



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:18 AM UTC

PDB ID : 5L5J / pdb_00005l5j
Title : Yeast 20S proteasome with human beta5i (1-138) and human beta6 (97-111; 118-133) in complex with epoxyketone inhibitor 14
Authors : Groll, M.; Huber, E.M.
Deposited on : 2016-05-28
Resolution : 2.90 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

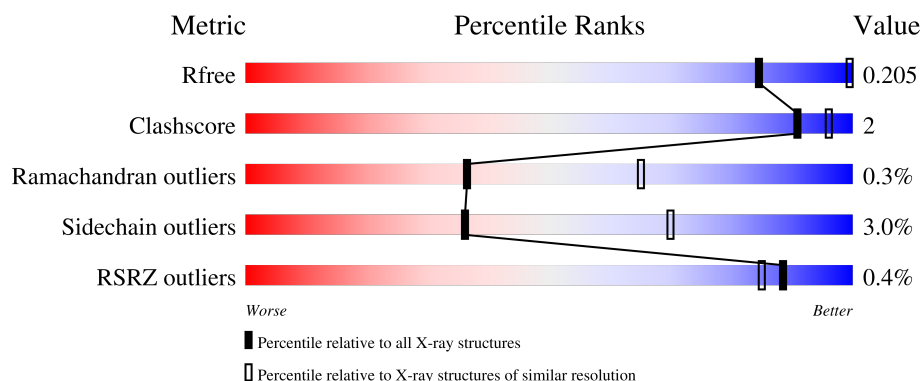
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

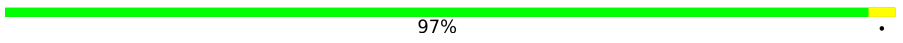
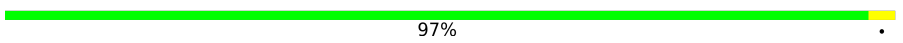
The reported resolution of this entry is 2.90 Å.

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.



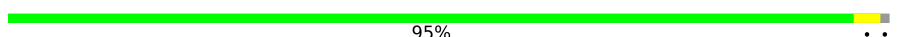
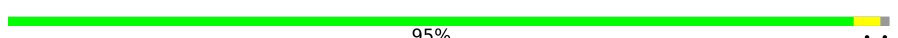
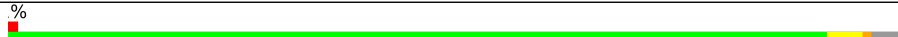
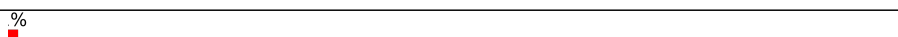
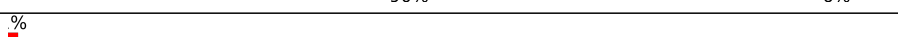
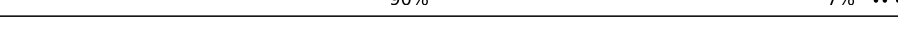
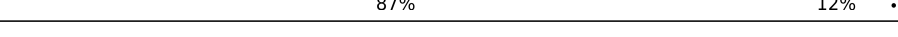
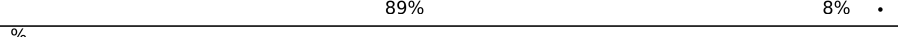
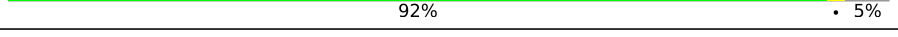
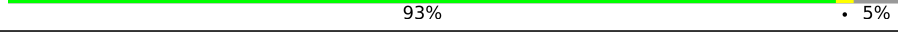
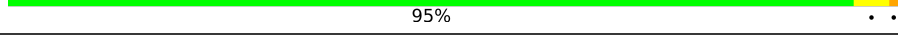
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	250	 97% .
1	O	250	 97% .
2	B	258	 87% 7% 5%
2	P	258	 86% 8% 5%
3	C	254	 87% 6% . 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49764 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

- 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	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-8,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1640	1035	282	311	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1640	1035	282	311	12			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	1	0
			1832	1159	315	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

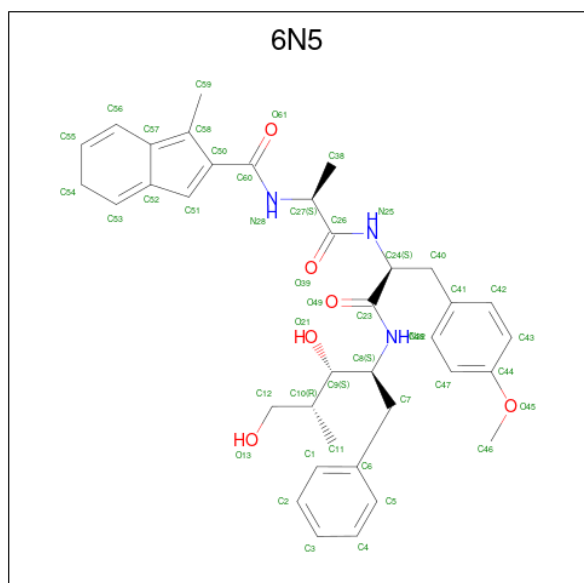
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	J	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

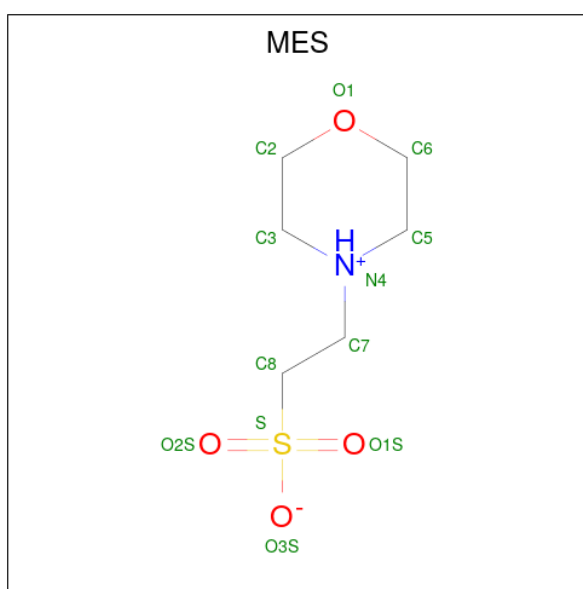
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is {N}-[(2 {S})-1-[(2 {S})-3-(4-methoxyphenyl)-1-[(2 {S},3 {S},4 {R})-4-methyl-3,5-bis(oxidanyl)-1-phenyl-pentan-2-yl]amino]-1-oxidanylidene-propan-2-yl]amino]-1-oxidanylidene-propan-2-yl]-1-methyl-5 {H}-indene-2-carboxamide (CCD ID: 6N5) (formula: C₃₆H₄₃N₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			45	36	3	6		
17	K	1	Total	C	N	O	0	0
			45	36	3	6		
17	V	1	Total	C	N	O	0	0
			45	36	3	6		
17	Y	1	Total	C	N	O	0	0
			45	36	3	6		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	3	Total	O	0	0
			3	3		
19	B	12	Total	O	0	0
			12	12		
19	C	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	2	Total O 2 2	0	0
19	E	2	Total O 2 2	0	0
19	F	7	Total O 7 7	0	0
19	G	7	Total O 7 7	0	0
19	H	6	Total O 6 6	0	0
19	I	5	Total O 5 5	0	0
19	J	6	Total O 6 6	0	0
19	K	4	Total O 4 4	0	0
19	L	10	Total O 10 10	0	0
19	M	11	Total O 11 11	0	0
19	N	8	Total O 8 8	0	0
19	O	1	Total O 1 1	0	0
19	P	5	Total O 5 5	0	0
19	Q	5	Total O 5 5	0	0
19	R	2	Total O 2 2	0	0
19	S	3	Total O 3 3	0	0
19	T	5	Total O 5 5	0	0
19	U	8	Total O 8 8	0	0
19	V	7	Total O 7 7	0	0
19	W	3	Total O 3 3	0	0
19	X	8	Total O 8 8	0	0

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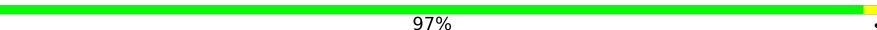
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	Y	7	Total 7	O 7	0	0
19	Z	8	Total 8	O 8	0	0
19	a	11	Total 11	O 11	0	0
19	b	7	Total 7	O 7	0	0

3 Residue-property plots [i](#)

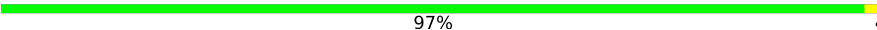
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain A:  97% .



- Molecule 1: Proteasome subunit alpha type-2

Chain O:  97% .



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  87% 7% 5% .



- Molecule 2: Proteasome subunit alpha type-3

Chain P:  86% 8% 5% .

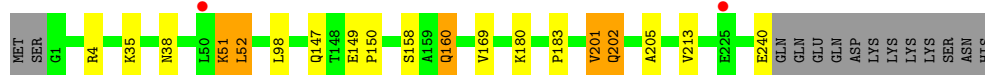
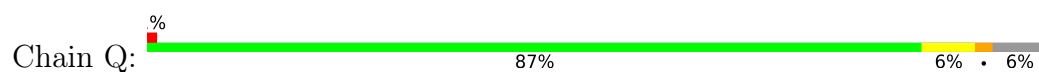


- Molecule 3: Proteasome subunit alpha type-4

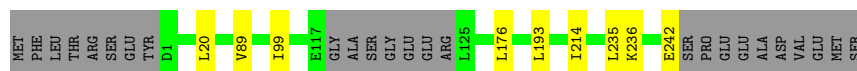
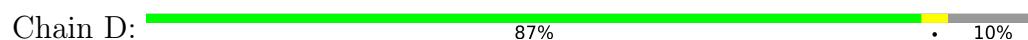
Chain C:  87% 6% 6% .



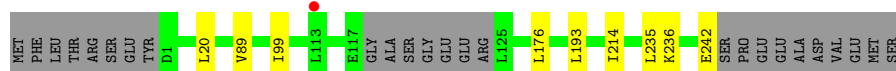
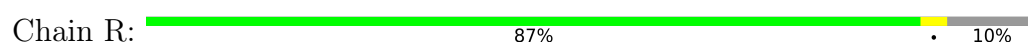
- Molecule 3: Proteasome subunit alpha type-4



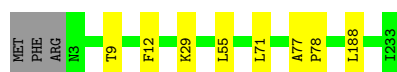
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



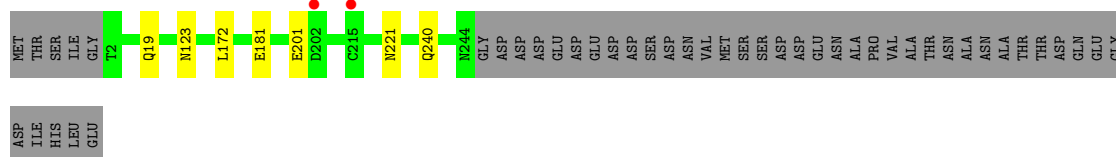
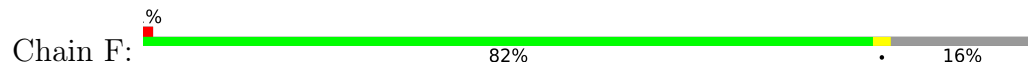
- Molecule 5: Proteasome subunit alpha type-6



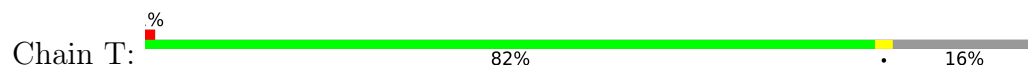
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7



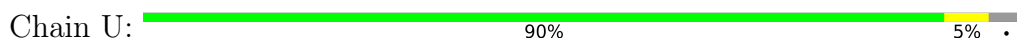
- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 7: Proteasome subunit alpha type-1



- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



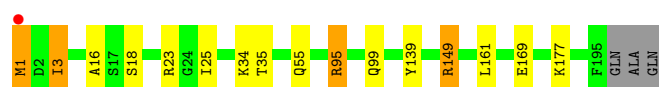
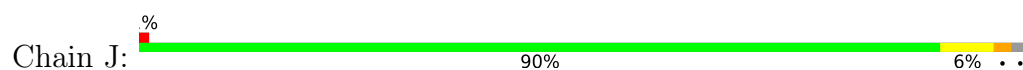
- Molecule 9: Proteasome subunit beta type-3



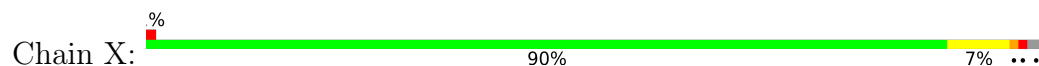
- Molecule 9: Proteasome subunit beta type-3



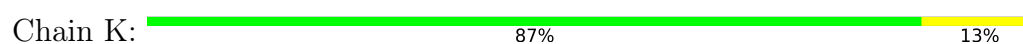
- Molecule 10: Proteasome subunit beta type-4



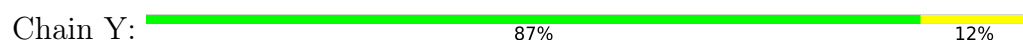
- Molecule 10: Proteasome subunit beta type-4



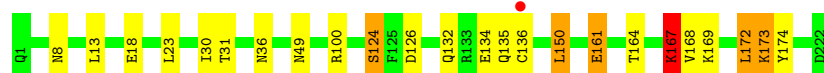
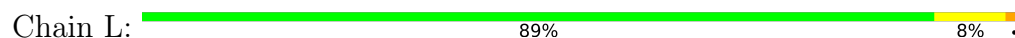
- Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

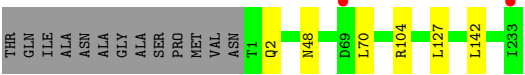


- Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6,Proteasome subunit beta type-1,Proteasome subunit beta type-6

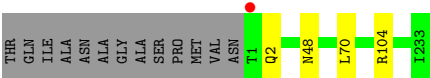
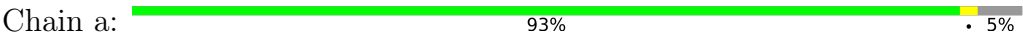


- Molecule 13: Proteasome subunit beta type-7

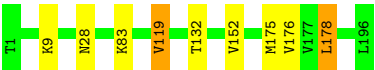




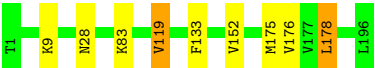
● Molecule 13: Proteasome subunit beta type-7



● Molecule 14: Proteasome subunit beta type-1



● Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.69Å 299.81Å 145.60Å 90.00° 112.76° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-2.90) 96.6 (15.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.172 , 0.200 0.178 , 0.205	Depositor DCC
R_{free} test set	11408 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.3	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	0.95	EDS
Total number of atoms	49764	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 6N5, MG, MES

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	0.40	0/1952	0.68	0/2642
1	O	0.40	0/1952	0.68	0/2642
2	B	0.41	0/1934	0.68	0/2618
2	P	0.41	0/1934	0.67	0/2618
3	C	0.40	0/1910	0.70	1/2586 (0.0%)
3	Q	0.41	0/1910	0.70	1/2586 (0.0%)
4	D	0.40	0/1837	0.66	0/2475
4	R	0.40	0/1837	0.66	0/2475
5	E	0.40	0/1800	0.65	0/2433
5	S	0.40	0/1800	0.65	0/2433
6	F	0.40	0/1932	0.69	0/2609
6	T	0.40	0/1932	0.69	0/2609
7	G	0.40	0/1945	0.68	0/2634
7	U	0.40	0/1945	0.68	0/2634
8	H	0.35	0/1750	0.69	1/2373 (0.0%)
8	V	0.35	0/1750	0.69	1/2373 (0.0%)
9	I	0.40	1/1611 (0.1%)	0.87	4/2174 (0.2%)
9	W	0.40	1/1611 (0.1%)	0.81	5/2174 (0.2%)
10	J	0.40	0/1589	0.84	6/2142 (0.3%)
10	X	0.40	0/1589	0.83	6/2142 (0.3%)
11	K	0.37	0/1677	0.74	0/2263
11	Y	0.38	0/1677	0.74	1/2263 (0.0%)
12	L	0.43	1/1802 (0.1%)	0.80	4/2430 (0.2%)
12	Z	0.44	1/1802 (0.1%)	0.78	2/2430 (0.1%)
13	M	0.36	0/1866	0.69	0/2528
13	a	0.36	0/1855	0.69	0/2514
14	N	0.34	0/1541	0.68	0/2087
14	b	0.34	0/1541	0.69	0/2087
All	All	0.39	4/50281 (0.0%)	0.71	32/67974 (0.0%)

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
10	J	0	2
10	X	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	126	ILE	CB-CG2	-6.49	1.31	1.52
12	Z	49	ASN	CG-ND2	-6.46	1.19	1.33
12	L	49	ASN	CG-ND2	-5.98	1.20	1.33
9	I	126	ILE	CB-CG2	-5.19	1.35	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	126	ILE	CG1-CB-CG2	-18.32	55.75	110.70
9	W	126	ILE	CA-CB-CG1	12.77	132.12	110.40
9	I	126	ILE	N-CA-CB	-11.22	98.98	112.33
10	J	149	ARG	NE-CZ-NH1	-11.16	110.33	121.50
10	X	95	ARG	NE-CZ-NH1	-10.57	110.93	121.50
9	I	126	ILE	CA-CB-CG1	10.55	128.34	110.40
10	J	95	ARG	NE-CZ-NH2	-10.43	109.81	119.20
10	J	149	ARG	NE-CZ-NH2	10.41	128.57	119.20
9	W	126	ILE	CG1-CB-CG2	-10.32	79.72	110.70
10	X	149	ARG	NE-CZ-NH2	-10.22	110.00	119.20
10	X	95	ARG	NE-CZ-NH2	10.14	128.32	119.20
10	J	95	ARG	CD-NE-CZ	10.06	138.49	124.40
12	L	167	LYS	CG-CD-CE	9.47	133.07	111.30
10	X	149	ARG	CD-NE-CZ	9.32	137.45	124.40
10	J	149	ARG	CD-NE-CZ	9.02	137.03	124.40
10	X	95	ARG	CD-NE-CZ	8.13	135.79	124.40
12	L	167	LYS	CD-CE-NZ	7.96	137.36	111.90
12	Z	173	LYS	CB-CG-CD	7.44	128.41	111.30
12	L	173	LYS	CB-CG-CD	7.35	128.20	111.30
9	W	126	ILE	CB-CA-C	-7.32	97.69	110.94
9	W	126	ILE	N-CA-C	6.54	121.27	113.22
9	I	126	ILE	CB-CA-C	6.41	117.55	110.62
10	X	149	ARG	NE-CZ-NH1	6.38	127.88	121.50
12	Z	167	LYS	CG-CD-CE	5.96	125.01	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	5.85	116.59	110.62
3	C	201	VAL	N-CA-C	5.81	116.54	110.62
12	L	167	LYS	CB-CG-CD	-5.75	98.09	111.30
10	J	95	ARG	NE-CZ-NH1	5.72	127.22	121.50
8	H	1	THR	N-CA-C	5.42	126.16	111.00
8	V	1	THR	N-CA-C	5.37	126.03	111.00
9	W	126	ILE	N-CA-CB	5.09	119.81	112.07
11	Y	31	VAL	CB-CA-C	-5.03	102.86	110.95

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	149	ARG	Sidechain
10	J	95	ARG	Sidechain
10	X	149	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	1	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	5	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	1	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1716	11	0
8	V	1719	0	1716	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1581	0	1574	12	0
9	W	1581	0	1574	10	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	10	0
11	K	1640	0	1578	19	0
11	Y	1640	0	1578	19	0
12	L	1764	0	1716	16	0
12	Z	1764	0	1716	19	0
13	M	1832	0	1845	1	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	5	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	45	0	0	0	0
17	K	45	0	0	2	0
17	V	45	0	0	0	0
17	Y	45	0	0	4	0
18	H	12	0	13	4	0
18	Y	12	0	13	1	0
19	A	3	0	0	0	0
19	B	12	0	0	0	0
19	C	7	0	0	0	0
19	D	2	0	0	0	0
19	E	2	0	0	0	0
19	F	7	0	0	0	0
19	G	7	0	0	0	0
19	H	6	0	0	0	0
19	I	5	0	0	0	0
19	J	6	0	0	0	0
19	K	4	0	0	0	0
19	L	10	0	0	0	0
19	M	11	0	0	0	0
19	N	8	0	0	0	0
19	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	5	0	0	0	0
19	Q	5	0	0	0	0
19	R	2	0	0	0	0
19	S	3	0	0	0	0
19	T	5	0	0	0	0
19	U	8	0	0	0	0
19	V	7	0	0	0	0
19	W	3	0	0	0	0
19	X	8	0	0	0	0
19	Y	7	0	0	0	0
19	Z	8	0	0	0	0
19	a	11	0	0	0	0
19	b	7	0	0	0	0
All	All	49764	0	49139	163	0

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

All (163) 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)
11:K:194:GLU:OE1	12:L:169:LYS:NZ	1.89	1.05
11:Y:194:GLU:OE1	12:Z:169:LYS:NZ	1.95	0.99
12:L:164:THR:O	12:L:167:LYS:HD2	1.75	0.87
9:I:98:ARG:HD2	9:I:126:ILE:HD11	1.57	0.86
12:Z:165:ASN:HB3	12:Z:167:LYS:HD2	1.59	0.83
8:H:128:GLY:H	18:H:302:MES:H31	1.45	0.81
12:L:164:THR:HG21	12:L:168:VAL:HB	1.63	0.81
12:Z:164:THR:HG21	12:Z:168:VAL:HB	1.63	0.81
17:Y:301:6N5:C46	17:Y:301:6N5:C59	2.62	0.78
10:J:23:ARG:NH2	11:K:119:THR:OG1	2.18	0.77
10:X:23:ARG:NH2	11:Y:119:THR:OG1	2.21	0.73
12:L:124:SER:OG	12:L:134:GLU:OE2	2.09	0.69
12:L:161:GLU:O	12:L:164:THR:OG1	2.12	0.68
8:H:128:GLY:N	18:H:302:MES:H31	2.08	0.67
12:Z:161:GLU:O	12:Z:164:THR:OG1	2.12	0.65
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.82	0.61
11:K:1:THR:HG22	11:K:2:THR:N	2.15	0.60
9:I:98:ARG:CD	9:I:126:ILE:HD11	2.31	0.60
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.82	0.60
9:I:98:ARG:HD2	9:I:126:ILE:CD1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:164:THR:O	12:Z:167:LYS:CD	2.53	0.57
9:W:98:ARG:HD2	9:W:126:ILE:HD12	1.87	0.56
12:Z:164:THR:HG21	12:Z:168:VAL:CB	2.36	0.55
4:D:89:VAL:HG12	11:K:61:LYS:HG3	1.87	0.55
8:H:128:GLY:H	18:H:302:MES:C3	2.19	0.54
11:Y:30:ARG:O	12:Z:132:GLN:NE2	2.40	0.54
10:J:25:ILE:O	10:X:139:TYR:OH	2.25	0.54
11:K:1:THR:CG2	11:K:2:THR:N	2.71	0.54
14:b:152:VAL:HA	14:b:175:MET:HE1	1.89	0.53
10:J:139:TYR:OH	10:X:25:ILE:O	2.25	0.53
12:L:164:THR:HG21	12:L:168:VAL:CB	2.36	0.53
7:U:23:PHE:O	7:U:26:THR:HB	2.08	0.53
14:N:152:VAL:HA	14:N:175:MET:HE1	1.90	0.53
11:K:30:ARG:O	12:L:132:GLN:NE2	2.39	0.53
9:W:98:ARG:CD	9:W:126:ILE:HD12	2.39	0.53
12:Z:172:LEU:HD23	12:Z:172:LEU:N	2.23	0.52
12:Z:164:THR:O	12:Z:167:LYS:HD3	2.09	0.52
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.74	0.52
7:G:23:PHE:O	7:G:26:THR:HB	2.09	0.52
17:K:301:6N5:C48	17:K:301:6N5:N25	2.72	0.52
12:L:172:LEU:N	12:L:172:LEU:HD23	2.24	0.52
11:K:20:ALA:HB3	11:K:28:ALA:HB3	1.92	0.52
11:Y:20:ALA:HB3	11:Y:28:ALA:HB3	1.92	0.52
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.75	0.51
8:H:35:HIS:CB	8:H:56:THR:HG21	2.40	0.51
11:Y:1:THR:HG22	11:Y:2:THR:N	2.26	0.51
17:Y:301:6N5:N25	17:Y:301:6N5:C48	2.73	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
8:V:35:HIS:CB	8:V:56:THR:HG21	2.40	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.50
17:Y:301:6N5:C59	17:Y:301:6N5:N28	2.74	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.50
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.94	0.49
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.42	0.49
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.94	0.49
11:Y:9:GLN:HG2	11:Y:10:HIS:CD2	2.46	0.49
2:B:50:LYS:O	2:B:51:VAL:C	2.55	0.49
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.94	0.48
11:Y:18:SER:O	11:Y:31:VAL:HG22	2.13	0.48
11:K:208:ASN:O	9:W:38:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:301:6N5:N28	17:K:301:6N5:C59	2.77	0.48
10:X:148:TYR:O	10:X:149:ARG:HD3	2.13	0.48
8:H:128:GLY:CA	18:H:302:MES:H31	2.43	0.47
8:H:112:SER:OG	8:H:120:ASP:HB3	2.15	0.47
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.97	0.47
10:J:55:GLN:NE2	11:K:88:CYS:SG	2.88	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.97	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.97	0.47
3:C:99:GLU:HG3	11:K:81:LYS:CD	2.45	0.47
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.15	0.47
12:L:8:ASN:HA	12:L:30:ILE:O	2.15	0.47
8:V:112:SER:OG	8:V:120:ASP:HB3	2.15	0.47
11:K:9:GLN:HG2	11:K:10:HIS:CD2	2.49	0.46
10:J:177:LYS:NZ	10:X:169:GLU:O	2.49	0.46
12:Z:124:SER:OG	12:Z:134:GLU:OE2	2.22	0.46
3:C:51:LYS:O	3:C:52:LEU:HB2	2.15	0.46
11:K:31:VAL:HA	12:L:132:GLN:NE2	2.30	0.46
11:Y:31:VAL:HA	12:Z:132:GLN:NE2	2.31	0.46
10:J:169:GLU:O	10:X:177:LYS:NZ	2.48	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.97	0.46
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.15	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
12:Z:18:GLU:HG3	12:Z:174:TYR:CD2	2.51	0.45
11:K:38:ASN:OD1	11:K:38:ASN:C	2.59	0.45
3:C:201:VAL:O	3:C:202:GLN:HB3	2.17	0.45
12:L:18:GLU:HG3	12:L:174:TYR:CD2	2.51	0.45
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.31	0.45
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.17	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.45
2:B:217:LYS:C	2:B:219:ALA:H	2.25	0.45
8:H:196:ARG:NH2	9:I:150:GLU:O	2.50	0.44
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.51	0.44
8:H:120:ASP:OD1	14:N:28:ASN:ND2	2.50	0.44
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	1.99	0.44
11:Y:1:THR:CG2	11:Y:2:THR:N	2.79	0.44
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.59	0.44
12:Z:161:GLU:OE2	12:Z:161:GLU:HA	2.18	0.44
17:Y:301:6N5:O13	18:Y:302:MES:H51	2.18	0.44
2:P:217:LYS:C	2:P:219:ALA:H	2.26	0.44
8:V:120:ASP:OD1	14:b:28:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.99	0.44
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.00	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.18	0.43
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.43
5:S:12:PHE:H	6:T:19:GLN:HE22	1.66	0.43
12:Z:18:GLU:CG	12:Z:174:TYR:CD2	3.02	0.43
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.54	0.43
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.87	0.43
12:L:18:GLU:CG	12:L:174:TYR:CD2	3.02	0.43
9:I:200:LYS:HE3	11:Y:197:TRP:CE2	2.54	0.42
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.42
9:I:148:MET:HE2	9:I:172:ASN:HB2	2.02	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.42
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.54	0.42
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.00	0.42
12:Z:164:THR:O	12:Z:167:LYS:HD2	2.19	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
11:K:197:TRP:CE2	9:W:200:LYS:HE3	2.54	0.42
14:N:132:THR:O	14:b:133:PHE:HA	2.19	0.42
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.02	0.42
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.84	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.42
11:K:125:MET:SD	11:K:139:LEU:HB3	2.60	0.42
9:W:148:MET:HE2	9:W:172:ASN:HB2	2.02	0.42
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.02	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
5:E:77:ALA:N	5:E:78:PRO:CD	2.83	0.42
11:Y:125:MET:SD	11:Y:139:LEU:HB3	2.60	0.42
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.85	0.41
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.56	0.41
12:Z:164:THR:HG21	12:Z:168:VAL:CG2	2.50	0.41
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.55	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.03	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.41
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.02	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
2:P:221:ASP:O	2:P:223:GLU:N	2.54	0.41
11:Y:37:ILE:HG23	11:Y:60:ALA:HA	2.03	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:PHE:H	6:F:19:GLN:HE22	1.68	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.41
2:B:221:ASP:O	2:B:223:GLU:N	2.54	0.41
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.03	0.41
12:L:126:ASP:OD1	12:L:126:ASP:C	2.64	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.03	0.41
10:X:55:GLN:NE2	11:Y:88:CYS:SG	2.93	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.03	0.41
11:K:37:ILE:HG23	11:K:60:ALA:HA	2.02	0.41
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.36	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.04	0.40
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.56	0.40
12:L:161:GLU:OE2	12:L:161:GLU:HA	2.20	0.40
2:P:145:TYR:OH	2:P:217:LYS:N	2.54	0.40
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.03	0.40
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.02	0.40
11:K:4:LEU:C	11:K:4:LEU:HD22	2.47	0.40
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.47	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	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	59
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	59
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	26
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	9	32
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	5 (2%)	1 (0%)	30	59
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	232/246 (94%)	220 (95%)	12 (5%)	0	100	100
13	a	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6283/6612 (95%)	6111 (97%)	156 (2%)	16 (0%)	36	65

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR

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Mol	Chain	Res	Type
2	B	218	GLY
2	B	222	GLY
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
2	B	220	ASN
3	C	205	ALA
3	Q	205	ALA
2	P	220	ASN
8	V	9	ASN
3	Q	183	PRO

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	209/209 (100%)	205 (98%)	4 (2%)	50	79
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	79
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	70
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	70
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	56
3	Q	212/226 (94%)	201 (95%)	11 (5%)	21	52
4	D	194/215 (90%)	186 (96%)	8 (4%)	27	61
4	R	194/215 (90%)	186 (96%)	8 (4%)	27	61
5	E	190/193 (98%)	185 (97%)	5 (3%)	40	73
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	73
6	F	201/239 (84%)	195 (97%)	6 (3%)	36	70
6	T	201/239 (84%)	195 (97%)	6 (3%)	36	70
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	66
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	66
8	H	185/190 (97%)	180 (97%)	5 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	185/190 (97%)	180 (97%)	5 (3%)	39	73
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	82
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	82
10	J	173/175 (99%)	169 (98%)	4 (2%)	44	76
10	X	173/175 (99%)	169 (98%)	4 (2%)	44	76
11	K	170/170 (100%)	166 (98%)	4 (2%)	43	75
11	Y	170/170 (100%)	166 (98%)	4 (2%)	43	75
12	L	186/186 (100%)	176 (95%)	10 (5%)	20	51
12	Z	186/186 (100%)	176 (95%)	10 (5%)	20	51
13	M	200/208 (96%)	196 (98%)	4 (2%)	48	78
13	a	199/208 (96%)	195 (98%)	4 (2%)	48	78
14	N	162/162 (100%)	159 (98%)	3 (2%)	50	79
14	b	162/162 (100%)	159 (98%)	3 (2%)	50	79
All	All	5325/5544 (96%)	5166 (97%)	159 (3%)	36	70

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	98	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL

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Mol	Chain	Res	Type
3	C	240	GLU
4	D	20	LEU
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	91	GLN
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	35	THR
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	35	ILE

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Mol	Chain	Res	Type
11	K	173	SER
12	L	23	LEU
12	L	100	ARG
12	L	124	SER
12	L	135	GLN
12	L	136	CYS
12	L	150	LEU
12	L	161	GLU
12	L	167	LYS
12	L	172	LEU
12	L	173	LYS
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
14	N	9	LYS
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	98	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	20	LEU
4	R	99	ILE
4	R	176	LEU

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Mol	Chain	Res	Type
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	188	LEU
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	91	GLN
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	35	THR
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	35	ILE
11	Y	173	SER
12	Z	23	LEU
12	Z	99	SER
12	Z	100	ARG

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Mol	Chain	Res	Type
12	Z	124	SER
12	Z	136	CYS
12	Z	150	LEU
12	Z	161	GLU
12	Z	167	LYS
12	Z	172	LEU
12	Z	173	LYS
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
14	b	9	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
3	C	17	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	180	HIS
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN

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Mol	Chain	Res	Type
6	F	123	ASN
6	F	143	HIS
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
8	H	30	ASN
8	H	189	ASN
9	I	63	ASN
9	I	88	GLN
9	I	203	GLN
10	J	55	GLN
10	J	61	GLN
10	J	63	ASN
11	K	9	GLN
11	K	142	ASN
11	K	189	ASN
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	70	ASN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	48	ASN
13	M	108	ASN
13	M	149	HIS
14	N	38	HIS
14	N	141	ASN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	220	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	165	ASN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	180	HIS

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Mol	Chain	Res	Type
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	143	HIS
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	172	ASN
8	V	30	ASN
8	V	114	HIS
8	V	189	ASN
9	W	63	ASN
9	W	88	GLN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	147	HIS
11	Y	142	ASN
11	Y	189	ASN
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	155	ASN
12	Z	165	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	108	ASN
13	a	149	HIS
14	b	38	HIS

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Mol	Chain	Res	Type
14	b	141	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	MES	Y	302	-	12,12,12	2.26	1 (8%)	15,16,16	1.13	1 (6%)
18	MES	H	302	-	12,12,12	2.42	1 (8%)	15,16,16	1.82	4 (26%)
17	6N5	K	301	11	47,48,48	2.00	10 (21%)	55,66,66	1.67	7 (12%)
17	6N5	Y	301	11	47,48,48	2.03	10 (21%)	55,66,66	1.75	11 (20%)
17	6N5	H	301	8	47,48,48	1.89	9 (19%)	55,66,66	1.57	12 (21%)
17	6N5	V	301	8	47,48,48	1.90	9 (19%)	55,66,66	1.54	11 (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
18	MES	Y	302	-	-	0/6/14/14	0/1/1/1
18	MES	H	302	-	-	4/6/14/14	0/1/1/1
17	6N5	K	301	11	-	10/44/67/67	0/4/4/4
17	6N5	Y	301	11	-	12/44/67/67	0/4/4/4
17	6N5	H	301	8	-	10/44/67/67	0/4/4/4
17	6N5	V	301	8	-	11/44/67/67	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	302	MES	C8-S	-8.34	1.65	1.77
18	Y	302	MES	C8-S	-7.42	1.67	1.77
17	V	301	6N5	C10-C9	6.31	1.64	1.53
17	H	301	6N5	C10-C9	6.30	1.64	1.53
17	K	301	6N5	C40-C41	-6.24	1.36	1.51
17	Y	301	6N5	C40-C41	-5.83	1.37	1.51
17	Y	301	6N5	C7-C6	-5.69	1.37	1.51
17	K	301	6N5	C50-C60	-5.48	1.33	1.49
17	Y	301	6N5	C50-C60	-5.30	1.34	1.49
17	K	301	6N5	C7-C6	-5.14	1.39	1.51
17	V	301	6N5	C50-C60	-5.05	1.35	1.49
17	H	301	6N5	C50-C60	-4.96	1.35	1.49
17	K	301	6N5	C57-C52	-4.91	1.32	1.47
17	Y	301	6N5	C57-C52	-4.79	1.32	1.47
17	H	301	6N5	C40-C41	-4.53	1.40	1.51
17	V	301	6N5	C40-C41	-4.46	1.40	1.51
17	V	301	6N5	C57-C52	-4.07	1.34	1.47
17	H	301	6N5	C57-C52	-4.04	1.34	1.47
17	V	301	6N5	C7-C6	-3.87	1.42	1.51
17	H	301	6N5	C7-C6	-3.87	1.42	1.51
17	Y	301	6N5	C56-C57	-3.42	1.32	1.40
17	K	301	6N5	C54-C53	-3.32	1.38	1.49
17	Y	301	6N5	C10-C9	3.30	1.59	1.53
17	K	301	6N5	C56-C57	-3.29	1.32	1.40
17	Y	301	6N5	C54-C53	-3.25	1.38	1.49
17	H	301	6N5	C54-C53	-2.88	1.39	1.49
17	V	301	6N5	C54-C53	-2.87	1.39	1.49
17	Y	301	6N5	C50-C58	-2.76	1.31	1.41
17	K	301	6N5	C50-C58	-2.75	1.31	1.41
17	H	301	6N5	C56-C57	-2.58	1.34	1.40
17	V	301	6N5	C56-C57	-2.55	1.34	1.40
17	V	301	6N5	C56-C55	2.55	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	6N5	C56-C55	2.50	1.39	1.33
17	Y	301	6N5	C57-C58	-2.31	1.32	1.37
17	K	301	6N5	C54-C55	-2.29	1.37	1.47
17	V	301	6N5	C50-C58	-2.27	1.33	1.41
17	K	301	6N5	C10-C9	2.24	1.57	1.53
17	Y	301	6N5	C54-C55	-2.19	1.37	1.47
17	H	301	6N5	C50-C58	-2.19	1.33	1.41
17	K	301	6N5	O21-C9	-2.12	1.37	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	6N5	C7-C8-N22	-6.61	100.70	110.08
17	Y	301	6N5	C7-C8-N22	-6.16	101.33	110.08
17	H	301	6N5	C50-C51-C52	-5.73	103.74	109.72
17	V	301	6N5	C50-C51-C52	-5.65	103.83	109.72
17	K	301	6N5	C50-C58-C57	4.55	111.22	107.98
17	Y	301	6N5	C50-C51-C52	-4.47	105.05	109.72
17	H	301	6N5	C26-C27-N28	-4.37	100.76	111.59
17	V	301	6N5	C26-C27-N28	-4.37	100.76	111.59
17	Y	301	6N5	C46-O45-C44	-4.26	108.37	117.50
17	K	301	6N5	C50-C51-C52	-3.73	105.82	109.72
17	Y	301	6N5	C50-C58-C57	3.73	110.64	107.98
17	H	301	6N5	C41-C40-C24	-3.71	103.48	113.36
17	V	301	6N5	C41-C40-C24	-3.69	103.53	113.36
18	H	302	MES	O3S-S-C8	3.52	112.90	106.00
18	H	302	MES	O2S-S-O1S	-3.29	103.11	113.82
18	H	302	MES	O1-C2-C3	-3.19	104.90	111.77
17	K	301	6N5	C50-C60-N28	3.17	120.37	116.25
17	Y	301	6N5	C41-C40-C24	-2.94	105.53	113.36
17	Y	301	6N5	C50-C60-N28	2.86	119.97	116.25
17	K	301	6N5	C6-C7-C8	2.63	117.86	113.40
17	Y	301	6N5	C6-C7-C8	2.60	117.82	113.40
17	V	301	6N5	C7-C6-C5	2.60	125.73	120.90
17	H	301	6N5	C7-C8-N22	-2.58	106.41	110.08
17	K	301	6N5	C41-C40-C24	-2.56	106.56	113.36
17	H	301	6N5	C51-C52-C57	2.50	110.14	107.00
17	H	301	6N5	C7-C6-C5	2.44	125.44	120.90
17	V	301	6N5	C51-C52-C57	2.42	110.03	107.00
17	V	301	6N5	C7-C8-N22	-2.37	106.72	110.08
18	H	302	MES	O1-C6-C5	-2.29	106.84	111.77
17	Y	301	6N5	O21-C9-C8	-2.27	103.83	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	6N5	C56-C57-C58	-2.24	131.22	134.07
17	Y	301	6N5	C56-C57-C58	-2.23	131.23	134.07
17	H	301	6N5	O13-C12-C10	-2.22	106.94	111.51
17	V	301	6N5	C7-C6-C1	-2.19	116.82	120.90
17	V	301	6N5	C56-C57-C58	-2.19	131.28	134.07
17	H	301	6N5	C54-C53-C52	-2.17	120.80	124.59
17	V	301	6N5	C54-C53-C52	-2.14	120.85	124.59
17	H	301	6N5	C7-C6-C1	-2.12	116.96	120.90
17	H	301	6N5	C59-C58-C57	-2.11	123.32	128.43
18	Y	302	MES	O1S-S-C8	2.11	109.92	106.73
17	V	301	6N5	C59-C58-C57	-2.10	123.33	128.43
17	Y	301	6N5	O13-C12-C10	2.10	115.83	111.51
17	H	301	6N5	C50-C58-C57	2.06	109.45	107.98
17	K	301	6N5	C38-C27-C26	-2.06	106.25	110.14
17	V	301	6N5	C50-C58-C57	2.05	109.44	107.98
17	Y	301	6N5	C54-C53-C52	-2.02	121.06	124.59

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	6N5	C11-C10-C9-C8
17	H	301	6N5	C12-C10-C9-C8
17	K	301	6N5	C11-C10-C9-C8
17	K	301	6N5	C12-C10-C9-C8
17	K	301	6N5	C9-C10-C12-O13
17	K	301	6N5	C11-C10-C12-O13
17	V	301	6N5	C11-C10-C9-C8
17	V	301	6N5	C12-C10-C9-C8
17	Y	301	6N5	C11-C10-C9-C8
17	Y	301	6N5	C12-C10-C9-C8
17	Y	301	6N5	C9-C10-C12-O13
17	Y	301	6N5	C11-C10-C12-O13
18	H	302	MES	C7-C8-S-O1S
18	H	302	MES	C7-C8-S-O3S
17	Y	301	6N5	C47-C44-O45-C46
17	Y	301	6N5	C43-C44-O45-C46
17	V	301	6N5	C5-C6-C7-C8
17	Y	301	6N5	C5-C6-C7-C8
17	H	301	6N5	C5-C6-C7-C8
17	V	301	6N5	C1-C6-C7-C8
17	K	301	6N5	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	H	301	6N5	C1-C6-C7-C8
17	Y	301	6N5	C1-C6-C7-C8
17	H	301	6N5	C12-C10-C9-O21
17	K	301	6N5	C12-C10-C9-O21
17	V	301	6N5	C12-C10-C9-O21
17	K	301	6N5	C1-C6-C7-C8
17	H	301	6N5	C11-C10-C9-O21
17	K	301	6N5	C11-C10-C9-O21
17	V	301	6N5	C11-C10-C9-O21
17	Y	301	6N5	C11-C10-C9-O21
17	Y	301	6N5	C12-C10-C9-O21
18	H	302	MES	C7-C8-S-O2S
17	H	301	6N5	C6-C7-C8-N22
17	V	301	6N5	C6-C7-C8-N22
18	H	302	MES	N4-C7-C8-S
17	K	301	6N5	O49-C23-C24-N25
17	K	301	6N5	N22-C23-C24-N25
17	Y	301	6N5	O49-C23-C24-N25
17	H	301	6N5	O49-C23-C24-N25
17	V	301	6N5	O49-C23-C24-N25
17	V	301	6N5	C11-C10-C12-O13
17	Y	301	6N5	N22-C23-C24-N25
17	H	301	6N5	N25-C26-C27-N28
17	H	301	6N5	N22-C23-C24-N25
17	V	301	6N5	N25-C26-C27-N28
17	V	301	6N5	N22-C23-C24-N25

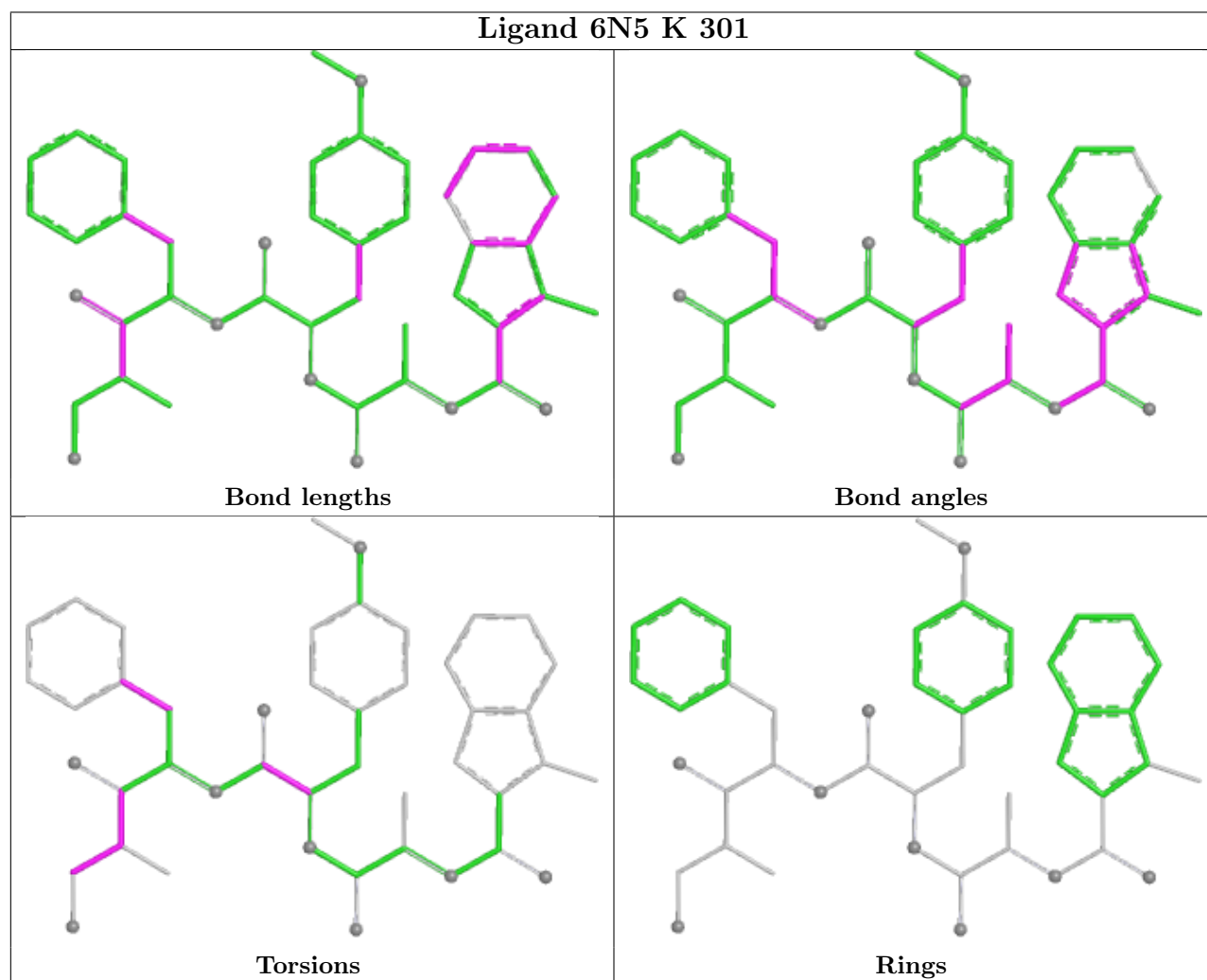
There are no ring outliers.

4 monomers are involved in 10 short contacts:

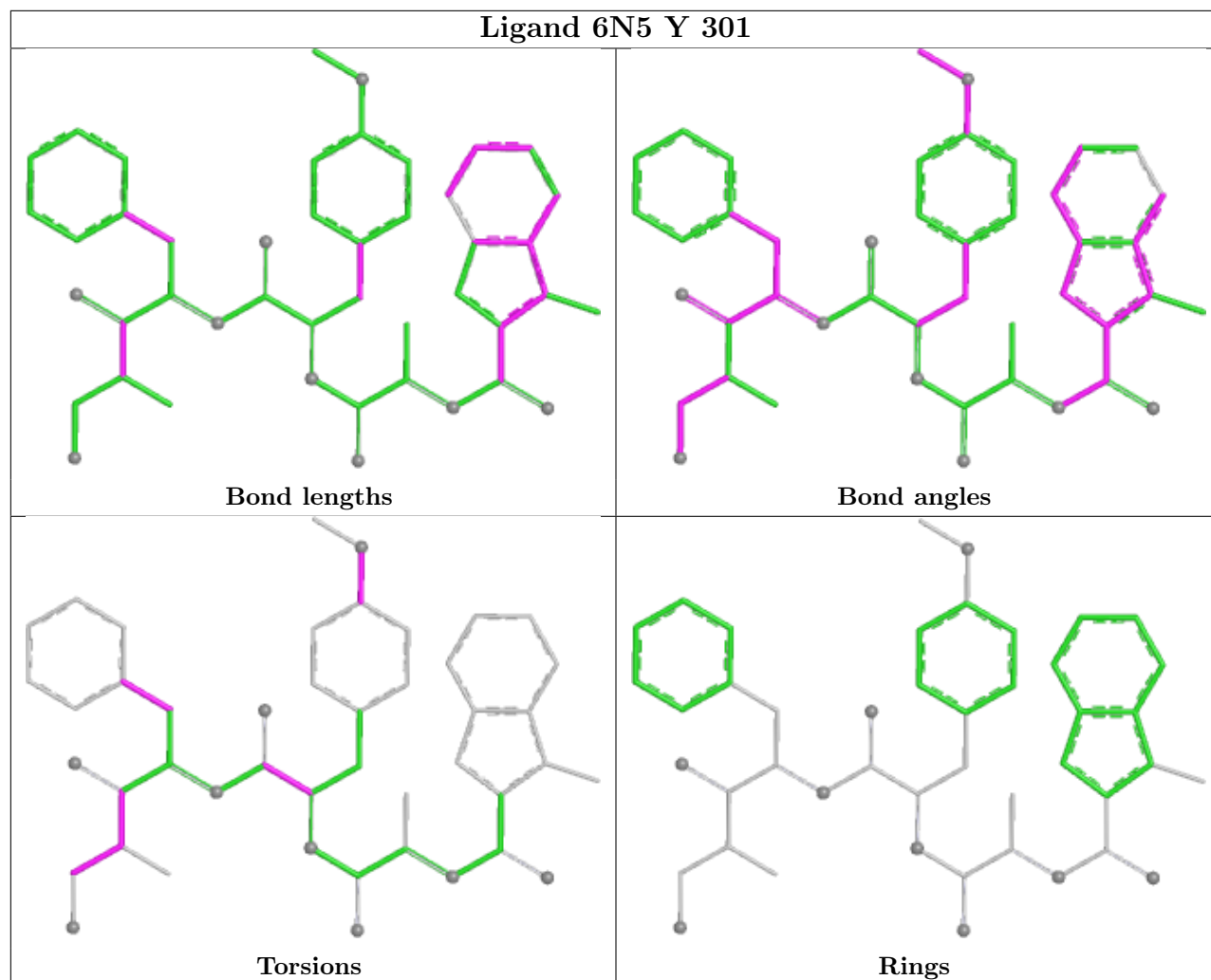
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Y	302	MES	1	0
18	H	302	MES	4	0
17	K	301	6N5	2	0
17	Y	301	6N5	4	0

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

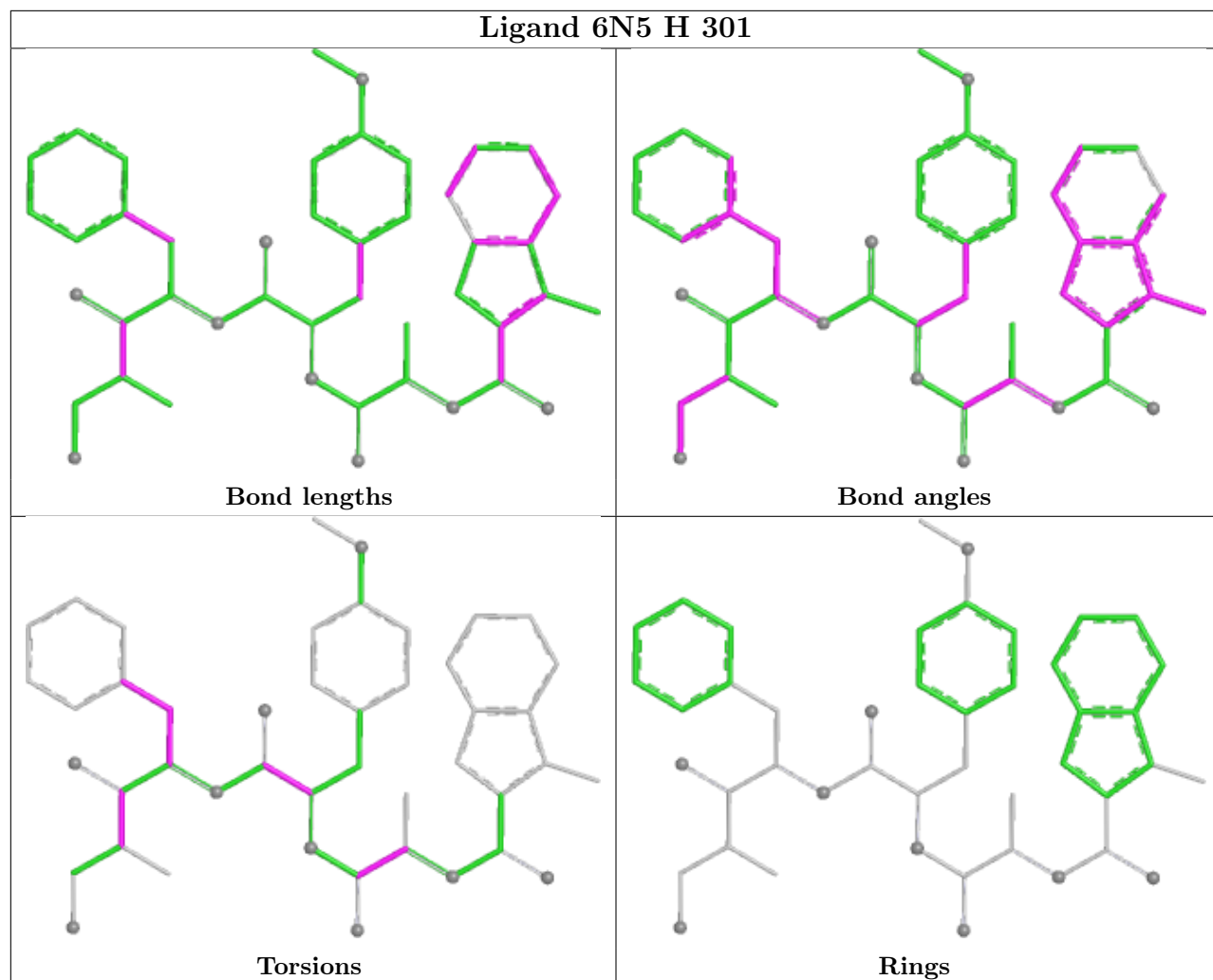
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

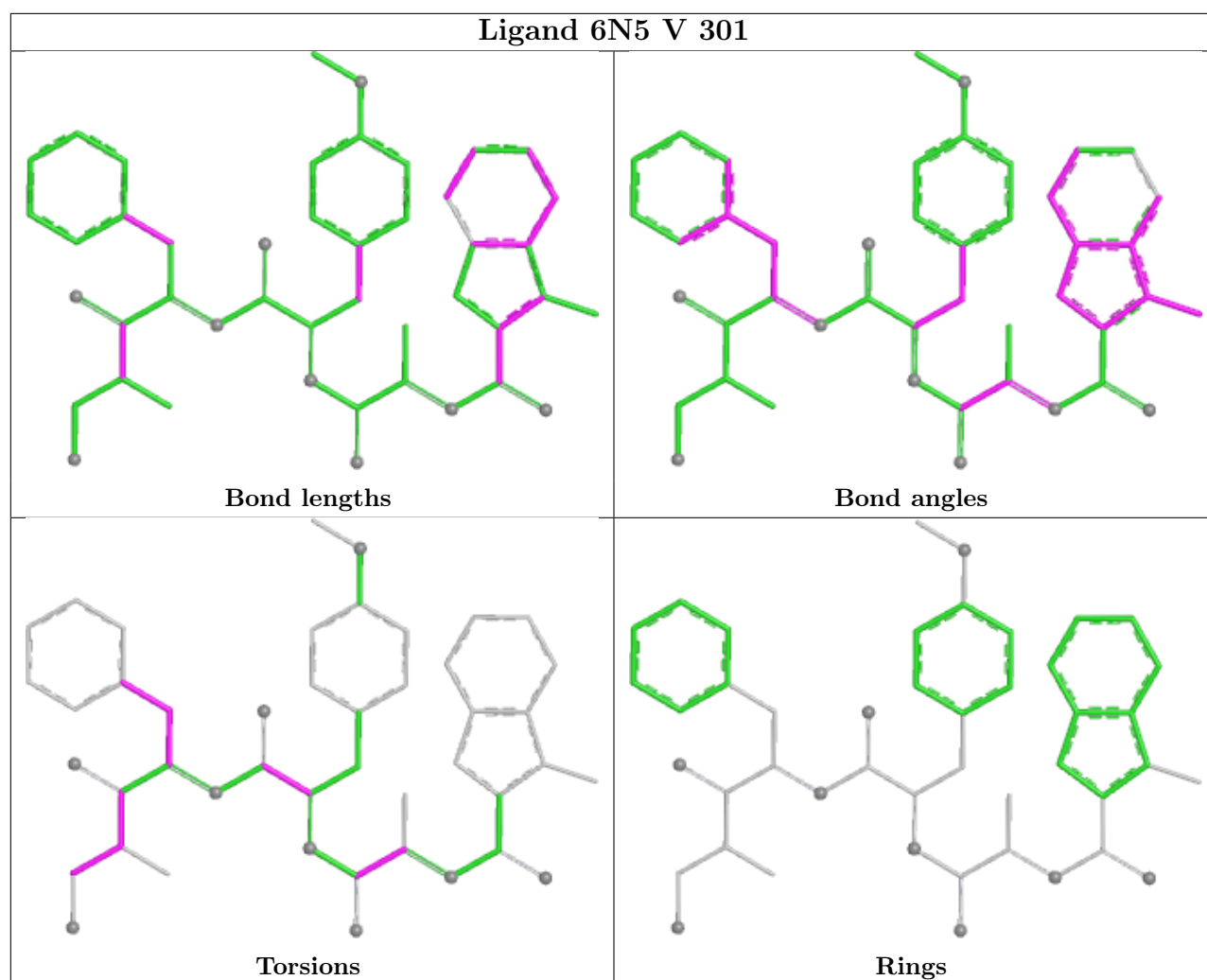


Ligand 6N5 Y 301



Ligand 6N5 H 301





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	250/250 (100%)	-0.52	0 100 100	38, 56, 96, 134	0
1	O	250/250 (100%)	-0.48	0 100 100	41, 60, 104, 141	0
2	B	244/258 (94%)	-0.36	2 (0%) 82 77	41, 62, 106, 157	0
2	P	244/258 (94%)	-0.37	1 (0%) 88 85	45, 63, 105, 158	0
3	C	240/254 (94%)	-0.16	5 (2%) 63 54	41, 69, 137, 169	0
3	Q	240/254 (94%)	-0.06	2 (0%) 82 77	28, 77, 152, 191	0
4	D	235/260 (90%)	-0.39	0 100 100	47, 66, 99, 129	0
4	R	235/260 (90%)	-0.30	1 (0%) 88 85	55, 76, 115, 145	0
5	E	231/234 (98%)	-0.41	0 100 100	45, 69, 110, 154	0
5	S	231/234 (98%)	-0.35	0 100 100	48, 71, 112, 143	0
6	F	243/288 (84%)	-0.50	2 (0%) 82 77	39, 62, 110, 142	0
6	T	243/288 (84%)	-0.39	3 (1%) 76 69	39, 65, 123, 148	0
7	G	241/252 (95%)	-0.45	0 100 100	38, 60, 101, 156	0
7	U	241/252 (95%)	-0.52	0 100 100	41, 57, 92, 133	0
8	H	226/232 (97%)	-0.49	2 (0%) 81 75	35, 54, 91, 145	0
8	V	226/232 (97%)	-0.42	2 (0%) 81 75	35, 55, 93, 162	0
9	I	204/205 (99%)	-0.62	0 100 100	35, 53, 86, 110	0
9	W	204/205 (99%)	-0.64	0 100 100	38, 54, 82, 106	0
10	J	195/198 (98%)	-0.50	1 (0%) 87 83	38, 58, 85, 129	0
10	X	195/198 (98%)	-0.50	1 (0%) 87 83	40, 62, 88, 140	0
11	K	211/211 (100%)	-0.33	1 (0%) 87 83	35, 64, 92, 126	0
11	Y	211/211 (100%)	-0.35	1 (0%) 87 83	26, 65, 93, 126	0
12	L	222/222 (100%)	-0.39	1 (0%) 87 83	44, 59, 101, 133	0
12	Z	222/222 (100%)	-0.35	0 100 100	43, 62, 104, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.55	2 (0%) 81 75	32, 56, 86, 106	1 (0%)
13	a	233/246 (94%)	-0.52	1 (0%) 88 85	39, 57, 84, 115	0
14	N	196/196 (100%)	-0.61	0 100 100	33, 51, 84, 108	0
14	b	196/196 (100%)	-0.63	0 100 100	33, 51, 84, 111	0
All	All	6342/6612 (95%)	-0.43	28 (0%) 88 85	26, 61, 106, 191	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	5.4
10	J	1	MET	4.8
3	Q	50	LEU	3.6
8	V	223	ILE	3.2
2	B	218	GLY	3.1
6	T	243	ILE	3.0
11	K	146	ASP	2.9
13	a	1	THR	2.8
3	C	58	THR	2.7
6	F	202	ASP	2.7
3	C	205	ALA	2.7
6	T	204	LYS	2.7
8	H	223	ILE	2.5
6	T	205	GLU	2.5
13	M	69	ASP	2.4
13	M	233	ILE	2.4
11	Y	146	ASP	2.4
2	P	93	HIS	2.4
3	C	238	LYS	2.4
4	R	113	LEU	2.4
8	H	224	GLN	2.2
8	V	224	GLN	2.2
3	Q	225	GLU	2.2
6	F	215	CYS	2.1
3	C	206	LYS	2.1
3	C	186	VAL	2.1
12	L	136	CYS	2.1
2	B	51	VAL	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

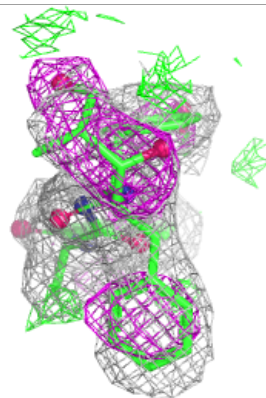
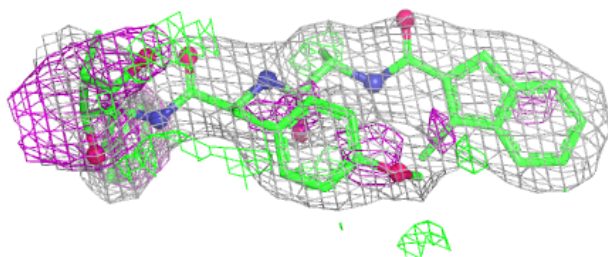
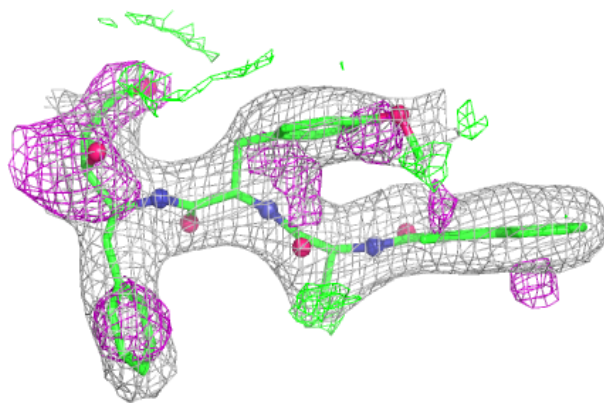
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	MES	Y	302	12/12	0.82	0.20	41,45,71,73	12
17	6N5	Y	301	45/45	0.87	0.13	25,51,70,73	0
17	6N5	K	301	45/45	0.89	0.11	35,51,69,77	0
18	MES	H	302	12/12	0.91	0.13	64,69,83,89	12
17	6N5	V	301	45/45	0.91	0.10	34,49,63,64	0
17	6N5	H	301	45/45	0.92	0.09	33,45,57,61	0
15	MG	I	301	1/1	0.98	0.08	59,59,59,59	0
15	MG	L	301	1/1	0.98	0.09	73,73,73,73	0
15	MG	Z	301	1/1	0.98	0.04	66,66,66,66	0
16	CL	G	302	1/1	0.98	0.11	47,47,47,47	0
15	MG	G	301	1/1	0.98	0.04	54,54,54,54	0
15	MG	N	201	1/1	0.99	0.03	56,56,56,56	0
15	MG	J	201	1/1	0.99	0.04	47,47,47,47	0
15	MG	K	302	1/1	0.99	0.09	63,63,63,63	0
16	CL	U	301	1/1	0.99	0.10	42,42,42,42	0
15	MG	I	302	1/1	0.99	0.08	64,64,64,64	0

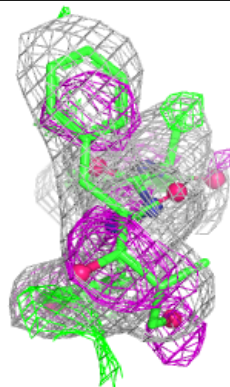
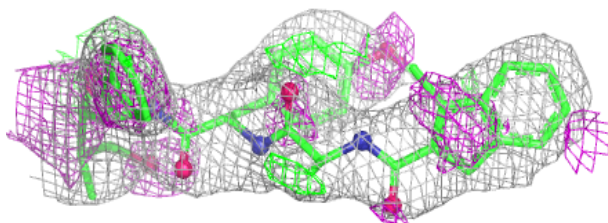
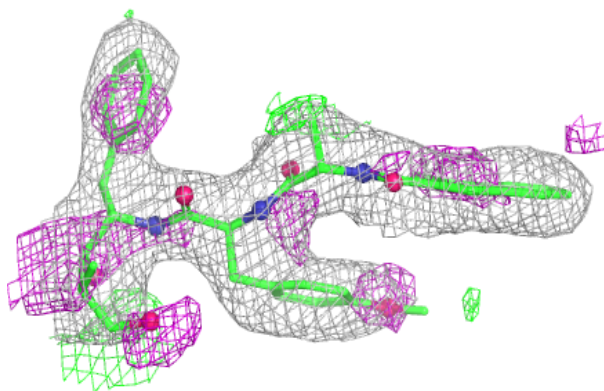
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6N5 Y 301:

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

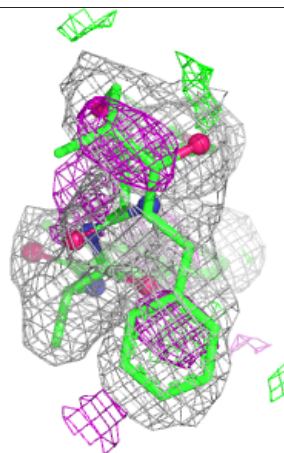
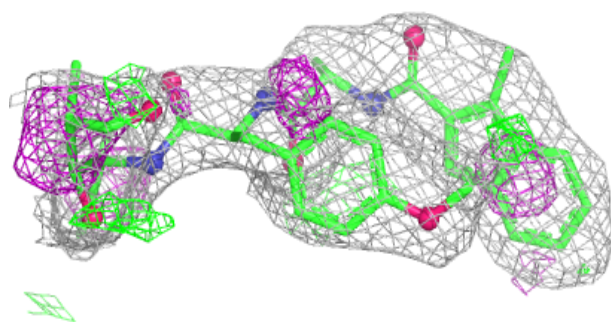
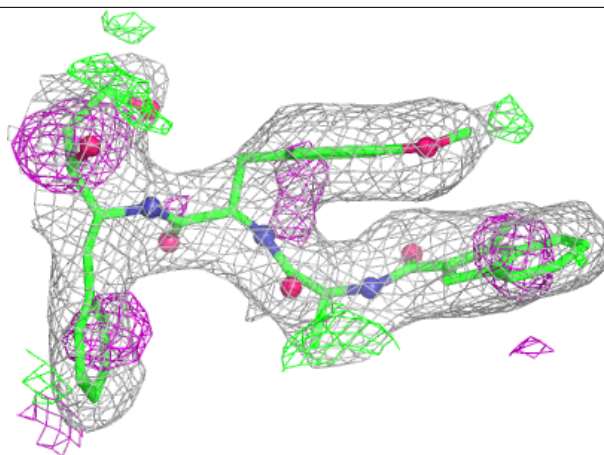
**Electron density around 6N5 K 301:**

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

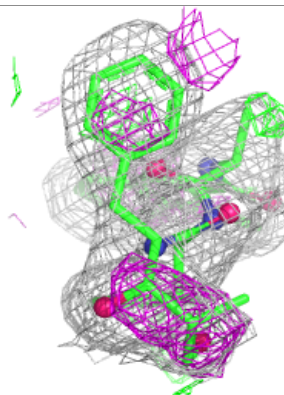
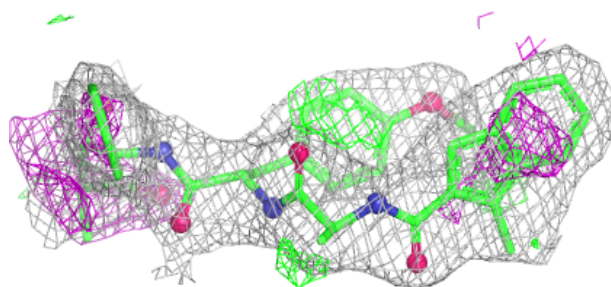
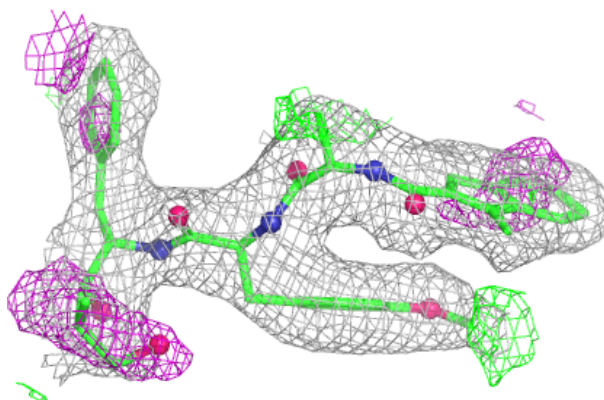


Electron density around 6N5 V 301:

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

**Electron density around 6N5 H 301:**

$2mF_o-DF_c$ (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.