



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:48 AM UTC

PDB ID : 4QLQ / pdb_00004qlq
Title : yCP in complex with tripeptidic epoxyketone inhibitor 8
Authors : De Bruin, G.; Huber, E.; Xin, B.; Van Rooden, E.; Al-Ayed, K.; Kim, K.; Kisselev, A.; Driessen, C.; Van der Marel, G.; Groll, M.; Overkleeft, H.
Deposited on : 2014-06-13
Resolution : 2.40 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

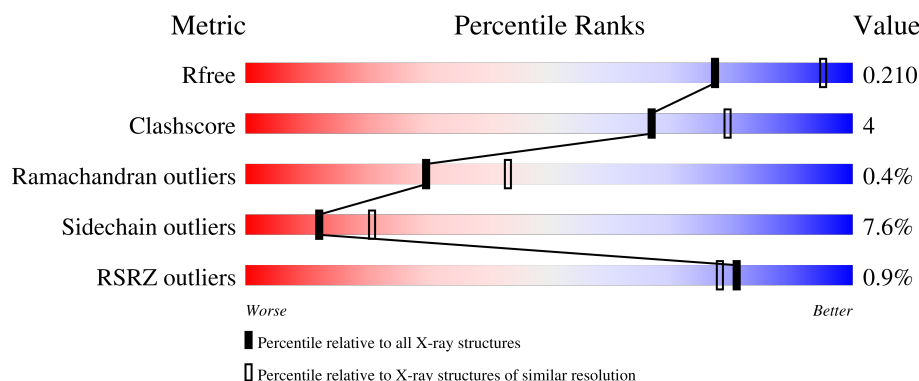
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	2% 92% 7% .
1	O	250	% 90% 8% .
2	B	258	2% 80% 13% 5%
2	P	258	3% 79% 14% 5%
3	C	254	2% 77% 15% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 3% 77% 15% • 6%
4	D	260	 76% 13% • 10%
4	R	260	 76% 13% • 10%
5	E	234	 80% 15% • •
5	S	234	 81% 15% • •
6	F	288	 74% 9% • 16%
6	T	288	 73% 10% • 16%
7	G	252	 83% 10% • •
7	U	252	 82% 11% • •
8	H	232	 89% 6% • •
8	V	232	 88% 6% • •
9	I	205	 88% 11% •
9	W	205	 88% 11% •
10	J	198	 85% 12% • •
10	X	198	 86% 11% • •
11	K	212	 89% 8% •
11	Y	212	 88% 9% •
12	L	222	 89% 9% •
12	Z	222	 87% 11% •
13	M	246	 84% 9% • 5%
13	a	246	 85% 9% • 5%
14	N	196	 88% 11% •
14	b	196	 88% 11% •

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50332 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	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	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-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	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	0	0
			1824	1154	312	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).

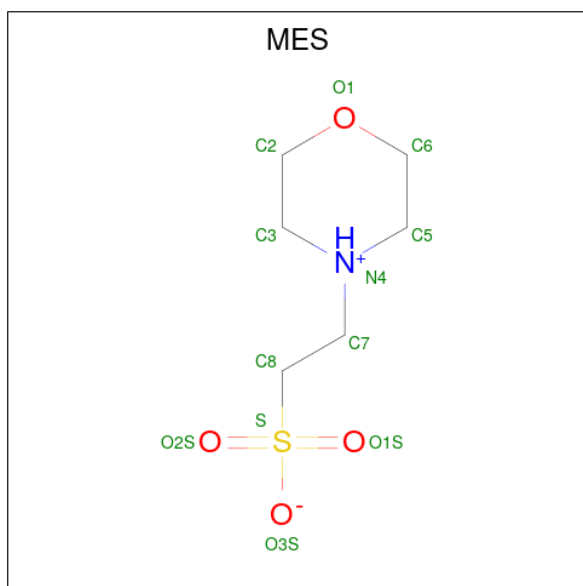
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

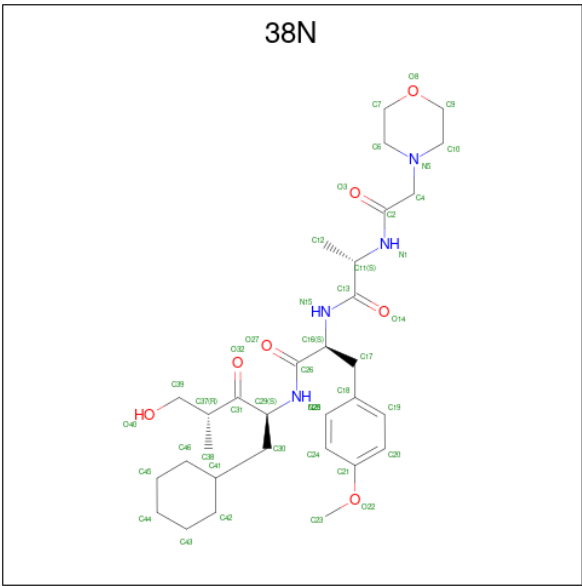
- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 17 is N-(morpholin-4-ylacetyl)-L-alanyl-N-[(2S,4R)-1-cyclohexyl-5-hydroxy-4-met

hyl-3-oxopentan-2-yl]-O-methyl-L-tyrosinamide (CCD ID: 38N) (formula: C₃₁H₄₈N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			42	31	4	7		
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	V	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	7		

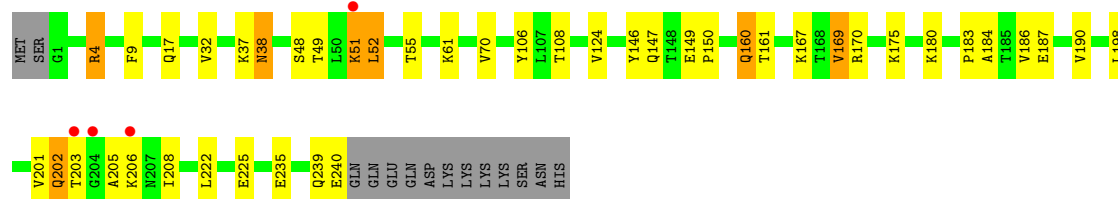
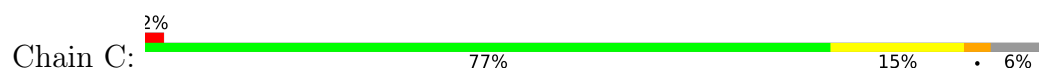
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	34	Total	O	0	0
			34	34		
18	B	29	Total	O	0	0
			29	29		
18	C	21	Total	O	0	0
			21	21		
18	D	12	Total	O	0	0
			12	12		
18	E	7	Total	O	0	0
			7	7		
18	F	17	Total	O	0	0
			17	17		
18	G	42	Total	O	0	0
			42	42		

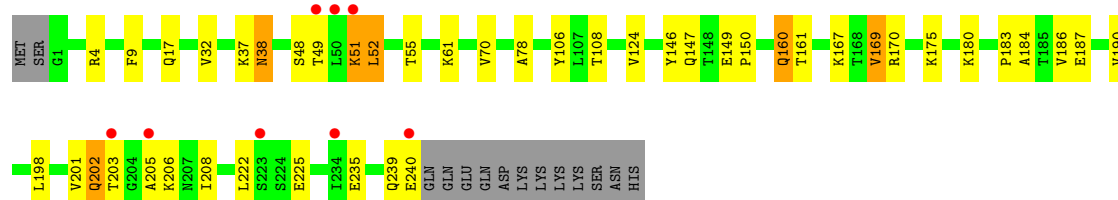
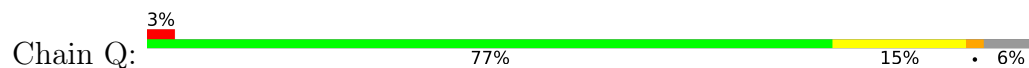
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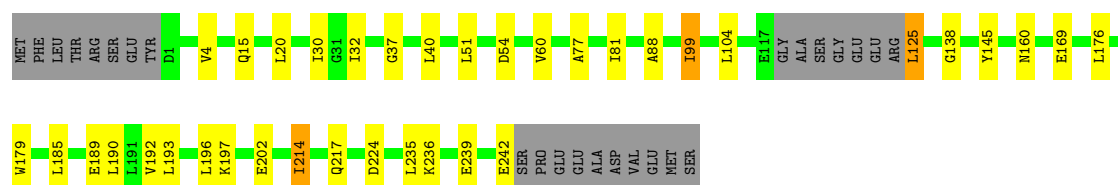
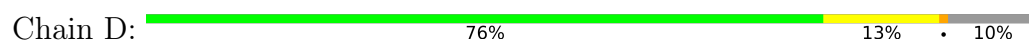
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	H	38	Total 38	O 38	0	0
18	I	46	Total 46	O 46	0	0
18	J	42	Total 42	O 42	0	0
18	K	43	Total 43	O 43	0	0
18	L	48	Total 48	O 48	0	0
18	M	28	Total 28	O 28	0	0
18	N	17	Total 17	O 17	0	0
18	O	20	Total 20	O 20	0	0
18	P	17	Total 17	O 17	0	0
18	Q	9	Total 9	O 9	0	0
18	R	14	Total 14	O 14	0	0
18	S	7	Total 7	O 7	0	0
18	T	23	Total 23	O 23	0	0
18	U	36	Total 36	O 36	0	0
18	V	34	Total 34	O 34	0	0
18	W	42	Total 42	O 42	0	0
18	X	34	Total 34	O 34	0	0
18	Y	38	Total 38	O 38	0	0
18	Z	40	Total 40	O 40	0	0
18	a	43	Total 43	O 43	0	0
18	b	31	Total 31	O 31	0	0



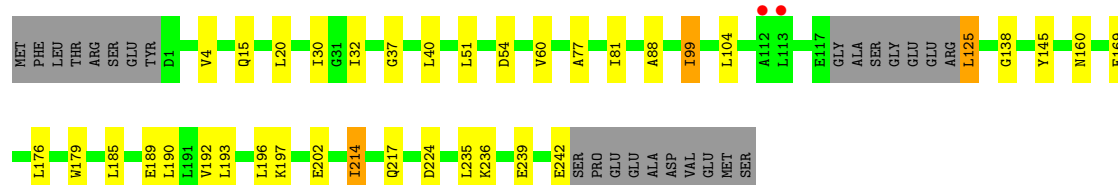
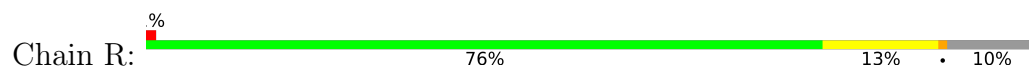
• Molecule 3: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-5



• Molecule 4: Proteasome subunit alpha type-5

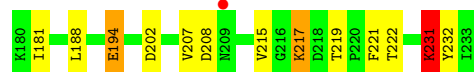
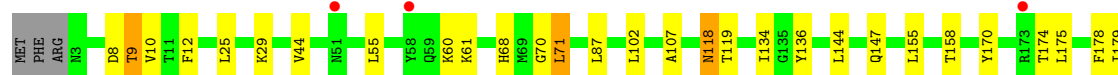
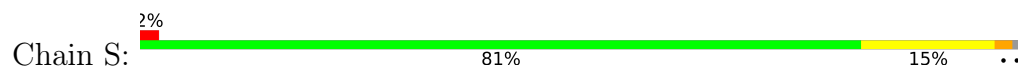


• Molecule 5: Proteasome subunit alpha type-6

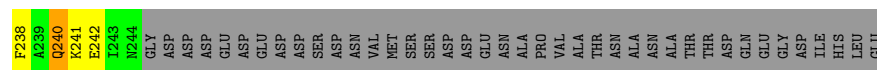
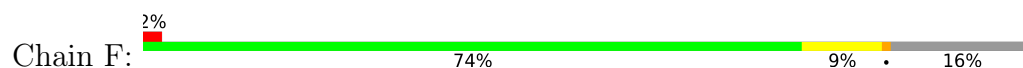




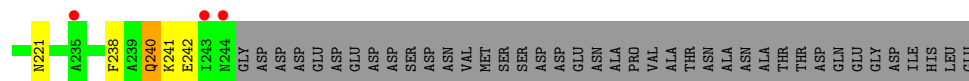
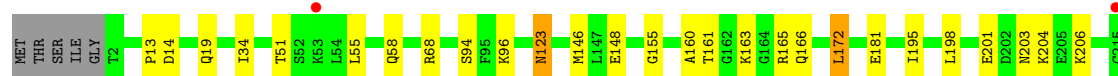
• Molecule 5: Proteasome subunit alpha type-6



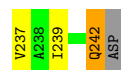
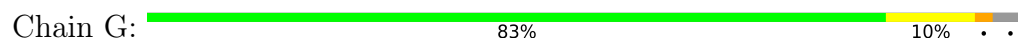
• Molecule 6: Probable proteasome subunit alpha type-7



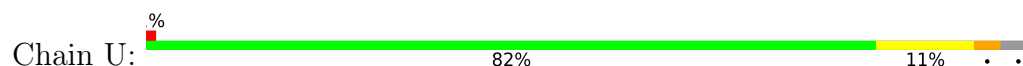
• Molecule 6: Probable proteasome subunit alpha type-7

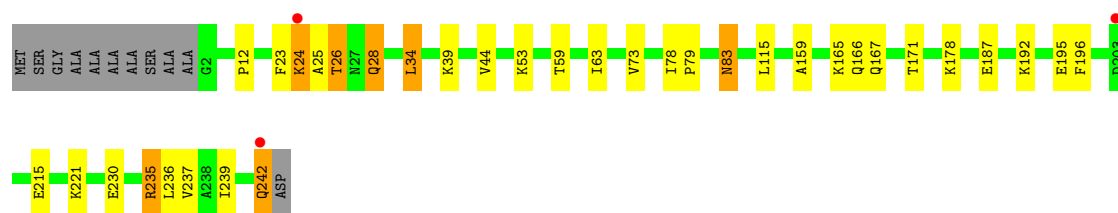


• Molecule 7: Proteasome subunit alpha type-1



• Molecule 7: Proteasome subunit alpha type-1





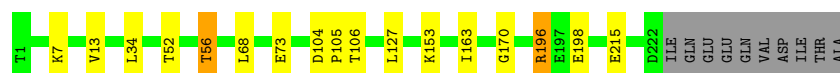
• Molecule 8: Proteasome subunit beta type-2

Chain H: 89% 6% . .



• Molecule 8: Proteasome subunit beta type-2

Chain V: 88% 6% . .



• Molecule 9: Proteasome subunit beta type-3

Chain I: 88% 11% .



• Molecule 9: Proteasome subunit beta type-3

Chain W: 88% 11% .



• Molecule 10: Proteasome subunit beta type-4

Chain J: 85% 12% . . .



• Molecule 10: Proteasome subunit beta type-4

Chain X: 86% 11% . . .



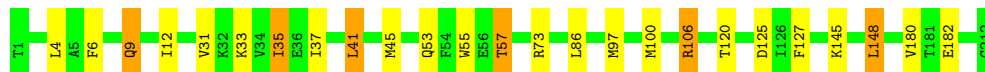
- Molecule 11: Proteasome subunit beta type-5

Chain K:  89% 8% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  88% 9% .



- Molecule 12: Proteasome subunit beta type-6

Chain L:  89% 9% .



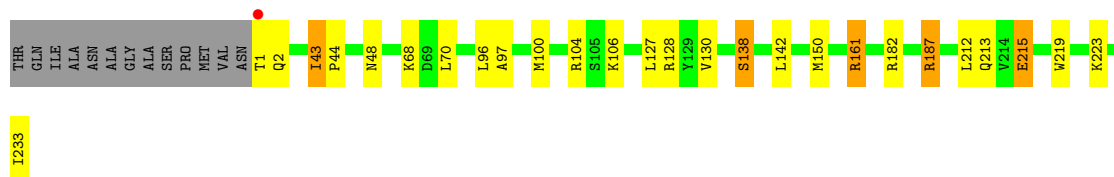
- Molecule 12: Proteasome subunit beta type-6

Chain Z:  87% 11% .



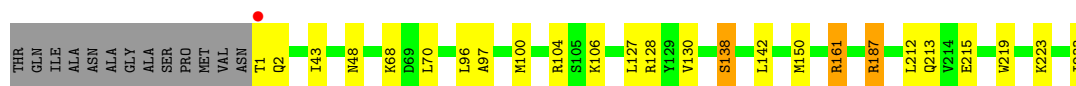
- Molecule 13: Proteasome subunit beta type-7

Chain M:  84% 9% 5% .



- Molecule 13: Proteasome subunit beta type-7

Chain a:  85% 9% 5% .

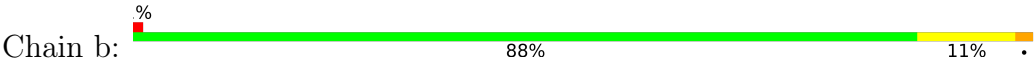


- Molecule 14: Proteasome subunit beta type-1

Chain N:  88% 11% .



● 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	136.65Å 299.59Å 144.82Å 90.00° 112.85° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (15.00-2.40) 98.0 (15.00-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.215 (Not available) , 0.210	Depositor DCC
R_{free} test set	20403 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	50332	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: MG, 38N, 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	0.42	0/1952	0.76	0/2642
1	O	0.42	0/1952	0.76	0/2642
2	B	0.43	0/1934	0.76	0/2618
2	P	0.43	0/1934	0.76	0/2618
3	C	0.44	0/1910	0.78	0/2586
3	Q	0.44	0/1910	0.79	0/2586
4	D	0.42	0/1837	0.74	0/2475
4	R	0.42	0/1837	0.74	0/2475
5	E	0.41	0/1800	0.73	0/2433
5	S	0.41	0/1800	0.73	0/2433
6	F	0.43	0/1932	0.76	0/2609
6	T	0.43	0/1932	0.76	0/2609
7	G	0.41	0/1945	0.74	0/2634
7	U	0.41	0/1945	0.74	0/2634
8	H	0.41	0/1715	0.74	0/2326
8	V	0.41	0/1715	0.74	0/2326
9	I	0.39	0/1611	0.74	0/2174
9	W	0.39	0/1611	0.74	0/2174
10	J	0.40	0/1589	0.71	0/2142
10	X	0.40	0/1589	0.71	0/2142
11	K	0.40	0/1681	0.71	0/2274
11	Y	0.40	0/1681	0.71	0/2274
12	L	0.40	0/1795	0.73	0/2420
12	Z	0.40	0/1795	0.73	0/2420
13	M	0.43	0/1855	0.72	0/2514
13	a	0.43	0/1855	0.73	0/2514
14	N	0.38	0/1541	0.71	1/2087 (0.0%)
14	b	0.38	0/1541	0.72	1/2087 (0.0%)
All	All	0.41	0/50194	0.74	2/67868 (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
9	I	0	1
9	W	0	1
12	L	0	1
12	Z	0	1
13	M	0	1
13	a	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	115	LEU	N-CA-C	5.20	117.35	111.11
14	N	115	LEU	N-CA-C	5.16	117.31	111.11

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	192	ASP	Peptide
12	L	135	GLN	Peptide
13	M	1	THR	Peptide
9	W	192	ASP	Peptide
12	Z	135	GLN	Peptide
13	a	1	THR	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	1915	0	1929	8	0
1	O	1915	0	1929	10	0
2	B	1904	0	1904	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1904	0	1904	20	0
3	C	1881	0	1895	21	0
3	Q	1881	0	1895	23	0
4	D	1813	0	1797	14	0
4	R	1813	0	1797	13	0
5	E	1773	0	1775	19	0
5	S	1773	0	1775	18	0
6	F	1892	0	1883	17	0
6	T	1892	0	1883	19	0
7	G	1907	0	1901	14	0
7	U	1907	0	1901	18	0
8	H	1684	0	1685	5	0
8	V	1684	0	1685	6	0
9	I	1581	0	1574	12	0
9	W	1581	0	1574	12	0
10	J	1561	0	1569	15	0
10	X	1561	0	1569	14	0
11	K	1644	0	1592	14	0
11	Y	1644	0	1592	16	0
12	L	1757	0	1711	12	0
12	Z	1757	0	1711	15	0
13	M	1824	0	1832	9	0
13	a	1824	0	1832	7	0
14	N	1512	0	1481	15	0
14	b	1512	0	1481	13	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	H	12	0	13	0	0
16	K	12	0	13	0	0
16	V	12	0	13	0	0
16	Y	12	0	13	1	0
17	H	42	0	47	1	0
17	K	42	0	47	2	0
17	V	42	0	47	1	0
17	Y	42	0	47	2	0
18	A	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	29	0	0	0	0
18	C	21	0	0	0	0
18	D	12	0	0	1	0
18	E	7	0	0	0	0
18	F	17	0	0	0	0
18	G	42	0	0	0	0
18	H	38	0	0	0	0
18	I	46	0	0	0	0
18	J	42	0	0	0	0
18	K	43	0	0	0	0
18	L	48	0	0	0	0
18	M	28	0	0	0	0
18	N	17	0	0	0	0
18	O	20	0	0	0	0
18	P	17	0	0	0	0
18	Q	9	0	0	0	0
18	R	14	0	0	0	0
18	S	7	0	0	0	0
18	T	23	0	0	0	0
18	U	36	0	0	0	0
18	V	34	0	0	0	0
18	W	42	0	0	0	0
18	X	34	0	0	0	0
18	Y	38	0	0	0	0
18	Z	40	0	0	0	0
18	a	43	0	0	0	0
18	b	31	0	0	0	0
All	All	50332	0	49296	362	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 4.

All (362) 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:100:MET:HE3	11:K:127:PHE:HB2	1.34	1.08
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.32	1.05
2:P:50:LYS:HE3	2:P:50:LYS:HA	1.49	0.94
2:B:50:LYS:HE3	2:B:50:LYS:HA	1.48	0.93
11:K:100:MET:CE	11:K:127:PHE:HB2	2.09	0.82
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:106:ARG:HH11	11:Y:106:ARG:HB3	1.45	0.81
11:K:106:ARG:HH11	11:K:106:ARG:HB3	1.45	0.79
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.51	0.76
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.51	0.75
6:T:146:MET:CE	6:T:161:THR:HB	2.17	0.74
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.18	0.73
6:F:146:MET:CE	6:F:161:THR:HB	2.17	0.73
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.18	0.73
3:C:51:LYS:O	3:C:52:LEU:HB2	1.89	0.72
11:K:100:MET:HE3	11:K:127:PHE:CB	2.18	0.72
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.89	0.71
2:B:12:PHE:H	3:C:17:GLN:HE22	1.39	0.70
11:K:53:GLN:O	11:K:57:THR:HG23	1.91	0.70
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.91	0.70
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.17	0.70
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.74	0.70
6:T:146:MET:HE3	6:T:161:THR:HB	1.74	0.69
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.74	0.69
6:F:146:MET:HE3	6:F:161:THR:HB	1.74	0.69
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.74	0.68
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.75	0.67
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.76	0.67
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.76	0.66
5:E:12:PHE:H	6:F:19:GLN:HE22	1.42	0.66
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.61	0.65
17:H:303:38N:O32	17:H:303:38N:O40	2.15	0.65
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.60	0.65
17:V:303:38N:O32	17:V:303:38N:O40	2.15	0.65
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.46	0.64
8:H:196:ARG:NH2	9:I:150:GLU:O	2.31	0.64
5:S:12:PHE:H	6:T:19:GLN:HE22	1.44	0.64
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.79	0.64
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.80	0.63
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.79	0.63
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.46	0.63
5:S:155:LEU:HD13	5:S:158:THR:HB	1.81	0.63
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.81	0.62
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.82	0.62
9:I:65:MET:HE1	9:I:93:SER:HB3	1.81	0.62
5:E:155:LEU:HD13	5:E:158:THR:HB	1.81	0.62
9:W:65:MET:HE1	9:W:93:SER:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:35:THR:HG21	14:N:45:ARG:HE	1.66	0.61
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.64	0.61
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.64	0.61
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.81	0.60
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.82	0.60
14:b:35:THR:HG21	14:b:45:ARG:HE	1.65	0.60
2:B:180:LYS:O	2:B:183:MET:HB2	2.02	0.60
2:P:180:LYS:O	2:P:183:MET:HB2	2.02	0.60
5:E:9:THR:HG21	5:E:119:THR:HA	1.85	0.59
8:V:196:ARG:NH2	9:W:150:GLU:O	2.37	0.58
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.39	0.58
6:F:123:ASN:C	6:F:123:ASN:HD22	2.12	0.57
14:b:20:THR:HG23	14:b:28:ASN:HB3	1.86	0.57
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.38	0.57
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.17	0.57
5:S:9:THR:HG21	5:S:119:THR:HA	1.85	0.57
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.69	0.57
6:T:123:ASN:C	6:T:123:ASN:HD22	2.12	0.57
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.69	0.57
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.87	0.57
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.53	0.57
12:L:8:ASN:HA	12:L:30:ILE:O	2.05	0.56
11:Y:106:ARG:HH11	11:Y:106:ARG:CB	2.16	0.56
1:O:12:PHE:H	2:P:20:GLN:HE22	1.53	0.56
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.70	0.56
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.05	0.56
3:C:201:VAL:O	3:C:202:GLN:HB2	2.05	0.56
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.19	0.56
7:U:23:PHE:O	7:U:26:THR:HB	2.06	0.56
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.88	0.56
3:C:201:VAL:O	3:C:202:GLN:CB	2.53	0.56
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.88	0.56
14:N:20:THR:HG22	14:N:31:THR:OG1	2.06	0.56
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.70	0.56
3:C:161:THR:HG21	3:C:169:VAL:HG22	1.87	0.55
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.05	0.55
14:b:20:THR:HG22	14:b:31:THR:OG1	2.06	0.55
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.52	0.55
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.88	0.55
10:J:23:ARG:NH2	11:K:120:THR:OG1	2.39	0.55
11:K:106:ARG:HH11	11:K:106:ARG:CB	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:202:GLN:CG	3:Q:203:THR:H	2.19	0.54
10:X:23:ARG:NH2	11:Y:120:THR:OG1	2.40	0.54
3:Q:161:THR:HG21	3:Q:169:VAL:HG22	1.88	0.54
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.89	0.54
7:G:23:PHE:O	7:G:26:THR:HB	2.06	0.54
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.89	0.54
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.88	0.54
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.22	0.54
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.38	0.54
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.38	0.54
3:C:202:GLN:CG	3:C:203:THR:H	2.19	0.54
8:H:52:THR:O	8:H:56:THR:HB	2.09	0.53
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.90	0.53
10:X:1:MET:HA	10:X:34:LYS:CE	2.39	0.53
4:R:77:ALA:O	4:R:81:ILE:HG12	2.08	0.53
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.91	0.53
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.57	0.52
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.90	0.52
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.57	0.52
3:C:202:GLN:HG3	3:C:203:THR:N	2.24	0.52
3:Q:51:LYS:HA	3:Q:51:LYS:HE3	1.91	0.52
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.91	0.52
8:V:52:THR:O	8:V:56:THR:HB	2.10	0.52
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.91	0.52
4:D:77:ALA:O	4:D:81:ILE:HG12	2.09	0.52
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.24	0.52
14:N:152:VAL:HA	14:N:175:MET:HE1	1.92	0.52
3:C:51:LYS:HE3	3:C:51:LYS:HA	1.91	0.51
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.91	0.51
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.75	0.51
3:C:202:GLN:HG3	3:C:203:THR:H	1.75	0.51
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.93	0.51
13:M:150:MET:HE1	13:M:187:ARG:HG2	1.91	0.51
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.91	0.51
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.93	0.51
10:J:1:MET:HA	10:J:34:LYS:CE	2.39	0.51
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.92	0.51
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.36	0.51
6:T:146:MET:HE1	6:T:161:THR:HB	1.92	0.51
14:b:152:VAL:HA	14:b:175:MET:HE1	1.92	0.51
7:G:34:LEU:C	7:G:34:LEU:HD23	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.93	0.51
12:L:195:HIS:HD2	12:L:197:GLN:H	1.57	0.51
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.93	0.51
11:K:86:LEU:C	11:K:86:LEU:HD13	2.36	0.50
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.45	0.50
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.44	0.50
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.93	0.50
3:C:9:PHE:H	4:D:15:GLN:HE22	1.58	0.50
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.46	0.50
14:N:103:ASP:HB2	14:N:106:ASN:HB2	1.93	0.50
14:b:103:ASP:HB2	14:b:106:ASN:HB2	1.93	0.50
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.93	0.50
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.46	0.50
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.94	0.50
7:U:34:LEU:C	7:U:34:LEU:HD23	2.36	0.50
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.92	0.50
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.93	0.49
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.48	0.49
3:C:37:LYS:HB2	3:C:184:ALA:HA	1.95	0.49
3:C:38:ASN:N	3:C:38:ASN:HD22	2.10	0.49
5:E:68:HIS:HE1	5:E:102:LEU:O	1.95	0.49
10:J:1:MET:O	10:J:2:ASP:HB2	2.12	0.49
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.95	0.49
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.95	0.49
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.47	0.49
6:F:146:MET:HE1	6:F:161:THR:HB	1.92	0.49
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.95	0.49
3:Q:37:LYS:HB2	3:Q:184:ALA:HA	1.95	0.49
7:G:242:GLN:HA	7:G:242:GLN:OE1	2.13	0.49
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.95	0.48
7:U:242:GLN:OE1	7:U:242:GLN:HA	2.13	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.48
10:X:139:TYR:CE2	10:X:172:MET:HE2	2.49	0.48
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.62	0.48
10:X:1:MET:O	10:X:2:ASP:HB2	2.12	0.48
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.78	0.48
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.78	0.48
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.78	0.48
14:N:20:THR:CG2	14:N:31:THR:OG1	2.61	0.48
11:Y:33:LYS:HE2	17:Y:303:38N:H34	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.78	0.48
1:O:30:GLN:HA	1:O:30:GLN:HE21	1.78	0.48
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.10	0.48
4:R:185:LEU:O	4:R:189:GLU:HG3	2.14	0.48
1:A:12:PHE:H	2:B:20:GLN:HE22	1.61	0.48
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.95	0.48
5:S:134:ILE:HD12	5:S:215:VAL:HG12	1.96	0.48
13:M:96:LEU:O	13:M:100:MET:HG2	2.14	0.48
1:O:55:LEU:HB3	7:U:159:ALA:O	2.14	0.48
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.77	0.48
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.79	0.48
5:S:68:HIS:HE1	5:S:102:LEU:O	1.96	0.48
4:D:185:LEU:O	4:D:189:GLU:HG3	2.14	0.47
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.49	0.47
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.94	0.47
5:S:170:TYR:CD1	5:S:170:TYR:C	2.92	0.47
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.49	0.47
10:J:158:LEU:O	10:J:162:LYS:HG3	2.15	0.47
10:X:1:MET:HA	10:X:34:LYS:HE3	1.96	0.47
14:b:20:THR:CG2	14:b:31:THR:OG1	2.61	0.47
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.96	0.47
5:S:71:LEU:C	5:S:71:LEU:HD23	2.40	0.47
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.95	0.47
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.95	0.47
9:I:65:MET:CE	9:I:93:SER:HB3	2.44	0.47
2:P:183:MET:HE1	2:P:191:LEU:HD12	1.97	0.47
9:W:65:MET:CE	9:W:93:SER:HB3	2.44	0.47
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.50	0.47
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.96	0.47
2:B:110:LEU:HD23	2:B:110:LEU:C	2.40	0.47
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.55	0.47
13:a:96:LEU:O	13:a:100:MET:HG2	2.15	0.47
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.97	0.47
5:E:134:ILE:HD12	5:E:215:VAL:HG12	1.96	0.46
10:J:1:MET:HA	10:J:34:LYS:HE3	1.95	0.46
10:J:139:TYR:CE2	10:J:172:MET:HE2	2.49	0.46
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.96	0.46
12:L:13:LEU:HD12	12:L:14:GLY:N	2.30	0.46
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.46
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.30	0.46
5:E:155:LEU:HD23	6:F:55:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.46
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.98	0.46
10:X:158:LEU:O	10:X:162:LYS:HG3	2.15	0.46
13:a:128:ARG:HH11	13:a:138:SER:HB2	1.81	0.46
2:B:183:MET:HE2	2:B:188:ALA:HA	1.97	0.46
11:K:33:LYS:HE2	17:K:303:38N:H34	1.96	0.46
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.51	0.46
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.51	0.46
2:P:110:LEU:C	2:P:110:LEU:HD23	2.40	0.46
2:P:183:MET:HE2	2:P:188:ALA:HA	1.97	0.46
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.97	0.46
1:A:149:GLN:O	1:A:156:TYR:HA	2.16	0.46
5:E:71:LEU:C	5:E:71:LEU:HD23	2.41	0.46
5:E:170:TYR:CD1	5:E:170:TYR:C	2.92	0.46
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.51	0.46
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.81	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.46
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.51	0.46
5:S:155:LEU:HD23	6:T:55:LEU:HD23	1.97	0.46
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.51	0.46
10:X:152:MET:HE3	10:X:156:GLU:HB3	1.98	0.46
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.81	0.46
9:W:14:MET:HB3	9:W:162:LEU:HD11	1.98	0.46
1:A:115:ALA:HB1	1:A:154:GLY:O	2.16	0.46
2:B:183:MET:HE1	2:B:191:LEU:HD12	1.96	0.46
5:E:170:TYR:CZ	5:E:194:GLU:HG2	2.50	0.46
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.46	0.46
5:S:170:TYR:CZ	5:S:194:GLU:HG2	2.51	0.46
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.46	0.45
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.81	0.45
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.46	0.45
7:G:78:ILE:N	7:G:79:PRO:CD	2.80	0.45
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.98	0.45
10:J:126:VAL:CG1	10:J:128:LEU:HG	2.44	0.45
11:K:55:TRP:CD1	11:K:97:MET:HE1	2.52	0.45
1:O:115:ALA:HB1	1:O:154:GLY:O	2.16	0.45
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.98	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.45
11:Y:55:TRP:CD1	11:Y:97:MET:HE1	2.51	0.45
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.98	0.45
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:126:VAL:CG1	10:X:128:LEU:HG	2.44	0.45
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.57	0.44
6:F:238:PHE:O	6:F:242:GLU:HG2	2.17	0.44
4:R:99:ILE:HD13	4:R:104:LEU:HB2	1.98	0.44
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.98	0.44
9:I:101:PRO:HB3	9:I:126:ILE:CD1	2.47	0.44
10:J:152:MET:HE3	10:J:156:GLU:HB3	1.98	0.44
7:U:83:ASN:C	7:U:83:ASN:HD22	2.26	0.44
7:G:83:ASN:C	7:G:83:ASN:HD22	2.26	0.44
9:W:101:PRO:HB3	9:W:126:ILE:CD1	2.47	0.44
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.99	0.44
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.46	0.44
6:T:238:PHE:O	6:T:242:GLU:HG2	2.17	0.44
6:T:240:GLN:HE21	6:T:240:GLN:CA	2.31	0.44
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.53	0.44
7:G:196:PHE:CD1	7:G:196:PHE:C	2.96	0.44
6:T:240:GLN:HA	6:T:240:GLN:NE2	2.33	0.44
12:Z:125:PHE:HA	12:Z:130:SER:O	2.18	0.44
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.53	0.44
7:U:78:ILE:N	7:U:79:PRO:CD	2.80	0.44
2:B:162:ILE:HG13	2:B:163:SER:N	2.33	0.43
10:J:193:ASP:OD1	10:J:193:ASP:N	2.51	0.43
3:C:186:VAL:O	3:C:190:VAL:HG23	2.18	0.43
6:T:13:PRO:O	7:U:24:LYS:HD2	2.18	0.43
6:F:240:GLN:HA	6:F:240:GLN:NE2	2.33	0.43
17:K:303:38N:O40	17:K:303:38N:H19	2.18	0.43
17:Y:303:38N:O40	17:Y:303:38N:H19	2.18	0.43
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.19	0.43
5:S:178:PHE:HA	5:S:181:ILE:HG13	2.00	0.43
2:P:162:ILE:HG13	2:P:163:SER:N	2.34	0.43
13:a:97:ALA:HA	13:a:130:VAL:HG21	2.01	0.43
6:F:240:GLN:HE21	6:F:240:GLN:CA	2.31	0.43
5:S:155:LEU:CD2	6:T:55:LEU:HD23	2.49	0.43
7:U:196:PHE:CD1	7:U:196:PHE:C	2.96	0.43
8:V:104:ASP:OD1	8:V:106:THR:HB	2.19	0.43
4:D:125:LEU:HD12	4:D:125:LEU:O	2.20	0.42
9:I:120:ILE:HD12	9:I:136:ILE:HG12	2.01	0.42
4:D:99:ILE:HG22	18:D:303:HOH:O	2.18	0.42
12:L:125:PHE:HA	12:L:130:SER:O	2.19	0.42
9:W:120:ILE:HD12	9:W:136:ILE:HG12	2.01	0.42
4:R:125:LEU:HD12	4:R:125:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:PHE:HA	5:E:181:ILE:HG13	2.01	0.42
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.02	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.42
5:E:118:ASN:N	5:E:118:ASN:HD22	2.18	0.42
4:D:99:ILE:HD13	4:D:104:LEU:HB2	1.98	0.42
6:F:201:GLU:O	6:F:204:LYS:HD2	2.20	0.42
9:W:98:ARG:HD2	9:W:126:ILE:HG12	2.02	0.42
10:X:152:MET:CE	10:X:156:GLU:HB3	2.50	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.20	0.42
12:Z:149:PHE:CE1	12:Z:153:GLN:HG3	2.55	0.42
8:H:104:ASP:OD1	8:H:106:THR:HB	2.20	0.42
10:J:1:MET:HE3	10:J:53:THR:OG1	2.20	0.42
11:K:6:PHE:HA	11:K:125:ASP:O	2.20	0.42
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.02	0.42
11:Y:97:MET:C	16:Y:302:MES:H21	2.45	0.42
9:I:98:ARG:HD2	9:I:126:ILE:HG12	2.02	0.42
10:J:152:MET:CE	10:J:156:GLU:HB3	2.50	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.42
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.49	0.41
14:N:13:ILE:HG21	14:N:175:MET:CE	2.48	0.41
2:P:119:GLN:HG3	3:Q:78:ALA:HB1	2.03	0.41
5:E:174:THR:O	5:E:175:LEU:C	2.63	0.41
11:K:35:ILE:HB	11:K:45:MET:CE	2.49	0.41
12:L:149:PHE:CE1	12:L:153:GLN:HG3	2.55	0.41
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.50	0.41
5:S:174:THR:O	5:S:175:LEU:C	2.62	0.41
10:X:193:ASP:OD1	10:X:193:ASP:N	2.51	0.41
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.50	0.41
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.02	0.41
12:Z:22:VAL:HG12	12:Z:206:ILE:HG13	2.02	0.41
5:E:155:LEU:CD2	6:F:55:LEU:HD23	2.50	0.41
12:L:43:VAL:HG12	12:L:205:LEU:HD22	2.02	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.02	0.41
3:Q:160:GLN:HE21	3:Q:161:THR:H	1.69	0.41
3:C:160:GLN:HE21	3:C:161:THR:H	1.69	0.41
1:O:247:LEU:O	1:O:250:LEU:HB2	2.21	0.41
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.99	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.03	0.41
7:G:83:ASN:C	7:G:83:ASN:ND2	2.79	0.41
5:S:118:ASN:HD22	5:S:118:ASN:N	2.19	0.41
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:25:ALA:O	7:G:28:GLN:HB2	2.20	0.41
13:M:182:ARG:NH2	13:M:215:GLU:O	2.51	0.41
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.02	0.41
6:T:238:PHE:CD2	6:T:238:PHE:C	2.99	0.41
5:E:60:LYS:H	5:E:60:LYS:HG2	1.69	0.41
7:U:25:ALA:O	7:U:28:GLN:HB2	2.21	0.41
7:G:239:ILE:O	7:G:242:GLN:HB3	2.20	0.41
14:N:140:LYS:HG3	14:b:137:TYR:CE1	2.56	0.41
7:U:83:ASN:C	7:U:83:ASN:ND2	2.79	0.41
7:U:239:ILE:O	7:U:242:GLN:HB3	2.20	0.41
12:Z:43:VAL:HG12	12:Z:205:LEU:HD22	2.02	0.41
3:C:106:TYR:CD1	3:C:106:TYR:C	2.99	0.41
5:E:61:LYS:O	5:E:72:SER:HA	2.21	0.41
5:S:170:TYR:CE2	5:S:194:GLU:HG2	2.56	0.41
6:T:201:GLU:O	6:T:204:LYS:HD2	2.20	0.41
8:V:215:GLU:HG2	9:W:197:ARG:HG2	2.03	0.41
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.86	0.40
1:O:158:PRO:HB2	2:P:57:GLU:HB3	2.01	0.40
14:N:35:THR:CG2	14:N:45:ARG:HE	2.32	0.40
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.68	0.40
7:U:44:VAL:HG21	7:U:73:VAL:HG11	2.03	0.40
9:I:176:ARG:NH2	12:Z:147:MET:HE2	2.36	0.40
14:N:137:TYR:CE1	14:b:140:LYS:HG3	2.56	0.40
3:Q:202:GLN:CG	3:Q:203:THR:N	2.81	0.40
6:F:238:PHE:C	6:F:238:PHE:CD2	2.99	0.40
5:S:231:LYS:HD2	5:S:232:TYR:CE2	2.56	0.40
5:E:231:LYS:HD2	5:E:232:TYR:CE2	2.56	0.40
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.87	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%)	240 (97%)	6 (2%)	2 (1%)	16	25
1	O	248/250 (99%)	241 (97%)	5 (2%)	2 (1%)	16	25
2	B	242/258 (94%)	230 (95%)	10 (4%)	2 (1%)	16	25
2	P	242/258 (94%)	231 (96%)	9 (4%)	2 (1%)	16	25
3	C	238/254 (94%)	227 (95%)	8 (3%)	3 (1%)	9	14
3	Q	238/254 (94%)	227 (95%)	8 (3%)	3 (1%)	9	14
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	213 (93%)	14 (6%)	2 (1%)	14	22
5	S	229/234 (98%)	213 (93%)	14 (6%)	2 (1%)	14	22
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
7	U	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
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%)	2 (1%)	1 (0%)	24	37
10	X	193/198 (98%)	190 (98%)	2 (1%)	1 (0%)	24	37
11	K	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	24	37
11	Y	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	24	37
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6276/6614 (95%)	6068 (97%)	186 (3%)	22 (0%)	30	43

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
3	C	202	GLN
3	C	205	ALA
10	J	2	ASP
1	O	2	THR
2	P	51	VAL
3	Q	202	GLN
3	Q	205	ALA
10	X	2	ASP
1	A	166	LYS
5	E	231	LYS
11	K	9	GLN
5	S	217	LYS
5	S	231	LYS
11	Y	9	GLN
3	C	183	PRO
5	E	217	LYS
1	O	166	LYS
3	Q	183	PRO
2	B	221	ASP
2	P	221	ASP

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%)	196 (94%)	13 (6%)	16	29
1	O	209/209 (100%)	196 (94%)	13 (6%)	16	29
2	B	203/216 (94%)	187 (92%)	16 (8%)	11	19
2	P	203/216 (94%)	187 (92%)	16 (8%)	11	19
3	C	212/226 (94%)	187 (88%)	25 (12%)	5	7
3	Q	212/226 (94%)	187 (88%)	25 (12%)	5	7
4	D	194/215 (90%)	173 (89%)	21 (11%)	6	9
4	R	194/215 (90%)	173 (89%)	21 (11%)	6	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	190/193 (98%)	168 (88%)	22 (12%)	5	8
5	S	190/193 (98%)	168 (88%)	22 (12%)	5	8
6	F	201/239 (84%)	182 (90%)	19 (10%)	8	13
6	T	201/239 (84%)	182 (90%)	19 (10%)	8	13
7	G	206/210 (98%)	188 (91%)	18 (9%)	9	16
7	U	206/210 (98%)	189 (92%)	17 (8%)	10	17
8	H	181/190 (95%)	171 (94%)	10 (6%)	19	34
8	V	181/190 (95%)	171 (94%)	10 (6%)	19	34
9	I	172/173 (99%)	163 (95%)	9 (5%)	21	36
9	W	172/173 (99%)	163 (95%)	9 (5%)	21	36
10	J	173/175 (99%)	163 (94%)	10 (6%)	18	32
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	36
11	K	169/169 (100%)	159 (94%)	10 (6%)	18	31
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	31
12	L	185/185 (100%)	178 (96%)	7 (4%)	29	49
12	Z	185/185 (100%)	178 (96%)	7 (4%)	29	49
13	M	199/208 (96%)	184 (92%)	15 (8%)	12	21
13	a	199/208 (96%)	184 (92%)	15 (8%)	12	21
14	N	162/162 (100%)	153 (94%)	9 (6%)	19	33
14	b	162/162 (100%)	153 (94%)	9 (6%)	19	33
All	All	5312/5540 (96%)	4906 (92%)	406 (8%)	12	21

All (406) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	29	LYS
1	A	30	GLN
1	A	44	VAL
1	A	59	GLU
1	A	61	LEU
1	A	108	LYS
1	A	122	THR
1	A	157	PHE

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Mol	Chain	Res	Type
1	A	184	GLU
1	A	231	LYS
1	A	238	LEU
2	B	50	LYS
2	B	54	THR
2	B	55	LEU
2	B	56	LEU
2	B	58	GLN
2	B	79	LEU
2	B	102	ASN
2	B	149	THR
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	237	ILE
2	B	238	LEU
2	B	239	VAL
2	B	244	THR
3	C	4	ARG
3	C	32	VAL
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	51	LYS
3	C	52	LEU
3	C	55	THR
3	C	61	LYS
3	C	70	VAL
3	C	124	VAL
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	206	LYS
3	C	208	ILE
3	C	222	LEU
3	C	225	GLU
3	C	235	GLU

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Mol	Chain	Res	Type
3	C	239	GLN
3	C	240	GLU
4	D	4	VAL
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	60	VAL
4	D	99	ILE
4	D	125	LEU
4	D	169	GLU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	197	LYS
4	D	202	GLU
4	D	214	ILE
4	D	217	GLN
4	D	224	ASP
4	D	235	LEU
4	D	236	LYS
4	D	239	GLU
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	44	VAL
5	E	55	LEU
5	E	60	LYS
5	E	61	LYS
5	E	71	LEU
5	E	118	ASN
5	E	144	LEU
5	E	147	GLN
5	E	179	ILE
5	E	188	LEU
5	E	194	GLU
5	E	202	ASP
5	E	207	VAL
5	E	208	ASP

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Mol	Chain	Res	Type
5	E	219	THR
5	E	222	THR
5	E	231	LYS
6	F	14	ASP
6	F	51	THR
6	F	58	GLN
6	F	68	ARG
6	F	94	SER
6	F	96	LYS
6	F	123	ASN
6	F	148	GLU
6	F	163	LYS
6	F	165	ARG
6	F	166	GLN
6	F	172	LEU
6	F	181	GLU
6	F	198	LEU
6	F	203	ASN
6	F	206	LYS
6	F	221	ASN
6	F	240	GLN
6	F	241	LYS
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	34	LEU
7	G	39	LYS
7	G	53	LYS
7	G	83	ASN
7	G	115	LEU
7	G	148	THR
7	G	165	LYS
7	G	166	GLN
7	G	178	LYS
7	G	221	LYS
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
7	G	237	VAL
7	G	242	GLN
8	H	7	LYS
8	H	13	VAL

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Mol	Chain	Res	Type
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	73	GLU
8	H	127	LEU
8	H	153	LYS
8	H	196	ARG
8	H	198	GLU
9	I	1	SER
9	I	37	ASN
9	I	38	LYS
9	I	92	SER
9	I	114	LYS
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	110	LYS
10	J	126	VAL
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
10	J	194	ASP
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	41	LEU
11	K	57	THR
11	K	73	ARG
11	K	106	ARG
11	K	148	LEU
11	K	182	GLU
12	L	1	GLN
12	L	13	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN

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Mol	Chain	Res	Type
12	L	150	LEU
12	L	167	LYS
13	M	2	GLN
13	M	43	ILE
13	M	48	ASN
13	M	68	LYS
13	M	70	LEU
13	M	104	ARG
13	M	106	LYS
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	212	LEU
13	M	213	GLN
13	M	215	GLU
13	M	223	LYS
13	M	233	ILE
14	N	9	LYS
14	N	20	THR
14	N	36	ARG
14	N	44	CYS
14	N	104	ASP
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	17	LYS
1	O	29	LYS
1	O	30	GLN
1	O	44	VAL
1	O	59	GLU
1	O	61	LEU
1	O	108	LYS
1	O	122	THR
1	O	157	PHE
1	O	184	GLU
1	O	231	LYS
1	O	238	LEU
2	P	50	LYS
2	P	54	THR
2	P	55	LEU

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Mol	Chain	Res	Type
2	P	56	LEU
2	P	58	GLN
2	P	79	LEU
2	P	102	ASN
2	P	149	THR
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	237	ILE
2	P	238	LEU
2	P	239	VAL
2	P	244	THR
3	Q	4	ARG
3	Q	32	VAL
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	51	LYS
3	Q	52	LEU
3	Q	55	THR
3	Q	61	LYS
3	Q	70	VAL
3	Q	124	VAL
3	Q	147	GLN
3	Q	160	GLN
3	Q	167	LYS
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	206	LYS
3	Q	208	ILE
3	Q	222	LEU
3	Q	225	GLU
3	Q	235	GLU
3	Q	239	GLN
3	Q	240	GLU
4	R	4	VAL
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU

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Mol	Chain	Res	Type
4	R	54	ASP
4	R	60	VAL
4	R	99	ILE
4	R	125	LEU
4	R	169	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	197	LYS
4	R	202	GLU
4	R	214	ILE
4	R	217	GLN
4	R	224	ASP
4	R	235	LEU
4	R	236	LYS
4	R	239	GLU
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	44	VAL
5	S	55	LEU
5	S	60	LYS
5	S	61	LYS
5	S	71	LEU
5	S	118	ASN
5	S	144	LEU
5	S	147	GLN
5	S	179	ILE
5	S	188	LEU
5	S	194	GLU
5	S	202	ASP
5	S	207	VAL
5	S	208	ASP
5	S	219	THR
5	S	222	THR
5	S	231	LYS
6	T	14	ASP
6	T	51	THR
6	T	58	GLN

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Mol	Chain	Res	Type
6	T	68	ARG
6	T	94	SER
6	T	96	LYS
6	T	123	ASN
6	T	148	GLU
6	T	163	LYS
6	T	165	ARG
6	T	166	GLN
6	T	172	LEU
6	T	181	GLU
6	T	198	LEU
6	T	203	ASN
6	T	206	LYS
6	T	221	ASN
6	T	240	GLN
6	T	241	LYS
7	U	24	LYS
7	U	26	THR
7	U	28	GLN
7	U	34	LEU
7	U	39	LYS
7	U	53	LYS
7	U	83	ASN
7	U	115	LEU
7	U	165	LYS
7	U	166	GLN
7	U	178	LYS
7	U	221	LYS
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
7	U	237	VAL
7	U	242	GLN
8	V	7	LYS
8	V	13	VAL
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	73	GLU
8	V	127	LEU
8	V	153	LYS
8	V	196	ARG

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Mol	Chain	Res	Type
8	V	198	GLU
9	W	1	SER
9	W	37	ASN
9	W	38	LYS
9	W	92	SER
9	W	114	LYS
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	110	LYS
10	X	126	VAL
10	X	144	LEU
10	X	163	LEU
10	X	194	ASP
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	35	ILE
11	Y	41	LEU
11	Y	57	THR
11	Y	73	ARG
11	Y	106	ARG
11	Y	148	LEU
11	Y	182	GLU
12	Z	1	GLN
12	Z	13	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	150	LEU
12	Z	167	LYS
13	a	2	GLN
13	a	43	ILE
13	a	48	ASN
13	a	68	LYS
13	a	70	LEU
13	a	104	ARG

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Mol	Chain	Res	Type
13	a	106	LYS
13	a	138	SER
13	a	161	ARG
13	a	187	ARG
13	a	212	LEU
13	a	213	GLN
13	a	215	GLU
13	a	223	LYS
13	a	233	ILE
14	b	9	LYS
14	b	20	THR
14	b	36	ARG
14	b	44	CYS
14	b	104	ASP
14	b	115	LEU
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	53	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS

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Mol	Chain	Res	Type
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	198	GLN
4	D	207	ASN
4	D	225	ASN
5	E	68	HIS
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	29	ASN
6	F	58	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
8	H	22	GLN
8	H	57	GLN
8	H	66	HIS
8	H	86	HIS
8	H	165	ASN
8	H	172	ASN
9	I	31	GLN
9	I	37	ASN
9	I	63	ASN
9	I	88	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN

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Mol	Chain	Res	Type
10	J	146	HIS
10	J	147	HIS
10	J	191	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	80	ASN
12	L	153	GLN
12	L	195	HIS
12	L	197	GLN
13	M	48	ASN
13	M	62	HIS
13	M	102	GLN
13	M	149	HIS
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	53	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN

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Mol	Chain	Res	Type
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	198	GLN
4	R	207	ASN
4	R	225	ASN
5	S	68	HIS
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	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	22	GLN
8	V	57	GLN
8	V	66	HIS
8	V	86	HIS
8	V	165	ASN
8	V	172	ASN
9	W	31	GLN
9	W	37	ASN
9	W	63	ASN
9	W	88	GLN
10	X	37	GLN

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Mol	Chain	Res	Type
10	X	55	GLN
10	X	63	ASN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	79	HIS
12	Z	80	ASN
12	Z	153	GLN
12	Z	197	GLN
13	a	26	ASN
13	a	48	ASN
13	a	62	HIS
13	a	102	GLN
13	a	149	HIS
13	a	179	ASN
13	a	194	ASN
13	a	203	ASN
13	a	213	GLN
14	b	38	HIS
14	b	69	GLN
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	MES	V	302	-	12,12,12	2.20	1 (8%)	15,16,16	1.22	1 (6%)
16	MES	K	302	-	12,12,12	2.35	1 (8%)	15,16,16	1.19	1 (6%)
17	38N	V	303	-	43,44,44	2.47	4 (9%)	51,58,58	1.45	5 (9%)
16	MES	H	302	-	12,12,12	2.25	1 (8%)	15,16,16	1.25	1 (6%)
17	38N	H	303	-	43,44,44	2.44	4 (9%)	51,58,58	1.46	6 (11%)
16	MES	Y	302	-	12,12,12	2.35	1 (8%)	15,16,16	1.22	1 (6%)
17	38N	K	303	-	43,44,44	2.52	4 (9%)	51,58,58	1.43	5 (9%)
17	38N	Y	303	-	43,44,44	2.48	4 (9%)	51,58,58	1.44	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MES	V	302	-	-	3/6/14/14	0/1/1/1
16	MES	K	302	-	-	0/6/14/14	0/1/1/1
17	38N	V	303	-	-	8/44/60/60	0/3/3/3
16	MES	H	302	-	-	3/6/14/14	0/1/1/1
17	38N	H	303	-	-	8/44/60/60	0/3/3/3
16	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	38N	K	303	-	-	10/44/60/60	0/3/3/3
17	38N	Y	303	-	-	10/44/60/60	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	303	38N	O32-C31	14.50	1.44	1.21
17	Y	303	38N	O32-C31	14.23	1.43	1.21
17	V	303	38N	O32-C31	14.17	1.43	1.21
17	H	303	38N	O32-C31	13.90	1.43	1.21
16	Y	302	MES	C8-S	-7.87	1.66	1.77
16	K	302	MES	C8-S	-7.87	1.66	1.77
16	H	302	MES	C8-S	-7.50	1.67	1.77
16	V	302	MES	C8-S	-7.34	1.67	1.77
17	H	303	38N	C17-C18	-4.62	1.40	1.51
17	V	303	38N	C17-C18	-4.61	1.40	1.51
17	Y	303	38N	C37-C31	4.16	1.65	1.52
17	K	303	38N	C17-C18	-4.08	1.41	1.51
17	Y	303	38N	C17-C18	-4.06	1.41	1.51
17	K	303	38N	C37-C31	4.04	1.64	1.52
17	V	303	38N	C37-C31	3.86	1.64	1.52
17	H	303	38N	C37-C31	3.78	1.64	1.52
17	K	303	38N	C29-C31	3.13	1.57	1.52
17	Y	303	38N	C29-C31	2.99	1.57	1.52
17	H	303	38N	C29-C31	2.95	1.57	1.52
17	V	303	38N	C29-C31	2.74	1.56	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	303	38N	O32-C31-C37	-6.52	109.53	121.30
17	K	303	38N	O32-C31-C37	-6.51	109.54	121.30
17	H	303	38N	O32-C31-C37	-5.81	110.80	121.30
17	V	303	38N	O32-C31-C37	-5.79	110.83	121.30
17	Y	303	38N	C4-N5-C10	4.35	117.90	111.14
17	K	303	38N	C4-N5-C10	4.30	117.84	111.14
17	V	303	38N	C7-C6-N5	-3.81	104.34	110.12
17	H	303	38N	C7-C6-N5	-3.78	104.38	110.12
16	H	302	MES	O2S-S-C8	3.45	111.94	106.73
17	H	303	38N	C2-C4-N5	-3.21	105.95	113.41
16	V	302	MES	O2S-S-C8	3.12	111.44	106.73
17	V	303	38N	C2-C4-N5	-3.12	106.16	113.41
16	Y	302	MES	O3S-S-C8	2.97	111.81	106.00
16	K	302	MES	O3S-S-C8	2.93	111.74	106.00
17	K	303	38N	O8-C9-C10	-2.88	105.58	111.77
17	V	303	38N	C9-C10-N5	2.85	114.45	110.12
17	H	303	38N	C9-C10-N5	2.83	114.41	110.12
17	Y	303	38N	O8-C9-C10	-2.77	105.81	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	303	38N	C30-C41-C46	-2.51	105.88	111.71
17	K	303	38N	C30-C41-C46	-2.50	105.89	111.71
17	H	303	38N	C30-C41-C46	-2.21	106.58	111.71
17	Y	303	38N	C43-C42-C41	-2.18	107.50	112.08
17	K	303	38N	C43-C42-C41	-2.16	107.53	112.08
17	V	303	38N	C30-C41-C46	-2.15	106.71	111.71
17	H	303	38N	O8-C7-C6	-2.09	107.27	111.77

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	H	302	MES	C7-C8-S-O1S
16	H	302	MES	C7-C8-S-O3S
17	H	303	38N	C29-C31-C37-C38
17	H	303	38N	O32-C31-C37-C38
17	H	303	38N	C31-C37-C39-O40
17	H	303	38N	C38-C37-C39-O40
17	K	303	38N	C2-C4-N5-C10
17	K	303	38N	C29-C31-C37-C38
17	K	303	38N	O32-C31-C37-C38
17	V	303	38N	C29-C31-C37-C38
17	V	303	38N	O32-C31-C37-C38
17	V	303	38N	C31-C37-C39-O40
17	V	303	38N	C38-C37-C39-O40
17	Y	303	38N	C2-C4-N5-C10
17	Y	303	38N	C29-C31-C37-C38
17	Y	303	38N	O32-C31-C37-C38
17	K	303	38N	C24-C21-O22-C23
17	K	303	38N	C20-C21-O22-C23
17	Y	303	38N	C20-C21-O22-C23
17	Y	303	38N	C24-C21-O22-C23
16	V	302	MES	C7-C8-S-O3S
17	K	303	38N	O3-C2-C4-N5
17	Y	303	38N	O3-C2-C4-N5
17	H	303	38N	N1-C2-C4-N5
17	K	303	38N	N1-C2-C4-N5
17	V	303	38N	N1-C2-C4-N5
17	Y	303	38N	N1-C2-C4-N5
16	H	302	MES	C7-C8-S-O2S
16	V	302	MES	C7-C8-S-O1S
16	V	302	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
17	H	303	38N	O3-C2-C4-N5
17	V	303	38N	O3-C2-C4-N5
17	H	303	38N	N28-C29-C31-C37
17	K	303	38N	N28-C29-C31-C37
17	V	303	38N	N28-C29-C31-C37
17	Y	303	38N	N28-C29-C31-C37
17	K	303	38N	C29-C31-C37-C39
17	Y	303	38N	C29-C31-C37-C39
17	H	303	38N	C30-C29-C31-O32
17	K	303	38N	C30-C29-C31-O32
17	V	303	38N	C30-C29-C31-O32
17	Y	303	38N	C30-C29-C31-O32

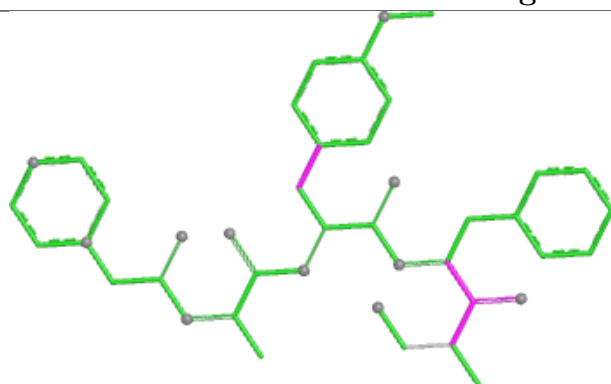
There are no ring outliers.

5 monomers are involved in 7 short contacts:

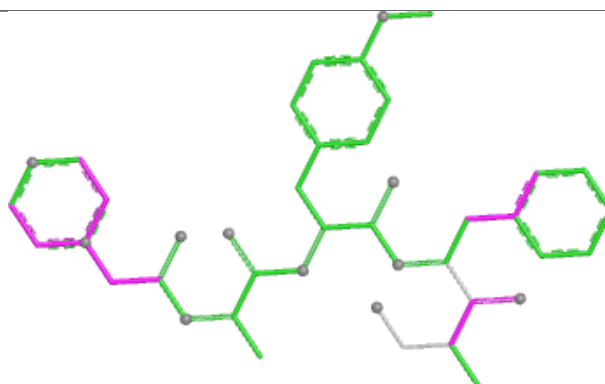
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	303	38N	1	0
17	H	303	38N	1	0
16	Y	302	MES	1	0
17	K	303	38N	2	0
17	Y	303	38N	2	0

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

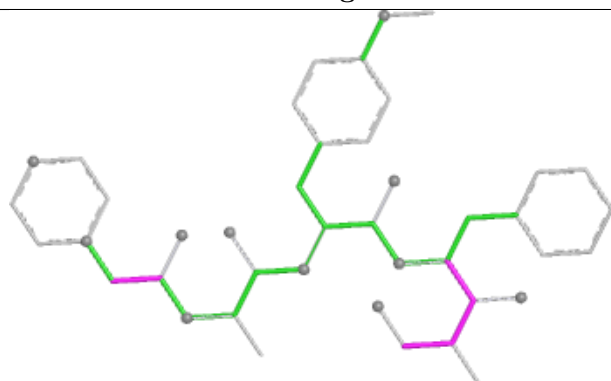
Ligand 38N V 303



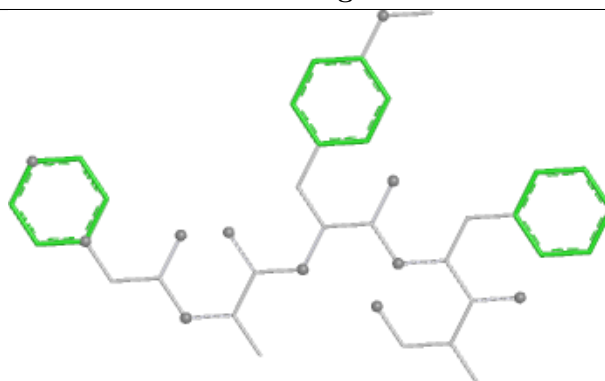
Bond lengths



Bond angles

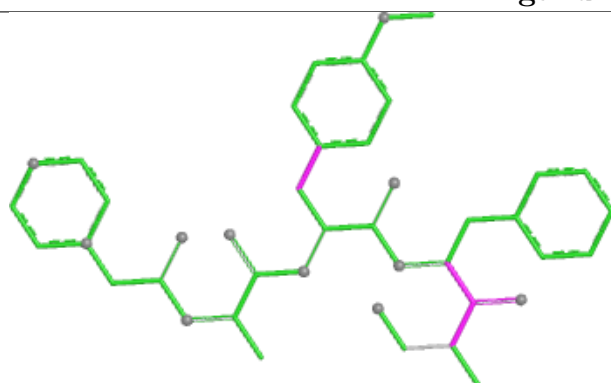


Torsions

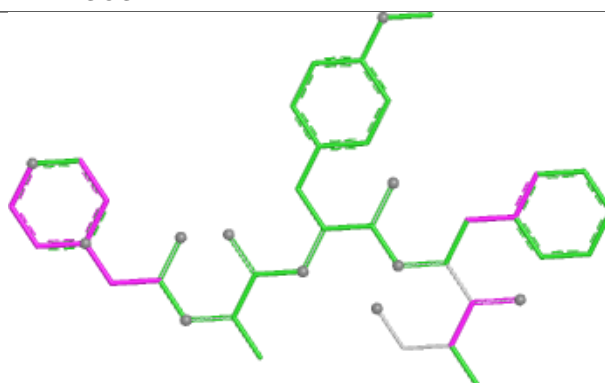


Rings

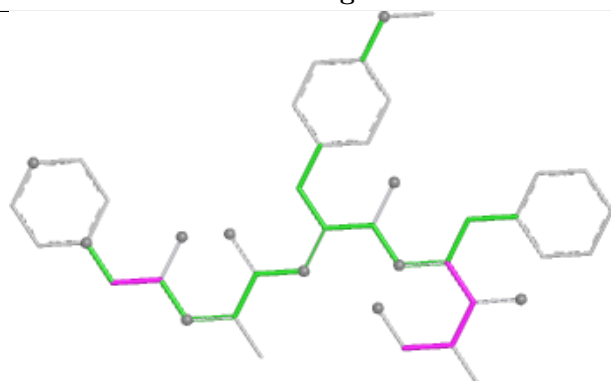
Ligand 38N H 303



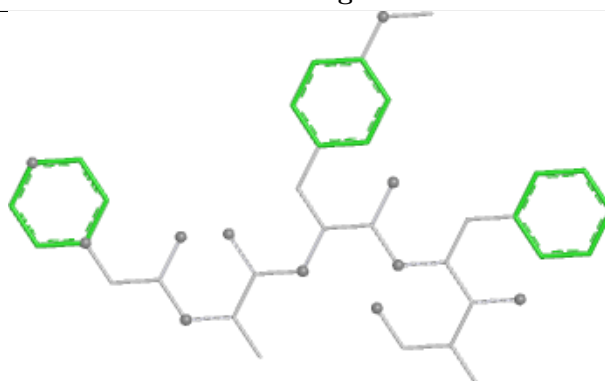
Bond lengths



Bond angles

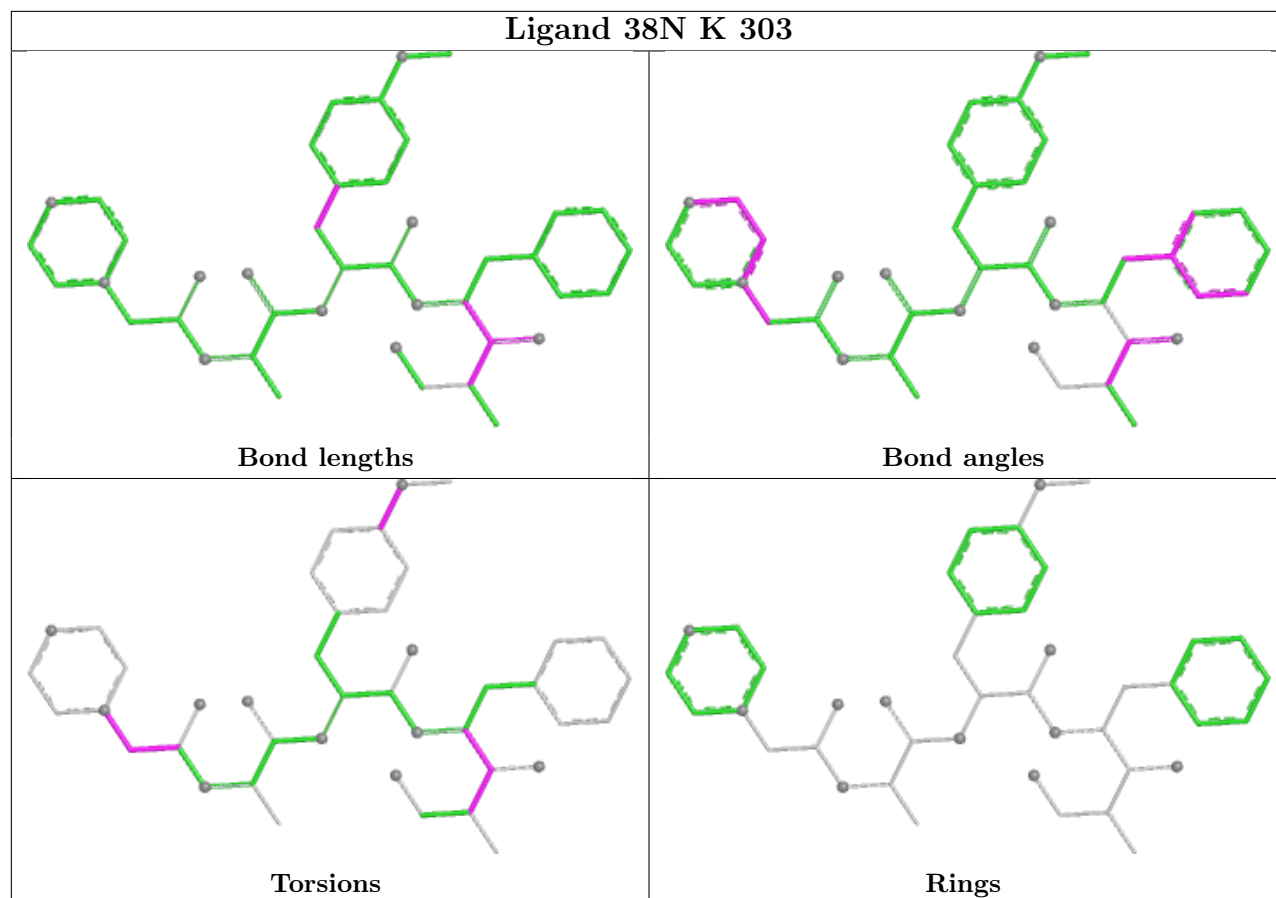


Torsions

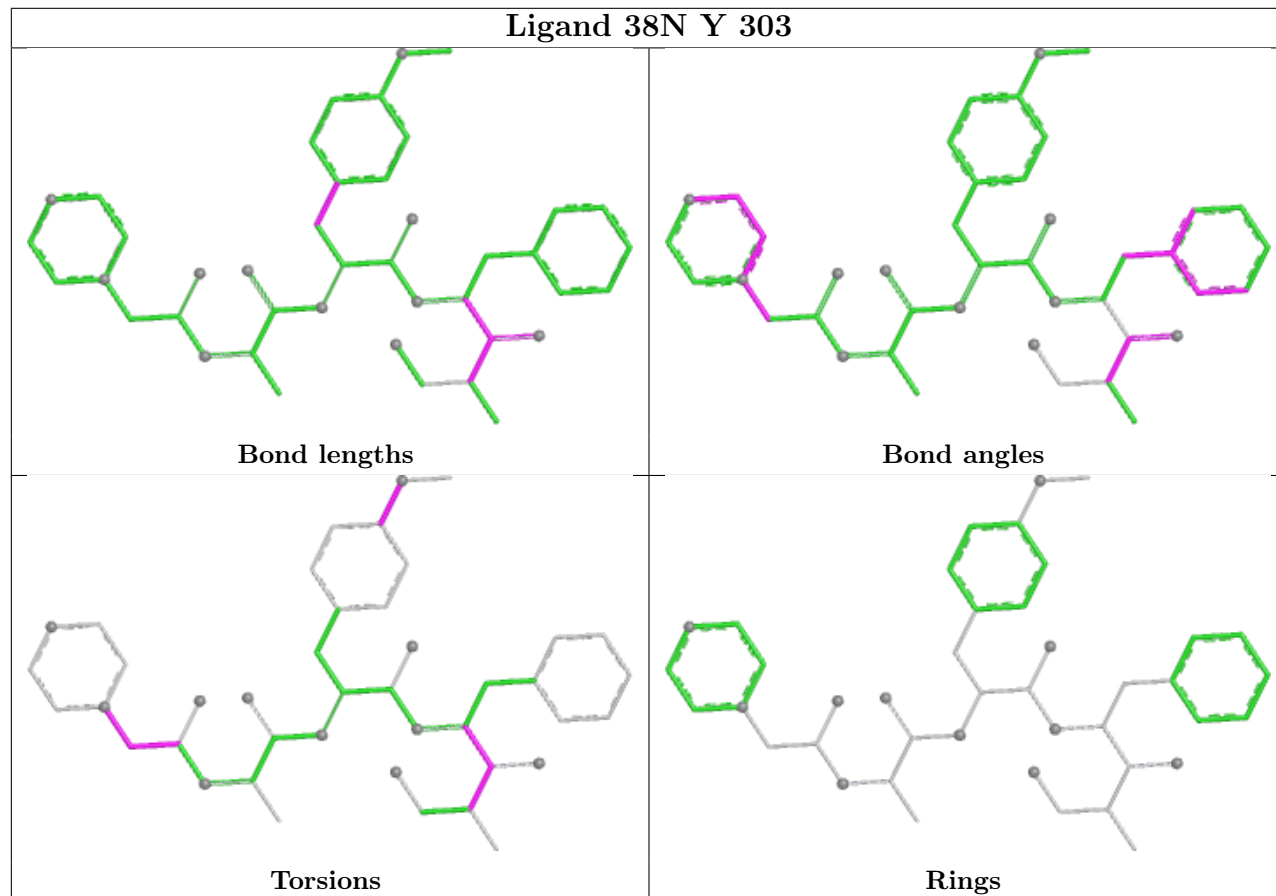


Rings

Ligand 38N K 303



Ligand 38N Y 303



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%)	-0.35	4 (1%) 70 66	37, 52, 85, 135	0
1	O	250/250 (100%)	-0.33	3 (1%) 76 73	40, 57, 102, 133	0
2	B	244/258 (94%)	-0.22	5 (2%) 65 60	35, 56, 105, 152	0
2	P	244/258 (94%)	-0.19	7 (2%) 53 50	41, 60, 108, 157	0
3	C	240/254 (94%)	-0.15	4 (1%) 69 65	37, 59, 121, 145	0
3	Q	240/254 (94%)	0.15	8 (3%) 49 45	44, 74, 146, 162	0
4	D	235/260 (90%)	-0.25	0 100 100	39, 60, 90, 129	0
4	R	235/260 (90%)	-0.15	2 (0%) 81 78	44, 65, 102, 130	0
5	E	231/234 (98%)	-0.14	1 (0%) 88 86	45, 64, 99, 151	0
5	S	231/234 (98%)	0.15	4 (1%) 69 65	48, 70, 111, 143	0
6	F	243/288 (84%)	-0.20	5 (2%) 63 59	41, 58, 109, 141	0
6	T	243/288 (84%)	-0.07	5 (2%) 63 59	43, 62, 107, 145	0
7	G	241/252 (95%)	-0.27	0 100 100	39, 55, 92, 144	0
7	U	241/252 (95%)	-0.32	3 (1%) 76 73	40, 55, 91, 112	0
8	H	222/232 (95%)	-0.52	0 100 100	37, 49, 71, 124	0
8	V	222/232 (95%)	-0.54	0 100 100	37, 51, 75, 124	0
9	I	204/205 (99%)	-0.65	0 100 100	35, 46, 74, 102	0
9	W	204/205 (99%)	-0.58	1 (0%) 87 85	33, 47, 74, 122	0
10	J	195/198 (98%)	-0.57	1 (0%) 87 85	32, 47, 74, 135	0
10	X	195/198 (98%)	-0.54	1 (0%) 87 85	36, 50, 79, 149	0
11	K	212/212 (100%)	-0.60	0 100 100	33, 48, 75, 103	0
11	Y	212/212 (100%)	-0.52	0 100 100	36, 50, 76, 111	0
12	L	222/222 (100%)	-0.59	1 (0%) 87 85	33, 50, 73, 87	0
12	Z	222/222 (100%)	-0.56	0 100 100	36, 50, 74, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.51	1 (0%) 88 86	34, 52, 76, 88	0
13	a	233/246 (94%)	-0.49	1 (0%) 88 86	34, 50, 75, 90	0
14	N	196/196 (100%)	-0.33	1 (0%) 87 85	33, 52, 81, 112	0
14	b	196/196 (100%)	-0.42	2 (1%) 79 76	34, 52, 80, 108	0
All	All	6336/6614 (95%)	-0.34	60 (0%) 81 78	32, 55, 98, 162	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	1	MET	6.0
10	X	1	MET	5.6
3	Q	50	LEU	4.4
2	B	219	ALA	3.9
2	P	218	GLY	3.8
2	P	219	ALA	3.6
1	O	1	MET	3.5
1	A	1	MET	3.4
13	M	1	THR	3.4
6	F	202	ASP	3.3
2	B	51	VAL	3.2
14	N	1	THR	3.2
6	F	215	CYS	3.1
2	P	51	VAL	2.9
14	b	103	ASP	2.9
3	Q	234	ILE	2.8
2	B	93	HIS	2.8
6	T	244	ASN	2.8
14	b	1	THR	2.8
13	a	1	THR	2.8
6	T	243	ILE	2.8
4	R	113	LEU	2.8
1	A	201	GLU	2.8
4	R	112	ALA	2.7
3	Q	51	LYS	2.7
6	T	215	CYS	2.7
3	C	206	LYS	2.7
3	Q	49	THR	2.7
1	O	53	SER	2.6
3	C	203	THR	2.6
5	S	58	TYR	2.6
3	C	204	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	93	HIS	2.5
6	T	235	ALA	2.5
7	U	203	ASP	2.5
6	F	203	ASN	2.3
3	Q	203	THR	2.3
2	P	222	GLY	2.3
6	T	53	LYS	2.3
5	S	209	ASN	2.2
2	P	244	THR	2.2
7	U	242	GLN	2.2
7	U	24	LYS	2.2
3	C	51	LYS	2.2
5	S	173	ARG	2.2
5	S	51	ASN	2.2
1	A	249	ALA	2.1
1	O	249	ALA	2.1
3	Q	205	ALA	2.1
3	Q	223	SER	2.1
6	F	176	VAL	2.1
1	A	53	SER	2.1
9	W	1	SER	2.1
3	Q	240	GLU	2.0
2	B	217	LYS	2.0
2	B	244	THR	2.0
12	L	136	CYS	2.0
6	F	204	LYS	2.0
2	P	52	THR	2.0
5	E	122	TYR	2.0

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,

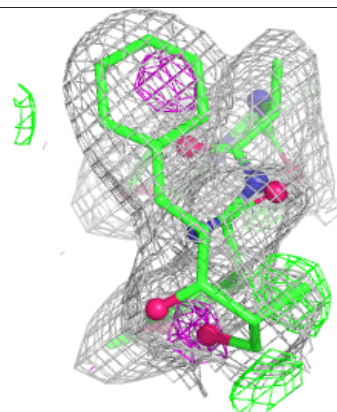
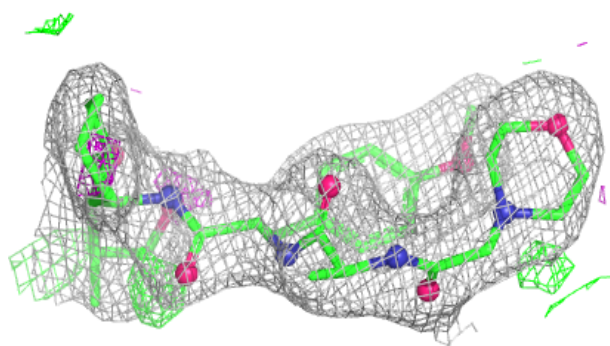
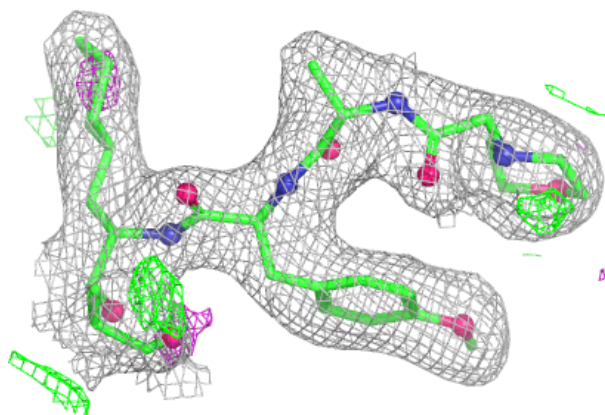
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	H	301	1/1	0.89	0.14	69,69,69,69	0
16	MES	V	302	12/12	0.91	0.12	70,75,80,81	0
15	MG	Z	301	1/1	0.93	0.10	57,57,57,57	0
15	MG	I	301	1/1	0.93	0.07	58,58,58,58	0
16	MES	H	302	12/12	0.94	0.10	60,72,79,83	0
17	38N	H	303	42/42	0.94	0.08	31,42,62,69	0
17	38N	V	303	42/42	0.94	0.08	34,44,60,69	0
17	38N	K	303	42/42	0.95	0.07	34,39,51,61	0
15	MG	V	301	1/1	0.96	0.10	54,54,54,54	0
16	MES	Y	302	12/12	0.96	0.07	42,45,53,56	0
15	MG	K	301	1/1	0.96	0.07	51,51,51,51	0
15	MG	N	201	1/1	0.96	0.05	48,48,48,48	0
16	MES	K	302	12/12	0.96	0.08	43,47,53,58	0
17	38N	Y	303	42/42	0.96	0.07	31,41,54,62	0
15	MG	G	301	1/1	0.97	0.04	54,54,54,54	0
15	MG	Y	301	1/1	0.99	0.05	49,49,49,49	0

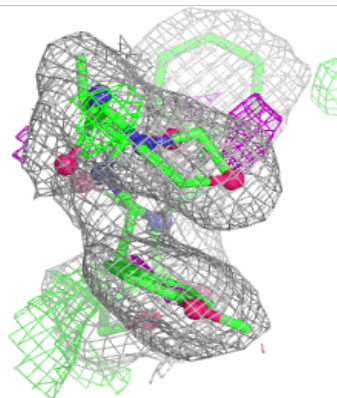
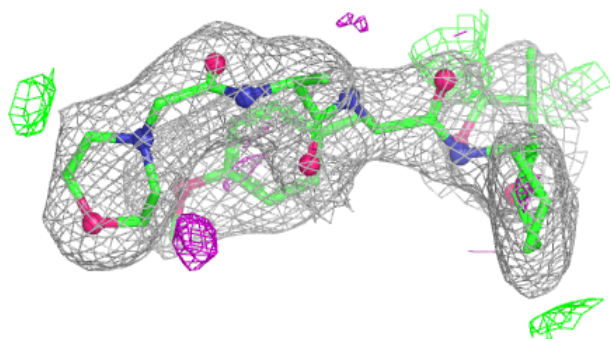
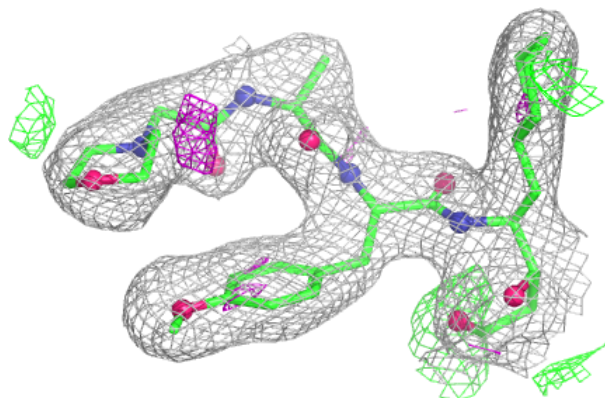
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 38N H 303:

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

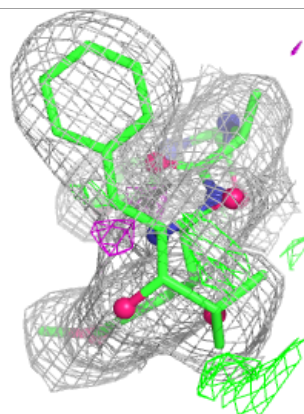
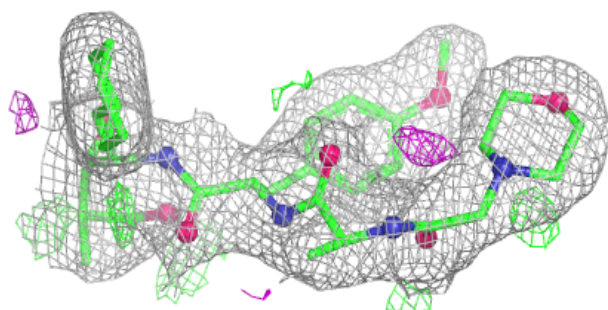
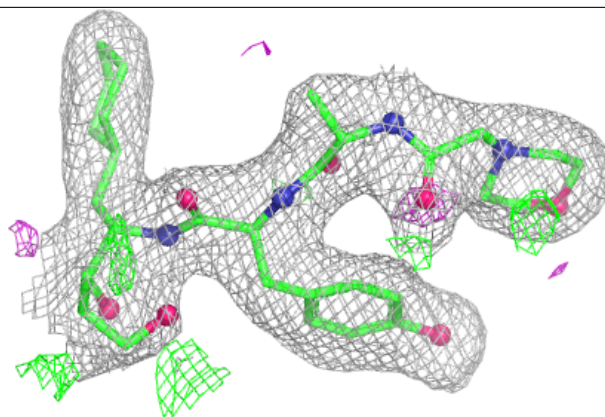
**Electron density around 38N V 303:**

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

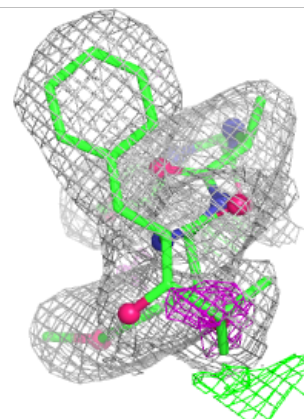
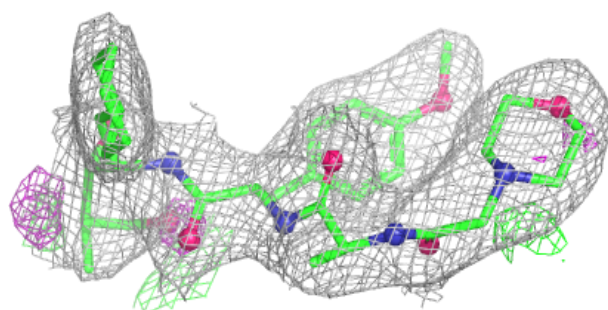
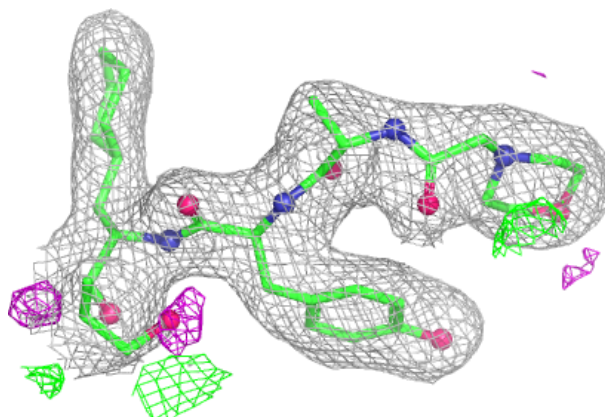


Electron density around 38N K 303:

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

**Electron density around 38N Y 303:**

$2mF_o-DF_c$ (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.