



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:28 AM UTC

PDB ID : 5LF7 / pdb_00005lf7
Title : Human 20S proteasome complex with Ixazomib at 2.0 Angstrom
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on : 2016-06-30
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

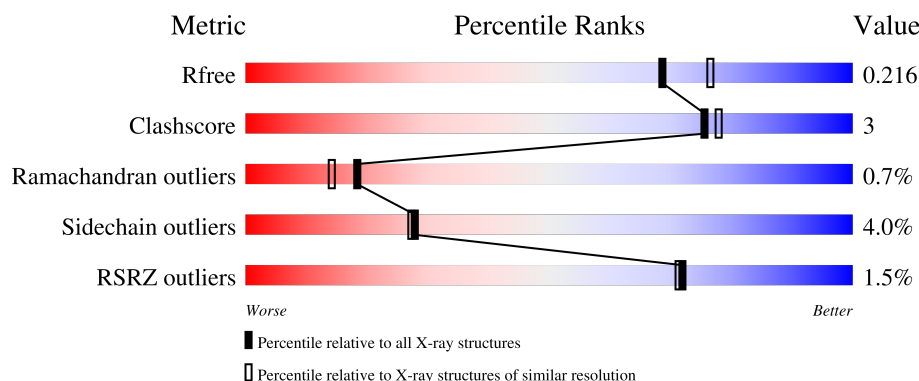
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	84% 12% ..
1	O	234	3% 88% 8% ..
2	B	261	85% 9% 5%
2	P	261	3% 83% 9% .. 5%
3	C	248	3% 81% 12% ..

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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 20 unique types of molecules in this entry. The entry contains 52085 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	247	Total	C	N	O	S	0	2	0
			1898	1200	321	366	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	1	0
			1822	1144	325	342	11			
5	S	238	Total	C	N	O	S	0	3	0
			1875	1175	340	349	11			

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

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

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

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

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

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

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	0	0
			1545	974	269	293	9			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

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

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

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

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

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

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

- Molecule 15 is CHLORIDE ION (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	1	Total 1	Cl 1	0	0
15	I	1	Total 1	Cl 1	0	0
15	K	3	Total 3	Cl 3	0	0
15	M	4	Total 4	Cl 4	0	0
15	N	2	Total 2	Cl 2	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	1	Total 1	Cl 1	0	0
15	W	1	Total 1	Cl 1	0	0
15	Y	4	Total 4	Cl 4	0	0
15	a	4	Total 4	Cl 4	0	0
15	b	1	Total 1	Cl 1	0	0

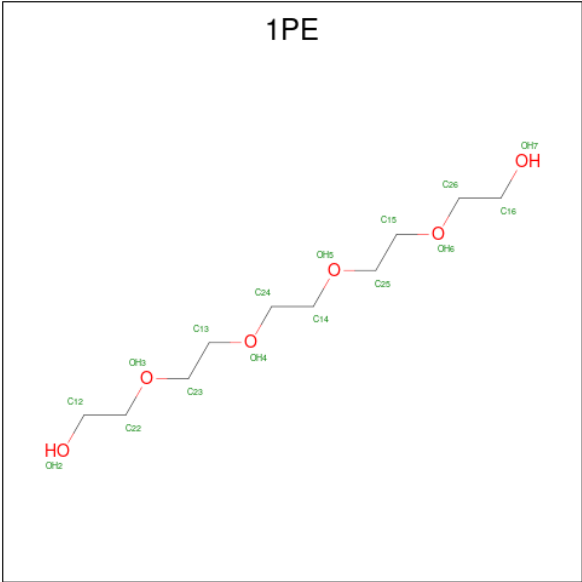
- Molecule 16 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

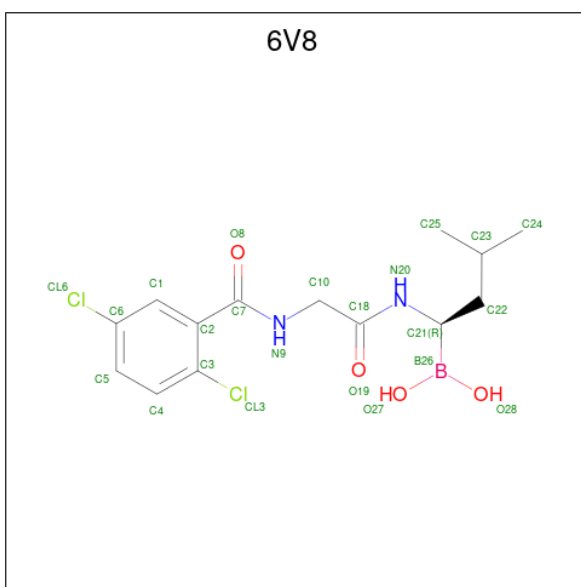
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	2	Total Mg 2 2	0	0
17	I	2	Total Mg 2 2	0	0
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0
17	V	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	X	1	Total Mg 1 1	0	0

- Molecule 18 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

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



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

- Molecule 20 is water.

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

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

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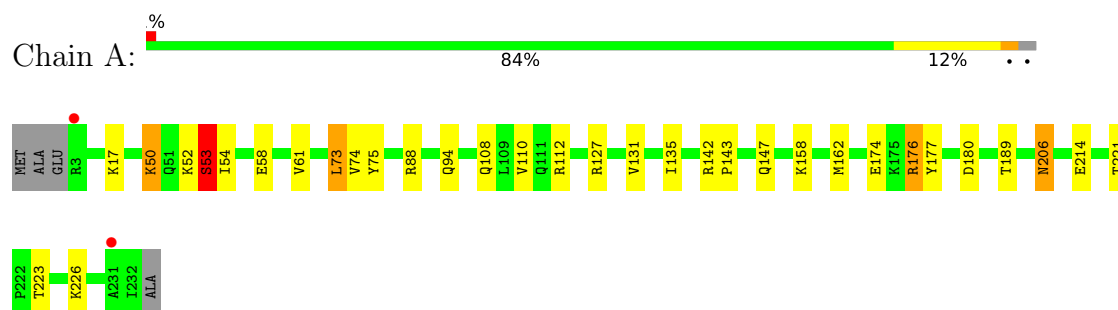
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	b	121	Total 121	O 121	0	0

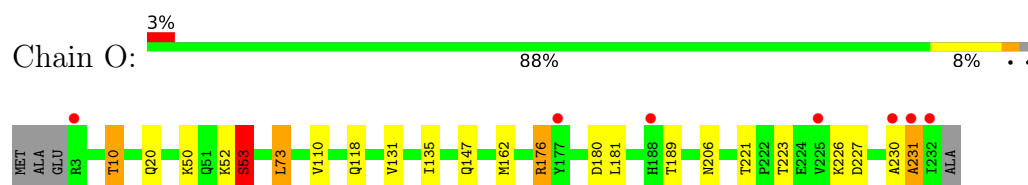
3 Residue-property plots

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

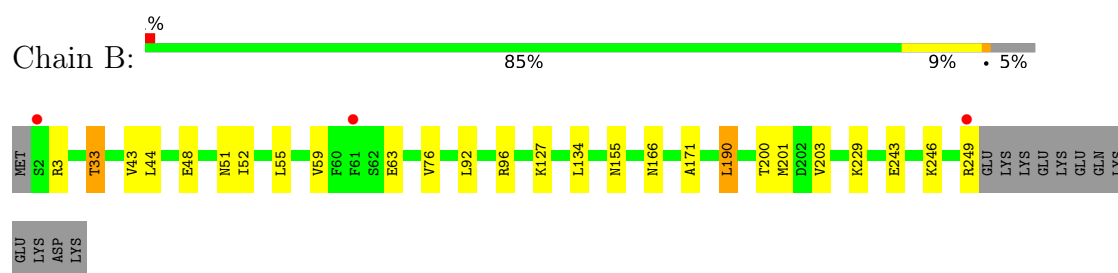
- Molecule 1: Proteasome subunit alpha type-2



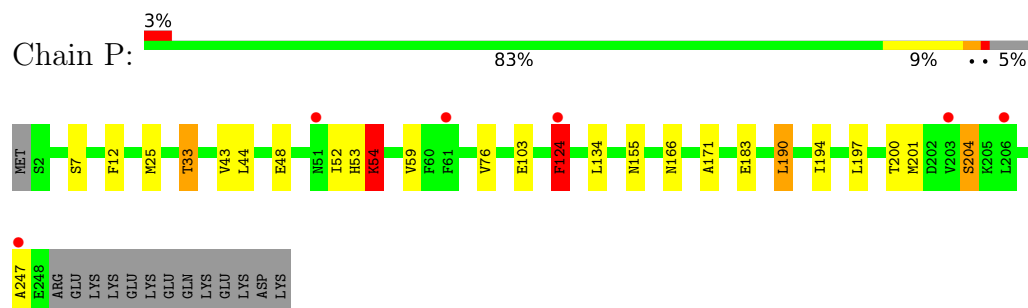
- Molecule 1: Proteasome subunit alpha type-2



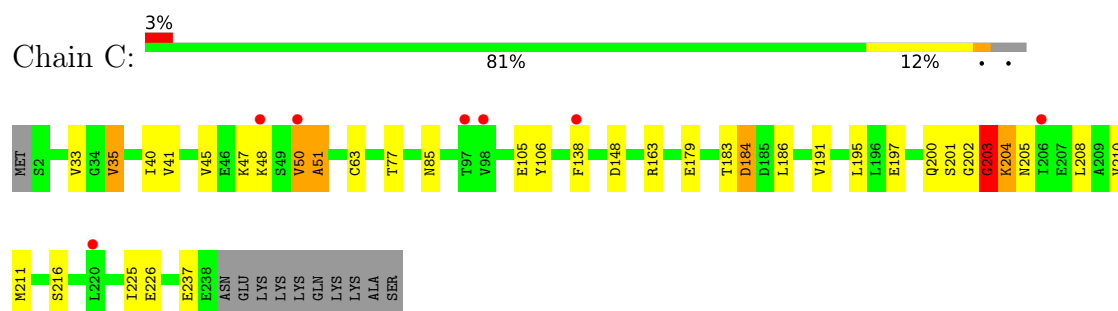
- Molecule 2: Proteasome subunit alpha type-4



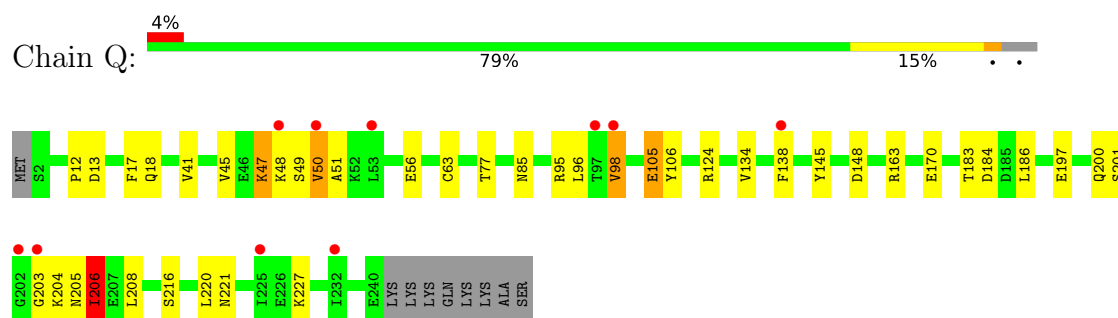
- Molecule 2: Proteasome subunit alpha type-4



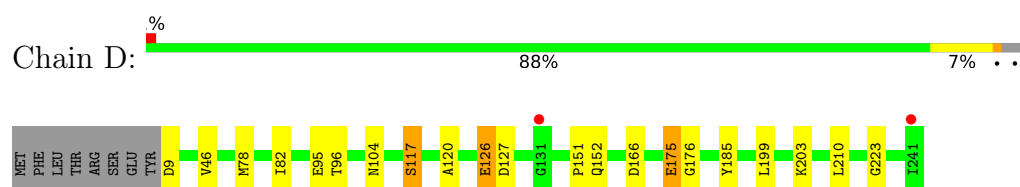
- Molecule 3: Proteasome subunit alpha type-7



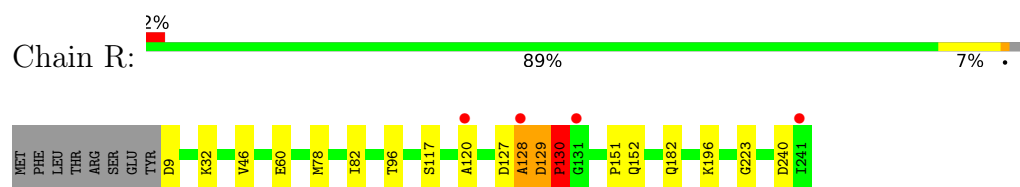
- Molecule 3: Proteasome subunit alpha type-7



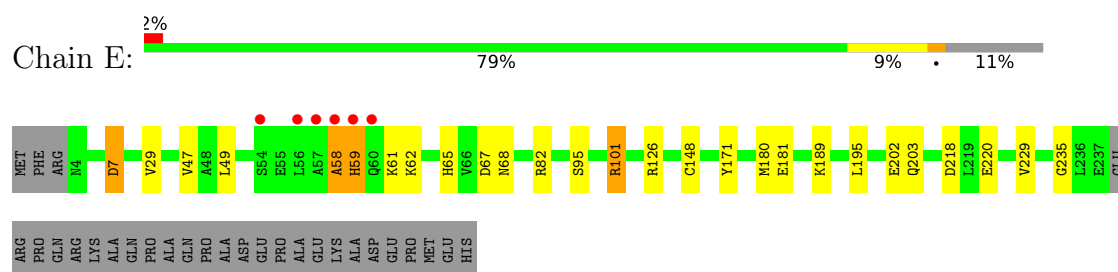
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5

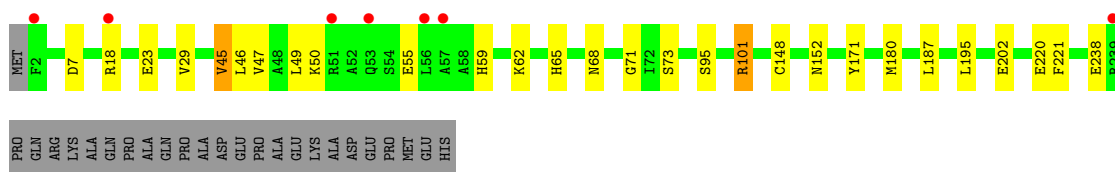


- Molecule 5: Proteasome subunit alpha type-1

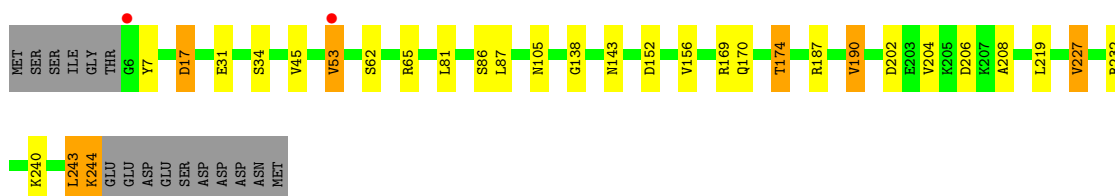
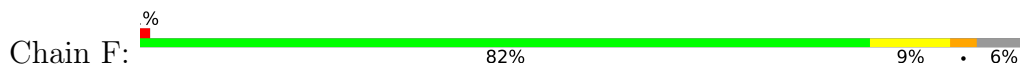


- Molecule 5: Proteasome subunit alpha type-1

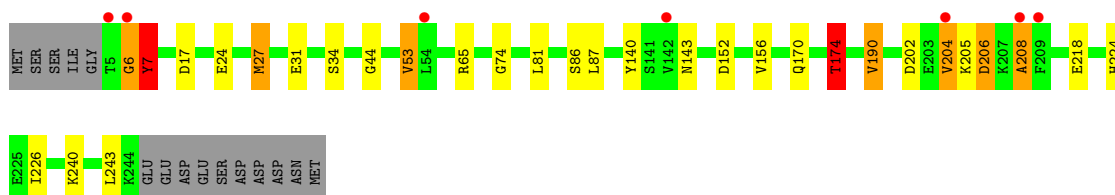
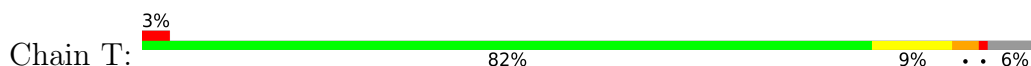




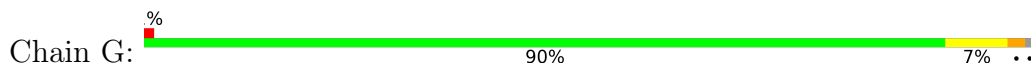
• Molecule 6: Proteasome subunit alpha type-3



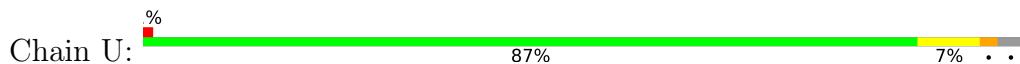
• Molecule 6: Proteasome subunit alpha type-3



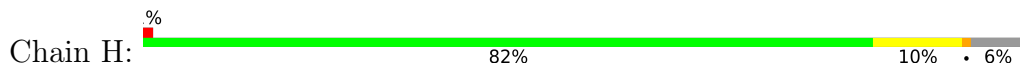
• Molecule 7: Proteasome subunit alpha type-6



• Molecule 7: Proteasome subunit alpha type-6



• Molecule 8: Proteasome subunit beta type-7



MET
ASP
THR
SER

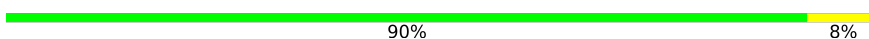
• Molecule 8: Proteasome subunit beta type-7

Chain V:  3% 84% 9% 6%



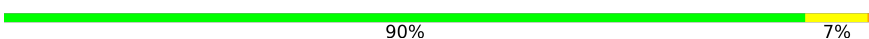
THR
SER

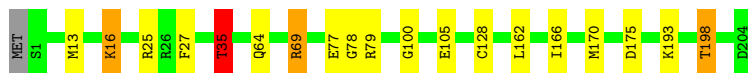
• Molecule 9: Proteasome subunit beta type-3

Chain I:  90% 8%



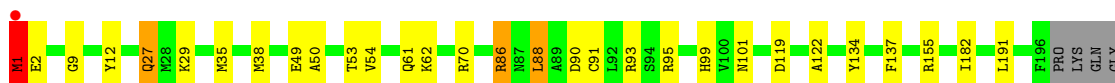
• Molecule 9: Proteasome subunit beta type-3

Chain W:  90% 7%



• Molecule 10: Proteasome subunit beta type-2

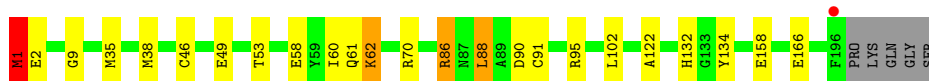
Chain J:  83% 13% ..



SER

• Molecule 10: Proteasome subunit beta type-2

Chain X:  86% 10% ..

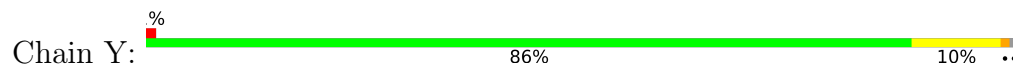


• Molecule 11: Proteasome subunit beta type-5

Chain K:  89% 6% ..



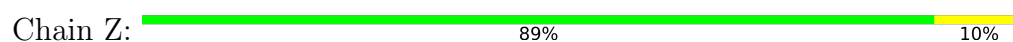
- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-1



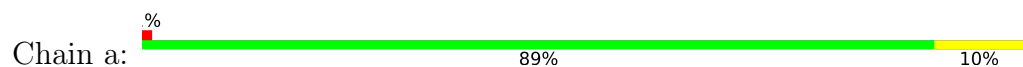
- Molecule 12: Proteasome subunit beta type-1



- Molecule 13: Proteasome subunit beta type-4



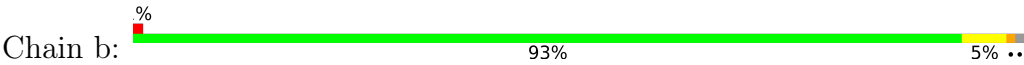
- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.41Å 202.61Å 314.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.33 – 2.00 170.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (170.33-2.00) 99.6 (170.33-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.175 , 0.213 0.182 , 0.216	Depositor DCC
R_{free} test set	24030 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52085	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YCM, 6V8, MG, K, CL, 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	1.24	1/1833 (0.1%)	1.11	3/2489 (0.1%)
1	O	1.06	0/1778	1.04	1/2419 (0.0%)
2	B	1.16	2/1962 (0.1%)	1.06	2/2649 (0.1%)
2	P	1.16	1/1934 (0.1%)	1.07	2/2617 (0.1%)
3	C	1.13	0/1818	1.16	2/2469 (0.1%)
3	Q	1.19	2/1834 (0.1%)	1.17	9/2490 (0.4%)
4	D	1.11	2/1789 (0.1%)	1.09	1/2424 (0.0%)
4	R	1.26	0/1780	1.16	3/2408 (0.1%)
5	E	1.27	1/1842 (0.1%)	1.14	3/2493 (0.1%)
5	S	1.15	0/1901	1.10	1/2571 (0.0%)
6	F	1.39	4/1935 (0.2%)	1.18	5/2605 (0.2%)
6	T	1.09	1/1894 (0.1%)	1.14	11/2556 (0.4%)
7	G	1.35	6/1909 (0.3%)	1.13	3/2579 (0.1%)
7	U	1.02	0/1804	1.00	1/2441 (0.0%)
8	H	1.47	8/1697 (0.5%)	1.21	6/2299 (0.3%)
8	V	1.24	1/1655 (0.1%)	1.12	5/2251 (0.2%)
9	I	1.32	6/1648 (0.4%)	1.26	10/2219 (0.5%)
9	W	1.26	4/1630 (0.2%)	1.18	9/2197 (0.4%)
10	J	1.27	3/1613 (0.2%)	1.08	4/2180 (0.2%)
10	X	1.31	4/1599 (0.3%)	1.11	4/2163 (0.2%)
11	K	1.28	4/1576 (0.3%)	1.11	2/2131 (0.1%)
11	Y	1.36	5/1620 (0.3%)	1.11	2/2185 (0.1%)
12	L	1.31	2/1672 (0.1%)	1.15	1/2257 (0.0%)
12	Z	1.42	8/1675 (0.5%)	1.18	6/2257 (0.3%)
13	M	1.27	1/1728 (0.1%)	1.12	3/2339 (0.1%)
13	a	1.30	6/1724 (0.3%)	1.11	3/2336 (0.1%)
14	N	1.35	5/1545 (0.3%)	1.15	2/2091 (0.1%)
14	b	1.21	2/1554 (0.1%)	1.11	1/2104 (0.0%)
All	All	1.25	79/48949 (0.2%)	1.13	105/66219 (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	2
3	C	0	2
3	Q	0	2
4	D	0	4
4	R	0	2
5	E	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
11	Y	0	1
13	a	0	1
All	All	1	20

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	86	ARG	CD-NE	-8.37	1.34	1.46
10	J	86	ARG	CD-NE	-8.05	1.34	1.46
6	F	17	ASP	CG-OD2	7.52	1.39	1.25
12	Z	171	ALA	N-CA	7.42	1.55	1.46
12	L	158	MET	N-CA	7.08	1.54	1.46
12	Z	158	MET	N-CA	6.86	1.54	1.46
4	D	126	GLU	N-CA	6.62	1.52	1.46
8	H	39	SER	N-CA	-6.50	1.40	1.46
7	G	108	GLU	CD-OE1	6.49	1.37	1.25
11	Y	187[A]	ARG	C-O	-6.43	1.16	1.24
11	Y	187[B]	ARG	C-O	-6.43	1.16	1.24
8	H	10	LYS	CA-CB	6.38	1.63	1.53
9	I	105	GLU	C-O	-6.34	1.17	1.24
14	b	165	MET	C-O	-6.19	1.16	1.24
8	H	39	SER	CA-C	6.17	1.58	1.52
9	W	105	GLU	C-O	-6.13	1.19	1.24
14	N	20	ARG	C-O	-6.11	1.16	1.24
7	G	76	ILE	C-O	6.09	1.30	1.24
10	X	9	GLY	N-CA	6.02	1.52	1.44
14	b	30	ARG	CD-NE	-6.02	1.37	1.46
9	W	175	ASP	CG-OD1	6.00	1.36	1.25
13	a	5	MET	CA-C	5.98	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	70	SER	N-CA	-5.95	1.39	1.46
8	H	101	LEU	N-CA	-5.94	1.39	1.46
10	J	35	MET	C-O	-5.92	1.17	1.23
1	A	50	LYS	CA-C	5.91	1.60	1.52
12	Z	3	SER	CB-OG	5.91	1.53	1.42
13	a	82	SER	CA-C	-5.88	1.45	1.52
11	Y	171	SER	C-O	5.84	1.31	1.24
2	B	3	ARG	C-O	-5.82	1.16	1.24
12	Z	102	PHE	N-CA	5.78	1.54	1.46
7	G	103	TYR	CA-C	5.72	1.60	1.52
11	K	159	ARG	CZ-NH2	-5.71	1.26	1.33
6	F	45	VAL	N-CA	-5.69	1.39	1.46
13	a	101	SER	C-O	-5.66	1.16	1.24
3	Q	206	ILE	CA-C	5.61	1.59	1.52
6	T	7	TYR	N-CA	5.61	1.56	1.46
9	I	96	GLU	C-O	-5.59	1.17	1.24
13	a	152	GLU	N-CA	-5.56	1.39	1.46
9	I	163	PHE	C-O	5.53	1.30	1.24
8	H	173	ASN	C-O	5.53	1.31	1.23
9	W	100	GLY	N-CA	5.48	1.52	1.44
7	G	103	TYR	C-O	-5.48	1.17	1.24
13	a	41	ARG	N-CA	-5.47	1.39	1.46
11	K	187	ARG	C-O	-5.44	1.17	1.24
14	N	89	TYR	C-O	-5.39	1.17	1.24
12	Z	55	SER	CA-C	-5.38	1.46	1.52
8	V	212	VAL	C-O	-5.38	1.18	1.24
4	D	104	ASN	C-O	-5.36	1.16	1.23
12	L	171	ALA	N-CA	5.36	1.52	1.46
9	I	175	ASP	CG-OD1	5.34	1.35	1.25
8	H	170	SER	CA-C	-5.34	1.46	1.52
9	I	75	LEU	C-O	-5.33	1.17	1.24
10	J	50	ALA	C-O	5.33	1.30	1.23
13	M	29	SER	C-O	-5.30	1.17	1.23
13	a	29	SER	C-O	-5.29	1.17	1.23
6	F	62	SER	CA-C	5.28	1.59	1.52
8	H	67	HIS	CA-C	5.27	1.59	1.52
11	K	171	SER	C-O	5.27	1.30	1.23
2	P	103	GLU	CD-OE2	5.25	1.35	1.25
10	X	60	ILE	CA-C	5.24	1.59	1.52
14	N	165	MET	C-O	-5.24	1.18	1.24
12	Z	170	ARG	CA-C	5.24	1.59	1.52
12	Z	206	GLU	C-O	5.24	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	127	LYS	CA-C	5.18	1.59	1.52
9	W	198	THR	C-O	5.17	1.29	1.23
14	N	59	ALA	N-CA	-5.13	1.40	1.46
3	Q	13	ASP	CB-CG	5.13	1.64	1.52
7	G	67	THR	N-CA	5.12	1.52	1.45
11	K	171	SER	CA-C	5.12	1.58	1.52
10	X	35	MET	C-O	-5.12	1.17	1.24
11	Y	38	ILE	C-O	-5.09	1.18	1.24
6	F	138	GLY	C-O	5.07	1.30	1.23
11	Y	130	GLY	N-CA	5.06	1.51	1.45
5	E	7	ASP	CB-CG	-5.05	1.39	1.52
12	Z	142	SER	CB-OG	-5.04	1.32	1.42
9	I	145	MET	N-CA	-5.03	1.40	1.46
7	G	45	LYS	CA-CB	5.02	1.61	1.53
14	N	36	THR	CB-CG2	-5.01	1.36	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-9.76	98.96	112.14
7	G	183	VAL	CB-CA-C	-9.32	99.56	112.14
6	T	6	GLY	CA-C-N	9.29	138.41	121.70
6	T	6	GLY	C-N-CA	9.29	138.41	121.70
6	T	190	VAL	CB-CA-C	-9.09	100.13	112.04
10	X	86	ARG	NE-CZ-NH2	-8.86	111.23	119.20
9	I	16[A]	LYS	CA-C-N	8.80	139.76	123.13
9	I	16[A]	LYS	C-N-CA	8.80	139.76	123.13
9	I	16[B]	LYS	CA-C-N	8.80	139.76	123.13
9	I	16[B]	LYS	C-N-CA	8.80	139.76	123.13
10	J	86	ARG	NE-CZ-NH2	-8.65	111.42	119.20
4	D	120	ALA	N-CA-C	8.45	120.49	111.28
4	R	120[A]	ALA	N-CA-C	-8.06	97.46	110.20
4	R	120[B]	ALA	N-CA-C	-8.06	97.46	110.20
14	b	23	THR	CB-CA-C	-7.90	97.51	110.14
3	Q	220	LEU	N-CA-C	-7.88	97.78	110.32
13	a	10	SER	N-CA-C	7.63	121.00	110.24
14	N	23	THR	CB-CA-C	-7.51	97.69	110.16
3	Q	12	PRO	N-CA-C	7.19	123.18	113.84
7	G	183	VAL	N-CA-CB	6.97	120.02	110.54
13	M	10	SER	N-CA-C	6.77	119.04	110.24
2	P	124	PHE	CA-CB-CG	6.72	120.52	113.80
3	Q	220	LEU	CA-C-N	6.65	133.66	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	220	LEU	C-N-CA	6.65	133.66	121.70
6	T	7	TYR	N-CA-CB	6.65	121.80	110.50
9	I	69	ARG	NE-CZ-NH1	6.62	128.12	121.50
3	C	197	GLU	N-CA-C	6.59	118.54	111.36
7	U	199	ILE	CB-CA-C	6.52	121.21	112.22
6	T	143	ASN	N-CA-C	6.46	118.40	111.36
9	W	79	ARG	N-CA-C	6.45	117.94	108.14
8	H	217	ILE	CB-CA-C	-6.43	102.94	110.91
12	Z	172	MET	CG-SD-CE	-6.30	87.03	100.90
9	I	35	THR	N-CA-CB	-6.26	101.20	111.66
13	M	19	GLY	N-CA-C	6.17	118.90	110.69
2	B	52	ILE	N-CA-C	6.06	118.97	113.10
9	I	79	ARG	N-CA-C	5.97	117.62	108.42
11	K	139	VAL	N-CA-CB	5.97	118.21	110.57
6	T	190	VAL	N-CA-CB	5.88	117.82	110.47
8	V	171	GLY	N-CA-C	5.81	118.99	110.80
2	P	246	LYS	N-CA-C	5.76	119.56	112.54
8	H	73	ARG	NE-CZ-NH2	-5.75	114.03	119.20
11	K	175	VAL	CB-CA-C	5.74	118.84	110.98
9	W	170	MET	N-CA-C	5.70	117.19	110.97
9	W	69	ARG	NE-CZ-NH1	5.70	127.20	121.50
12	L	172	MET	CG-SD-CE	-5.69	88.39	100.90
4	R	127	ASP	N-CA-C	-5.65	104.76	111.03
9	I	77	GLU	CA-C-N	-5.64	110.36	121.41
9	I	77	GLU	C-N-CA	-5.64	110.36	121.41
12	Z	156	LYS	N-CA-C	5.64	118.63	110.28
9	W	35	THR	N-CA-CB	-5.63	102.26	111.66
6	T	27	MET	CG-SD-CE	5.63	113.28	100.90
13	M	133	GLU	CB-CA-C	5.62	120.40	109.33
9	I	77	GLU	O-C-N	-5.60	116.12	122.68
3	Q	220	LEU	CA-C-O	-5.58	114.66	121.36
10	X	58	GLU	N-CA-C	5.58	117.44	111.36
6	F	190	VAL	N-CA-CB	5.57	118.12	110.54
8	V	39	SER	CA-C-N	-5.53	113.20	119.28
8	V	39	SER	C-N-CA	-5.53	113.20	119.28
2	B	55	LEU	N-CA-C	5.51	119.75	113.19
12	Z	85	THR	CA-C-N	5.50	126.08	119.98
12	Z	85	THR	C-N-CA	5.50	126.08	119.98
9	W	77	GLU	O-C-N	-5.50	116.25	122.68
5	E	58	ALA	N-CA-C	5.49	117.97	111.33
6	T	44	GLY	N-CA-C	5.47	117.56	110.45
6	F	227	VAL	N-CA-C	-5.47	103.94	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	54	VAL	N-CA-CB	5.43	118.73	110.58
1	A	53	SER	N-CA-C	5.42	122.35	110.80
10	J	86	ARG	NE-CZ-NH1	5.39	126.89	121.50
13	a	71	VAL	N-CA-CB	5.39	118.66	110.58
3	Q	17	PHE	N-CA-C	5.33	117.78	111.33
8	V	82	ARG	CB-CA-C	-5.30	102.55	110.88
8	V	217	ILE	CB-CA-C	-5.30	104.34	110.91
6	F	206	ASP	CB-CA-C	5.29	118.60	110.14
1	A	127	ARG	CA-C-N	-5.27	115.15	120.21
1	A	127	ARG	C-N-CA	-5.27	115.15	120.21
10	J	86	ARG	CD-NE-CZ	5.26	131.77	124.40
6	T	226	ILE	CB-CA-C	-5.25	103.36	111.08
6	F	143	ASN	N-CA-C	5.24	117.07	111.36
1	O	53	SER	N-CA-C	5.20	121.87	110.80
6	T	174	THR	N-CA-CB	5.20	118.22	110.22
13	a	19	GLY	N-CA-C	5.20	117.86	110.74
6	T	204	VAL	CB-CA-C	5.19	118.57	111.87
10	X	86	ARG	NE-CZ-NH1	5.19	126.69	121.50
3	Q	12	PRO	CA-C-N	-5.18	114.94	122.86
3	Q	12	PRO	C-N-CA	-5.18	114.94	122.86
3	Q	98	VAL	CB-CA-C	5.17	116.20	110.62
11	Y	200	TYR	CA-C-N	5.13	130.94	121.70
11	Y	200	TYR	C-N-CA	5.13	130.94	121.70
5	S	7	ASP	N-CA-C	5.12	119.48	112.88
9	W	16[A]	LYS	CA-C-N	5.11	132.79	123.13
9	W	16[A]	LYS	C-N-CA	5.11	132.79	123.13
9	W	16[B]	LYS	CA-C-N	5.11	132.79	123.13
9	W	16[B]	LYS	C-N-CA	5.11	132.79	123.13
3	C	184	ASP	N-CA-C	5.11	116.53	111.07
12	Z	71	ARG	NE-CZ-NH2	5.10	123.79	119.20
7	G	88	ARG	CG-CD-NE	-5.10	100.78	112.00
14	N	12	GLY	N-CA-C	5.08	117.45	110.69
8	H	171	GLY	N-CA-C	5.08	117.96	110.80
8	H	23	GLU	N-CA-C	-5.07	100.03	108.34
12	Z	3	SER	CB-CA-C	-5.04	103.11	109.31
10	X	86	ARG	CD-NE-CZ	5.03	131.44	124.40
5	E	126	ARG	CA-C-N	-5.02	114.55	119.92
5	E	126	ARG	C-N-CA	-5.02	114.55	119.92
8	H	73	ARG	CB-CG-CD	5.01	122.82	111.30
8	H	87	MET	CG-SD-CE	-5.00	89.90	100.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	203	GLY	Peptide
3	C	237	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
4	D	223	GLY	Peptide
5	E	235	GLY	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	245	ALA	Peptide
2	P	54	LYS	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
11	Y	200	TYR	Peptide
13	a	215	ILE	Peptide

5.2 Too-close contacts [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	14	0
1	O	1741	0	1683	8	0
2	B	1926	0	1924	10	0
2	P	1898	0	1861	15	0
3	C	1798	0	1718	18	0
3	Q	1820	0	1749	14	0
4	D	1762	0	1709	6	0
4	R	1753	0	1726	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1822	0	1779	13	0
5	S	1875	0	1818	18	0
6	F	1888	0	1882	13	0
6	T	1856	0	1816	11	0
7	G	1912	0	1882	9	0
7	U	1815	0	1748	13	0
8	H	1664	0	1677	11	0
8	V	1622	0	1591	7	0
9	I	1613	0	1646	9	0
9	W	1599	0	1621	11	0
10	J	1590	0	1581	18	0
10	X	1576	0	1561	15	0
11	K	1545	0	1494	7	0
11	Y	1580	0	1554	15	0
12	L	1636	0	1625	7	0
12	Z	1642	0	1635	6	0
13	M	1692	0	1670	7	0
13	a	1688	0	1658	8	0
14	N	1516	0	1483	7	0
14	b	1524	0	1492	7	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	1	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	3	0	0	0	0
15	M	4	0	0	1	0
15	N	2	0	0	0	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	1	0
15	R	2	0	0	0	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	4	0	0	0	0
15	a	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	16	0	22	0	0
18	I	32	0	44	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0
18	N	16	0	22	1	0
18	W	16	0	22	0	0
18	Y	16	0	22	0	0
18	b	16	0	22	0	0
19	H	23	0	0	0	0
19	K	23	0	0	0	0
19	N	23	0	0	0	0
19	V	23	0	0	0	0
19	Y	23	0	0	0	0
19	b	23	0	0	0	0
20	A	110	0	0	2	0
20	B	124	0	0	0	0
20	C	76	0	0	0	0
20	D	88	0	0	1	0
20	E	143	0	0	2	0
20	F	189	0	0	5	0
20	G	190	0	0	2	0
20	H	158	0	0	5	0
20	I	153	0	0	1	0
20	J	137	0	0	2	0
20	K	100	0	0	0	0
20	L	131	0	0	0	0
20	M	146	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	158	0	0	1	0
20	O	92	0	0	2	0
20	P	117	0	0	0	0
20	Q	73	0	0	1	0
20	R	124	0	0	2	0
20	S	122	0	0	3	0
20	T	89	0	0	0	0
20	U	106	0	0	2	0
20	V	114	0	0	0	0
20	W	114	0	0	2	0
20	X	128	0	0	1	0
20	Y	150	0	0	2	0
20	Z	169	0	0	1	0
20	a	173	0	0	1	0
20	b	121	0	0	0	0
All	All	52085	0	47542	284	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 (284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.17	1.06
10:X:1:MET:HE1	10:X:134:TYR:H	1.22	1.03
11:Y:36:ILE:HD11	11:Y:46:MET:SD	2.12	0.90
8:H:78:VAL:HB	20:H:540:HOH:O	1.72	0.88
11:K:36:ILE:HD11	11:K:46:MET:SD	2.15	0.85
10:X:1:MET:HE1	10:X:134:TYR:N	1.93	0.82
2:P:155:ASN:OD1	3:Q:77:THR:OG1	1.98	0.82
10:J:1[A]:MET:HE1	10:J:134:TYR:N	1.92	0.82
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.26	0.80
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.65	0.78
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.64	0.78
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.66	0.78
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	1.66	0.78
11:Y:200:TYR:HA	11:Y:201:SER:HB2	1.68	0.76
9:W:13:MET:HE2	9:W:166:ILE:HB	1.67	0.76
14:N:36:THR:CG2	14:N:46:ARG:HE	2.00	0.75
5:S:152[B]:ASN:OD1	20:S:401:HOH:O	2.06	0.73
1:O:10:THR:HG23	20:O:403:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:301:CL:CL	20:F:401:HOH:O	2.47	0.69
9:W:16[B]:LYS:NZ	20:W:401:HOH:O	2.25	0.69
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.74	0.69
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.10	0.69
4:D:96:THR:OG1	20:D:401:HOH:O	2.10	0.69
6:F:169[A]:ARG:NH1	20:F:401:HOH:O	2.26	0.68
14:b:36:THR:CG2	14:b:46:ARG:HE	2.06	0.68
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.77	0.67
3:C:47:LYS:CB	3:C:48:LYS:HA	2.25	0.67
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.43	0.66
10:J:99[A]:HIS:CD2	20:J:414:HOH:O	2.49	0.66
1:A:88[B]:ARG:NH2	20:A:401:HOH:O	2.28	0.65
5:E:68:ASN:ND2	5:E:220:GLU:OE1	2.28	0.65
13:a:5:MET:HE2	14:b:117:MET:HB3	1.79	0.65
13:M:5:MET:HE2	14:N:117:MET:HB3	1.79	0.65
8:V:55:MET:HE1	20:W:437:HOH:O	1.95	0.65
5:E:58:ALA:O	5:E:59:HIS:CB	2.45	0.64
7:U:195:VAL:O	7:U:199:ILE:HG23	1.98	0.63
7:U:118:ILE:HG13	7:U:138:MET:HE1	1.81	0.63
5:E:101[A]:ARG:NH1	20:E:401:HOH:O	2.32	0.62
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.14	0.62
1:A:108:GLN:NE2	1:A:112:ARG:HH12	1.96	0.62
11:Y:41:TYR:HB3	11:Y:74:ARG:NH1	2.14	0.62
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.81	0.62
9:W:13:MET:HE1	9:W:166:ILE:N	2.15	0.62
9:I:13[A]:MET:CE	9:I:166:ILE:HB	2.30	0.61
4:R:129:ASP:CB	4:R:130:PRO:CD	2.79	0.61
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.33	0.61
15:M:302:CL:CL	15:M:303:CL:CL	2.92	0.61
3:C:47:LYS:CB	3:C:48:LYS:CA	2.79	0.60
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.83	0.60
15:a:302:CL:CL	15:a:303:CL:CL	2.93	0.60
5:S:68:ASN:ND2	5:S:220:GLU:OE1	2.35	0.59
11:Y:159:ARG:HE	11:Y:163:GLN:HE21	1.50	0.59
5:S:65[A]:HIS:CE1	20:Z:414:HOH:O	2.55	0.59
8:H:78:VAL:HG13	20:H:428:HOH:O	2.02	0.59
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.83	0.59
7:U:58:ASP:O	7:U:59:LYS:CB	2.51	0.59
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.85	0.58
11:Y:41:TYR:CZ	11:Y:74:ARG:HB3	2.38	0.58
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:41:TYR:HB3	11:K:74:ARG:NH1	2.19	0.58
8:H:154:ASN:ND2	20:H:404:HOH:O	2.37	0.58
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.69	0.57
10:J:27[A]:GLN:HE21	10:J:29:LYS:N	2.02	0.57
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.86	0.57
10:X:38:MET:HE1	10:X:61:GLN:HB2	1.86	0.57
9:I:35:THR:HG21	20:I:487:HOH:O	2.04	0.57
9:W:13:MET:HE3	9:W:162:LEU:HD12	1.86	0.57
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.35	0.57
2:P:48:GLU:HB2	2:P:201:MET:HE2	1.87	0.57
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.86	0.57
6:T:6:GLY:HA3	6:T:7:TYR:CD2	2.39	0.57
13:a:112:ILE:HD12	13:a:112:ILE:N	2.20	0.57
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.35	0.56
9:W:13:MET:CE	9:W:166:ILE:HB	2.33	0.56
11:K:41:TYR:CZ	11:K:74:ARG:HB3	2.42	0.55
12:L:144:MET:CE	12:L:185:ARG:HB2	2.34	0.55
14:N:15:LEU:HD23	14:N:45:CYS:SG	2.46	0.55
14:b:191:LEU:H	14:b:194:GLN:HE21	1.54	0.55
2:B:92[B]:LEU:HG	2:B:96:ARG:NH1	2.22	0.55
14:b:15:LEU:HD23	14:b:45:CYS:SG	2.46	0.55
10:J:182:ILE:CD1	10:J:191:LEU:HD11	2.37	0.55
4:R:129:ASP:CB	4:R:130:PRO:HD3	2.37	0.55
2:P:246:LYS:HE3	2:P:246:LYS:N	2.22	0.55
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.47	0.54
7:U:185:LYS:HD3	20:U:402:HOH:O	2.07	0.54
7:U:43:ARG:HB3	7:U:151:VAL:HG13	1.89	0.54
11:Y:39:ASN:ND2	11:Y:41:TYR:CZ	2.76	0.54
2:B:243:GLU:OE2	2:B:246:LYS:HD3	2.08	0.54
20:S:461:HOH:O	12:Z:66:LYS:HE3	2.07	0.54
6:T:53:VAL:HG12	6:T:208:ALA:HB1	1.90	0.54
15:B:301:CL:CL	15:B:302:CL:CL	2.99	0.54
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.90	0.54
13:a:86:ARG:NH1	13:a:133:GLU:OE1	2.40	0.54
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.89	0.53
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.90	0.53
8:H:78:VAL:CB	20:H:540:HOH:O	2.41	0.53
7:U:196:GLU:HG2	7:U:242:LEU:HD21	1.90	0.53
7:G:11:ARG:HG2	7:G:11:ARG:HH11	1.74	0.53
12:L:148:LEU:HD23	12:L:178:VAL:HG12	1.91	0.53
2:B:44:LEU:C	2:B:44:LEU:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.58	0.52
3:Q:95:ARG:HG2	15:Q:301:CL:CL	2.46	0.52
13:a:96:MET:HE3	13:a:127:MET:HA	1.90	0.52
4:R:96:THR:OG1	20:R:401:HOH:O	2.19	0.52
20:G:504:HOH:O	8:H:73:ARG:HD3	2.10	0.52
8:V:203:TYR:O	8:V:205:CYS:N	2.42	0.52
10:J:38:MET:HE1	10:J:61:GLN:HB2	1.90	0.52
13:a:38:ASN:N	15:a:301:CL:CL	2.75	0.52
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.91	0.51
13:M:47:ASN:ND2	20:M:404:HOH:O	2.43	0.51
1:O:227:ASP:HB2	20:O:468:HOH:O	2.09	0.51
3:Q:96:LEU:HD13	10:X:62:LYS:HG2	1.92	0.51
1:A:158:LYS:HB3	1:A:177:TYR:CZ	2.45	0.51
13:M:112:ILE:HD12	13:M:112:ILE:N	2.25	0.51
1:O:10:THR:HB	1:O:20:GLN:HB2	1.92	0.51
11:Y:200:TYR:HA	11:Y:201:SER:CB	2.39	0.51
3:C:35:VAL:HG13	3:C:191:VAL:HG22	1.93	0.51
11:Y:41:TYR:HD1	20:Y:413:HOH:O	1.93	0.51
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.40	0.50
1:A:58[B]:GLU:CD	1:A:58[B]:GLU:H	2.18	0.50
2:P:44:LEU:C	2:P:44:LEU:HD12	2.36	0.50
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.93	0.50
6:F:7:TYR:HH	7:G:11:ARG:HD3	1.76	0.50
13:a:5:MET:HE2	14:b:117:MET:CB	2.42	0.50
2:P:197:LEU:HD22	2:P:201:MET:HE3	1.92	0.50
4:R:182:GLN:OE1	5:S:55:GLU:HB3	2.11	0.50
5:S:49:LEU:O	5:S:62:LYS:HD2	2.11	0.50
11:Y:10:ARG:NH2	11:Y:147:ASP:OD1	2.42	0.50
13:a:47:ASN:ND2	20:a:402:HOH:O	2.45	0.50
13:M:96:MET:HE3	13:M:127:MET:HA	1.94	0.50
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.60	0.49
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.44	0.49
6:T:24:GLU:HA	6:T:27:MET:HE3	1.94	0.49
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.94	0.49
5:E:49:LEU:O	5:E:62:LYS:HD2	2.11	0.49
5:E:202:GLU:HG2	5:E:203:GLN:N	2.27	0.49
6:F:105:ASN:ND2	20:F:402:HOH:O	2.44	0.49
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.94	0.49
6:F:243:LEU:O	6:F:244:LYS:C	2.55	0.49
5:S:18[B]:ARG:CG	5:S:23:GLU:OE2	2.60	0.49
8:V:214:THR:HB	9:W:198:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:37:GLU:OE2	11:Y:187[A]:ARG:NH2	2.46	0.49
3:C:183:THR:OG1	3:C:184:ASP:N	2.46	0.49
9:W:25[A]:ARG:HG2	9:W:25[A]:ARG:HH11	1.78	0.48
6:F:219:LEU:HD22	20:F:447:HOH:O	2.13	0.48
13:M:92:LEU:HD23	13:M:112:ILE:HD11	1.96	0.48
6:T:202:ASP:OD1	6:T:204:VAL:HG12	2.13	0.48
3:C:183:THR:HG23	3:C:186:LEU:H	1.78	0.48
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.13	0.48
13:M:5:MET:HE2	14:N:117:MET:CB	2.43	0.48
14:N:191:LEU:H	14:N:194:GLN:HE21	1.62	0.48
13:a:92:LEU:HD12	13:a:112:ILE:HD11	1.96	0.48
10:X:132:HIS:HD2	20:X:481:HOH:O	1.97	0.47
13:M:92:LEU:CD2	13:M:112:ILE:HD11	2.45	0.47
6:T:205:LYS:O	6:T:206:ASP:CG	2.57	0.47
9:I:13[A]:MET:HE1	9:I:166:ILE:CA	2.45	0.47
1:A:214:GLU:HB3	20:A:499:HOH:O	2.14	0.47
14:b:145:ARG:O	14:b:148[B]:MET:SD	2.73	0.47
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.97	0.47
9:I:27:PHE:HB3	9:I:35:THR:HG22	1.97	0.47
7:G:192:GLU:HG2	7:G:193:GLN:OE1	2.14	0.47
11:K:39:ASN:ND2	11:K:41:TYR:CZ	2.82	0.47
10:J:182:ILE:HD12	10:J:191:LEU:HD11	1.98	0.46
3:Q:183:THR:HG23	3:Q:186:LEU:H	1.80	0.46
6:F:34:SER:OG	6:F:65:ARG:NH1	2.48	0.46
2:P:53:HIS:O	2:P:54:LYS:HB2	2.14	0.46
5:S:50:LYS:CB	5:S:59:HIS:HB3	2.45	0.46
7:G:192:GLU:HG3	20:G:407:HOH:O	2.15	0.46
10:J:86:ARG:HD3	10:J:90:ASP:OD1	2.15	0.46
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.98	0.46
6:F:170:GLN:O	6:F:174:THR:HG23	2.16	0.46
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.98	0.46
18:N:303:1PE:H222	20:N:480:HOH:O	2.16	0.46
10:X:49:GLU:O	10:X:53:THR:HG23	2.16	0.46
3:C:201:SER:O	3:C:202:GLY:C	2.59	0.46
6:T:170:GLN:O	6:T:174:THR:HG23	2.16	0.46
8:V:98:ALA:HB1	8:V:128[B]:MET:SD	2.56	0.45
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.41	0.45
10:X:86:ARG:HD3	10:X:90:ASP:OD1	2.16	0.45
5:E:65:HIS:HB2	20:E:435:HOH:O	2.16	0.45
2:P:171:ALA:HB2	2:P:200:THR:HG21	1.99	0.45
10:X:1:MET:HE2	10:X:1:MET:HB3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:42:VAL:HG13	7:G:198:ALA:HB2	1.99	0.45
1:A:94:GLN:HG3	8:H:66:LEU:HD13	1.99	0.45
5:E:171:TYR:CD2	5:E:171:TYR:C	2.95	0.45
8:H:133:LEU:HD22	14:N:26:TYR:CZ	2.51	0.45
2:P:124:PHE:CD1	3:Q:124:ARG:HG2	2.52	0.45
10:J:49:GLU:O	10:J:53:THR:HG23	2.16	0.45
9:I:25[A]:ARG:HG2	9:I:25[A]:ARG:HH11	1.80	0.45
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	2.17	0.45
3:Q:183:THR:OG1	3:Q:184:ASP:N	2.50	0.45
4:D:166:ASP:HB3	4:D:185:TYR:CZ	2.52	0.44
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.46	0.44
3:C:41:VAL:CG2	3:C:211:MET:HB3	2.47	0.44
2:P:76:VAL:HG12	2:P:134:LEU:HG	1.98	0.44
9:W:27:PHE:HB3	9:W:35:THR:HG22	1.99	0.44
6:F:7:TYR:OH	7:G:11:ARG:HD3	2.16	0.44
8:H:9:TYR:O	8:H:10:LYS:C	2.61	0.44
2:P:190:LEU:HG	2:P:236:LEU:HD21	1.99	0.44
4:R:151:PRO:O	4:R:152:GLN:HG3	2.18	0.44
6:T:206:ASP:OD1	6:T:206:ASP:O	2.35	0.44
5:E:218:ASP:OD1	5:E:218:ASP:N	2.47	0.44
6:T:34:SER:OG	6:T:65:ARG:NH1	2.49	0.44
3:C:50:VAL:O	3:C:51:ALA:HB3	2.17	0.44
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.95	0.44
20:Q:463:HOH:O	4:R:60:GLU:HG3	2.17	0.44
6:T:152:ASP:OD1	6:T:156:VAL:HG12	2.18	0.44
7:U:51:VAL:HG12	7:U:198:ALA:HB1	2.00	0.44
10:X:1:MET:HG2	10:X:2:GLU:H	1.83	0.44
11:Y:68:GLU:HB2	20:Y:401:HOH:O	2.18	0.43
12:Z:148:LEU:HD23	12:Z:178:VAL:HG12	1.99	0.43
2:P:194:ILE:CD1	2:P:236:LEU:HB3	2.48	0.43
11:Y:13:VAL:HG13	11:Y:180:VAL:HB	1.99	0.43
1:A:158:LYS:HB3	1:A:177:TYR:CE1	2.53	0.43
12:L:184:GLU:OE2	12:L:211:ARG:HD2	2.18	0.43
2:B:33:THR:HB	2:B:166:ASN:O	2.17	0.43
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.18	0.43
1:A:74:VAL:HG22	1:A:75:TYR:H	1.84	0.43
6:F:202:ASP:OD1	6:F:204:VAL:HG22	2.19	0.43
8:H:78:VAL:CG1	20:H:540:HOH:O	2.67	0.43
5:E:7:ASP:OD1	5:E:7:ASP:C	2.60	0.43
7:G:188:ASP:O	7:G:190:THR:HG22	2.17	0.43
2:P:33:THR:HB	2:P:166:ASN:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:172:MET:HE1	12:Z:197:ILE:HD11	2.01	0.43
5:S:71:GLY:HA3	5:S:221:PHE:CZ	2.54	0.43
4:R:196:LYS:HE3	4:R:240:ASP:HB3	2.00	0.43
1:A:147:GLN:HG3	1:A:162:MET:HE1	2.01	0.42
1:O:147:GLN:HG3	1:O:162:MET:HE1	2.00	0.42
3:Q:204:LYS:HA	3:Q:205:ASN:C	2.43	0.42
2:B:76:VAL:HG12	2:B:134:LEU:HG	2.00	0.42
3:C:40:ILE:HD11	3:C:210:VAL:CG1	2.48	0.42
5:E:67:ASP:OD1	12:L:73:LYS:HE2	2.20	0.42
5:E:202:GLU:CG	5:E:203:GLN:N	2.82	0.42
4:D:151:PRO:O	4:D:152:GLN:HG3	2.19	0.42
8:H:205:CYS:SG	12:Z:158:MET:HE2	2.59	0.42
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.19	0.42
14:N:36:THR:HG21	14:N:46:ARG:HE	1.77	0.42
7:U:195:VAL:HG13	7:U:196:GLU:OE1	2.20	0.42
3:C:35:VAL:CG1	3:C:191:VAL:HG22	2.50	0.42
3:C:106:TYR:CD1	3:C:106:TYR:C	2.97	0.42
11:K:142:ARG:NH1	10:X:166:GLU:OE2	2.53	0.42
8:V:140:GLU:HA	8:V:140:GLU:OE2	2.20	0.42
4:R:128:ALA:HB1	20:R:435:HOH:O	2.19	0.42
3:C:33:VAL:HG21	3:C:195:LEU:HD12	2.02	0.42
1:O:230:ALA:O	1:O:231:ALA:CB	2.68	0.42
1:A:142:ARG:NH1	1:A:143:PRO:O	2.49	0.42
4:D:203:LYS:HE2	4:D:210:LEU:HB3	2.00	0.42
6:F:53:VAL:HG12	6:F:208:ALA:HB3	2.01	0.42
5:S:101:ARG:NH1	20:S:405:HOH:O	2.52	0.42
7:U:42:VAL:HG13	7:U:198:ALA:HB2	2.01	0.42
7:U:199:ILE:HD11	7:U:239:LEU:CD2	2.46	0.42
10:J:1[A]:MET:HG2	10:J:2:GLU:H	1.84	0.41
5:S:46:LEU:HD13	5:S:73:SER:HB2	2.01	0.41
2:B:171:ALA:HB2	2:B:200:THR:HG21	2.02	0.41
9:W:13:MET:HE1	9:W:166:ILE:CA	2.50	0.41
10:X:46[B]:CYS:SG	10:X:102:LEU:CD2	3.09	0.41
12:L:172:MET:HE1	12:L:197:ILE:HD11	2.03	0.41
5:S:45:VAL:CG1	5:S:187:LEU:HD23	2.50	0.41
3:C:203:GLY:CA	3:C:204:LYS:CB	2.99	0.41
5:S:171:TYR:CD1	5:S:171:TYR:C	2.98	0.41
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.55	0.41
7:U:186:LYS:HA	20:U:432:HOH:O	2.21	0.41
11:Y:200:TYR:CA	11:Y:201:SER:CB	2.99	0.41
10:J:9:GLY:HA3	10:J:12:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:118:GLN:NE2	1:O:118:GLN:C	2.78	0.41
7:G:183:VAL:HG13	7:G:191:PHE:CZ	2.56	0.41
1:A:206:ASN:HD22	1:A:206:ASN:C	2.29	0.41
11:K:13:VAL:HG13	11:K:180:VAL:HB	2.02	0.41
10:J:93:ARG:HD2	20:J:485:HOH:O	2.21	0.41
11:Y:36:ILE:CD1	11:Y:46:MET:SD	2.98	0.41
2:B:48:GLU:HG3	2:B:201:MET:HE3	2.03	0.40
4:D:117:SER:OG	5:E:82:ARG:NH2	2.54	0.40
6:F:169[A]:ARG:NH1	20:F:409:HOH:O	2.54	0.40
10:J:137:PHE:HB3	11:Y:134:VAL:HG21	2.03	0.40
11:K:53:CYS:SG	11:K:98:MET:HG3	2.61	0.40
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.21	0.40
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.53	0.40
3:Q:105:GLU:HG3	3:Q:145:TYR:OH	2.22	0.40
6:T:140:TYR:CE2	6:T:218:GLU:HG2	2.55	0.40
8:V:50:ALA:HB1	9:W:128:CYS:SG	2.61	0.40
8:V:133:LEU:HD22	14:b:26:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/234 (99%)	220 (95%)	7 (3%)	4 (2%)	7	3
1	O	228/234 (97%)	215 (94%)	8 (4%)	5 (2%)	5	2
2	B	248/261 (95%)	239 (96%)	8 (3%)	1 (0%)	30	27
2	P	247/261 (95%)	233 (94%)	10 (4%)	4 (2%)	7	3
3	C	236/248 (95%)	222 (94%)	7 (3%)	7 (3%)	3	1
3	Q	236/248 (95%)	219 (93%)	7 (3%)	10 (4%)	2	0
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	9	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	232/241 (96%)	225 (97%)	4 (2%)	3 (1%)	9	5
5	E	232/263 (88%)	228 (98%)	3 (1%)	1 (0%)	30	27
5	S	238/263 (90%)	232 (98%)	5 (2%)	1 (0%)	30	27
6	F	241/255 (94%)	237 (98%)	4 (2%)	0	100	100
6	T	239/255 (94%)	234 (98%)	2 (1%)	3 (1%)	9	5
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
8	H	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	24	21
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	24	21
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100	100
9	W	204/205 (100%)	200 (98%)	4 (2%)	0	100	100
10	J	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	198/204 (97%)	195 (98%)	3 (2%)	0	100	100
11	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	24	21
12	L	213/213 (100%)	210 (99%)	3 (1%)	0	100	100
12	Z	212/213 (100%)	209 (99%)	3 (1%)	0	100	100
13	M	215/219 (98%)	210 (98%)	5 (2%)	0	100	100
13	a	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	201 (100%)	1 (0%)	0	100	100
All	All	6211/6458 (96%)	6043 (97%)	123 (2%)	45 (1%)	18	14

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	53	SER
5	E	59	HIS
1	O	52	LYS
1	O	53	SER
2	P	54	LYS
3	Q	47	LYS
3	Q	201	SER
3	Q	206	ILE

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Mol	Chain	Res	Type
3	Q	221	ASN
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
6	T	7	TYR
8	V	204	ARG
11	Y	201	SER
1	A	50	LYS
3	C	200	GLN
4	D	176	GLY
1	O	176	ARG
1	O	231	ALA
2	P	204	SER
2	P	247	ALA
3	Q	138	PHE
3	Q	200	GLN
6	T	206	ASP
1	A	176	ARG
2	B	203	VAL
3	C	50	VAL
3	C	138	PHE
8	H	204	ARG
1	O	50	LYS
3	Q	50	VAL
6	T	208	ALA
3	C	51	ALA
3	C	204	LYS
3	Q	48	LYS
3	C	203	GLY
3	C	216	SER
4	D	175[A]	GLU
4	D	175[B]	GLU
2	P	52	ILE
3	Q	216	SER
3	Q	203	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	171 (92%)	14 (8%)	12	9
1	O	176/191 (92%)	164 (93%)	12 (7%)	14	11
2	B	200/221 (90%)	194 (97%)	6 (3%)	36	38
2	P	196/221 (89%)	184 (94%)	12 (6%)	17	14
3	C	179/210 (85%)	169 (94%)	10 (6%)	19	16
3	Q	184/210 (88%)	173 (94%)	11 (6%)	17	14
4	D	189/203 (93%)	183 (97%)	6 (3%)	34	35
4	R	187/203 (92%)	183 (98%)	4 (2%)	47	52
5	E	192/223 (86%)	183 (95%)	9 (5%)	23	22
5	S	197/223 (88%)	191 (97%)	6 (3%)	36	38
6	F	199/212 (94%)	187 (94%)	12 (6%)	17	14
6	T	192/212 (91%)	182 (95%)	10 (5%)	21	18
7	G	202/207 (98%)	195 (96%)	7 (4%)	32	32
7	U	186/207 (90%)	179 (96%)	7 (4%)	29	29
8	H	181/195 (93%)	173 (96%)	8 (4%)	25	24
8	V	172/195 (88%)	162 (94%)	10 (6%)	18	15
9	I	176/174 (101%)	173 (98%)	3 (2%)	53	60
9	W	173/174 (99%)	170 (98%)	3 (2%)	53	60
10	J	166/170 (98%)	158 (95%)	8 (5%)	23	21
10	X	165/170 (97%)	160 (97%)	5 (3%)	36	38
11	K	154/159 (97%)	146 (95%)	8 (5%)	21	18
11	Y	159/159 (100%)	152 (96%)	7 (4%)	25	24
12	L	175/178 (98%)	169 (97%)	6 (3%)	32	33
12	Z	175/178 (98%)	169 (97%)	6 (3%)	32	33
13	M	180/181 (99%)	174 (97%)	6 (3%)	33	34
13	a	178/181 (98%)	174 (98%)	4 (2%)	45	50
14	N	157/159 (99%)	155 (99%)	2 (1%)	61	68
14	b	158/159 (99%)	155 (98%)	3 (2%)	50	56
All	All	5033/5366 (94%)	4828 (96%)	205 (4%)	28	26

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	53	SER
1	A	54	ILE
1	A	61	VAL
1	A	73	LEU
1	A	131	VAL
1	A	174	GLU
1	A	176	ARG
1	A	180	ASP
1	A	189	THR
1	A	206	ASN
1	A	221	THR
1	A	223	THR
1	A	226	LYS
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	35	VAL
3	C	45	VAL
3	C	105	GLU
3	C	148	ASP
3	C	163	ARG
3	C	179	GLU
3	C	205	ASN
3	C	208	LEU
3	C	225	ILE
3	C	226	GLU
4	D	9	ASP
4	D	46	VAL
4	D	95	GLU
4	D	117	SER
4	D	126	GLU
4	D	199	LEU
5	E	29	VAL
5	E	61	LYS
5	E	95	SER
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	180	MET
5	E	181	GLU

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Mol	Chain	Res	Type
5	E	189	LYS
5	E	229	VAL
6	F	17	ASP
6	F	31	GLU
6	F	53	VAL
6	F	81	LEU
6	F	86	SER
6	F	87	LEU
6	F	174	THR
6	F	187	ARG
6	F	190	VAL
6	F	240	LYS
6	F	243	LEU
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
7	G	232	GLU
8	H	7	VAL
8	H	13	ILE
8	H	66	LEU
8	H	69	LEU
8	H	74	LEU
8	H	184	LEU
8	H	200	LEU
8	H	216	LYS
9	I	35	THR
9	I	69	ARG
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	27[A]	GLN
10	J	27[B]	GLN
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	155	ARG
11	K	13	VAL
11	K	43	LEU

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Mol	Chain	Res	Type
11	K	139	VAL
11	K	142	ARG
11	K	148	LEU
11	K	159	ARG
11	K	175	VAL
11	K	188	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	169	ASP
12	L	172	MET
12	L	174	LEU
12	L	207	THR
13	M	119	GLU
13	M	154	LEU
13	M	155	GLU
13	M	198	GLU
13	M	206	GLU
13	M	216	SER
14	N	23	THR
14	N	36	THR
1	O	10	THR
1	O	53	SER
1	O	73	LEU
1	O	131	VAL
1	O	176	ARG
1	O	180	ASP
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	221	THR
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	43	VAL
2	P	59	VAL
2	P	124	PHE
2	P	183	GLU
2	P	190	LEU
2	P	204	SER
2	P	235	GLN

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Mol	Chain	Res	Type
2	P	236	LEU
2	P	246	LYS
3	Q	45	VAL
3	Q	56	GLU
3	Q	98	VAL
3	Q	105	GLU
3	Q	148	ASP
3	Q	163	ARG
3	Q	170	GLU
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	227	LYS
4	R	9	ASP
4	R	32	LYS
4	R	46	VAL
4	R	117	SER
5	S	29	VAL
5	S	45	VAL
5	S	95	SER
5	S	101	ARG
5	S	180	MET
5	S	202	GLU
6	T	17	ASP
6	T	31	GLU
6	T	53	VAL
6	T	81	LEU
6	T	86	SER
6	T	87	LEU
6	T	174	THR
6	T	190	VAL
6	T	240	LYS
6	T	243	LEU
7	U	42	VAL
7	U	78	CYS
7	U	151	VAL
7	U	182	LYS
7	U	196	GLU
7	U	199	ILE
7	U	206	LEU
8	V	7	VAL
8	V	13	ILE

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Mol	Chain	Res	Type
8	V	66	LEU
8	V	69	LEU
8	V	74	LEU
8	V	105[A]	ASP
8	V	105[B]	ASP
8	V	184	LEU
8	V	200	LEU
8	V	214	THR
9	W	35	THR
9	W	69	ARG
9	W	193	LYS
10	X	1	MET
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	158	GLU
11	Y	13	VAL
11	Y	107	LYS
11	Y	139	VAL
11	Y	142[A]	ARG
11	Y	142[B]	ARG
11	Y	148	LEU
11	Y	193	VAL
12	Z	73	LYS
12	Z	169	ASP
12	Z	172	MET
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
13	a	119	GLU
13	a	154	LEU
13	a	198	GLU
13	a	216	SER
14	b	23	THR
14	b	30	ARG
14	b	36	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	94	GLN

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Mol	Chain	Res	Type
1	A	108	GLN
1	A	111	GLN
1	A	206	ASN
2	B	40	ASN
2	B	51	ASN
2	B	100	GLN
2	B	102	GLN
2	B	146	GLN
3	C	54	GLN
3	C	94	HIS
3	C	175	ASN
5	E	8	ASN
5	E	65	HIS
6	F	143	ASN
7	G	33	ASN
7	G	100	ASN
7	G	128	ASN
8	H	81	ASN
8	H	154	ASN
9	I	80	GLN
9	I	161	HIS
9	I	172	ASN
10	J	61	GLN
10	J	63	ASN
10	J	101	ASN
10	J	132	HIS
10	J	186	ASN
11	K	63	GLN
11	K	120	ASN
11	K	163	GLN
13	M	65	GLN
13	M	162	GLN
14	N	194	GLN
1	O	62	HIS
1	O	94	GLN
1	O	111	GLN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	102	GLN
2	P	146	GLN
2	P	235	GLN

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Mol	Chain	Res	Type
3	Q	18	GLN
3	Q	175	ASN
4	R	152	GLN
4	R	186	HIS
5	S	86	ASN
6	T	68	ASN
6	T	110	HIS
6	T	143	ASN
7	U	33	ASN
7	U	100	ASN
7	U	172	GLN
8	V	58	GLN
8	V	81	ASN
9	W	168	GLN
10	X	24	ASN
10	X	61	GLN
10	X	63	ASN
10	X	174	ASN
11	Y	63	GLN
11	Y	120	ASN
11	Y	163	GLN
12	Z	79	ASN
13	a	65	GLN
13	a	89	HIS
13	a	162	GLN
14	b	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	6V1	G	161	7	13,15,16	1.59	4 (30%)	10,20,22	3.11	7 (70%)
7	6V1	U	161	7	13,15,16	1.90	3 (23%)	10,20,22	2.73	4 (40%)
3	YCM	C	63	3	7,9,10	0.93	0	5,10,12	1.12	1 (20%)
7	YCM	G	137	7	7,9,10	2.27	3 (42%)	5,10,12	2.56	2 (40%)
7	YCM	U	137	7	7,9,10	1.01	0	5,10,12	1.82	1 (20%)
10	6V1	J	91	10	13,15,16	2.26	4 (30%)	10,20,22	5.44	7 (70%)
7	6V1	G	47	7	13,15,16	2.72	4 (30%)	10,20,22	1.50	2 (20%)
5	6V1	S	148	5	13,15,16	1.62	4 (30%)	10,20,22	2.86	4 (40%)
10	6V1	X	91	10	13,15,16	1.99	5 (38%)	10,20,22	5.82	7 (70%)
7	6V1	U	47	7	13,15,16	2.09	2 (15%)	10,20,22	1.98	3 (30%)
3	YCM	Q	63	3	7,9,10	1.10	1 (14%)	5,10,12	2.96	4 (80%)
5	6V1	E	148	5	13,15,16	1.67	3 (23%)	10,20,22	3.20	5 (50%)

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

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-7.29	1.74	1.82
7	U	47	6V1	CB-SG	-6.18	1.76	1.82
10	J	91	6V1	CB-SG	-5.88	1.76	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	91	6V1	CB-SG	-4.82	1.77	1.82
7	U	161	6V1	CB-SG	-4.45	1.77	1.82
7	G	137	YCM	CD-SG	3.97	1.91	1.81
7	G	47	6V1	C4-N3	-3.90	1.32	1.38
7	U	161	6V1	C4-N3	-3.49	1.33	1.38
5	E	148	6V1	CB-SG	-3.48	1.78	1.82
7	G	137	YCM	CE-NZ2	3.37	1.43	1.32
5	S	148	6V1	CB-SG	-3.33	1.78	1.82
7	G	47	6V1	C1-SG	3.30	1.86	1.83
10	J	91	6V1	C1-SG	-3.29	1.79	1.83
7	G	161	6V1	C2-N3	-3.11	1.34	1.38
10	J	91	6V1	C4-N3	-2.96	1.34	1.38
5	E	148	6V1	C4-N3	-2.93	1.34	1.38
10	X	91	6V1	C1-C2	2.88	1.55	1.52
7	G	161	6V1	C4-N3	-2.82	1.34	1.38
7	G	47	6V1	C2-N3	-2.76	1.34	1.38
5	E	148	6V1	C2-N3	-2.72	1.35	1.38
7	U	47	6V1	C4-N3	-2.71	1.34	1.38
7	G	161	6V1	CB-SG	2.65	1.84	1.82
5	S	148	6V1	C4-N3	-2.59	1.34	1.38
10	X	91	6V1	C4-N3	-2.58	1.34	1.38
7	U	161	6V1	C2-N3	-2.57	1.35	1.38
7	G	137	YCM	CB-SG	-2.41	1.71	1.81
10	J	91	6V1	O7-C2	2.28	1.26	1.22
5	S	148	6V1	C2-N3	-2.24	1.35	1.38
3	Q	63	YCM	CD-SG	-2.21	1.76	1.81
10	X	91	6V1	C5-C4	2.13	1.54	1.50
7	G	161	6V1	O-C	2.11	1.28	1.20
5	S	148	6V1	C1-C2	2.07	1.54	1.52
10	X	91	6V1	O7-C2	2.00	1.26	1.22

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	C5-C4-N3	8.78	113.60	108.07
10	X	91	6V1	C2-N3-C4	-8.30	108.21	113.07
10	X	91	6V1	O7-C2-N3	8.21	134.10	124.14
10	J	91	6V1	C5-C4-N3	8.04	113.13	108.07
10	J	91	6V1	C6-N3-C2	8.03	132.78	123.37
10	J	91	6V1	O7-C2-N3	7.92	133.75	124.14
10	X	91	6V1	C6-N3-C2	7.88	132.60	123.37
5	E	148	6V1	C2-N3-C4	-7.70	108.56	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	91	6V1	C2-N3-C4	-7.19	108.86	113.07
7	U	161	6V1	C2-N3-C4	-5.52	109.84	113.07
5	S	148	6V1	C2-N3-C4	-5.51	109.85	113.07
5	S	148	6V1	C5-C4-N3	5.46	111.51	108.07
7	G	161	6V1	C2-N3-C4	-4.78	110.27	113.07
7	G	161	6V1	O8-C4-N3	4.71	128.99	123.94
7	U	161	6V1	C5-C4-N3	4.66	111.00	108.07
10	X	91	6V1	O7-C2-C1	-4.58	114.55	124.52
10	X	91	6V1	O8-C4-C5	-4.49	120.71	127.28
3	Q	63	YCM	CE-CD-SG	-4.37	100.03	113.81
7	G	137	YCM	CE-CD-SG	4.35	127.54	113.81
10	J	91	6V1	C6-N3-C4	-4.32	117.41	122.52
10	X	91	6V1	C6-N3-C4	-4.23	117.52	122.52
7	U	47	6V1	C2-N3-C4	-4.14	110.64	113.07
7	G	161	6V1	O8-C4-C5	-4.11	121.27	127.28
10	J	91	6V1	O7-C2-C1	-3.92	115.98	124.52
10	J	91	6V1	O8-C4-C5	-3.85	121.64	127.28
7	G	161	6V1	C6-N3-C2	3.78	127.80	123.37
5	E	148	6V1	C5-C4-N3	3.77	110.44	108.07
7	G	47	6V1	C2-N3-C4	-3.68	110.92	113.07
7	U	137	YCM	CE-CD-SG	3.40	124.55	113.81
5	E	148	6V1	CB-CA-C	-3.24	101.99	110.80
7	U	47	6V1	C5-C4-N3	3.22	110.09	108.07
7	U	47	6V1	C6-N3-C2	3.05	126.95	123.37
5	E	148	6V1	C6-N3-C4	3.03	126.11	122.52
7	U	161	6V1	O8-C4-C5	-2.93	122.99	127.28
3	Q	63	YCM	CB-SG-CD	2.92	130.26	104.24
5	S	148	6V1	CB-CA-C	-2.83	103.11	110.80
3	Q	63	YCM	CB-CA-C	-2.78	103.26	110.80
3	Q	63	YCM	CA-CB-SG	-2.76	103.33	113.51
7	G	137	YCM	OZ1-CE-NZ2	-2.71	115.30	122.53
7	G	161	6V1	C5-C4-N3	2.66	109.74	108.07
7	U	161	6V1	C6-N3-C2	2.65	126.47	123.37
5	S	148	6V1	O8-C4-C5	-2.59	123.49	127.28
7	G	161	6V1	O7-C2-C1	-2.59	118.88	124.52
7	G	161	6V1	O7-C2-N3	2.39	127.04	124.14
7	G	47	6V1	C6-N3-C2	2.15	125.89	123.37
3	C	63	YCM	CB-CA-C	-2.06	105.20	110.80
5	E	148	6V1	O8-C4-C5	-2.06	124.27	127.28

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-OZ1
7	G	137	YCM	SG-CD-CE-NZ2
7	G	161	6V1	C3-C6-N3-C2
7	G	161	6V1	C3-C6-N3-C4
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
5	S	148	6V1	C3-C6-N3-C4
7	U	137	YCM	CE-CD-SG-CB
10	X	91	6V1	C3-C6-N3-C2
10	X	91	6V1	C3-C6-N3-C4
5	E	148	6V1	C3-C6-N3-C4
5	E	148	6V1	C3-C6-N3-C2
3	C	63	YCM	CE-CD-SG-CB
7	U	161	6V1	N-CA-CB-SG
7	G	137	YCM	CE-CD-SG-CB

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, 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$
19	6V8	K	305	11	19,23,23	1.64	3 (15%)	25,31,31	2.19	8 (32%)
18	1PE	M	305	-	15,15,15	0.51	0	14,14,14	0.43	0
19	6V8	Y	306	11	19,23,23	1.72	3 (15%)	25,31,31	2.80	9 (36%)
18	1PE	N	303	-	15,15,15	0.51	0	14,14,14	0.77	0
18	1PE	I	304	-	15,15,15	0.50	0	14,14,14	0.77	0
19	6V8	b	304	14	19,23,23	1.72	1 (5%)	25,31,31	1.62	5 (20%)
18	1PE	b	302	-	15,15,15	0.63	0	14,14,14	1.06	1 (7%)
18	1PE	W	303	-	15,15,15	0.58	0	14,14,14	0.47	0
18	1PE	H	304	-	15,15,15	0.44	0	14,14,14	0.46	0
18	1PE	I	303	-	15,15,15	0.57	0	14,14,14	0.89	0
18	1PE	L	301	-	15,15,15	0.61	0	14,14,14	0.75	0
19	6V8	H	305	8	19,23,23	2.44	3 (15%)	25,31,31	2.90	10 (40%)
19	6V8	V	303	8	19,23,23	2.78	3 (15%)	25,31,31	2.96	10 (40%)
19	6V8	N	305	14	19,23,23	1.35	2 (10%)	25,31,31	2.11	7 (28%)
18	1PE	Y	305	-	15,15,15	0.57	0	14,14,14	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	6V8	K	305	11	-	0/16/21/21	0/1/1/1
18	1PE	M	305	-	-	7/13/13/13	-
19	6V8	Y	306	11	-	0/16/21/21	0/1/1/1
18	1PE	N	303	-	-	5/13/13/13	-
18	1PE	I	304	-	-	8/13/13/13	-
19	6V8	b	304	14	-	0/16/21/21	0/1/1/1
18	1PE	b	302	-	-	7/13/13/13	-
18	1PE	W	303	-	-	8/13/13/13	-
18	1PE	H	304	-	-	5/13/13/13	-
18	1PE	I	303	-	-	6/13/13/13	-
18	1PE	L	301	-	-	6/13/13/13	-
19	6V8	H	305	8	-	3/16/21/21	0/1/1/1
19	6V8	V	303	8	-	2/16/21/21	0/1/1/1
19	6V8	N	305	14	-	0/16/21/21	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	Y	305	-	-	6/13/13/13	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	V	303	6V8	C2-C3	10.68	1.54	1.39
19	H	305	6V8	C2-C3	9.00	1.52	1.39
19	b	304	6V8	C2-C3	6.73	1.48	1.39
19	K	305	6V8	C2-C3	5.30	1.46	1.39
19	Y	306	6V8	C1-C2	-4.98	1.32	1.39
19	N	305	6V8	C2-C3	3.86	1.44	1.39
19	V	303	6V8	C3-CL3	3.69	1.82	1.73
19	Y	306	6V8	C5-C4	-3.37	1.33	1.38
19	N	305	6V8	C3-CL3	3.09	1.80	1.73
19	H	305	6V8	C3-CL3	3.07	1.80	1.73
19	H	305	6V8	C6-CL6	2.92	1.81	1.74
19	K	305	6V8	C1-C2	-2.68	1.35	1.39
19	V	303	6V8	C6-CL6	2.52	1.80	1.74
19	K	305	6V8	C6-CL6	2.40	1.80	1.74
19	Y	306	6V8	C2-C3	2.20	1.42	1.39

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	303	6V8	C2-C3-CL3	7.74	132.44	121.01
19	V	303	6V8	C3-C2-C7	7.11	134.08	122.56
19	H	305	6V8	C2-C3-CL3	7.07	131.44	121.01
19	Y	306	6V8	C2-C3-CL3	-6.74	111.06	121.01
19	Y	306	6V8	C4-C3-C2	6.32	128.36	121.36
19	H	305	6V8	C3-C2-C7	6.11	132.45	122.56
19	Y	306	6V8	C1-C6-CL6	-5.90	111.77	119.17
19	K	305	6V8	C2-C3-CL3	-5.89	112.31	121.01
19	N	305	6V8	C5-C6-C1	5.47	128.69	121.53
19	H	305	6V8	O8-C7-C2	-5.05	111.77	121.03
19	K	305	6V8	C4-C3-C2	4.93	126.82	121.36
19	H	305	6V8	C4-C3-C2	-4.66	116.20	121.36
19	V	303	6V8	C4-C3-C2	-4.23	116.68	121.36
19	V	303	6V8	C1-C2-C7	-4.00	105.85	117.21
19	Y	306	6V8	C1-C2-C3	-3.99	113.44	117.84
19	H	305	6V8	C10-N9-C7	3.97	130.88	121.29
19	V	303	6V8	C4-C3-CL3	-3.83	110.88	118.42
19	K	305	6V8	C5-C4-C3	-3.82	114.70	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	304	6V8	C5-C6-C1	3.80	126.50	121.53
19	N	305	6V8	C1-C6-CL6	-3.75	114.47	119.17
19	Y	306	6V8	C5-C6-C1	3.71	126.38	121.53
19	Y	306	6V8	C5-C4-C3	-3.66	114.93	119.98
19	V	303	6V8	C10-N9-C7	3.65	130.11	121.29
19	N	305	6V8	O8-C7-C2	-3.61	114.41	121.03
19	H	305	6V8	C4-C5-C6	3.51	122.78	119.24
19	V	303	6V8	C4-C5-C6	3.36	122.62	119.24
19	H	305	6V8	O8-C7-N9	3.19	128.81	122.59
19	K	305	6V8	C1-C6-CL6	-3.16	115.20	119.17
19	H	305	6V8	C4-C3-CL3	-3.08	112.36	118.42
18	b	302	1PE	C26-OH6-C15	3.05	126.63	113.26
19	H	305	6V8	C1-C2-C7	-3.01	108.68	117.21
19	Y	306	6V8	C3-C2-C7	2.97	127.37	122.56
19	N	305	6V8	C2-C1-C6	-2.88	114.65	119.53
19	b	304	6V8	O8-C7-C2	-2.87	115.77	121.03
19	K	305	6V8	C5-C6-C1	2.78	125.17	121.53
19	K	305	6V8	C10-N9-C7	2.77	127.99	121.29
19	V	303	6V8	C5-C6-CL6	2.72	123.37	119.36
19	b	304	6V8	C21-C22-C23	2.72	118.79	115.32
19	N	305	6V8	C21-C22-C23	2.66	118.72	115.32
19	V	303	6V8	C1-C6-CL6	-2.64	115.86	119.17
19	N	305	6V8	C4-C5-C6	-2.64	116.59	119.24
19	Y	306	6V8	O8-C7-C2	-2.62	116.24	121.03
19	b	304	6V8	C1-C6-CL6	-2.56	115.96	119.17
19	Y	306	6V8	C10-N9-C7	2.36	126.98	121.29
19	N	305	6V8	C4-C3-C2	2.32	123.93	121.36
19	V	303	6V8	O8-C7-C2	-2.25	116.91	121.03
19	b	304	6V8	C5-C4-C3	-2.08	117.10	119.98
19	H	305	6V8	C5-C6-C1	-2.08	118.81	121.53
19	K	305	6V8	O8-C7-C2	-2.03	117.31	121.03
19	K	305	6V8	C1-C2-C3	-2.02	115.62	117.84

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	b	302	1PE	C25-C15-OH6-C26
18	L	301	1PE	C16-C26-OH6-C15
18	N	303	1PE	C13-C23-OH3-C22
18	I	304	1PE	C24-C14-OH5-C25
18	I	303	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
18	M	305	1PE	OH5-C14-C24-OH4
18	Y	305	1PE	OH6-C15-C25-OH5
18	I	304	1PE	OH4-C13-C23-OH3
18	L	301	1PE	OH5-C14-C24-OH4
18	b	302	1PE	OH4-C13-C23-OH3
18	L	301	1PE	OH6-C15-C25-OH5
18	M	305	1PE	OH4-C13-C23-OH3
18	I	304	1PE	OH2-C12-C22-OH3
18	H	304	1PE	OH4-C13-C23-OH3
18	W	303	1PE	OH6-C15-C25-OH5
18	N	303	1PE	OH2-C12-C22-OH3
18	W	303	1PE	OH7-C16-C26-OH6
18	Y	305	1PE	C16-C26-OH6-C15
18	I	303	1PE	OH2-C12-C22-OH3
18	I	304	1PE	OH7-C16-C26-OH6
18	N	303	1PE	OH7-C16-C26-OH6
18	Y	305	1PE	OH2-C12-C22-OH3
18	M	305	1PE	OH6-C15-C25-OH5
18	I	303	1PE	C15-C25-OH5-C14
18	L	301	1PE	OH2-C12-C22-OH3
18	M	305	1PE	OH2-C12-C22-OH3
18	N	303	1PE	OH4-C13-C23-OH3
18	H	304	1PE	OH5-C14-C24-OH4
18	W	303	1PE	C12-C22-OH3-C23
18	I	304	1PE	C16-C26-OH6-C15
18	M	305	1PE	C23-C13-OH4-C24
18	W	303	1PE	C13-C23-OH3-C22
18	L	301	1PE	C13-C23-OH3-C22
18	Y	305	1PE	C15-C25-OH5-C14
18	I	303	1PE	C14-C24-OH4-C13
18	b	302	1PE	OH5-C14-C24-OH4
18	H	304	1PE	OH6-C15-C25-OH5
18	Y	305	1PE	C12-C22-OH3-C23
18	H	304	1PE	OH2-C12-C22-OH3
18	b	302	1PE	OH2-C12-C22-OH3
18	W	303	1PE	C14-C24-OH4-C13
18	W	303	1PE	C16-C26-OH6-C15
18	I	303	1PE	C12-C22-OH3-C23
18	W	303	1PE	C25-C15-OH6-C26
18	I	303	1PE	C24-C14-OH5-C25
18	I	304	1PE	C23-C13-OH4-C24
18	L	301	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
18	b	302	1PE	C16-C26-OH6-C15
18	H	304	1PE	C25-C15-OH6-C26
18	I	304	1PE	OH5-C14-C24-OH4
18	I	304	1PE	OH6-C15-C25-OH5
19	H	305	6V8	N9-C10-C18-N20
19	V	303	6V8	N9-C10-C18-N20
18	W	303	1PE	C24-C14-OH5-C25
18	N	303	1PE	C23-C13-OH4-C24
18	M	305	1PE	C24-C14-OH5-C25
18	b	302	1PE	C24-C14-OH5-C25
18	b	302	1PE	OH6-C15-C25-OH5
19	V	303	6V8	N9-C10-C18-O19
19	H	305	6V8	N9-C10-C18-O19
18	Y	305	1PE	C13-C23-OH3-C22
19	H	305	6V8	C1-C2-C7-N9
18	M	305	1PE	C16-C26-OH6-C15

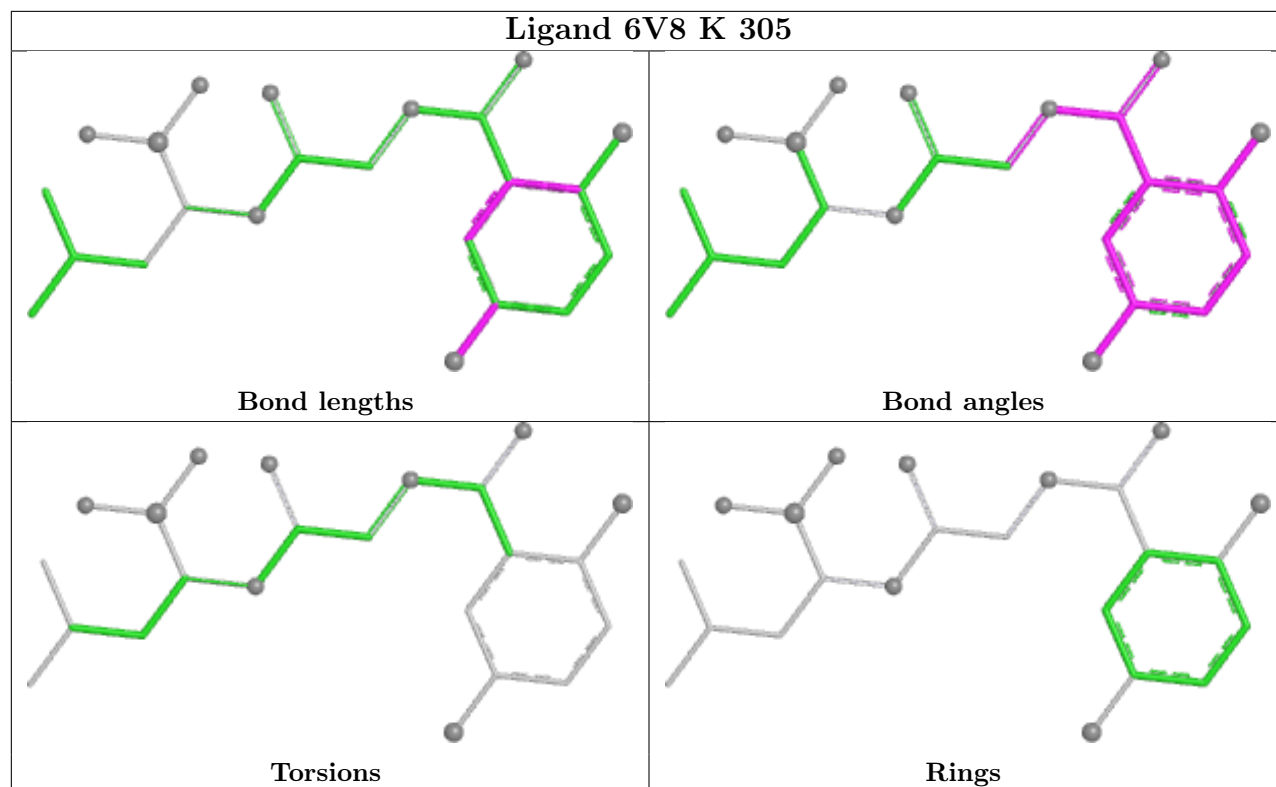
There are no ring outliers.

1 monomer is involved in 1 short contact:

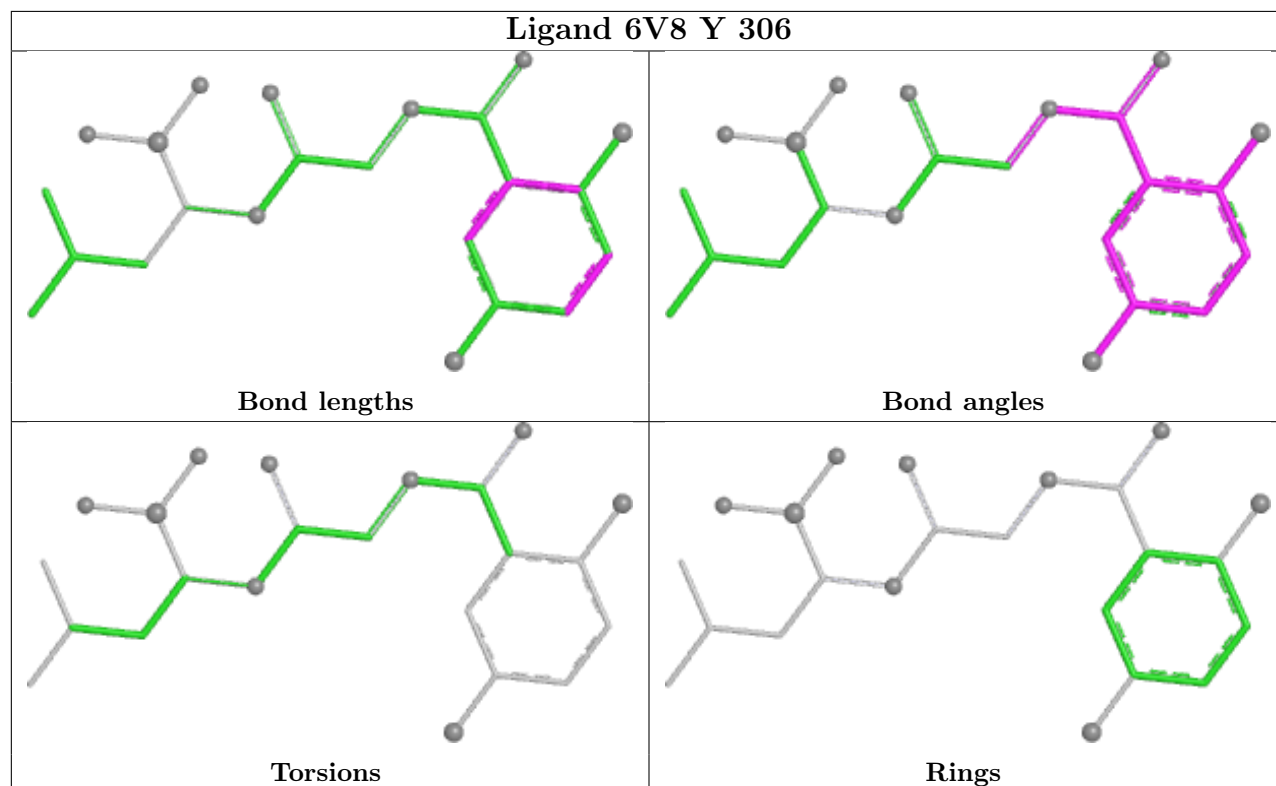
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	303	1PE	1	0

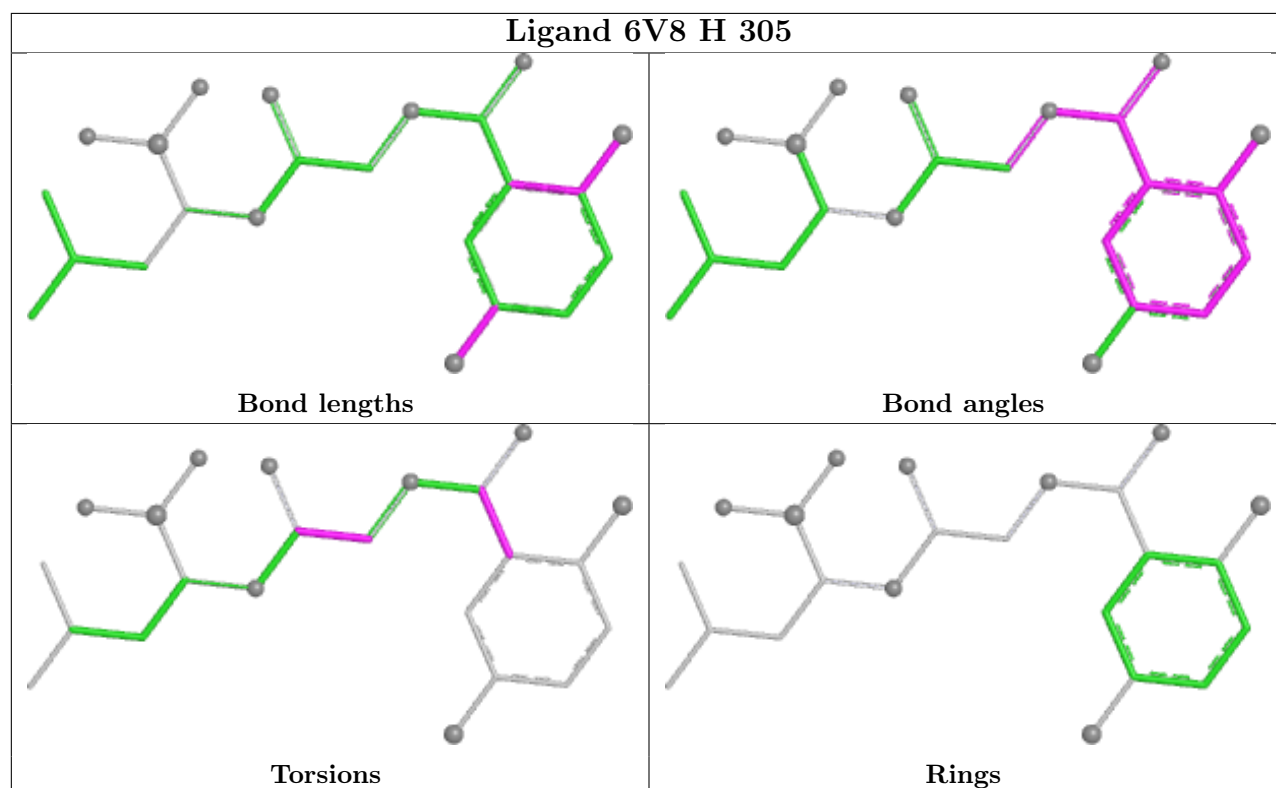
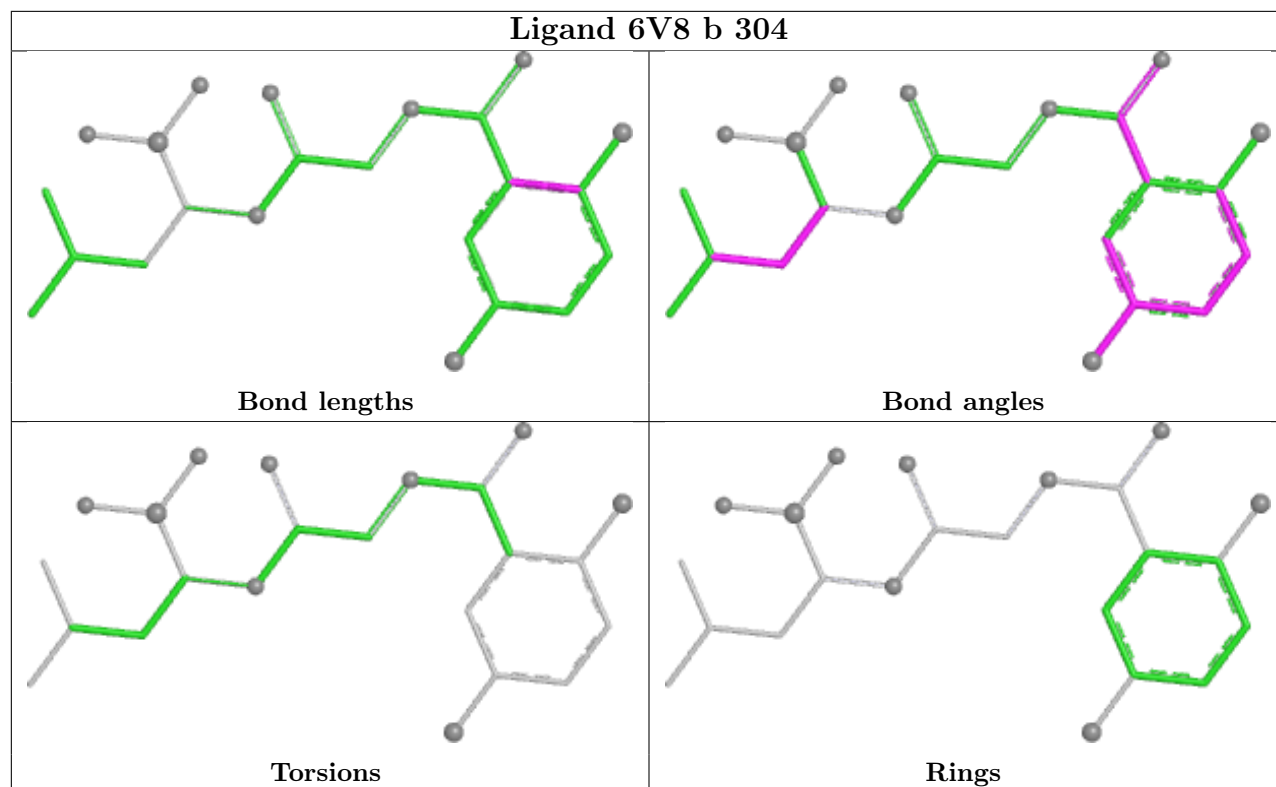
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

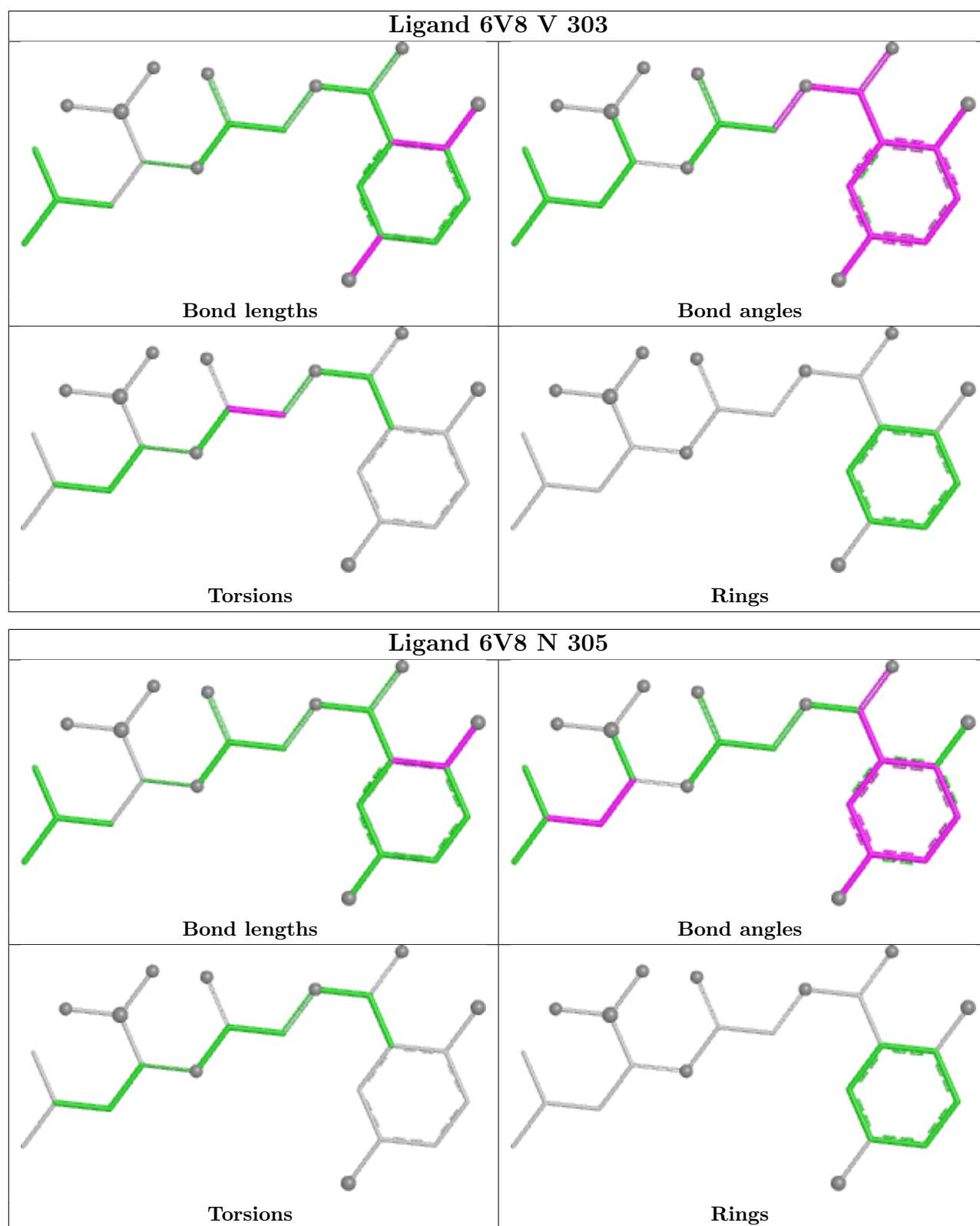
Ligand 6V8 K 305



Ligand 6V8 Y 306







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, 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%)	-0.17	2 (0%) 81 80	25, 45, 86, 98	3 (1%)
1	O	230/234 (98%)	0.34	7 (3%) 52 51	43, 67, 110, 149	0
2	B	248/261 (95%)	0.01	3 (1%) 76 76	21, 54, 98, 137	2 (0%)
2	P	247/261 (94%)	0.20	7 (2%) 55 54	34, 60, 107, 154	2 (0%)
3	C	236/248 (95%)	0.33	7 (2%) 52 51	27, 64, 106, 136	2 (0%)
3	Q	238/248 (95%)	0.44	10 (4%) 40 39	37, 66, 126, 160	0
4	D	233/241 (96%)	0.21	2 (0%) 81 80	33, 61, 91, 135	1 (0%)
4	R	233/241 (96%)	0.06	4 (1%) 69 68	23, 48, 76, 116	1 (0%)
5	E	233/263 (88%)	-0.13	6 (2%) 57 56	26, 43, 91, 112	1 (0%)
5	S	237/263 (90%)	0.10	7 (2%) 52 51	24, 53, 88, 113	3 (1%)
6	F	239/255 (93%)	-0.37	2 (0%) 82 82	21, 36, 60, 82	4 (1%)
6	T	240/255 (94%)	0.36	7 (2%) 53 52	34, 61, 96, 135	1 (0%)
7	G	241/246 (97%)	-0.30	3 (1%) 76 76	19, 40, 72, 110	2 (0%)
7	U	235/246 (95%)	0.32	3 (1%) 75 74	36, 70, 106, 140	1 (0%)
8	H	220/234 (94%)	-0.34	2 (0%) 81 80	22, 37, 75, 126	2 (0%)
8	V	220/234 (94%)	0.07	6 (2%) 56 55	26, 52, 83, 120	2 (0%)
9	I	204/205 (99%)	-0.39	1 (0%) 87 87	22, 38, 60, 77	3 (1%)
9	W	204/205 (99%)	-0.10	0 100 100	29, 50, 76, 88	2 (0%)
10	J	195/201 (97%)	-0.27	1 (0%) 87 87	18, 43, 62, 78	3 (1%)
10	X	195/201 (97%)	-0.23	1 (0%) 87 87	21, 44, 60, 81	2 (1%)
11	K	200/204 (98%)	-0.19	1 (0%) 87 87	33, 47, 76, 88	0
11	Y	201/204 (98%)	-0.33	3 (1%) 72 71	22, 39, 64, 84	3 (1%)
12	L	213/213 (100%)	-0.14	0 100 100	26, 48, 71, 91	2 (0%)
12	Z	213/213 (100%)	-0.33	1 (0%) 87 87	28, 39, 65, 81	1 (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%)	87 87	28, 41, 67, 96	1 (0%)
13	a	216/219 (98%)	-0.26	2 (0%)	81 80	28, 43, 64, 86	2 (0%)
14	N	202/205 (98%)	-0.38	3 (1%)	72 71	20, 38, 60, 101	1 (0%)
14	b	203/205 (99%)	-0.16	3 (1%)	72 71	36, 47, 72, 111	1 (0%)
All	All	6222/6458 (96%)	-0.06	95 (1%)	72 71	18, 49, 91, 160	48 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	41	TYR	5.0
14	N	203	LEU	4.9
5	S	57	ALA	4.6
11	Y	202	GLY	4.2
4	R	241	ILE	4.2
5	S	2	PHE	4.1
14	N	201	ALA	3.9
13	a	216	SER	3.8
8	V	205	CYS	3.8
2	P	61	PHE	3.7
11	Y	41	TYR	3.7
7	U	186	LYS	3.6
5	S	18[A]	ARG	3.5
3	C	97	THR	3.5
4	R	131	GLY	3.3
1	O	232	ILE	3.3
5	E	57	ALA	3.2
6	T	5	THR	3.2
2	P	203	VAL	3.1
8	V	221	GLU	3.1
3	C	138	PHE	3.1
4	D	241	ILE	3.1
5	E	59	HIS	3.1
8	V	204	ARG	3.1
4	D	131	GLY	3.0
5	E	56	LEU	3.0
5	E	58	ALA	2.9
3	Q	50	VAL	2.9
2	P	51	ASN	2.9
3	Q	203	GLY	2.9
1	O	188	HIS	2.8
6	T	208	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
5	S	56	LEU	2.8
2	P	206	LEU	2.8
4	R	120[A]	ALA	2.7
14	b	200	VAL	2.7
2	B	61	PHE	2.7
5	S	239	ARG	2.7
1	A	231	ALA	2.6
8	H	205	CYS	2.6
1	A	3	ARG	2.6
6	T	6	GLY	2.5
5	E	54	SER	2.5
14	b	204	PRO	2.5
13	a	215	ILE	2.5
1	O	177	TYR	2.5
3	Q	97	THR	2.5
2	P	245	ALA	2.5
3	Q	53	LEU	2.5
10	J	1[A]	MET	2.5
3	C	98	VAL	2.4
13	M	215	ILE	2.4
2	B	2	SER	2.4
5	S	53	GLN	2.3
6	T	209	PHE	2.3
3	Q	98	VAL	2.3
1	O	230	ALA	2.3
12	Z	169	ASP	2.3
7	U	185	LYS	2.3
10	X	196	PHE	2.3
2	P	124	PHE	2.3
8	V	203	TYR	2.3
7	G	189	TRP	2.3
3	C	206	ILE	2.2
1	O	225	VAL	2.2
7	U	193	GLN	2.2
1	O	3	ARG	2.2
8	V	202	ARG	2.2
3	Q	48	LYS	2.2
6	T	142	VAL	2.2
3	Q	202	GLY	2.2
6	F	6	GLY	2.2
2	P	247	ALA	2.2
9	I	16[A]	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	Q	138	PHE	2.2
3	Q	225	ILE	2.2
8	V	217	ILE	2.2
4	R	128	ALA	2.2
6	F	53	VAL	2.1
5	S	51	ARG	2.1
14	b	201	ALA	2.1
11	Y	201	SER	2.1
3	Q	232	ILE	2.1
6	T	54	LEU	2.1
2	B	249	ARG	2.1
3	C	48	LYS	2.1
7	G	187	PHE	2.1
1	O	231	ALA	2.1
7	G	208	ILE	2.0
3	C	50	VAL	2.0
6	T	204	VAL	2.0
14	N	200	VAL	2.0
3	C	220	LEU	2.0
5	E	60	GLN	2.0
8	H	203	TYR	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	0.86	0.15	85,120,126,126	0
7	YCM	G	137	10/11	0.88	0.14	32,40,55,61	0
3	YCM	C	63	10/11	0.89	0.10	58,60,68,69	0
7	YCM	U	137	10/11	0.90	0.12	59,67,78,79	0
5	6V1	S	148	15/16	0.91	0.14	45,78,85,86	0
7	6V1	U	161	15/16	0.92	0.11	66,88,97,97	0
7	6V1	G	47	15/16	0.93	0.12	37,63,69,70	0
5	6V1	E	148	15/16	0.93	0.13	32,66,78,78	0
3	YCM	Q	63	10/11	0.94	0.09	56,59,73,73	0
10	6V1	X	91	15/16	0.94	0.14	37,67,74,80	0
7	6V1	G	161	15/16	0.95	0.10	33,53,59,61	0
10	6V1	J	91	15/16	0.95	0.12	35,59,70,71	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
19	6V8	V	303	23/23	0.79	0.15	60,69,96,114	0
15	CL	Q	301	1/1	0.83	0.12	92,92,92,92	0
18	1PE	I	304	16/16	0.84	0.17	60,79,98,99	0
19	6V8	H	305	23/23	0.84	0.14	47,57,91,103	0
15	CL	O	304	1/1	0.84	0.20	77,77,77,77	0
18	1PE	M	305	16/16	0.85	0.16	68,77,95,97	0
15	CL	D	301	1/1	0.87	0.18	84,84,84,84	0
15	CL	C	302	1/1	0.89	0.20	76,76,76,76	0
17	MG	V	301	1/1	0.89	0.09	75,75,75,75	0
18	1PE	W	303	16/16	0.89	0.13	62,71,82,82	0
18	1PE	H	304	16/16	0.89	0.14	59,66,97,97	0
18	1PE	I	303	16/16	0.89	0.12	54,61,77,87	0
15	CL	Y	304	1/1	0.90	0.21	77,77,77,77	0
18	1PE	Y	305	16/16	0.90	0.14	56,74,81,83	0
15	CL	K	303	1/1	0.90	0.16	78,78,78,78	0
15	CL	O	303	1/1	0.90	0.10	103,103,103,103	0
19	6V8	K	305	23/23	0.91	0.10	41,45,60,77	0
18	1PE	b	302	16/16	0.91	0.14	50,59,91,96	0
15	CL	K	302	1/1	0.92	0.12	80,80,80,80	0
15	CL	D	302	1/1	0.92	0.18	71,71,71,71	0
15	CL	Q	302	1/1	0.92	0.19	72,72,72,72	0
15	CL	E	303	1/1	0.92	0.13	62,62,62,62	0
18	1PE	L	301	16/16	0.92	0.13	59,76,84,85	0
17	MG	H	301	1/1	0.92	0.09	69,69,69,69	0
19	6V8	Y	306	23/23	0.92	0.10	35,37,53,63	0
16	K	L	302	1/1	0.93	0.16	57,57,57,57	0
16	K	Z	301	1/1	0.93	0.12	48,48,48,48	0
15	CL	B	302	1/1	0.93	0.20	64,64,64,64	0
15	CL	a	301	1/1	0.93	0.14	73,73,73,73	0
19	6V8	b	304	23/23	0.93	0.09	39,41,48,54	0
15	CL	M	301	1/1	0.94	0.27	70,70,70,70	0
18	1PE	N	303	16/16	0.94	0.10	43,48,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CL	M	302	1/1	0.94	0.24	62,62,62,62	0
16	K	b	303	1/1	0.94	0.16	54,54,54,54	0
15	CL	R	302	1/1	0.94	0.22	69,69,69,69	0
15	CL	S	301	1/1	0.94	0.21	77,77,77,77	0
15	CL	Y	302	1/1	0.94	0.12	76,76,76,76	0
19	6V8	N	305	23/23	0.94	0.08	32,34,37,43	0
15	CL	Y	303	1/1	0.94	0.12	60,60,60,60	0
15	CL	C	301	1/1	0.94	0.10	72,72,72,72	0
15	CL	K	304	1/1	0.94	0.25	70,70,70,70	0
17	MG	H	302	1/1	0.95	0.13	34,34,34,34	0
17	MG	K	301	1/1	0.95	0.09	37,37,37,37	0
15	CL	F	301	1/1	0.95	0.14	58,58,58,58	0
15	CL	A	302	1/1	0.95	0.07	72,72,72,72	0
15	CL	a	304	1/1	0.95	0.09	68,68,68,68	0
15	CL	S	302	1/1	0.95	0.14	75,75,75,75	0
15	CL	V	302	1/1	0.95	0.15	66,66,66,66	0
15	CL	O	301	1/1	0.95	0.10	64,64,64,64	0
15	CL	O	302	1/1	0.95	0.10	67,67,67,67	0
15	CL	M	304	1/1	0.96	0.15	59,59,59,59	0
15	CL	E	301	1/1	0.96	0.12	69,69,69,69	0
15	CL	a	302	1/1	0.96	0.16	67,67,67,67	0
15	CL	E	302	1/1	0.96	0.10	57,57,57,57	0
15	CL	b	301	1/1	0.96	0.19	61,61,61,61	0
15	CL	A	304	1/1	0.96	0.15	68,68,68,68	0
15	CL	S	303	1/1	0.96	0.15	63,63,63,63	0
15	CL	A	301	1/1	0.96	0.11	50,50,50,50	0
15	CL	W	302	1/1	0.96	0.06	55,55,55,55	0
15	CL	Y	301	1/1	0.96	0.17	65,65,65,65	0
17	MG	I	305	1/1	0.96	0.09	33,33,33,33	0
15	CL	P	301	1/1	0.96	0.09	57,57,57,57	0
17	MG	L	303	1/1	0.96	0.13	42,42,42,42	0
15	CL	G	301	1/1	0.96	0.18	58,58,58,58	0
17	MG	W	301	1/1	0.96	0.10	38,38,38,38	0
15	CL	N	301	1/1	0.97	0.07	40,40,40,40	0
16	K	U	302	1/1	0.97	0.14	53,53,53,53	0
15	CL	U	301	1/1	0.97	0.08	68,68,68,68	0
15	CL	R	301	1/1	0.97	0.11	64,64,64,64	0
15	CL	N	302	1/1	0.97	0.22	58,58,58,58	0
15	CL	a	303	1/1	0.97	0.12	49,49,49,49	0
17	MG	I	301	1/1	0.97	0.11	34,34,34,34	0
15	CL	A	303	1/1	0.97	0.08	56,56,56,56	0
15	CL	G	302	1/1	0.97	0.07	64,64,64,64	0

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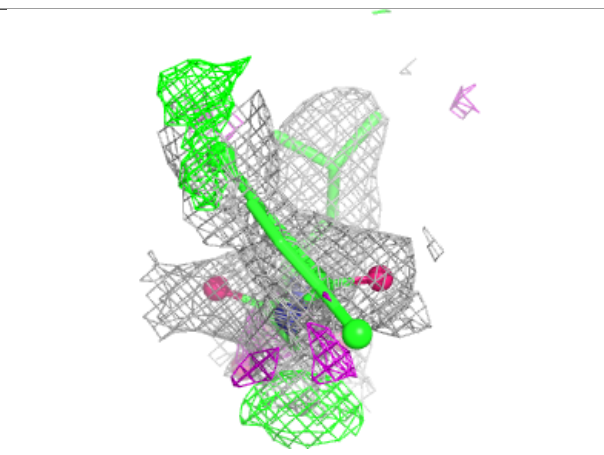
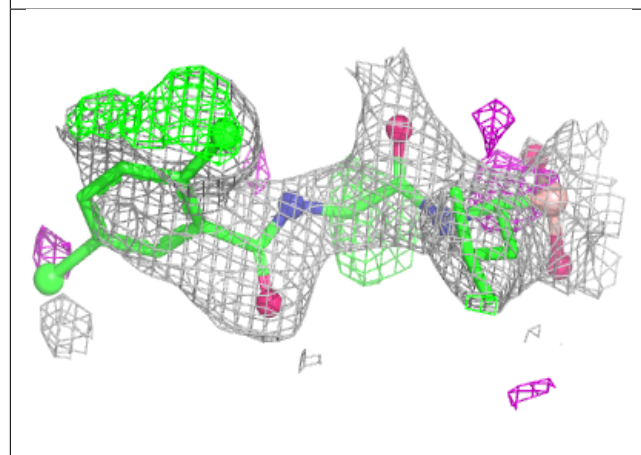
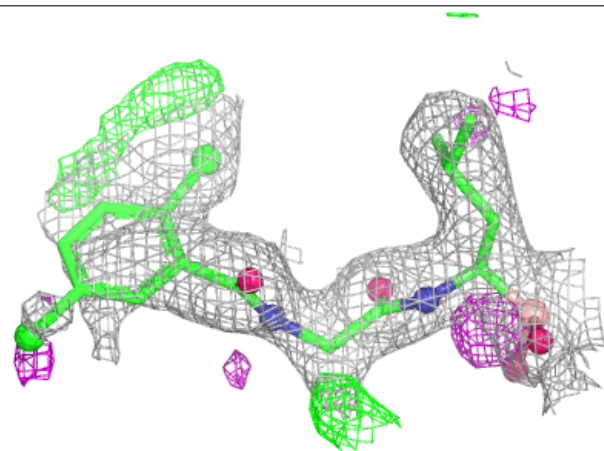
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CL	I	302	1/1	0.98	0.07	46,46,46,46	0
15	CL	B	301	1/1	0.98	0.11	44,44,44,44	0
15	CL	H	303	1/1	0.98	0.11	50,50,50,50	0
16	K	G	303	1/1	0.98	0.14	41,41,41,41	0
15	CL	M	303	1/1	0.98	0.14	45,45,45,45	0
17	MG	X	301	1/1	0.98	0.04	49,49,49,49	0
16	K	N	304	1/1	0.98	0.12	49,49,49,49	0
17	MG	J	301	1/1	0.99	0.03	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

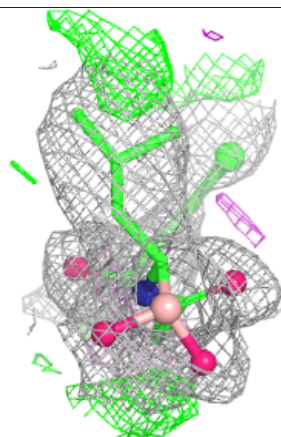
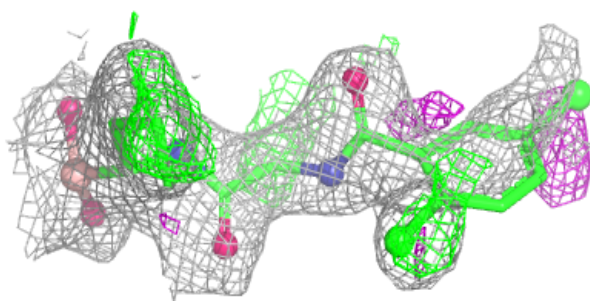
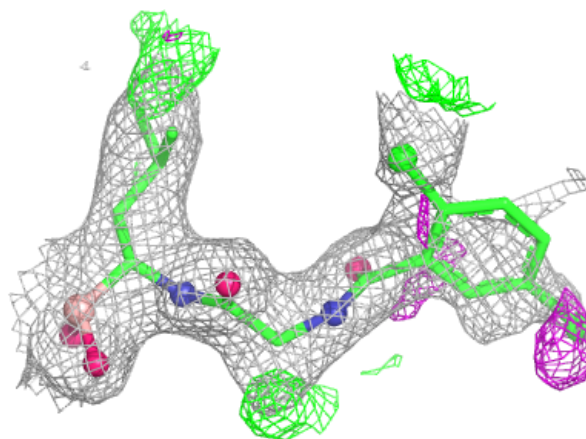
Electron density around 6V8 V 303:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

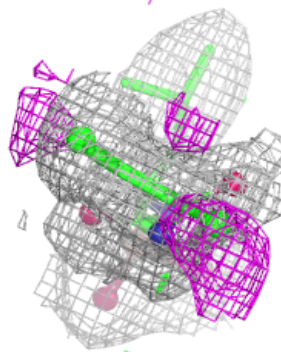
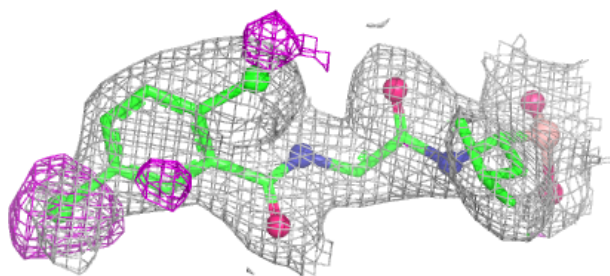
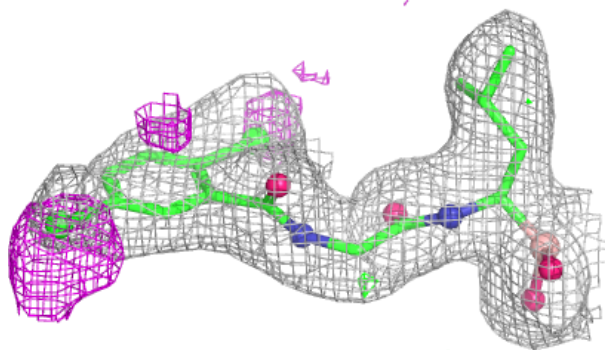


Electron density around 6V8 H 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

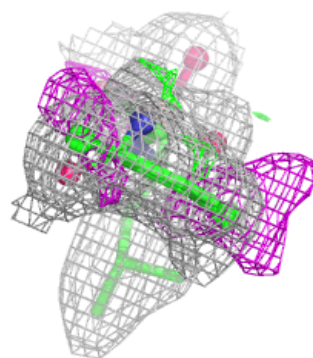
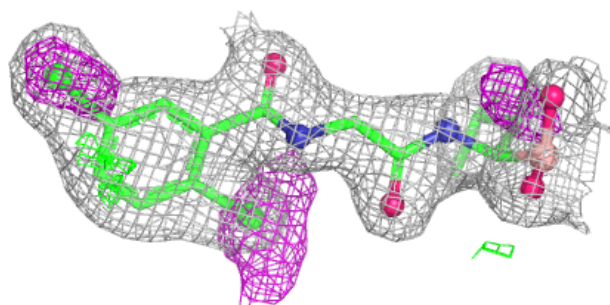
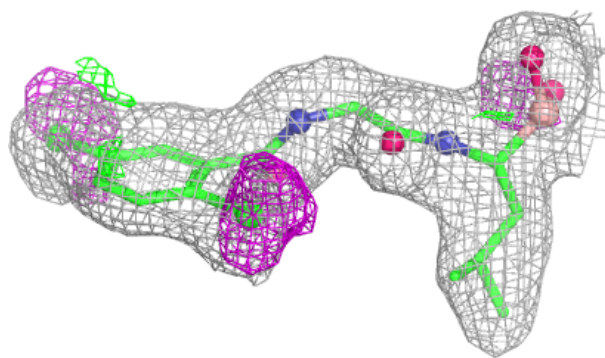
**Electron density around 6V8 K 305:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

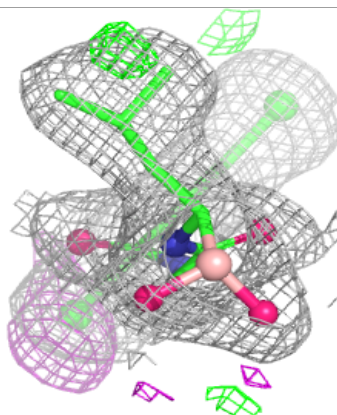
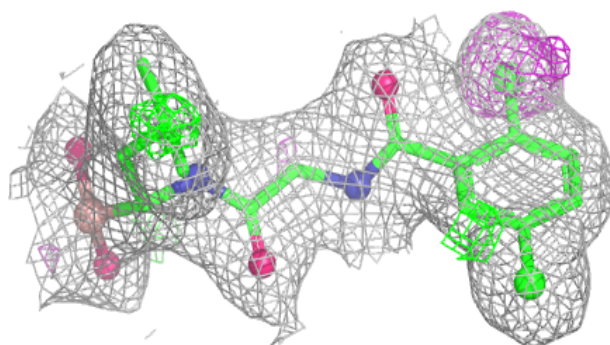
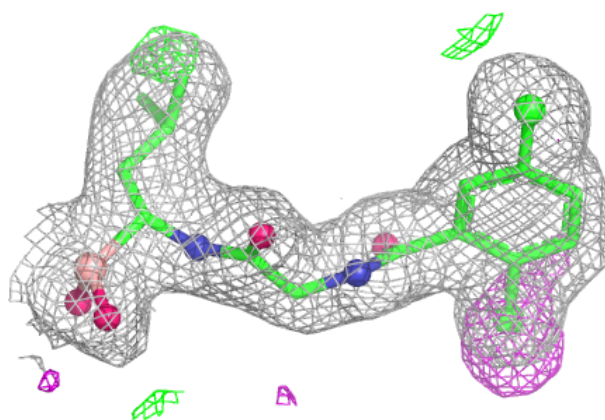


Electron density around 6V8 Y 306:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

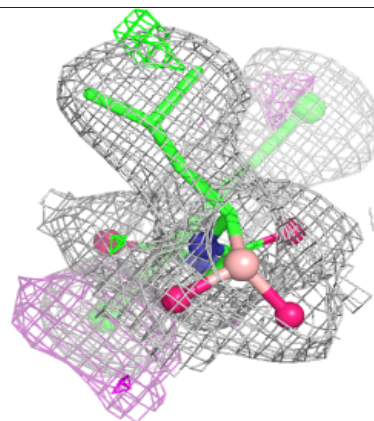
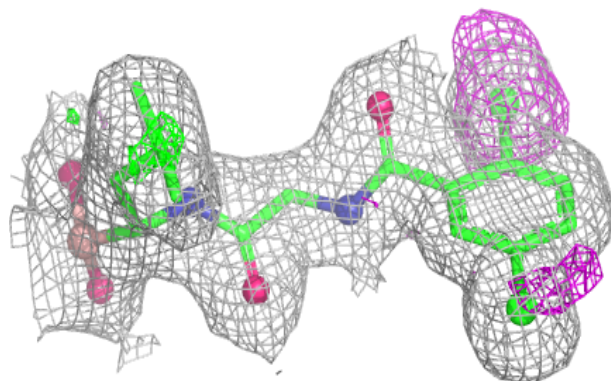
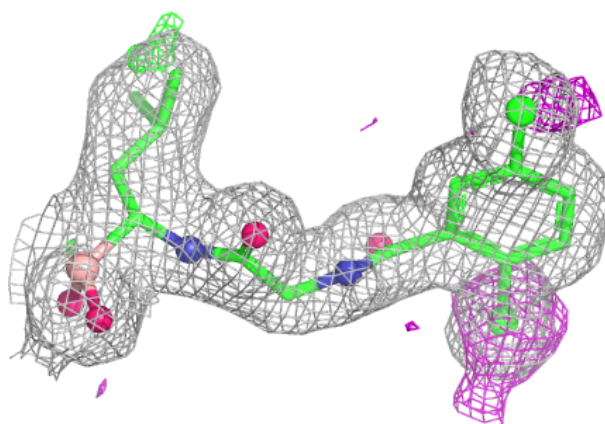
**Electron density around 6V8 b 304:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6V8 N 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.