



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:51 AM UTC

PDB ID : 5LF4 / pdb_00005lf4
Title : Human 20S proteasome complex with Delanzomib 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 : 1.99 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

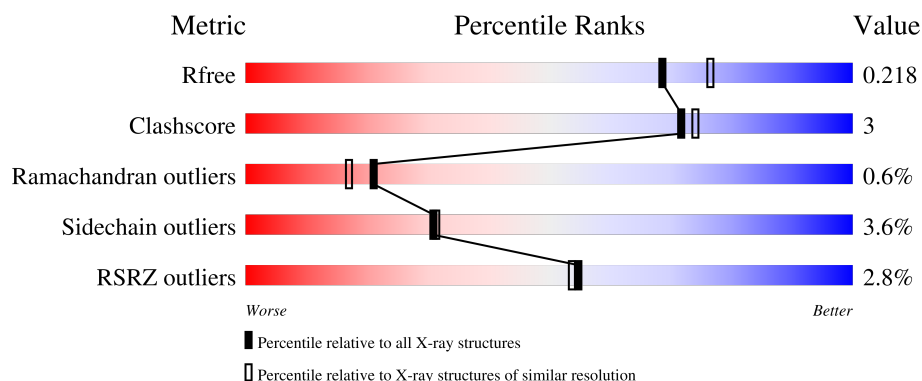
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	3% 86% 10% • •
1	O	234	3% 90% 6% • •
2	B	261	3% 84% 10% • 5%
2	P	261	6% 82% 11% • • 5%
3	C	248	6% 80% 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
19	6V7	N	307	X	-	-	-
19	6V7	Y	306	X	-	-	-
7	6V1	U	47	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 52186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	11			

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

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

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

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

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

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

- 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	1	0
			1550	978	269	293	10			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	2	Total 2	Cl 2	0	0
15	D	2	Total 2	Cl 2	0	0
15	E	3	Total 3	Cl 3	0	0
15	F	1	Total 1	Cl 1	0	0
15	G	2	Total 2	Cl 2	0	0
15	H	2	Total 2	Cl 2	0	0
15	I	1	Total 1	Cl 1	0	0
15	K	3	Total 3	Cl 3	0	0
15	M	3	Total 3	Cl 3	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	2	Total 2	Cl 2	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

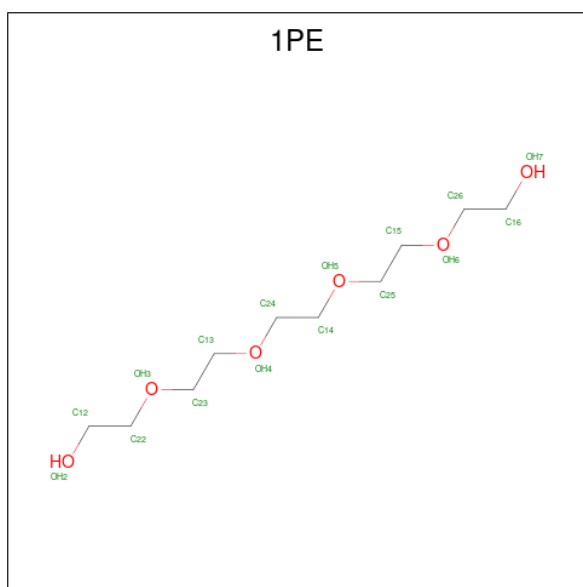
- Molecule 16 is POTASSIUM ION (CCD ID: K) (formula: K).

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	2	Total K 2 2	0	0
16	U	1	Total K 1 1	0	0
16	Z	1	Total K 1 1	0	0
16	b	2	Total K 2 2	0	0

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

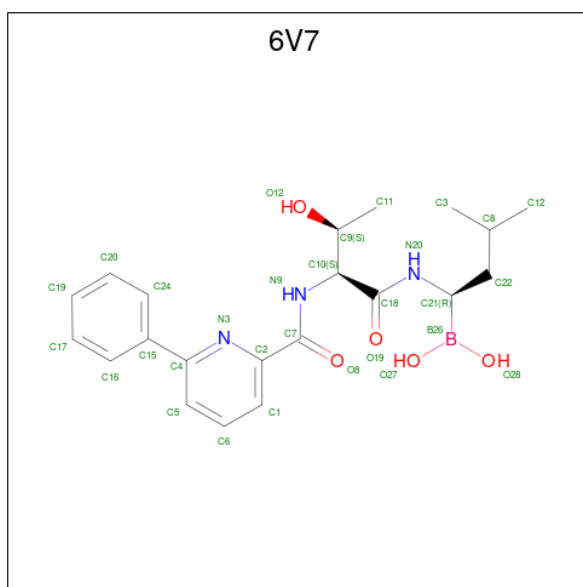
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	2	Total Mg 2 2	0	0
17	I	2	Total Mg 2 2	0	0
17	J	1	Total Mg 1 1	0	0
17	K	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0
17	V	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	X	1	Total Mg 1 1	0	0

- 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	L	1	Total	C	O	0	0
			16	10	6		
18	L	1	Total	C	O	0	0
			16	10	6		
18	N	1	Total	C	O	0	0
			16	10	6		
18	N	1	Total	C	O	0	0
			16	10	6		
18	U	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		

- Molecule 19 is [(1 {R})-3-methyl-1-[[[(2 {S},3 {S})-3-oxidanyl-2-[(6-phenylpyridin-2-yl)carbonylamino]butanoyl]amino]butyl]boronic acid (CCD ID: 6V7) (formula: C₂₁H₂₈BN₃O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	K	1	Total	B	C	N	O	0	0
			30	1	21	3	5		
19	N	1	Total	B	C	N	O	0	0
			30	1	21	3	5		
19	Y	1	Total	B	C	N	O	0	0
			30	1	21	3	5		
19	b	1	Total	B	C	N	O	0	0
			30	1	21	3	5		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	115	Total	O	0	0
			115	115		
20	B	129	Total	O	0	0
			129	129		
20	C	78	Total	O	0	0
			78	78		
20	D	98	Total	O	0	0
			98	98		
20	E	143	Total	O	0	0
			143	143		
20	F	186	Total	O	0	0
			186	186		
20	G	195	Total	O	0	0
			195	195		
20	H	164	Total	O	0	0
			164	164		

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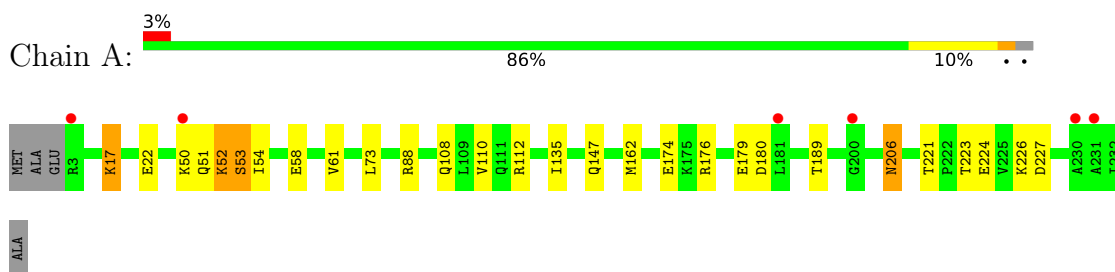
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	I	155	Total 155	O 155	0	0
20	J	141	Total 141	O 141	0	0
20	K	102	Total 102	O 102	0	0
20	L	124	Total 124	O 124	0	0
20	M	148	Total 148	O 148	0	0
20	N	168	Total 168	O 168	0	0
20	O	95	Total 95	O 95	0	0
20	P	124	Total 124	O 124	0	0
20	Q	75	Total 75	O 75	0	0
20	R	129	Total 129	O 129	0	0
20	S	128	Total 128	O 128	0	0
20	T	96	Total 96	O 96	0	0
20	U	113	Total 113	O 113	0	0
20	V	117	Total 117	O 117	0	0
20	W	123	Total 123	O 123	0	0
20	X	128	Total 128	O 128	0	0
20	Y	149	Total 149	O 149	0	0
20	Z	171	Total 171	O 171	0	0
20	a	172	Total 172	O 172	0	0
20	b	126	Total 126	O 126	0	0

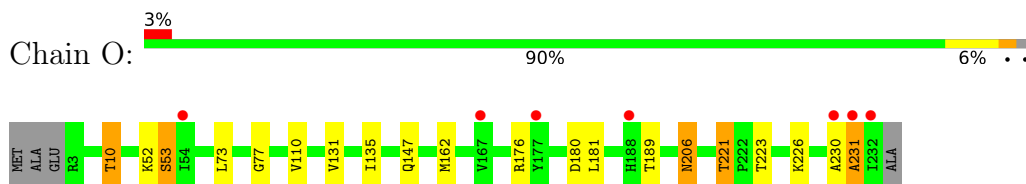
3 Residue-property plots [i](#)

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.

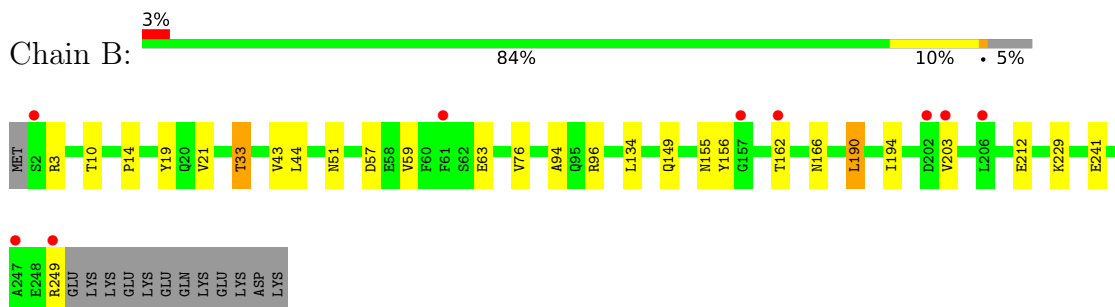
- Molecule 1: Proteasome subunit alpha type-2



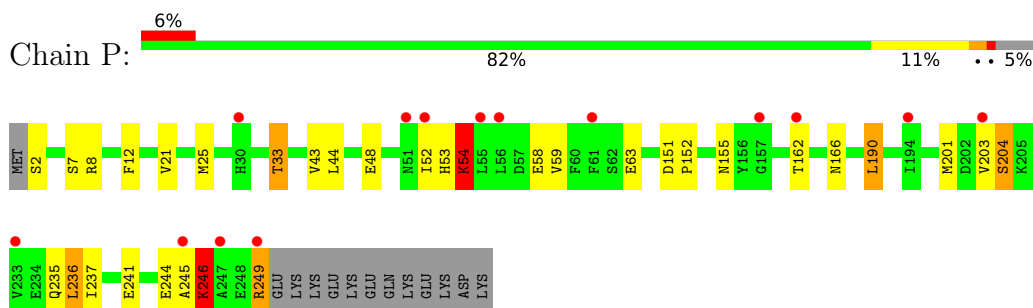
- Molecule 1: Proteasome subunit alpha type-2



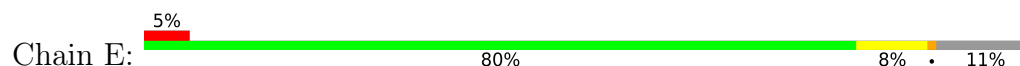
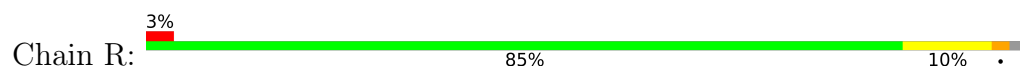
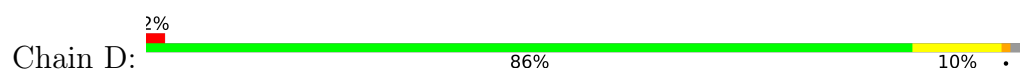
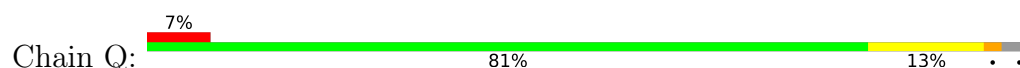
- Molecule 2: Proteasome subunit alpha type-4



- Molecule 2: Proteasome subunit alpha type-4



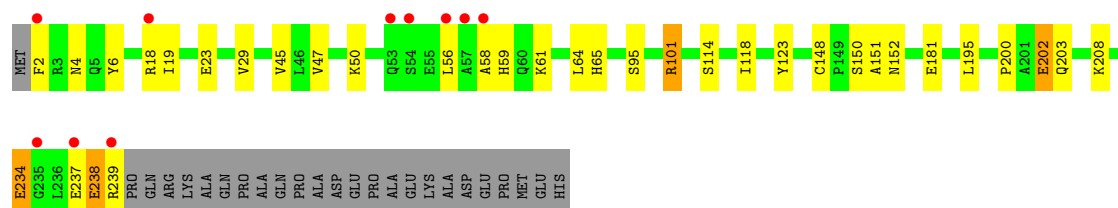
Chain C: 6% 80% 12% . .



GLN
ARG
LYS
ALA
GLN
PRO
ALA
GLN
PRO
ALA
ASP
GLU
PRO
ALA
GLU
LYS
ALA
ASP
GLU
PRO
GLU
MET
GLU
HIS

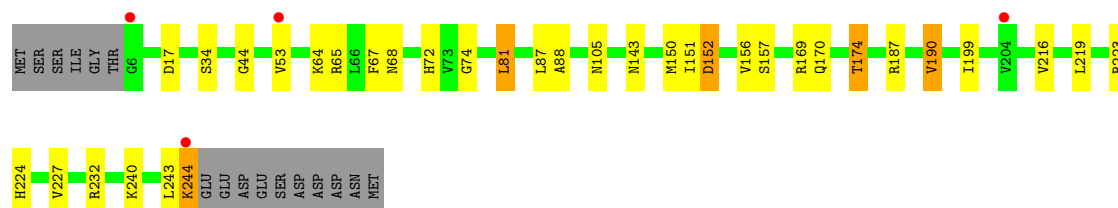
• Molecule 5: Proteasome subunit alpha type-1

Chain S: 4% 77% 12% 10%



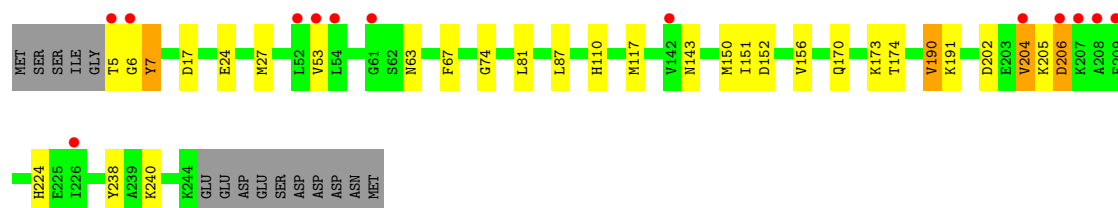
• Molecule 6: Proteasome subunit alpha type-3

Chain F: 2% 80% 12% 6%



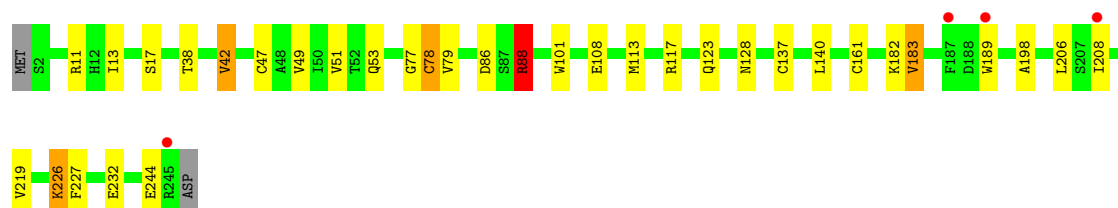
• Molecule 6: Proteasome subunit alpha type-3

Chain T: 5% 82% 11% 6%



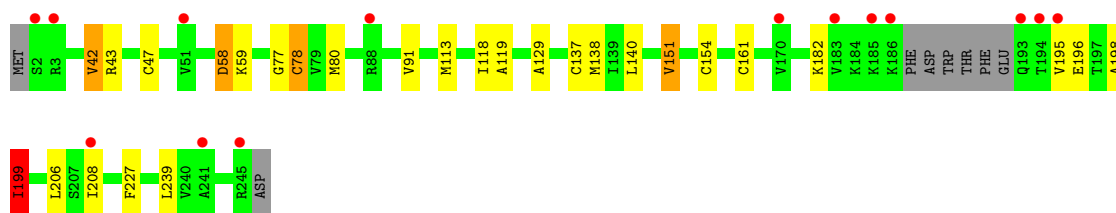
• Molecule 7: Proteasome subunit alpha type-6

Chain G: 2% 85% 12% 2%

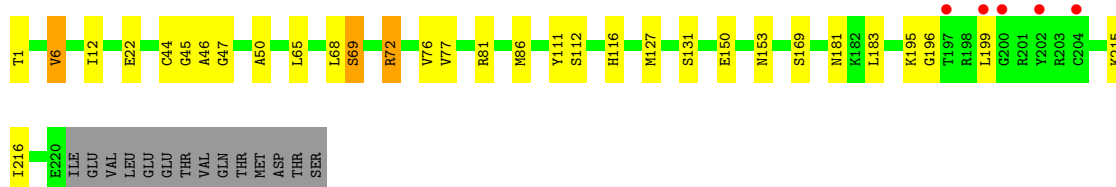
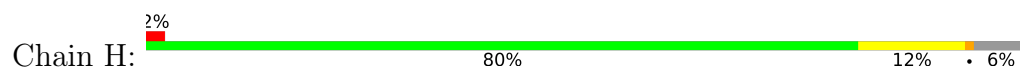


• Molecule 7: Proteasome subunit alpha type-6

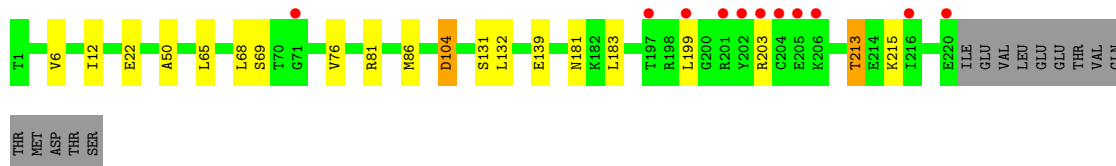
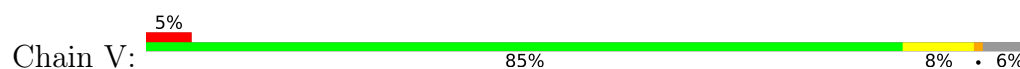
Chain U: 6% 85% 9% 2%



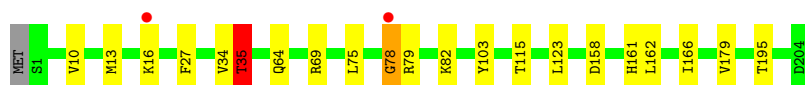
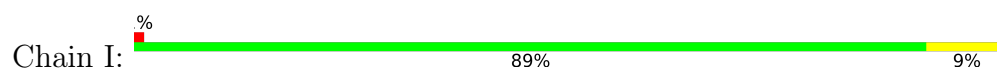
• Molecule 8: Proteasome subunit beta type-7



• Molecule 8: Proteasome subunit beta type-7



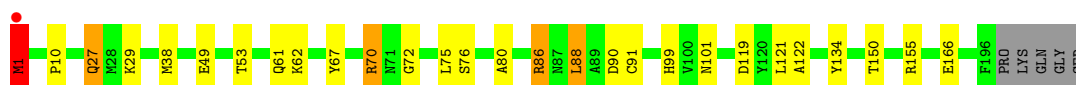
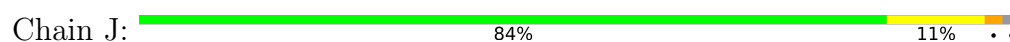
• Molecule 9: Proteasome subunit beta type-3



• Molecule 9: Proteasome subunit beta type-3

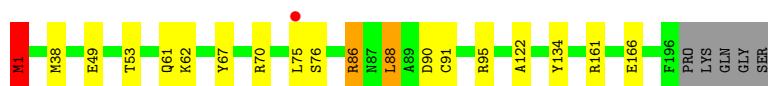


• Molecule 10: Proteasome subunit beta type-2



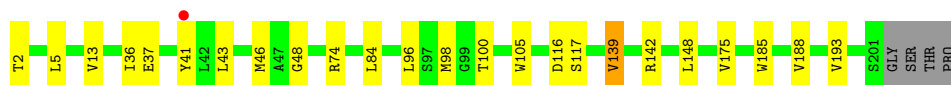
- Molecule 10: Proteasome subunit beta type-2

Chain X:  88% 8% ..



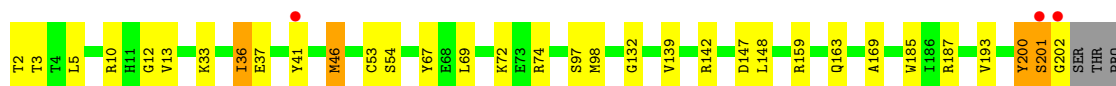
- Molecule 11: Proteasome subunit beta type-5

Chain K:  86% 11% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  82% 14% ..

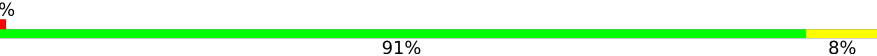


- Molecule 12: Proteasome subunit beta type-1

Chain L:  90% 9%



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  91% 8%



- Molecule 13: Proteasome subunit beta type-4

Chain M:  89% 8% ..



- Molecule 13: Proteasome subunit beta type-4

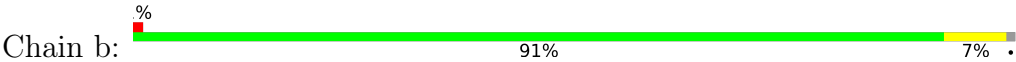
Chain a:  87% 10% ..



● 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	113.45Å 202.76Å 314.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.38 – 1.99 170.38 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (170.38-1.99) 99.0 (170.38-1.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.181 , 0.216 0.187 , 0.218	Depositor DCC
R_{free} test set	24259 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52186	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: 6V7, CL, K, YCM, MG, 6V1, 1PE

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	1.19	0/1833	1.07	0/2489
1	O	1.01	1/1778 (0.1%)	1.03	1/2419 (0.0%)
2	B	1.23	6/1962 (0.3%)	1.10	4/2649 (0.2%)
2	P	1.08	2/1945 (0.1%)	1.07	3/2631 (0.1%)
3	C	1.13	2/1818 (0.1%)	1.15	1/2469 (0.0%)
3	Q	1.09	2/1834 (0.1%)	1.18	11/2490 (0.4%)
4	D	1.09	1/1789 (0.1%)	1.08	2/2424 (0.1%)
4	R	1.31	5/1780 (0.3%)	1.13	4/2408 (0.2%)
5	E	1.27	2/1842 (0.1%)	1.15	8/2493 (0.3%)
5	S	1.18	0/1901	1.16	9/2571 (0.4%)
6	F	1.44	9/1935 (0.5%)	1.22	3/2605 (0.1%)
6	T	1.18	2/1894 (0.1%)	1.18	10/2556 (0.4%)
7	G	1.36	13/1909 (0.7%)	1.15	5/2579 (0.2%)
7	U	1.10	2/1804 (0.1%)	1.06	2/2441 (0.1%)
8	H	1.43	8/1697 (0.5%)	1.22	10/2299 (0.4%)
8	V	1.17	0/1655	1.10	4/2251 (0.2%)
9	I	1.36	6/1648 (0.4%)	1.27	12/2219 (0.5%)
9	W	1.12	0/1630	1.11	7/2197 (0.3%)
10	J	1.29	2/1613 (0.1%)	1.17	6/2180 (0.3%)
10	X	1.20	1/1599 (0.1%)	1.08	3/2163 (0.1%)
11	K	1.21	2/1584 (0.1%)	1.11	1/2141 (0.0%)
11	Y	1.37	4/1620 (0.2%)	1.18	4/2185 (0.2%)
12	L	1.22	3/1672 (0.2%)	1.08	2/2257 (0.1%)
12	Z	1.43	5/1675 (0.3%)	1.13	2/2257 (0.1%)
13	M	1.35	3/1728 (0.2%)	1.13	3/2339 (0.1%)
13	a	1.45	6/1724 (0.3%)	1.17	1/2336 (0.0%)
14	N	1.48	6/1548 (0.4%)	1.23	3/2095 (0.1%)
14	b	1.34	6/1554 (0.4%)	1.18	2/2104 (0.1%)
All	All	1.26	99/48971 (0.2%)	1.14	123/66247 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	3
3	C	0	1
3	Q	0	3
4	D	0	4
4	R	0	2
5	E	0	1
6	T	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
13	a	0	1
All	All	1	21

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	162	THR	C-N	8.74	1.44	1.33
6	F	44	GLY	N-CA	8.66	1.53	1.45
2	P	162	THR	C-N	8.22	1.44	1.33
14	b	87	MET	CA-C	7.72	1.62	1.52
7	G	108	GLU	CD-OE1	7.70	1.40	1.25
6	F	81	LEU	CA-C	7.52	1.62	1.52
5	E	76	GLY	C-O	-7.35	1.19	1.24
10	J	76	SER	CA-C	7.24	1.61	1.53
6	F	72	HIS	CA-C	7.17	1.62	1.52
12	Z	6	VAL	C-O	7.00	1.31	1.23
12	Z	32	GLY	N-CA	6.95	1.55	1.45
2	B	162	THR	C-O	6.92	1.31	1.24
7	G	101	TRP	N-CA	-6.69	1.38	1.46
8	H	45	GLY	CA-C	6.54	1.57	1.52
6	F	68	ASN	N-CA	6.53	1.54	1.46
13	a	3	ASN	C-O	-6.49	1.19	1.25
14	b	36	THR	CB-CG2	-6.47	1.31	1.52
14	N	139	TYR	CA-C	6.47	1.61	1.52
12	Z	96	LEU	N-CA	6.46	1.54	1.46
14	N	36	THR	CB-CG2	-6.41	1.31	1.52
9	I	103	TYR	CA-C	-6.40	1.46	1.53
8	H	86	MET	CA-C	6.39	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	ARG	C-O	-6.33	1.16	1.24
8	H	46	ALA	C-N	-6.20	1.29	1.33
13	a	57	TYR	N-CA	-6.19	1.38	1.46
4	R	133	MET	N-CA	6.19	1.54	1.46
14	N	17	ALA	CA-C	-6.14	1.45	1.52
6	F	88	ALA	N-CA	-6.14	1.39	1.46
11	Y	169	ALA	CA-C	6.11	1.61	1.52
14	b	91	TYR	CA-C	5.97	1.61	1.52
6	F	223	ARG	CA-C	5.95	1.60	1.52
8	H	69	SER	N-CA	-5.93	1.39	1.46
6	F	67	PHE	N-CA	5.84	1.53	1.45
3	Q	206	ILE	CA-C	5.83	1.60	1.52
12	L	6	VAL	C-O	5.79	1.30	1.23
8	H	169	SER	C-O	-5.75	1.16	1.23
10	X	76	SER	CA-C	5.75	1.60	1.53
3	Q	13	ASP	CB-CG	5.72	1.66	1.52
13	a	114	GLY	N-CA	-5.71	1.39	1.45
6	T	67	PHE	N-CA	5.68	1.53	1.45
2	B	162	THR	CA-CB	5.62	1.62	1.53
4	D	82	ILE	C-O	-5.62	1.17	1.24
14	b	131	SER	CA-C	5.62	1.60	1.52
7	G	79	VAL	C-O	-5.61	1.18	1.24
11	Y	12	GLY	C-O	-5.59	1.21	1.24
14	N	116	PRO	C-O	5.58	1.32	1.23
13	M	22	ILE	N-CA	-5.57	1.39	1.46
13	a	182	ARG	NE-CZ	5.56	1.39	1.33
2	P	162	THR	CA-CB	5.55	1.62	1.53
14	N	131	SER	CA-C	5.54	1.59	1.52
9	I	123	LEU	C-O	-5.52	1.17	1.23
2	B	96	ARG	CD-NE	-5.51	1.38	1.46
6	F	152	ASP	CA-CB	5.50	1.62	1.53
7	G	123	GLN	C-O	5.50	1.30	1.24
9	I	34	VAL	N-CA	5.49	1.53	1.46
12	L	67	ILE	C-O	5.48	1.30	1.24
6	T	7	TYR	N-CA	5.47	1.56	1.46
7	G	13	ILE	N-CA	5.45	1.52	1.46
7	U	129	ALA	N-CA	5.43	1.53	1.46
9	I	75	LEU	C-O	-5.42	1.17	1.24
9	I	10	VAL	N-CA	-5.37	1.40	1.46
13	a	45	VAL	CA-C	5.36	1.59	1.52
12	Z	3	SER	CB-OG	5.35	1.52	1.42
13	a	68	GLY	CA-C	5.34	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	51	VAL	N-CA	5.28	1.52	1.46
9	I	82	LYS	CA-C	5.28	1.59	1.53
7	G	17	SER	N-CA	5.22	1.53	1.45
4	R	75	GLY	N-CA	5.22	1.49	1.44
11	Y	33	LYS	C-O	-5.21	1.17	1.24
8	H	76	VAL	CA-CB	-5.17	1.48	1.54
13	M	3	ASN	C-O	-5.17	1.20	1.25
3	C	109	ARG	CA-C	5.17	1.59	1.52
8	H	44	CYS	N-CA	5.14	1.52	1.46
10	J	70	ARG	CD-NE	-5.14	1.39	1.46
12	Z	200	LYS	C-O	-5.14	1.17	1.24
5	E	4	ASN	N-CA	5.14	1.56	1.46
12	L	46	LEU	C-O	-5.13	1.17	1.23
14	b	101	ILE	N-CA	5.12	1.52	1.46
7	G	53	GLN	C-O	-5.12	1.17	1.23
7	G	86	ASP	N-CA	-5.11	1.40	1.46
6	F	199	ILE	C-O	-5.11	1.18	1.24
7	G	88	ARG	N-CA	-5.11	1.40	1.46
1	O	77	GLY	C-O	-5.09	1.21	1.24
11	K	105	TRP	C-O	-5.09	1.18	1.23
14	N	86	GLU	C-O	-5.09	1.18	1.24
4	R	179	SER	N-CA	-5.09	1.40	1.46
7	U	119	ALA	N-CA	-5.08	1.40	1.46
11	Y	202	GLY	CA-C	5.07	1.61	1.52
2	B	94	ALA	C-O	-5.07	1.18	1.24
13	M	139	THR	N-CA	-5.04	1.40	1.45
3	C	13	ASP	CA-C	-5.04	1.46	1.52
14	b	139	TYR	CA-C	5.03	1.59	1.52
11	K	48	GLY	C-O	-5.03	1.21	1.24
7	G	108	GLU	CD-OE2	5.02	1.34	1.25
4	R	135	ARG	N-CA	-5.02	1.40	1.46
7	G	38	THR	CA-C	5.02	1.58	1.52
4	R	82	ILE	C-O	-5.01	1.18	1.24
8	H	116	HIS	CA-C	5.01	1.59	1.52
7	G	128	ASN	CG-ND2	-5.01	1.22	1.33

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	190	VAL	CB-CA-C	-11.30	97.24	112.04
6	T	190	VAL	CB-CA-C	-10.55	98.22	112.04
7	G	183	VAL	CB-CA-C	-9.84	98.65	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	86	ARG	NE-CZ-NH2	-9.45	110.70	119.20
9	I	16[A]	LYS	CA-C-N	8.86	135.11	122.08
9	I	16[A]	LYS	C-N-CA	8.86	135.11	122.08
9	I	16[B]	LYS	CA-C-N	8.86	135.11	122.08
9	I	16[B]	LYS	C-N-CA	8.86	135.11	122.08
8	H	72	ARG	NE-CZ-NH2	-8.55	111.50	119.20
10	X	86	ARG	NE-CZ-NH2	-8.55	111.50	119.20
6	T	6	GLY	CA-C-N	8.27	136.59	121.70
6	T	6	GLY	C-N-CA	8.27	136.59	121.70
8	H	47	GLY	N-CA-C	-8.15	102.73	111.21
10	J	86	ARG	NE-CZ-NH1	7.92	129.41	121.50
9	I	69	ARG	NE-CZ-NH1	7.84	129.34	121.50
2	P	204	SER	N-CA-C	7.62	119.28	110.97
4	D	120	ALA	N-CA-C	7.59	120.22	111.11
2	B	162	THR	CA-C-O	7.42	129.34	121.25
3	Q	12	PRO	CA-C-N	-7.32	111.66	122.86
3	Q	12	PRO	C-N-CA	-7.32	111.66	122.86
7	G	183	VAL	N-CA-CB	7.12	121.26	110.58
7	G	244	GLU	N-CA-C	7.09	119.71	109.71
8	H	81	ARG	CB-CA-C	-7.04	99.11	110.79
2	B	19	TYR	N-CA-C	7.00	118.91	111.28
11	Y	200	TYR	CA-C-N	6.94	134.20	121.70
11	Y	200	TYR	C-N-CA	6.94	134.20	121.70
5	S	118	ILE	CA-C-N	-6.94	112.66	119.87
5	S	118	ILE	C-N-CA	-6.94	112.66	119.87
8	V	81	ARG	CB-CA-C	-6.92	100.01	110.88
7	G	183	VAL	N-CA-C	6.77	117.56	110.72
3	Q	220	LEU	CA-C-N	6.74	133.84	121.70
3	Q	220	LEU	C-N-CA	6.74	133.84	121.70
13	a	71	VAL	N-CA-CB	6.73	120.68	110.58
5	S	234	GLU	N-CA-C	6.71	118.64	109.11
6	F	190	VAL	N-CA-CB	6.68	118.82	110.47
10	J	86	ARG	CD-NE-CZ	6.68	133.75	124.40
9	I	79	ARG	N-CA-C	6.67	118.28	108.14
6	T	190	VAL	N-CA-CB	6.65	118.79	110.47
8	H	72	ARG	CD-NE-CZ	6.64	133.69	124.40
6	T	143	ASN	N-CA-C	6.61	118.57	111.36
9	I	78	GLY	N-CA-C	6.61	123.50	115.31
5	S	58	ALA	N-CA-C	-6.55	101.71	110.55
2	P	246	LYS	N-CA-C	6.51	120.49	112.54
3	C	197	GLU	N-CA-C	6.49	118.36	111.28
8	H	86	MET	CG-SD-CE	-6.47	86.66	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	13	ASP	CB-CA-C	6.47	121.54	111.13
10	J	86	ARG	N-CA-C	-6.41	104.29	111.28
11	Y	46	MET	CG-SD-CE	-6.36	86.92	100.90
9	W	69	ARG	NE-CZ-NH1	6.30	127.80	121.50
9	W	79	ARG	N-CA-C	6.28	117.77	108.60
9	W	16[A]	LYS	CA-C-N	6.27	134.98	123.13
9	W	16[A]	LYS	C-N-CA	6.27	134.98	123.13
9	W	16[B]	LYS	CA-C-N	6.27	134.98	123.13
9	W	16[B]	LYS	C-N-CA	6.27	134.98	123.13
10	X	86	ARG	CD-NE-CZ	6.21	133.10	124.40
9	I	35	THR	N-CA-CB	-6.17	101.36	111.66
3	Q	98	VAL	CB-CA-C	6.14	117.25	110.62
9	I	35	THR	OG1-CB-CG2	6.11	121.51	109.30
12	Z	172	MET	CG-SD-CE	-6.06	87.58	100.90
10	X	86	ARG	NE-CZ-NH1	6.01	127.51	121.50
10	J	72	GLY	N-CA-C	5.97	123.90	115.30
5	E	126	ARG	CA-C-N	-5.95	113.56	119.92
5	E	126	ARG	C-N-CA	-5.95	113.56	119.92
8	H	72	ARG	NE-CZ-NH1	5.94	127.44	121.50
3	Q	220	LEU	N-CA-C	-5.94	100.88	110.32
6	T	204	VAL	CB-CA-C	5.93	119.22	111.81
11	K	139	VAL	N-CA-CB	5.93	119.05	110.52
7	G	208	ILE	N-CA-C	5.87	116.61	111.56
3	Q	11	SER	O-C-N	5.83	125.34	121.14
9	I	69	ARG	NE-CZ-NH2	-5.76	114.01	119.20
5	S	114	SER	CB-CA-C	-5.72	101.89	110.88
14	N	23	THR	OG1-CB-CG2	-5.72	97.86	109.30
7	U	199	ILE	CB-CA-C	5.68	120.06	112.22
11	Y	36	ILE	CA-CB-CG1	-5.64	100.80	110.40
10	J	80	ALA	N-CA-C	-5.63	105.28	111.82
5	S	114	SER	CA-CB-OG	-5.62	99.86	111.10
12	L	172	MET	CG-SD-CE	-5.57	88.65	100.90
6	F	143	ASN	N-CA-C	5.56	117.42	111.36
6	T	7	TYR	N-CA-CB	5.55	119.93	110.50
9	W	35	THR	N-CA-CB	-5.54	102.42	111.66
14	b	136	ILE	N-CA-C	5.53	117.42	112.17
9	I	69	ARG	CB-CG-CD	5.53	124.01	111.30
14	N	167	ARG	N-CA-C	5.49	120.10	112.90
12	Z	80	ASN	N-CA-C	5.48	119.14	111.74
5	E	114	SER	CA-CB-OG	-5.48	100.15	111.10
8	V	86	MET	CG-SD-CE	-5.46	88.88	100.90
12	L	2	PHE	CA-C-O	-5.46	115.01	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	31	ILE	CB-CA-C	-5.42	103.47	112.26
4	R	120[A]	ALA	N-CA-C	5.40	117.17	111.28
4	R	120[B]	ALA	N-CA-C	5.40	117.17	111.28
6	T	117	MET	CG-SD-CE	5.39	112.76	100.90
5	E	6	TYR	CA-C-N	-5.36	114.12	122.37
5	E	6	TYR	C-N-CA	-5.36	114.12	122.37
5	E	118	ILE	CA-C-N	-5.36	114.30	119.87
5	E	118	ILE	C-N-CA	-5.36	114.30	119.87
8	H	181	ASN	N-CA-C	5.35	119.96	113.38
13	M	5	MET	CG-SD-CE	5.34	112.66	100.90
3	Q	220	LEU	O-C-N	-5.32	117.10	123.06
3	Q	220	LEU	CA-C-O	-5.30	115.00	121.36
8	H	50	ALA	N-CA-C	-5.30	105.68	111.82
13	M	10	SER	N-CA-C	5.29	117.11	110.24
1	O	221	THR	CB-CA-C	-5.28	99.89	109.45
5	S	6	TYR	CA-C-N	-5.27	114.25	122.37
5	S	6	TYR	C-N-CA	-5.27	114.25	122.37
2	B	57	ASP	N-CA-C	5.26	119.98	113.50
8	H	150	GLU	CB-CA-C	-5.24	102.65	110.88
9	I	179	VAL	N-CA-C	5.24	116.57	111.91
13	M	106	LEU	N-CA-C	-5.24	100.63	108.96
8	H	6	VAL	N-CA-CB	-5.20	102.92	111.45
4	R	152	GLN	N-CA-C	5.20	116.85	108.32
2	B	21	VAL	O-C-N	5.16	126.97	121.91
7	U	208	ILE	N-CA-C	5.15	115.99	111.56
14	N	199	ALA	N-CA-C	5.14	117.55	110.35
4	D	125	GLU	N-CA-C	5.13	119.08	112.41
6	T	6	GLY	N-CA-C	5.13	125.34	113.18
5	E	236	LEU	N-CA-C	-5.12	101.95	109.62
2	P	21	VAL	N-CA-C	-5.11	105.52	110.42
5	S	4	ASN	N-CA-C	5.05	116.78	111.28
14	b	36	THR	CB-CA-C	5.05	115.43	109.47
8	V	50	ALA	N-CA-C	-5.04	105.78	111.28
8	V	181	ASN	N-CA-C	5.02	119.55	113.38
6	T	63	ASN	CB-CA-C	-5.01	104.77	111.89
3	Q	206	ILE	N-CA-C	5.00	119.74	109.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	46	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,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	203	VAL	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
3	Q	46	GLU	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
4	R	223	GLY	Peptide
6	T	5	THR	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
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	16	0
1	O	1741	0	1683	7	0
2	B	1926	0	1924	12	0
2	P	1909	0	1874	18	0
3	C	1798	0	1718	24	0
3	Q	1820	0	1749	11	0
4	D	1762	0	1709	9	0
4	R	1753	0	1726	11	0
5	E	1822	0	1779	7	0
5	S	1875	0	1818	21	0
6	F	1888	0	1882	14	0
6	T	1856	0	1816	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1912	0	1882	10	0
7	U	1815	0	1748	12	0
8	H	1664	0	1681	12	0
8	V	1622	0	1595	6	0
9	I	1613	0	1646	10	0
9	W	1599	0	1621	9	0
10	J	1590	0	1581	18	0
10	X	1576	0	1561	14	0
11	K	1550	0	1503	11	0
11	Y	1580	0	1554	30	0
12	L	1636	0	1625	10	0
12	Z	1642	0	1635	5	0
13	M	1692	0	1670	8	0
13	a	1688	0	1658	11	0
14	N	1519	0	1492	8	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	0	0
15	G	2	0	0	0	0
15	H	2	0	0	1	0
15	I	1	0	0	0	0
15	K	3	0	0	0	0
15	M	3	0	0	1	0
15	N	2	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	2	0	0	0	0
15	W	1	0	0	0	0
15	Y	4	0	0	0	0
15	a	4	0	0	1	0
15	b	1	0	0	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	2	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	16	0	22	0	0
18	L	32	0	44	0	0
18	N	32	0	44	0	0
18	U	16	0	22	1	0
18	W	16	0	22	0	0
18	Y	16	0	22	0	0
19	K	30	0	0	1	0
19	N	30	0	0	0	0
19	Y	30	0	0	1	0
19	b	30	0	0	0	0
20	A	115	0	0	3	0
20	B	129	0	0	2	0
20	C	78	0	0	2	0
20	D	98	0	0	1	0
20	E	143	0	0	1	0
20	F	186	0	0	4	0
20	G	195	0	0	3	0
20	H	164	0	0	5	0
20	I	155	0	0	1	0
20	J	141	0	0	1	0
20	K	102	0	0	0	0
20	L	124	0	0	2	0
20	M	148	0	0	0	0
20	N	168	0	0	1	0
20	O	95	0	0	1	0
20	P	124	0	0	0	0
20	Q	75	0	0	0	0
20	R	129	0	0	4	0
20	S	128	0	0	6	0
20	T	96	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	U	113	0	0	1	0
20	V	117	0	0	0	0
20	W	123	0	0	1	0
20	X	128	0	0	1	0
20	Y	149	0	0	0	0
20	Z	171	0	0	0	0
20	a	172	0	0	0	0
20	b	126	0	0	0	0
All	All	52186	0	47581	320	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 (320) 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	1.41	1.02
11:Y:46:MET:HE1	11:Y:54:SER:HA	1.45	0.99
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.28	0.96
10:X:1:MET:HE1	10:X:134:TYR:H	1.28	0.96
11:Y:36:ILE:HD12	11:Y:46:MET:HE3	1.52	0.92
11:Y:36:ILE:CD1	11:Y:46:MET:HE3	2.06	0.84
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	1.61	0.81
5:S:65[A]:HIS:CE1	20:S:402:HOH:O	2.32	0.81
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.63	0.80
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.29	0.80
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.62	0.80
6:F:169[A]:ARG:NH1	20:F:401:HOH:O	2.13	0.79
5:S:152[B]:ASN:OD1	20:S:401:HOH:O	2.01	0.78
14:N:36:THR:CG2	14:N:46:ARG:HE	1.99	0.75
13:a:86:ARG:NH1	13:a:133:GLU:OE1	2.19	0.75
9:W:13:MET:HE2	9:W:166:ILE:HB	1.67	0.75
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.68	0.74
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.05	0.74
8:H:77:VAL:HB	20:H:549:HOH:O	1.87	0.72
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.01	0.72
10:X:1:MET:HE1	10:X:134:TYR:N	2.02	0.72
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.23	0.71
9:I:35:THR:HG21	20:I:428:HOH:O	1.90	0.71
11:Y:200:TYR:HA	11:Y:201:SER:HB2	1.73	0.71
14:b:36:THR:CG2	14:b:46:ARG:HE	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	1.94	0.68
1:O:10:THR:HG23	20:O:403:HOH:O	1.92	0.68
5:E:58:ALA:O	5:E:59:HIS:CB	2.41	0.67
1:A:17:LYS:HE2	1:A:22:GLU:OE2	1.94	0.67
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.77	0.67
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.77	0.67
11:Y:36:ILE:CD1	11:Y:46:MET:CE	2.72	0.67
2:B:10:THR:OG1	20:B:401:HOH:O	2.13	0.66
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.78	0.66
3:C:47:LYS:CB	3:C:48:LYS:HA	2.26	0.66
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.45	0.65
3:C:47:LYS:CB	3:C:48:LYS:CA	2.75	0.65
11:K:36:ILE:HD11	11:K:46:MET:SD	2.37	0.64
11:Y:46:MET:HE1	11:Y:54:SER:CA	2.24	0.64
11:Y:36:ILE:HD11	11:Y:46:MET:SD	2.37	0.64
2:P:25[B]:MET:HA	2:P:25[B]:MET:CE	2.25	0.64
4:R:96:THR:OG1	20:R:401:HOH:O	2.15	0.63
11:Y:159:ARG:HE	11:Y:163:GLN:HE21	1.47	0.63
9:W:13:MET:HE1	9:W:166:ILE:N	2.13	0.63
3:C:5:ARG:NH1	4:D:125:GLU:OE2	2.29	0.62
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.80	0.62
6:F:105:ASN:ND2	20:F:402:HOH:O	2.32	0.62
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.14	0.62
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.81	0.62
15:a:302:CL:CL	15:a:303:CL:CL	2.92	0.61
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.33	0.61
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.82	0.61
9:W:13:MET:HE3	9:W:162:LEU:HD12	1.83	0.61
5:E:101[A]:ARG:NH1	20:E:401:HOH:O	2.34	0.59
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.49	0.59
6:F:151:ILE:N	6:F:151:ILE:HD12	2.17	0.59
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.85	0.59
4:R:129:ASP:CB	4:R:130:PRO:CD	2.81	0.59
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.35	0.58
9:W:27:PHE:HB3	9:W:35:THR:HG22	1.86	0.58
5:S:101:ARG:NH1	20:S:403:HOH:O	2.34	0.58
5:S:65[A]:HIS:ND1	20:S:402:HOH:O	2.31	0.58
7:U:195:VAL:O	7:U:199:ILE:HG23	2.04	0.58
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.69	0.58
11:K:142:ARG:NH1	10:X:166:GLU:OE2	2.36	0.58
8:V:139:GLU:OE1	14:b:30:ARG:HD3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:118:ILE:HG13	7:U:138:MET:HE1	1.86	0.57
9:I:27:PHE:HB3	9:I:35:THR:HG22	1.86	0.57
2:P:246:LYS:HE3	2:P:246:LYS:N	2.20	0.57
10:X:38:MET:HE1	10:X:61:GLN:HB2	1.87	0.56
3:C:35:VAL:HG13	3:C:191:VAL:HG22	1.88	0.56
14:b:15:LEU:HD23	14:b:45:CYS:SG	2.46	0.56
9:I:13[A]:MET:CE	9:I:166:ILE:HB	2.33	0.56
6:T:205:LYS:O	6:T:206:ASP:CG	2.49	0.56
8:V:213:THR:HB	9:W:198:THR:OG1	2.06	0.56
5:S:152[B]:ASN:ND2	20:S:405:HOH:O	2.38	0.55
11:Y:46:MET:HE2	11:Y:53:CYS:C	2.32	0.55
13:M:5:MET:HE2	14:N:117:MET:HB3	1.89	0.55
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.90	0.54
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.38	0.54
13:a:5:MET:HE2	14:b:117:MET:HB3	1.88	0.54
10:J:166:GLU:OE2	11:Y:142[A]:ARG:NH1	2.41	0.54
5:S:18[B]:ARG:HG3	5:S:19:ILE:N	2.05	0.54
2:P:48:GLU:HB2	2:P:201:MET:HE2	1.90	0.53
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.38	0.53
3:C:47:LYS:CB	3:C:48:LYS:C	2.82	0.53
20:G:572:HOH:O	14:N:72:ASN:HB2	2.08	0.53
10:J:38:MET:HE1	10:J:61:GLN:HB2	1.90	0.53
6:F:219:LEU:HD22	20:F:486:HOH:O	2.08	0.53
8:H:77:VAL:HG12	8:H:111:TYR:OH	2.09	0.53
11:K:98[B]:MET:HE3	11:K:117:SER:HB3	1.91	0.53
4:D:203:LYS:HE2	4:D:210:LEU:HB3	1.91	0.52
8:H:77:VAL:CB	20:H:549:HOH:O	2.52	0.52
6:F:150:MET:C	6:F:151:ILE:HD12	2.34	0.52
1:A:58[B]:GLU:CD	1:A:58[B]:GLU:H	2.17	0.52
15:B:301:CL:CL	15:B:302:CL:CL	3.01	0.52
10:J:99[A]:HIS:CD2	20:J:429:HOH:O	2.62	0.52
11:Y:37:GLU:HG2	11:Y:185:TRP:CZ2	2.44	0.52
2:B:63:GLU:N	2:B:212:GLU:OE2	2.38	0.52
2:B:33:THR:HB	2:B:166:ASN:O	2.09	0.52
2:B:44:LEU:C	2:B:44:LEU:HD12	2.36	0.51
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.92	0.51
3:Q:12:PRO:HA	4:R:26:TYR:CD2	2.45	0.51
1:A:206:ASN:C	1:A:206:ASN:HD22	2.18	0.51
5:S:237:GLU:O	5:S:238:GLU:CB	2.58	0.51
3:C:203:GLY:CA	3:C:204:LYS:CB	2.89	0.51
14:N:15:LEU:HD23	14:N:45:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:202:ASP:OD1	6:T:204:VAL:HG12	2.11	0.51
8:H:112:SER:HB2	8:H:127[B]:MET:HE3	1.92	0.51
12:L:25:SER:OG	20:L:401:HOH:O	2.19	0.51
10:J:49:GLU:O	10:J:53:THR:HG23	2.11	0.51
3:C:42:VAL:HG22	3:C:210:VAL:HG22	1.92	0.50
7:G:113:MET:HE1	8:H:69:SER:OG	2.11	0.50
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.40	0.50
4:D:96:THR:OG1	20:D:401:HOH:O	2.19	0.50
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.11	0.50
2:P:44:LEU:C	2:P:44:LEU:HD12	2.37	0.50
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.60	0.50
11:Y:46:MET:HE2	11:Y:53:CYS:O	2.12	0.50
8:H:77:VAL:CG1	20:H:549:HOH:O	2.60	0.50
11:Y:46:MET:HE2	11:Y:53:CYS:HB3	1.94	0.50
7:U:58:ASP:O	7:U:59:LYS:CB	2.59	0.50
13:a:92:LEU:HD12	13:a:112:ILE:HD11	1.92	0.50
12:L:72:LEU:HD22	12:L:83:MET:SD	2.52	0.50
10:J:38:MET:HE2	10:J:38:MET:HA	1.94	0.50
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.44	0.49
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.93	0.49
2:P:33:THR:HB	2:P:166:ASN:O	2.11	0.49
6:F:243:LEU:O	6:F:244:LYS:C	2.56	0.49
11:K:37:GLU:HG2	11:K:185:TRP:CZ2	2.47	0.49
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.95	0.49
3:C:106:TYR:CD1	3:C:106:TYR:C	2.90	0.49
7:G:42:VAL:HG13	7:G:198:ALA:HB2	1.95	0.49
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.42	0.49
6:T:24:GLU:HA	6:T:27:MET:HE3	1.93	0.49
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.94	0.49
1:O:206:ASN:C	1:O:206:ASN:HD22	2.21	0.49
12:Z:72:LEU:HD22	12:Z:83:MET:SD	2.52	0.49
10:J:67:TYR:CE2	10:J:75:LEU:HD21	2.47	0.49
4:R:151:PRO:O	4:R:152:GLN:HG3	2.13	0.49
4:R:203:LYS:HE2	4:R:210:LEU:HB3	1.95	0.49
11:K:36:ILE:CD1	11:K:46:MET:SD	3.01	0.48
13:M:114:GLY:HA2	13:M:192:VAL:HG11	1.95	0.48
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.94	0.48
7:G:11:ARG:HG2	7:G:11:ARG:HH11	1.78	0.48
10:X:49:GLU:O	10:X:53:THR:HG23	2.13	0.48
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.95	0.48
20:H:428:HOH:O	13:a:216:SER:HB3	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:92:LEU:CD2	13:M:112:ILE:HD11	2.44	0.48
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.44	0.48
12:L:144:MET:CE	12:L:185:ARG:HB2	2.42	0.48
2:P:53:HIS:O	2:P:54:LYS:HB2	2.13	0.48
6:T:152:ASP:OD1	6:T:156:VAL:HG12	2.14	0.48
11:Y:41:TYR:CD2	11:Y:74:ARG:CZ	2.97	0.48
13:M:5:MET:HE3	14:N:117:MET:HB2	1.95	0.48
2:B:33:THR:HG22	2:B:166:ASN:HB3	1.95	0.48
3:C:50:VAL:O	3:C:51:ALA:HB3	2.14	0.48
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.13	0.48
11:Y:69:LEU:O	11:Y:72:LYS:CE	2.62	0.48
2:P:63:GLU:N	2:P:212:GLU:OE2	2.39	0.48
9:W:35:THR:HG21	20:W:450:HOH:O	2.14	0.47
11:Y:200:TYR:HA	11:Y:201:SER:CB	2.44	0.47
2:P:33:THR:HG22	2:P:166:ASN:HB3	1.96	0.47
13:a:96:MET:HE3	13:a:127:MET:HA	1.96	0.47
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.96	0.47
9:W:13:MET:CE	9:W:166:ILE:HB	2.42	0.47
14:N:36:THR:HB	20:N:553:HOH:O	2.13	0.47
10:X:38:MET:HE2	10:X:38:MET:HA	1.96	0.47
13:a:112:ILE:HD12	13:a:112:ILE:N	2.29	0.47
10:J:27[A]:GLN:HE21	10:J:29:LYS:N	2.13	0.47
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.92	0.47
1:A:88[B]:ARG:NH2	20:A:404:HOH:O	2.43	0.47
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.26	0.47
4:D:164:GLN:OE1	5:E:58:ALA:HB2	2.14	0.47
8:H:195:LYS:HG2	8:H:196:GLY:O	2.14	0.47
15:R:301:CL:CL	20:R:510:HOH:O	2.58	0.47
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	2.14	0.47
6:T:170:GLN:O	6:T:174:THR:HG23	2.15	0.47
5:E:150:SER:O	5:E:151:ALA:HB3	2.15	0.47
4:R:32:LYS:HG2	20:R:510:HOH:O	2.14	0.47
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.03	0.47
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.96	0.47
4:R:204:GLN:NE2	20:R:404:HOH:O	2.46	0.47
6:T:24:GLU:HA	6:T:27:MET:CE	2.45	0.47
5:E:171:TYR:C	5:E:171:TYR:CD2	2.93	0.47
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.97	0.46
7:G:117:ARG:NH2	20:G:401:HOH:O	2.35	0.46
11:K:96:LEU:HB3	11:K:98[B]:MET:HE2	1.96	0.46
11:Y:37:GLU:OE2	11:Y:187[A]:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:46:MET:CE	11:Y:53:CYS:C	2.89	0.46
1:A:17:LYS:CE	1:A:22:GLU:OE2	2.62	0.46
6:T:151:ILE:N	6:T:151:ILE:HD12	2.30	0.46
7:U:42:VAL:HG13	7:U:198:ALA:HB2	1.96	0.46
4:D:151:PRO:O	4:D:152:GLN:HG3	2.16	0.46
2:P:237:ILE:O	2:P:241:GLU:HG2	2.16	0.46
8:H:216:ILE:HD13	9:I:195:THR:HG23	1.96	0.46
13:a:114:GLY:HA2	13:a:192:VAL:HG11	1.97	0.46
10:X:86:ARG:HD3	10:X:90:ASP:OD1	2.15	0.46
5:E:202:GLU:HG2	5:E:203:GLN:N	2.30	0.46
20:G:462:HOH:O	8:H:72:ARG:HD3	2.15	0.46
11:Y:10:ARG:NH2	11:Y:147:ASP:OD1	2.44	0.46
14:N:191:LEU:H	14:N:194:GLN:HE21	1.62	0.46
5:S:238:GLU:CB	5:S:239:ARG:C	2.88	0.46
7:G:49[B]:VAL:HG22	7:G:219:VAL:HG12	1.98	0.46
12:L:125:ASP:CG	12:L:129:SER:HB3	2.41	0.45
5:S:61:LYS:HD2	5:S:64:LEU:HD21	1.97	0.45
6:T:173:LYS:HB3	6:T:173:LYS:HE2	1.63	0.45
11:Y:97:SER:O	11:Y:98[B]:MET:HG3	2.15	0.45
4:R:182:GLN:HA	5:S:56:LEU:HD11	1.97	0.45
6:T:150:MET:C	6:T:151:ILE:HD12	2.41	0.45
6:F:170:GLN:O	6:F:174:THR:HG23	2.17	0.45
3:Q:204:LYS:HA	3:Q:205:ASN:C	2.41	0.45
10:J:86:ARG:HD3	10:J:90:ASP:OD1	2.16	0.45
13:M:96:MET:HE3	13:M:127:MET:HA	1.98	0.45
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.45	0.45
11:Y:36:ILE:CD1	11:Y:46:MET:SD	3.03	0.45
1:A:221:THR:HG22	1:A:224:GLU:HG3	1.98	0.45
13:M:126:ASP:OD2	13:M:126:ASP:C	2.57	0.45
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.51	0.45
10:X:1:MET:HE2	10:X:1:MET:HB3	1.71	0.45
3:C:47:LYS:HA	3:C:205:ASN:HB2	1.98	0.45
14:N:173:GLY:HA2	13:a:209:TRP:CH2	2.51	0.45
5:S:150:SER:O	5:S:151:ALA:HB3	2.16	0.45
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.99	0.45
7:U:113:MET:HE1	8:V:69:SER:OG	2.16	0.45
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.47	0.44
10:X:67:TYR:CD1	10:X:75:LEU:HG	2.53	0.44
12:Z:172:MET:HE1	12:Z:197:ILE:HD11	1.98	0.44
1:A:51:GLN:HE22	1:A:58[B]:GLU:HB3	1.81	0.44
6:F:64:LYS:NZ	20:F:407:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2:PHE:HE2	20:S:406:HOH:O	1.99	0.44
10:X:161:ARG:HD3	20:X:514:HOH:O	2.16	0.44
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.99	0.44
11:Y:36:ILE:HD11	11:Y:46:MET:CE	2.48	0.44
8:H:153:ASN:ND2	20:H:405:HOH:O	2.51	0.44
1:A:54:ILE:HD11	7:G:189:TRP:CD2	2.52	0.44
3:C:40:ILE:HD11	3:C:210:VAL:CG1	2.47	0.44
10:J:67:TYR:CD1	10:J:75:LEU:HG	2.53	0.44
11:Y:3:THR:OG1	11:Y:132:GLY:HA3	2.18	0.44
9:I:13[A]:MET:HE1	9:I:166:ILE:CA	2.47	0.44
2:P:246:LYS:O	2:P:249:ARG:NH2	2.51	0.44
13:a:1:THR:OG1	13:a:59:ASP:OD2	2.34	0.44
2:B:149:GLN:O	2:B:156:TYR:HA	2.17	0.43
5:S:202:GLU:CD	5:S:202:GLU:H	2.25	0.43
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.99	0.43
4:D:35:SER:OG	4:D:66:LYS:NZ	2.49	0.43
10:X:67:TYR:CE2	10:X:75:LEU:HD21	2.54	0.43
5:S:50:LYS:CB	5:S:59:HIS:HB3	2.47	0.43
11:Y:2:THR:N	19:Y:306:6V7:O28	2.52	0.43
11:Y:46:MET:CE	11:Y:53:CYS:O	2.66	0.43
11:Y:67:TYR:CD2	11:Y:67:TYR:C	2.97	0.43
1:A:52:LYS:CB	20:A:423:HOH:O	2.66	0.43
14:b:191:LEU:H	14:b:194:GLN:HE21	1.65	0.43
3:C:169:ARG:NH2	20:C:403:HOH:O	2.51	0.43
5:S:200:PRO:HB2	5:S:203:GLN:HG2	2.00	0.43
14:b:36:THR:HG21	14:b:46:ARG:HE	1.82	0.43
1:A:73:LEU:CD2	1:A:135:ILE:HG12	2.49	0.42
11:K:5:LEU:HD12	11:K:5:LEU:C	2.44	0.42
3:C:47:LYS:CB	3:C:48:LYS:O	2.68	0.42
9:I:158:ASP:OD1	9:I:161:HIS:HD2	2.02	0.42
7:U:138:MET:HE2	7:U:154:CYS:SG	2.60	0.42
12:Z:125:ASP:CG	12:Z:129:SER:HB3	2.45	0.42
2:B:76:VAL:HG12	2:B:134:LEU:HG	2.00	0.42
11:K:41:TYR:CD2	11:K:74:ARG:CZ	3.02	0.42
11:Y:187[A]:ARG:HE	11:Y:187[A]:ARG:HB2	1.69	0.42
13:a:214:MET:O	13:a:216:SER:N	2.53	0.42
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.54	0.42
13:M:60:PHE:CZ	13:M:64:LYS:HD2	2.55	0.42
2:P:8:ARG:HH21	3:Q:5:ARG:HD2	1.85	0.42
4:R:35:SER:OG	4:R:66:LYS:NZ	2.52	0.42
1:A:179:GLU:CB	20:A:424:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:60:PHE:CZ	13:a:64:LYS:HD2	2.55	0.42
11:Y:69:LEU:O	11:Y:72:LYS:HE3	2.19	0.42
15:M:302:CL:CL	15:N:301:CL:CL	3.11	0.42
1:O:73:LEU:CD2	1:O:135:ILE:HG12	2.49	0.42
7:U:195:VAL:HG13	7:U:196:GLU:OE1	2.19	0.42
7:G:77:GLY:HA3	7:G:227:PHE:CD1	2.55	0.41
10:J:10:PRO:HG3	10:J:150:THR:HA	2.01	0.41
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.20	0.41
18:U:302:1PE:H252	20:U:498:HOH:O	2.21	0.41
8:H:1:THR:HB	15:H:303:CL:CL	2.57	0.41
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.51	0.41
7:U:80[A]:MET:CE	7:U:91:VAL:HG23	2.51	0.41
6:F:157:SER:O	7:G:88:ARG:NH2	2.54	0.41
10:J:121:LEU:O	10:J:122:ALA:HB3	2.21	0.41
11:K:84:LEU:HD21	11:K:100:THR:HG21	2.02	0.41
11:K:116:ASP:OD1	11:K:116:ASP:C	2.63	0.41
12:L:148:LEU:CD2	12:L:178:VAL:HG12	2.51	0.41
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.51	0.41
2:P:232:GLU:O	2:P:236:LEU:HD13	2.21	0.41
6:T:191:LYS:HB3	6:T:238:TYR:CD1	2.56	0.41
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	2.21	0.41
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.21	0.41
2:B:14:PRO:HA	3:C:21:TYR:CD1	2.55	0.41
3:C:201:SER:O	3:C:202:GLY:C	2.63	0.41
6:F:216:VAL:O	6:F:216:VAL:HG13	2.21	0.41
11:K:2:THR:N	19:K:305:6V7:O28	2.54	0.41
9:W:124:ASP:OD1	9:W:124:ASP:C	2.64	0.41
4:D:69:GLU:HB2	4:D:226:PHE:CE2	2.56	0.41
7:G:226:LYS:HE2	7:G:226:LYS:HB2	1.94	0.41
12:L:172:MET:HE1	12:L:197:ILE:HD11	2.02	0.40
12:L:146:GLN:HB3	12:L:147:PRO:HD3	2.02	0.40
7:U:43:ARG:HB3	7:U:151:VAL:HG13	2.03	0.40
11:Y:5:LEU:HD12	11:Y:5:LEU:C	2.46	0.40
11:Y:159:ARG:HE	11:Y:163:GLN:NE2	2.15	0.40
2:B:241:GLU:HG2	20:B:514:HOH:O	2.21	0.40
1:O:230:ALA:O	1:O:231:ALA:CB	2.69	0.40
7:U:77:GLY:HA3	7:U:227:PHE:CD1	2.57	0.40
6:F:34:SER:OG	6:F:65:ARG:NH1	2.54	0.40
2:P:2:SER:HB3	5:S:123:TYR:CE2	2.56	0.40
3:C:41:VAL:CG2	3:C:211:MET:HB3	2.51	0.40
3:C:85[B]:ASN:HB3	20:C:427:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:88:LEU:HB3	10:J:122:ALA:HB2	2.02	0.40
12:L:41:PRO:HB3	20:L:401:HOH:O	2.21	0.40
6:T:110:HIS:HD2	20:T:358:HOH:O	2.04	0.40
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.21	0.40
14:b:148[B]:MET:HE1	14:b:156:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/234 (99%)	221 (96%)	6 (3%)	4 (2%)	7	3
1	O	228/234 (97%)	217 (95%)	7 (3%)	4 (2%)	6	3
2	B	248/261 (95%)	238 (96%)	9 (4%)	1 (0%)	30	27
2	P	248/261 (95%)	235 (95%)	10 (4%)	3 (1%)	10	6
3	C	236/248 (95%)	223 (94%)	7 (3%)	6 (2%)	4	1
3	Q	236/248 (95%)	221 (94%)	6 (2%)	9 (4%)	2	1
4	D	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	9	5
4	R	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	9	5
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	30	27
5	S	238/263 (90%)	228 (96%)	9 (4%)	1 (0%)	30	27
6	F	241/255 (94%)	238 (99%)	3 (1%)	0	100	100
6	T	239/255 (94%)	233 (98%)	4 (2%)	2 (1%)	16	11
7	G	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	30	27
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	24	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	199/204 (98%)	197 (99%)	2 (1%)	0	100	100
11	Y	202/204 (99%)	199 (98%)	2 (1%)	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%)	209 (97%)	6 (3%)	0	100	100
13	a	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
14	N	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
14	b	202/205 (98%)	201 (100%)	1 (0%)	0	100	100
All	All	6213/6458 (96%)	6039 (97%)	134 (2%)	40 (1%)	21	17

All (40) 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
1	O	231	ALA
2	P	52	ILE
2	P	54	LYS
3	Q	206	ILE
3	Q	221	ASN
4	R	128	ALA
4	R	130	PRO
5	S	238	GLU
11	Y	201	SER
1	A	176	ARG
2	B	203	VAL
3	C	50	VAL
3	C	200	GLN
3	C	204	LYS
3	C	216	SER
4	D	176	GLY

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Mol	Chain	Res	Type
1	O	176	ARG
3	Q	47	LYS
3	Q	50	VAL
3	Q	201	SER
3	Q	216	SER
6	T	7	TYR
6	T	206	ASP
8	V	203	ARG
3	C	51	ALA
4	D	175[A]	GLU
4	D	175[B]	GLU
4	R	129	ASP
7	U	58	ASP
1	A	50	LYS
3	Q	48	LYS
3	Q	51	ALA
3	C	203	GLY
3	Q	203	GLY
2	P	58	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	175 (95%)	10 (5%)	20	17
1	O	176/191 (92%)	166 (94%)	10 (6%)	18	15
2	B	200/221 (90%)	193 (96%)	7 (4%)	32	32
2	P	197/221 (89%)	185 (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%)	182 (96%)	7 (4%)	30	30
4	R	187/203 (92%)	183 (98%)	4 (2%)	47	52
5	E	192/223 (86%)	184 (96%)	8 (4%)	26	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	197/223 (88%)	189 (96%)	8 (4%)	27	26
6	F	199/212 (94%)	190 (96%)	9 (4%)	24	23
6	T	192/212 (91%)	186 (97%)	6 (3%)	35	37
7	G	202/207 (98%)	194 (96%)	8 (4%)	28	27
7	U	186/207 (90%)	180 (97%)	6 (3%)	34	35
8	H	181/195 (93%)	173 (96%)	8 (4%)	25	24
8	V	172/195 (88%)	160 (93%)	12 (7%)	14	10
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%)	159 (96%)	7 (4%)	26	25
10	X	165/170 (97%)	161 (98%)	4 (2%)	43	47
11	K	155/159 (98%)	148 (96%)	7 (4%)	24	23
11	Y	159/159 (100%)	155 (98%)	4 (2%)	42	45
12	L	175/178 (98%)	169 (97%)	6 (3%)	32	33
12	Z	175/178 (98%)	170 (97%)	5 (3%)	37	40
13	M	180/181 (99%)	176 (98%)	4 (2%)	45	50
13	a	178/181 (98%)	174 (98%)	4 (2%)	45	50
14	N	158/159 (99%)	156 (99%)	2 (1%)	61	68
14	b	158/159 (99%)	156 (99%)	2 (1%)	61	68
All	All	5036/5366 (94%)	4851 (96%)	185 (4%)	31	30

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	53	SER
1	A	61	VAL
1	A	174	GLU
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

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Mol	Chain	Res	Type
2	B	43	VAL
2	B	59	VAL
2	B	190	LEU
2	B	194	ILE
2	B	229	LYS
2	B	249	ARG
3	C	2	SER
3	C	35	VAL
3	C	45	VAL
3	C	113	SER
3	C	163	ARG
3	C	179	GLU
3	C	205	ASN
3	C	208	LEU
3	C	210	VAL
3	C	225	ILE
4	D	9	ASP
4	D	46	VAL
4	D	126	GLU
4	D	139	VAL
4	D	182	GLN
4	D	199	LEU
4	D	231	LYS
5	E	29	VAL
5	E	61	LYS
5	E	95	SER
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	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

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Mol	Chain	Res	Type
7	G	88	ARG
7	G	182	LYS
7	G	183	VAL
7	G	206	LEU
7	G	226	LYS
7	G	232	GLU
8	H	6	VAL
8	H	12	ILE
8	H	22	GLU
8	H	65	LEU
8	H	68	LEU
8	H	183	LEU
8	H	199	LEU
8	H	215	LYS
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	155	ARG
11	K	13	VAL
11	K	43	LEU
11	K	139	VAL
11	K	148	LEU
11	K	175	VAL
11	K	188	VAL
11	K	193	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	72	LEU
12	L	172	MET
12	L	174	LEU
12	L	207	THR
13	M	133	GLU
13	M	154	LEU
13	M	156	LYS
13	M	216	SER
14	N	36	THR
14	N	146	GLU

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Mol	Chain	Res	Type
1	O	10	THR
1	O	53	SER
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	235	GLN
2	P	236	LEU
2	P	246	LYS
2	P	249	ARG
3	Q	2	SER
3	Q	45	VAL
3	Q	98	VAL
3	Q	113	SER
3	Q	163	ARG
3	Q	170	GLU
3	Q	179	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	225	ILE
3	Q	227	LYS
4	R	9	ASP
4	R	46	VAL
4	R	139	VAL
4	R	182	GLN
5	S	29	VAL
5	S	45	VAL
5	S	95	SER
5	S	101	ARG
5	S	181	GLU

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Mol	Chain	Res	Type
5	S	202	GLU
5	S	208	LYS
5	S	234	GLU
6	T	17	ASP
6	T	53	VAL
6	T	81	LEU
6	T	87	LEU
6	T	190	VAL
6	T	240	LYS
7	U	42	VAL
7	U	78	CYS
7	U	151	VAL
7	U	182	LYS
7	U	199	ILE
7	U	206	LEU
8	V	6	VAL
8	V	12	ILE
8	V	22	GLU
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	132	LEU
8	V	183	LEU
8	V	199	LEU
8	V	213	THR
8	V	215	LYS
9	W	35	THR
9	W	69	ARG
10	X	1	MET
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
11	Y	13	VAL
11	Y	139	VAL
11	Y	148	LEU
11	Y	193	VAL
12	Z	72	LEU
12	Z	172	MET
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL

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Mol	Chain	Res	Type
13	a	71	VAL
13	a	92	LEU
13	a	154	LEU
13	a	198	GLU
14	b	30	ARG
14	b	36	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	94	GLN
1	A	108	GLN
1	A	111	GLN
1	A	206	ASN
2	B	40	ASN
2	B	51	ASN
2	B	102	GLN
2	B	109	GLN
2	B	146	GLN
2	B	198	ASN
2	B	240	HIS
3	C	54	GLN
3	C	175	ASN
4	D	204	GLN
4	D	227	HIS
5	E	8	ASN
5	E	65	HIS
6	F	143	ASN
7	G	100	ASN
7	G	193	GLN
8	H	80	ASN
8	H	153	ASN
8	H	172	ASN
9	I	80	GLN
9	I	161	HIS
10	J	61	GLN
10	J	63	ASN
10	J	101	ASN
10	J	132	HIS
11	K	63	GLN
11	K	120	ASN

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Mol	Chain	Res	Type
12	L	77	HIS
12	L	163	HIS
13	M	47	ASN
13	M	65	GLN
13	M	162	GLN
13	M	188	GLN
14	N	111	GLN
14	N	194	GLN
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	109	GLN
2	P	142	HIS
2	P	198	ASN
2	P	235	GLN
2	P	240	HIS
3	Q	18	GLN
3	Q	94	HIS
3	Q	175	ASN
4	R	97	GLN
4	R	186	HIS
4	R	227	HIS
5	S	8	ASN
5	S	86	ASN
6	T	68	ASN
6	T	110	HIS
6	T	143	ASN
7	U	128	ASN
8	V	172	ASN
9	W	32	GLN
10	X	24	ASN
10	X	61	GLN
10	X	63	ASN
10	X	174	ASN
11	Y	63	GLN
11	Y	163	GLN
12	Z	79	ASN
13	a	47	ASN
13	a	65	GLN

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Mol	Chain	Res	Type
13	a	89	HIS
13	a	162	GLN
13	a	188	GLN
14	b	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	YCM	Q	63	3	7,9,10	1.54	1 (14%)	5,10,12	3.02	4 (80%)
3	YCM	C	63	3	7,9,10	1.12	1 (14%)	5,10,12	1.55	2 (40%)
5	6V1	S	148	5	13,15,16	1.99	4 (30%)	10,20,22	2.93	5 (50%)
10	6V1	J	91	10	13,15,16	2.28	4 (30%)	10,20,22	4.48	7 (70%)
10	6V1	X	91	10	13,15,16	1.75	3 (23%)	10,20,22	4.83	7 (70%)
7	6V1	U	161	7	13,15,16	1.83	3 (23%)	10,20,22	3.27	5 (50%)
7	YCM	U	137	7	7,9,10	1.11	0	5,10,12	1.89	2 (40%)
5	6V1	E	148	5	13,15,16	2.13	2 (15%)	10,20,22	3.51	5 (50%)
7	6V1	G	161	7	13,15,16	1.38	3 (23%)	10,20,22	2.58	6 (60%)
7	6V1	U	47	7	13,15,16	2.22	4 (30%)	10,20,22	1.99	2 (20%)
7	YCM	G	137	7	7,9,10	1.96	3 (42%)	5,10,12	2.21	2 (40%)
7	6V1	G	47	7	13,15,16	2.06	3 (23%)	10,20,22	1.19	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YCM	Q	63	3	-	3/6/8/10	-
3	YCM	C	63	3	-	1/6/8/10	-
5	6V1	S	148	5	-	1/6/25/27	0/1/1/1
10	6V1	J	91	10	-	2/6/25/27	0/1/1/1
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
7	6V1	U	161	7	-	3/6/25/27	0/1/1/1
7	YCM	U	137	7	-	2/6/8/10	-
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1
7	6V1	G	161	7	-	3/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	0/6/25/27	0/1/1/1
7	YCM	G	137	7	-	2/6/8/10	-
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	C1-SG	-6.56	1.76	1.83
5	E	148	6V1	CB-SG	-5.80	1.76	1.82
7	U	47	6V1	CB-SG	-5.65	1.76	1.82
5	S	148	6V1	CB-SG	-4.90	1.77	1.82
7	G	47	6V1	CB-SG	-4.63	1.77	1.82
7	U	161	6V1	CB-SG	-4.47	1.77	1.82
10	X	91	6V1	C1-SG	-4.32	1.78	1.83
7	G	47	6V1	C2-N3	-3.79	1.33	1.38
7	G	47	6V1	C4-N3	-3.52	1.33	1.38
3	Q	63	YCM	CD-SG	-3.28	1.73	1.81
7	U	47	6V1	C1-SG	-3.28	1.79	1.83
7	G	137	YCM	CD-SG	3.26	1.89	1.81
7	G	137	YCM	CE-NZ2	3.04	1.42	1.32
5	S	148	6V1	C2-N3	-3.02	1.34	1.38
7	U	47	6V1	C2-N3	-2.99	1.34	1.38
7	U	161	6V1	C4-N3	-2.88	1.34	1.38
5	S	148	6V1	C5-C4	2.86	1.55	1.50
10	X	91	6V1	C4-N3	-2.84	1.34	1.38
5	E	148	6V1	C4-N3	-2.82	1.34	1.38
7	G	161	6V1	C4-N3	-2.72	1.34	1.38
7	U	47	6V1	C4-N3	-2.65	1.34	1.38
7	U	161	6V1	C1-SG	-2.64	1.80	1.83
5	S	148	6V1	C4-N3	-2.57	1.34	1.38
10	J	91	6V1	C4-N3	-2.44	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	CB-SG	2.42	1.84	1.82
10	X	91	6V1	O7-C2	2.41	1.26	1.22
3	C	63	YCM	CD-SG	-2.22	1.76	1.81
7	G	137	YCM	CB-SG	-2.18	1.72	1.81
7	G	161	6V1	C2-N3	-2.16	1.35	1.38
7	G	161	6V1	C1-SG	-2.12	1.80	1.83
10	J	91	6V1	C2-N3	2.08	1.41	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	O7-C2-N3	7.77	133.57	124.14
10	J	91	6V1	O7-C2-N3	7.62	133.38	124.14
10	X	91	6V1	C5-C4-N3	7.20	112.60	108.07
5	E	148	6V1	C2-N3-C4	-7.18	108.86	113.07
10	J	91	6V1	C5-C4-N3	6.82	112.36	108.07
10	X	91	6V1	C2-N3-C4	-6.46	109.29	113.07
10	X	91	6V1	C6-N3-C2	6.39	130.86	123.37
7	U	161	6V1	C2-N3-C4	-6.27	109.40	113.07
10	J	91	6V1	C6-N3-C2	6.25	130.69	123.37
5	S	148	6V1	C2-N3-C4	-6.19	109.45	113.07
5	E	148	6V1	C6-N3-C2	5.32	129.60	123.37
7	U	161	6V1	C5-C4-N3	5.31	111.41	108.07
10	J	91	6V1	C2-N3-C4	-5.29	109.98	113.07
5	E	148	6V1	C5-C4-N3	5.09	111.27	108.07
5	S	148	6V1	C5-C4-N3	4.71	111.03	108.07
7	U	47	6V1	C5-C4-N3	4.43	110.85	108.07
7	G	161	6V1	O8-C4-N3	4.05	128.28	123.94
10	X	91	6V1	O7-C2-C1	-4.04	115.73	124.52
7	U	161	6V1	O8-C4-C5	-3.82	121.68	127.28
7	G	161	6V1	O8-C4-C5	-3.81	121.70	127.28
7	U	161	6V1	C6-N3-C2	3.75	127.76	123.37
7	G	137	YCM	CE-CD-SG	3.72	125.57	113.81
3	Q	63	YCM	CA-CB-SG	-3.47	100.72	113.51
10	J	91	6V1	O7-C2-C1	-3.41	117.09	124.52
10	J	91	6V1	C6-N3-C4	-3.40	118.50	122.52
7	U	47	6V1	C2-N3-C4	-3.39	111.08	113.07
10	X	91	6V1	O8-C4-C5	-3.38	122.33	127.28
3	Q	63	YCM	CE-CD-SG	-3.34	103.25	113.81
7	U	137	YCM	CE-CD-SG	3.27	124.13	113.81
3	Q	63	YCM	CB-CA-C	-3.26	101.96	110.80
10	X	91	6V1	C6-N3-C4	-3.26	118.67	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	63	YCM	CB-SG-CD	3.23	133.01	104.24
7	G	161	6V1	O7-C2-N3	3.11	127.92	124.14
5	E	148	6V1	CB-CA-C	-3.11	102.36	110.80
7	G	47	6V1	C2-N3-C4	-3.02	111.30	113.07
5	S	148	6V1	C6-N3-C4	2.98	126.05	122.52
7	G	161	6V1	C5-C4-N3	2.92	109.91	108.07
5	S	148	6V1	CB-CA-C	-2.83	103.12	110.80
7	U	161	6V1	O8-C4-N3	2.76	126.90	123.94
7	G	161	6V1	C2-N3-C4	-2.71	111.49	113.07
3	C	63	YCM	CB-CA-C	-2.45	104.16	110.80
10	J	91	6V1	O8-C4-C5	-2.33	123.88	127.28
7	G	161	6V1	C6-N3-C2	2.30	126.07	123.37
5	E	148	6V1	C3-C6-N3	2.12	118.94	111.66
3	C	63	YCM	CE-CD-SG	-2.12	107.13	113.81
5	S	148	6V1	O7-C2-N3	-2.03	121.68	124.14
7	G	137	YCM	CA-CB-SG	-2.02	106.05	113.51
7	U	137	YCM	CA-CB-SG	-2.02	106.05	113.51

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (21) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
7	G	137	YCM	CE-CD-SG-CB
7	U	137	YCM	CE-CD-SG-CB
5	S	148	6V1	C3-C6-N3-C4
7	G	161	6V1	N-CA-CB-SG
7	U	161	6V1	N-CA-CB-SG

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 83 ligands modelled in this entry, 70 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	1PE	W	303	-	15,15,15	0.56	0	14,14,14	0.40	0
18	1PE	Y	305	-	15,15,15	0.53	0	14,14,14	0.52	0
18	1PE	L	301	-	15,15,15	0.55	0	14,14,14	0.69	0
18	1PE	U	302	-	15,15,15	0.57	0	14,14,14	0.84	0
18	1PE	N	304	-	15,15,15	0.53	0	14,14,14	0.38	0
18	1PE	N	303	-	15,15,15	0.50	0	14,14,14	0.73	0
18	1PE	L	302	-	15,15,15	0.52	0	14,14,14	0.41	0
19	6V7	b	304	14	27,31,31	0.97	1 (3%)	37,42,42	1.62	5 (13%)
19	6V7	K	305	11	27,31,31	1.45	4 (14%)	37,42,42	1.86	11 (29%)
18	1PE	H	305	-	15,15,15	0.46	0	14,14,14	0.57	0
18	1PE	I	303	-	15,15,15	0.55	0	14,14,14	1.10	2 (14%)
19	6V7	Y	306	11	27,31,31	1.09	1 (3%)	37,42,42	1.55	7 (18%)
19	6V7	N	307	14	27,31,31	0.96	1 (3%)	37,42,42	1.64	8 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	W	303	-	-	6/13/13/13	-
18	1PE	Y	305	-	-	6/13/13/13	-
18	1PE	L	301	-	-	6/13/13/13	-
18	1PE	U	302	-	-	7/13/13/13	-
18	1PE	N	304	-	-	7/13/13/13	-
18	1PE	N	303	-	-	4/13/13/13	-
18	1PE	L	302	-	-	8/13/13/13	-
19	6V7	b	304	14	-	8/27/32/32	0/2/2/2
19	6V7	K	305	11	-	8/27/32/32	0/2/2/2
18	1PE	I	303	-	-	8/13/13/13	-
18	1PE	H	305	-	-	9/13/13/13	-
19	6V7	N	307	14	1/1/7/9	4/27/32/32	0/2/2/2
19	6V7	Y	306	11	1/1/7/9	5/27/32/32	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	305	6V7	C2-N3	4.16	1.40	1.34
19	Y	306	6V7	O12-C9	-3.52	1.33	1.43
19	K	305	6V7	C11-C9	-2.81	1.43	1.51
19	b	304	6V7	C10-C18	-2.25	1.47	1.52
19	K	305	6V7	C24-C15	2.10	1.43	1.39
19	N	307	6V7	C2-N3	-2.09	1.31	1.34
19	K	305	6V7	C5-C4	2.02	1.43	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	304	6V7	C11-C9-C10	5.49	123.15	112.29
19	K	305	6V7	C6-C1-C2	-4.64	113.08	118.63
19	b	304	6V7	C2-C7-N9	4.07	123.00	115.19
19	K	305	6V7	C21-C22-C8	3.95	120.36	115.32
19	N	307	6V7	O12-C9-C10	3.84	116.81	109.07
19	N	307	6V7	C2-C7-N9	3.79	122.48	115.19
19	N	307	6V7	B26-C21-C22	-3.76	105.22	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	306	6V7	C21-C22-C8	3.73	120.08	115.32
19	Y	306	6V7	O12-C9-C11	-3.59	98.94	109.68
19	K	305	6V7	O12-C9-C11	-3.42	99.45	109.68
19	K	305	6V7	C1-C2-N3	3.38	126.85	122.92
19	b	304	6V7	B26-C21-C22	-3.26	106.16	112.31
19	K	305	6V7	C7-C2-N3	-3.24	112.30	117.43
19	Y	306	6V7	B26-C21-C22	-2.88	106.88	112.31
19	Y	306	6V7	C11-C9-C10	2.86	117.95	112.29
19	K	305	6V7	C6-C5-C4	2.75	122.60	118.90
18	I	303	1PE	C25-OH5-C14	2.74	125.24	113.26
19	K	305	6V7	C5-C4-N3	-2.61	118.53	121.97
19	Y	306	6V7	C12-C8-C22	2.54	120.22	111.08
19	K	305	6V7	O12-C9-C10	2.53	114.18	109.07
19	b	304	6V7	O8-C7-C2	-2.37	115.85	121.08
19	N	307	6V7	C9-C10-N9	-2.36	105.44	111.70
19	N	307	6V7	C20-C24-C15	-2.33	117.88	120.54
19	K	305	6V7	C2-C7-N9	2.32	119.65	115.19
18	I	303	1PE	OH5-C25-C15	2.31	120.89	110.35
19	b	304	6V7	C9-C10-C18	2.24	116.20	111.32
19	N	307	6V7	C11-C9-C10	2.22	116.68	112.29
19	Y	306	6V7	C19-C17-C16	2.21	122.97	120.24
19	N	307	6V7	C1-C2-C7	2.17	123.09	119.57
19	Y	306	6V7	C2-C7-N9	2.16	119.33	115.19
19	N	307	6V7	C7-C2-N3	-2.12	114.08	117.43
19	K	305	6V7	C12-C8-C22	2.09	118.58	111.08
19	K	305	6V7	B26-C21-C22	-2.06	108.43	112.31

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	N	307	6V7	C9
19	Y	306	6V7	C9

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	K	305	6V7	C21-C22-C8-C12
19	Y	306	6V7	C21-C22-C8-C12
19	b	304	6V7	C18-C10-C9-C11
19	b	304	6V7	C18-C10-C9-O12
19	b	304	6V7	N9-C10-C9-C11
19	b	304	6V7	N9-C10-C9-O12

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Mol	Chain	Res	Type	Atoms
19	N	307	6V7	N3-C2-C7-O8
19	b	304	6V7	N3-C2-C7-O8
19	N	307	6V7	C1-C2-C7-O8
19	b	304	6V7	C1-C2-C7-O8
19	N	307	6V7	N3-C2-C7-N9
19	b	304	6V7	N3-C2-C7-N9
19	N	307	6V7	C1-C2-C7-N9
19	b	304	6V7	C1-C2-C7-N9
18	I	303	1PE	C15-C25-OH5-C14
19	Y	306	6V7	C1-C2-C7-O8
19	K	305	6V7	C1-C2-C7-O8
19	K	305	6V7	N3-C2-C7-O8
19	Y	306	6V7	N3-C2-C7-O8
19	K	305	6V7	N3-C2-C7-N9
19	Y	306	6V7	N3-C2-C7-N9
19	K	305	6V7	C1-C2-C7-N9
19	Y	306	6V7	C1-C2-C7-N9
18	L	302	1PE	OH4-C13-C23-OH3
18	L	301	1PE	C16-C26-OH6-C15
18	U	302	1PE	C24-C14-OH5-C25
18	N	304	1PE	OH4-C13-C23-OH3
18	Y	305	1PE	OH6-C15-C25-OH5
18	U	302	1PE	OH4-C13-C23-OH3
18	H	305	1PE	OH4-C13-C23-OH3
18	N	304	1PE	OH5-C14-C24-OH4
18	L	302	1PE	OH5-C14-C24-OH4
18	W	303	1PE	OH6-C15-C25-OH5
18	N	303	1PE	OH4-C13-C23-OH3
18	I	303	1PE	OH2-C12-C22-OH3
18	N	303	1PE	OH2-C12-C22-OH3
18	U	302	1PE	OH6-C15-C25-OH5
19	K	305	6V7	N9-C10-C9-O12
18	N	304	1PE	OH7-C16-C26-OH6
18	H	305	1PE	C24-C14-OH5-C25
18	L	302	1PE	OH7-C16-C26-OH6
18	Y	305	1PE	C16-C26-OH6-C15
18	L	302	1PE	OH6-C15-C25-OH5
18	H	305	1PE	OH7-C16-C26-OH6
18	L	302	1PE	OH2-C12-C22-OH3
18	N	303	1PE	OH7-C16-C26-OH6
18	H	305	1PE	OH5-C14-C24-OH4
19	K	305	6V7	C18-C10-C9-O12

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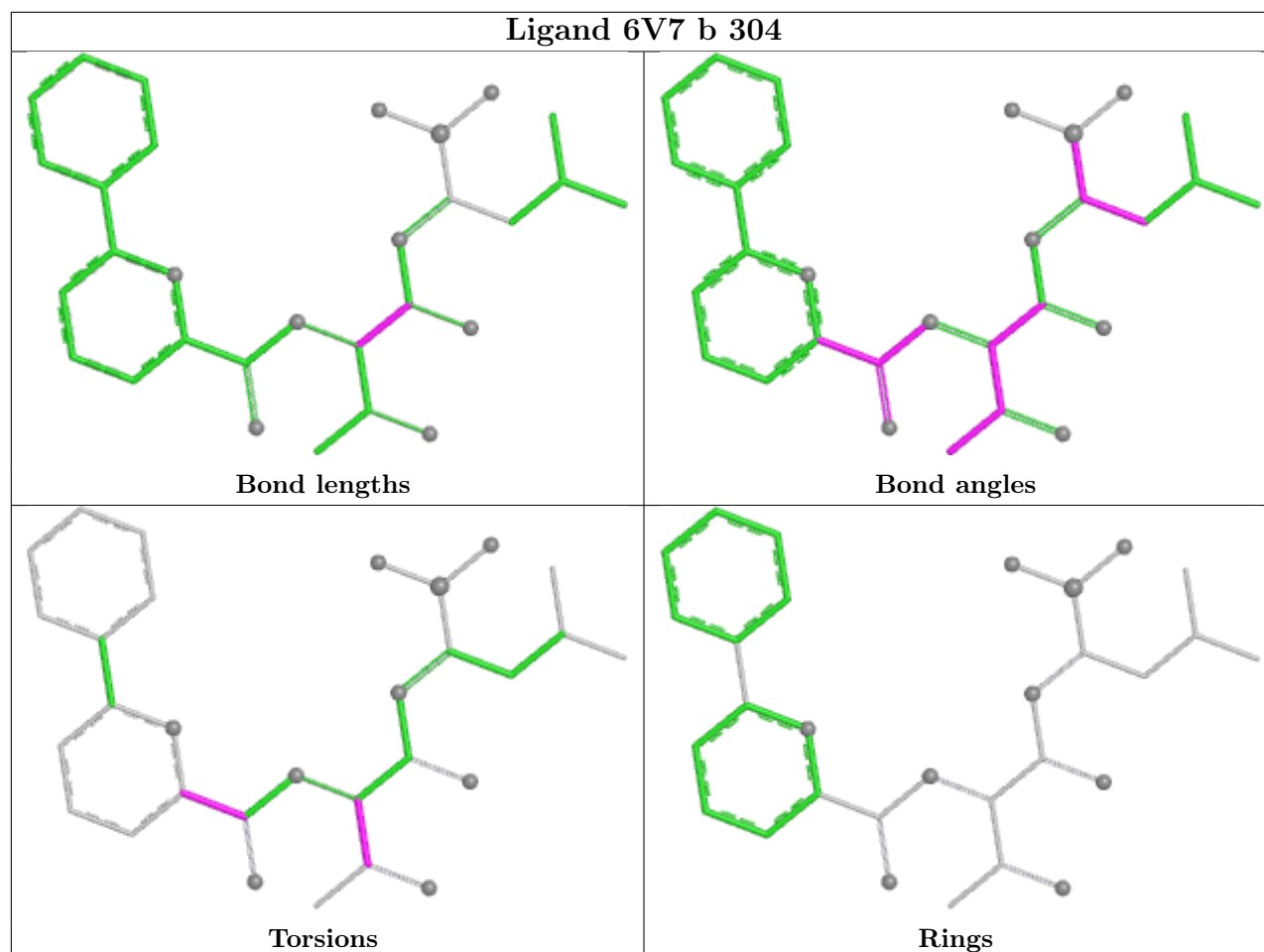
Mol	Chain	Res	Type	Atoms
18	U	302	1PE	OH7-C16-C26-OH6
18	I	303	1PE	OH6-C15-C25-OH5
18	H	305	1PE	OH2-C12-C22-OH3
18	N	304	1PE	OH2-C12-C22-OH3
18	W	303	1PE	OH7-C16-C26-OH6
18	U	302	1PE	C25-C15-OH6-C26
18	L	301	1PE	C13-C23-OH3-C22
18	L	301	1PE	C25-C15-OH6-C26
18	L	301	1PE	C24-C14-OH5-C25
18	L	302	1PE	C14-C24-OH4-C13
18	N	304	1PE	C25-C15-OH6-C26
18	I	303	1PE	C25-C15-OH6-C26
18	I	303	1PE	C24-C14-OH5-C25
18	H	305	1PE	C23-C13-OH4-C24
18	Y	305	1PE	C12-C22-OH3-C23
18	H	305	1PE	C16-C26-OH6-C15
18	H	305	1PE	C15-C25-OH5-C14
18	W	303	1PE	C24-C14-OH5-C25
18	I	303	1PE	C14-C24-OH4-C13
18	L	301	1PE	C23-C13-OH4-C24
18	W	303	1PE	C12-C22-OH3-C23
18	L	302	1PE	C23-C13-OH4-C24
18	W	303	1PE	C23-C13-OH4-C24
18	N	304	1PE	C23-C13-OH4-C24
18	I	303	1PE	C13-C23-OH3-C22
18	N	304	1PE	C14-C24-OH4-C13
18	H	305	1PE	OH6-C15-C25-OH5
18	Y	305	1PE	OH4-C13-C23-OH3
18	N	303	1PE	C12-C22-OH3-C23
18	I	303	1PE	OH5-C14-C24-OH4
18	Y	305	1PE	C15-C25-OH5-C14
18	L	301	1PE	OH2-C12-C22-OH3
18	L	302	1PE	C15-C25-OH5-C14
18	W	303	1PE	OH2-C12-C22-OH3
19	K	305	6V7	C18-C10-C9-C11
18	U	302	1PE	C14-C24-OH4-C13
18	U	302	1PE	OH5-C14-C24-OH4
18	Y	305	1PE	OH7-C16-C26-OH6

There are no ring outliers.

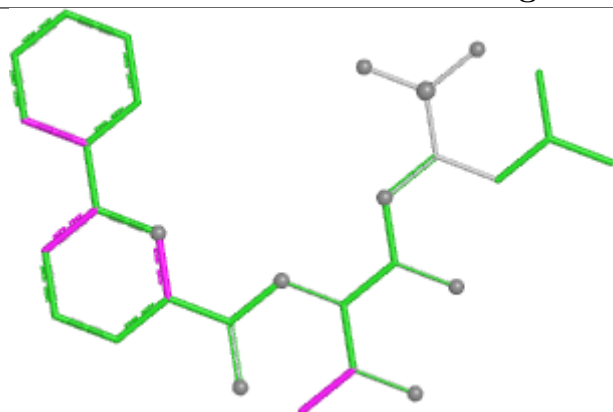
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	U	302	1PE	1	0
19	K	305	6V7	1	0
19	Y	306	6V7	1	0

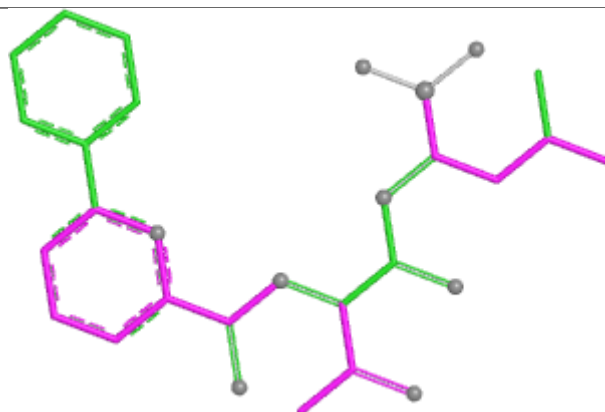
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



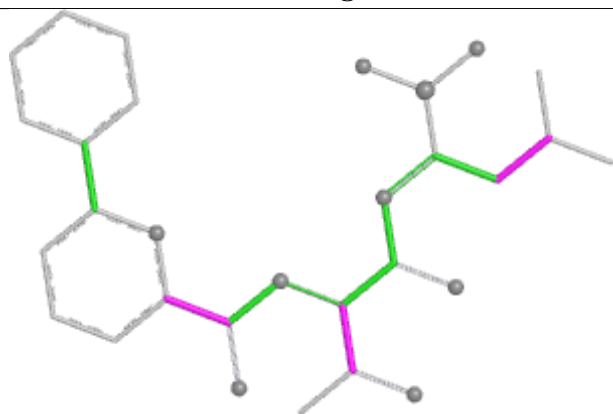
Ligand 6V7 K 305



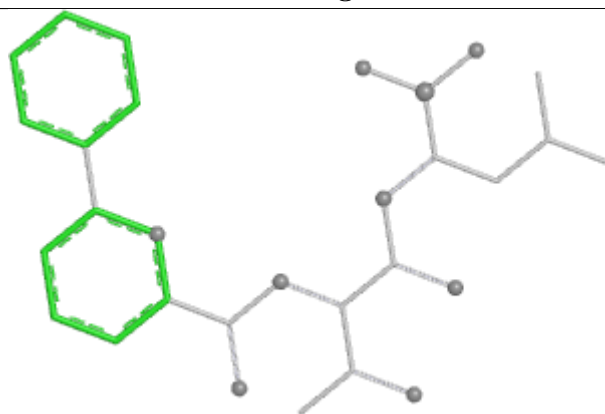
Bond lengths



Bond angles

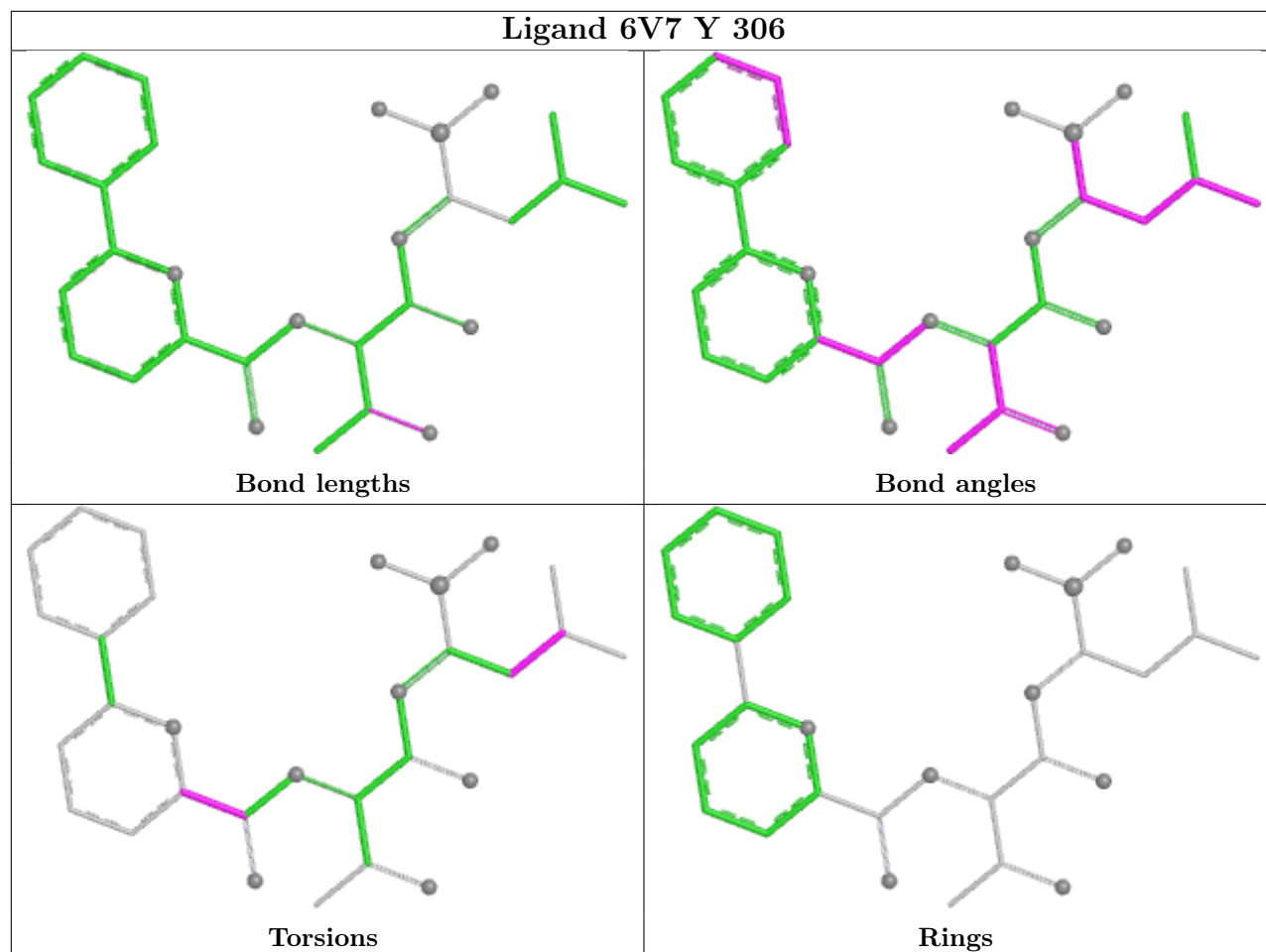


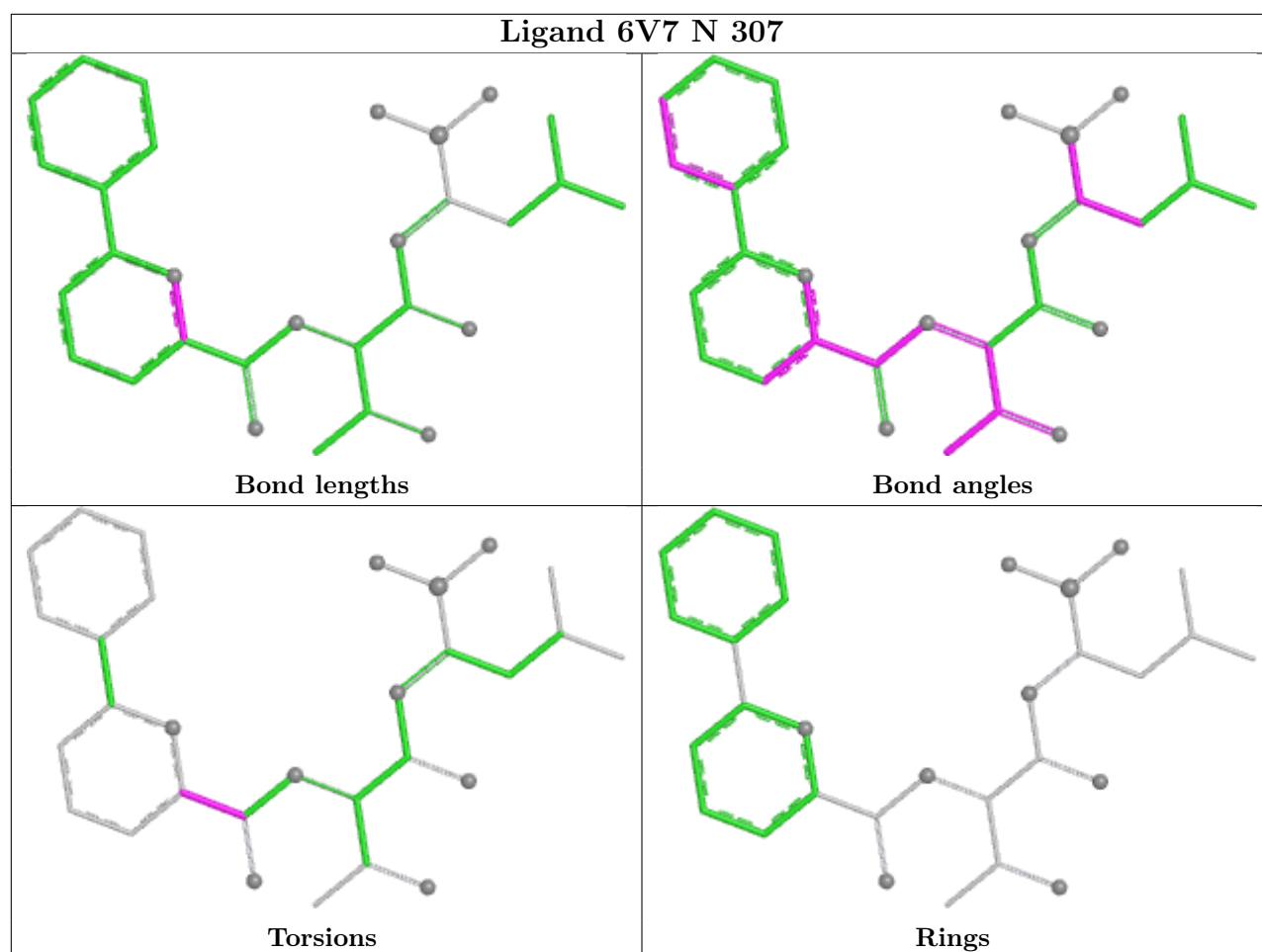
Torsions



Rings

Ligand 6V7 Y 306





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%)	0.06	6 (2%) 57 56	23, 46, 86, 102	3 (1%)
1	O	230/234 (98%)	0.51	7 (3%) 52 51	40, 68, 117, 148	0
2	B	248/261 (95%)	0.22	9 (3%) 46 45	20, 53, 98, 144	2 (0%)
2	P	248/261 (95%)	0.52	15 (6%) 27 26	32, 64, 127, 174	2 (0%)
3	C	236/248 (95%)	0.54	14 (5%) 28 27	27, 65, 112, 146	2 (0%)
3	Q	238/248 (95%)	0.68	17 (7%) 22 20	33, 66, 138, 175	0
4	D	233/241 (96%)	0.32	5 (2%) 63 63	33, 62, 95, 139	1 (0%)
4	R	233/241 (96%)	0.11	7 (3%) 52 51	19, 44, 75, 106	1 (0%)
5	E	233/263 (88%)	0.13	12 (5%) 33 31	24, 41, 92, 116	1 (0%)
5	S	237/263 (90%)	0.18	10 (4%) 40 39	22, 48, 86, 118	3 (1%)
6	F	239/255 (93%)	-0.21	4 (1%) 69 68	17, 33, 59, 77	4 (1%)
6	T	240/255 (94%)	0.39	13 (5%) 31 30	28, 57, 97, 137	1 (0%)
7	G	241/246 (97%)	-0.08	4 (1%) 69 68	17, 39, 73, 110	2 (0%)
7	U	235/246 (95%)	0.44	14 (5%) 27 26	33, 67, 107, 136	1 (0%)
8	H	220/234 (94%)	-0.17	5 (2%) 61 60	19, 35, 77, 133	2 (0%)
8	V	220/234 (94%)	0.23	11 (5%) 34 33	25, 50, 91, 130	2 (0%)
9	I	204/205 (99%)	-0.28	2 (0%) 79 79	22, 36, 61, 81	3 (1%)
9	W	204/205 (99%)	0.10	2 (0%) 79 79	30, 51, 80, 92	2 (0%)
10	J	195/201 (97%)	-0.15	1 (0%) 87 87	16, 43, 61, 84	3 (1%)
10	X	195/201 (97%)	-0.07	1 (0%) 87 87	19, 44, 60, 84	2 (1%)
11	K	200/204 (98%)	-0.03	1 (0%) 87 87	24, 47, 76, 97	1 (0%)
11	Y	201/204 (98%)	-0.25	3 (1%) 72 71	20, 35, 60, 81	3 (1%)
12	L	213/213 (100%)	0.03	0 100 100	22, 49, 75, 95	2 (0%)
12	Z	213/213 (100%)	-0.20	3 (1%) 73 73	22, 36, 63, 86	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.21	2 (0%)	81	80	23, 37, 65, 98	1 (0%)
13	a	216/219 (98%)	-0.20	2 (0%)	81	80	24, 38, 60, 86	2 (0%)
14	N	202/205 (98%)	-0.33	3 (1%)	72	71	19, 32, 55, 81	1 (0%)
14	b	203/205 (99%)	-0.12	3 (1%)	72	71	29, 41, 69, 97	1 (0%)
All	All	6223/6458 (96%)	0.09	176 (2%)	55	54	16, 47, 93, 175	49 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	204	CYS	5.5
11	K	41	TYR	5.0
5	S	2	PHE	4.9
11	Y	202	GLY	4.4
4	R	241	ILE	4.4
11	Y	41	TYR	4.1
5	E	57	ALA	4.0
5	E	52	ALA	4.0
2	P	61	PHE	3.9
5	E	56	LEU	3.9
3	Q	50	VAL	3.9
1	O	232	ILE	3.8
3	C	138	PHE	3.8
13	M	215	ILE	3.7
2	P	51	ASN	3.7
5	E	59	HIS	3.6
5	E	58	ALA	3.5
13	a	215	ILE	3.5
13	a	216	SER	3.5
5	E	54	SER	3.5
14	b	200	VAL	3.5
3	Q	232	ILE	3.4
2	B	61	PHE	3.4
4	R	131	GLY	3.4
6	T	6	GLY	3.4
8	V	199	LEU	3.4
3	Q	225	ILE	3.4
8	V	220	GLU	3.4
6	T	208	ALA	3.4
4	D	131	GLY	3.4
7	U	186	LYS	3.3
3	Q	48	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
5	S	18[A]	ARG	3.2
7	G	208	ILE	3.2
6	T	5	THR	3.2
6	T	53	VAL	3.2
5	S	57	ALA	3.2
4	R	130	PRO	3.2
3	Q	217	LEU	3.1
1	A	3	ARG	3.1
1	A	181	LEU	3.1
2	P	157	GLY	3.1
5	S	56	LEU	3.0
2	P	245	ALA	3.0
5	S	239	ARG	3.0
5	E	53	GLN	2.9
2	P	249	ARG	2.9
7	G	245	ARG	2.9
3	C	206	ILE	2.9
2	B	202	ASP	2.9
2	B	203	VAL	2.9
6	T	209	PHE	2.9
1	O	231	ALA	2.9
2	B	249	ARG	2.9
10	J	1[A]	MET	2.9
1	O	188	HIS	2.8
6	T	142	VAL	2.8
2	P	203	VAL	2.8
3	Q	98	VAL	2.8
5	E	51	ARG	2.7
5	S	53	GLN	2.7
8	V	206	LYS	2.7
9	I	78	GLY	2.7
2	P	162	THR	2.7
2	P	206	LEU	2.7
3	Q	49	SER	2.7
6	F	204	VAL	2.7
4	R	128	ALA	2.7
3	C	220	LEU	2.7
14	b	204	PRO	2.7
7	U	185	LYS	2.7
2	P	247	ALA	2.7
6	T	61	GLY	2.7
8	V	202	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
3	Q	138	PHE	2.7
7	G	187	PHE	2.7
4	D	241	ILE	2.7
8	V	216	ILE	2.7
2	B	247	ALA	2.6
6	F	6	GLY	2.6
8	V	203	ARG	2.6
8	H	204	CYS	2.6
3	C	97	THR	2.6
3	Q	53	LEU	2.6
3	Q	220	LEU	2.6
3	Q	206	ILE	2.6
2	B	157	GLY	2.6
1	O	230	ALA	2.6
5	S	58	ALA	2.6
5	E	60	GLN	2.6
1	O	177	TYR	2.6
3	C	48	LYS	2.6
2	P	56	LEU	2.6
6	T	204	VAL	2.6
7	U	183	VAL	2.6
7	G	189	TRP	2.5
1	A	230	ALA	2.5
14	N	203	LEU	2.5
8	V	201	ARG	2.5
8	V	197	THR	2.5
1	A	231	ALA	2.4
7	U	51	VAL	2.4
2	P	30	HIS	2.4
7	U	2	SER	2.4
8	H	202	TYR	2.4
1	O	54	ILE	2.4
3	C	98	VAL	2.4
8	V	205	GLU	2.4
3	C	102	VAL	2.4
5	S	235	GLY	2.4
2	P	55	LEU	2.3
3	C	196	LEU	2.3
6	T	54	LEU	2.3
9	W	84	TYR	2.3
14	N	201	ALA	2.3
4	D	184	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
7	U	194	THR	2.3
7	U	208	ILE	2.3
2	B	2	SER	2.3
6	T	206	ASP	2.3
5	E	233	LEU	2.3
8	H	199	LEU	2.3
2	P	52	ILE	2.3
2	P	233	VAL	2.3
6	F	53	VAL	2.3
7	U	170	VAL	2.3
7	U	195	VAL	2.3
3	C	53	LEU	2.3
7	U	3	ARG	2.2
3	Q	203	GLY	2.2
11	Y	201	SER	2.2
6	T	226	ILE	2.2
5	E	61	LYS	2.2
1	A	50	LYS	2.2
6	T	207	LYS	2.2
8	H	197	THR	2.2
3	Q	202	GLY	2.2
13	M	216	SER	2.2
4	R	132	ALA	2.2
4	R	54	ILE	2.2
12	Z	160	ASN	2.2
3	Q	183	THR	2.2
6	T	52	LEU	2.2
4	R	120[A]	ALA	2.2
9	I	16[A]	LYS	2.2
12	Z	80	ASN	2.1
3	C	225	ILE	2.1
7	U	193	GLN	2.1
1	O	167	VAL	2.1
3	Q	229	VAL	2.1
14	b	203	LEU	2.1
2	P	194	ILE	2.1
9	W	73	TYR	2.1
3	C	183	THR	2.1
8	V	71	GLY	2.1
12	Z	161	VAL	2.1
6	F	244	LYS	2.1
2	B	206	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
7	U	241	ALA	2.1
3	C	49	SER	2.1
5	S	54	SER	2.1
7	U	88	ARG	2.1
5	S	237	GLU	2.1
1	A	200	GLY	2.1
14	N	199	ALA	2.1
7	U	245	ARG	2.1
3	Q	59	VAL	2.0
3	C	195	LEU	2.0
10	X	75	LEU	2.0
4	D	128	ALA	2.0
5	E	201	ALA	2.0
4	D	129	ASP	2.0
3	Q	236	LYS	2.0
3	C	11	SER	2.0
2	B	162	THR	2.0
8	H	200	GLY	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	YCM	G	137	10/11	0.87	0.14	27,36,52,53	0
7	6V1	U	47	15/16	0.90	0.14	81,117,124,127	0
7	YCM	U	137	10/11	0.91	0.12	54,64,77,80	0
3	YCM	C	63	10/11	0.92	0.10	58,62,76,78	0
5	6V1	S	148	15/16	0.92	0.13	38,70,77,78	0
5	6V1	E	148	15/16	0.92	0.13	31,59,70,71	0
7	6V1	G	47	15/16	0.92	0.12	39,60,67,69	0
10	6V1	X	91	15/16	0.94	0.13	34,57,64,68	0
10	6V1	J	91	15/16	0.95	0.11	32,51,60,60	0
7	6V1	U	161	15/16	0.95	0.09	58,74,81,82	0
3	YCM	Q	63	10/11	0.95	0.08	53,58,69,69	0
7	6V1	G	161	15/16	0.96	0.10	32,53,59,62	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
15	CL	O	304	1/1	0.79	0.20	77,77,77,77	0
18	1PE	H	305	16/16	0.81	0.17	60,83,112,113	0
15	CL	Q	301	1/1	0.84	0.15	84,84,84,84	0
15	CL	D	301	1/1	0.85	0.22	81,81,81,81	0
15	CL	O	303	1/1	0.86	0.12	99,99,99,99	0
18	1PE	W	303	16/16	0.86	0.13	65,69,85,87	0
18	1PE	L	302	16/16	0.87	0.18	75,84,119,120	0
15	CL	M	303	1/1	0.88	0.15	65,65,65,65	0
18	1PE	L	301	16/16	0.88	0.14	60,77,83,91	0
15	CL	C	302	1/1	0.88	0.18	76,76,76,76	0
18	1PE	N	304	16/16	0.88	0.18	72,74,112,114	0
15	CL	Q	302	1/1	0.88	0.21	72,72,72,72	0
18	1PE	Y	305	16/16	0.88	0.14	59,75,81,84	0
15	CL	E	303	1/1	0.89	0.17	74,74,74,74	0
18	1PE	U	302	16/16	0.90	0.14	50,57,92,92	0
18	1PE	I	303	16/16	0.90	0.12	60,62,82,83	0
15	CL	S	301	1/1	0.90	0.18	81,81,81,81	0
15	CL	D	302	1/1	0.91	0.21	72,72,72,72	0
15	CL	Y	304	1/1	0.91	0.27	75,75,75,75	0
15	CL	a	304	1/1	0.91	0.12	67,67,67,67	0
17	MG	V	301	1/1	0.91	0.06	85,85,85,85	0
15	CL	K	302	1/1	0.92	0.12	84,84,84,84	0
15	CL	a	302	1/1	0.92	0.23	69,69,69,69	0
18	1PE	N	303	16/16	0.92	0.11	39,48,65,68	0
15	CL	K	304	1/1	0.92	0.23	80,80,80,80	0
15	CL	B	302	1/1	0.92	0.22	64,64,64,64	0
15	CL	C	301	1/1	0.92	0.14	76,76,76,76	0
15	CL	S	302	1/1	0.92	0.13	72,72,72,72	0
15	CL	U	301	1/1	0.93	0.16	67,67,67,67	0
15	CL	V	302	1/1	0.93	0.12	68,68,68,68	0
15	CL	V	303	1/1	0.93	0.20	62,62,62,62	0
15	CL	Y	301	1/1	0.93	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CL	K	303	1/1	0.93	0.16	74,74,74,74	0
15	CL	a	301	1/1	0.93	0.20	74,74,74,74	0
15	CL	R	301	1/1	0.93	0.13	67,67,67,67	0
15	CL	H	303	1/1	0.93	0.15	63,63,63,63	0
15	CL	B	301	1/1	0.93	0.11	44,44,44,44	0
15	CL	R	302	1/1	0.94	0.23	61,61,61,61	0
15	CL	E	302	1/1	0.94	0.15	62,62,62,62	0
15	CL	G	301	1/1	0.94	0.24	53,53,53,53	0
15	CL	S	303	1/1	0.94	0.14	59,59,59,59	0
15	CL	b	301	1/1	0.94	0.19	69,69,69,69	0
16	K	N	305	1/1	0.95	0.09	41,41,41,41	0
16	K	b	302	1/1	0.95	0.11	43,43,43,43	0
15	CL	A	304	1/1	0.95	0.12	63,63,63,63	0
15	CL	G	302	1/1	0.95	0.09	68,68,68,68	0
15	CL	M	301	1/1	0.95	0.35	62,62,62,62	0
15	CL	Y	303	1/1	0.95	0.10	68,68,68,68	0
15	CL	A	302	1/1	0.95	0.10	72,72,72,72	0
15	CL	N	301	1/1	0.95	0.20	68,68,68,68	0
15	CL	O	302	1/1	0.95	0.09	72,72,72,72	0
15	CL	a	303	1/1	0.95	0.10	46,46,46,46	0
15	CL	I	302	1/1	0.95	0.10	51,51,51,51	0
15	CL	A	303	1/1	0.95	0.11	57,57,57,57	0
19	6V7	K	305	30/30	0.95	0.07	34,37,46,49	0
19	6V7	Y	306	30/30	0.95	0.07	24,28,34,37	0
15	CL	A	301	1/1	0.96	0.10	55,55,55,55	0
15	CL	F	301	1/1	0.96	0.11	61,61,61,61	0
16	K	U	303	1/1	0.96	0.10	46,46,46,46	0
15	CL	O	301	1/1	0.96	0.14	61,61,61,61	0
16	K	b	303	1/1	0.96	0.10	48,48,48,48	0
17	MG	H	301	1/1	0.96	0.05	71,71,71,71	0
17	MG	I	301	1/1	0.96	0.08	33,33,33,33	0
17	MG	I	304	1/1	0.96	0.09	29,29,29,29	0
15	CL	Y	302	1/1	0.96	0.09	68,68,68,68	0
15	CL	P	301	1/1	0.96	0.09	56,56,56,56	0
19	6V7	b	304	30/30	0.96	0.07	32,36,44,45	0
16	K	N	306	1/1	0.97	0.05	40,40,40,40	0
15	CL	H	304	1/1	0.97	0.10	50,50,50,50	0
17	MG	K	301	1/1	0.97	0.08	37,37,37,37	0
17	MG	L	304	1/1	0.97	0.12	39,39,39,39	0
15	CL	W	302	1/1	0.97	0.06	61,61,61,61	0
17	MG	W	301	1/1	0.97	0.06	37,37,37,37	0
16	K	L	303	1/1	0.97	0.09	53,53,53,53	0

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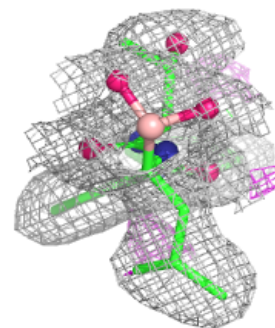
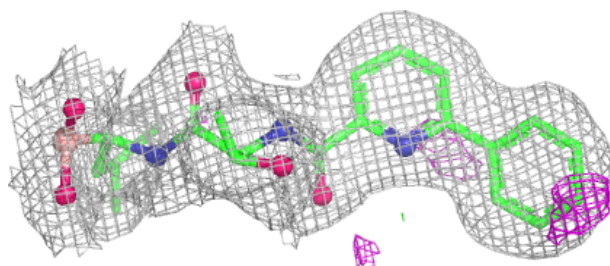
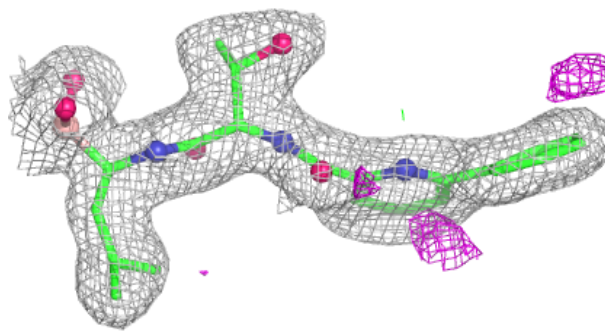
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	6V7	N	307	30/30	0.97	0.06	25,26,37,38	0
15	CL	E	301	1/1	0.97	0.10	68,68,68,68	0
17	MG	H	302	1/1	0.97	0.11	32,32,32,32	0
16	K	Z	301	1/1	0.98	0.07	41,41,41,41	0
15	CL	N	302	1/1	0.98	0.14	59,59,59,59	0
15	CL	M	302	1/1	0.98	0.07	42,42,42,42	0
17	MG	J	301	1/1	0.99	0.06	59,59,59,59	0
17	MG	X	301	1/1	0.99	0.03	58,58,58,58	0
16	K	G	303	1/1	0.99	0.07	36,36,36,36	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.

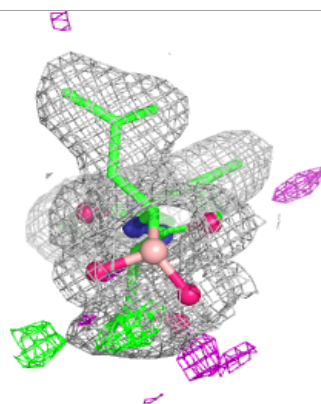
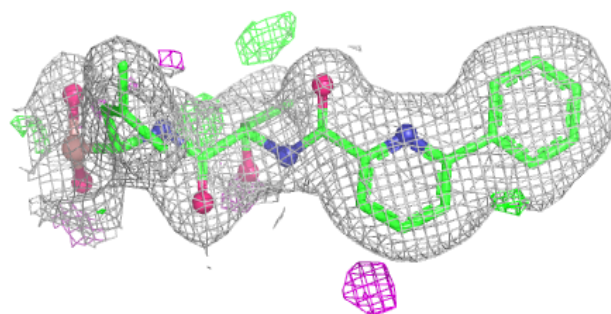
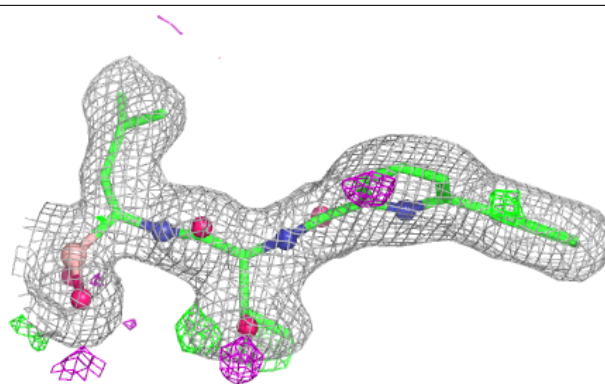
Electron density around 6V7 K 305:

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

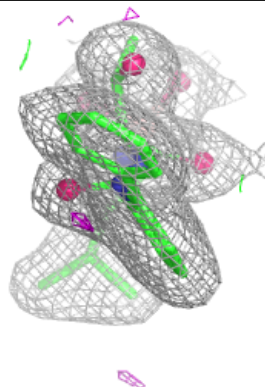
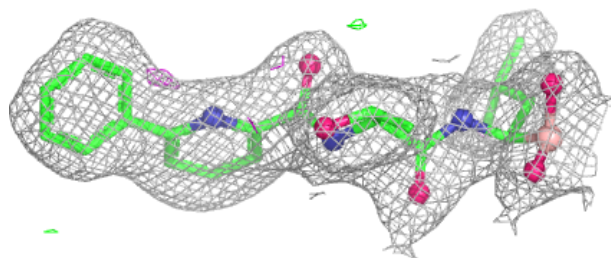
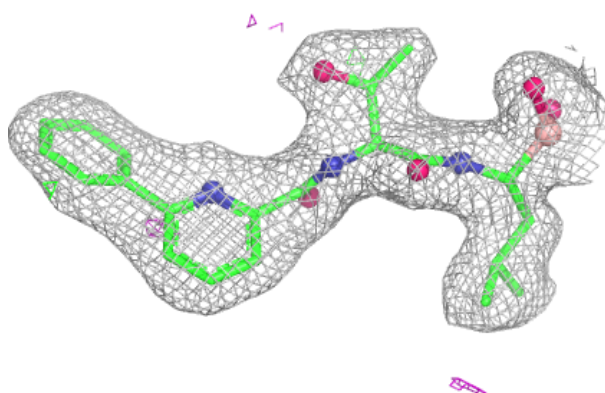


Electron density around 6V7 Y 306:

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

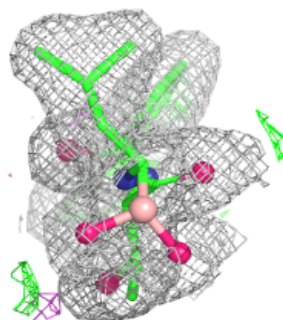
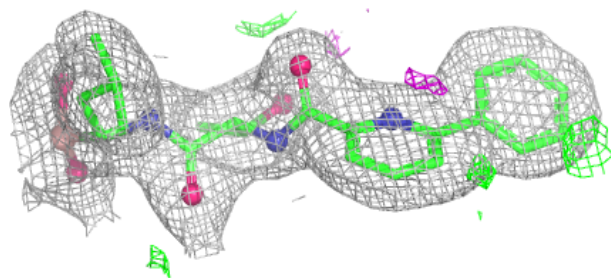
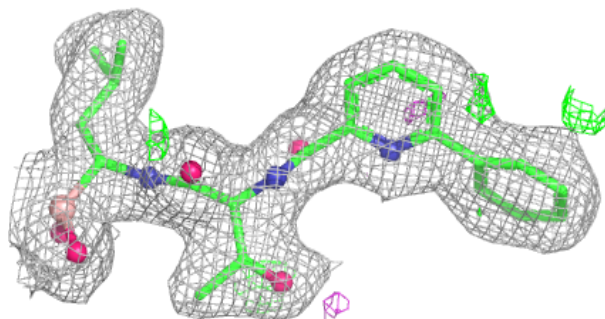
**Electron density around 6V7 b 304:**

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



Electron density around 6V7 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.