



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:50 AM UTC

PDB ID : 5LE5 / pdb_00005le5
Title : Native human 20S proteasome at 1.8 Angstrom
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on : 2016-06-29
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

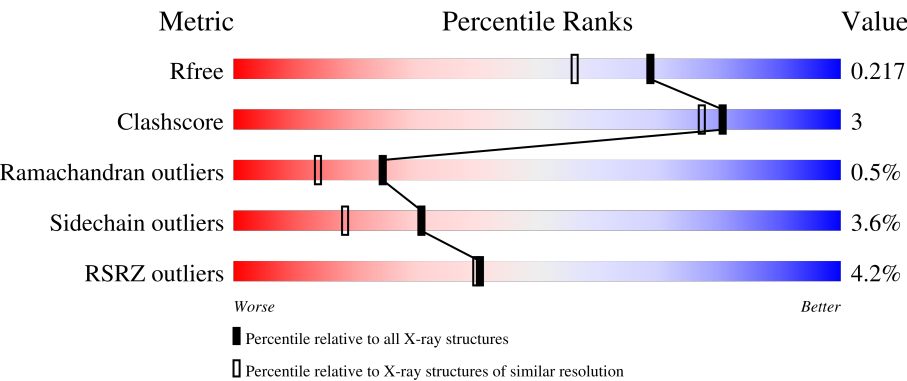
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	234	4% 89% 7% ...
1	O	234	8% 88% 9% ...
2	B	261	3% 87% 7% 5%
2	P	261	7% 84% 9% 5%
3	C	248	10% 79% 14% ..

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

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

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

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 52161 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	2	0
			1799	1151	307	335	6			
1	O	230	Total	C	N	O	S	0	0	0
			1779	1136	301	336	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	1	0
			1942	1226	332	373	11			
2	P	247	Total	C	N	O	S	0	2	0
			1919	1211	326	371	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	0	0
			1836	1152	328	351	5			
3	Q	234	Total	C	N	O	S	0	0	0
			1821	1143	319	354	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	2	0
			1783	1118	294	360	11			
4	R	233	Total	C	N	O	S	0	1	0
			1773	1115	295	352	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	0	0
			1833	1150	328	344	11			
5	S	238	Total	C	N	O	S	0	3	0
			1880	1179	339	351	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
			1890	1200	323	355	12			
6	T	240	Total	C	N	O	S	0	1	0
			1867	1186	320	349	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
			1928	1223	322	370	13			
7	U	235	Total	C	N	O	S	0	0	0
			1820	1151	306	350	13			

- 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
			1672	1053	286	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1655	1042	278	322	13			

- 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	6	0
			1633	1039	274	301	19			
9	W	204	Total	C	N	O	S	0	2	0
			1604	1021	269	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	2	0
			1585	1017	268	290	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1590	1019	270	291	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1543	974	267	293	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1564	988	275	291	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1656	1048	283	314	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1644	1043	281	309	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	0	0
			1687	1064	291	320	12			
13	a	216	Total	C	N	O	S	0	1	0
			1688	1065	291	320	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
			1515	951	258	293	13			
14	b	203	Total	C	N	O	S	0	1	0
			1526	958	259	296	13			

- Molecule 15 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

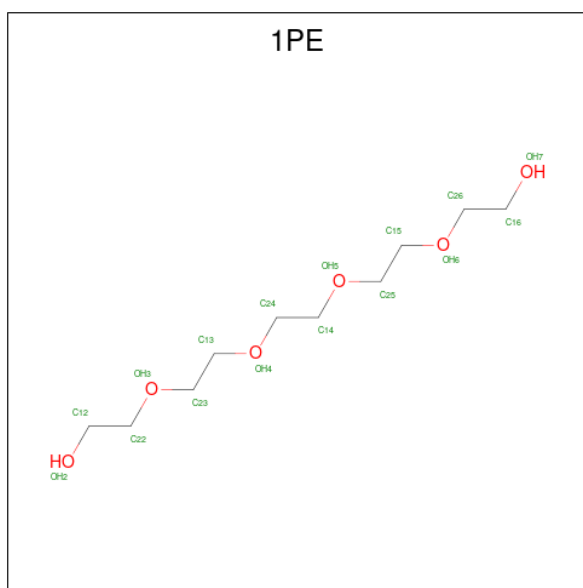
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	4	Total	Cl	0	0
			4	4		
15	B	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	2	Total 2	Cl 2	0	0
15	D	2	Total 2	Cl 2	0	0
15	E	3	Total 3	Cl 3	0	0
15	F	1	Total 1	Cl 1	0	0
15	G	2	Total 2	Cl 2	0	0
15	H	2	Total 2	Cl 2	0	0
15	I	1	Total 1	Cl 1	0	0
15	K	4	Total 4	Cl 4	0	0
15	M	4	Total 4	Cl 4	0	0
15	N	3	Total 3	Cl 3	0	0
15	O	4	Total 4	Cl 4	0	0
15	P	1	Total 1	Cl 1	0	0
15	Q	2	Total 2	Cl 2	0	0
15	R	2	Total 2	Cl 2	0	0
15	S	3	Total 3	Cl 3	0	0
15	U	1	Total 1	Cl 1	0	0
15	V	2	Total 2	Cl 2	0	0
15	W	1	Total 1	Cl 1	0	0
15	Y	5	Total 5	Cl 5	0	0
15	a	3	Total 3	Cl 3	0	0
15	b	3	Total 3	Cl 3	0	0

- Molecule 16 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 17 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	K	0	0
			1	1		
17	L	1	Total	K	0	0
			1	1		

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

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	112	Total 112	O 112	0	0
19	B	123	Total 123	O 123	0	0
19	C	75	Total 75	O 75	0	0
19	D	83	Total 83	O 83	0	0
19	E	134	Total 134	O 134	0	0

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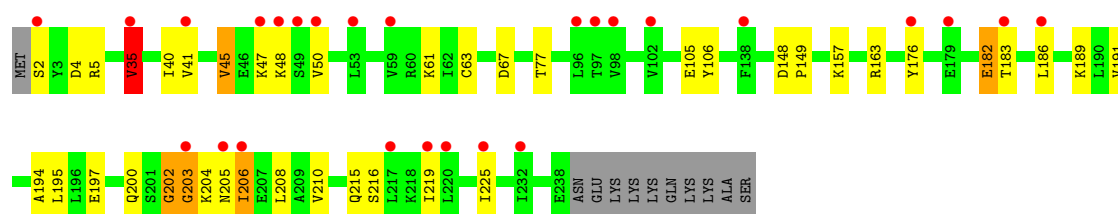
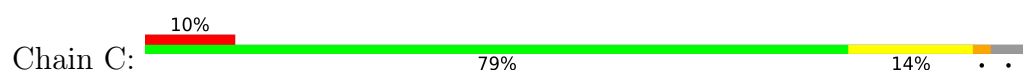
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	F	189	Total 189	O 189	0	0
19	G	190	Total 190	O 190	0	0
19	H	151	Total 151	O 151	0	0
19	I	149	Total 149	O 149	0	0
19	J	127	Total 127	O 127	0	0
19	K	108	Total 108	O 108	0	0
19	L	115	Total 115	O 115	0	0
19	M	155	Total 155	O 155	0	0
19	N	164	Total 164	O 164	0	0
19	O	85	Total 85	O 85	0	0
19	P	111	Total 111	O 111	0	0
19	Q	66	Total 66	O 66	0	0
19	R	126	Total 126	O 126	0	0
19	S	115	Total 115	O 115	0	0
19	T	85	Total 85	O 85	0	0
19	U	100	Total 100	O 100	0	0
19	V	108	Total 108	O 108	0	0
19	W	117	Total 117	O 117	0	0
19	X	120	Total 120	O 120	0	0
19	Y	145	Total 145	O 145	0	0
19	Z	168	Total 168	O 168	0	0

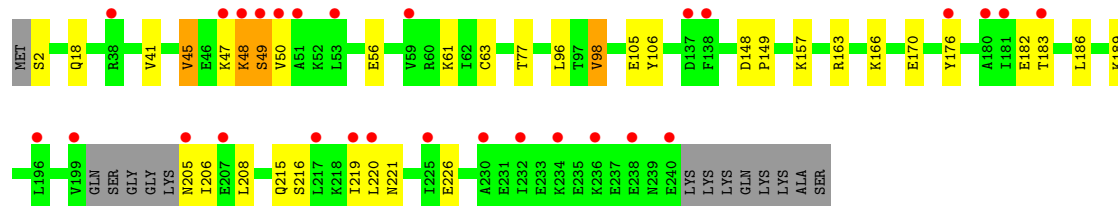
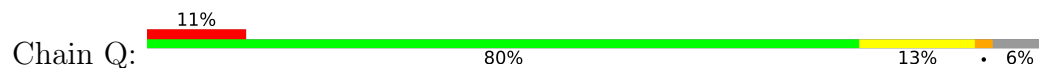
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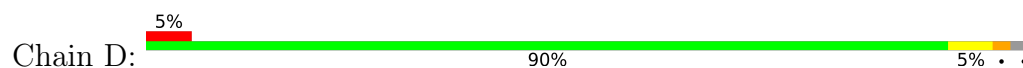
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	a	164	Total 164	O 164	0	0
19	b	127	Total 127	O 127	0	0



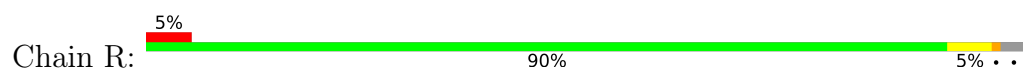
- Molecule 3: Proteasome subunit alpha type-7



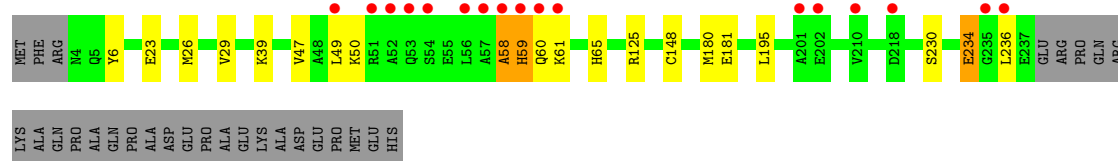
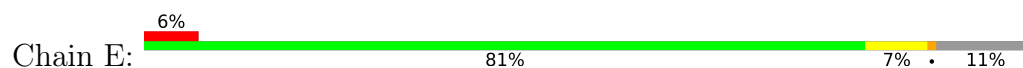
- Molecule 4: Proteasome subunit alpha type-5



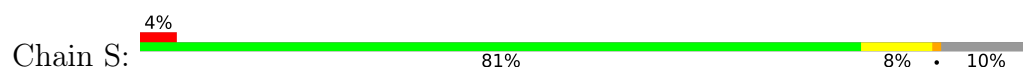
- Molecule 4: Proteasome subunit alpha type-5

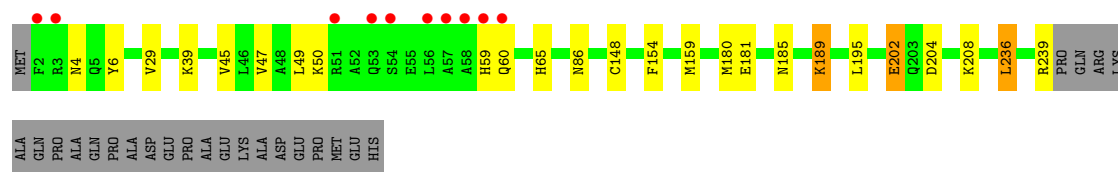


- Molecule 5: Proteasome subunit alpha type-1

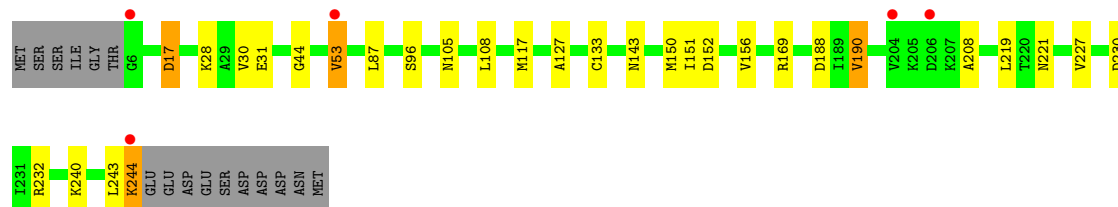
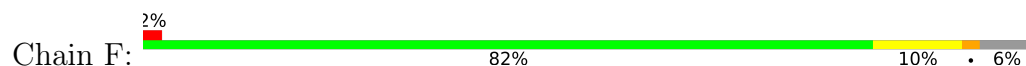


- Molecule 5: Proteasome subunit alpha type-1

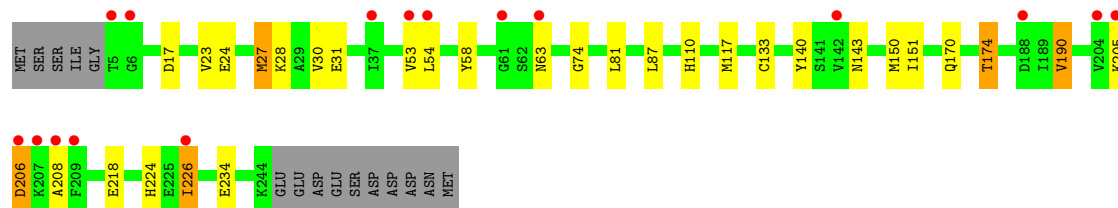
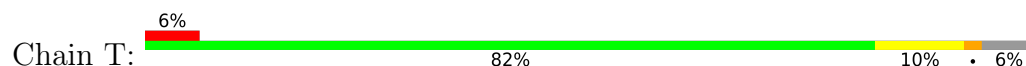




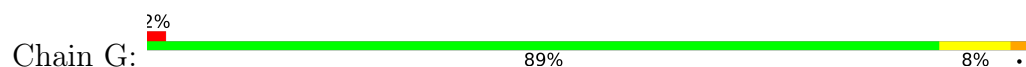
• Molecule 6: Proteasome subunit alpha type-3



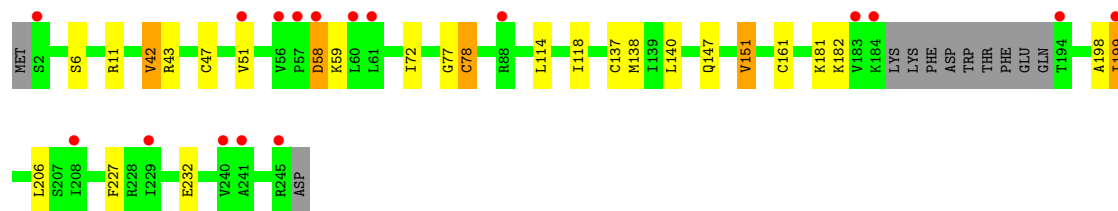
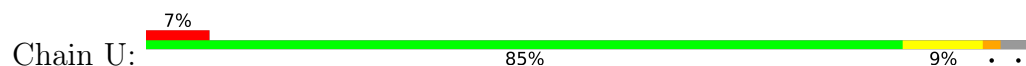
• Molecule 6: Proteasome subunit alpha type-3



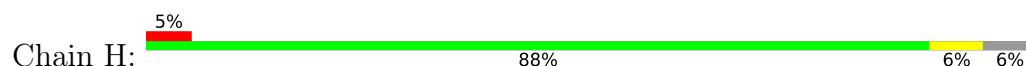
• Molecule 7: Proteasome subunit alpha type-6

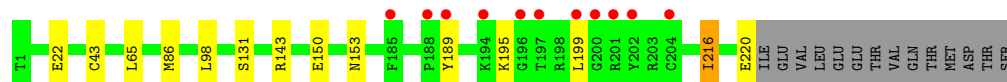


• Molecule 7: Proteasome subunit alpha type-6

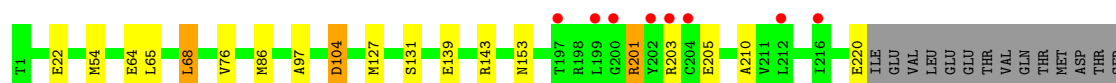
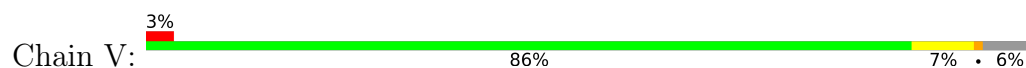


• Molecule 8: Proteasome subunit beta type-7

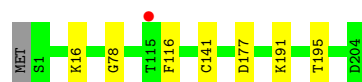




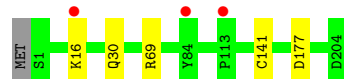
- Molecule 8: Proteasome subunit beta type-7



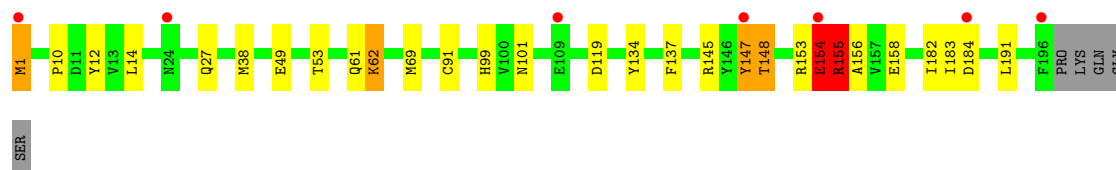
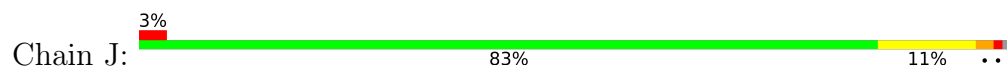
- Molecule 9: Proteasome subunit beta type-3



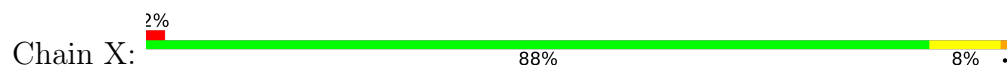
- Molecule 9: Proteasome subunit beta type-3



- 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

Chain Y:  90% 7% .

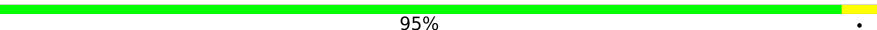


- Molecule 12: Proteasome subunit beta type-1

Chain L:  93% 6% .

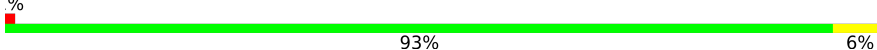


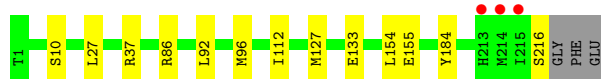
- Molecule 12: Proteasome subunit beta type-1

Chain Z:  95% . .



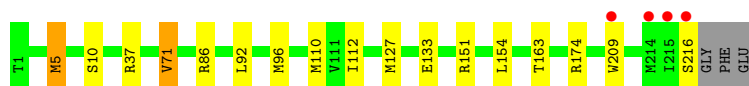
- Molecule 13: Proteasome subunit beta type-4

Chain M:  93% 6% .

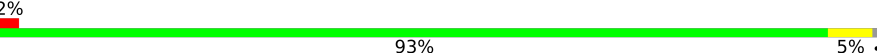


- Molecule 13: Proteasome subunit beta type-4

Chain a:  91% 7% ..

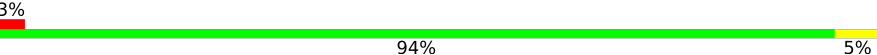


- Molecule 14: Proteasome subunit beta type-6

Chain N:  93% 5% .



- Molecule 14: Proteasome subunit beta type-6

Chain b:  94% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.44Å 202.77Å 316.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.66 – 1.80 170.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (170.66-1.80) 99.9 (170.66-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.182 , 0.212 0.190 , 0.217	Depositor DCC
R_{free} test set	33208 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52161	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: YCM, CL, MG, K, 1PE, 6V1

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	1/1844 (0.1%)	0.96	1/2500 (0.0%)
1	O	0.85	0/1818	0.96	1/2467 (0.0%)
2	B	1.06	3/1975 (0.2%)	1.07	6/2665 (0.2%)
2	P	0.97	3/1955 (0.2%)	0.98	0/2642
3	C	1.18	4/1851 (0.2%)	1.09	6/2502 (0.2%)
3	Q	1.07	3/1835 (0.2%)	1.07	1/2485 (0.0%)
4	D	0.95	0/1810	1.01	7/2448 (0.3%)
4	R	1.03	0/1800	1.06	6/2431 (0.2%)
5	E	0.99	0/1851	1.03	3/2502 (0.1%)
5	S	0.94	0/1908	0.99	4/2577 (0.2%)
6	F	1.12	4/1937 (0.2%)	1.07	4/2607 (0.2%)
6	T	0.99	0/1905	1.06	6/2567 (0.2%)
7	G	1.08	1/1925 (0.1%)	1.05	8/2598 (0.3%)
7	U	0.90	0/1806	0.94	2/2438 (0.1%)
8	H	1.09	1/1705 (0.1%)	1.01	2/2307 (0.1%)
8	V	0.89	0/1688	0.97	1/2288 (0.0%)
9	I	1.04	0/1668	0.97	0/2247
9	W	0.89	0/1636	0.95	7/2205 (0.3%)
10	J	1.30	8/1605 (0.5%)	1.05	3/2170 (0.1%)
10	X	1.08	2/1613 (0.1%)	1.02	5/2180 (0.2%)
11	K	1.04	1/1574 (0.1%)	1.02	3/2128 (0.1%)
11	Y	1.07	0/1604	0.98	1/2165 (0.0%)
12	L	0.90	0/1692	0.94	0/2281
12	Z	1.03	0/1677	1.01	3/2260 (0.1%)
13	M	1.01	0/1720	1.00	1/2328 (0.0%)
13	a	1.06	0/1724	1.02	5/2334 (0.2%)
14	N	1.18	2/1544 (0.1%)	1.04	1/2090 (0.0%)
14	b	1.07	4/1556 (0.3%)	1.03	1/2107 (0.0%)
All	All	1.03	37/49226 (0.1%)	1.01	88/66519 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
3	C	0	1
3	Q	0	2
4	D	0	3
7	U	1	0
9	I	0	1
10	X	0	1
12	Z	0	1
All	All	1	10

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	182	GLU	CG-CD	16.72	1.93	1.52
3	Q	189	LYS	C-O	16.44	1.44	1.24
3	C	182	GLU	CD-OE2	-14.01	0.98	1.25
10	J	154	GLU	CA-C	12.91	1.69	1.52
10	J	10	PRO	C-O	-12.48	1.08	1.24
10	J	155	ARG	N-CA	-10.13	1.33	1.46
7	G	108	GLU	CD-OE1	8.82	1.42	1.25
3	C	41	VAL	C-O	8.30	1.32	1.24
3	C	189	LYS	C-O	8.25	1.34	1.24
14	b	181	GLU	C-O	7.45	1.33	1.24
2	B	162	THR	C-O	7.30	1.31	1.23
10	J	147	TYR	C-N	6.54	1.40	1.33
10	J	158	GLU	CA-C	6.36	1.60	1.52
10	X	184	ASP	CG-OD1	6.35	1.37	1.25
2	P	37	ILE	C-O	6.29	1.30	1.24
10	J	156	ALA	N-CA	5.88	1.53	1.46
3	Q	41	VAL	C-O	5.83	1.29	1.24
10	J	14	LEU	CA-C	-5.68	1.45	1.52
3	Q	182	GLU	C-O	5.68	1.30	1.24
14	b	164	MET	C-O	-5.66	1.17	1.24
14	b	150	GLU	CD-OE1	5.63	1.36	1.25
8	H	189	TYR	CA-C	-5.63	1.45	1.53
2	P	184	MET	C-O	5.62	1.30	1.24
11	K	147	LEU	C-O	5.47	1.30	1.23
14	b	180	ALA	CA-C	5.43	1.59	1.52
10	X	158	GLU	CA-C	5.43	1.59	1.52
6	F	188	ASP	CG-OD1	5.41	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	52	ILE	CA-C	-5.39	1.46	1.52
1	A	3	ARG	CZ-NH2	5.32	1.40	1.33
6	F	44	GLY	N-CA	5.26	1.50	1.45
14	N	62	GLN	CA-C	5.24	1.59	1.52
2	B	97	TYR	CA-C	5.13	1.59	1.52
6	F	96	SER	C-O	-5.11	1.18	1.24
6	F	17	ASP	CG-OD2	5.09	1.35	1.25
14	N	148	THR	CA-CB	5.08	1.61	1.53
2	B	103	GLU	C-O	5.08	1.28	1.24
10	J	145	ARG	C-O	5.03	1.30	1.24

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	183	VAL	CB-CA-C	-11.30	96.88	112.14
6	F	190	VAL	CB-CA-C	-10.78	97.59	112.14
6	T	190	VAL	CB-CA-C	-9.52	99.56	112.04
10	X	1	MET	CB-CG-SD	-9.42	84.45	112.70
5	E	58	ALA	N-CA-C	8.49	121.48	111.71
12	Z	99	ARG	NE-CZ-NH2	-8.37	111.67	119.20
3	C	203	GLY	N-CA-C	8.25	122.58	111.03
6	T	27	MET	CG-SD-CE	7.24	116.82	100.90
6	T	226	ILE	CB-CA-C	-7.23	100.45	111.08
12	Z	99	ARG	NE-CZ-NH1	6.97	128.47	121.50
11	K	86	MET	CG-SD-CE	6.95	116.20	100.90
6	T	190	VAL	N-CA-CB	6.87	119.06	110.47
4	R	129	ASP	CA-C-N	-6.67	111.50	119.84
4	R	129	ASP	C-N-CA	-6.67	111.50	119.84
7	G	183	VAL	N-CA-CB	6.66	119.60	110.54
13	a	5	MET	CG-SD-CE	6.63	115.48	100.90
7	G	183	VAL	N-CA-C	6.62	117.37	110.62
4	D	125	GLU	N-CA-C	6.50	120.85	112.41
3	Q	98	VAL	CB-CA-C	6.46	118.92	110.84
9	W	16[A]	LYS	CA-C-N	6.45	135.33	123.13
9	W	16[A]	LYS	C-N-CA	6.45	135.33	123.13
9	W	16[B]	LYS	CA-C-N	6.45	135.33	123.13
9	W	16[B]	LYS	C-N-CA	6.45	135.33	123.13
11	K	47	GLY	N-CA-C	-6.40	105.78	111.67
2	B	247	ALA	N-CA-C	6.38	119.91	111.75
7	G	88	ARG	NE-CZ-NH1	-6.37	115.13	121.50
10	X	155	ARG	CB-CA-C	-6.34	100.26	110.79
3	C	35	VAL	CB-CA-C	6.28	120.18	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	12	VAL	CB-CA-C	6.28	119.50	110.33
7	U	58	ASP	N-CA-C	6.26	117.98	111.03
10	J	10	PRO	CB-CA-C	-6.22	102.35	112.62
10	J	158	GLU	O-C-N	6.21	128.46	122.07
14	N	6	VAL	CB-CA-C	-6.17	100.53	110.28
14	b	6	VAL	CB-CA-C	-6.16	100.55	110.28
6	F	190	VAL	N-CA-CB	6.14	118.90	110.54
9	W	69	ARG	NE-CZ-NH1	6.14	127.64	121.50
12	Z	99	ARG	CD-NE-CZ	6.13	132.98	124.40
11	Y	71	LYS	CD-CE-NZ	6.05	131.27	111.90
8	H	86	MET	CG-SD-CE	-5.98	87.75	100.90
4	R	120[A]	ALA	N-CA-C	5.98	117.88	111.36
4	R	120[B]	ALA	N-CA-C	5.98	117.88	111.36
9	W	69	ARG	NE-CZ-NH2	-5.97	113.83	119.20
10	X	154	GLU	CA-C-O	5.87	126.64	120.42
10	X	154	GLU	O-C-N	-5.84	115.50	122.15
3	C	200	GLN	N-CA-C	5.77	118.04	111.11
2	B	162	THR	CA-C-O	5.75	127.47	121.31
3	C	189	LYS	N-CA-C	5.73	118.30	111.71
9	W	69	ARG	CB-CG-CD	5.66	124.33	111.30
6	T	143	ASN	N-CA-C	5.62	117.40	111.28
13	a	71	VAL	N-CA-CB	5.62	119.00	110.58
5	S	236	LEU	N-CA-C	-5.59	95.36	111.00
4	D	120[A]	ALA	N-CA-C	-5.55	100.93	109.76
4	D	120[B]	ALA	N-CA-C	-5.55	100.93	109.76
8	V	86	MET	CG-SD-CE	-5.54	88.72	100.90
10	X	155	ARG	N-CA-C	5.52	117.30	111.28
3	C	189	LYS	CA-C-O	5.48	126.30	120.10
3	C	182	GLU	CG-CD-OE2	-5.47	105.82	118.40
13	a	10	SER	N-CA-C	5.43	117.30	110.24
2	B	168	SER	CB-CA-C	-5.42	101.47	110.68
2	B	204	SER	N-CA-C	5.39	122.29	110.80
5	E	6	TYR	CA-C-N	-5.39	114.20	122.60
5	E	6	TYR	C-N-CA	-5.39	114.20	122.60
2	B	43	VAL	CB-CA-C	-5.38	101.50	111.18
7	G	88	ARG	CG-CD-NE	-5.37	100.18	112.00
5	S	4	ASN	N-CA-C	5.34	117.10	111.28
6	F	117	MET	CG-SD-CE	5.34	112.65	100.90
13	a	110	MET	N-CA-C	5.31	117.89	109.50
13	M	10	SER	N-CA-C	5.30	117.13	110.24
8	H	216	ILE	CB-CA-C	-5.29	103.64	110.84
4	R	31	ILE	CB-CA-C	-5.25	105.05	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	199	ILE	CB-CA-C	5.24	119.45	112.22
1	O	180	ASP	N-CA-C	5.23	121.94	110.80
10	J	148	THR	O-C-N	5.22	125.05	121.71
1	A	53	SER	N-CA-C	5.17	121.82	110.80
7	G	244	GLU	N-CA-C	5.16	118.62	111.55
7	G	196	GLU	CB-CG-CD	5.15	121.36	112.60
4	D	120[A]	ALA	CA-C-N	5.14	131.40	122.56
4	D	120[A]	ALA	C-N-CA	5.14	131.40	122.56
4	D	120[B]	ALA	CA-C-N	5.14	131.40	122.56
4	D	120[B]	ALA	C-N-CA	5.14	131.40	122.56
2	B	55	LEU	N-CA-C	5.13	119.30	113.19
5	S	6	TYR	CA-C-N	-5.12	114.61	122.60
5	S	6	TYR	C-N-CA	-5.12	114.61	122.60
7	G	11	ARG	CG-CD-NE	5.12	123.26	112.00
6	T	117	MET	CG-SD-CE	5.10	112.12	100.90
6	F	143	ASN	N-CA-C	5.02	116.75	111.28
4	R	128	ALA	N-CA-C	5.02	121.49	110.80
13	a	151	ARG	CB-CG-CD	5.01	122.83	111.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	202	GLY	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide,Mainchain
9	I	78[B]	GLY	Peptide
2	P	54	LYS	Peptide
3	Q	220	LEU	Peptide
3	Q	49	SER	Peptide
10	X	10	PRO	Mainchain
12	Z	99	ARG	Sidechain

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	1799	0	1793	9	0
1	O	1779	0	1747	12	0
2	B	1942	0	1938	8	0
2	P	1919	0	1895	18	0
3	C	1836	0	1821	21	0
3	Q	1821	0	1788	12	0
4	D	1783	0	1751	6	0
4	R	1773	0	1760	9	0
5	E	1833	0	1797	9	0
5	S	1880	0	1850	13	0
6	F	1890	0	1886	12	0
6	T	1867	0	1847	12	0
7	G	1928	0	1905	11	0
7	U	1820	0	1792	12	0
8	H	1672	0	1703	6	0
8	V	1655	0	1661	10	0
9	I	1633	0	1660	4	0
9	W	1604	0	1626	2	0
10	J	1585	0	1568	22	0
10	X	1590	0	1580	9	0
11	K	1543	0	1495	4	0
11	Y	1564	0	1539	9	0
12	L	1656	0	1655	7	0
12	Z	1644	0	1644	3	0
13	M	1687	0	1666	6	0
13	a	1688	0	1666	12	0
14	N	1515	0	1492	4	0
14	b	1526	0	1503	8	0
15	A	4	0	0	0	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	0	0
15	G	2	0	0	0	0
15	H	2	0	0	1	0
15	I	1	0	0	0	0
15	K	4	0	0	0	0
15	M	4	0	0	1	0
15	N	3	0	0	0	0
15	O	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	2	0	0	1	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	2	0	0	0	0
15	W	1	0	0	0	0
15	Y	5	0	0	1	0
15	a	3	0	0	1	0
15	b	3	0	0	1	0
16	G	16	0	22	1	0
16	I	32	0	44	0	0
16	L	16	0	22	0	0
16	W	16	0	22	0	0
16	Z	16	0	22	0	0
16	a	16	0	22	0	0
16	b	32	0	44	0	0
17	G	1	0	0	0	0
17	L	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	Z	1	0	0	0	0
17	b	1	0	0	0	0
18	H	2	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	K	1	0	0	0	0
18	L	1	0	0	0	0
18	V	1	0	0	0	0
18	W	1	0	0	0	0
18	X	1	0	0	0	0
19	A	112	0	0	1	0
19	B	123	0	0	0	0
19	C	75	0	0	0	0
19	D	83	0	0	0	0
19	E	134	0	0	1	0
19	F	189	0	0	5	0
19	G	190	0	0	5	0
19	H	151	0	0	2	0
19	I	149	0	0	1	0
19	J	127	0	0	1	0
19	K	108	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	115	0	0	2	0
19	M	155	0	0	0	0
19	N	164	0	0	0	0
19	O	85	0	0	1	0
19	P	111	0	0	0	0
19	Q	66	0	0	0	0
19	R	126	0	0	2	0
19	S	115	0	0	3	0
19	T	85	0	0	1	0
19	U	100	0	0	0	0
19	V	108	0	0	2	0
19	W	117	0	0	2	0
19	X	120	0	0	1	0
19	Y	145	0	0	0	0
19	Z	168	0	0	0	0
19	a	164	0	0	2	0
19	b	127	0	0	0	0
All	All	52161	0	48226	251	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 (251) 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)
3:C:182:GLU:CD	3:C:182:GLU:CG	1.93	1.39
10:J:1:MET:HG3	10:J:134:TYR:CD2	1.92	1.04
10:J:183:ILE:O	10:J:184:ASP:OD1	1.83	0.97
9:I:16[A]:LYS:O	19:I:401:HOH:O	1.85	0.95
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.52	0.91
10:J:1:MET:HG3	10:J:134:TYR:HD2	1.36	0.91
2:P:155:ASN:OD1	3:Q:77:THR:OG1	1.89	0.88
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.58	0.84
10:J:153:ARG:NH2	10:J:184:ASP:OD2	2.11	0.84
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.61	0.82
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.62	0.80
5:S:65[A]:HIS:CE1	19:S:401:HOH:O	2.34	0.80
7:G:192:GLU:OE2	19:G:401:HOH:O	2.01	0.77
4:R:129:ASP:CB	4:R:130:PRO:HD3	2.15	0.77
2:P:194:ILE:CD1	2:P:236:LEU:HB3	2.15	0.77
3:C:35:VAL:HG13	3:C:191:VAL:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:301:CL:CL	19:R:515:HOH:O	2.42	0.75
2:P:52:ILE:O	2:P:53:HIS:HB2	1.87	0.75
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.04	0.74
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.35	0.74
10:J:1:MET:CG	10:J:134:TYR:CD2	2.71	0.73
1:O:73:LEU:CD2	1:O:135:ILE:HG12	2.19	0.73
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.71	0.73
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.38	0.72
1:A:3:ARG:HG2	6:F:127:ALA:HB2	1.71	0.71
7:U:118:ILE:HG13	7:U:138:MET:HE1	1.73	0.69
10:J:99[A]:HIS:CD2	19:J:408:HOH:O	2.45	0.69
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.74	0.68
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.74	0.68
10:J:153:ARG:NH1	10:J:184:ASP:OD2	2.28	0.67
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.40	0.66
10:J:183:ILE:C	10:J:184:ASP:OD1	2.39	0.66
13:a:86:ARG:NH1	13:a:133:GLU:OE1	2.29	0.65
13:a:5:MET:HE2	14:b:116:MET:HB3	1.78	0.64
1:O:181:LEU:CD2	1:O:185:ASP:HB2	2.27	0.64
8:H:153:ASN:ND2	19:H:401:HOH:O	2.30	0.63
6:T:205:LYS:O	6:T:206:ASP:CG	2.41	0.63
10:J:153:ARG:CZ	10:J:184:ASP:OD2	2.47	0.63
8:H:143:ARG:NH2	8:H:150:GLU:OE1	2.29	0.62
10:J:182:ILE:CD1	10:J:191:LEU:HD11	2.31	0.61
2:P:201:MET:HE1	2:P:211:VAL:HG12	1.83	0.60
1:O:180:ASP:N	1:O:180:ASP:OD1	2.34	0.60
3:Q:157:LYS:HB3	3:Q:176:TYR:CE2	2.37	0.60
10:J:12:TYR:CB	10:J:184:ASP:OD1	2.51	0.59
3:Q:157:LYS:HB3	3:Q:176:TYR:CZ	2.38	0.59
16:G:303:1PE:H222	19:G:457:HOH:O	2.02	0.58
5:S:65[A]:HIS:ND1	19:S:401:HOH:O	2.32	0.58
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.44	0.58
13:a:112:ILE:HD12	13:a:112:ILE:N	2.20	0.56
12:L:144:MET:CE	12:L:185:ARG:HB2	2.29	0.56
10:J:12:TYR:HB2	10:J:184:ASP:OD1	2.05	0.56
3:C:182:GLU:CG	3:C:182:GLU:OE2	2.40	0.56
2:P:48:GLU:HB2	2:P:201:MET:HE2	1.88	0.56
6:T:24:GLU:HA	6:T:27:MET:HE3	1.88	0.56
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.86	0.55
2:P:194:ILE:HD12	2:P:236:LEU:HB3	1.88	0.55
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:58:ASP:O	7:U:59:LYS:HB3	2.06	0.55
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.06	0.55
10:J:147:TYR:CE1	10:J:148:THR:C	2.85	0.55
12:L:72:LEU:HD22	12:L:83:MET:SD	2.47	0.55
10:X:1:MET:HG2	10:X:134:TYR:H	1.71	0.55
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.37	0.55
5:E:39:LYS:HE3	5:E:180:MET:HE1	1.88	0.55
3:Q:47:LYS:O	3:Q:48:LYS:CB	2.53	0.55
3:C:195:LEU:HD22	3:C:206:ILE:HG13	1.88	0.55
6:T:87:LEU:HD12	6:T:133[A]:CYS:SG	2.46	0.55
4:R:129:ASP:CB	4:R:130:PRO:CD	2.85	0.54
14:N:165:GLU:OE2	13:a:37:ARG:NH1	2.41	0.54
13:a:5:MET:HE3	14:b:116:MET:HB2	1.90	0.54
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	2.07	0.54
2:P:197:LEU:HD22	2:P:201:MET:HE3	1.90	0.54
2:P:194:ILE:HD13	2:P:236:LEU:HB3	1.89	0.54
6:F:87:LEU:HD12	6:F:133[A]:CYS:SG	2.48	0.54
15:a:302:CL:CL	15:b:502:CL:CL	3.00	0.54
15:H:304:CL:CL	19:H:533:HOH:O	2.55	0.54
5:S:185:ASN:HD21	5:S:189:LYS:HE2	1.72	0.54
13:a:96:MET:HE3	13:a:127:MET:HA	1.89	0.54
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.48	0.53
12:Z:72:LEU:HD22	12:Z:83:MET:SD	2.48	0.53
13:M:96:MET:HE3	13:M:127:MET:HA	1.91	0.53
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.91	0.53
14:N:190:LEU:H	14:N:193:GLN:HE21	1.57	0.53
3:C:182:GLU:CD	3:C:182:GLU:CB	2.76	0.52
5:S:39:LYS:HE3	5:S:180:MET:HE1	1.91	0.52
5:E:23:GLU:HA	5:E:26:MET:HE2	1.91	0.52
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.91	0.52
13:M:37:ARG:NH1	14:b:165:GLU:OE2	2.43	0.52
13:M:112:ILE:HD12	13:M:112:ILE:N	2.25	0.52
7:U:43:ARG:HB3	7:U:151:VAL:HG13	1.91	0.52
1:A:206:ASN:C	1:A:206:ASN:HD22	2.18	0.52
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.91	0.51
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.93	0.51
3:Q:183:THR:HG23	3:Q:186:LEU:H	1.75	0.51
11:Y:141[A]:ARG:NE	11:Y:141[A]:ARG:HA	2.25	0.51
14:b:190:LEU:H	14:b:193:GLN:HE21	1.58	0.51
3:C:47:LYS:HB2	3:C:205:ASN:HB3	1.93	0.51
1:O:181:LEU:HD21	1:O:185:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:54:MET:HE1	19:W:495:HOH:O	2.10	0.50
3:C:157:LYS:HB3	3:C:176:TYR:CE2	2.46	0.50
7:G:43:ARG:HB3	7:G:151:VAL:HG23	1.93	0.50
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.94	0.50
11:K:176:LEU:HD23	11:K:187:VAL:HG22	1.93	0.50
1:A:221:THR:HG21	19:A:509:HOH:O	2.12	0.50
10:J:182:ILE:HD12	10:J:191:LEU:HD11	1.93	0.50
15:M:302:CL:CL	15:M:303:CL:CL	3.04	0.50
8:V:201:ARG:NH1	19:V:401:HOH:O	2.39	0.50
10:J:38:MET:HE1	10:J:61:GLN:HB2	1.94	0.49
4:D:164:GLN:OE1	5:E:58:ALA:HB2	2.12	0.49
10:X:38:MET:HE1	10:X:61:GLN:HB2	1.93	0.49
5:S:185:ASN:ND2	5:S:189:LYS:HE2	2.27	0.49
10:X:49:GLU:O	10:X:53:THR:HG23	2.13	0.49
13:a:5:MET:HE2	14:b:116:MET:CB	2.41	0.49
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.42	0.49
8:H:195:LYS:HD2	12:Z:184:GLU:HG3	1.95	0.49
2:P:25[B]:MET:HA	2:P:25[B]:MET:CE	2.36	0.49
4:R:213:THR:HG22	4:R:231:LYS:HE3	1.95	0.49
3:C:40:ILE:HD11	3:C:210:VAL:CG1	2.42	0.49
3:C:203:GLY:HA3	3:C:206:ILE:HG22	1.94	0.49
6:F:105:ASN:ND2	19:F:405:HOH:O	2.44	0.49
7:G:192:GLU:HG3	19:G:401:HOH:O	2.12	0.49
6:F:169:ARG:NH1	19:F:406:HOH:O	2.46	0.49
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.94	0.48
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.53	0.48
1:O:206:ASN:C	1:O:206:ASN:HD22	2.21	0.48
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.91	0.48
7:G:88:ARG:NH1	19:G:406:HOH:O	2.46	0.48
6:T:170:GLN:O	6:T:174:THR:HG22	2.14	0.48
13:a:5:MET:CE	14:b:116:MET:HB2	2.43	0.48
6:F:221:ASN:HB2	19:F:566:HOH:O	2.12	0.48
8:H:216:ILE:HD13	9:I:195:THR:HG23	1.94	0.48
11:K:141:ARG:HA	11:K:141:ARG:NE	2.28	0.48
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.10	0.48
2:B:194:ILE:HD12	2:B:236:LEU:HB3	1.96	0.47
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.44	0.47
11:Y:158:ARG:HE	11:Y:162:GLN:NE2	2.08	0.47
12:L:81:LYS:NZ	19:L:401:HOH:O	2.46	0.47
10:J:49:GLU:O	10:J:53:THR:HG23	2.14	0.47
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:186[A]:ARG:HE	11:Y:186[A]:ARG:HB2	1.58	0.47
6:T:23:VAL:HG12	6:T:27:MET:HE2	1.96	0.47
7:G:11:ARG:HG2	7:G:11:ARG:HH11	1.80	0.47
5:S:86:ASN:ND2	19:S:403:HOH:O	2.48	0.47
13:a:163:THR:HG23	19:a:531:HOH:O	2.14	0.47
5:S:49:LEU:HG	5:S:195:LEU:HD21	1.96	0.46
5:E:230:SER:O	5:E:234:GLU:HG2	2.14	0.46
6:F:30:VAL:HG22	6:F:133[A]:CYS:HA	1.98	0.46
6:F:243:LEU:O	6:F:244:LYS:C	2.57	0.46
4:R:204:GLN:NE2	19:R:403:HOH:O	2.47	0.46
6:T:140:TYR:CZ	6:T:218:GLU:HG2	2.50	0.46
7:U:138:MET:HE3	7:U:140:LEU:HD11	1.98	0.46
9:I:141:CYS:HB3	9:I:177:ASP:HB2	1.97	0.46
12:L:159:GLN:HG3	8:V:210:ALA:HB2	1.98	0.46
3:Q:96:LEU:HD13	10:X:62:LYS:HG2	1.98	0.46
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.42	0.45
10:J:137:PHE:HB3	11:Y:133:VAL:HG21	1.98	0.45
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.46	0.45
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.46	0.45
13:a:5:MET:CE	14:b:116:MET:CB	2.94	0.45
1:A:58:GLU:CD	1:A:58:GLU:H	2.25	0.45
2:B:194:ILE:CD1	2:B:236:LEU:HB3	2.46	0.45
3:C:106:TYR:CD1	3:C:106:TYR:C	2.94	0.45
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.50	0.45
2:B:248:GLU:N	2:B:248:GLU:OE1	2.50	0.45
5:S:154:PHE:HD2	6:T:63:ASN:HD21	1.65	0.45
5:E:50:LYS:HB3	5:E:59:HIS:HB3	1.98	0.45
1:O:179:GLU:O	1:O:181:LEU:N	2.50	0.45
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.99	0.44
8:V:64:GLU:HG2	8:V:68:LEU:HD22	1.99	0.44
3:C:67:ASP:OD1	10:J:69:MET:HE1	2.18	0.44
6:F:219:LEU:HD22	19:F:525:HOH:O	2.17	0.44
1:O:17:LYS:HE2	1:O:19:VAL:HG12	1.99	0.44
5:S:202:GLU:CD	5:S:202:GLU:H	2.26	0.44
3:C:194:ALA:O	3:C:197:GLU:HB2	2.17	0.44
3:Q:45:VAL:HG21	3:Q:61:LYS:HB2	1.99	0.44
7:G:72:ILE:HG21	7:G:114:LEU:HD21	2.00	0.44
4:R:78:MET:HG3	4:R:82:ILE:HD12	2.00	0.44
14:N:172:GLY:HA2	13:a:209:TRP:CH2	2.52	0.44
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.98	0.44
7:G:192:GLU:CD	19:G:401:HOH:O	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:133:VAL:HG21	10:X:137:PHE:HB3	2.00	0.44
7:U:58:ASP:O	7:U:59:LYS:CB	2.65	0.44
8:V:143:ARG:HE	8:V:143:ARG:HB2	1.67	0.44
15:B:301:CL:CL	15:B:302:CL:CL	3.10	0.43
5:E:65:HIS:HB2	19:E:494:HOH:O	2.17	0.43
6:F:150:MET:C	6:F:151:ILE:HD12	2.42	0.43
6:T:30:VAL:HG22	6:T:133[A]:CYS:HA	1.99	0.43
2:P:52:ILE:O	2:P:53:HIS:CB	2.64	0.43
4:R:96:THR:HG22	4:R:112:VAL:HG22	2.00	0.43
2:B:44:LEU:C	2:B:44:LEU:HD12	2.44	0.43
10:J:154:GLU:H	10:J:154:GLU:CD	2.26	0.43
4:R:199:LEU:HD12	4:R:237:VAL:HG12	2.01	0.43
11:Y:68:LEU:O	11:Y:71:LYS:CE	2.66	0.43
4:D:127:ASP:HB3	5:E:125:ARG:HD3	2.00	0.43
8:V:153:ASN:HB2	19:V:493:HOH:O	2.18	0.43
5:S:189:LYS:HG2	5:S:236:LEU:HD13	2.01	0.43
2:B:97:TYR:CD1	2:B:97:TYR:C	2.96	0.43
7:G:49[B]:VAL:HG22	7:G:219:VAL:HG12	2.00	0.43
2:P:50:ARG:O	2:P:52:ILE:N	2.52	0.43
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.49	0.43
7:U:6:SER:OG	7:U:11:ARG:NH1	2.45	0.43
13:a:174:ARG:NH2	19:a:401:HOH:O	2.52	0.43
8:V:97:ALA:HB1	8:V:127[B]:MET:CE	2.49	0.42
3:C:183:THR:HG23	3:C:186:LEU:H	1.84	0.42
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.19	0.42
5:E:49:LEU:HG	5:E:195:LEU:HD21	2.00	0.42
9:I:116:PHE:CD2	9:I:191:LYS:HE3	2.54	0.42
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.42
3:C:4:ASP:O	4:D:125:GLU:HB2	2.20	0.42
4:R:199:LEU:HD12	4:R:237:VAL:CG1	2.49	0.42
1:A:164:LYS:HE2	1:A:164:LYS:HB3	1.81	0.42
3:C:5:ARG:NH1	4:D:125:GLU:OE2	2.44	0.42
1:O:147:GLN:HG3	1:O:162:MET:HE1	2.00	0.42
7:U:43:ARG:HB3	7:U:151:VAL:CG1	2.50	0.42
7:U:77:GLY:HA3	7:U:227:PHE:CD1	2.55	0.42
2:P:51:ASN:HB3	2:P:56:LEU:HD13	2.02	0.42
6:T:150:MET:C	6:T:151:ILE:HD12	2.44	0.42
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.20	0.42
2:P:190:LEU:HG	2:P:236:LEU:HD21	2.01	0.42
12:L:49:LYS:NZ	19:L:404:HOH:O	2.52	0.42
6:T:110:HIS:HD2	19:T:364:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:448:HOH:O	7:G:88:ARG:HD2	2.20	0.41
8:H:43:CYS:SG	8:H:98:LEU:HB3	2.60	0.41
7:U:42:VAL:HG13	7:U:198:ALA:HB2	2.02	0.41
10:X:132:HIS:HD2	19:X:488:HOH:O	2.03	0.41
1:O:181:LEU:HD23	1:O:185:ASP:HB2	2.00	0.41
2:P:197:LEU:HB3	2:P:201:MET:HE3	2.01	0.41
2:B:160:LYS:HE2	2:B:181:GLU:HG3	2.02	0.41
6:F:53:VAL:HG12	6:F:208:ALA:HB3	2.03	0.41
9:W:141:CYS:HB3	9:W:177:ASP:HB2	2.02	0.41
9:W:30:GLN:NE2	19:W:403:HOH:O	2.45	0.41
10:X:62:LYS:HA	10:X:62:LYS:HD3	1.81	0.41
7:G:192:GLU:OE1	7:G:193:GLN:OE1	2.39	0.41
11:Y:1:THR:HB	15:Y:301:CL:CL	2.58	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.03	0.41
12:L:184:GLU:OE2	12:L:211:ARG:HD2	2.21	0.41
3:Q:183:THR:HG22	3:Q:186:LEU:HD22	2.02	0.41
7:U:51:VAL:HG12	7:U:198:ALA:HB1	2.03	0.41
11:Y:9:ARG:NH2	11:Y:146:ASP:OD1	2.53	0.41
3:C:45:VAL:HG21	3:C:61:LYS:HB2	2.04	0.40
10:J:155:ARG:HD2	10:J:155:ARG:HA	1.95	0.40
5:S:159:MET:HE3	6:T:58:TYR:CE2	2.56	0.40
13:M:27:LEU:HD22	13:M:184:TYR:HB2	2.02	0.40
10:J:62:LYS:HD3	10:J:62:LYS:HA	1.84	0.40
13:M:92:LEU:O	13:M:96:MET:HG2	2.22	0.40
1:O:227:ASP:HB2	19:O:471:HOH:O	2.20	0.40
4:D:203:LYS:HE2	4:D:210:LEU:HB3	2.03	0.40
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.56	0.40
10:X:147:TYR:CE1	10:X:148:THR:C	3.00	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	230/234 (98%)	220 (96%)	6 (3%)	4 (2%)	7	2
1	O	228/234 (97%)	214 (94%)	7 (3%)	7 (3%)	3	0
2	B	247/261 (95%)	238 (96%)	9 (4%)	0	100	100
2	P	247/261 (95%)	234 (95%)	11 (4%)	2 (1%)	16	6
3	C	234/248 (94%)	224 (96%)	6 (3%)	4 (2%)	7	2
3	Q	229/248 (92%)	218 (95%)	6 (3%)	5 (2%)	5	1
4	D	233/241 (97%)	223 (96%)	6 (3%)	4 (2%)	7	2
4	R	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	9	3
5	E	231/263 (88%)	226 (98%)	4 (2%)	1 (0%)	30	19
5	S	238/263 (90%)	234 (98%)	4 (2%)	0	100	100
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100	100
6	T	239/255 (94%)	233 (98%)	4 (2%)	2 (1%)	16	6
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	228/246 (93%)	224 (98%)	4 (2%)	0	100	100
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	215 (98%)	4 (2%)	1 (0%)	24	14
9	I	208/205 (102%)	204 (98%)	4 (2%)	0	100	100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100	100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
11	K	199/204 (98%)	195 (98%)	4 (2%)	0	100	100
11	Y	200/204 (98%)	197 (98%)	3 (2%)	0	100	100
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
13	a	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	6196/6458 (96%)	6031 (97%)	132 (2%)	33 (0%)	24	14

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
4	D	127	ASP
4	D	176	GLY
1	O	52	LYS
1	O	53	SER
1	O	179	GLU
1	O	180	ASP
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
3	C	50	VAL
4	D	175[A]	GLU
4	D	175[B]	GLU
5	E	59	HIS
1	O	4	GLY
1	O	231	ALA
2	P	53	HIS
2	P	54	LYS
3	Q	48	LYS
1	A	50	LYS
3	C	48	LYS
3	C	202	GLY
3	C	216	SER
3	Q	49	SER
3	Q	216	SER
6	T	208	ALA
8	V	203	ARG
1	A	201	GLN
3	Q	50	VAL
1	O	201	GLN
6	T	206	ASP
3	Q	221	ASN

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	188/191 (98%)	178 (95%)	10 (5%)	20	9
1	O	184/191 (96%)	172 (94%)	12 (6%)	15	5
2	B	205/221 (93%)	197 (96%)	8 (4%)	28	16
2	P	201/221 (91%)	188 (94%)	13 (6%)	15	5
3	C	189/210 (90%)	179 (95%)	10 (5%)	20	9
3	Q	189/210 (90%)	175 (93%)	14 (7%)	13	4
4	D	194/203 (96%)	187 (96%)	7 (4%)	31	18
4	R	192/203 (95%)	190 (99%)	2 (1%)	68	64
5	E	195/223 (87%)	189 (97%)	6 (3%)	35	23
5	S	201/223 (90%)	192 (96%)	9 (4%)	24	12
6	F	200/212 (94%)	191 (96%)	9 (4%)	24	12
6	T	194/212 (92%)	184 (95%)	10 (5%)	21	9
7	G	206/207 (100%)	197 (96%)	9 (4%)	25	13
7	U	192/207 (93%)	183 (95%)	9 (5%)	23	11
8	H	183/195 (94%)	179 (98%)	4 (2%)	45	34
8	V	180/195 (92%)	172 (96%)	8 (4%)	25	13
9	I	178/174 (102%)	178 (100%)	0	100	100
9	W	174/174 (100%)	174 (100%)	0	100	100
10	J	166/170 (98%)	161 (97%)	5 (3%)	36	24
10	X	168/170 (99%)	165 (98%)	3 (2%)	51	43
11	K	153/159 (96%)	144 (94%)	9 (6%)	18	7
11	Y	157/159 (99%)	153 (98%)	4 (2%)	42	30
12	L	179/178 (101%)	171 (96%)	8 (4%)	24	12
12	Z	176/178 (99%)	170 (97%)	6 (3%)	32	20
13	M	179/181 (99%)	176 (98%)	3 (2%)	53	45
13	a	179/181 (99%)	175 (98%)	4 (2%)	45	34
14	N	157/159 (99%)	155 (99%)	2 (1%)	61	54
14	b	159/159 (100%)	159 (100%)	0	100	100
All	All	5118/5366 (95%)	4934 (96%)	184 (4%)	31	18

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	53	SER
1	A	61	VAL
1	A	109	LEU
1	A	164	LYS
1	A	176	ARG
1	A	178	ASN
1	A	189	THR
1	A	206	ASN
1	A	227	ASP
2	B	43	VAL
2	B	59	VAL
2	B	65	ILE
2	B	190	LEU
2	B	204	SER
2	B	207	SER
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	163	ARG
3	C	206	ILE
3	C	208	LEU
3	C	215	GLN
3	C	219	ILE
3	C	225	ILE
4	D	46	VAL
4	D	95	GLU
4	D	126	GLU
4	D	129	ASP
4	D	187	LYS
4	D	199	LEU
4	D	217	LEU
5	E	29	VAL
5	E	60	GLN
5	E	61	LYS
5	E	181	GLU
5	E	234	GLU
5	E	236	LEU
6	F	17	ASP
6	F	28	LYS

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Mol	Chain	Res	Type
6	F	31	GLU
6	F	53	VAL
6	F	108	LEU
6	F	190	VAL
6	F	230	ASP
6	F	240	LYS
6	F	244	LYS
7	G	11	ARG
7	G	42	VAL
7	G	78	CYS
7	G	146	GLU
7	G	147	GLN
7	G	183	VAL
7	G	196	GLU
7	G	206	LEU
7	G	232	GLU
8	H	22	GLU
8	H	65	LEU
8	H	199	LEU
8	H	220	GLU
10	J	1	MET
10	J	27	GLN
10	J	62	LYS
10	J	154	GLU
10	J	155	ARG
11	K	12	VAL
11	K	42	LEU
11	K	58	LEU
11	K	81	LYS
11	K	106	LYS
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	49	LYS
12	L	72	LEU
12	L	161	VAL
12	L	169	ASP
12	L	174	LEU
12	L	207	THR

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Mol	Chain	Res	Type
13	M	154	LEU
13	M	155	GLU
13	M	216	SER
14	N	201	THR
14	N	202	LEU
1	O	3	ARG
1	O	50	LYS
1	O	53	SER
1	O	131	VAL
1	O	174	GLU
1	O	176	ARG
1	O	178	ASN
1	O	179	GLU
1	O	180	ASP
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
2	P	7[A]	SER
2	P	7[B]	SER
2	P	43	VAL
2	P	53	HIS
2	P	54	LYS
2	P	59	VAL
2	P	65	ILE
2	P	160	LYS
2	P	190	LEU
2	P	207	SER
2	P	226	ARG
2	P	235	GLN
2	P	236	LEU
3	Q	2	SER
3	Q	45	VAL
3	Q	56	GLU
3	Q	98	VAL
3	Q	105	GLU
3	Q	163	ARG
3	Q	166	LYS
3	Q	170	GLU
3	Q	205	ASN
3	Q	206	ILE
3	Q	208	LEU
3	Q	215	GLN

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Mol	Chain	Res	Type
3	Q	219	ILE
3	Q	226	GLU
4	R	46	VAL
4	R	217	LEU
5	S	29	VAL
5	S	45	VAL
5	S	60	GLN
5	S	181	GLU
5	S	189	LYS
5	S	202	GLU
5	S	204	ASP
5	S	208	LYS
5	S	239	ARG
6	T	17	ASP
6	T	28	LYS
6	T	31	GLU
6	T	53	VAL
6	T	54	LEU
6	T	81	LEU
6	T	174	THR
6	T	190	VAL
6	T	226	ILE
6	T	234	GLU
7	U	42	VAL
7	U	78	CYS
7	U	147	GLN
7	U	151	VAL
7	U	181	LYS
7	U	182	LYS
7	U	199	ILE
7	U	206	LEU
7	U	232	GLU
8	V	22	GLU
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	201	ARG
8	V	205	GLU
8	V	220	GLU
10	X	62	LYS
10	X	95	ARG

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Mol	Chain	Res	Type
10	X	155	ARG
11	Y	58	LEU
11	Y	81	LYS
11	Y	89	GLN
11	Y	147	LEU
12	Z	49	LYS
12	Z	72	LEU
12	Z	161	VAL
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
13	a	71	VAL
13	a	92	LEU
13	a	154	LEU
13	a	216	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	94	GLN
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
2	B	88	ASN
2	B	100	GLN
2	B	102	GLN
2	B	146	GLN
3	C	54	GLN
3	C	92	GLN
3	C	175	ASN
3	C	215	GLN
4	D	152	GLN
4	D	204	GLN
4	D	227	HIS
5	E	8	ASN
5	E	16	GLN
5	E	65	HIS
5	E	185	ASN
5	E	203	GLN
6	F	143	ASN
7	G	128	ASN

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Mol	Chain	Res	Type
7	G	193	GLN
8	H	153	ASN
9	I	32	GLN
9	I	161	HIS
9	I	168	GLN
9	I	172	ASN
10	J	61	GLN
10	J	63	ASN
10	J	101	ASN
11	K	62	GLN
13	M	47	ASN
13	M	65	GLN
13	M	162	GLN
14	N	193	GLN
1	O	118	GLN
1	O	178	ASN
1	O	206	ASN
2	P	40	ASN
2	P	88	ASN
2	P	102	GLN
2	P	109	GLN
2	P	177	GLN
3	Q	15	HIS
3	Q	18	GLN
3	Q	92	GLN
3	Q	94	HIS
3	Q	175	ASN
3	Q	239	ASN
4	R	97	GLN
4	R	186	HIS
4	R	204	GLN
4	R	227	HIS
5	S	86	ASN
5	S	185	ASN
6	T	63	ASN
6	T	110	HIS
6	T	143	ASN
9	W	161	HIS
9	W	168	GLN
10	X	24	ASN
10	X	61	GLN
10	X	63	ASN

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Mol	Chain	Res	Type
10	X	174	ASN
11	Y	119	ASN
11	Y	162	GLN
12	Z	77	HIS
12	Z	79	ASN
13	a	65	GLN
13	a	89	HIS
13	a	162	GLN
14	b	193	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	$\# Z > 2$
7	6V1	G	47	7	13,15,16	3.29	5 (38%)	10,20,22	2.22	4 (40%)
7	6V1	U	47	7	13,15,16	2.26	2 (15%)	10,20,22	2.84	4 (40%)
5	6V1	S	148	5	13,15,16	2.03	3 (23%)	10,20,22	3.20	5 (50%)
5	6V1	E	148	5	13,15,16	1.94	5 (38%)	10,20,22	2.94	3 (30%)
7	6V1	U	161	7	13,15,16	1.88	4 (30%)	10,20,22	2.38	4 (40%)
3	YCM	Q	63	3	7,9,10	1.68	1 (14%)	5,10,12	3.49	3 (60%)
7	6V1	G	161	7	13,15,16	1.99	4 (30%)	10,20,22	2.08	3 (30%)
3	YCM	C	63	3	7,9,10	1.12	1 (14%)	5,10,12	0.82	0
7	YCM	G	137	7	7,9,10	2.25	3 (42%)	5,10,12	2.30	3 (60%)
10	6V1	X	91	10	13,15,16	2.72	4 (30%)	10,20,22	5.42	8 (80%)
7	YCM	U	137	7	7,9,10	1.30	1 (14%)	5,10,12	1.82	2 (40%)
10	6V1	J	91	10	13,15,16	2.39	2 (15%)	10,20,22	5.65	7 (70%)

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
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	2/6/25/27	0/1/1/1
5	6V1	S	148	5	-	2/6/25/27	0/1/1/1
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1
3	YCM	Q	63	3	-	4/6/8/10	-
7	6V1	G	161	7	-	1/6/25/27	0/1/1/1
3	YCM	C	63	3	-	1/6/8/10	-
7	YCM	G	137	7	-	2/6/8/10	-
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
7	YCM	U	137	7	-	2/6/8/10	-
10	6V1	J	91	10	-	2/6/25/27	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-8.81	1.73	1.82
10	X	91	6V1	C1-SG	-7.89	1.74	1.83
10	J	91	6V1	C1-SG	-7.53	1.75	1.83
7	U	47	6V1	CB-SG	-6.76	1.75	1.82
5	S	148	6V1	CB-SG	-4.97	1.77	1.82
7	G	47	6V1	C4-N3	-4.60	1.31	1.38
5	E	148	6V1	CB-SG	-4.49	1.77	1.82
7	G	47	6V1	C1-SG	3.93	1.87	1.83
3	Q	63	YCM	CD-SG	-3.82	1.72	1.81
10	X	91	6V1	CB-SG	-3.79	1.78	1.82
7	G	47	6V1	C2-N3	-3.78	1.33	1.38
7	G	161	6V1	CB-SG	-3.60	1.78	1.82
5	S	148	6V1	C2-N3	-3.60	1.33	1.38
7	G	137	YCM	CE-NZ2	3.56	1.44	1.32
7	U	161	6V1	CB-SG	-3.44	1.78	1.82
7	U	161	6V1	C4-N3	-3.37	1.33	1.38
7	G	161	6V1	C2-N3	-3.34	1.34	1.38
7	U	161	6V1	C1-SG	-3.19	1.79	1.83
7	G	161	6V1	C1-SG	-3.18	1.79	1.83
7	G	137	YCM	CD-SG	3.02	1.89	1.81
7	G	137	YCM	CB-SG	-2.95	1.69	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	161	6V1	C4-N3	-2.91	1.34	1.38
7	U	47	6V1	C4-N3	-2.86	1.34	1.38
7	U	161	6V1	C2-N3	-2.86	1.34	1.38
5	E	148	6V1	C4-N3	-2.73	1.34	1.38
10	X	91	6V1	O7-C2	2.66	1.27	1.22
10	J	91	6V1	CB-SG	-2.65	1.79	1.82
7	G	47	6V1	C5-C4	2.58	1.54	1.50
5	S	148	6V1	C1-C2	2.54	1.54	1.52
5	E	148	6V1	C2-N3	-2.47	1.35	1.38
5	E	148	6V1	C1-SG	-2.46	1.80	1.83
10	X	91	6V1	C4-N3	-2.30	1.35	1.38
5	E	148	6V1	C1-C2	2.28	1.54	1.52
3	C	63	YCM	CD-SG	-2.23	1.76	1.81
7	U	137	YCM	CA-N	-2.19	1.41	1.48

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	91	6V1	C6-N3-C2	10.00	135.09	123.37
10	J	91	6V1	C5-C4-N3	9.49	114.04	108.07
10	X	91	6V1	C6-N3-C2	9.18	134.12	123.37
10	X	91	6V1	C5-C4-N3	8.57	113.46	108.07
10	X	91	6V1	O7-C2-N3	6.25	131.72	124.14
3	Q	63	YCM	CE-CD-SG	-6.12	94.49	113.81
10	J	91	6V1	C6-N3-C4	-6.12	115.29	122.52
10	J	91	6V1	C2-N3-C4	-6.03	109.54	113.07
5	S	148	6V1	C5-C4-N3	5.82	111.73	108.07
10	X	91	6V1	C6-N3-C4	-5.64	115.85	122.52
5	S	148	6V1	C2-N3-C4	-5.59	109.80	113.07
5	E	148	6V1	C5-C4-N3	5.57	111.57	108.07
7	U	47	6V1	C5-C4-N3	5.53	111.55	108.07
7	U	47	6V1	C2-N3-C4	-5.48	109.86	113.07
10	X	91	6V1	C2-N3-C4	-5.44	109.89	113.07
10	J	91	6V1	O7-C2-N3	5.15	130.38	124.14
5	E	148	6V1	C2-N3-C4	-5.01	110.14	113.07
7	G	47	6V1	C2-N3-C4	-4.98	110.15	113.07
5	S	148	6V1	C6-N3-C2	4.75	128.94	123.37
5	E	148	6V1	C6-N3-C2	4.32	128.43	123.37
7	G	161	6V1	O8-C4-N3	4.26	128.51	123.94
10	X	91	6V1	O8-C4-C5	-4.14	121.23	127.28
7	U	161	6V1	C2-N3-C4	-4.13	110.65	113.07
10	J	91	6V1	O8-C4-C5	-4.03	121.39	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	161	6V1	C5-C4-N3	3.65	110.37	108.07
3	Q	63	YCM	CA-CB-SG	-3.23	101.60	113.51
7	U	161	6V1	O8-C4-C5	-3.21	122.59	127.28
7	G	161	6V1	O8-C4-C5	-3.12	122.71	127.28
3	Q	63	YCM	CB-SG-CD	3.04	131.39	104.24
10	X	91	6V1	C3-C6-N3	3.01	122.01	111.66
10	J	91	6V1	C3-C6-N3	2.98	121.89	111.66
7	G	137	YCM	CE-CD-SG	2.94	123.10	113.81
7	U	47	6V1	O8-C4-C5	-2.89	123.05	127.28
7	U	161	6V1	O8-C4-N3	2.88	127.03	123.94
7	G	47	6V1	O7-C2-N3	-2.71	120.85	124.14
10	X	91	6V1	O7-C2-C1	-2.60	118.85	124.52
7	G	137	YCM	CA-CB-SG	-2.56	104.06	113.51
5	S	148	6V1	O8-C4-C5	-2.41	123.75	127.28
7	U	137	YCM	CA-CB-SG	-2.35	104.84	113.51
7	G	161	6V1	O7-C2-N3	2.22	126.84	124.14
7	G	47	6V1	C6-N3-C4	2.22	125.15	122.52
7	U	137	YCM	CE-CD-SG	2.18	120.69	113.81
7	G	47	6V1	O8-C4-C5	2.10	130.36	127.28
7	U	47	6V1	C6-N3-C2	2.09	125.82	123.37
7	G	137	YCM	OZ1-CE-NZ2	-2.07	116.99	122.53
5	S	148	6V1	C3-C6-N3	2.01	118.57	111.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	63	YCM	CE-CD-SG-CB
5	E	148	6V1	C3-C6-N3-C2
5	E	148	6V1	C3-C6-N3-C4
7	G	137	YCM	CE-CD-SG-CB
7	G	137	YCM	SG-CD-CE-NZ2
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2
5	S	148	6V1	C3-C6-N3-C2

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Mol	Chain	Res	Type	Atoms
5	S	148	6V1	C3-C6-N3-C4
7	U	47	6V1	C3-C6-N3-C2
7	U	47	6V1	C3-C6-N3-C4
10	X	91	6V1	C3-C6-N3-C2
10	X	91	6V1	C3-C6-N3-C4
7	U	137	YCM	CE-CD-SG-CB
7	G	161	6V1	N-CA-CB-SG
7	U	161	6V1	N-CA-CB-SG
3	Q	63	YCM	CA-CB-SG-CD
7	U	137	YCM	SG-CD-CE-NZ2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 73 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	1PE	W	303	-	15,15,15	0.56	0	14,14,14	0.49	0
16	1PE	L	301	-	15,15,15	0.61	0	14,14,14	0.72	1 (7%)
16	1PE	Z	301	-	15,15,15	0.63	0	14,14,14	0.61	0
16	1PE	a	304	-	15,15,15	0.54	0	14,14,14	0.56	0
16	1PE	G	303	-	15,15,15	0.58	0	14,14,14	0.69	0
16	1PE	b	504	-	15,15,15	0.61	0	14,14,14	0.77	0
16	1PE	I	304	-	15,15,15	0.53	0	14,14,14	0.63	0
16	1PE	I	303	-	15,15,15	0.55	0	14,14,14	0.85	1 (7%)
16	1PE	b	505	-	15,15,15	0.66	0	14,14,14	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	1PE	W	303	-	-	6/13/13/13	-
16	1PE	L	301	-	-	6/13/13/13	-
16	1PE	Z	301	-	-	6/13/13/13	-
16	1PE	a	304	-	-	4/13/13/13	-
16	1PE	G	303	-	-	3/13/13/13	-
16	1PE	b	504	-	-	5/13/13/13	-
16	1PE	I	304	-	-	5/13/13/13	-
16	1PE	I	303	-	-	8/13/13/13	-
16	1PE	b	505	-	-	9/13/13/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	303	1PE	C25-OH5-C14	2.11	122.49	113.26
16	L	301	1PE	C26-OH6-C15	2.10	122.45	113.26

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	L	301	1PE	OH6-C15-C25-OH5
16	W	303	1PE	OH6-C15-C25-OH5
16	Z	301	1PE	OH6-C15-C25-OH5
16	b	505	1PE	OH5-C14-C24-OH4
16	I	303	1PE	C15-C25-OH5-C14
16	I	304	1PE	C24-C14-OH5-C25
16	b	504	1PE	OH6-C15-C25-OH5
16	G	303	1PE	C13-C23-OH3-C22
16	L	301	1PE	C16-C26-OH6-C15
16	a	304	1PE	OH4-C13-C23-OH3
16	I	304	1PE	OH4-C13-C23-OH3
16	L	301	1PE	OH5-C14-C24-OH4
16	a	304	1PE	OH5-C14-C24-OH4
16	Z	301	1PE	C16-C26-OH6-C15

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Mol	Chain	Res	Type	Atoms
16	I	303	1PE	OH6-C15-C25-OH5
16	b	505	1PE	OH4-C13-C23-OH3
16	b	504	1PE	OH4-C13-C23-OH3
16	I	303	1PE	OH2-C12-C22-OH3
16	a	304	1PE	OH7-C16-C26-OH6
16	b	505	1PE	OH7-C16-C26-OH6
16	G	303	1PE	OH7-C16-C26-OH6
16	Z	301	1PE	OH4-C13-C23-OH3
16	b	505	1PE	OH6-C15-C25-OH5
16	b	504	1PE	C24-C14-OH5-C25
16	L	301	1PE	C25-C15-OH6-C26
16	I	303	1PE	OH4-C13-C23-OH3
16	I	303	1PE	C14-C24-OH4-C13
16	L	301	1PE	C13-C23-OH3-C22
16	W	303	1PE	C23-C13-OH4-C24
16	b	505	1PE	C12-C22-OH3-C23
16	W	303	1PE	C13-C23-OH3-C22
16	b	505	1PE	C23-C13-OH4-C24
16	W	303	1PE	C14-C24-OH4-C13
16	I	303	1PE	C24-C14-OH5-C25
16	I	304	1PE	C23-C13-OH4-C24
16	W	303	1PE	C24-C14-OH5-C25
16	Z	301	1PE	C15-C25-OH5-C14
16	G	303	1PE	OH2-C12-C22-OH3
16	a	304	1PE	C25-C15-OH6-C26
16	I	304	1PE	OH7-C16-C26-OH6
16	b	505	1PE	OH2-C12-C22-OH3
16	b	505	1PE	C14-C24-OH4-C13
16	W	303	1PE	C12-C22-OH3-C23
16	Z	301	1PE	C12-C22-OH3-C23
16	b	504	1PE	C14-C24-OH4-C13
16	I	303	1PE	C25-C15-OH6-C26
16	I	303	1PE	C12-C22-OH3-C23
16	Z	301	1PE	OH2-C12-C22-OH3
16	b	505	1PE	C15-C25-OH5-C14
16	L	301	1PE	OH2-C12-C22-OH3
16	I	304	1PE	C25-C15-OH6-C26
16	b	504	1PE	C13-C23-OH3-C22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	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%)	0.19	9 (3%) 43 43	18, 42, 75, 87	2 (0%)
1	O	230/234 (98%)	0.74	18 (7%) 19 17	36, 56, 92, 119	0
2	B	248/261 (95%)	0.44	7 (2%) 55 55	27, 48, 85, 130	1 (0%)
2	P	247/261 (94%)	0.61	19 (7%) 19 17	28, 53, 91, 133	2 (0%)
3	C	236/248 (95%)	0.87	26 (11%) 10 9	32, 57, 97, 128	0
3	Q	233/248 (93%)	0.85	28 (12%) 9 7	31, 54, 95, 127	0
4	D	233/241 (96%)	0.67	11 (4%) 36 35	21, 55, 85, 106	2 (0%)
4	R	233/241 (96%)	0.32	13 (5%) 30 29	18, 40, 62, 82	1 (0%)
5	E	233/263 (88%)	0.26	17 (7%) 21 19	25, 39, 82, 98	0
5	S	237/263 (90%)	0.30	10 (4%) 40 40	23, 43, 72, 94	3 (1%)
6	F	239/255 (93%)	-0.12	5 (2%) 63 64	17, 31, 52, 72	4 (1%)
6	T	240/255 (94%)	0.57	16 (6%) 24 22	25, 49, 79, 105	1 (0%)
7	G	241/246 (97%)	0.00	6 (2%) 58 58	16, 35, 65, 89	2 (0%)
7	U	232/246 (94%)	0.68	17 (7%) 21 19	38, 56, 86, 122	0
8	H	220/234 (94%)	0.02	11 (5%) 34 33	18, 32, 62, 87	2 (0%)
8	V	220/234 (94%)	0.33	8 (3%) 46 46	23, 44, 78, 100	2 (0%)
9	I	204/205 (99%)	-0.27	1 (0%) 87 88	18, 32, 51, 64	6 (2%)
9	W	204/205 (99%)	0.16	3 (1%) 72 72	24, 44, 65, 72	2 (0%)
10	J	195/201 (97%)	0.12	7 (3%) 46 46	15, 38, 55, 70	2 (1%)
10	X	195/201 (97%)	0.14	4 (2%) 63 64	18, 38, 54, 69	2 (1%)
11	K	201/204 (98%)	0.09	2 (0%) 79 80	32, 41, 65, 90	0
11	Y	199/204 (97%)	-0.19	1 (0%) 87 88	19, 33, 51, 62	3 (1%)
12	L	213/213 (100%)	0.23	1 (0%) 87 88	23, 45, 65, 83	2 (0%)
12	Z	213/213 (100%)	-0.13	1 (0%) 87 88	24, 34, 55, 73	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.09	3 (1%)	73 73	24, 35, 59, 94	0
13	a	216/219 (98%)	-0.05	4 (1%)	66 66	24, 35, 57, 82	1 (0%)
14	N	202/205 (98%)	-0.11	4 (1%)	65 65	18, 32, 52, 91	1 (0%)
14	b	203/205 (99%)	0.05	7 (3%)	48 48	30, 38, 63, 90	1 (0%)
All	All	6213/6458 (96%)	0.25	259 (4%)	40 40	15, 42, 78, 133	43 (0%)

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	202	LEU	7.8
5	E	57	ALA	6.3
3	Q	50	VAL	5.7
4	R	241	ILE	5.5
10	J	184	ASP	5.5
2	B	203	VAL	5.1
5	S	2	PHE	5.1
4	R	131	GLY	5.0
2	P	61	PHE	5.0
13	a	215	ILE	5.0
1	A	231	ALA	4.9
2	P	203	VAL	4.8
5	E	56	LEU	4.7
3	C	138	PHE	4.7
6	T	5	THR	4.6
3	Q	138	PHE	4.6
1	O	232	ILE	4.5
13	M	215	ILE	4.5
5	E	54	SER	4.4
5	E	52	ALA	4.4
14	b	199	VAL	4.3
4	R	120[A]	ALA	4.3
3	Q	199	VAL	4.2
5	E	58	ALA	4.2
6	T	208	ALA	4.2
4	R	130	PRO	4.2
1	O	54	ILE	4.1
7	G	187	PHE	4.0
3	Q	49	SER	3.8
2	P	205	LYS	3.8
1	A	3	ARG	3.8
8	V	204	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
6	T	6	GLY	3.7
4	D	241	ILE	3.7
3	Q	48	LYS	3.7
7	U	194	THR	3.7
1	A	230	ALA	3.7
2	P	53	HIS	3.7
3	Q	53	LEU	3.6
14	b	198	ALA	3.6
2	B	61	PHE	3.6
1	O	231	ALA	3.5
3	C	50	VAL	3.5
10	J	147	TYR	3.5
8	H	204	CYS	3.5
3	C	53	LEU	3.5
8	V	199	LEU	3.5
3	C	49	SER	3.4
5	E	53	GLN	3.4
3	C	48	LYS	3.4
14	N	198	ALA	3.4
3	C	176	TYR	3.3
5	S	57	ALA	3.3
3	Q	47	LYS	3.3
3	C	97	THR	3.3
4	R	129	ASP	3.3
4	D	131	GLY	3.3
6	T	204	VAL	3.2
7	U	240	VAL	3.2
7	U	245	ARG	3.2
14	N	200	ALA	3.2
3	C	183	THR	3.2
6	T	54	LEU	3.2
10	X	147	TYR	3.2
7	G	189	TRP	3.1
1	A	232	ILE	3.1
8	V	197	THR	3.1
7	U	51	VAL	3.1
9	W	16[A]	LYS	3.1
4	D	120[A]	ALA	3.1
2	B	2	SER	3.1
5	S	53	GLN	3.1
5	E	59	HIS	3.1
14	b	203	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	P	245	ALA	3.1
6	T	61	GLY	3.1
5	E	60	GLN	3.0
8	H	197	THR	3.0
3	C	59	VAL	3.0
8	V	203	ARG	3.0
1	O	230	ALA	3.0
3	Q	51	ALA	3.0
2	P	248	GLU	3.0
2	P	52	ILE	3.0
10	J	1	MET	2.9
3	Q	220	LEU	2.9
14	b	202	LEU	2.9
3	C	41	VAL	2.9
10	X	196	PHE	2.9
5	E	201	ALA	2.9
3	C	225	ILE	2.9
3	Q	232	ILE	2.9
10	X	1	MET	2.9
3	Q	59	VAL	2.9
8	H	189	TYR	2.9
4	R	128	ALA	2.9
3	C	47	LYS	2.9
13	a	216	SER	2.9
2	P	55	LEU	2.9
14	N	199	VAL	2.8
8	H	185	PHE	2.8
5	S	54	SER	2.8
3	Q	217	LEU	2.8
6	T	63	ASN	2.8
11	K	201	GLY	2.8
6	T	209	PHE	2.8
3	C	186	LEU	2.8
1	O	50	LYS	2.8
2	P	206	LEU	2.8
5	S	56	LEU	2.8
4	D	184	VAL	2.8
9	W	84	TYR	2.7
3	Q	205	ASN	2.7
3	Q	238	GLU	2.7
1	O	181	LEU	2.7
7	G	208	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
13	a	214	MET	2.7
7	U	183	VAL	2.7
12	Z	161	VAL	2.7
5	S	51	ARG	2.7
6	F	53	VAL	2.7
6	T	53	VAL	2.7
6	T	206	ASP	2.7
3	C	220	LEU	2.7
3	C	206	ILE	2.7
10	J	24	ASN	2.7
1	O	167	VAL	2.7
4	R	127	ASP	2.6
11	Y	40	TYR	2.6
4	D	128	ALA	2.6
6	T	205	LYS	2.6
5	E	202	GLU	2.6
6	T	142	VAL	2.6
2	B	205	LYS	2.6
1	O	177	TYR	2.6
1	A	181	LEU	2.6
4	R	9	ASP	2.6
3	Q	236	LYS	2.6
4	D	47	CYS	2.5
1	O	198	PHE	2.5
4	D	54	ILE	2.5
8	V	216	ILE	2.5
2	P	211	VAL	2.5
5	E	218	ASP	2.5
7	G	188	ASP	2.5
3	Q	225	ILE	2.5
7	G	243	ALA	2.5
1	O	189	THR	2.5
8	H	200	GLY	2.5
6	T	37	ILE	2.5
3	Q	207	GLU	2.5
2	P	54	LYS	2.5
6	F	244	LYS	2.5
3	C	203	GLY	2.4
4	R	54	ILE	2.4
3	C	98	VAL	2.4
4	D	130	PRO	2.4
7	U	57	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	249	ARG	2.4
5	E	51	ARG	2.4
2	P	56	LEU	2.4
5	E	236	LEU	2.4
6	T	207	LYS	2.4
3	C	35	VAL	2.4
4	R	223	GLY	2.4
7	U	2	SER	2.4
1	O	73	LEU	2.4
10	X	148	THR	2.4
7	U	184	LYS	2.4
5	E	49	LEU	2.3
3	Q	240	GLU	2.3
3	C	232	ILE	2.3
7	U	208	ILE	2.3
7	U	241	ALA	2.3
8	H	196	GLY	2.3
5	E	61	LYS	2.3
1	O	157	TRP	2.3
8	V	202	TYR	2.3
14	b	200	ALA	2.3
6	T	226	ILE	2.3
8	H	201	ARG	2.3
4	R	60	GLU	2.3
3	Q	196	LEU	2.3
8	H	199	LEU	2.3
8	H	188	PRO	2.3
1	A	54	ILE	2.3
3	C	219	ILE	2.3
5	E	235	GLY	2.3
3	C	217	LEU	2.3
4	D	86	LYS	2.3
1	O	3	ARG	2.2
5	S	58	ALA	2.2
2	P	237	ILE	2.2
7	U	199	ILE	2.2
7	U	61	LEU	2.2
6	F	6	GLY	2.2
3	Q	137	ASP	2.2
12	L	41	PRO	2.2
13	a	209	TRP	2.2
5	S	59	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
6	F	204	VAL	2.2
9	I	115	THR	2.2
9	W	113	PRO	2.2
2	P	208	ALA	2.2
3	Q	180	ALA	2.2
10	J	196	PHE	2.2
3	C	205	ASN	2.2
4	R	86	LYS	2.2
6	F	206	ASP	2.2
3	C	2	SER	2.2
2	B	206	LEU	2.2
7	U	60	LEU	2.2
2	B	247	ALA	2.2
10	J	154	GLU	2.1
3	C	102	VAL	2.1
14	b	201	THR	2.1
1	O	55	LEU	2.1
3	C	96	LEU	2.1
1	A	50	LYS	2.1
5	S	3	ARG	2.1
3	Q	230	ALA	2.1
5	S	60	GLN	2.1
8	H	202	TYR	2.1
2	P	2	SER	2.1
1	O	4	GLY	2.1
2	P	59	VAL	2.1
3	Q	38	ARG	2.1
2	P	236	LEU	2.1
4	R	132	ALA	2.1
7	U	58	ASP	2.1
11	K	40	TYR	2.1
1	A	221	THR	2.1
2	P	162	THR	2.1
8	V	200	GLY	2.1
13	M	214	MET	2.1
7	U	56	VAL	2.1
1	O	51	GLN	2.1
1	O	149	ASP	2.1
6	T	188	ASP	2.1
7	U	88	ARG	2.1
1	A	199	GLU	2.0
3	C	179	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	Q	181	ILE	2.0
3	Q	234	LYS	2.0
7	U	229	ILE	2.0
14	b	150	GLU	2.0
3	Q	176	TYR	2.0
3	Q	183	THR	2.0
13	M	213	HIS	2.0
4	D	234	LEU	2.0
8	V	212	LEU	2.0
7	G	245	ARG	2.0
10	J	109	GLU	2.0
8	H	194	LYS	2.0
2	P	174	MET	2.0
3	Q	219	ILE	2.0
4	D	176	GLY	2.0
1	O	61	VAL	2.0
5	E	210	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	6V1	U	47	15/16	0.84	0.18	64,96,103,104	0
7	YCM	U	137	10/11	0.86	0.15	46,54,72,72	0
7	YCM	G	137	10/11	0.87	0.15	27,34,48,49	0
3	YCM	C	63	10/11	0.88	0.13	48,50,59,60	0
7	6V1	G	47	15/16	0.90	0.14	33,52,55,55	0
5	6V1	S	148	15/16	0.90	0.14	35,56,62,64	0
3	YCM	Q	63	10/11	0.91	0.10	45,48,59,60	0
5	6V1	E	148	15/16	0.91	0.14	29,45,55,55	0
10	6V1	J	91	15/16	0.94	0.12	31,44,50,50	0
7	6V1	U	161	15/16	0.94	0.11	48,62,69,70	0
10	6V1	X	91	15/16	0.94	0.13	32,47,53,53	0
7	6V1	G	161	15/16	0.95	0.10	28,44,50,52	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	1PE	b	505	16/16	0.78	0.18	64,67,78,78	0
16	1PE	I	304	16/16	0.81	0.17	48,61,71,75	0
15	CL	O	303	1/1	0.82	0.17	74,74,74,74	0
16	1PE	a	304	16/16	0.83	0.17	57,62,69,71	0
15	CL	b	502	1/1	0.86	0.20	59,59,59,59	0
15	CL	K	305	1/1	0.86	0.30	60,60,60,60	0
16	1PE	W	303	16/16	0.87	0.13	55,58,64,66	0
16	1PE	Z	301	16/16	0.87	0.14	51,61,64,64	0
15	CL	M	302	1/1	0.87	0.25	62,62,62,62	0
16	1PE	b	504	16/16	0.87	0.14	41,50,67,68	0
16	1PE	L	301	16/16	0.87	0.14	49,62,66,69	0
15	CL	D	301	1/1	0.88	0.22	61,61,61,61	0
15	CL	C	301	1/1	0.88	0.19	56,56,56,56	0
15	CL	B	302	1/1	0.89	0.27	54,54,54,54	0
15	CL	C	302	1/1	0.89	0.20	63,63,63,63	0
15	CL	H	303	1/1	0.90	0.23	51,51,51,51	0
15	CL	Y	305	1/1	0.90	0.24	54,54,54,54	0
15	CL	D	302	1/1	0.90	0.20	53,53,53,53	0
16	1PE	G	303	16/16	0.90	0.11	34,42,51,56	0
16	1PE	I	303	16/16	0.90	0.12	48,52,60,68	0
15	CL	E	303	1/1	0.90	0.19	54,54,54,54	0
18	MG	V	301	1/1	0.91	0.11	48,48,48,48	0
15	CL	A	302	1/1	0.92	0.11	61,61,61,61	0
15	CL	M	301	1/1	0.92	0.29	52,52,52,52	0
15	CL	O	304	1/1	0.92	0.22	55,55,55,55	0
15	CL	V	303	1/1	0.92	0.16	59,59,59,59	0
15	CL	S	302	1/1	0.93	0.15	54,54,54,54	0
18	MG	H	301	1/1	0.93	0.08	45,45,45,45	0
15	CL	K	303	1/1	0.93	0.14	62,62,62,62	0
15	CL	K	304	1/1	0.94	0.19	52,52,52,52	0
15	CL	V	302	1/1	0.94	0.17	50,50,50,50	0
15	CL	F	301	1/1	0.94	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CL	Y	304	1/1	0.94	0.15	51,51,51,51	0
15	CL	Q	302	1/1	0.94	0.29	54,54,54,54	0
15	CL	a	301	1/1	0.94	0.24	53,53,53,53	0
15	CL	W	302	1/1	0.95	0.09	49,49,49,49	0
15	CL	Y	303	1/1	0.95	0.10	56,56,56,56	0
15	CL	M	304	1/1	0.95	0.12	49,49,49,49	0
15	CL	R	301	1/1	0.95	0.17	50,50,50,50	0
15	CL	S	301	1/1	0.95	0.32	59,59,59,59	0
15	CL	a	303	1/1	0.95	0.13	52,52,52,52	0
15	CL	B	301	1/1	0.95	0.11	37,37,37,37	0
15	CL	G	302	1/1	0.95	0.11	56,56,56,56	0
18	MG	K	301	1/1	0.95	0.10	33,33,33,33	0
15	CL	Q	301	1/1	0.95	0.14	62,62,62,62	0
15	CL	S	303	1/1	0.96	0.15	48,48,48,48	0
15	CL	a	302	1/1	0.96	0.11	42,42,42,42	0
15	CL	N	501	1/1	0.96	0.10	42,42,42,42	0
15	CL	O	301	1/1	0.96	0.11	49,49,49,49	0
15	CL	O	302	1/1	0.96	0.10	59,59,59,59	0
17	K	L	302	1/1	0.96	0.14	42,42,42,42	0
17	K	U	302	1/1	0.96	0.13	38,38,38,38	0
17	K	b	506	1/1	0.96	0.17	38,38,38,38	0
15	CL	R	302	1/1	0.96	0.25	48,48,48,48	0
15	CL	E	302	1/1	0.96	0.13	49,49,49,49	0
15	CL	K	302	1/1	0.96	0.15	41,41,41,41	0
15	CL	b	503	1/1	0.97	0.13	44,44,44,44	0
15	CL	I	302	1/1	0.97	0.10	40,40,40,40	0
15	CL	A	304	1/1	0.97	0.18	52,52,52,52	0
15	CL	A	301	1/1	0.97	0.10	45,45,45,45	0
15	CL	N	502	1/1	0.97	0.13	43,43,43,43	0
15	CL	Y	301	1/1	0.97	0.09	33,33,33,33	0
18	MG	I	301	1/1	0.97	0.12	29,29,29,29	0
18	MG	J	301	1/1	0.97	0.04	41,41,41,41	0
15	CL	b	501	1/1	0.97	0.21	44,44,44,44	0
15	CL	N	503	1/1	0.97	0.15	40,40,40,40	0
18	MG	X	301	1/1	0.97	0.06	44,44,44,44	0
17	K	Z	302	1/1	0.98	0.08	34,34,34,34	0
15	CL	M	303	1/1	0.98	0.10	38,38,38,38	0
15	CL	G	301	1/1	0.98	0.23	41,41,41,41	0
15	CL	A	303	1/1	0.98	0.17	42,42,42,42	0
18	MG	I	305	1/1	0.98	0.11	26,26,26,26	0
15	CL	Y	302	1/1	0.98	0.15	47,47,47,47	0
15	CL	U	301	1/1	0.98	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	MG	L	303	1/1	0.98	0.15	33,33,33,33	0
17	K	N	504	1/1	0.98	0.13	37,37,37,37	0
18	MG	W	301	1/1	0.98	0.11	34,34,34,34	0
15	CL	P	301	1/1	0.98	0.12	45,45,45,45	0
15	CL	E	301	1/1	0.99	0.19	54,54,54,54	0
15	CL	H	304	1/1	0.99	0.16	47,47,47,47	0
17	K	G	304	1/1	0.99	0.10	28,28,28,28	0
18	MG	H	302	1/1	0.99	0.09	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.