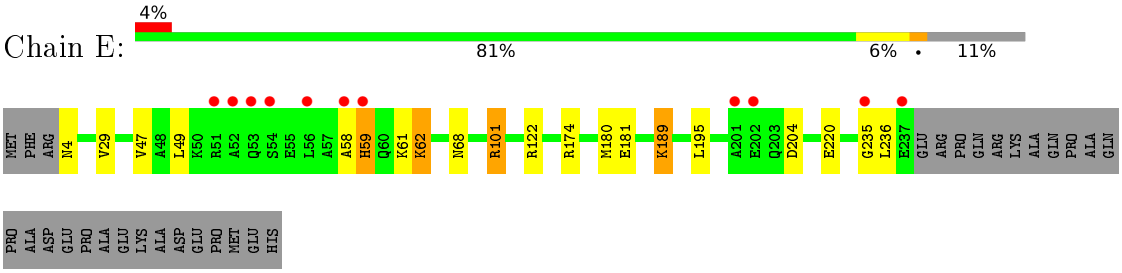
• Molecule 4: Proteasome subunit alpha type-5



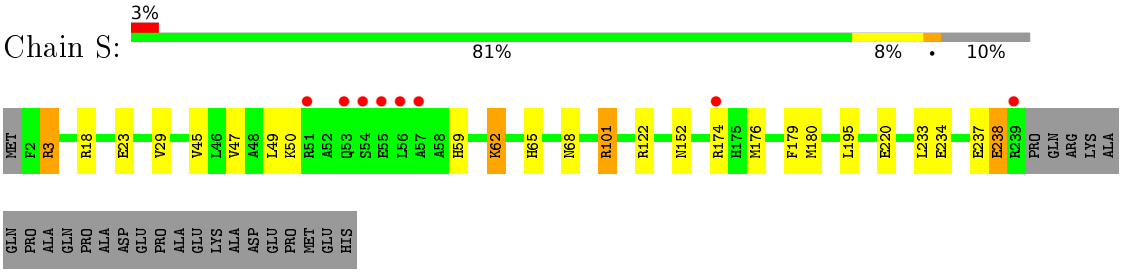
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 5: Proteasome subunit alpha type-1

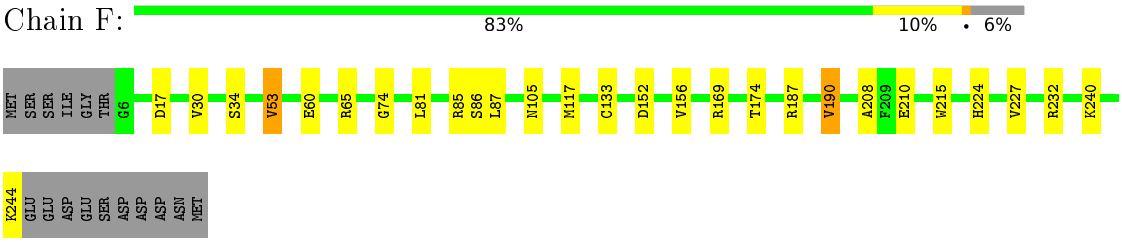


• Molecule 5: Proteasome subunit alpha type-1



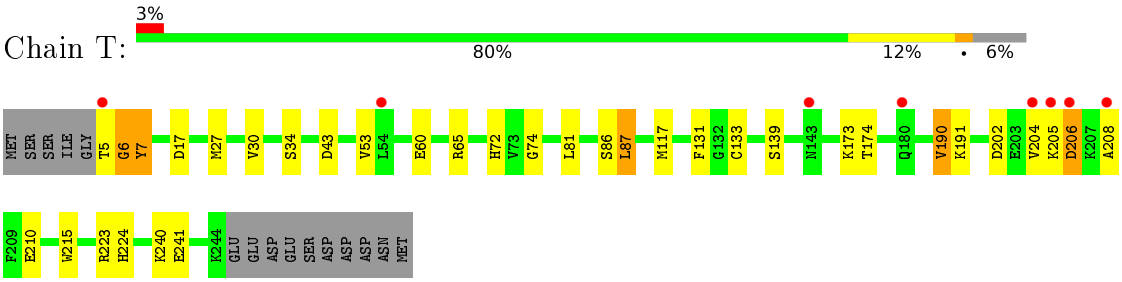
• Molecule 6: Proteasome subunit alpha type-3

Chain F:



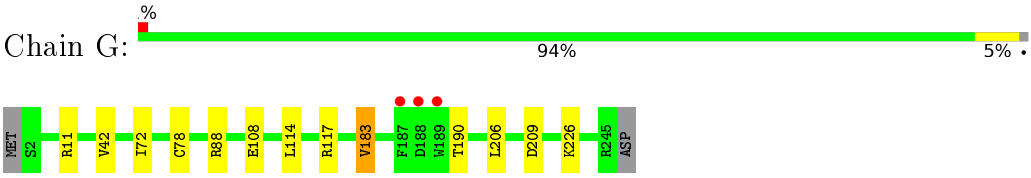
- Molecule 6: Proteasome subunit alpha type-3

Chain T:



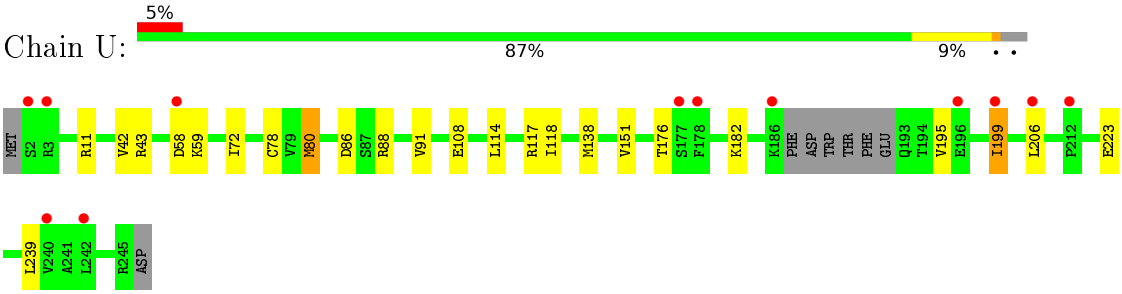
- Molecule 7: Proteasome subunit alpha type-6

Chain G:



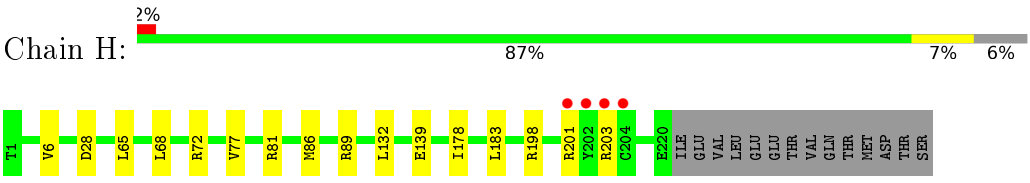
- Molecule 7: Proteasome subunit alpha type-6

Chain U:



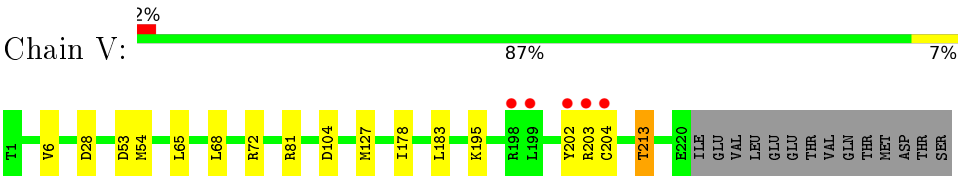
- Molecule 8: Proteasome subunit beta type-7

Chain H:



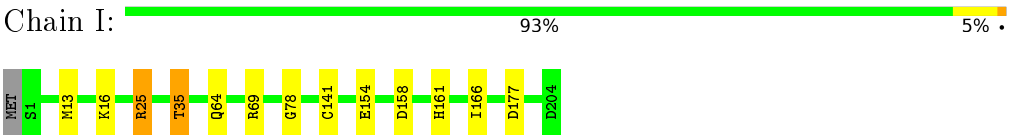
- Molecule 8: Proteasome subunit beta type-7

Chain V:



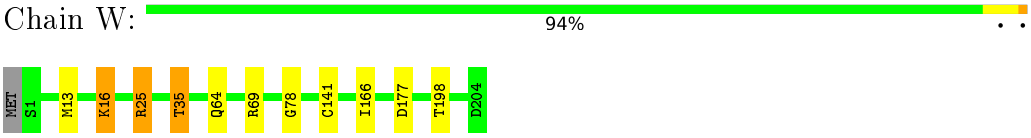
• Molecule 9: Proteasome subunit beta type-3

Chain I:



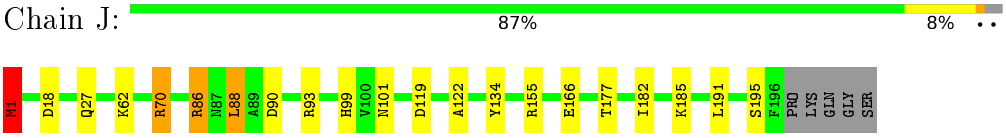
• Molecule 9: Proteasome subunit beta type-3

Chain W:



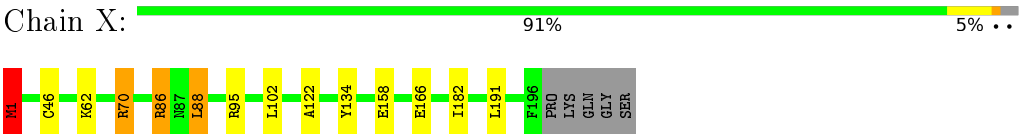
• Molecule 10: Proteasome subunit beta type-2

Chain J:



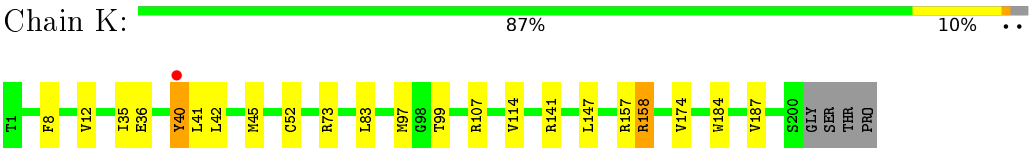
• Molecule 10: Proteasome subunit beta type-2

Chain X:



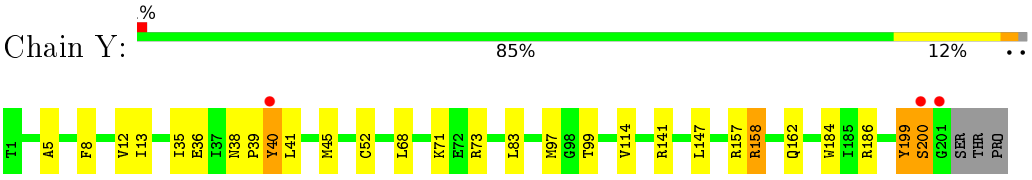
• Molecule 11: Proteasome subunit beta type-5

Chain K:



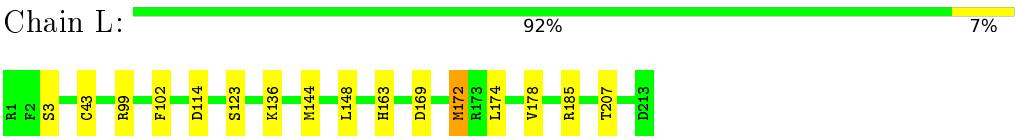
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



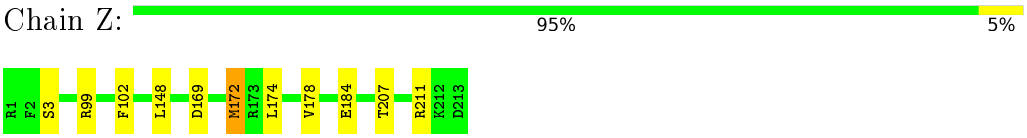
• Molecule 12: Proteasome subunit beta type-1

Chain L:



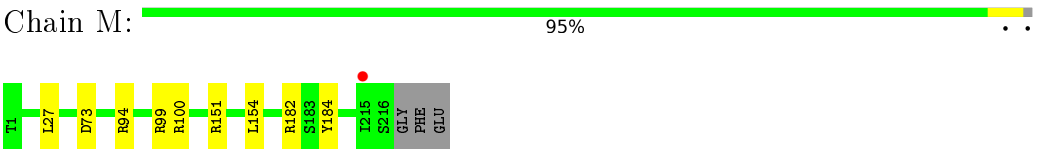
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



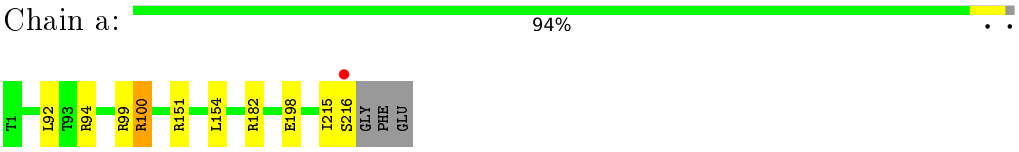
• Molecule 13: Proteasome subunit beta type-4

Chain M:



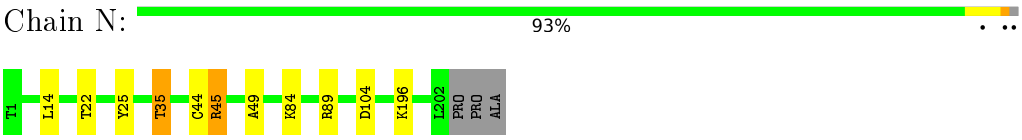
• Molecule 13: Proteasome subunit beta type-4

Chain a:



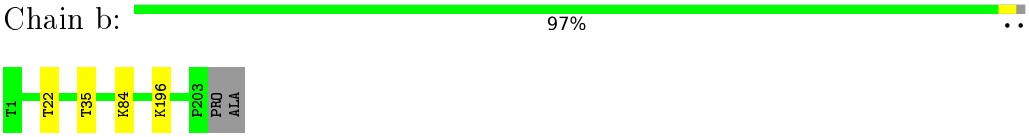
• Molecule 14: Proteasome subunit beta type-6

Chain N:



• Molecule 14: 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	113.37Å 202.72Å 314.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.45 – 2.10 170.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (170.45-2.10) 98.6 (170.45-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.184 , 0.226 0.191 , 0.230	Depositor DCC
R_{free} test set	20644 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52211	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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: MG, CL, BO2, 6V1, 1PE, YCM, K

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	0.83	1/2489 (0.0%)
1	O	0.63	0/1778	0.81	0/2419
2	B	0.70	0/1962	0.85	3/2649 (0.1%)
2	P	0.69	0/1945	0.89	4/2631 (0.2%)
3	C	0.66	0/1818	0.89	1/2469 (0.0%)
3	Q	0.67	0/1834	0.89	4/2490 (0.2%)
4	D	0.70	0/1789	0.81	2/2424 (0.1%)
4	R	0.73	0/1780	0.89	3/2408 (0.1%)
5	E	0.71	0/1842	0.86	2/2493 (0.1%)
5	S	0.68	0/1901	0.85	3/2571 (0.1%)
6	F	0.78	0/1935	0.90	3/2605 (0.1%)
6	T	0.68	1/1894 (0.1%)	0.92	6/2556 (0.2%)
7	G	0.78	1/1909 (0.1%)	0.83	2/2579 (0.1%)
7	U	0.64	0/1804	0.81	6/2441 (0.2%)
8	H	0.80	0/1697	0.97	8/2299 (0.3%)
8	V	0.69	0/1655	0.89	5/2251 (0.2%)
9	I	0.73	0/1648	0.97	5/2219 (0.2%)
9	W	0.66	0/1630	0.92	6/2197 (0.3%)
10	J	0.71	0/1613	0.99	5/2180 (0.2%)
10	X	0.72	0/1597	0.98	3/2160 (0.1%)
11	K	0.75	2/1584 (0.1%)	0.89	4/2141 (0.2%)
11	Y	0.79	1/1620 (0.1%)	0.94	4/2185 (0.2%)
12	L	0.73	0/1672	0.89	4/2257 (0.2%)
12	Z	0.80	1/1675 (0.1%)	0.91	3/2257 (0.1%)
13	M	0.74	0/1728	0.91	6/2339 (0.3%)
13	a	0.76	0/1724	0.91	5/2336 (0.2%)
14	N	0.81	0/1548	0.84	3/2095 (0.1%)
14	b	0.70	0/1554	0.83	0/2104
All	All	0.72	6/48969 (0.0%)	0.89	101/66244 (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	3
3	C	0	1
3	Q	0	2
4	D	0	4
4	R	0	2
5	E	0	1
6	T	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	21

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Z	3	SER	CB-OG	7.53	1.52	1.42
7	G	108	GLU	CD-OE1	7.45	1.33	1.25
11	Y	40	TYR	CE1-CZ	6.05	1.46	1.38
11	K	40	TYR	CE1-CZ	5.66	1.46	1.38
11	K	40	TYR	CG-CD1	5.44	1.46	1.39
6	T	7	TYR	N-CA	5.17	1.56	1.46

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	86	ARG	NE-CZ-NH2	-16.38	112.11	120.30
10	X	86	ARG	NE-CZ-NH2	-15.92	112.34	120.30
10	J	86	ARG	NE-CZ-NH1	13.76	127.18	120.30
10	X	86	ARG	NE-CZ-NH1	13.18	126.89	120.30
2	P	124	PHE	CB-CG-CD1	-10.33	113.57	120.80
8	H	72	ARG	NE-CZ-NH2	-10.16	115.22	120.30
9	I	25[A]	ARG	NE-CZ-NH1	9.71	125.16	120.30
9	I	25[B]	ARG	NE-CZ-NH1	9.71	125.16	120.30
4	R	120[A]	ALA	C-N-CA	9.40	145.21	121.70
4	R	120[B]	ALA	C-N-CA	9.40	145.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	69	ARG	NE-CZ-NH1	9.34	124.97	120.30
2	P	124	PHE	CB-CG-CD2	9.26	127.28	120.80
9	W	16[A]	LYS	C-N-CA	8.74	143.54	121.70
9	W	16[B]	LYS	C-N-CA	8.74	143.54	121.70
9	I	69	ARG	NE-CZ-NH1	8.51	124.55	120.30
11	Y	158	ARG	NE-CZ-NH1	8.49	124.55	120.30
9	I	16[A]	LYS	C-N-CA	8.44	142.80	121.70
9	I	16[B]	LYS	C-N-CA	8.44	142.80	121.70
2	B	96	ARG	NE-CZ-NH1	7.72	124.16	120.30
11	Y	158	ARG	NE-CZ-NH2	-7.67	116.47	120.30
7	U	11	ARG	NE-CZ-NH1	7.57	124.08	120.30
8	H	72	ARG	NE-CZ-NH1	7.41	124.00	120.30
6	T	43	ASP	CB-CG-OD2	7.13	124.72	118.30
13	M	151	ARG	NE-CZ-NH1	6.97	123.79	120.30
13	M	182	ARG	NE-CZ-NH1	6.90	123.75	120.30
9	W	25[A]	ARG	NE-CZ-NH1	6.83	123.72	120.30
9	W	25[B]	ARG	NE-CZ-NH1	6.83	123.72	120.30
6	T	27	MET	CG-SD-CE	6.82	111.12	100.20
3	Q	13	ASP	CB-CG-OD2	6.74	124.37	118.30
11	Y	157	ARG	NE-CZ-NH2	-6.70	116.95	120.30
2	B	4	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	P	96	ARG	NE-CZ-NH1	6.56	123.58	120.30
5	E	122	ARG	NE-CZ-NH2	-6.55	117.03	120.30
10	J	93	ARG	NE-CZ-NH1	6.51	123.56	120.30
8	H	28	ASP	CB-CG-OD1	6.47	124.12	118.30
12	L	172	MET	CG-SD-CE	-6.39	89.97	100.20
7	U	88	ARG	NE-CZ-NH1	6.39	123.49	120.30
12	Z	172	MET	CG-SD-CE	-6.33	90.08	100.20
7	U	117	ARG	NE-CZ-NH1	6.30	123.45	120.30
5	S	122	ARG	NE-CZ-NH2	-6.28	117.16	120.30
8	V	28	ASP	CB-CG-OD1	6.24	123.92	118.30
8	H	198	ARG	NE-CZ-NH2	-6.21	117.20	120.30
13	M	151	ARG	NE-CZ-NH2	-6.15	117.22	120.30
8	H	89	ARG	NE-CZ-NH1	6.15	123.38	120.30
13	a	182	ARG	NE-CZ-NH1	6.08	123.34	120.30
12	L	99	ARG	NE-CZ-NH1	6.01	123.30	120.30
2	P	4	ARG	NE-CZ-NH1	6.01	123.30	120.30
7	G	117	ARG	NE-CZ-NH1	5.96	123.28	120.30
7	U	80[A]	MET	CG-SD-CE	5.94	109.70	100.20
7	U	80[B]	MET	CG-SD-CE	5.94	109.70	100.20
11	Y	157	ARG	NE-CZ-NH1	5.93	123.27	120.30
8	V	72	ARG	NE-CZ-NH1	5.92	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	198	ARG	NE-CZ-NH1	5.90	123.25	120.30
7	G	183	VAL	CB-CA-C	-5.86	100.28	111.40
13	M	94	ARG	NE-CZ-NH1	5.78	123.19	120.30
6	T	117	MET	CG-SD-CE	5.77	109.44	100.20
7	U	86	ASP	CB-CG-OD2	5.72	123.45	118.30
13	a	94	ARG	NE-CZ-NH1	5.70	123.15	120.30
6	F	190	VAL	CB-CA-C	-5.69	100.58	111.40
13	M	99	ARG	NE-CZ-NH1	5.68	123.14	120.30
14	N	45	ARG	NE-CZ-NH2	-5.68	117.46	120.30
5	S	122	ARG	NE-CZ-NH1	5.68	123.14	120.30
6	T	6	GLY	C-N-CA	5.67	135.87	121.70
4	D	175[A]	GLU	N-CA-C	-5.65	95.75	111.00
4	D	175[B]	GLU	N-CA-C	-5.65	95.75	111.00
10	X	70	ARG	NE-CZ-NH1	5.57	123.09	120.30
12	Z	99	ARG	NE-CZ-NH1	5.54	123.07	120.30
6	T	190	VAL	CB-CA-C	-5.52	100.92	111.40
2	B	96	ARG	NE-CZ-NH2	-5.47	117.57	120.30
11	K	107	ARG	NE-CZ-NH1	5.46	123.03	120.30
12	Z	99	ARG	NE-CZ-NH2	-5.46	117.57	120.30
5	E	174	ARG	NE-CZ-NH1	5.41	123.00	120.30
6	T	7	TYR	N-CA-CB	5.38	120.29	110.60
11	K	158	ARG	NE-CZ-NH1	5.38	122.99	120.30
11	K	157	ARG	NE-CZ-NH2	-5.36	117.62	120.30
8	V	53	ASP	CB-CG-OD2	5.35	123.12	118.30
3	Q	137	ASP	CB-CG-OD2	-5.35	113.49	118.30
14	N	104	ASP	CB-CG-OD2	5.34	123.11	118.30
14	N	89	ARG	NE-CZ-NH1	5.34	122.97	120.30
13	a	99	ARG	NE-CZ-NH1	5.33	122.97	120.30
10	J	70	ARG	NE-CZ-NH1	5.33	122.96	120.30
10	J	86	ARG	CD-NE-CZ	5.30	131.02	123.60
9	W	69	ARG	NE-CZ-NH2	-5.29	117.66	120.30
12	L	99	ARG	NE-CZ-NH2	-5.23	117.69	120.30
13	a	100	ARG	NE-CZ-NH1	5.22	122.91	120.30
12	L	114	ASP	CB-CG-OD1	5.20	122.98	118.30
4	R	168	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	Q	220	LEU	CA-C-N	5.17	128.58	117.20
8	V	72	ARG	NE-CZ-NH2	-5.17	117.71	120.30
8	V	81	ARG	NE-CZ-NH2	-5.17	117.71	120.30
8	H	86	MET	CG-SD-CE	-5.16	91.95	100.20
6	F	117	MET	CG-SD-CE	5.13	108.40	100.20
8	H	81	ARG	NE-CZ-NH2	-5.11	117.74	120.30
3	C	117	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	174	ARG	NE-CZ-NH1	5.08	122.84	120.30
13	M	73	ASP	CB-CG-OD2	-5.06	113.75	118.30
13	a	151	ARG	NE-CZ-NH1	5.03	122.82	120.30
11	K	42	LEU	CA-CB-CG	5.03	126.87	115.30
6	F	85	ARG	NE-CZ-NH2	-5.02	117.79	120.30
3	Q	220	LEU	C-N-CA	5.02	134.25	121.70
1	A	73	LEU	CB-CA-C	-5.01	100.69	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	244	GLU	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
6	T	5	THR	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
11	Y	199	TYR	Peptide
13	a	215	ILE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1761	10	0
1	O	1741	0	1683	6	0
2	B	1926	0	1924	7	0
2	P	1909	0	1874	13	0
3	C	1798	0	1718	14	0
3	Q	1820	0	1749	14	0
4	D	1762	0	1709	7	0
4	R	1753	0	1726	6	0
5	E	1822	0	1779	8	0
5	S	1875	0	1818	17	0
6	F	1888	0	1882	10	0
6	T	1856	0	1816	10	0
7	G	1912	0	1882	3	0
7	U	1815	0	1748	9	0
8	H	1664	0	1680	11	0
8	V	1622	0	1594	6	0
9	I	1613	0	1646	8	0
9	W	1599	0	1621	8	0
10	J	1590	0	1581	18	0
10	X	1574	0	1561	11	0
11	K	1550	0	1506	10	0
11	Y	1580	0	1557	19	0
12	L	1636	0	1625	6	0
12	Z	1642	0	1635	2	0
13	M	1692	0	1670	1	0
13	a	1688	0	1658	0	0
14	N	1519	0	1495	6	0
14	b	1524	0	1495	0	0
15	A	4	0	0	1	0
15	B	2	0	0	2	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	0	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0

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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	0	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	3	0	0	0	0
15	b	2	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	32	0	44	0	0
18	I	32	0	44	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0
18	W	16	0	22	0	0
18	Z	16	0	22	0	0
18	b	16	0	22	0	0
19	H	28	0	25	1	0
19	K	28	0	25	0	0
19	N	28	0	25	1	0
19	V	28	0	25	0	0
19	Y	28	0	25	0	0
19	b	28	0	25	0	0
20	A	115	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	131	0	0	2	0
20	C	75	0	0	0	0
20	D	95	0	0	1	0
20	E	147	0	0	2	0
20	F	186	0	0	3	0
20	G	196	0	0	0	0
20	H	159	0	0	6	0
20	I	157	0	0	1	0
20	J	138	0	0	4	0
20	K	105	0	0	0	0
20	L	125	0	0	1	0
20	M	147	0	0	0	0
20	N	162	0	0	0	0
20	O	95	0	0	1	0
20	P	125	0	0	0	0
20	Q	75	0	0	2	0
20	R	132	0	0	0	0
20	S	130	0	0	3	0
20	T	100	0	0	1	0
20	U	107	0	0	1	0
20	V	120	0	0	1	0
20	W	118	0	0	3	0
20	X	125	0	0	0	0
20	Y	142	0	0	0	0
20	Z	169	0	0	0	0
20	a	174	0	0	0	0
20	b	124	0	0	0	0
All	All	52211	0	47741	225	0

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

All (225) 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)
6:F:169[A]:ARG:NH1	20:F:401:HOH:O	2.02	0.92
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.57	0.86
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.01	0.79
11:Y:35:ILE:HD11	11:Y:45:MET:SD	2.24	0.77
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.67	0.77
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.33	0.74
11:K:35:ILE:HD11	11:K:45:MET:SD	2.26	0.74
11:K:141:ARG:NH1	10:X:166:GLU:OE2	2.22	0.73
7:U:108:GLU:OE1	20:U:401:HOH:O	2.06	0.72
8:V:54:MET:HE1	20:W:440:HOH:O	1.91	0.69
1:O:10:THR:HG23	20:O:402:HOH:O	1.93	0.67
5:S:152[B]:ASN:ND2	20:S:402:HOH:O	2.27	0.67
10:J:99[A]:HIS:CD2	20:J:411:HOH:O	2.48	0.67
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	1.95	0.66
14:N:35:THR:CG2	14:N:45:ARG:HE	2.09	0.65
2:B:10:THR:OG1	20:B:401:HOH:O	2.14	0.64
8:V:195:LYS:CB	20:V:503:HOH:O	2.44	0.64
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.45	0.64
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.80	0.63
11:Y:199:TYR:HA	11:Y:200:SER:HB2	1.81	0.63
5:S:65[A]:HIS:CE1	20:S:407:HOH:O	2.52	0.62
3:C:5:ARG:NH1	4:D:125:GLU:OE2	2.32	0.62
12:L:144:MET:CE	12:L:185:ARG:HB2	2.29	0.62
3:C:47:LYS:CB	3:C:48:LYS:HA	2.30	0.61
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.48	0.61
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.34	0.61
5:S:233:LEU:HB2	5:S:234:GLU:OE2	2.00	0.61
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.82	0.61
5:E:58:ALA:O	5:E:59:HIS:CB	2.48	0.60
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.66	0.60
9:W:16[B]:LYS:NZ	20:W:401:HOH:O	2.33	0.60
10:J:166:GLU:OE2	11:Y:141[A]:ARG:NH1	2.34	0.60
7:U:195:VAL:O	7:U:199:ILE:HG23	2.01	0.60
9:W:13:MET:HE1	9:W:166:ILE:N	2.17	0.60
4:D:96:THR:OG1	20:D:401:HOH:O	2.16	0.59
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.50	0.59
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.18	0.59
6:F:105:ASN:ND2	20:F:403:HOH:O	2.35	0.58
10:J:185:LYS:NZ	20:J:401:HOH:O	2.36	0.58
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.84	0.58
9:I:35:THR:HG21	20:I:415:HOH:O	2.03	0.58
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.84	0.57
3:C:47:LYS:CB	3:C:48:LYS:CA	2.82	0.57
2:P:25[B]:MET:CE	2:P:25[B]:MET:HA	2.32	0.57
11:K:99:THR:HG22	11:K:114:VAL:O	2.05	0.57
11:Y:99:THR:HG22	11:Y:114:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:129:ASP:CB	4:R:130:PRO:HD3	2.34	0.57
5:E:49:LEU:O	5:E:62:LYS:HD2	2.05	0.57
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.38	0.57
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.87	0.56
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.87	0.56
5:S:49:LEU:O	5:S:62:LYS:HD2	2.05	0.56
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.20	0.56
5:E:101[A]:ARG:NH1	20:E:401:HOH:O	2.39	0.56
10:X:1:MET:HE1	10:X:134:TYR:H	1.71	0.56
6:T:191:LYS:NZ	20:T:302:HOH:O	2.38	0.56
7:U:58:ASP:O	7:U:59:LYS:CB	2.55	0.55
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.89	0.55
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.47	0.55
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.88	0.54
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.36	0.54
15:B:301:CL:CL	15:B:302:CL:CL	2.99	0.54
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	2.08	0.54
5:S:234:GLU:N	5:S:234:GLU:OE2	2.41	0.54
14:N:49:ALA:HB3	19:N:304:BO2:H3	1.89	0.54
2:P:194:ILE:CD1	2:P:236:LEU:HB3	2.39	0.53
4:R:129:ASP:CB	4:R:130:PRO:CD	2.87	0.53
5:S:101:ARG:NH1	20:S:406:HOH:O	2.41	0.53
1:A:51:GLN:HE22	1:A:58[B]:GLU:HB3	1.75	0.52
20:Q:406:HOH:O	4:R:128:ALA:HB1	2.09	0.52
10:X:1:MET:C	10:X:1:MET:HE3	2.31	0.51
11:Y:40:TYR:HB3	11:Y:73:ARG:NH1	2.25	0.51
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.92	0.51
15:M:302:CL:CL	15:M:303:CL:CL	3.03	0.51
2:P:190:LEU:HG	2:P:236:LEU:HD21	1.93	0.51
3:C:50:VAL:O	3:C:51:ALA:HB3	2.11	0.51
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.91	0.51
7:U:80[A]:MET:HE3	7:U:91:VAL:HG23	1.91	0.51
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.93	0.51
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.12	0.50
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.76	0.50
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.43	0.50
7:U:43:ARG:HB3	7:U:151:VAL:HG13	1.94	0.49
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.42	0.49
6:T:205:LYS:O	6:T:206:ASP:CG	2.51	0.49
10:J:177:THR:HG22	10:J:195:SER:CB	2.43	0.49
19:H:306:BO2:H16	20:H:407:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.94	0.49
3:Q:85:ASN:OD1	10:X:70:ARG:NH2	2.46	0.49
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.95	0.49
10:X:1:MET:HE1	10:X:134:TYR:N	2.27	0.49
6:F:34:SER:OG	6:F:65:ARG:NH1	2.45	0.48
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.96	0.48
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.93	0.48
11:K:40:TYR:HB3	11:K:73:ARG:NH1	2.29	0.48
6:T:173:LYS:HB3	6:T:173:LYS:HE2	1.61	0.48
6:T:202:ASP:OD1	6:T:204:VAL:HG12	2.14	0.48
8:H:201:ARG:NH1	20:H:405:HOH:O	2.45	0.48
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.48	0.48
5:E:68:ASN:ND2	5:E:220:GLU:OE1	2.48	0.47
7:G:11:ARG:HH11	7:G:11:ARG:HG2	1.80	0.47
3:Q:204:LYS:HA	3:Q:205:ASN:O	2.14	0.47
9:I:158:ASP:OD1	9:I:161:HIS:HD2	1.97	0.47
8:H:203:ARG:NH2	9:I:154:GLU:OE1	2.45	0.47
6:T:87:LEU:HD13	6:T:131:PHE:CE1	2.48	0.47
11:Y:40:TYR:CZ	11:Y:73:ARG:HB3	2.49	0.47
15:A:302:CL:CL	15:B:301:CL:CL	40.78	0.47
6:F:53:VAL:HG12	6:F:208:ALA:HB3	1.97	0.47
9:W:35:THR:HG21	20:W:428:HOH:O	2.14	0.47
6:F:169[A]:ARG:NH1	20:F:408:HOH:O	2.47	0.47
11:Y:40:TYR:CD2	11:Y:73:ARG:CZ	2.98	0.47
8:H:132:LEU:HD22	14:N:25:TYR:CE2	2.50	0.47
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.45	0.47
10:J:182:ILE:CD1	10:J:191:LEU:HD11	2.45	0.47
3:Q:63:YCM:HD2	3:Q:84:ILE:HD13	1.96	0.46
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.08	0.46
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.30	0.46
8:H:77:VAL:HG12	20:H:542:HOH:O	2.16	0.46
11:K:40:TYR:CZ	11:K:73:ARG:HB3	2.51	0.46
3:Q:199:VAL:O	3:Q:201:SER:N	2.48	0.46
9:W:25[A]:ARG:HH11	9:W:25[A]:ARG:HG2	1.81	0.46
1:A:158:LYS:NZ	20:A:404:HOH:O	2.48	0.46
4:D:164:GLN:OE1	5:E:58:ALA:HB2	2.15	0.46
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	1.97	0.46
4:R:96:THR:HG22	4:R:112:VAL:HG22	1.97	0.46
1:O:10:THR:HB	1:O:20:GLN:HB2	1.98	0.45
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.47	0.45
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:TYR:CD2	11:K:73:ARG:CZ	3.00	0.45
10:X:182:ILE:CD1	10:X:191:LEU:HD11	2.47	0.45
3:C:40:ILE:HD11	3:C:210:VAL:CG1	2.46	0.45
11:Y:199:TYR:HA	11:Y:200:SER:CB	2.46	0.45
8:V:213:THR:HB	9:W:198:THR:OG1	2.16	0.45
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.57	0.45
8:H:77:VAL:HG13	20:H:414:HOH:O	2.16	0.44
5:S:237:GLU:O	5:S:238:GLU:CB	2.64	0.44
6:T:34:SER:OG	6:T:65:ARG:NH1	2.47	0.44
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.63	0.44
5:E:189:LYS:HG3	5:E:236:LEU:HD23	1.99	0.44
9:I:25[A]:ARG:HG2	9:I:25[A]:ARG:HH11	1.82	0.44
10:J:27[A]:GLN:NE2	20:J:404:HOH:O	2.47	0.44
9:W:141:CYS:HB3	9:W:177:ASP:HB2	2.00	0.44
3:C:47:LYS:HA	3:C:205:ASN:HB3	2.00	0.44
8:H:77:VAL:HB	20:H:542:HOH:O	2.17	0.44
1:A:17:LYS:HE2	1:A:22:GLU:OE2	2.18	0.44
7:G:72:ILE:HG21	7:G:114:LEU:HD21	2.00	0.44
3:Q:63:YCM:HD2	3:Q:84:ILE:CD1	2.48	0.44
8:V:202:TYR:O	8:V:204:CYS:N	2.51	0.44
2:B:33:THR:HB	2:B:166:ASN:O	2.17	0.44
10:X:1:MET:CE	10:X:134:TYR:H	2.30	0.44
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.53	0.44
5:S:233:LEU:CB	5:S:234:GLU:OE2	2.66	0.43
7:U:118:ILE:HG21	7:U:138:MET:HE2	1.98	0.43
11:Y:36:GLU:HG2	11:Y:184:TRP:CZ2	2.53	0.43
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.19	0.43
8:H:77:VAL:CG1	20:H:542:HOH:O	2.66	0.43
11:Y:52:CYS:SG	11:Y:97[A]:MET:HG3	2.58	0.43
3:C:35:VAL:HG13	3:C:191:VAL:HG22	2.00	0.43
8:V:127[B]:MET:HB3	8:V:127[B]:MET:HE2	1.88	0.43
4:D:195:ILE:O	4:D:199:LEU:HD22	2.19	0.43
9:I:141:CYS:HB3	9:I:177:ASP:HB2	2.00	0.43
6:T:60:GLU:HA	6:T:210:GLU:OE1	2.18	0.43
8:H:201:ARG:HD2	8:H:203:ARG:HB2	2.01	0.43
2:P:246:LYS:N	2:P:246:LYS:HE3	2.34	0.43
2:P:33:THR:HB	2:P:166:ASN:O	2.18	0.42
4:D:96:THR:HG22	4:D:112:VAL:HG22	2.02	0.42
8:V:178:ILE:HG12	8:V:183:LEU:HD12	2.01	0.42
11:Y:40:TYR:OH	11:Y:73:ARG:HA	2.19	0.42
1:A:147:GLN:HG3	1:A:162:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASP:HB2	2:B:152:PRO:CD	2.49	0.42
2:B:92[B]:LEU:HD23	20:B:424:HOH:O	2.18	0.42
6:F:30:VAL:HG22	6:F:133[A]:CYS:HA	2.02	0.42
7:G:226:LYS:HE2	7:G:226:LYS:HB2	1.96	0.42
11:K:83:LEU:HD21	11:K:99:THR:HG21	2.02	0.42
13:M:27:LEU:HD22	13:M:184:TYR:HB2	2.01	0.42
1:O:147:GLN:HG3	1:O:162:MET:HE1	2.01	0.42
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.20	0.42
2:P:63:GLU:N	2:P:212:GLU:OE2	2.44	0.42
2:P:8:ARG:NH2	3:Q:5:ARG:HD2	2.35	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.20	0.42
6:F:60:GLU:HA	6:F:210:GLU:OE1	2.20	0.42
10:J:1[A]:MET:CE	10:J:134:TYR:H	2.32	0.42
11:K:52:CYS:SG	11:K:97[A]:MET:HG3	2.60	0.42
12:L:43[B]:CYS:SG	20:L:402:HOH:O	2.62	0.42
14:N:35:THR:CG2	14:N:45:ARG:NE	2.81	0.42
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.19	0.42
10:J:1[A]:MET:CE	20:J:483:HOH:O	2.67	0.41
12:L:144:MET:HE2	12:L:144:MET:HB3	1.94	0.41
3:C:203:GLY:CA	3:C:204:LYS:CB	2.99	0.41
5:E:4:ASN:ND2	20:E:405:HOH:O	2.52	0.41
8:H:132:LEU:HD22	14:N:25:TYR:CZ	2.55	0.41
12:L:123:SER:CB	12:L:136:LYS:HG2	2.50	0.41
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.50	0.41
11:Y:186[A]:ARG:HB2	11:Y:186[A]:ARG:HE	1.76	0.41
11:Y:68:LEU:O	11:Y:71:LYS:HE3	2.20	0.41
8:H:178:ILE:HG12	8:H:183:LEU:HD12	2.02	0.41
6:T:30:VAL:HG22	6:T:133[A]:CYS:HA	2.02	0.41
10:J:177:THR:HG22	10:J:195:SER:HB2	2.02	0.41
3:Q:106:TYR:C	3:Q:106:TYR:CD1	2.94	0.41
5:S:50:LYS:CB	5:S:59:HIS:HB3	2.48	0.41
5:S:68:ASN:ND2	5:S:220:GLU:OE1	2.52	0.41
6:T:72:HIS:O	6:T:139:SER:HB2	2.21	0.41
9:W:13:MET:HE1	9:W:166:ILE:CA	2.51	0.41
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.45	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.41
3:C:106:TYR:C	3:C:106:TYR:CD1	2.94	0.40
10:J:86:ARG:HD3	10:J:90:ASP:OD1	2.21	0.40
20:Q:465:HOH:O	4:R:60:GLU:HG3	2.21	0.40
1:O:55:LEU:HD12	7:U:176:THR:HG23	2.03	0.40
11:Y:68:LEU:O	11:Y:71:LYS:CE	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:36:GLU:HG2	11:K:184:TRP:CZ2	2.56	0.40
11:K:35:ILE:CD1	11:K:45:MET:SD	3.05	0.40
2:P:25[B]:MET:HE3	2:P:28:ILE:HD12	2.02	0.40
3:Q:221:ASN:ND2	3:Q:224:GLU:HB2	2.36	0.40
5:S:176:MET:HA	5:S:179:PHE:CD2	2.56	0.40
11:Y:141[B]:ARG:HD2	11:Y:141[B]:ARG:HA	1.88	0.40
1:A:206:ASN:HD22	1:A:206:ASN:C	2.25	0.40
4:D:146:VAL:HG11	4:D:222:PRO:HA	2.04	0.40
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.21	0.40
11:Y:83:LEU:HD21	11:Y:99:THR:HG21	2.03	0.40
1:A:36:GLY:O	1:A:159:ALA:HA	2.21	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%)	222 (96%)	4 (2%)	5 (2%)	8 3
1	O	228/234 (97%)	218 (96%)	4 (2%)	6 (3%)	7 2
2	B	248/261 (95%)	239 (96%)	7 (3%)	2 (1%)	24 17
2	P	248/261 (95%)	232 (94%)	13 (5%)	3 (1%)	16 10
3	C	236/248 (95%)	224 (95%)	6 (2%)	6 (2%)	7 2
3	Q	236/248 (95%)	218 (92%)	8 (3%)	10 (4%)	3 1
4	D	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	11 5
4	R	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	15 9
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	39 37
5	S	238/263 (90%)	230 (97%)	6 (2%)	2 (1%)	24 17
6	F	241/255 (94%)	240 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	T	239/255 (94%)	233 (98%)	2 (1%)	4 (2%)	11 5
7	G	241/246 (98%)	235 (98%)	5 (2%)	1 (0%)	39 37
7	U	232/246 (94%)	228 (98%)	4 (2%)	0	100 100
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100 100
8	V	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	34 30
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100 100
9	W	204/205 (100%)	199 (98%)	5 (2%)	0	100 100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100 100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100 100
11	K	199/204 (98%)	196 (98%)	3 (2%)	0	100 100
11	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	34 30
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100 100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100 100
13	M	215/219 (98%)	208 (97%)	7 (3%)	0	100 100
13	a	216/219 (99%)	209 (97%)	7 (3%)	0	100 100
14	N	201/205 (98%)	199 (99%)	2 (1%)	0	100 100
14	b	202/205 (98%)	200 (99%)	2 (1%)	0	100 100
All	All	6213/6458 (96%)	6040 (97%)	124 (2%)	49 (1%)	24 17

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	52	LYS
1	A	53	SER
4	D	176	GLY
5	E	59	HIS
1	O	52	LYS
1	O	53	SER
2	P	204	SER
3	Q	47	LYS
3	Q	201	SER
3	Q	206	ILE
3	Q	221	ASN
4	R	130	PRO
5	S	238	GLU

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Mol	Chain	Res	Type
6	T	208	ALA
11	Y	200	SER
3	C	200	GLN
1	O	50	LYS
1	O	231	ALA
2	P	52	ILE
2	P	54	LYS
3	Q	200	GLN
6	T	7	TYR
6	T	206	ASP
8	V	203	ARG
1	A	176	ARG
3	C	50	VAL
3	C	204	LYS
4	D	175[A]	GLU
4	D	175[B]	GLU
1	O	176	ARG
4	R	128	ALA
3	C	216	SER
4	D	126	GLU
3	Q	48	LYS
3	Q	50	VAL
5	S	3	ARG
6	T	6	GLY
1	A	201	GLN
3	C	51	ALA
7	G	209	ASP
1	O	201	GLN
3	Q	216	SER
4	R	129	ASP
2	B	204	SER
3	Q	51	ALA
3	C	203	GLY
2	B	203	VAL
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%)	172 (93%)	13 (7%)	19	15
1	O	176/191 (92%)	166 (94%)	10 (6%)	25	22
2	B	200/221 (90%)	194 (97%)	6 (3%)	48	51
2	P	197/221 (89%)	186 (94%)	11 (6%)	26	22
3	C	179/210 (85%)	170 (95%)	9 (5%)	30	27
3	Q	184/210 (88%)	171 (93%)	13 (7%)	18	14
4	D	189/203 (93%)	184 (97%)	5 (3%)	54	58
4	R	187/203 (92%)	185 (99%)	2 (1%)	80	85
5	E	192/223 (86%)	183 (95%)	9 (5%)	32	30
5	S	197/223 (88%)	191 (97%)	6 (3%)	48	51
6	F	199/212 (94%)	188 (94%)	11 (6%)	27	23
6	T	192/212 (91%)	181 (94%)	11 (6%)	25	22
7	G	202/207 (98%)	196 (97%)	6 (3%)	48	51
7	U	186/207 (90%)	180 (97%)	6 (3%)	46	48
8	H	181/195 (93%)	178 (98%)	3 (2%)	68	74
8	V	172/195 (88%)	166 (96%)	6 (4%)	43	44
9	I	176/174 (101%)	175 (99%)	1 (1%)	90	94
9	W	173/174 (99%)	172 (99%)	1 (1%)	90	94
10	J	166/170 (98%)	160 (96%)	6 (4%)	42	43
10	X	164/170 (96%)	159 (97%)	5 (3%)	48	51
11	K	155/159 (98%)	148 (96%)	7 (4%)	34	32
11	Y	159/159 (100%)	155 (98%)	4 (2%)	55	59
12	L	175/178 (98%)	167 (95%)	8 (5%)	33	31
12	Z	175/178 (98%)	170 (97%)	5 (3%)	50	53
13	M	180/181 (99%)	178 (99%)	2 (1%)	80	85
13	a	178/181 (98%)	173 (97%)	5 (3%)	51	55
14	N	158/159 (99%)	154 (98%)	4 (2%)	55	59
14	b	158/159 (99%)	154 (98%)	4 (2%)	55	59
All	All	5035/5366 (94%)	4856 (96%)	179 (4%)	43	43

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	50	LYS
1	A	53	SER
1	A	61	VAL
1	A	69	LYS
1	A	142	ARG
1	A	174	GLU
1	A	176	ARG
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	43	VAL
2	B	59	VAL
2	B	190	LEU
2	B	229	LYS
2	B	249	ARG
3	C	2	SER
3	C	35	VAL
3	C	45	VAL
3	C	105	GLU
3	C	113	SER
3	C	148	ASP
3	C	183	THR
3	C	205	ASN
3	C	208	LEU
4	D	46	VAL
4	D	65	GLU
4	D	95	GLU
4	D	126	GLU
4	D	199	LEU
5	E	29	VAL
5	E	61	LYS
5	E	62	LYS
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	180	MET
5	E	181	GLU
5	E	189	LYS
5	E	204	ASP
6	F	17	ASP

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Mol	Chain	Res	Type
6	F	53	VAL
6	F	81	LEU
6	F	86	SER
6	F	87	LEU
6	F	174	THR
6	F	187	ARG
6	F	190	VAL
6	F	215	TRP
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
8	H	6	VAL
8	H	65	LEU
8	H	68	LEU
9	I	35	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	18	ASP
10	J	62	LYS
10	J	88	LEU
10	J	155	ARG
11	K	8	PHE
11	K	12	VAL
11	K	41	LEU
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	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

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Mol	Chain	Res	Type
13	M	154	LEU
14	N	22	THR
14	N	35	THR
14	N	84	LYS
14	N	196	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	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	43	VAL
2	P	59	VAL
2	P	124	PHE
2	P	190	LEU
2	P	204	SER
2	P	235	GLN
2	P	246	LYS
2	P	249	ARG
3	Q	2	SER
3	Q	45	VAL
3	Q	56	GLU
3	Q	98	VAL
3	Q	105	GLU
3	Q	113	SER
3	Q	148	ASP
3	Q	170	GLU
3	Q	183	THR
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	227	LYS
4	R	32	LYS
4	R	46	VAL
5	S	3	ARG

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Mol	Chain	Res	Type
5	S	29	VAL
5	S	45	VAL
5	S	62	LYS
5	S	101	ARG
5	S	180	MET
6	T	17	ASP
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	223	ARG
6	T	240	LYS
6	T	241	GLU
7	U	42	VAL
7	U	78	CYS
7	U	182	LYS
7	U	199	ILE
7	U	206	LEU
7	U	223	GLU
8	V	6	VAL
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	213	THR
9	W	35	THR
10	X	1	MET
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	158	GLU
11	Y	8	PHE
11	Y	12	VAL
11	Y	41	LEU
11	Y	147	LEU
12	Z	102	PHE
12	Z	169	ASP
12	Z	172	MET
12	Z	174	LEU

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Mol	Chain	Res	Type
12	Z	207	THR
13	a	92	LEU
13	a	100	ARG
13	a	154	LEU
13	a	198	GLU
13	a	216	SER
14	b	22	THR
14	b	35	THR
14	b	84	LYS
14	b	196	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) 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
5	E	16	GLN
5	E	65	HIS
6	F	143	ASN
7	G	68	HIS
8	H	116	HIS
8	H	153	ASN
8	H	193	ASN
9	I	161	HIS
10	J	87	ASN
10	J	101	ASN
11	K	162	GLN
12	L	157	ASN
13	M	162	GLN
1	O	62	HIS
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	109	GLN
2	P	146	GLN
3	Q	18	GLN
4	R	186	HIS
5	S	86	ASN
6	T	68	ASN
6	T	143	ASN

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Mol	Chain	Res	Type
8	V	116	HIS
8	V	193	ASN
9	W	172	ASN
10	X	24	ASN
11	Y	162	GLN
12	Z	79	ASN
12	Z	157	ASN
13	a	89	HIS
13	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	$\#\|Z\|>2$
3	YCM	C	63	3	7,9,10	1.12	0	5,10,12	1.25	1 (20%)
5	6V1	E	148	5	11,15,16	1.33	2 (18%)	11,20,22	1.91	4 (36%)
7	YCM	G	137	7	7,9,10	2.83	2 (28%)	5,10,12	2.66	3 (60%)
7	6V1	G	161	7	11,15,16	1.29	1 (9%)	11,20,22	2.85	8 (72%)
7	6V1	G	47	7	11,15,16	1.25	2 (18%)	11,20,22	2.39	2 (18%)
10	6V1	J	91	10	11,15,16	2.07	2 (18%)	11,20,22	3.39	5 (45%)
3	YCM	Q	63	3	7,9,10	1.74	2 (28%)	5,10,12	3.05	3 (60%)
5	6V1	S	148	5	11,15,16	1.38	3 (27%)	11,20,22	1.95	4 (36%)
7	YCM	U	137	7	7,9,10	1.85	1 (14%)	5,10,12	1.59	2 (40%)
7	6V1	U	161	7	11,15,16	1.23	1 (9%)	11,20,22	2.54	6 (54%)
7	6V1	U	47	7	11,15,16	1.46	3 (27%)	11,20,22	3.92	4 (36%)
10	6V1	X	91	10	11,15,16	1.57	2 (18%)	11,20,22	3.69	6 (54%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CB-SG	-6.58	1.68	1.81
10	J	91	6V1	C1-SG	-5.71	1.76	1.83
7	U	137	YCM	CB-SG	-4.64	1.72	1.81
10	X	91	6V1	C1-SG	-4.06	1.78	1.83
7	G	161	6V1	C2-N3	-3.19	1.34	1.38
3	Q	63	YCM	CD-SG	-3.13	1.74	1.81
5	E	148	6V1	C2-N3	-3.12	1.34	1.38
5	S	148	6V1	C2-N3	-3.08	1.34	1.38
3	Q	63	YCM	CB-SG	-2.96	1.75	1.81
7	G	47	6V1	C4-N3	-2.90	1.33	1.38
7	U	47	6V1	C1-SG	-2.85	1.79	1.83
7	U	47	6V1	C2-N3	-2.71	1.34	1.38
7	G	47	6V1	C2-N3	-2.61	1.35	1.38
10	J	91	6V1	C4-N3	-2.27	1.34	1.38
5	S	148	6V1	C4-N3	-2.24	1.34	1.38
7	U	47	6V1	C4-N3	-2.20	1.34	1.38
7	U	161	6V1	C2-N3	-2.12	1.35	1.38
5	E	148	6V1	C1-SG	-2.06	1.80	1.83
10	X	91	6V1	C4-N3	-2.05	1.35	1.38
5	S	148	6V1	C5-C4	2.16	1.54	1.50
7	G	137	YCM	CD-CE	2.16	1.57	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	63	YCM	CA-CB-SG	-5.01	101.00	112.84
7	G	47	6V1	C5-C1-C2	-4.56	100.51	103.98
10	X	91	6V1	O8-C4-C5	-4.31	121.60	127.38
10	X	91	6V1	O7-C2-C1	-4.09	117.79	125.18
7	U	161	6V1	C5-C1-C2	-3.90	101.02	103.98
7	U	161	6V1	O8-C4-C5	-3.83	122.24	127.38
10	J	91	6V1	O8-C4-C5	-3.42	122.79	127.38
10	J	91	6V1	O7-C2-C1	-3.26	119.29	125.18
7	U	47	6V1	C5-C1-C2	-3.20	101.55	103.98
5	S	148	6V1	C5-C1-C2	-2.98	101.71	103.98
5	E	148	6V1	O8-C4-C5	-2.92	123.46	127.38
7	G	161	6V1	O8-C4-C5	-2.87	123.53	127.38
7	U	47	6V1	O8-C4-C5	-2.87	123.53	127.38
7	G	161	6V1	C5-C1-C2	-2.85	101.81	103.98
7	G	137	YCM	CA-CB-SG	-2.84	106.14	112.84
7	G	161	6V1	C3-C6-N3	-2.69	103.08	111.79
7	G	161	6V1	C6-N3-C4	-2.60	120.48	123.24
7	U	137	YCM	CA-CB-SG	-2.48	106.99	112.84
5	E	148	6V1	O-C-CA	-2.40	119.27	125.72
5	S	148	6V1	O8-C4-C5	-2.39	124.18	127.38
5	S	148	6V1	O-C-CA	-2.29	119.57	125.72
7	U	137	YCM	O-C-CA	-2.28	119.61	125.72
3	Q	63	YCM	O-C-CA	-2.22	119.78	125.72
3	C	63	YCM	O-C-CA	-2.19	119.85	125.72
7	G	137	YCM	O-C-CA	-2.19	119.86	125.72
10	X	91	6V1	C6-N3-C4	-2.05	121.06	123.24
7	U	161	6V1	O-C-CA	-2.05	120.24	125.72
7	G	161	6V1	O7-C2-N3	2.01	126.97	124.19
5	E	148	6V1	C3-C6-N3	2.07	118.49	111.79
7	U	161	6V1	C6-N3-C4	2.37	125.76	123.24
7	G	161	6V1	O8-C4-N3	2.68	127.23	123.91
7	U	47	6V1	C6-N3-C2	3.32	126.00	123.42
7	U	161	6V1	O8-C4-N3	3.66	128.46	123.91
7	U	161	6V1	CB-SG-C1	3.77	109.07	101.58
5	S	148	6V1	C6-N3-C4	3.78	127.27	123.24
3	Q	63	YCM	CD-CE-NZ2	3.96	119.84	115.48
7	G	161	6V1	CB-SG-C1	4.09	109.72	101.58
5	E	148	6V1	C6-N3-C2	4.32	126.77	123.42
7	G	137	YCM	CD-CE-NZ2	4.36	120.29	115.48
7	G	161	6V1	C6-N3-C2	4.65	127.03	123.42
10	X	91	6V1	CB-SG-C1	4.68	110.88	101.58
10	J	91	6V1	O7-C2-N3	5.00	131.09	124.19
10	J	91	6V1	CB-SG-C1	5.03	111.59	101.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	X	91	6V1	O7-C2-N3	5.10	131.24	124.19
7	G	47	6V1	CB-SG-C1	5.84	113.19	101.58
10	J	91	6V1	C6-N3-C2	6.71	128.64	123.42
10	X	91	6V1	C6-N3-C2	7.53	129.27	123.42
7	U	47	6V1	CB-SG-C1	11.54	124.54	101.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	63	YCM	2	0

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	0.52	0	14,14,14	0.54	0
18	1PE	H	305	-	15,15,15	0.57	0	14,14,14	0.39	0
19	BO2	H	306	8	28,29,29	1.08	1 (3%)	32,38,38	1.22	2 (6%)
18	1PE	I	303	-	15,15,15	0.56	0	14,14,14	0.86	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	1PE	I	304	-	15,15,15	0.54	0	14,14,14	0.45	0
19	BO2	K	305	11	28,29,29	0.77	0	32,38,38	1.28	4 (12%)
18	1PE	L	301	-	15,15,15	0.58	0	14,14,14	0.68	0
18	1PE	M	305	-	15,15,15	0.54	0	14,14,14	0.33	0
19	BO2	N	304	14	28,29,29	1.01	1 (3%)	32,38,38	1.72	10 (31%)
19	BO2	V	303	8	28,29,29	0.87	0	32,38,38	1.47	4 (12%)
18	1PE	W	303	-	15,15,15	0.59	0	14,14,14	0.38	0
19	BO2	Y	305	11	28,29,29	0.77	0	32,38,38	1.08	2 (6%)
18	1PE	Z	301	-	15,15,15	0.59	0	14,14,14	0.46	0
18	1PE	b	303	-	15,15,15	0.62	0	14,14,14	0.66	0
19	BO2	b	305	14	28,29,29	0.95	0	32,38,38	1.23	4 (12%)

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
18	1PE	H	305	-	-	0/13/13/13	0/0/0/0
19	BO2	H	306	8	-	0/22/28/28	0/2/2/2
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	BO2	K	305	11	-	0/22/28/28	0/2/2/2
18	1PE	L	301	-	-	0/13/13/13	0/0/0/0
18	1PE	M	305	-	-	0/13/13/13	0/0/0/0
19	BO2	N	304	14	-	0/22/28/28	0/2/2/2
19	BO2	V	303	8	-	0/22/28/28	0/2/2/2
18	1PE	W	303	-	-	0/13/13/13	0/0/0/0
19	BO2	Y	305	11	-	0/22/28/28	0/2/2/2
18	1PE	Z	301	-	-	0/13/13/13	0/0/0/0
18	1PE	b	303	-	-	0/13/13/13	0/0/0/0
19	BO2	b	305	14	-	0/22/28/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	306	BO2	C11-C10	-2.17	1.48	1.54
19	N	304	BO2	O8-C7	-2.02	1.19	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	N	304	BO2	C3-C2-N1	-3.45	117.42	121.69
19	K	305	BO2	C2-C3-N4	-3.32	118.01	122.05
19	b	305	BO2	C6-C5-N4	-2.77	118.19	121.95
19	N	304	BO2	O8-C7-C2	-2.74	115.50	121.23
19	K	305	BO2	C3-C2-C7	-2.72	116.71	119.58
19	N	304	BO2	C6-C5-N4	-2.63	118.38	121.95
19	V	303	BO2	C22-C21-N20	-2.61	106.56	110.99
19	b	305	BO2	C3-C2-N1	-2.36	118.76	121.69
19	N	304	BO2	C5-C6-N1	-2.35	119.29	122.23
19	V	303	BO2	C3-C2-C7	-2.19	117.27	119.58
19	V	303	BO2	C15-C16-C17	-2.17	117.19	120.20
19	N	304	BO2	C2-C3-N4	-2.16	119.42	122.05
19	H	306	BO2	C22-C21-N20	-2.11	107.42	110.99
19	Y	305	BO2	C2-C3-N4	-2.08	119.52	122.05
18	I	303	1PE	C25-OH5-C14	2.10	122.27	113.31
19	Y	305	BO2	C7-C2-N1	2.12	120.18	117.67
19	b	305	BO2	C7-C2-N1	2.22	120.30	117.67
19	N	304	BO2	C7-C2-N1	2.24	120.31	117.67
19	K	305	BO2	C5-N4-C3	2.44	121.31	116.82
19	b	305	BO2	C5-N4-C3	2.48	121.37	116.82
19	N	304	BO2	C3-C2-C7	2.48	122.19	119.58
19	N	304	BO2	C2-C7-N9	2.53	120.73	115.07
19	N	304	BO2	C5-N4-C3	3.05	122.43	116.82
19	K	305	BO2	C7-C2-N1	3.13	121.37	117.67
19	H	306	BO2	C7-C2-N1	3.99	122.39	117.67
19	N	304	BO2	C6-N1-C2	4.52	122.94	116.93
19	V	303	BO2	C7-C2-N1	4.75	123.29	117.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	306	BO2	1	0
19	N	304	BO2	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.26	1 (0%) 93 94	31, 46, 82, 94	0
1	O	230/234 (98%)	0.06	9 (3%) 43 52	43, 63, 103, 122	0
2	B	248/261 (95%)	-0.20	4 (1%) 74 79	34, 52, 94, 132	0
2	P	248/261 (95%)	0.02	12 (4%) 34 43	39, 57, 100, 142	0
3	C	236/248 (95%)	0.03	8 (3%) 49 58	35, 62, 101, 125	0
3	Q	238/248 (95%)	0.38	25 (10%) 8 11	38, 66, 116, 153	0
4	D	233/241 (96%)	-0.05	4 (1%) 73 78	38, 57, 85, 118	0
4	R	233/241 (96%)	-0.18	3 (1%) 79 84	33, 47, 75, 97	0
5	E	233/263 (88%)	-0.07	11 (4%) 35 44	29, 43, 89, 116	0
5	S	237/263 (90%)	-0.11	8 (3%) 49 58	38, 51, 89, 114	0
6	F	239/255 (93%)	-0.25	0 100 100	27, 37, 59, 74	0
6	T	240/255 (94%)	0.08	8 (3%) 50 59	40, 60, 90, 114	0
7	G	241/246 (97%)	-0.20	3 (1%) 81 85	28, 42, 74, 108	0
7	U	235/246 (95%)	0.18	12 (5%) 32 40	45, 68, 100, 131	0
8	H	220/234 (94%)	-0.24	4 (1%) 71 76	29, 38, 69, 109	0
8	V	220/234 (94%)	-0.17	5 (2%) 64 70	37, 49, 79, 105	0
9	I	204/205 (99%)	-0.35	0 100 100	29, 38, 58, 76	0
9	W	204/205 (99%)	-0.25	0 100 100	34, 47, 71, 77	0
10	J	195/201 (97%)	-0.35	0 100 100	32, 43, 60, 75	0
10	X	195/201 (97%)	-0.37	0 100 100	33, 43, 58, 73	0
11	K	200/204 (98%)	-0.33	1 (0%) 91 93	32, 44, 69, 81	0
11	Y	201/204 (98%)	-0.27	3 (1%) 76 81	28, 40, 63, 80	0
12	L	213/213 (100%)	-0.32	0 100 100	32, 46, 68, 82	0
12	Z	213/213 (100%)	-0.34	0 100 100	29, 39, 61, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	216/219 (98%)	-0.29	1 (0%) 91 93	28, 41, 64, 90	0
13	a	216/219 (98%)	-0.32	1 (0%) 91 93	30, 43, 64, 83	0
14	N	202/205 (98%)	-0.33	0 100 100	29, 38, 57, 87	0
14	b	203/205 (99%)	-0.26	0 100 100	34, 46, 72, 101	0
All	All	6223/6458 (96%)	-0.16	123 (1%) 68 73	27, 48, 87, 153	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	204	SER	12.9
1	O	232	ILE	9.5
4	D	241	ILE	9.0
3	Q	202	GLY	7.6
2	P	203	VAL	7.2
5	E	54	SER	7.0
3	Q	238	GLU	6.7
3	Q	232	ILE	6.6
7	U	2	SER	6.5
3	Q	233	GLU	6.3
8	V	203	ARG	6.1
3	Q	236	LYS	6.0
3	Q	234	LYS	5.9
3	C	49	SER	5.9
11	K	40	TYR	5.7
13	a	216	SER	5.6
2	P	61	PHE	5.5
6	T	208	ALA	5.1
8	H	204	CYS	4.8
3	Q	240	GLU	4.6
5	E	201	ALA	4.6
5	E	53	GLN	4.4
2	P	205	LYS	4.3
4	R	241	ILE	4.2
5	E	52	ALA	4.1
5	S	239	ARG	4.1
3	Q	48	LYS	4.1
3	C	201	SER	4.0
7	U	242	LEU	3.9
1	O	201	GLN	3.8
11	Y	40	TYR	3.8
3	C	138	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
3	Q	229	VAL	3.8
11	Y	200	SER	3.8
3	Q	239	ASN	3.8
2	B	61	PHE	3.7
8	H	203	ARG	3.7
5	S	57	ALA	3.6
2	P	51	ASN	3.6
7	G	187	PHE	3.5
2	B	202	ASP	3.5
3	Q	205	ASN	3.5
5	E	56	LEU	3.5
2	B	203	VAL	3.4
3	Q	201	SER	3.4
3	Q	203	GLY	3.4
4	R	127	ASP	3.3
3	Q	200	GLN	3.2
8	V	204	CYS	3.2
2	P	202	ASP	3.2
3	Q	225	ILE	3.2
5	E	58	ALA	3.2
6	T	206	ASP	3.2
4	R	128	ALA	3.1
7	G	188	ASP	3.1
6	T	205	LYS	3.1
1	O	225	VAL	3.0
8	H	201	ARG	3.0
7	U	212	PRO	3.0
7	U	199	ILE	3.0
8	V	198	ARG	3.0
8	V	199	LEU	3.0
5	S	54	SER	2.9
5	S	56	LEU	2.8
11	Y	201	GLY	2.8
7	U	206	LEU	2.8
8	V	202	TYR	2.8
3	C	225	ILE	2.7
4	D	131	GLY	2.7
5	S	53	GLN	2.7
3	Q	230	ALA	2.7
1	O	181	LEU	2.7
3	Q	138	PHE	2.6
3	Q	47	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	130	PRO	2.6
2	P	220	ASN	2.6
7	U	3	ARG	2.6
3	Q	223	GLU	2.6
3	C	202	GLY	2.5
6	T	5	THR	2.5
2	P	234	GLU	2.5
1	O	157	TRP	2.5
6	T	143	ASN	2.4
3	C	236	LYS	2.4
1	O	56	TYR	2.4
1	O	3	ARG	2.4
6	T	204	VAL	2.4
5	E	237	GLU	2.4
2	P	247	ALA	2.4
7	U	177	SER	2.4
3	C	203	GLY	2.4
2	P	230	GLN	2.4
5	E	202	GLU	2.4
7	U	58	ASP	2.4
3	Q	181	ILE	2.4
7	U	186	LYS	2.3
2	P	52	ILE	2.3
5	S	55	GLU	2.3
1	O	177	TYR	2.3
3	C	48	LYS	2.3
2	P	249	ARG	2.3
3	Q	192	ILE	2.3
5	E	235	GLY	2.3
3	Q	237	GLU	2.3
6	T	180	GLN	2.3
5	S	51	ARG	2.2
8	H	202	TYR	2.2
13	M	215	ILE	2.2
7	U	240	VAL	2.2
6	T	54	LEU	2.2
7	U	196	GLU	2.2
4	D	127	ASP	2.2
1	O	59	ARG	2.1
5	S	174	ARG	2.1
3	Q	226	GLU	2.1
5	E	51	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	189	TRP	2.1
3	Q	213	ARG	2.0
1	A	232	ILE	2.0
3	Q	219	ILE	2.0
5	E	59	HIS	2.0
7	U	178	PHE	2.0
2	B	205	LYS	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	YCM	C	63	10/11	0.89	0.10	-	55,60,68,69	0
5	6V1	S	148	15/16	0.92	0.15	-	39,63,69,69	0
7	6V1	G	161	15/16	0.94	0.16	-	33,54,60,63	0
7	YCM	G	137	10/11	0.91	0.14	-	35,43,60,61	0
7	6V1	U	161	15/16	0.92	0.14	-	58,72,79,80	0
7	6V1	G	47	15/16	0.93	0.13	-	42,58,60,61	0
10	6V1	J	91	15/16	0.92	0.16	-	36,55,59,59	0
10	6V1	X	91	15/16	0.92	0.16	-	38,59,64,70	0
3	YCM	Q	63	10/11	0.93	0.09	-	54,57,66,68	0
7	YCM	U	137	10/11	0.90	0.15	-	57,65,83,84	0
5	6V1	E	148	15/16	0.93	0.11	-	32,51,59,59	0
7	6V1	U	47	15/16	0.77	0.29	-	82,108,112,115	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
18	1PE	I	304	16/16	0.79	0.29	22.51	62,76,88,88	0
15	CL	M	301	1/1	0.98	0.22	12.19	68,68,68,68	0
18	1PE	M	305	16/16	0.79	0.19	8.53	75,80,95,96	0
15	CL	S	301	1/1	0.95	0.22	8.20	75,75,75,75	0
18	1PE	L	301	16/16	0.82	0.17	6.12	55,70,75,76	0
15	CL	b	301	1/1	0.96	0.15	5.30	68,68,68,68	0
18	1PE	Z	301	16/16	0.83	0.16	4.57	57,71,80,80	0
17	MG	H	302	1/1	0.97	0.14	4.45	34,34,34,34	0
18	1PE	H	305	16/16	0.84	0.20	4.40	65,69,89,90	0
15	CL	M	302	1/1	0.97	0.15	4.00	65,65,65,65	0
15	CL	b	302	1/1	0.96	0.17	3.79	64,64,64,64	0
18	1PE	I	303	16/16	0.88	0.15	3.59	56,60,68,72	0
19	BO2	b	305	28/28	0.93	0.14	2.68	37,43,53,55	0
18	1PE	b	303	16/16	0.87	0.16	2.01	52,59,77,78	0
19	BO2	V	303	28/28	0.91	0.15	1.96	49,54,66,67	0
15	CL	B	302	1/1	0.96	0.13	1.89	62,62,62,62	0
18	1PE	W	303	16/16	0.87	0.12	1.75	56,63,79,79	0
19	BO2	N	304	28/28	0.94	0.12	1.71	35,37,44,47	0
19	BO2	H	306	28/28	0.91	0.15	1.49	38,45,67,67	0
15	CL	D	301	1/1	0.96	0.16	1.09	73,73,73,73	0
18	1PE	H	304	16/16	0.93	0.13	0.84	46,51,64,67	0
15	CL	Q	302	1/1	0.89	0.15	0.79	70,70,70,70	0
15	CL	G	301	1/1	0.99	0.13	0.74	50,50,50,50	0
15	CL	U	301	1/1	0.94	0.12	0.52	64,64,64,64	0
19	BO2	K	305	28/28	0.97	0.10	0.51	32,37,41,42	0
15	CL	A	304	1/1	0.98	0.11	0.37	59,59,59,59	0
15	CL	N	302	1/1	0.96	0.10	0.24	59,59,59,59	0
19	BO2	Y	305	28/28	0.97	0.11	-0.07	29,32,37,38	0
15	CL	N	301	1/1	0.97	0.10	-0.18	37,37,37,37	0
17	MG	L	303	1/1	0.96	0.09	-0.61	37,37,37,37	0
15	CL	S	302	1/1	0.91	0.11	-0.66	69,69,69,69	0
15	CL	C	301	1/1	0.87	0.08	-0.76	66,66,66,66	0
16	K	N	303	1/1	0.97	0.08	-0.97	45,45,45,45	0
15	CL	O	301	1/1	0.96	0.09	-1.18	59,59,59,59	0
15	CL	A	301	1/1	0.98	0.08	-1.27	48,48,48,48	0
15	CL	K	302	1/1	0.98	0.08	-1.36	74,74,74,74	0
15	CL	E	301	1/1	0.98	0.09	-1.38	65,65,65,65	0
15	CL	F	301	1/1	0.98	0.09	-1.53	56,56,56,56	0
15	CL	G	302	1/1	0.94	0.05	-1.82	62,62,62,62	0
16	K	Z	302	1/1	0.98	0.08	-1.95	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
17	MG	I	301	1/1	0.91	0.07	-2.14	37,37,37,37	0
15	CL	S	303	1/1	0.96	0.06	-2.14	61,61,61,61	0
16	K	b	304	1/1	0.93	0.07	-2.27	46,46,46,46	0
17	MG	I	305	1/1	0.98	0.07	-2.27	31,31,31,31	0
15	CL	Y	302	1/1	0.99	0.04	-2.47	68,68,68,68	0
15	CL	E	303	1/1	0.96	0.06	-2.76	60,60,60,60	0
16	K	L	302	1/1	0.98	0.05	-3.47	49,49,49,49	0
16	K	G	303	1/1	1.00	0.07	-3.62	37,37,37,37	0
17	MG	W	301	1/1	0.96	0.06	-4.01	36,36,36,36	0
15	CL	a	301	1/1	0.96	0.07	-4.43	67,67,67,67	0
17	MG	K	301	1/1	0.97	0.05	-6.05	34,34,34,34	0
16	K	U	302	1/1	0.98	0.04	-7.35	46,46,46,46	0
15	CL	O	303	1/1	0.82	0.12	-	87,87,87,87	0
15	CL	M	303	1/1	0.99	0.08	-	47,47,47,47	0
17	MG	H	301	1/1	0.99	0.06	-	53,53,53,53	0
15	CL	Y	301	1/1	0.96	0.10	-	67,67,67,67	0
15	CL	H	303	1/1	0.96	0.08	-	47,47,47,47	0
15	CL	Y	304	1/1	0.91	0.19	-	70,70,70,70	0
17	MG	X	301	1/1	0.97	0.04	-	49,49,49,49	0
17	MG	V	301	1/1	0.90	0.09	-	57,57,57,57	0
15	CL	R	302	1/1	0.96	0.18	-	58,58,58,58	0
15	CL	B	301	1/1	0.97	0.10	-	45,45,45,45	0
15	CL	a	302	1/1	0.98	0.08	-	49,49,49,49	0
17	MG	J	301	1/1	0.99	0.06	-	48,48,48,48	0
15	CL	M	304	1/1	0.97	0.09	-	58,58,58,58	0
15	CL	D	302	1/1	0.96	0.07	-	65,65,65,65	0
15	CL	I	302	1/1	0.96	0.08	-	44,44,44,44	0
15	CL	O	304	1/1	0.92	0.12	-	70,70,70,70	0
15	CL	Y	303	1/1	0.94	0.07	-	64,64,64,64	0
15	CL	V	302	1/1	0.89	0.10	-	60,60,60,60	0
15	CL	O	302	1/1	0.97	0.12	-	60,60,60,60	0
15	CL	K	304	1/1	0.89	0.13	-	71,71,71,71	0
15	CL	P	301	1/1	0.95	0.06	-	51,51,51,51	0
15	CL	Q	301	1/1	0.85	0.17	-	78,78,78,78	0
15	CL	R	301	1/1	0.96	0.09	-	61,61,61,61	0
15	CL	a	303	1/1	0.95	0.07	-	66,66,66,66	0
15	CL	W	302	1/1	0.97	0.06	-	52,52,52,52	0
15	CL	A	303	1/1	0.98	0.06	-	52,52,52,52	0
15	CL	E	302	1/1	0.97	0.09	-	53,53,53,53	0
15	CL	C	302	1/1	0.93	0.08	-	69,69,69,69	0
15	CL	A	302	1/1	0.83	0.11	-	69,69,69,69	0
15	CL	K	303	1/1	0.91	0.12	-	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.