



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:45 AM UTC

PDB ID : 5LF1 / pdb_00005lf1
Title : Human 20S proteasome complex with Dihydroeponemycin 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

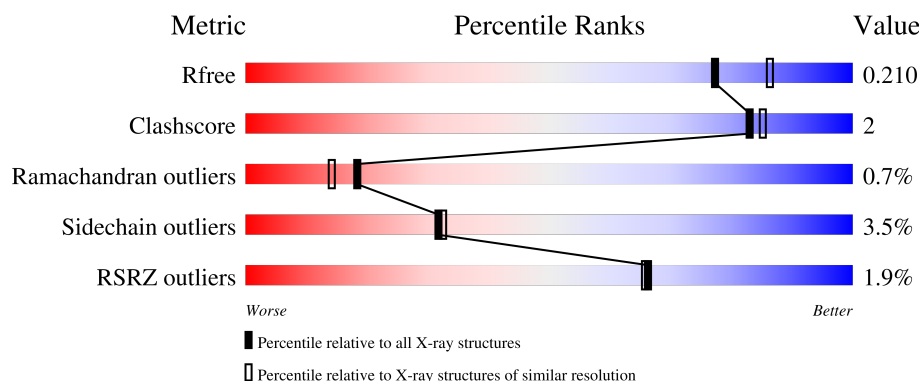
1 Overall quality at a glance

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	2% 89% 8% ..
1	O	234	3% 91% 6% ..
2	B	261	2% 88% 7% 5%
2	P	261	3% 83% 10% .. 5%
3	C	248	3% 84% 9% ..

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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 52156 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
			1922	1217	331	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	11			

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	47	6V1	CYS	conflict	UNP P60900
G	161	6V1	CYS	conflict	UNP P60900
U	47	6V1	CYS	conflict	UNP P60900
U	161	6V1	CYS	conflict	UNP P60900

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			
10	X	196	Total	C	N	O	S	0	2	0
			1576	1012	267	287	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	91	6V1	CYS	conflict	UNP P49721
X	91	6V1	CYS	conflict	UNP P49721

- 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			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- 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		
15	C	2	Total	Cl	0	0
			2	2		
15	D	1	Total	Cl	0	0
			1	1		
15	E	4	Total	Cl	0	0
			4	4		
15	F	1	Total	Cl	0	0
			1	1		
15	G	2	Total	Cl	0	0
			2	2		
15	H	1	Total	Cl	0	0
			1	1		
15	I	1	Total	Cl	0	0
			1	1		
15	K	4	Total	Cl	0	0
			4	4		
15	M	3	Total	Cl	0	0
			3	3		
15	N	4	Total	Cl	0	0
			4	4		
15	O	4	Total	Cl	0	0
			4	4		
15	P	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	5	Total 5	Cl 5	0	0
15	a	3	Total 3	Cl 3	0	0
15	b	4	Total 4	Cl 4	0	0

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

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

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

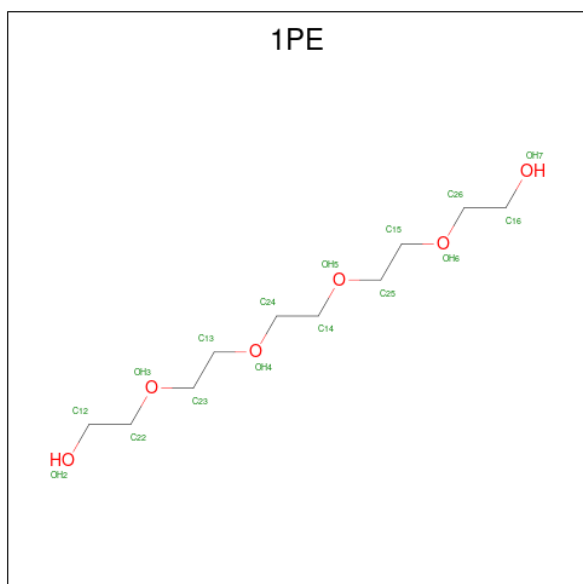
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	2	Total 2	Mg 2	0	0
17	I	1	Total 1	Mg 1	0	0

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

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



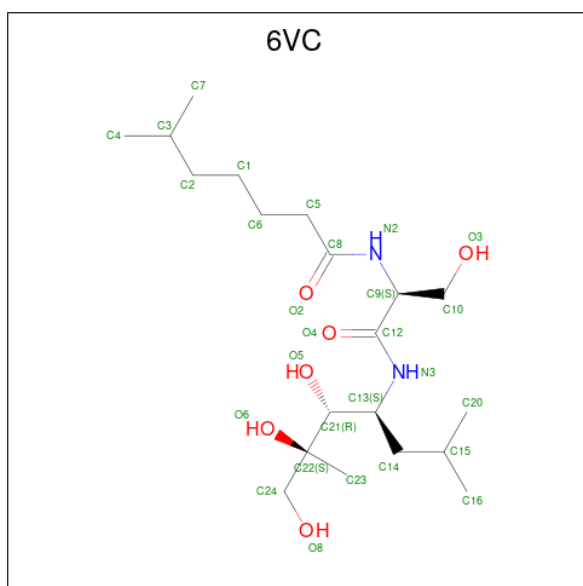
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	H	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	L	1	Total	C	O	0	0
			16	10	6		
18	M	1	Total	C	O	0	0
			16	10	6		
18	N	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	U	1	Total	C	O	0	0
			16	10	6		
18	W	1	Total	C	O	0	0
			16	10	6		
18	Z	1	Total	C	O	0	0
			16	10	6		
18	a	1	Total	C	O	0	0
			16	10	6		

- Molecule 19 is {N}-[(2 {S})-1-[(2 {S},3 {R},4 {S})-2,6-dimethyl-1,2,3-tris(oxidanyl)heptan-4-yl]amino]-3-oxidanyl-1-oxidanylidene-propan-2-yl]-6-methyl-heptanamide (CCD ID: 6VC) (formula: C₂₀H₄₀N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	H	1	Total	C	N	O	0	0
			28	20	2	6		
19	K	1	Total	C	N	O	0	0
			28	20	2	6		
19	N	1	Total	C	N	O	0	0
			28	20	2	6		
19	V	1	Total	C	N	O	0	0
			28	20	2	6		
19	Y	1	Total	C	N	O	0	0
			28	20	2	6		
19	b	1	Total	C	N	O	0	0
			28	20	2	6		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	110	Total O 110 110	0	0
20	B	127	Total O 127 127	0	0
20	C	82	Total O 82 82	0	0
20	D	91	Total O 91 91	0	0
20	E	140	Total O 140 140	0	0
20	F	186	Total O 186 186	0	0
20	G	191	Total O 191 191	0	0
20	H	156	Total O 156 156	0	0
20	I	153	Total O 153 153	0	0
20	J	138	Total O 138 138	0	0
20	K	98	Total O 98 98	0	0
20	L	130	Total O 130 130	0	0
20	M	149	Total O 149 149	0	0
20	N	165	Total O 165 165	0	0
20	O	91	Total O 91 91	0	0
20	P	123	Total O 123 123	0	0
20	Q	75	Total O 75 75	0	0
20	R	127	Total O 127 127	0	0
20	S	122	Total O 122 122	0	0
20	T	93	Total O 93 93	0	0
20	U	112	Total O 112 112	0	0

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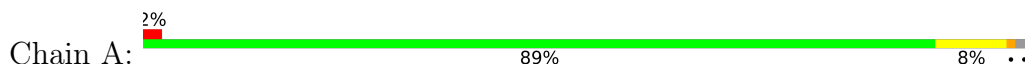
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	V	109	Total 109	O 109	0	0
20	W	116	Total 116	O 116	0	0
20	X	127	Total 127	O 127	0	0
20	Y	141	Total 141	O 141	0	0
20	Z	171	Total 171	O 171	0	0
20	a	174	Total 174	O 174	0	0
20	b	124	Total 124	O 124	0	0

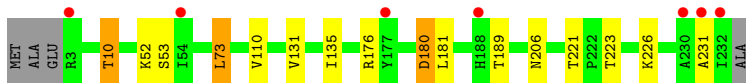
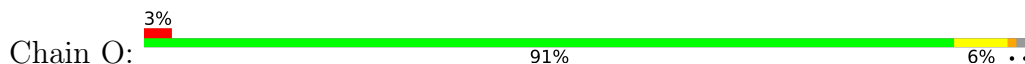
3 Residue-property plots [i](#)

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

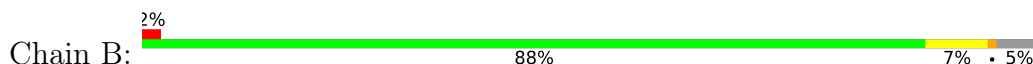
- Molecule 1: Proteasome subunit alpha type-2



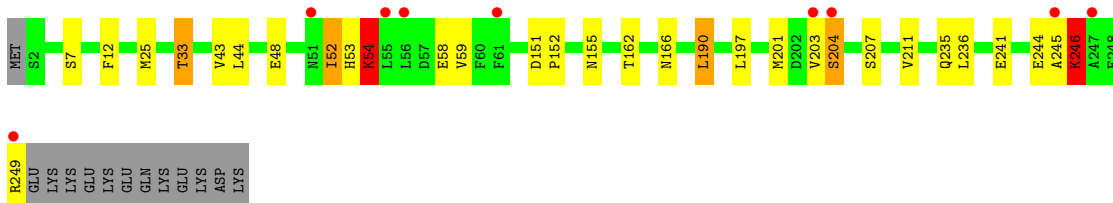
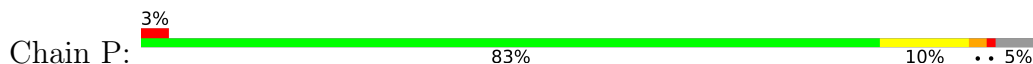
- Molecule 1: Proteasome subunit alpha type-2



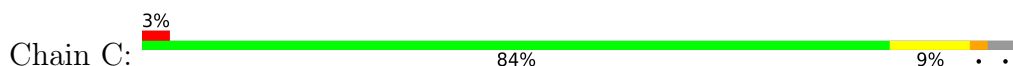
- Molecule 2: Proteasome subunit alpha type-4

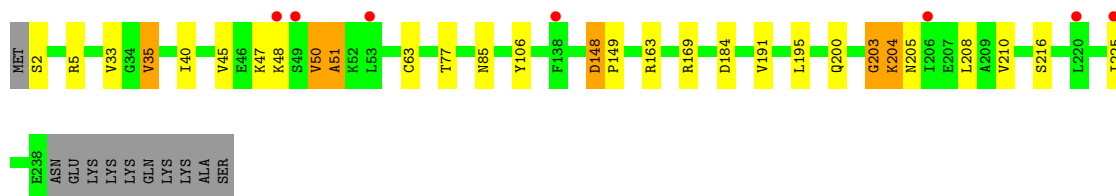


- Molecule 2: Proteasome subunit alpha type-4

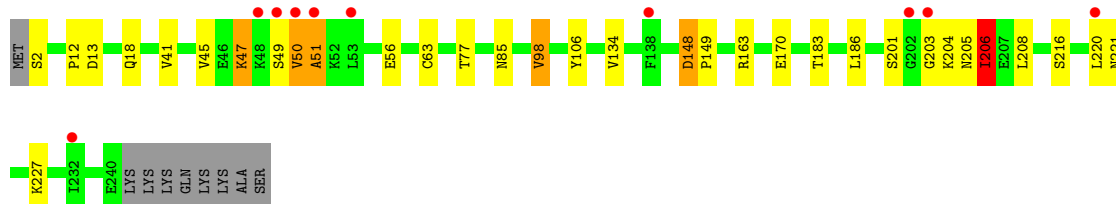
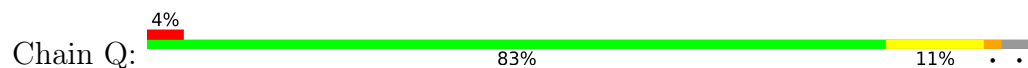


- Molecule 3: Proteasome subunit alpha type-7

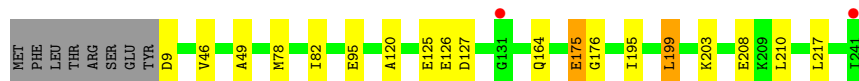
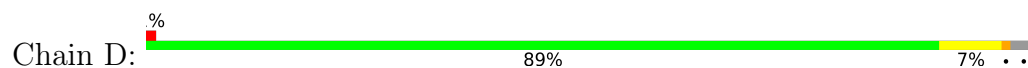




• Molecule 3: Proteasome subunit alpha type-7



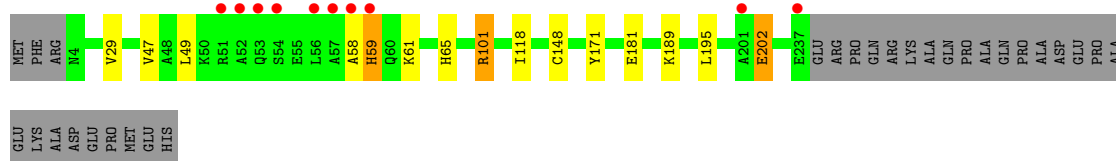
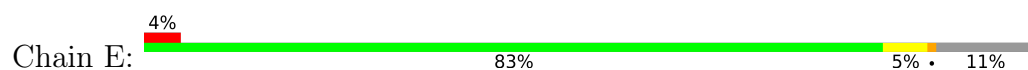
• Molecule 4: Proteasome subunit alpha type-5



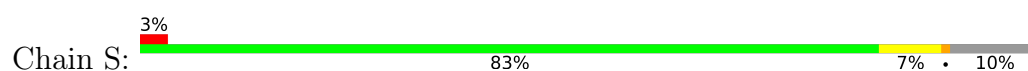
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 5: Proteasome subunit alpha type-1



• Molecule 5: Proteasome subunit alpha type-1



PRO
ALA
GLU
LYS
ALA
ASP
GLU
PRO
MET
GLU
HIS

• Molecule 6: Proteasome subunit alpha type-3

Chain F:  83% 10% • 6%

MET SER SER ILE GLY THR G6 D17 E31 S34 G44 V53 R65 G74 L81 L87 N105 M117 N143 D152 V156 R169 Q170 T174 K182 R187 V190 D202 E203 V204 H224 V227 R232 K240 K244

GLU
GLU
ASP
GLU
SER
ASP
ASP
ASN
MET

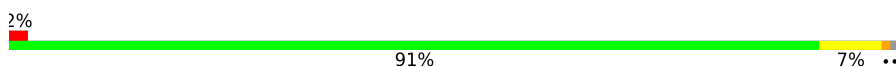
• Molecule 6: Proteasome subunit alpha type-3

Chain T:  82% 9% • 6%

MET SER SER ILE GLY T5 G6 Y7 D17 E24 M27 E31 S34 V53 G61 R65 G74 L81 L87 M117 V142 N143 D152 V156 Q170 T174 V190 K191 D202 E203 V204 K205 D206 K207 A208 R223 H224 Y238 A239

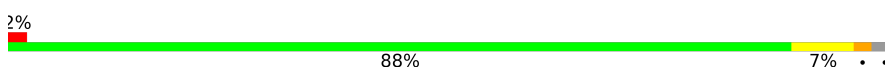
K240 E241 K244 GLU ASP GLU SER ASP ASP ASP ASN MET

• Molecule 7: Proteasome subunit alpha type-6

Chain G:  91% 7% • 2%

MET S2 V42 C47 V61 I72 C78 R88 E108 M113 L114 R117 C137 C161 V183 F187 D188 Q189 T190 A198 L206 S207 L208 K226 E232 E244 R245 ASP

• Molecule 7: Proteasome subunit alpha type-6

Chain U:  88% 7% • 2%

MET S2 V42 R43 C47 D58 K59 I72 C78 L114 I118 M138 I139 L140 V151 C161 V183 K184 K185 K186 PHE ASP TRP PHE GLU Q193 T194 V195 E196 T197 A198 I199 L206 L239 E244 R245 ASP

• Molecule 8: Proteasome subunit beta type-7

Chain H:  86% 6% • 6%

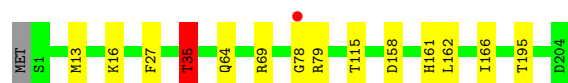
T1 V6 E22 E64 L65 L68 S69 R72 V77 R81 S112 M127 S131 L132 G170 L183 Y202 R203 C204 I216 E220 ILE GLU VAL LEU GLU GLU THR VAL GLN MET ASP THR SER

• Molecule 8: Proteasome subunit beta type-7

Chain V:  86% 7% • 3%



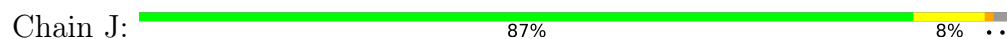
- Molecule 9: Proteasome subunit beta type-3



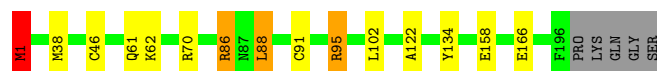
- Molecule 9: Proteasome subunit beta type-3



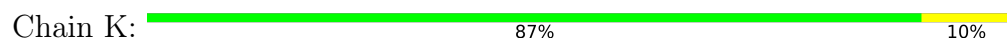
- Molecule 10: Proteasome subunit beta type-2



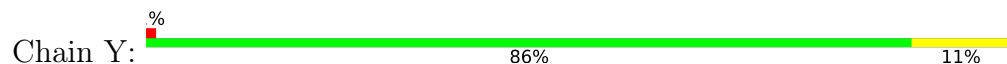
- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-1

Chain L:  92% 8%



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  93% 7%



- Molecule 13: Proteasome subunit beta type-4

Chain M:  92% 6%



- Molecule 13: Proteasome subunit beta type-4

Chain a:  93% 5% ..



- Molecule 14: Proteasome subunit beta type-6

Chain N:  94% ..



- Molecule 14: Proteasome subunit beta type-6

Chain b:  93% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.89Å 203.49Å 316.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.09 – 2.00 171.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (171.09-2.00) 99.4 (171.09-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.178 , 0.213 (Not available) , 0.210	Depositor DCC
R_{free} test set	24379 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52156	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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: 1PE, CL, 6VC, K, MG, 6V1, YCM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	0/1833	0.97	0/2489
1	O	0.81	0/1778	0.94	0/2419
2	B	0.95	0/1958	0.98	1/2645 (0.0%)
2	P	0.85	1/1945 (0.1%)	0.97	1/2631 (0.0%)
3	C	0.93	0/1818	1.06	1/2469 (0.0%)
3	Q	0.92	1/1834 (0.1%)	1.08	10/2490 (0.4%)
4	D	0.90	0/1789	0.98	1/2424 (0.0%)
4	R	1.00	0/1780	1.03	2/2408 (0.1%)
5	E	0.94	1/1842 (0.1%)	1.00	0/2493
5	S	0.90	0/1901	0.97	1/2571 (0.0%)
6	F	1.00	1/1935 (0.1%)	1.05	4/2605 (0.2%)
6	T	0.95	1/1894 (0.1%)	1.06	9/2556 (0.4%)
7	G	1.00	2/1909 (0.1%)	1.00	4/2579 (0.2%)
7	U	0.90	0/1804	0.95	0/2441
8	H	1.01	0/1697	1.06	5/2299 (0.2%)
8	V	0.89	0/1655	0.98	2/2251 (0.1%)
9	I	0.98	1/1648 (0.1%)	1.10	7/2219 (0.3%)
9	W	0.84	0/1630	0.99	6/2197 (0.3%)
10	J	0.99	0/1613	0.99	2/2180 (0.1%)
10	X	0.94	0/1599	0.94	1/2163 (0.0%)
11	K	0.93	0/1576	1.03	1/2131 (0.0%)
11	Y	1.03	0/1620	1.05	2/2185 (0.1%)
12	L	0.89	1/1672 (0.1%)	0.94	1/2257 (0.0%)
12	Z	1.03	1/1675 (0.1%)	0.99	2/2257 (0.1%)
13	M	0.99	1/1728 (0.1%)	0.98	1/2339 (0.0%)
13	a	1.04	0/1724	1.01	1/2336 (0.0%)
14	N	1.09	1/1548 (0.1%)	1.08	1/2095 (0.0%)
14	b	1.00	0/1554	1.06	2/2104 (0.1%)
All	All	0.95	12/48959 (0.0%)	1.01	68/66233 (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	4
3	Q	0	2
4	D	0	4
4	R	0	2
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
13	a	0	1
All	All	1	18

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Z	102	PHE	N-CA	7.68	1.55	1.46
6	F	44	GLY	N-CA	6.43	1.51	1.45
14	N	73	PRO	CA-C	6.06	1.55	1.51
13	M	3	ASN	C-O	-5.77	1.20	1.25
7	G	51	VAL	N-CA	5.72	1.53	1.46
12	L	102	PHE	N-CA	5.65	1.53	1.46
6	T	7	TYR	N-CA	5.55	1.56	1.46
3	Q	206	ILE	CA-C	5.44	1.59	1.52
7	G	108	GLU	CD-OE1	5.16	1.35	1.25
9	I	69	ARG	CD-NE	-5.13	1.39	1.46
2	P	162	THR	C-O	5.07	1.29	1.23
5	E	118	ILE	CA-CB	5.04	1.56	1.54

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-9.88	99.10	112.04
9	I	16[A]	LYS	CA-C-N	9.68	135.91	122.07
9	I	16[A]	LYS	C-N-CA	9.68	135.91	122.07
9	I	16[B]	LYS	CA-C-N	9.68	135.91	122.07
9	I	16[B]	LYS	C-N-CA	9.68	135.91	122.07
14	b	22	THR	CB-CA-C	-9.56	95.34	110.74
6	T	190	VAL	CB-CA-C	-8.87	100.43	112.04
14	N	22	THR	CB-CA-C	-8.75	96.65	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	246	LYS	N-CA-C	8.73	123.19	112.54
6	T	6	GLY	CA-C-N	8.14	136.36	121.70
6	T	6	GLY	C-N-CA	8.14	136.36	121.70
7	G	183	VAL	CB-CA-C	-7.96	99.82	112.16
10	J	86	ARG	NE-CZ-NH2	-7.28	112.65	119.20
8	H	77	VAL	CB-CA-C	-6.97	102.73	112.14
11	Y	199	TYR	CA-C-N	6.94	134.19	121.70
11	Y	199	TYR	C-N-CA	6.94	134.19	121.70
10	X	86	ARG	NE-CZ-NH2	-6.86	113.02	119.20
4	D	120	ALA	N-CA-C	6.79	119.26	111.11
3	Q	220	LEU	CA-C-N	6.62	133.61	121.70
3	Q	220	LEU	C-N-CA	6.62	133.61	121.70
6	F	190	VAL	N-CA-CB	6.38	118.45	110.47
6	T	143	ASN	N-CA-C	6.31	118.24	111.36
7	G	244	GLU	N-CA-C	6.29	118.58	109.71
6	T	190	VAL	N-CA-CB	6.29	118.33	110.47
4	R	120[A]	ALA	N-CA-C	6.28	118.12	111.28
4	R	120[B]	ALA	N-CA-C	6.28	118.12	111.28
13	a	71	VAL	N-CA-CB	6.19	119.86	110.58
8	H	81	ARG	CB-CA-C	-6.15	101.23	110.88
3	Q	98	VAL	CB-CA-C	6.11	117.53	110.88
3	Q	13	ASP	CB-CA-C	6.08	120.48	111.06
8	H	72	ARG	NE-CZ-NH2	-6.03	113.77	119.20
6	F	143	ASN	N-CA-C	5.99	117.89	111.36
9	I	79	ARG	N-CA-C	5.97	117.21	108.14
3	Q	12	PRO	N-CA-C	5.93	122.40	113.81
7	G	183	VAL	N-CA-C	5.89	118.42	111.05
9	I	69	ARG	NE-CZ-NH1	5.88	127.39	121.50
8	V	81	ARG	CB-CA-C	-5.85	101.70	110.88
7	G	183	VAL	N-CA-CB	5.84	120.65	110.65
6	T	7	TYR	N-CA-CB	5.83	120.41	110.50
9	W	79	ARG	N-CA-C	5.80	117.07	108.60
8	V	170	GLY	N-CA-C	5.71	118.86	110.80
9	I	35	THR	N-CA-CB	-5.69	102.16	111.66
2	B	55	LEU	N-CA-C	5.65	119.91	113.19
8	H	72	ARG	CD-NE-CZ	5.64	132.29	124.40
6	F	117	MET	CG-SD-CE	5.62	113.26	100.90
3	Q	220	LEU	CA-C-O	-5.60	114.64	121.36
10	J	86	ARG	NE-CZ-NH1	5.60	127.10	121.50
14	b	135	ILE	N-CA-C	5.56	117.55	112.43
13	M	19	GLY	N-CA-C	5.51	118.30	110.74
9	W	16[A]	LYS	CA-C-N	5.42	133.37	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	16[A]	LYS	C-N-CA	5.42	133.37	123.13
9	W	16[B]	LYS	CA-C-N	5.42	133.37	123.13
9	W	16[B]	LYS	C-N-CA	5.42	133.37	123.13
6	T	117	MET	CG-SD-CE	5.37	112.71	100.90
3	Q	220	LEU	N-CA-C	-5.36	101.79	110.32
8	H	170	GLY	N-CA-C	5.36	118.35	110.80
6	T	204	VAL	CB-CA-C	5.35	118.77	111.87
6	T	27	MET	CG-SD-CE	5.27	112.50	100.90
12	Z	71	ARG	NE-CZ-NH2	5.26	123.93	119.20
9	W	69	ARG	NE-CZ-NH1	5.22	126.72	121.50
3	Q	220	LEU	O-C-N	-5.16	117.28	123.06
3	C	184	ASP	N-CA-C	5.14	116.58	111.07
12	L	80	ASN	N-CA-C	5.14	118.83	112.24
11	K	174	VAL	CB-CA-C	5.13	118.01	110.98
12	Z	80	ASN	N-CA-C	5.04	118.69	112.24
3	Q	12	PRO	CA-C-N	-5.02	115.10	122.83
3	Q	12	PRO	C-N-CA	-5.02	115.10	122.83
5	S	7	ASP	N-CA-C	5.01	119.35	112.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide,Mainchain
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	203	VAL	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
2	P	52	ILE	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

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Mol	Chain	Res	Type	Group
10	X	1	MET	Peptide
13	a	215	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1761	7	0
1	O	1741	0	1683	4	0
2	B	1922	0	1913	8	0
2	P	1909	0	1874	13	1
3	C	1798	0	1718	18	0
3	Q	1820	0	1749	11	0
4	D	1762	0	1709	6	0
4	R	1753	0	1726	5	0
5	E	1822	0	1779	8	0
5	S	1875	0	1818	14	1
6	F	1888	0	1882	9	0
6	T	1856	0	1816	9	0
7	G	1912	0	1882	5	0
7	U	1815	0	1748	11	0
8	H	1664	0	1678	11	0
8	V	1622	0	1592	10	0
9	I	1613	0	1646	8	0
9	W	1599	0	1621	7	0
10	J	1590	0	1581	14	0
10	X	1576	0	1561	10	0
11	K	1545	0	1495	8	0
11	Y	1580	0	1555	15	0
12	L	1636	0	1625	8	0
12	Z	1642	0	1635	4	0
13	M	1692	0	1670	8	0
13	a	1688	0	1658	6	0
14	N	1519	0	1493	6	0
14	b	1524	0	1493	8	0
15	A	4	0	0	0	0
15	B	2	0	0	1	0
15	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	D	1	0	0	0	0
15	E	4	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	4	0	0	0	0
15	M	3	0	0	1	0
15	N	4	0	0	1	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	2	0	0	1	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	5	0	0	0	0
15	a	3	0	0	1	0
15	b	4	0	0	1	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	1	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	V	2	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
17	Y	1	0	0	0	0
18	H	16	0	22	0	0
18	I	16	0	22	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0
18	N	16	0	22	0	0
18	U	16	0	22	0	0
18	W	16	0	22	0	0
18	Z	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	a	16	0	22	0	0
19	H	28	0	0	0	0
19	K	28	0	0	0	0
19	N	28	0	0	0	0
19	V	28	0	0	0	0
19	Y	28	0	0	0	0
19	b	28	0	0	2	0
20	A	110	0	0	0	0
20	B	127	0	0	0	0
20	C	82	0	0	1	0
20	D	91	0	0	0	0
20	E	140	0	0	3	0
20	F	186	0	0	3	0
20	G	191	0	0	2	0
20	H	156	0	0	3	0
20	I	153	0	0	1	0
20	J	138	0	0	2	0
20	K	98	0	0	0	0
20	L	130	0	0	2	0
20	M	149	0	0	0	0
20	N	165	0	0	0	0
20	O	91	0	0	1	0
20	P	123	0	0	0	0
20	Q	75	0	0	0	0
20	R	127	0	0	2	0
20	S	122	0	0	2	0
20	T	93	0	0	0	0
20	U	112	0	0	0	0
20	V	109	0	0	0	0
20	W	116	0	0	2	0
20	X	127	0	0	0	0
20	Y	141	0	0	0	0
20	Z	171	0	0	1	0
20	a	174	0	0	0	0
20	b	124	0	0	0	0
All	All	52156	0	47559	230	1

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

All (230) 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)
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.36	1.06
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.31	0.91
10:X:1:MET:HE1	10:X:134:TYR:H	1.33	0.91
10:J:185:LYS:NZ	20:J:401:HOH:O	2.05	0.84
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.60	0.83
5:E:202:GLU:OE2	20:E:401:HOH:O	1.98	0.81
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.64	0.80
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.65	0.79
11:Y:199:TYR:HA	11:Y:200:SER:HB2	1.66	0.79
13:a:86:ARG:NH1	13:a:133:GLU:OE1	2.17	0.77
9:I:35:THR:HG21	20:I:483:HOH:O	1.85	0.74
2:P:25[B]:MET:HA	2:P:25[B]:MET:CE	2.17	0.74
7:G:188:ASP:O	7:G:190:THR:HG22	1.88	0.74
11:K:35:ILE:HD11	11:K:45:MET:SD	2.29	0.73
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.06	0.73
11:Y:35:ILE:HD11	11:Y:45:MET:SD	2.29	0.73
14:N:35:THR:CG2	14:N:45:ARG:HE	2.03	0.72
14:b:35:THR:CG2	14:b:45:ARG:HE	2.02	0.71
8:H:77:VAL:HG12	20:H:539:HOH:O	1.88	0.71
13:M:5:MET:HE2	14:N:116:MET:HB3	1.70	0.71
15:R:301:CL:CL	20:R:506:HOH:O	2.44	0.71
6:F:169[A]:ARG:NH1	20:F:402:HOH:O	2.23	0.70
7:U:118:ILE:HG13	7:U:138:MET:HE1	1.75	0.69
13:a:5:MET:HE2	14:b:116:MET:HB3	1.74	0.68
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.41	0.68
5:S:65[A]:HIS:CE1	20:Z:402:HOH:O	2.46	0.68
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.07	0.67
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.28	0.67
1:O:10:THR:HG23	20:O:402:HOH:O	1.94	0.67
4:R:129:ASP:CB	4:R:130:PRO:CD	2.72	0.66
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.42	0.66
10:X:1:MET:HE1	10:X:134:TYR:N	2.09	0.66
3:C:47:LYS:CB	3:C:48:LYS:HA	2.25	0.66
5:E:58:ALA:O	5:E:59:HIS:CB	2.43	0.65
13:M:5:MET:HE2	14:N:116:MET:CB	2.26	0.65
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	1.98	0.64
7:U:195:VAL:O	7:U:199:ILE:HG23	1.97	0.64
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.81	0.63
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.45	0.63
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	1.99	0.63
7:U:58:ASP:O	7:U:59:LYS:CB	2.48	0.62
13:a:5:MET:HE2	14:b:116:MET:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LYS:CB	3:C:48:LYS:CA	2.77	0.61
8:H:77:VAL:CG1	20:H:539:HOH:O	2.47	0.60
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.49	0.60
15:B:301:CL:CL	15:B:302:CL:CL	2.93	0.59
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.51	0.59
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.20	0.59
11:Y:36:GLU:HG2	11:Y:184:TRP:CZ2	2.38	0.59
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.83	0.59
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.33	0.59
6:F:105:ASN:ND2	20:F:404:HOH:O	2.36	0.58
8:V:54:MET:HE1	20:W:477:HOH:O	2.03	0.58
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.84	0.58
10:J:99[A]:HIS:CD2	20:J:426:HOH:O	2.57	0.58
6:T:205:LYS:O	6:T:206:ASP:CG	2.47	0.58
12:L:144:MET:CE	12:L:185:ARG:HB2	2.34	0.57
3:C:35:VAL:HG13	3:C:191:VAL:HG22	1.87	0.56
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.87	0.56
11:K:36:GLU:HG2	11:K:184:TRP:CZ2	2.41	0.56
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.88	0.55
11:K:141:ARG:NH1	10:X:166:GLU:OE2	2.40	0.55
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.40	0.55
11:Y:199:TYR:HA	11:Y:200:SER:CB	2.36	0.55
3:C:50:VAL:O	3:C:51:ALA:HB3	2.07	0.54
10:J:177:THR:HG22	10:J:195:SER:CB	2.37	0.54
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.89	0.54
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.42	0.53
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.91	0.53
15:a:302:CL:CL	15:b:302:CL:CL	3.00	0.53
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	2.09	0.53
5:S:101:ARG:NH1	20:S:404:HOH:O	2.41	0.53
7:G:117:ARG:NH2	20:G:401:HOH:O	2.28	0.52
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.75	0.52
9:W:13:MET:HE3	9:W:162:LEU:HD12	1.91	0.52
15:M:302:CL:CL	15:N:303:CL:CL	3.02	0.52
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.92	0.52
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.91	0.52
9:W:35:THR:HG21	20:W:432:HOH:O	2.10	0.52
4:R:129:ASP:CB	4:R:130:PRO:HD2	2.40	0.52
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.92	0.51
1:A:58[B]:GLU:CD	1:A:58[B]:GLU:H	2.19	0.51
3:C:5:ARG:NH1	4:D:125:GLU:OE2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:101[A]:ARG:NH1	20:E:402:HOH:O	2.44	0.51
10:X:38:MET:HE1	10:X:61:GLN:HB2	1.92	0.51
7:U:195:VAL:HG13	7:U:196:GLU:OE1	2.11	0.50
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.10	0.50
14:b:22:THR:OG1	19:b:306:6VC:C7	2.60	0.49
8:H:204:CYS:SG	12:Z:158:MET:HE2	2.53	0.49
2:P:48:GLU:HB2	2:P:201:MET:HE2	1.94	0.49
14:N:190:LEU:H	14:N:193:GLN:HE21	1.61	0.49
14:b:190:LEU:H	14:b:193:GLN:HE21	1.60	0.49
6:F:182:LYS:HE3	20:F:561:HOH:O	2.12	0.48
10:J:38:MET:HE1	10:J:61:GLN:HB2	1.94	0.48
2:P:246:LYS:HE3	2:P:246:LYS:N	2.28	0.48
13:a:112:ILE:HD12	13:a:112:ILE:N	2.28	0.48
12:Z:172:MET:HE1	12:Z:197:ILE:HD11	1.93	0.48
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.94	0.48
2:P:53:HIS:O	2:P:54:LYS:HB2	2.13	0.48
4:D:195:ILE:O	4:D:199:LEU:HD22	2.13	0.48
11:Y:40:TYR:CD2	11:Y:73:ARG:CZ	2.96	0.48
20:G:464:HOH:O	8:H:72:ARG:HD3	2.13	0.48
8:H:112:SER:HB2	8:H:127[A]:MET:HE2	1.96	0.48
2:P:197:LEU:HD22	2:P:201:MET:HE3	1.95	0.48
3:C:203:GLY:CA	3:C:204:LYS:CB	2.91	0.48
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.91	0.48
6:T:170:GLN:O	6:T:174:THR:HG23	2.14	0.47
11:Y:52:CYS:SG	11:Y:97[A]:MET:HG3	2.54	0.47
8:V:112:SER:HB2	8:V:127[A]:MET:HE2	1.95	0.47
13:a:92:LEU:HD12	13:a:112:ILE:HD11	1.97	0.47
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.44	0.47
13:a:96:MET:HE3	13:a:127:MET:HA	1.97	0.47
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.10	0.47
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.45	0.47
5:E:65:HIS:HB2	20:E:493:HOH:O	2.13	0.47
10:J:177:THR:HG22	10:J:195:SER:HB3	1.95	0.47
3:Q:204:LYS:HA	3:Q:205:ASN:C	2.40	0.47
6:T:24:GLU:HA	6:T:27:MET:HE3	1.95	0.47
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.55	0.47
2:P:201:MET:HE1	2:P:211:VAL:HG12	1.96	0.47
9:W:27:PHE:HB3	9:W:35:THR:HG22	1.97	0.47
6:F:170:GLN:O	6:F:174:THR:HG23	2.15	0.46
3:C:33:VAL:HG21	3:C:195:LEU:HD12	1.97	0.46
11:K:52:CYS:SG	11:K:97:MET:HG3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:112:ILE:HD12	13:M:112:ILE:N	2.30	0.46
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.98	0.46
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.98	0.46
5:S:18[B]:ARG:CG	5:S:23:GLU:OE2	2.64	0.46
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.46	0.46
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.96	0.46
2:B:33:THR:HB	2:B:166:ASN:O	2.15	0.46
3:C:50:VAL:O	3:C:51:ALA:CB	2.64	0.46
7:G:113:MET:HE1	8:H:69:SER:OG	2.15	0.45
5:S:237:GLU:O	5:S:238:GLU:CB	2.64	0.45
12:L:172:MET:HE1	12:L:197:ILE:HD11	1.97	0.45
8:V:213:THR:HB	9:W:198:THR:OG1	2.16	0.45
9:I:27:PHE:HB3	9:I:35:THR:HG22	1.98	0.45
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.98	0.45
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.49	0.45
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.99	0.45
14:b:35:THR:HG21	14:b:45:ARG:HE	1.80	0.45
10:X:95:ARG:HH11	10:X:95:ARG:HB2	1.82	0.45
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.98	0.45
6:T:202:ASP:OD1	6:T:204:VAL:HG12	2.16	0.45
3:C:106:TYR:CD1	3:C:106:TYR:C	2.94	0.45
4:R:32:LYS:HG2	20:R:506:HOH:O	2.16	0.45
11:Y:158:ARG:HE	11:Y:162:GLN:NE2	2.13	0.45
2:B:44:LEU:C	2:B:44:LEU:HD12	2.42	0.45
6:F:34:SER:OG	6:F:65:ARG:NH1	2.49	0.44
11:Y:9:ARG:NH2	11:Y:146:ASP:OD1	2.48	0.44
7:G:72:ILE:HG21	7:G:114:LEU:HD21	2.00	0.44
1:A:180:ASP:OD1	1:A:180:ASP:N	2.50	0.44
5:S:65[B]:HIS:CE1	5:S:223:ILE:HD12	2.53	0.44
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.99	0.44
13:M:184:TYR:OH	14:b:165:GLU:OE2	2.27	0.44
2:P:33:THR:HB	2:P:166:ASN:O	2.17	0.44
4:D:164:GLN:OE1	5:E:58:ALA:HB2	2.17	0.44
8:V:132:LEU:HD22	14:b:25:TYR:CZ	2.52	0.44
1:A:17:LYS:HE2	1:A:22:GLU:OE2	2.18	0.44
7:G:42:VAL:HG13	7:G:198:ALA:HB2	2.00	0.44
9:I:158:ASP:OD1	9:I:161:HIS:HD2	2.00	0.44
1:O:180:ASP:N	1:O:180:ASP:OD1	2.49	0.44
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.47	0.44
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.18	0.44
13:M:96:MET:HE3	13:M:127:MET:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:43[B]:CYS:SG	20:L:401:HOH:O	2.62	0.43
5:S:49:LEU:HG	5:S:195:LEU:HD21	1.99	0.43
3:Q:85:ASN:OD1	10:X:70:ARG:NH2	2.51	0.43
11:Y:68:LEU:O	11:Y:71:LYS:CE	2.66	0.43
7:U:138:MET:HE3	7:U:140:LEU:HD11	2.00	0.43
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.54	0.43
8:H:216:ILE:HD13	9:I:195:THR:HG23	2.00	0.43
11:K:40:TYR:CD2	11:K:73:ARG:CZ	3.01	0.43
11:K:83:LEU:HD21	11:K:99:THR:HG21	2.01	0.43
2:P:44:LEU:C	2:P:44:LEU:HD12	2.44	0.43
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.49	0.43
8:V:97:ALA:HB1	8:V:127[B]:MET:CE	2.49	0.43
8:H:64:GLU:HG2	8:H:68:LEU:HD22	2.01	0.42
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	2.01	0.42
8:V:64:GLU:HG2	8:V:68:LEU:HD22	2.01	0.42
10:J:166:GLU:OE2	11:Y:141[A]:ARG:NH1	2.53	0.42
13:M:27:LEU:HD22	13:M:184:TYR:HB2	2.01	0.42
7:U:42:VAL:HG13	7:U:198:ALA:HB2	2.02	0.42
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.19	0.42
2:B:25[B]:MET:HE3	2:B:25[B]:MET:HB3	1.83	0.42
12:L:184:GLU:OE2	12:L:211:ARG:HD2	2.20	0.42
7:U:43:ARG:HB3	7:U:151:VAL:HG13	2.01	0.42
8:V:114:TYR:CE1	8:V:127[B]:MET:HE3	2.54	0.42
11:Y:40:TYR:CD2	11:Y:73:ARG:NH1	2.87	0.42
8:H:132:LEU:HD22	14:N:25:TYR:CZ	2.55	0.42
11:Y:199:TYR:CA	11:Y:200:SER:CB	2.98	0.42
9:W:13:MET:HE1	9:W:166:ILE:N	2.35	0.42
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.19	0.42
3:Q:50:VAL:O	3:Q:51:ALA:CB	2.68	0.42
6:T:191:LYS:HB3	6:T:238:TYR:CD1	2.55	0.42
3:C:169:ARG:NH2	20:C:404:HOH:O	2.51	0.41
7:U:244:GLU:O	7:U:245:ARG:C	2.63	0.41
12:L:81:LYS:NZ	20:L:406:HOH:O	2.50	0.41
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.46	0.41
6:T:205:LYS:O	6:T:206:ASP:OD1	2.37	0.41
7:U:199:ILE:HD11	7:U:239:LEU:CD2	2.48	0.41
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.50	0.41
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.36	0.41
2:B:48:GLU:HG3	2:B:201:MET:HE3	2.02	0.41
6:T:152:ASP:OD1	6:T:156:VAL:HG12	2.21	0.41
8:H:77:VAL:HB	20:H:539:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:148:LEU:HD23	12:L:178:VAL:HG12	2.03	0.41
9:W:13:MET:HE1	9:W:165:THR:HB	2.01	0.41
5:E:49:LEU:HG	5:E:195:LEU:HD21	2.02	0.41
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.56	0.41
6:F:202:ASP:OD1	6:F:204:VAL:HG22	2.20	0.41
2:B:151:ASP:HB2	2:B:152:PRO:CD	2.51	0.41
5:E:171:TYR:CD2	5:E:171:TYR:C	2.99	0.41
5:S:152[B]:ASN:ND2	20:S:406:HOH:O	2.53	0.41
6:T:34:SER:OG	6:T:65:ARG:NH1	2.51	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.03	0.41
10:J:27[A]:GLN:HE21	10:J:29:LYS:N	2.18	0.41
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.51	0.41
11:Y:144:SER:HB3	11:Y:147:LEU:HD13	2.03	0.40
4:D:203:LYS:HE2	4:D:210:LEU:HB3	2.02	0.40
13:M:5:MET:CE	14:N:116:MET:HB2	2.51	0.40
5:S:234:GLU:HA	5:S:235:GLY:C	2.46	0.40
8:V:114:TYR:CE1	19:b:306:6VC:C3	3.05	0.40
3:C:47:LYS:CB	3:C:48:LYS:C	2.94	0.40
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.02	0.40
11:K:42:LEU:CD2	11:K:179:VAL:HG22	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:241:GLU:OE1	5:S:234:GLU:OE2[1_455]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	231/234 (99%)	221 (96%)	6 (3%)	4 (2%)	7 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	228/234 (97%)	217 (95%)	7 (3%)	4 (2%)	6	3
2	B	248/261 (95%)	238 (96%)	10 (4%)	0	100	100
2	P	248/261 (95%)	233 (94%)	11 (4%)	4 (2%)	7	3
3	C	236/248 (95%)	223 (94%)	7 (3%)	6 (2%)	4	1
3	Q	236/248 (95%)	221 (94%)	7 (3%)	8 (3%)	3	1
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	9	5
4	R	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	9	5
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	30	27
5	S	238/263 (90%)	231 (97%)	5 (2%)	2 (1%)	16	11
6	F	241/255 (94%)	239 (99%)	2 (1%)	0	100	100
6	T	239/255 (94%)	233 (98%)	3 (1%)	3 (1%)	9	5
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	3 (1%)	2 (1%)	14	9
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	216 (98%)	4 (2%)	0	100	100
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	5 (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%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
13	a	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
14	N	201/205 (98%)	198 (98%)	2 (1%)	1 (0%)	24	21
14	b	202/205 (98%)	198 (98%)	3 (2%)	1 (0%)	24	21
All	All	6212/6458 (96%)	6040 (97%)	129 (2%)	43 (1%)	18	14

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS

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Mol	Chain	Res	Type
3	C	204	LYS
4	D	176	GLY
1	O	52	LYS
2	P	54	LYS
3	Q	206	ILE
3	Q	221	ASN
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
11	Y	200	SER
1	A	53	SER
3	C	50	VAL
4	D	175[A]	GLU
4	D	175[B]	GLU
5	E	59	HIS
14	N	198	ALA
1	O	53	SER
1	O	231	ALA
3	Q	47	LYS
3	Q	50	VAL
3	Q	201	SER
3	Q	203	GLY
5	S	236	LEU
6	T	7	TYR
1	A	176	ARG
3	C	51	ALA
3	C	200	GLN
3	C	216	SER
1	O	176	ARG
3	Q	51	ALA
3	Q	216	SER
7	U	58	ASP
7	U	59	LYS
14	b	198	ALA
1	A	50	LYS
2	P	58	GLU
2	P	204	SER
6	T	208	ALA
3	C	203	GLY
2	P	52	ILE
6	T	6	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%)	174 (94%)	11 (6%)	18	14
1	O	176/191 (92%)	166 (94%)	10 (6%)	18	15
2	B	199/221 (90%)	191 (96%)	8 (4%)	28	27
2	P	197/221 (89%)	184 (93%)	13 (7%)	15	12
3	C	179/210 (85%)	171 (96%)	8 (4%)	24	23
3	Q	184/210 (88%)	174 (95%)	10 (5%)	20	17
4	D	189/203 (93%)	183 (97%)	6 (3%)	34	35
4	R	187/203 (92%)	184 (98%)	3 (2%)	55	62
5	E	192/223 (86%)	185 (96%)	7 (4%)	31	31
5	S	197/223 (88%)	193 (98%)	4 (2%)	48	54
6	F	199/212 (94%)	189 (95%)	10 (5%)	22	20
6	T	192/212 (91%)	182 (95%)	10 (5%)	21	18
7	G	202/207 (98%)	194 (96%)	8 (4%)	28	27
7	U	186/207 (90%)	181 (97%)	5 (3%)	39	42
8	H	181/195 (93%)	174 (96%)	7 (4%)	28	28
8	V	172/195 (88%)	164 (95%)	8 (5%)	23	22
9	I	176/174 (101%)	174 (99%)	2 (1%)	65	73
9	W	173/174 (99%)	171 (99%)	2 (1%)	63	70
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%)	147 (96%)	7 (4%)	24	23
11	Y	159/159 (100%)	153 (96%)	6 (4%)	29	29
12	L	175/178 (98%)	170 (97%)	5 (3%)	37	40
12	Z	175/178 (98%)	171 (98%)	4 (2%)	44	49
13	M	180/181 (99%)	176 (98%)	4 (2%)	45	50
13	a	178/181 (98%)	173 (97%)	5 (3%)	38	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	158/159 (99%)	156 (99%)	2 (1%)	61	68
14	b	158/159 (99%)	154 (98%)	4 (2%)	42	45
All	All	5034/5366 (94%)	4852 (96%)	182 (4%)	32	31

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	VAL
1	A	69	LYS
1	A	73	LEU
1	A	131	VAL
1	A	180	ASP
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP
2	B	33	THR
2	B	43	VAL
2	B	59	VAL
2	B	190	LEU
2	B	207	SER
2	B	229	LYS
2	B	238	LYS
2	B	249	ARG
3	C	2	SER
3	C	35	VAL
3	C	45	VAL
3	C	148	ASP
3	C	163	ARG
3	C	205	ASN
3	C	208	LEU
3	C	225	ILE
4	D	9	ASP
4	D	46	VAL
4	D	95	GLU
4	D	126	GLU
4	D	199	LEU
4	D	208	GLU
5	E	29	VAL

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Mol	Chain	Res	Type
5	E	61	LYS
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	181	GLU
5	E	189	LYS
5	E	202	GLU
6	F	17	ASP
6	F	31	GLU
6	F	53	VAL
6	F	81	LEU
6	F	87	LEU
6	F	174	THR
6	F	187	ARG
6	F	190	VAL
6	F	240	LYS
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
7	G	226	LYS
7	G	232	GLU
8	H	6	VAL
8	H	22	GLU
8	H	65	LEU
8	H	68	LEU
8	H	132	LEU
8	H	183	LEU
8	H	220	GLU
9	I	35	THR
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	27[A]	GLN
10	J	27[B]	GLN
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	155	ARG
11	K	12	VAL

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Mol	Chain	Res	Type
11	K	138	VAL
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	VAL
11	K	192	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	174	LEU
12	L	207	THR
12	L	212	LYS
13	M	154	LEU
13	M	156	LYS
13	M	198	GLU
13	M	216	SER
14	N	22	THR
14	N	35	THR
1	O	10	THR
1	O	73	LEU
1	O	131	VAL
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	54	LYS
2	P	59	VAL
2	P	190	LEU
2	P	204	SER
2	P	207	SER
2	P	235	GLN
2	P	236	LEU
2	P	246	LYS
2	P	249	ARG
3	Q	2	SER
3	Q	45	VAL

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Mol	Chain	Res	Type
3	Q	56	GLU
3	Q	98	VAL
3	Q	148	ASP
3	Q	163	ARG
3	Q	170	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	227	LYS
4	R	9	ASP
4	R	46	VAL
4	R	117	SER
5	S	29	VAL
5	S	45	VAL
5	S	101	ARG
5	S	202	GLU
6	T	17	ASP
6	T	31	GLU
6	T	53	VAL
6	T	81	LEU
6	T	87	LEU
6	T	174	THR
6	T	190	VAL
6	T	223	ARG
6	T	240	LYS
6	T	241	GLU
7	U	42	VAL
7	U	78	CYS
7	U	151	VAL
7	U	199	ILE
7	U	206	LEU
8	V	6	VAL
8	V	22	GLU
8	V	65	LEU
8	V	68	LEU
8	V	132	LEU
8	V	183	LEU
8	V	199	LEU
8	V	213	THR
9	W	35	THR
9	W	69	ARG
10	X	1	MET
10	X	62	LYS

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Mol	Chain	Res	Type
10	X	88	LEU
10	X	95	ARG
10	X	158	GLU
11	Y	12	VAL
11	Y	41	LEU
11	Y	81	LYS
11	Y	138	VAL
11	Y	147	LEU
11	Y	192	VAL
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
12	Z	212	LYS
13	a	71	VAL
13	a	92	LEU
13	a	154	LEU
13	a	198	GLU
13	a	216	SER
14	b	22	THR
14	b	29	ARG
14	b	35	THR
14	b	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	62	HIS
1	A	94	GLN
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
2	B	100	GLN
2	B	102	GLN
3	C	175	ASN
4	D	227	HIS
5	E	16	GLN
5	E	65	HIS
5	E	175	HIS
5	E	185	ASN
6	F	143	ASN
7	G	68	HIS

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Mol	Chain	Res	Type
7	G	193	GLN
8	H	80	ASN
8	H	116	HIS
8	H	153	ASN
8	H	172	ASN
9	I	161	HIS
10	J	63	ASN
10	J	101	ASN
11	K	62	GLN
11	K	162	GLN
12	L	157	ASN
13	M	65	GLN
13	M	162	GLN
13	M	208	ASN
14	N	193	GLN
1	O	101	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
3	Q	18	GLN
3	Q	94	HIS
3	Q	175	ASN
4	R	97	GLN
4	R	152	GLN
4	R	186	HIS
4	R	227	HIS
5	S	8	ASN
5	S	86	ASN
5	S	175	HIS
6	T	63	ASN
6	T	68	ASN
6	T	110	HIS
6	T	143	ASN
8	V	80	ASN
8	V	172	ASN
9	W	172	ASN
10	X	24	ASN
10	X	63	ASN
10	X	174	ASN

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Mol	Chain	Res	Type
11	Y	62	GLN
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	U	161	7	13,15,16	1.91	4 (30%)	10,20,22	2.77	4 (40%)
5	6V1	S	148	5	13,15,16	1.74	4 (30%)	10,20,22	3.00	6 (60%)
7	6V1	G	161	7	13,15,16	1.61	4 (30%)	10,20,22	2.44	4 (40%)
5	6V1	E	148	5	13,15,16	1.82	3 (23%)	10,20,22	3.73	4 (40%)
3	YCM	C	63	3	7,9,10	1.01	0	5,10,12	1.36	1 (20%)
7	YCM	U	137	7	7,9,10	0.99	0	5,10,12	1.13	0
7	6V1	U	47	7	13,15,16	1.93	3 (23%)	10,20,22	1.89	3 (30%)
10	6V1	X	91	10	13,15,16	1.73	3 (23%)	10,20,22	5.52	7 (70%)
7	YCM	G	137	7	7,9,10	1.79	3 (42%)	5,10,12	2.16	1 (20%)
10	6V1	J	91	10	13,15,16	1.76	3 (23%)	10,20,22	5.53	7 (70%)
3	YCM	Q	63	3	7,9,10	1.32	1 (14%)	5,10,12	3.04	4 (80%)
7	6V1	G	47	7	13,15,16	2.26	4 (30%)	10,20,22	2.13	2 (20%)

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	47	6V1	CB-SG	-5.93	1.76	1.82
7	U	47	6V1	CB-SG	-5.26	1.76	1.82
10	J	91	6V1	C1-SG	-5.16	1.77	1.83
10	X	91	6V1	C1-SG	-4.68	1.78	1.83
5	E	148	6V1	CB-SG	-4.45	1.77	1.82
7	U	161	6V1	CB-SG	-3.96	1.78	1.82
5	S	148	6V1	CB-SG	-3.71	1.78	1.82
7	G	47	6V1	C2-N3	-3.51	1.33	1.38
7	U	161	6V1	C4-N3	-3.32	1.33	1.38
5	S	148	6V1	C2-N3	-3.31	1.34	1.38
7	G	47	6V1	C4-N3	-3.31	1.33	1.38
7	U	161	6V1	C2-N3	-3.25	1.34	1.38
7	G	161	6V1	CB-SG	-3.17	1.78	1.82
7	G	161	6V1	C2-N3	-3.13	1.34	1.38
7	G	137	YCM	CE-NZ2	3.08	1.42	1.32
5	E	148	6V1	C4-N3	-3.00	1.34	1.38
3	Q	63	YCM	CD-SG	-2.83	1.74	1.81
10	X	91	6V1	O7-C2	2.61	1.27	1.22
5	E	148	6V1	C2-N3	-2.53	1.35	1.38
7	U	161	6V1	C1-SG	-2.51	1.80	1.83
7	U	47	6V1	C1-C2	2.51	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CD-SG	2.50	1.87	1.81
10	X	91	6V1	C4-N3	-2.47	1.34	1.38
5	S	148	6V1	C5-C4	2.35	1.54	1.50
7	G	137	YCM	CB-SG	-2.23	1.72	1.81
7	U	47	6V1	C4-N3	-2.20	1.35	1.38
7	G	161	6V1	C4-N3	-2.18	1.35	1.38
5	S	148	6V1	C4-N3	-2.14	1.35	1.38
10	J	91	6V1	O7-C2	2.14	1.26	1.22
10	J	91	6V1	C4-N3	-2.10	1.35	1.38
7	G	161	6V1	C1-SG	-2.07	1.81	1.83
7	G	47	6V1	C5-C4	2.05	1.54	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	91	6V1	C5-C4-N3	9.13	113.82	108.07
10	X	91	6V1	C6-N3-C2	8.54	133.38	123.37
10	J	91	6V1	C6-N3-C2	8.46	133.28	123.37
10	X	91	6V1	O7-C2-N3	8.10	133.96	124.14
10	X	91	6V1	C5-C4-N3	7.77	112.96	108.07
5	E	148	6V1	C2-N3-C4	-7.62	108.61	113.07
10	J	91	6V1	O7-C2-N3	7.41	133.13	124.14
10	J	91	6V1	C2-N3-C4	-7.06	108.94	113.07
5	E	148	6V1	C5-C4-N3	6.61	112.23	108.07
10	X	91	6V1	C2-N3-C4	-6.41	109.32	113.07
7	U	161	6V1	C2-N3-C4	-6.10	109.50	113.07
7	G	47	6V1	C2-N3-C4	-5.66	109.76	113.07
5	S	148	6V1	C5-C4-N3	5.66	111.63	108.07
5	S	148	6V1	C2-N3-C4	-5.63	109.77	113.07
10	X	91	6V1	C6-N3-C4	-5.36	116.19	122.52
5	E	148	6V1	C6-N3-C2	5.06	129.29	123.37
10	J	91	6V1	C6-N3-C4	-4.70	116.96	122.52
3	Q	63	YCM	CE-CD-SG	-4.59	99.31	113.81
7	U	161	6V1	C5-C4-N3	4.16	110.69	108.07
10	X	91	6V1	O8-C4-C5	-4.02	121.40	127.28
10	X	91	6V1	O7-C2-C1	-3.98	115.84	124.52
7	G	161	6V1	C2-N3-C4	-3.96	110.75	113.07
7	G	161	6V1	O8-C4-N3	3.93	128.15	123.94
7	G	137	YCM	CE-CD-SG	3.92	126.20	113.81
7	G	161	6V1	O8-C4-C5	-3.65	121.94	127.28
7	U	47	6V1	C5-C4-N3	3.55	110.31	108.07
10	J	91	6V1	O8-C4-C5	-3.25	122.53	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	91	6V1	O7-C2-C1	-3.20	117.55	124.52
7	U	47	6V1	C2-N3-C4	-3.19	111.20	113.07
3	Q	63	YCM	CA-CB-SG	-3.11	102.06	113.51
5	S	148	6V1	C6-N3-C4	3.02	126.09	122.52
7	U	161	6V1	O8-C4-C5	-3.02	122.86	127.28
7	G	161	6V1	C5-C4-N3	2.85	109.86	108.07
3	Q	63	YCM	CB-CA-C	-2.84	103.08	110.80
3	C	63	YCM	CB-CA-C	-2.71	103.44	110.80
3	Q	63	YCM	CB-SG-CD	2.53	126.85	104.24
5	S	148	6V1	O8-C4-C5	-2.45	123.69	127.28
7	U	161	6V1	O8-C4-N3	2.34	126.44	123.94
5	S	148	6V1	O7-C2-N3	-2.32	121.33	124.14
5	S	148	6V1	CB-CA-C	-2.24	104.72	110.80
7	G	47	6V1	C6-N3-C4	2.24	125.17	122.52
5	E	148	6V1	CB-CA-C	-2.16	104.94	110.80
7	U	47	6V1	O8-C4-C5	-2.13	124.16	127.28

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (18) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
7	U	47	6V1	C3-C6-N3-C4

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 87 ligands modelled in this entry, 72 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	6VC	V	304	8	27,27,27	1.04	2 (7%)	34,36,36	1.33	5 (14%)
18	1PE	N	305	-	15,15,15	0.54	0	14,14,14	0.53	0
18	1PE	U	302	-	15,15,15	0.62	0	14,14,14	0.96	1 (7%)
19	6VC	Y	307	11	27,27,27	1.28	4 (14%)	34,36,36	1.24	4 (11%)
18	1PE	M	304	-	15,15,15	0.63	0	14,14,14	0.35	0
18	1PE	H	304	-	15,15,15	0.60	0	14,14,14	0.58	0
18	1PE	a	304	-	15,15,15	0.70	0	14,14,14	0.46	0
19	6VC	H	305	8	27,27,27	1.02	2 (7%)	34,36,36	1.38	5 (14%)
19	6VC	N	307	14	27,27,27	1.19	1 (3%)	34,36,36	1.58	5 (14%)
18	1PE	Z	301	-	15,15,15	0.62	0	14,14,14	0.53	0
18	1PE	L	301	-	15,15,15	0.62	0	14,14,14	0.64	0
19	6VC	b	306	14	27,27,27	1.22	4 (14%)	34,36,36	1.93	10 (29%)
18	1PE	W	303	-	15,15,15	0.57	0	14,14,14	0.35	0
19	6VC	K	306	11	27,27,27	0.67	0	34,36,36	1.38	7 (20%)
18	1PE	I	303	-	15,15,15	0.57	0	14,14,14	0.84	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	6VC	V	304	8	-	5/38/38/38	-
18	1PE	N	305	-	-	4/13/13/13	-
18	1PE	U	302	-	-	8/13/13/13	-
19	6VC	Y	307	11	-	4/38/38/38	-
18	1PE	M	304	-	-	8/13/13/13	-
18	1PE	H	304	-	-	10/13/13/13	-
18	1PE	a	304	-	-	7/13/13/13	-
19	6VC	H	305	8	-	5/38/38/38	-
19	6VC	N	307	14	-	2/38/38/38	-
18	1PE	Z	301	-	-	8/13/13/13	-
18	1PE	L	301	-	-	7/13/13/13	-
19	6VC	b	306	14	-	5/38/38/38	-
18	1PE	W	303	-	-	7/13/13/13	-
19	6VC	K	306	11	-	5/38/38/38	-
18	1PE	I	303	-	-	6/13/13/13	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	307	6VC	C22-C21	4.53	1.60	1.55
19	Y	307	6VC	C22-C21	4.51	1.60	1.55
19	H	305	6VC	C23-C22	3.51	1.58	1.52
19	V	304	6VC	C22-C21	3.36	1.58	1.55
19	b	306	6VC	C22-C21	3.30	1.58	1.55
19	b	306	6VC	C23-C22	3.20	1.57	1.52
19	Y	307	6VC	C13-N3	-2.49	1.42	1.46
19	b	306	6VC	C14-C13	2.28	1.56	1.53
19	b	306	6VC	C9-C12	-2.24	1.47	1.52
19	H	305	6VC	C22-C21	2.19	1.57	1.55
19	V	304	6VC	C23-C22	2.17	1.56	1.52
19	Y	307	6VC	C9-C12	-2.14	1.47	1.52
19	Y	307	6VC	O4-C12	-2.08	1.19	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	307	6VC	C10-C9-N2	-5.34	97.52	110.78
19	b	306	6VC	O3-C10-C9	-4.79	98.18	111.18
19	b	306	6VC	C1-C6-C5	-4.64	96.06	113.13
19	b	306	6VC	O2-C8-C5	-3.90	114.95	122.02
19	N	307	6VC	C10-C9-C12	3.63	119.30	110.12
19	H	305	6VC	O3-C10-C9	-3.58	101.47	111.18
19	b	306	6VC	O4-C12-N3	3.36	128.97	122.96
19	H	305	6VC	O2-C8-C5	-3.20	116.23	122.02
19	K	306	6VC	O3-C10-C9	-3.12	102.72	111.18
19	b	306	6VC	C10-C9-C12	-3.11	102.26	110.12
19	N	307	6VC	C23-C22-C21	2.89	114.92	110.04
18	U	302	1PE	C26-OH6-C15	2.88	125.86	113.26
19	b	306	6VC	O2-C8-N2	2.86	127.80	122.95
19	Y	307	6VC	O3-C10-C9	-2.81	103.55	111.18
19	Y	307	6VC	C10-C9-C12	-2.77	103.11	110.12
19	V	304	6VC	O3-C10-C9	-2.69	103.87	111.18
19	K	306	6VC	C23-C22-C21	2.62	114.47	110.04
19	V	304	6VC	C10-C9-C12	-2.60	103.54	110.12
19	K	306	6VC	C10-C9-C12	-2.56	103.65	110.12
19	K	306	6VC	C6-C5-C8	-2.56	106.10	113.19
19	b	306	6VC	C10-C9-N2	2.54	117.08	110.78
19	Y	307	6VC	O2-C8-C5	-2.47	117.55	122.02
19	Y	307	6VC	C5-C8-N2	2.42	120.14	115.86
19	H	305	6VC	C10-C9-C12	-2.41	104.03	110.12
19	H	305	6VC	O4-C12-N3	2.41	127.27	122.96
19	N	307	6VC	O3-C10-C9	-2.39	104.68	111.18
19	V	304	6VC	O2-C8-C5	-2.32	117.83	122.02
19	K	306	6VC	O2-C8-C5	-2.30	117.86	122.02
19	b	306	6VC	C23-C22-C21	2.28	113.89	110.04
19	V	304	6VC	C10-C9-N2	2.26	116.39	110.78
19	H	305	6VC	C10-C9-N2	2.24	116.34	110.78
19	b	306	6VC	C6-C1-C2	2.23	122.04	113.62
19	b	306	6VC	C9-C12-N3	-2.23	111.88	116.63
19	K	306	6VC	C5-C8-N2	2.22	119.78	115.86
19	K	306	6VC	C1-C6-C5	2.22	121.27	113.13
19	V	304	6VC	C20-C15-C14	2.07	118.52	111.08
19	N	307	6VC	O2-C8-C5	-2.05	118.31	122.02

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	b	306	6VC	O3-C10-C9-N2

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Mol	Chain	Res	Type	Atoms
18	U	302	1PE	C25-C15-OH6-C26
18	L	301	1PE	C16-C26-OH6-C15
18	U	302	1PE	OH4-C13-C23-OH3
18	a	304	1PE	OH4-C13-C23-OH3
18	I	303	1PE	C15-C25-OH5-C14
18	Z	301	1PE	OH6-C15-C25-OH5
18	Z	301	1PE	C16-C26-OH6-C15
18	L	301	1PE	OH5-C14-C24-OH4
18	a	304	1PE	OH5-C14-C24-OH4
18	H	304	1PE	C24-C14-OH5-C25
19	V	304	6VC	C6-C1-C2-C3
18	H	304	1PE	OH4-C13-C23-OH3
18	L	301	1PE	OH6-C15-C25-OH5
18	a	304	1PE	OH2-C12-C22-OH3
18	M	304	1PE	OH5-C14-C24-OH4
19	N	307	6VC	C2-C1-C6-C5
18	I	303	1PE	OH6-C15-C25-OH5
18	M	304	1PE	OH4-C13-C23-OH3
18	H	304	1PE	OH7-C16-C26-OH6
18	N	305	1PE	OH2-C12-C22-OH3
18	a	304	1PE	OH7-C16-C26-OH6
19	Y	307	6VC	C6-C1-C2-C3
18	W	303	1PE	OH6-C15-C25-OH5
18	Z	301	1PE	OH2-C12-C22-OH3
18	N	305	1PE	OH4-C13-C23-OH3
19	V	304	6VC	C1-C2-C3-C7
19	H	305	6VC	C1-C2-C3-C7
18	W	303	1PE	OH7-C16-C26-OH6
19	V	304	6VC	C2-C1-C6-C5
18	N	305	1PE	OH7-C16-C26-OH6
18	M	304	1PE	OH6-C15-C25-OH5
19	H	305	6VC	C1-C2-C3-C4
19	b	306	6VC	C6-C1-C2-C3
18	L	301	1PE	OH2-C12-C22-OH3
19	K	306	6VC	C1-C2-C3-C4
19	K	306	6VC	C2-C1-C6-C5
19	H	305	6VC	C6-C1-C2-C3
19	Y	307	6VC	C2-C1-C6-C5
19	H	305	6VC	C2-C1-C6-C5
18	I	303	1PE	OH4-C13-C23-OH3
19	b	306	6VC	O3-C10-C9-C12
19	K	306	6VC	C1-C2-C3-C7

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Mol	Chain	Res	Type	Atoms
19	V	304	6VC	C1-C2-C3-C4
18	L	301	1PE	C25-C15-OH6-C26
19	b	306	6VC	C2-C1-C6-C5
18	H	304	1PE	C12-C22-OH3-C23
18	M	304	1PE	C15-C25-OH5-C14
18	U	302	1PE	C16-C26-OH6-C15
18	L	301	1PE	C13-C23-OH3-C22
18	I	303	1PE	C24-C14-OH5-C25
18	M	304	1PE	C23-C13-OH4-C24
18	H	304	1PE	OH2-C12-C22-OH3
18	I	303	1PE	OH2-C12-C22-OH3
19	Y	307	6VC	C6-C5-C8-O2
18	H	304	1PE	C16-C26-OH6-C15
18	W	303	1PE	C12-C22-OH3-C23
18	a	304	1PE	C23-C13-OH4-C24
19	N	307	6VC	O5-C21-C22-C24
19	b	306	6VC	O5-C21-C22-C24
18	H	304	1PE	C23-C13-OH4-C24
18	a	304	1PE	C16-C26-OH6-C15
18	U	302	1PE	C24-C14-OH5-C25
18	M	304	1PE	C14-C24-OH4-C13
19	H	305	6VC	O3-C10-C9-N2
19	V	304	6VC	O3-C10-C9-N2
18	Z	301	1PE	C12-C22-OH3-C23
18	W	303	1PE	C13-C23-OH3-C22
18	Z	301	1PE	C15-C25-OH5-C14
18	a	304	1PE	OH6-C15-C25-OH5
18	U	302	1PE	OH6-C15-C25-OH5
18	N	305	1PE	C12-C22-OH3-C23
18	M	304	1PE	OH2-C12-C22-OH3
18	Z	301	1PE	OH5-C14-C24-OH4
18	U	302	1PE	OH5-C14-C24-OH4
18	H	304	1PE	OH6-C15-C25-OH5
18	Z	301	1PE	C13-C23-OH3-C22
19	Y	307	6VC	C6-C5-C8-N2
19	K	306	6VC	C6-C5-C8-O2
18	Z	301	1PE	OH4-C13-C23-OH3
18	W	303	1PE	C14-C24-OH4-C13
18	H	304	1PE	C13-C23-OH3-C22
18	W	303	1PE	C23-C13-OH4-C24
18	H	304	1PE	OH5-C14-C24-OH4
18	M	304	1PE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
19	K	306	6VC	C6-C5-C8-N2
18	I	303	1PE	OH5-C14-C24-OH4
18	W	303	1PE	C24-C14-OH5-C25
18	U	302	1PE	OH2-C12-C22-OH3
18	U	302	1PE	C14-C24-OH4-C13
18	L	301	1PE	C14-C24-OH4-C13

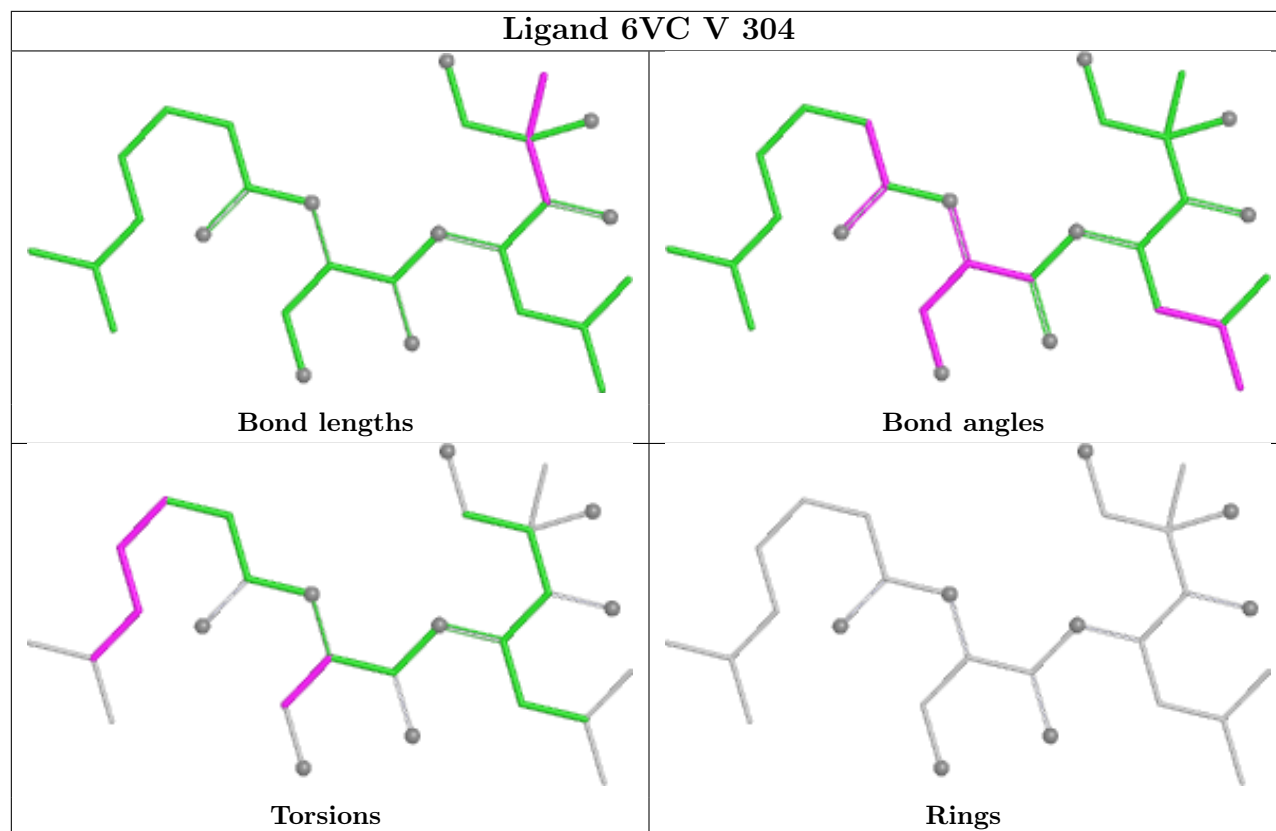
There are no ring outliers.

1 monomer is involved in 2 short contacts:

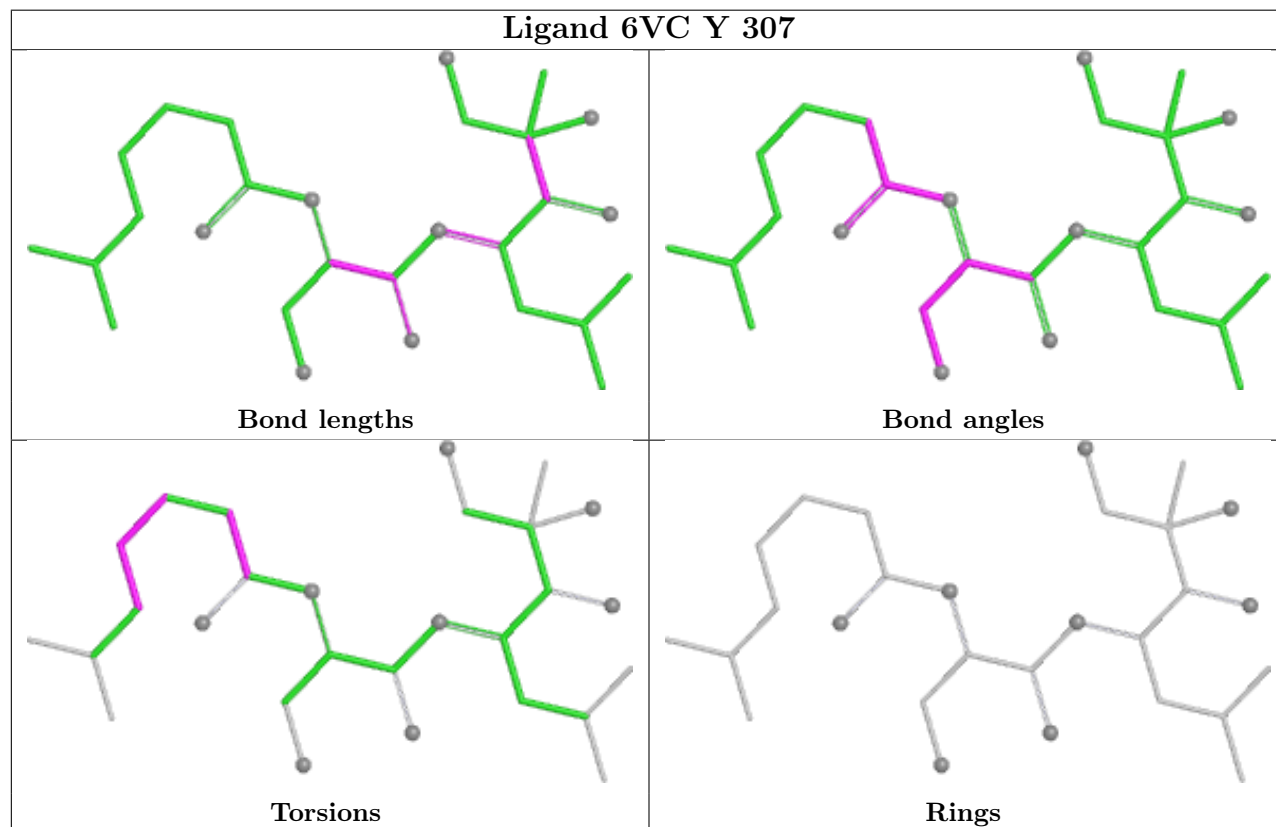
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	306	6VC	2	0

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.

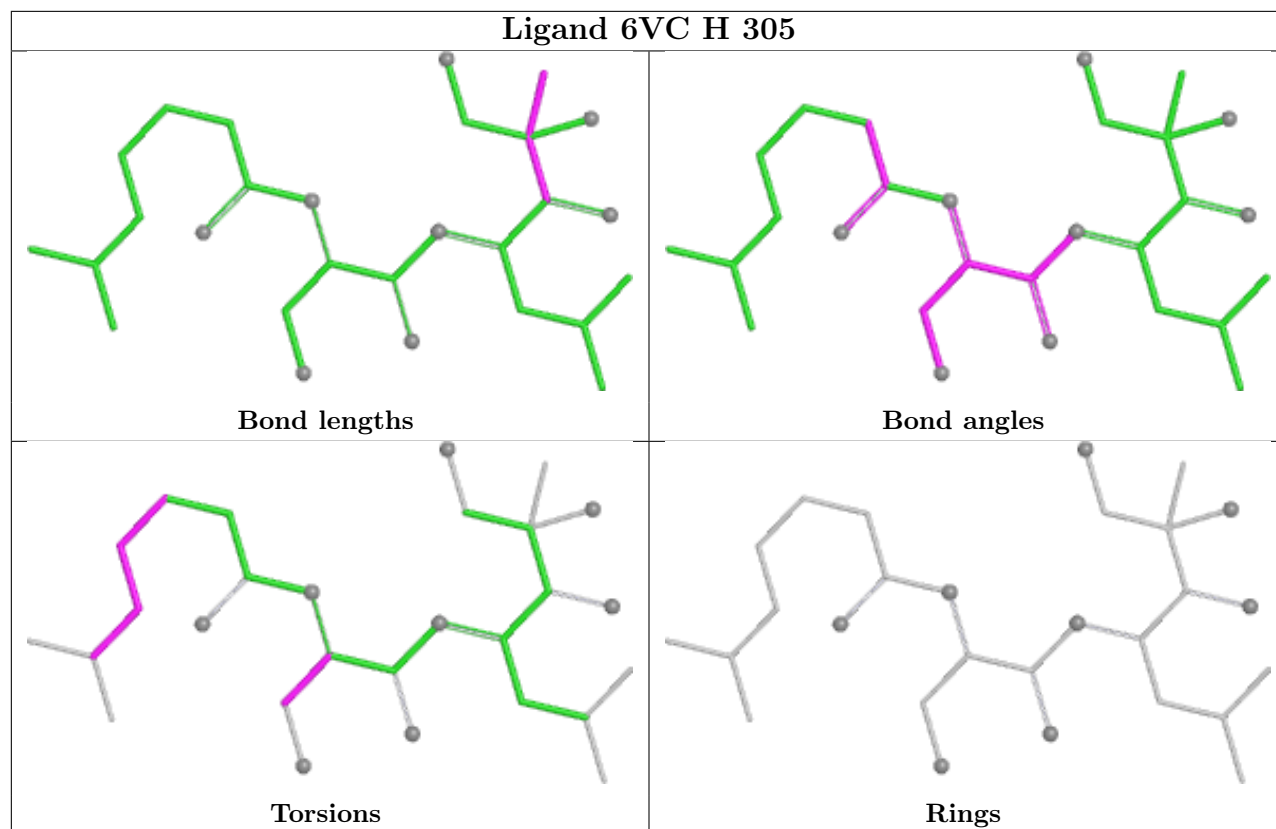
Ligand 6VC V 304



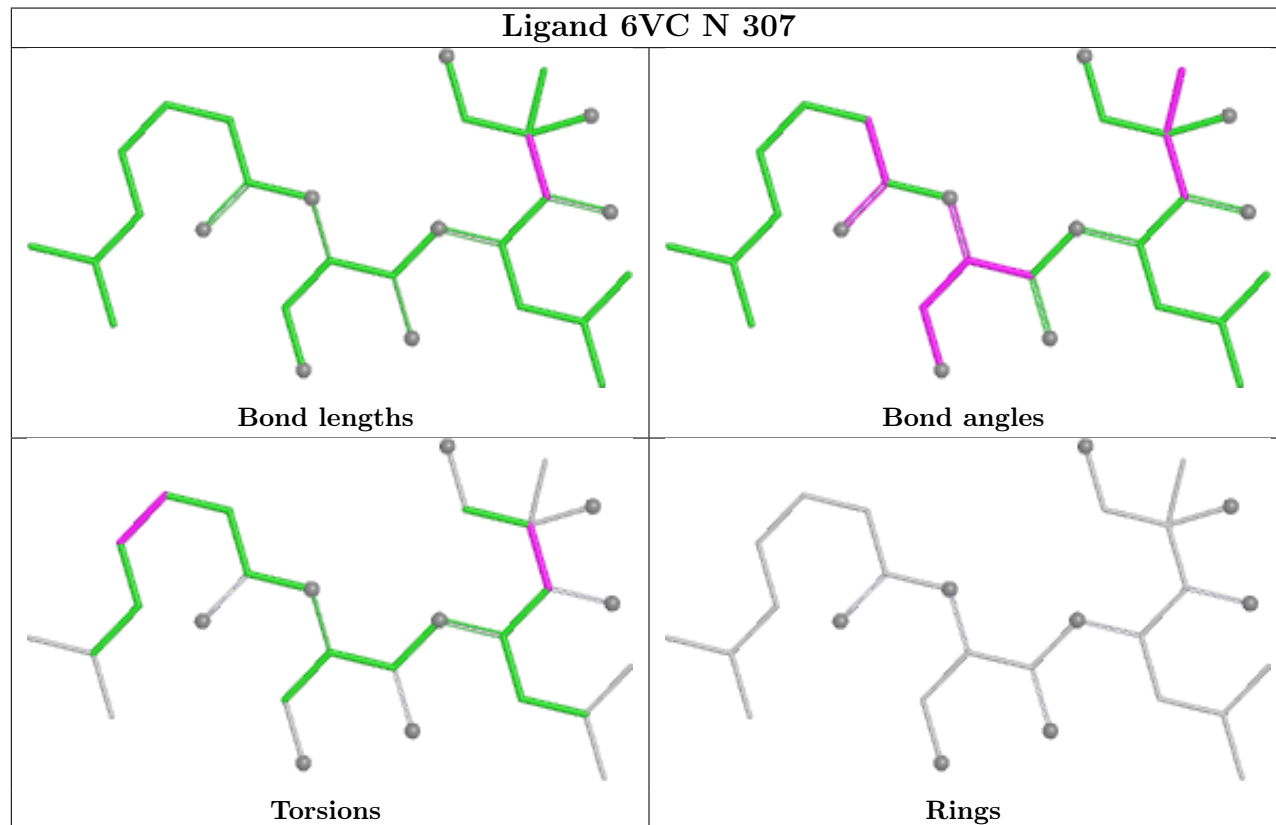
Ligand 6VC Y 307

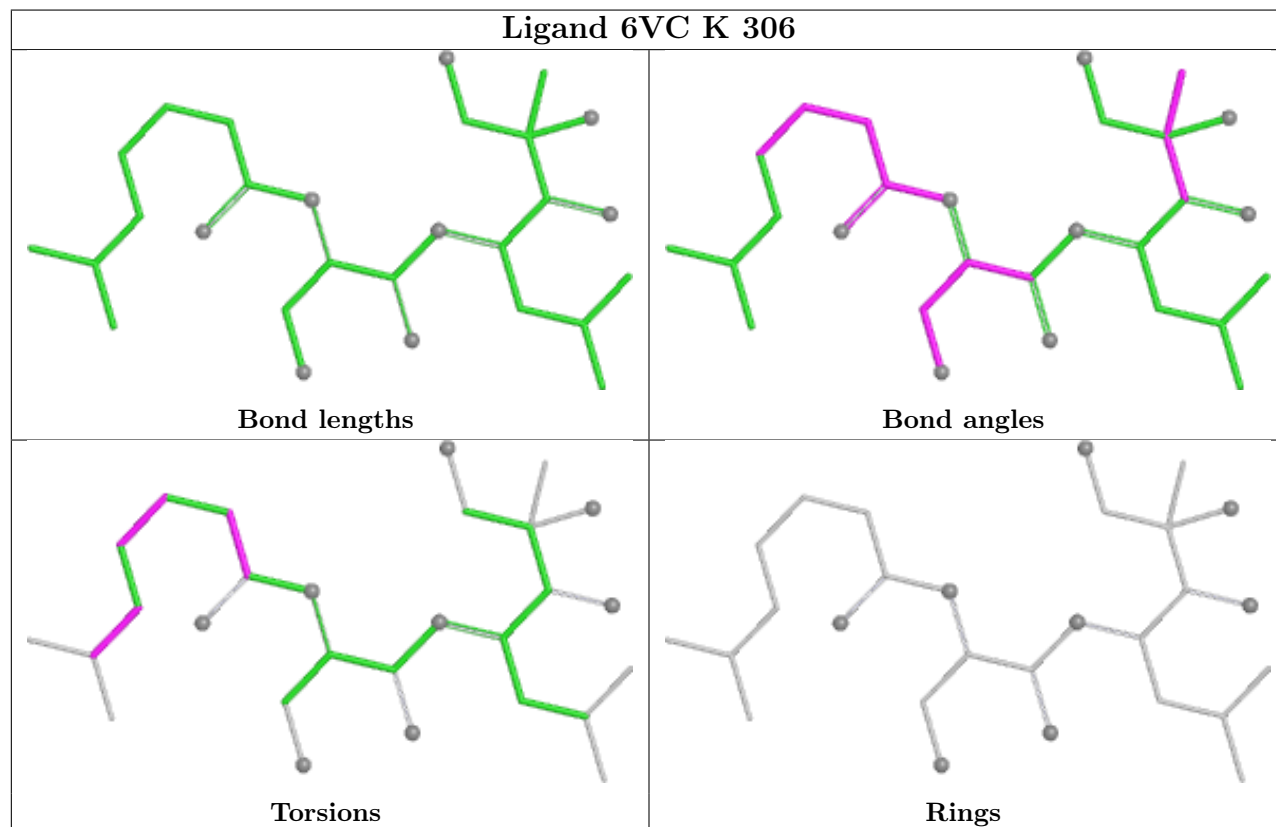
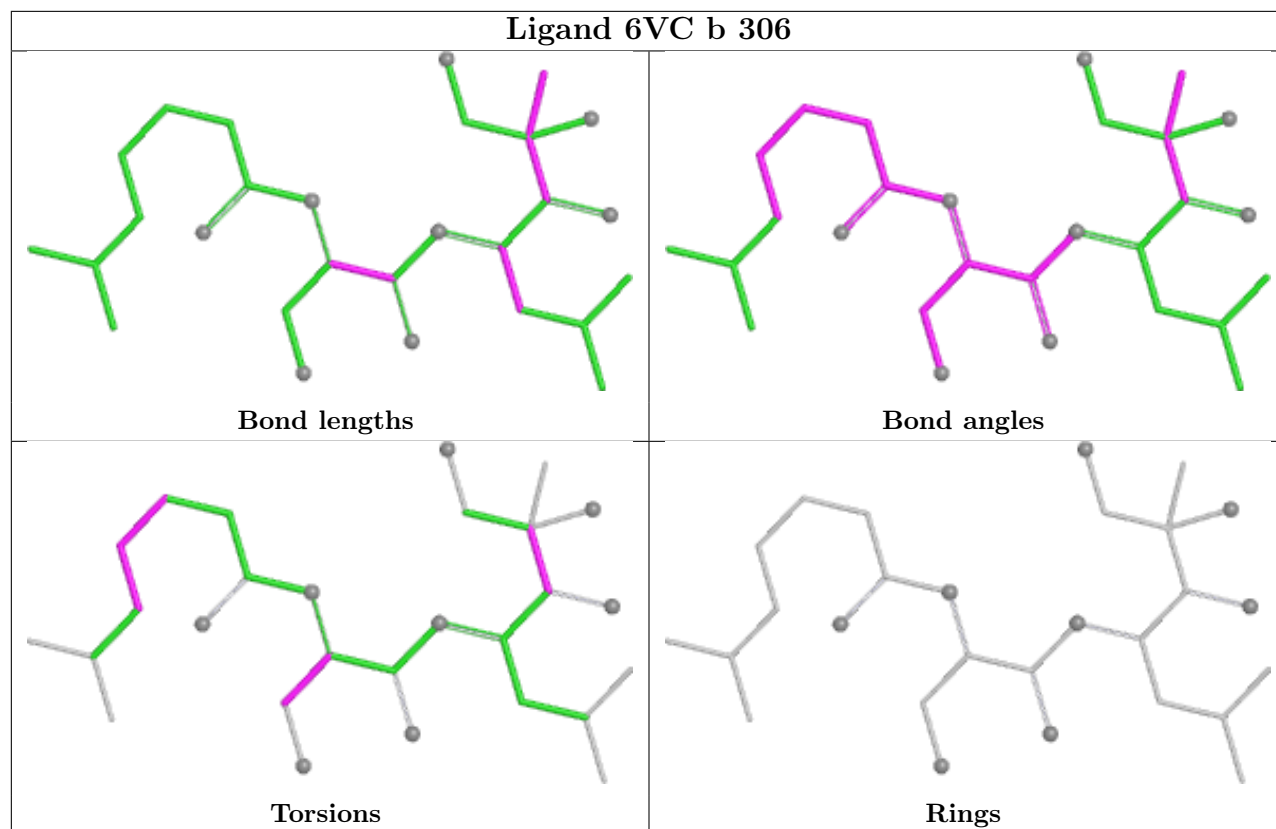


Ligand 6VC H 305



Ligand 6VC N 307





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%)	-0.05	5 (2%) 62 61	24, 46, 82, 92	3 (1%)
1	O	230/234 (98%)	0.43	7 (3%) 52 51	41, 63, 100, 120	0
2	B	248/261 (95%)	0.12	6 (2%) 59 59	21, 52, 89, 136	2 (0%)
2	P	248/261 (95%)	0.34	9 (3%) 46 45	32, 61, 106, 142	2 (0%)
3	C	236/248 (95%)	0.45	7 (2%) 52 51	27, 60, 100, 139	2 (0%)
3	Q	238/248 (95%)	0.42	10 (4%) 40 39	34, 61, 112, 149	0
4	D	233/241 (96%)	0.34	2 (0%) 81 80	31, 58, 88, 114	1 (0%)
4	R	233/241 (96%)	0.04	6 (2%) 57 56	20, 44, 71, 93	1 (0%)
5	E	233/263 (88%)	-0.00	10 (4%) 40 39	25, 43, 86, 100	1 (0%)
5	S	237/263 (90%)	0.09	9 (3%) 44 43	23, 47, 81, 104	3 (1%)
6	F	239/255 (93%)	-0.26	2 (0%) 82 82	20, 36, 58, 74	4 (1%)
6	T	240/255 (94%)	0.27	8 (3%) 49 48	28, 52, 85, 107	1 (0%)
7	G	241/246 (97%)	-0.16	5 (2%) 63 63	19, 40, 73, 101	2 (0%)
7	U	235/246 (95%)	0.33	4 (1%) 69 68	29, 60, 95, 124	1 (0%)
8	H	220/234 (94%)	-0.22	2 (0%) 81 80	21, 36, 66, 100	2 (0%)
8	V	220/234 (94%)	0.09	7 (3%) 50 49	25, 48, 84, 97	2 (0%)
9	I	204/205 (99%)	-0.34	1 (0%) 87 87	22, 37, 58, 74	3 (1%)
9	W	204/205 (99%)	-0.01	1 (0%) 87 87	29, 50, 73, 81	2 (0%)
10	J	195/201 (97%)	-0.22	1 (0%) 87 87	17, 42, 60, 76	3 (1%)
10	X	195/201 (97%)	-0.15	0 100 100	21, 44, 59, 74	2 (1%)
11	K	200/204 (98%)	-0.12	1 (0%) 87 87	36, 46, 71, 84	0
11	Y	201/204 (98%)	-0.31	3 (1%) 72 71	21, 37, 59, 70	3 (1%)
12	L	213/213 (100%)	0.00	1 (0%) 87 87	25, 49, 71, 85	2 (0%)
12	Z	213/213 (100%)	-0.24	0 100 100	26, 38, 60, 74	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.28	1 (0%)	87 87	27, 39, 62, 95	1 (0%)
13	a	216/219 (98%)	-0.27	2 (0%)	81 80	25, 39, 60, 82	2 (0%)
14	N	202/205 (98%)	-0.37	4 (1%)	65 64	22, 35, 56, 94	1 (0%)
14	b	203/205 (99%)	-0.19	4 (1%)	65 64	32, 41, 66, 97	1 (0%)
All	All	6223/6458 (96%)	0.00	118 (1%)	66 66	17, 46, 84, 149	48 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	40	TYR	5.1
5	S	2	PHE	4.7
13	a	216	SER	4.4
8	V	204	CYS	4.3
11	Y	40	TYR	4.3
11	Y	201	GLY	4.1
4	R	241	ILE	4.1
7	U	186	LYS	4.0
5	E	54	SER	4.0
5	E	59	HIS	4.0
5	E	52	ALA	3.9
2	P	203	VAL	3.9
5	S	57	ALA	3.8
5	S	239	ARG	3.8
5	S	18[A]	ARG	3.8
14	b	199	VAL	3.7
3	Q	48	LYS	3.6
13	a	215	ILE	3.5
4	D	241	ILE	3.5
2	P	61	PHE	3.5
5	E	57	ALA	3.5
2	P	51	ASN	3.4
3	Q	50	VAL	3.4
8	V	220	GLU	3.4
1	A	231	ALA	3.4
13	M	215	ILE	3.4
2	B	61	PHE	3.3
5	E	56	LEU	3.3
14	b	198	ALA	3.3
6	T	5	THR	3.2
4	R	131	GLY	3.2
5	E	58	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
14	N	198	ALA	3.2
1	O	232	ILE	3.1
3	C	138	PHE	3.0
1	A	230	ALA	3.0
1	O	3	ARG	2.9
4	D	131	GLY	2.9
14	N	199	VAL	2.9
2	B	203	VAL	2.8
1	O	188	HIS	2.8
14	N	202	LEU	2.8
8	H	204	CYS	2.8
7	G	187	PHE	2.8
3	Q	53	LEU	2.8
2	P	249	ARG	2.7
6	T	6	GLY	2.7
8	V	203	ARG	2.7
2	P	204	SER	2.7
1	O	231	ALA	2.7
3	Q	138	PHE	2.7
4	R	128	ALA	2.6
2	B	202	ASP	2.6
6	T	53	VAL	2.6
2	B	249	ARG	2.6
4	R	130	PRO	2.6
14	b	203	PRO	2.6
5	S	54	SER	2.6
2	P	245	ALA	2.6
7	G	189	TRP	2.6
14	N	200	ALA	2.6
2	P	56	LEU	2.6
10	J	1[A]	MET	2.6
1	A	3	ARG	2.6
5	S	53	GLN	2.5
2	B	2	SER	2.5
7	U	193	GLN	2.5
3	C	206	ILE	2.5
1	O	230	ALA	2.5
6	T	208	ALA	2.5
8	V	199	LEU	2.5
14	b	202	LEU	2.5
6	T	204	VAL	2.4
5	S	56	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	Q	202	GLY	2.4
6	T	142	VAL	2.4
5	E	51	ARG	2.4
7	U	185	LYS	2.4
3	Q	203	GLY	2.4
11	Y	200	SER	2.4
3	C	48	LYS	2.4
7	G	245	ARG	2.4
1	O	177	TYR	2.4
7	G	208	ILE	2.4
5	E	53	GLN	2.3
6	F	6	GLY	2.3
4	R	127	ASP	2.3
6	F	53	VAL	2.3
7	U	183	VAL	2.3
1	O	54	ILE	2.3
8	V	197	THR	2.3
3	Q	220	LEU	2.3
9	I	78	GLY	2.3
3	Q	49	SER	2.3
2	B	247	ALA	2.2
3	C	225	ILE	2.2
6	T	206	ASP	2.2
2	P	247	ALA	2.2
3	Q	51	ALA	2.2
4	R	120[A]	ALA	2.2
8	V	202	TYR	2.2
9	W	84	TYR	2.2
5	S	51	ARG	2.2
3	Q	232	ILE	2.1
3	C	53	LEU	2.1
5	S	235	GLY	2.1
2	P	55	LEU	2.1
5	E	201	ALA	2.1
5	E	237	GLU	2.0
1	A	181	LEU	2.0
3	C	220	LEU	2.0
7	G	188	ASP	2.0
8	V	201	ARG	2.0
3	C	49	SER	2.0
12	L	177	ASP	2.0
1	A	221	THR	2.0

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Mol	Chain	Res	Type	RSRZ
6	T	61	GLY	2.0
8	H	202	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.83	0.17	72,103,109,110	0
7	YCM	U	137	10/11	0.86	0.14	51,59,75,76	0
7	YCM	G	137	10/11	0.87	0.14	33,39,51,53	0
5	6V1	E	148	15/16	0.88	0.16	32,54,64,65	0
3	YCM	C	63	10/11	0.89	0.11	55,56,63,64	0
7	6V1	G	47	15/16	0.90	0.15	39,61,64,65	0
5	6V1	S	148	15/16	0.90	0.15	37,63,68,70	0
10	6V1	X	91	15/16	0.91	0.15	36,54,57,61	0
7	6V1	U	161	15/16	0.92	0.11	53,73,78,78	0
10	6V1	J	91	15/16	0.93	0.13	33,53,58,59	0
3	YCM	Q	63	10/11	0.93	0.09	51,54,64,67	0
7	6V1	G	161	15/16	0.94	0.12	33,51,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	1PE	M	304	16/16	0.80	0.19	78,83,97,98	0
18	1PE	H	304	16/16	0.81	0.15	58,69,77,79	0
18	1PE	a	304	16/16	0.81	0.17	66,70,86,87	0
18	1PE	W	303	16/16	0.85	0.13	59,64,71,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CL	O	304	1/1	0.85	0.16	67,67,67,67	0
18	1PE	I	303	16/16	0.87	0.11	55,58,68,71	0
18	1PE	U	302	16/16	0.87	0.14	46,56,73,75	0
15	CL	D	301	1/1	0.88	0.26	69,69,69,69	0
18	1PE	L	301	16/16	0.88	0.13	60,70,74,76	0
18	1PE	Z	301	16/16	0.88	0.12	57,66,72,73	0
15	CL	O	303	1/1	0.88	0.11	87,87,87,87	0
15	CL	E	303	1/1	0.90	0.22	64,64,64,64	0
15	CL	K	303	1/1	0.90	0.14	69,69,69,69	0
19	6VC	V	304	28/28	0.90	0.11	42,45,60,61	0
15	CL	Y	306	1/1	0.91	0.26	63,63,63,63	0
15	CL	E	304	1/1	0.91	0.15	63,63,63,63	0
18	1PE	N	305	16/16	0.91	0.11	41,49,62,64	0
15	CL	C	302	1/1	0.91	0.20	71,71,71,71	0
15	CL	Q	301	1/1	0.92	0.17	67,67,67,67	0
15	CL	C	301	1/1	0.92	0.13	60,60,60,60	0
15	CL	B	302	1/1	0.92	0.23	57,57,57,57	0
15	CL	A	302	1/1	0.93	0.10	64,64,64,64	0
15	CL	Q	302	1/1	0.93	0.24	64,64,64,64	0
15	CL	K	305	1/1	0.93	0.24	65,65,65,65	0
15	CL	a	303	1/1	0.93	0.10	60,60,60,60	0
15	CL	M	303	1/1	0.93	0.14	59,59,59,59	0
15	CL	G	302	1/1	0.93	0.12	60,60,60,60	0
15	CL	I	302	1/1	0.93	0.12	48,48,48,48	0
15	CL	E	302	1/1	0.94	0.16	55,55,55,55	0
15	CL	S	301	1/1	0.94	0.30	64,64,64,64	0
15	CL	V	303	1/1	0.94	0.21	59,59,59,59	0
15	CL	K	304	1/1	0.94	0.16	60,60,60,60	0
19	6VC	H	305	28/28	0.94	0.10	33,37,55,60	0
15	CL	N	303	1/1	0.94	0.21	56,56,56,56	0
19	6VC	Y	307	28/28	0.94	0.09	27,29,51,56	0
15	CL	Y	304	1/1	0.95	0.09	64,64,64,64	0
15	CL	Y	305	1/1	0.95	0.12	57,57,57,57	0
15	CL	M	301	1/1	0.95	0.33	56,56,56,56	0
15	CL	a	301	1/1	0.95	0.20	59,59,59,59	0
15	CL	R	301	1/1	0.95	0.14	58,58,58,58	0
16	K	b	305	1/1	0.95	0.12	41,41,41,41	0
15	CL	R	302	1/1	0.95	0.26	57,57,57,57	0
19	6VC	K	306	28/28	0.95	0.09	36,39,61,62	0
19	6VC	N	307	28/28	0.95	0.09	25,29,49,52	0
15	CL	N	304	1/1	0.95	0.26	52,52,52,52	0
15	CL	O	302	1/1	0.95	0.09	63,63,63,63	0

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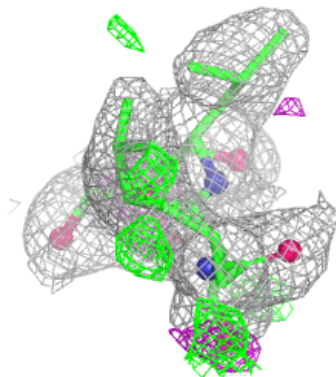
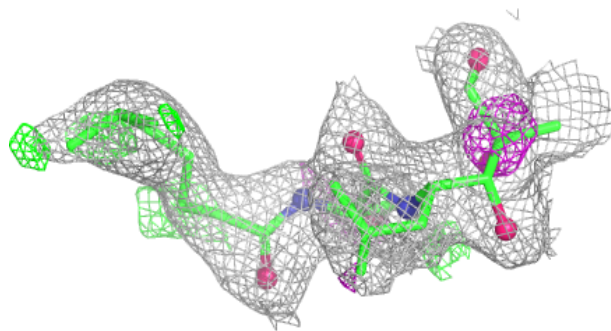
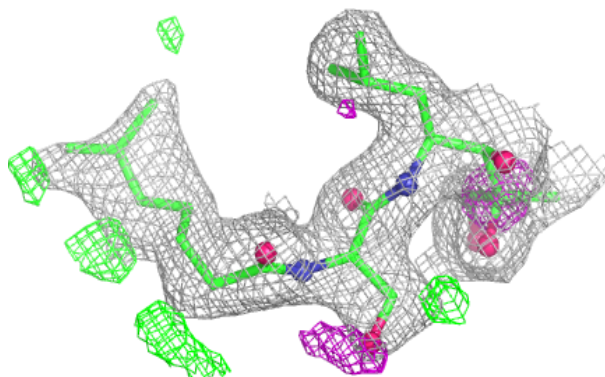
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	6VC	b	306	28/28	0.95	0.09	31,34,55,56	0
15	CL	W	302	1/1	0.96	0.09	54,54,54,54	0
15	CL	H	303	1/1	0.96	0.15	53,53,53,53	0
15	CL	F	301	1/1	0.96	0.15	51,51,51,51	0
15	CL	S	302	1/1	0.96	0.16	63,63,63,63	0
15	CL	S	303	1/1	0.96	0.13	55,55,55,55	0
15	CL	B	301	1/1	0.96	0.12	41,41,41,41	0
15	CL	b	302	1/1	0.96	0.16	55,55,55,55	0
15	CL	b	303	1/1	0.96	0.22	56,56,56,56	0
16	K	U	303	1/1	0.97	0.11	41,41,41,41	0
15	CL	Y	303	1/1	0.97	0.19	59,59,59,59	0
17	MG	I	301	1/1	0.97	0.10	33,33,33,33	0
17	MG	V	302	1/1	0.97	0.09	58,58,58,58	0
17	MG	Y	301	1/1	0.97	0.10	30,30,30,30	0
15	CL	a	302	1/1	0.97	0.09	43,43,43,43	0
15	CL	A	304	1/1	0.97	0.17	57,57,57,57	0
15	CL	A	303	1/1	0.97	0.08	50,50,50,50	0
15	CL	O	301	1/1	0.97	0.13	55,55,55,55	0
15	CL	b	304	1/1	0.97	0.08	42,42,42,42	0
15	CL	A	301	1/1	0.98	0.11	52,52,52,52	0
15	CL	b	301	1/1	0.98	0.15	45,45,45,45	0
15	CL	Y	302	1/1	0.98	0.08	38,38,38,38	0
15	CL	N	302	1/1	0.98	0.13	45,45,45,45	0
15	CL	E	301	1/1	0.98	0.15	61,61,61,61	0
16	K	G	303	1/1	0.98	0.11	33,33,33,33	0
16	K	L	302	1/1	0.98	0.13	47,47,47,47	0
16	K	N	306	1/1	0.98	0.08	38,38,38,38	0
15	CL	P	301	1/1	0.98	0.08	53,53,53,53	0
15	CL	G	301	1/1	0.98	0.30	48,48,48,48	0
17	MG	H	301	1/1	0.98	0.07	57,57,57,57	0
15	CL	U	301	1/1	0.98	0.18	54,54,54,54	0
17	MG	K	301	1/1	0.98	0.08	36,36,36,36	0
17	MG	V	301	1/1	0.98	0.10	37,37,37,37	0
15	CL	K	302	1/1	0.98	0.10	42,42,42,42	0
17	MG	W	301	1/1	0.98	0.10	38,38,38,38	0
16	K	Z	302	1/1	0.99	0.08	39,39,39,39	0
17	MG	X	301	1/1	0.99	0.04	49,49,49,49	0
17	MG	J	301	1/1	0.99	0.02	48,48,48,48	0
15	CL	M	302	1/1	0.99	0.11	40,40,40,40	0
15	CL	N	301	1/1	0.99	0.04	35,35,35,35	0
17	MG	H	302	1/1	0.99	0.10	33,33,33,33	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.

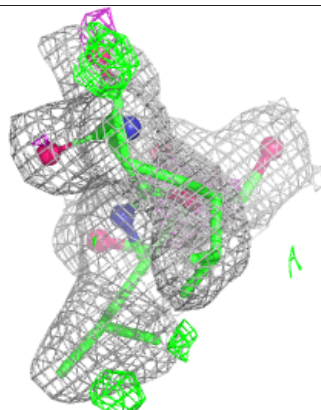
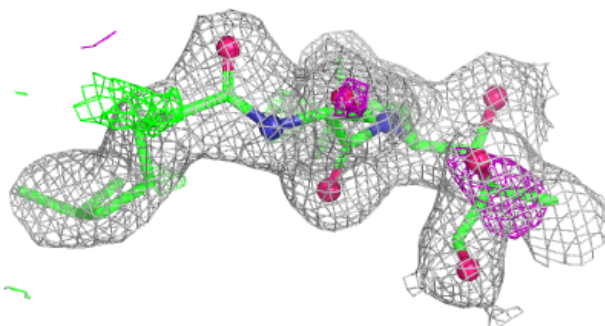
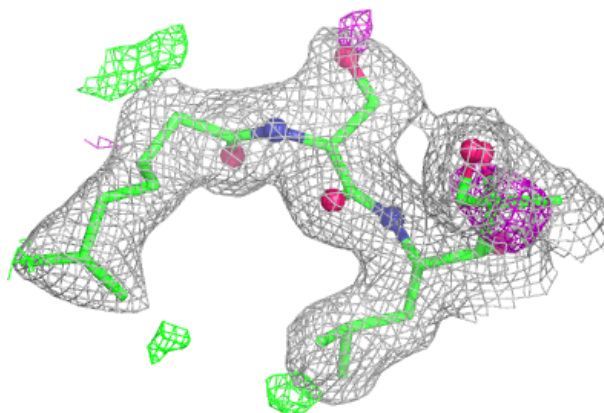
Electron density around 6VC V 304:

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

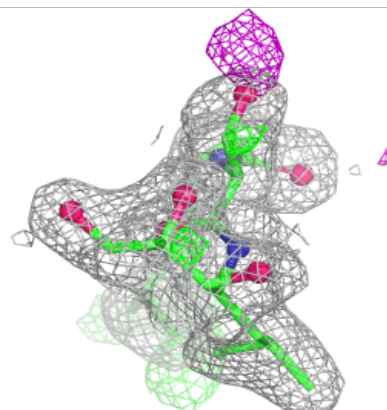
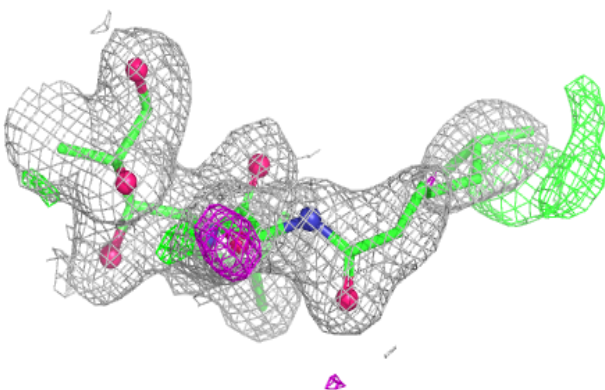
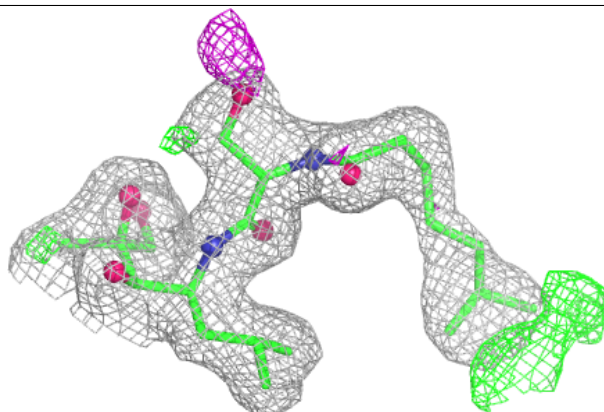


Electron density around 6VC H 305:

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

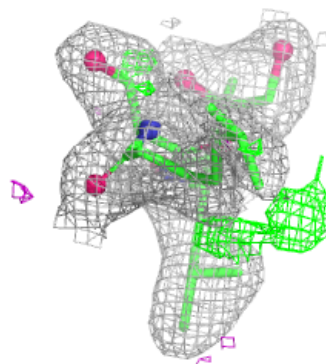
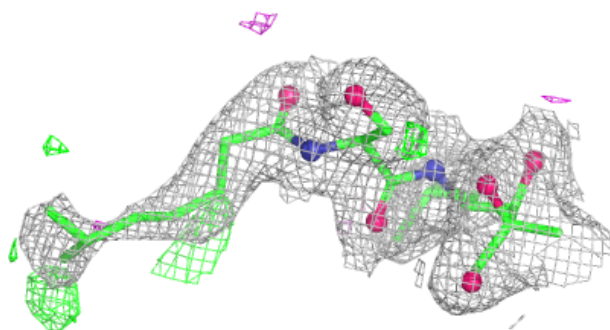
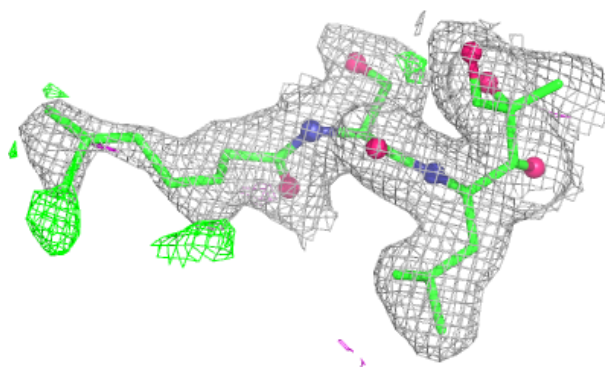
**Electron density around 6VC Y 307:**

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

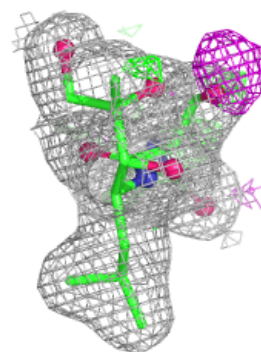
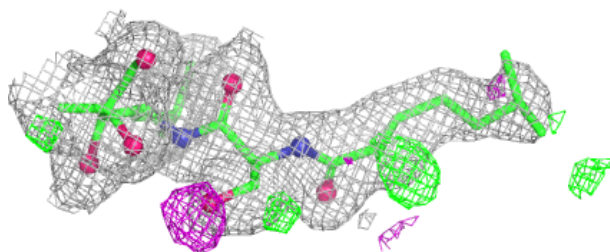
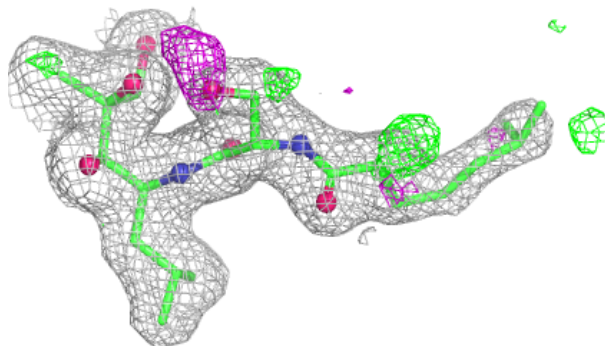


Electron density around 6VC K 306:

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

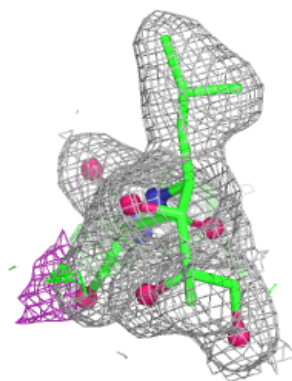
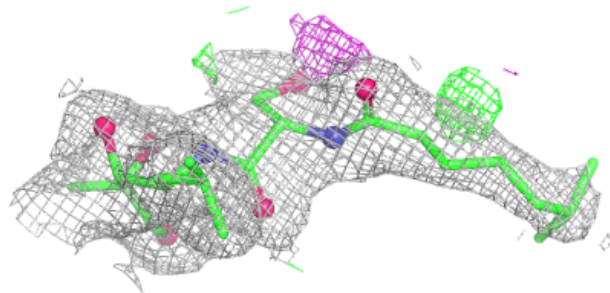
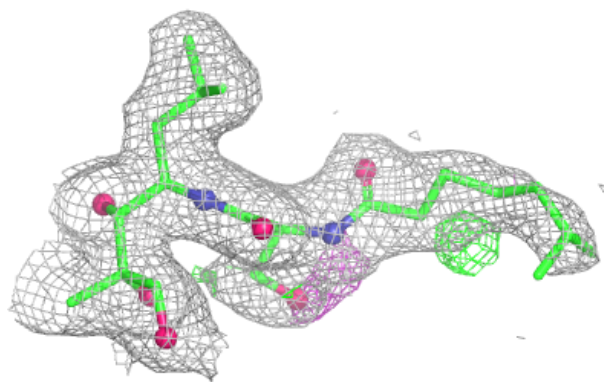
**Electron density around 6VC N 307:**

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



Electron density around 6VC b 306:

$2mF_o-DF_c$ (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.