



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:20 PM UTC

PDB ID : 4QLT / pdb_00004qlt
Title : yCP in complex with tripeptidic epoxyketone inhibitor 2 (PR924)
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 : 2.80 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

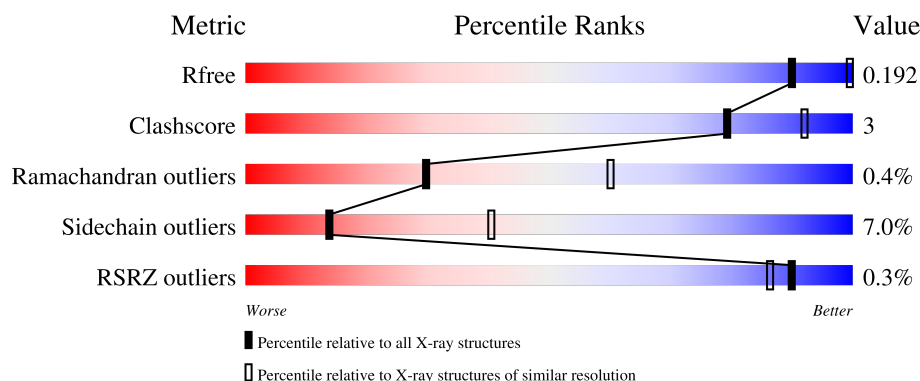
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



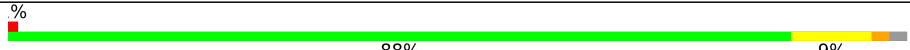
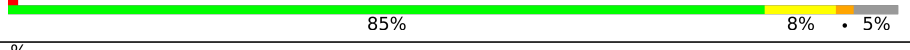
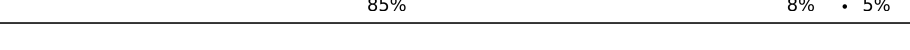
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	93% 6% .
1	O	250	92% 8% .
2	B	258	% 80% 14% . 5%
2	P	258	% 80% 14% . 5%
3	C	254	% 81% 10% . 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	%  81% 11% 6%
4	D	260	 78% 12% 10%
4	R	260	 78% 12% 10%
5	E	234	 85% 13% ..
5	S	234	 85% 13% ..
6	F	288	 77% 6% 16%
6	T	288	 76% 7% 16%
7	G	252	 85% 10% ..
7	U	252	 85% 10% ..
8	H	232	 88% 7% ..
8	V	232	 88% 6% ..
9	I	205	 87% 12%
9	W	205	 88% 11%
10	J	198	%  88% 9% ..
10	X	198	%  88% 9% ..
11	K	212	 86% 12% .
11	Y	212	 87% 11% .
12	L	222	 87% 11% .
12	Z	222	 87% 11% .
13	M	246	%  85% 8% 5%
13	a	246	%  85% 8% 5%
14	N	196	 90% 9% .
14	b	196	 90% 9% .

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49987 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).

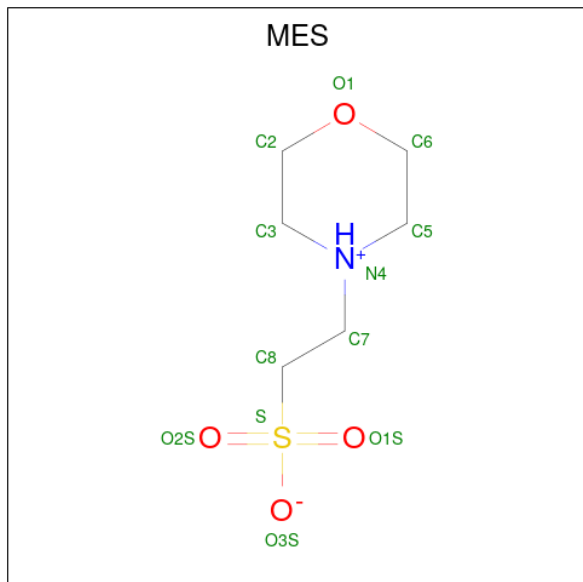
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

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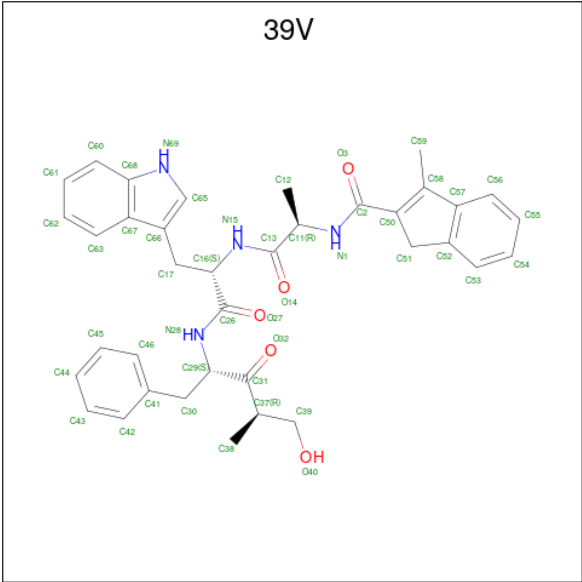
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	Mg	0	0
			1	1		
15	N	2	Total	Mg	0	0
			2	2		
15	V	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	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-[(3-methyl-1H-inden-2-yl)carbonyl]-D-alanyl-N-[(2S,4R)-5-hydroxy-4-methyl-3-oxo-1-phenylpentan-2-yl]-L-tryptophanamide (CCD ID: 39V) (formula: $C_{37}H_{40}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	K	1	Total	C	N	O	0	0
			46	37	4	5		
17	Y	1	Total	C	N	O	0	0
			46	37	4	5		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	24	Total	O	0	0
			24	24		
18	B	23	Total	O	0	0
			23	23		
18	C	14	Total	O	0	0
			14	14		
18	D	12	Total	O	0	0
			12	12		
18	E	11	Total	O	0	0
			11	11		
18	F	23	Total	O	0	0
			23	23		
18	G	27	Total	O	0	0
			27	27		
18	H	21	Total	O	0	0
			21	21		
18	I	26	Total	O	0	0
			26	26		
18	J	23	Total	O	0	0
			23	23		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	24	Total 24	O 24	0	0
18	L	23	Total 23	O 23	0	0
18	M	27	Total 27	O 27	0	0
18	N	16	Total 16	O 16	0	0
18	O	20	Total 20	O 20	0	0
18	P	11	Total 11	O 11	0	0
18	Q	12	Total 12	O 12	0	0
18	R	17	Total 17	O 17	0	0
18	S	7	Total 7	O 7	0	0
18	T	19	Total 19	O 19	0	0
18	U	30	Total 30	O 30	0	0
18	V	22	Total 22	O 22	0	0
18	W	25	Total 25	O 25	0	0
18	X	26	Total 26	O 26	0	0
18	Y	20	Total 20	O 20	0	0
18	Z	21	Total 21	O 21	0	0
18	a	21	Total 21	O 21	0	0
18	b	22	Total 22	O 22	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.

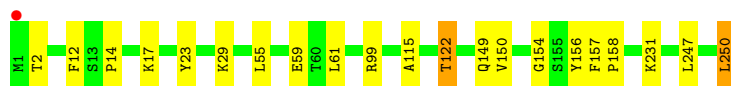
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  93% 6% .



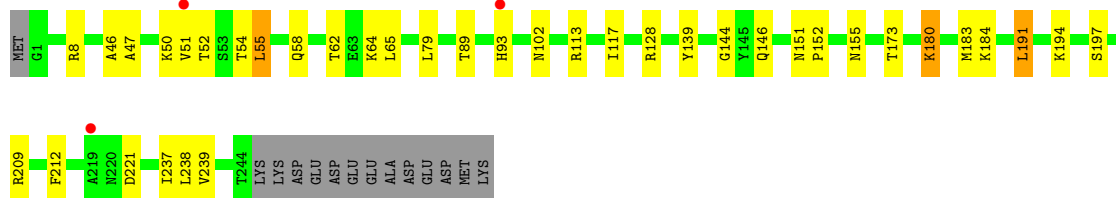
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  92% 8% .



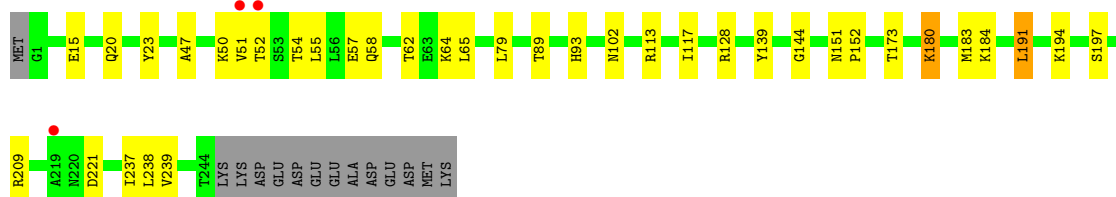
- Molecule 2: Proteasome subunit alpha type-3

Chain B:  80% 14% 5% .

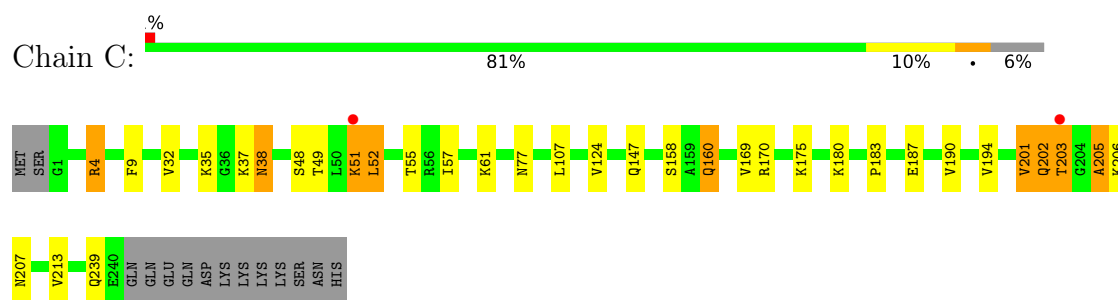


- Molecule 2: Proteasome subunit alpha type-3

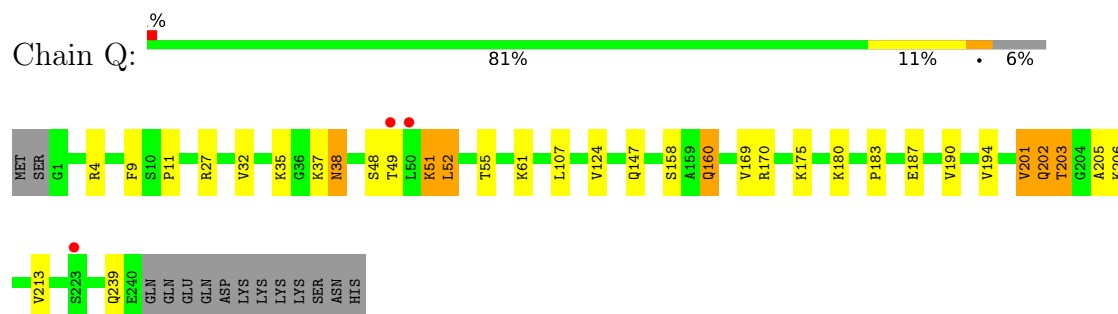
Chain P:  80% 14% 5% .



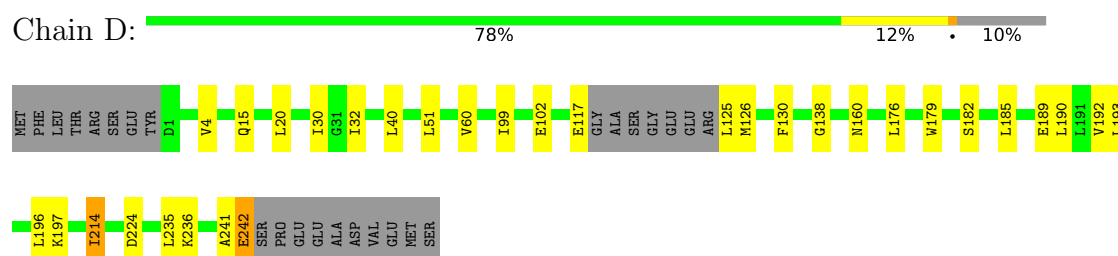
- Molecule 3: Proteasome subunit alpha type-4



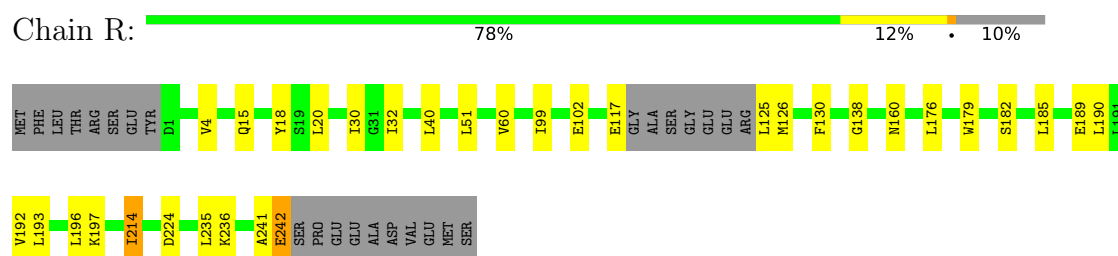
- Molecule 3: Proteasome subunit alpha type-4



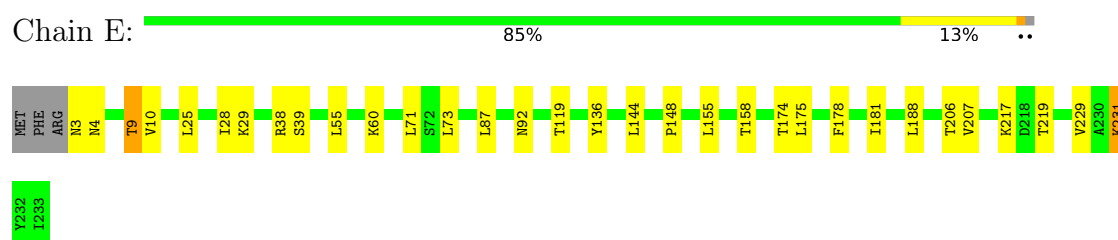
- Molecule 4: Proteasome subunit alpha type-5



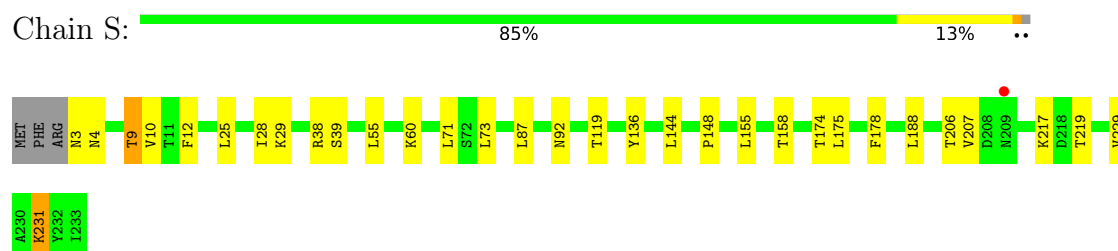
- Molecule 4: Proteasome subunit alpha type-5



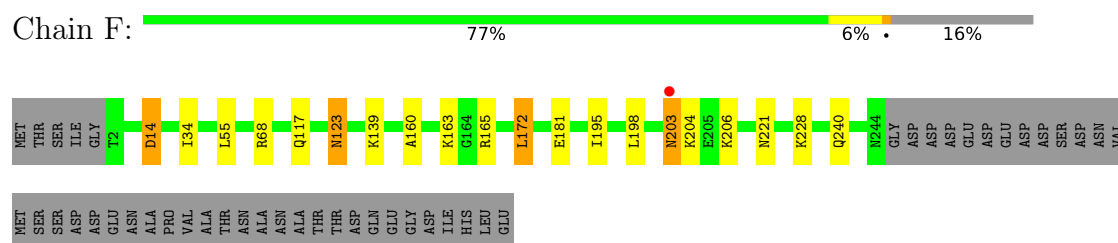
- Molecule 5: Proteasome subunit alpha type-6



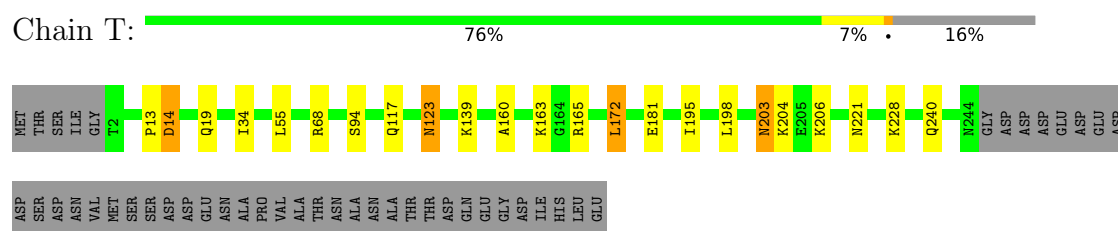
- Molecule 5: Proteasome subunit alpha type-6



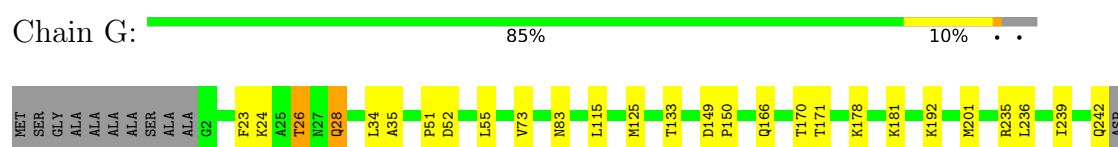
- Molecule 6: Probable proteasome subunit alpha type-7



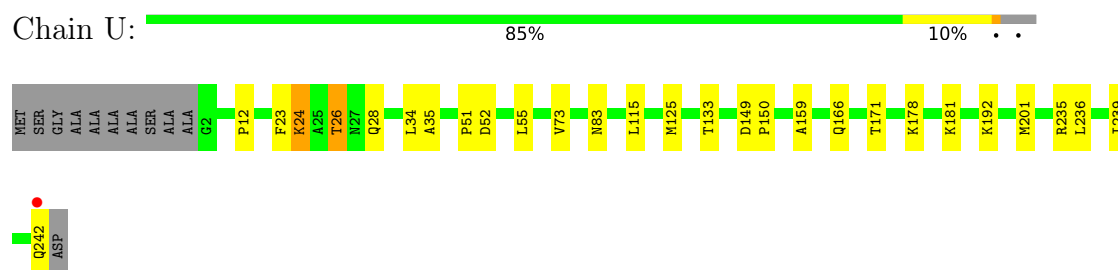
- Molecule 6: Probable proteasome subunit alpha type-7



- 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

Chain V: 88% 6% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I: 87% 12%



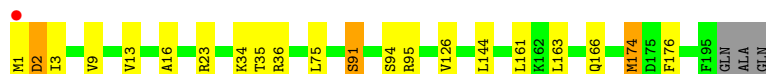
- Molecule 9: Proteasome subunit beta type-3

Chain W: 88% 11%



- Molecule 10: Proteasome subunit beta type-4

Chain J: 88% 9% . .



- Molecule 10: Proteasome subunit beta type-4

Chain X: 88% 9% . .



- Molecule 11: Proteasome subunit beta type-5

Chain K: 86% 12% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 87% 11% .



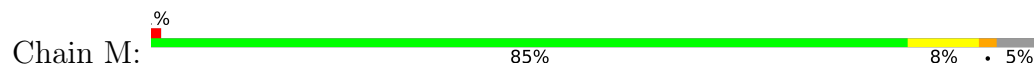
- Molecule 12: Proteasome subunit beta type-6



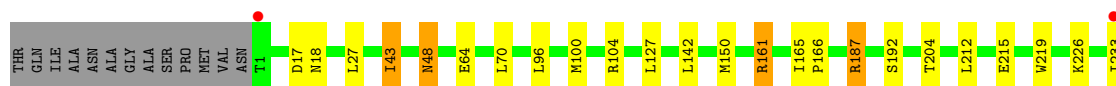
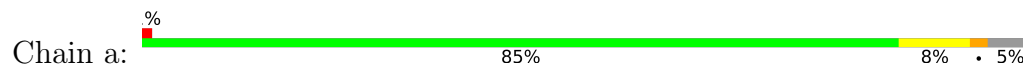
- Molecule 12: Proteasome subunit beta type-6



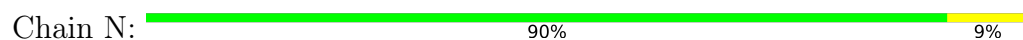
- Molecule 13: Proteasome subunit beta type-7



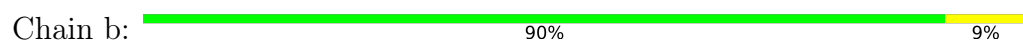
- Molecule 13: Proteasome subunit beta type-7



- 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	135.65Å 298.66Å 145.46Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (15.00-2.80) 94.3 (15.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.202 (Not available) , 0.192	Depositor DCC
R_{free} test set	12298 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.2	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	0.95	EDS
Total number of atoms	49987	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: MES, MG, 39V

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	0.72	0/2642
1	O	0.40	0/1952	0.72	0/2642
2	B	0.41	0/1934	0.73	0/2618
2	P	0.41	0/1934	0.73	0/2618
3	C	0.41	0/1910	0.78	0/2586
3	Q	0.41	0/1910	0.78	0/2586
4	D	0.39	0/1837	0.71	0/2475
4	R	0.40	0/1837	0.71	0/2475
5	E	0.39	0/1800	0.71	0/2433
5	S	0.39	0/1800	0.71	0/2433
6	F	0.40	0/1932	0.72	0/2609
6	T	0.40	0/1932	0.73	0/2609
7	G	0.39	0/1945	0.73	0/2634
7	U	0.39	0/1945	0.73	0/2634
8	H	0.37	0/1715	0.69	0/2326
8	V	0.37	0/1715	0.69	0/2326
9	I	0.38	0/1611	0.72	0/2174
9	W	0.38	0/1611	0.72	0/2174
10	J	0.38	0/1589	0.69	0/2142
10	X	0.38	0/1589	0.69	0/2142
11	K	0.39	0/1681	0.69	0/2274
11	Y	0.40	1/1681 (0.1%)	0.70	0/2274
12	L	0.38	0/1795	0.69	0/2420
12	Z	0.38	0/1795	0.69	0/2420
13	M	0.40	0/1855	0.70	0/2514
13	a	0.41	0/1855	0.71	0/2514
14	N	0.36	0/1541	0.69	0/2087
14	b	0.36	0/1541	0.69	0/2087
All	All	0.39	1/50194 (0.0%)	0.71	0/67868

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
12	L	0	1
12	Z	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1	THR	CB-OG1	-5.56	1.34	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	135	GLN	Peptide
12	Z	135	GLN	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	7	0
1	O	1915	0	1929	11	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	13	0
3	C	1881	0	1895	15	0
3	Q	1881	0	1895	12	0
4	D	1813	0	1797	8	0
4	R	1813	0	1797	9	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	8	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1907	0	1901	10	0
7	U	1907	0	1901	11	0
8	H	1684	0	1688	6	0
8	V	1684	0	1688	5	0
9	I	1581	0	1574	10	0
9	W	1581	0	1574	9	0
10	J	1561	0	1569	8	0
10	X	1561	0	1569	8	0
11	K	1644	0	1593	15	0
11	Y	1644	0	1593	16	0
12	L	1757	0	1711	13	0
12	Z	1757	0	1711	13	0
13	M	1824	0	1832	10	0
13	a	1824	0	1832	11	0
14	N	1512	0	1481	10	0
14	b	1512	0	1481	11	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	2	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	K	12	0	13	0	0
16	Y	12	0	13	0	0
17	K	46	0	39	5	0
17	Y	46	0	39	10	0
18	A	24	0	0	0	0
18	B	23	0	0	0	0
18	C	14	0	0	0	0
18	D	12	0	0	0	0
18	E	11	0	0	0	0
18	F	23	0	0	1	0
18	G	27	0	0	0	0
18	H	21	0	0	0	0
18	I	26	0	0	0	0
18	J	23	0	0	0	0
18	K	24	0	0	0	0
18	L	23	0	0	0	0
18	M	27	0	0	0	0
18	N	16	0	0	0	0
18	O	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	11	0	0	0	0
18	Q	12	0	0	0	0
18	R	17	0	0	0	0
18	S	7	0	0	0	0
18	T	19	0	0	0	0
18	U	30	0	0	0	0
18	V	22	0	0	0	0
18	W	25	0	0	0	0
18	X	26	0	0	0	0
18	Y	20	0	0	2	0
18	Z	21	0	0	0	0
18	a	21	0	0	0	0
18	b	22	0	0	0	0
All	All	49987	0	49168	263	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (263) 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)
17:Y:303:39V:H24	18:Y:416:HOH:O	1.54	1.08
17:Y:303:39V:C65	18:Y:416:HOH:O	2.01	1.05
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.58	0.86
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.58	0.86
11:K:53:GLN:O	11:K:57:THR:HG23	1.82	0.79
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.83	0.79
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.49	0.77
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.68	0.76
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.50	0.75
10:X:1:MET:HA	10:X:34:LYS:HE3	1.69	0.75
10:J:1:MET:HA	10:J:34:LYS:HE3	1.69	0.74
14:N:152:VAL:HA	14:N:175:MET:HE1	1.76	0.67
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.25	0.67
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.60	0.67
3:C:202:GLN:HG3	3:C:203:THR:H	1.60	0.66
14:b:152:VAL:HA	14:b:175:MET:HE1	1.76	0.66
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.29	0.65
11:K:100:MET:CE	11:K:127:PHE:HB2	2.26	0.65
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.98	0.63
17:K:303:39V:O40	17:K:303:39V:N28	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.81	0.62
3:C:51:LYS:O	3:C:52:LEU:HB2	1.98	0.62
17:K:303:39V:O40	17:K:303:39V:H2	1.98	0.62
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.82	0.61
5:E:9:THR:HG21	5:E:119:THR:HA	1.84	0.60
9:W:65:MET:HE1	9:W:93:SER:HB3	1.83	0.60
17:Y:303:39V:O32	17:Y:303:39V:O40	2.17	0.60
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.28	0.60
14:N:20:THR:HG22	14:N:31:THR:OG1	2.01	0.60
7:G:23:PHE:O	7:G:26:THR:HB	2.02	0.59
7:U:23:PHE:O	7:U:26:THR:HB	2.02	0.59
14:b:20:THR:HG22	14:b:31:THR:OG1	2.01	0.59
11:K:100:MET:HE3	11:K:127:PHE:CB	2.29	0.59
5:S:9:THR:HG21	5:S:119:THR:HA	1.84	0.58
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.68	0.58
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.68	0.58
9:I:65:MET:HE1	9:I:93:SER:HB3	1.84	0.58
11:K:170:TYR:O	17:K:303:39V:H37	2.04	0.57
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.87	0.57
9:I:101:PRO:HB3	9:I:126:ILE:CD1	2.35	0.57
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.87	0.56
9:W:101:PRO:HB3	9:W:126:ILE:CD1	2.35	0.56
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.88	0.56
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.88	0.55
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.88	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.88	0.55
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.90	0.55
11:Y:33:LYS:HZ3	17:Y:303:39V:H38	1.72	0.54
10:X:1:MET:HA	10:X:34:LYS:CE	2.37	0.54
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.90	0.54
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.89	0.54
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.90	0.54
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.90	0.54
10:J:1:MET:HA	10:J:34:LYS:CE	2.37	0.53
5:S:155:LEU:HD13	5:S:158:THR:HB	1.91	0.53
2:B:180:LYS:O	2:B:183:MET:HB2	2.09	0.53
5:E:155:LEU:HD13	5:E:158:THR:HB	1.90	0.52
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.24	0.52
3:C:201:VAL:O	3:C:202:GLN:HB2	2.10	0.52
3:C:201:VAL:HG13	3:C:202:GLN:N	2.25	0.52
10:J:174:MET:HA	10:X:174:MET:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.25	0.51
6:T:123:ASN:C	6:T:123:ASN:HD22	2.18	0.51
12:L:8:ASN:HA	12:L:30:ILE:O	2.11	0.51
17:K:303:39V:H16	17:K:303:39V:O3	2.10	0.51
2:P:180:LYS:O	2:P:183:MET:HB2	2.09	0.51
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.10	0.51
4:R:185:LEU:O	4:R:189:GLU:HG3	2.11	0.51
6:T:14:ASP:OD2	6:T:14:ASP:N	2.41	0.51
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.91	0.51
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.92	0.50
11:Y:107:LYS:HE2	11:Y:108:GLU:HG3	1.93	0.50
6:F:123:ASN:C	6:F:123:ASN:HD22	2.19	0.50
4:D:185:LEU:O	4:D:189:GLU:HG3	2.11	0.50
13:M:43:ILE:HG12	13:M:43:ILE:O	2.11	0.50
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.41	0.50
13:a:43:ILE:HG12	13:a:43:ILE:O	2.11	0.50
11:K:107:LYS:HE2	11:K:108:GLU:HG3	1.93	0.50
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.92	0.50
11:Y:33:LYS:NZ	17:Y:303:39V:H38	2.27	0.49
6:F:14:ASP:OD2	6:F:14:ASP:N	2.42	0.49
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.43	0.49
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.11	0.49
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.61	0.49
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.43	0.49
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.48	0.49
5:S:155:LEU:HD23	6:T:55:LEU:HD23	1.95	0.48
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.48	0.48
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.42	0.48
11:Y:31:VAL:HG11	17:Y:303:39V:C43	2.44	0.48
2:B:155:ASN:ND2	3:C:77:ASN:HB2	2.29	0.48
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.96	0.48
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.49	0.48
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.79	0.48
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.79	0.48
2:B:183:MET:HE1	2:B:191:LEU:HD12	1.96	0.48
13:a:27:LEU:HB2	13:a:192:SER:HB3	1.96	0.48
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.96	0.47
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.49	0.47
9:I:14:MET:HB2	9:I:162:LEU:HD11	1.97	0.47
7:G:239:ILE:O	7:G:242:GLN:HB3	2.14	0.47
11:K:1:THR:HG22	11:K:2:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.50	0.47
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.96	0.47
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.50	0.47
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.50	0.47
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.79	0.47
7:U:239:ILE:O	7:U:242:GLN:HB3	2.15	0.47
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.97	0.47
7:G:73:VAL:CG1	7:G:133:THR:HB	2.45	0.47
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.97	0.47
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.96	0.47
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.79	0.47
9:W:14:MET:HB2	9:W:162:LEU:HD11	1.97	0.46
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.45	0.46
7:U:73:VAL:CG1	7:U:133:THR:HB	2.44	0.46
8:H:218:VAL:CG2	9:I:196:LYS:HB2	2.46	0.46
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.79	0.46
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.96	0.46
17:Y:303:39V:O3	17:Y:303:39V:H6	2.16	0.46
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.46
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.97	0.46
2:P:183:MET:HE1	2:P:191:LEU:HD12	1.96	0.46
3:C:9:PHE:H	4:D:15:GLN:HE22	1.64	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.46	0.46
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.45	0.46
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.97	0.46
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.29	0.46
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.97	0.46
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.51	0.45
17:K:303:39V:O3	17:K:303:39V:H6	2.16	0.45
13:M:150:MET:HE1	13:M:187:ARG:HG2	1.98	0.45
1:O:247:LEU:O	1:O:250:LEU:HB2	2.16	0.45
12:Z:62:ASP:O	12:Z:66:LYS:HB2	2.16	0.45
1:O:99:ARG:HE	8:V:61:SER:HG	1.65	0.45
17:Y:303:39V:O27	17:Y:303:39V:H33	2.16	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.45
6:T:13:PRO:O	7:U:24:LYS:HD2	2.17	0.45
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.51	0.45
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.99	0.45
1:O:149:GLN:O	1:O:156:TYR:HA	2.17	0.45
10:X:91:SER:HA	10:X:94:SER:OG	2.17	0.45
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.45
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.82	0.45
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.52	0.45
14:N:32:ASP:OD2	14:N:185:ARG:NH2	2.50	0.45
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.51	0.45
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.52	0.45
14:b:32:ASP:OD2	14:b:185:ARG:NH2	2.50	0.45
12:L:62:ASP:O	12:L:66:LYS:HB2	2.16	0.44
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.52	0.44
4:R:241:ALA:O	4:R:242:GLU:HB2	2.17	0.44
1:A:247:LEU:O	1:A:250:LEU:HB2	2.17	0.44
8:H:52:THR:O	8:H:56:THR:HB	2.17	0.44
1:A:149:GLN:O	1:A:156:TYR:HA	2.17	0.44
9:W:7:ASN:HA	9:W:29:GLY:O	2.18	0.44
13:M:17:ASP:OD1	13:M:18:ASN:N	2.50	0.44
5:S:38:ARG:HD2	5:S:39:SER:O	2.18	0.44
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.00	0.44
17:Y:303:39V:O3	17:Y:303:39V:H16	2.16	0.44
11:K:5:ALA:HB3	11:K:100:MET:HE2	2.00	0.44
10:J:91:SER:HA	10:J:94:SER:OG	2.17	0.44
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.51	0.44
8:V:52:THR:O	8:V:56:THR:HB	2.17	0.44
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.00	0.44
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.51	0.44
5:E:38:ARG:HD2	5:E:39:SER:O	2.18	0.43
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.81	0.43
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.66	0.43
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.32	0.43
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.82	0.43
5:E:155:LEU:HD23	6:F:55:LEU:HD23	2.00	0.43
7:G:52:ASP:HB3	7:G:55:LEU:HG	2.00	0.43
4:D:241:ALA:O	4:D:242:GLU:HB2	2.17	0.43
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.65	0.43
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.00	0.43
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.01	0.43
13:a:127:LEU:HG	13:a:142:LEU:HD12	2.00	0.43
3:C:38:ASN:N	3:C:38:ASN:HD22	2.16	0.43
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.00	0.43
7:U:34:LEU:HD23	7:U:35:ALA:N	2.34	0.43
13:a:17:ASP:OD1	13:a:18:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.43
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.01	0.43
7:U:73:VAL:HG12	7:U:133:THR:HB	2.00	0.43
8:V:7:LYS:HG3	8:V:123:TYR:HA	2.01	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.43
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.01	0.43
8:H:7:LYS:HG3	8:H:123:TYR:HA	2.01	0.43
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.54	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.43
18:F:317:HOH:O	7:G:28:GLN:HG3	2.19	0.42
11:K:116:ASP:OD1	11:K:116:ASP:C	2.61	0.42
7:U:52:ASP:HB3	7:U:55:LEU:HG	2.01	0.42
3:C:202:GLN:CG	3:C:203:THR:H	2.31	0.42
7:G:34:LEU:HD23	7:G:35:ALA:N	2.33	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.42
12:L:126:ASP:OD1	12:L:126:ASP:C	2.61	0.42
12:L:149:PHE:CE1	12:L:153:GLN:HG3	2.54	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.42
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.00	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
17:Y:303:39V:H39	17:Y:303:39V:H26	1.90	0.42
12:Z:126:ASP:OD1	12:Z:126:ASP:C	2.62	0.42
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.49	0.42
7:G:73:VAL:HG12	7:G:133:THR:HB	2.00	0.42
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.20	0.42
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.34	0.42
14:b:20:THR:CG2	14:b:31:THR:OG1	2.67	0.42
4:D:126:MET:HE1	4:D:130:PHE:CE2	2.55	0.42
12:L:13:LEU:HD12	12:L:14:GLY:N	2.34	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.02	0.42
1:O:12:PHE:H	2:P:20:GLN:HE22	1.67	0.42
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.55	0.42
12:Z:149:PHE:CE1	12:Z:153:GLN:HG3	2.54	0.42
8:H:206:PRO:O	8:H:209:THR:OG1	2.36	0.42
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.00	0.42
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	2.00	0.42
3:C:190:VAL:O	3:C:194:VAL:HG23	2.20	0.42
1:O:158:PRO:HB2	2:P:57:GLU:HB3	2.02	0.42
11:Y:116:ASP:OD1	11:Y:116:ASP:C	2.63	0.42
11:K:6:PHE:HA	11:K:125:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:12:ILE:HB	11:K:180:VAL:HB	2.00	0.42
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.16	0.41
4:R:126:MET:HE1	4:R:130:PHE:CE2	2.55	0.41
13:M:48:ASN:H	13:M:48:ASN:HD22	1.68	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.67	0.41
1:O:55:LEU:HB3	7:U:159:ALA:O	2.21	0.41
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.49	0.41
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	2.01	0.41
14:b:20:THR:HG23	14:b:28:ASN:HB3	2.02	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.02	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.03	0.41
12:L:210:ASP:OD1	12:L:210:ASP:N	2.54	0.41
5:E:178:PHE:HA	5:E:181:ILE:HG13	2.03	0.41
7:G:34:LEU:HD23	7:G:34:LEU:C	2.45	0.41
14:N:38:HIS:O	14:N:39:ASP:C	2.63	0.41
7:U:34:LEU:HD23	7:U:34:LEU:C	2.46	0.41
13:a:48:ASN:H	13:a:48:ASN:HD22	1.69	0.41
14:b:38:HIS:O	14:b:39:ASP:C	2.63	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.41
2:B:46:ALA:HB2	2:B:212:PHE:CE1	2.56	0.41
9:I:7:ASN:HA	9:I:29:GLY:O	2.20	0.41
13:a:96:LEU:O	13:a:100:MET:HG2	2.20	0.41
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.01	0.41
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.56	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.56	0.41
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.68	0.41
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.56	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.40
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.03	0.40
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.52	0.40
12:L:195:HIS:HD2	12:L:197:GLN:H	1.68	0.40
13:M:43:ILE:HG21	13:M:64:GLU:HG2	2.03	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.21	0.40
12:Z:210:ASP:OD1	12:Z:210:ASP:N	2.54	0.40
3:C:205:ALA:C	3:C:207:ASN:H	2.29	0.40
13:a:43:ILE:HG21	13:a:64:GLU:HG2	2.02	0.40
1:A:49:LYS:HG3	1:A:210:GLU:HB2	2.04	0.40
14:N:20:THR:HG23	14:N:28:ASN:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	241 (97%)	6 (2%)	1 (0%)	30	60
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	60
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	16	44
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	16	44
3	C	238/254 (94%)	227 (95%)	6 (2%)	5 (2%)	5	20
3	Q	238/254 (94%)	227 (95%)	6 (2%)	5 (2%)	5	20
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	221 (96%)	7 (3%)	1 (0%)	30	60
5	S	229/234 (98%)	221 (96%)	7 (3%)	1 (0%)	30	60
6	F	241/288 (84%)	234 (97%)	6 (2%)	1 (0%)	30	60
6	T	241/288 (84%)	234 (97%)	6 (2%)	1 (0%)	30	60
7	G	239/252 (95%)	236 (99%)	2 (1%)	1 (0%)	30	60
7	U	239/252 (95%)	236 (99%)	2 (1%)	1 (0%)	30	60
8	H	220/232 (95%)	211 (96%)	9 (4%)	0	100	100
8	V	220/232 (95%)	211 (96%)	9 (4%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	189 (98%)	2 (1%)	2 (1%)	12	38
10	X	193/198 (98%)	189 (98%)	2 (1%)	2 (1%)	12	38
11	K	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	55
11	Y	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	24	55
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	225 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6276/6614 (95%)	6087 (97%)	161 (3%)	28 (0%)	30	60

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
11	K	9	GLN
11	Y	9	GLN
2	B	221	ASP
3	C	183	PRO
3	C	205	ALA
5	E	231	LYS
2	P	221	ASP
3	Q	183	PRO
3	Q	205	ALA
5	S	231	LYS
6	F	203	ASN
6	T	203	ASN
1	A	2	THR
3	C	206	LYS
1	O	2	THR
3	Q	206	LYS
7	G	51	PRO
10	J	9	VAL
7	U	51	PRO
10	X	9	VAL
3	C	201	VAL
3	Q	201	VAL

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%)	200 (96%)	9 (4%)	26	60
1	O	209/209 (100%)	200 (96%)	9 (4%)	26	60
2	B	203/216 (94%)	184 (91%)	19 (9%)	8	27
2	P	203/216 (94%)	184 (91%)	19 (9%)	8	27
3	C	212/226 (94%)	191 (90%)	21 (10%)	7	24
3	Q	212/226 (94%)	191 (90%)	21 (10%)	7	24
4	D	194/215 (90%)	175 (90%)	19 (10%)	7	25
4	R	194/215 (90%)	175 (90%)	19 (10%)	7	25
5	E	190/193 (98%)	170 (90%)	20 (10%)	6	22
5	S	190/193 (98%)	170 (90%)	20 (10%)	6	22
6	F	201/239 (84%)	185 (92%)	16 (8%)	11	34
6	T	201/239 (84%)	184 (92%)	17 (8%)	10	31
7	G	206/210 (98%)	192 (93%)	14 (7%)	14	42
7	U	206/210 (98%)	192 (93%)	14 (7%)	14	42
8	H	181/190 (95%)	171 (94%)	10 (6%)	19	51
8	V	181/190 (95%)	171 (94%)	10 (6%)	19	51
9	I	172/173 (99%)	162 (94%)	10 (6%)	18	49
9	W	172/173 (99%)	162 (94%)	10 (6%)	18	49
10	J	173/175 (99%)	161 (93%)	12 (7%)	14	41
10	X	173/175 (99%)	161 (93%)	12 (7%)	14	41
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	52
11	Y	169/169 (100%)	160 (95%)	9 (5%)	20	52
12	L	185/185 (100%)	175 (95%)	10 (5%)	20	51
12	Z	185/185 (100%)	175 (95%)	10 (5%)	20	51
13	M	199/208 (96%)	187 (94%)	12 (6%)	17	47
13	a	199/208 (96%)	188 (94%)	11 (6%)	19	51
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	65
14	b	162/162 (100%)	156 (96%)	6 (4%)	30	65
All	All	5312/5540 (96%)	4938 (93%)	374 (7%)	14	40

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	29	LYS
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	150	VAL
1	A	157	PHE
1	A	231	LYS
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	62	THR
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN
2	B	173	THR
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	197	SER
2	B	209	ARG
2	B	237	ILE
2	B	238	LEU
2	B	239	VAL
3	C	4	ARG
3	C	32	VAL
3	C	37	LYS
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	107	LEU
3	C	124	VAL
3	C	147	GLN
3	C	160	GLN

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Mol	Chain	Res	Type
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	213	VAL
3	C	239	GLN
4	D	4	VAL
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	102	GLU
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	182	SER
4	D	190	LEU
4	D	193	LEU
4	D	197	LYS
4	D	214	ILE
4	D	224	ASP
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	4	ASN
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	60	LYS
5	E	71	LEU
5	E	73	LEU
5	E	87	LEU
5	E	92	ASN
5	E	144	LEU
5	E	174	THR
5	E	188	LEU
5	E	206	THR

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Mol	Chain	Res	Type
5	E	207	VAL
5	E	219	THR
5	E	229	VAL
5	E	231	LYS
6	F	14	ASP
6	F	68	ARG
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	163	LYS
6	F	165	ARG
6	F	172	LEU
6	F	181	GLU
6	F	198	LEU
6	F	203	ASN
6	F	204	LYS
6	F	206	LYS
6	F	221	ASN
6	F	228	LYS
6	F	240	GLN
7	G	24	LYS
7	G	26	THR
7	G	28	GLN
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	192	LYS
7	G	201	MET
7	G	235	ARG
7	G	236	LEU
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	113	ILE
8	H	191	LEU

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Mol	Chain	Res	Type
8	H	196	ARG
8	H	198	GLU
9	I	31	GLN
9	I	37	ASN
9	I	92	SER
9	I	126	ILE
9	I	133	LYS
9	I	151	SER
9	I	171	LEU
9	I	182	TRP
9	I	193	GLU
9	I	195	VAL
10	J	2	ASP
10	J	13	VAL
10	J	23	ARG
10	J	35	THR
10	J	36	ARG
10	J	75	LEU
10	J	91	SER
10	J	95	ARG
10	J	144	LEU
10	J	163	LEU
10	J	166	GLN
10	J	174	MET
11	K	4	LEU
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	118	ASP
11	K	148	LEU
12	L	1	GLN
12	L	11	THR
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
12	L	173	LYS
12	L	181	ILE

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Mol	Chain	Res	Type
12	L	210	ASP
13	M	10	SER
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	204	THR
13	M	212	LEU
13	M	215	GLU
13	M	226	LYS
13	M	233	ILE
14	N	9	LYS
14	N	20	THR
14	N	44	CYS
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	17	LYS
1	O	29	LYS
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	150	VAL
1	O	157	PHE
1	O	231	LYS
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	62	THR
2	P	65	LEU
2	P	79	LEU
2	P	102	ASN
2	P	173	THR
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS

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Mol	Chain	Res	Type
2	P	197	SER
2	P	209	ARG
2	P	237	ILE
2	P	238	LEU
2	P	239	VAL
3	Q	4	ARG
3	Q	32	VAL
3	Q	37	LYS
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	107	LEU
3	Q	124	VAL
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	203	THR
3	Q	213	VAL
3	Q	239	GLN
4	R	4	VAL
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	102	GLU
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	182	SER
4	R	190	LEU
4	R	193	LEU
4	R	197	LYS
4	R	214	ILE
4	R	224	ASP

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Mol	Chain	Res	Type
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	4	ASN
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	60	LYS
5	S	71	LEU
5	S	73	LEU
5	S	87	LEU
5	S	92	ASN
5	S	144	LEU
5	S	174	THR
5	S	188	LEU
5	S	206	THR
5	S	207	VAL
5	S	219	THR
5	S	229	VAL
5	S	231	LYS
6	T	14	ASP
6	T	68	ARG
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	163	LYS
6	T	165	ARG
6	T	172	LEU
6	T	181	GLU
6	T	198	LEU
6	T	203	ASN
6	T	204	LYS
6	T	206	LYS
6	T	221	ASN
6	T	228	LYS
6	T	240	GLN
7	U	24	LYS
7	U	26	THR

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Mol	Chain	Res	Type
7	U	28	GLN
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	171	THR
7	U	178	LYS
7	U	181	LYS
7	U	192	LYS
7	U	201	MET
7	U	235	ARG
7	U	236	LEU
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	113	ILE
8	V	191	LEU
8	V	196	ARG
8	V	198	GLU
9	W	31	GLN
9	W	37	ASN
9	W	92	SER
9	W	126	ILE
9	W	133	LYS
9	W	151	SER
9	W	171	LEU
9	W	182	TRP
9	W	193	GLU
9	W	195	VAL
10	X	2	ASP
10	X	13	VAL
10	X	23	ARG
10	X	35	THR
10	X	36	ARG
10	X	75	LEU
10	X	91	SER
10	X	95	ARG
10	X	144	LEU
10	X	163	LEU

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Mol	Chain	Res	Type
10	X	166	GLN
10	X	174	MET
11	Y	4	LEU
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	118	ASP
11	Y	148	LEU
12	Z	1	GLN
12	Z	11	THR
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	173	LYS
12	Z	181	ILE
12	Z	210	ASP
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	204	THR
13	a	212	LEU
13	a	215	GLU
13	a	226	LYS
13	a	233	ILE
14	b	9	LYS
14	b	20	THR
14	b	44	CYS
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 (171) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	149	GLN
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	53	GLN
3	C	115	GLN
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
4	D	100	ASN
4	D	106	GLN
4	D	160	ASN
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	147	GLN
5	E	151	ASN
5	E	165	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	27	ASN
7	G	30	ASN
7	G	83	ASN

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Mol	Chain	Res	Type
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	175	ASN
8	H	9	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	172	ASN
8	H	189	ASN
9	I	31	GLN
9	I	37	ASN
9	I	63	ASN
9	I	172	ASN
10	J	37	GLN
10	J	55	GLN
10	J	61	GLN
10	J	63	ASN
10	J	112	ASN
10	J	147	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	153	GLN
12	L	155	ASN
13	M	18	ASN
13	M	26	ASN
13	M	48	ASN
13	M	108	ASN
14	N	38	HIS
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN

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Mol	Chain	Res	Type
1	O	94	HIS
1	O	149	GLN
2	P	20	GLN
2	P	58	GLN
2	P	102	ASN
2	P	119	GLN
2	P	123	GLN
2	P	146	GLN
2	P	155	ASN
2	P	176	GLN
2	P	232	GLN
3	Q	38	ASN
3	Q	115	GLN
3	Q	116	GLN
3	Q	120	GLN
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	160	ASN
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	147	GLN
5	S	151	ASN
5	S	165	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	140	ASN
6	T	191	GLN
6	T	240	GLN
7	U	27	ASN
7	U	30	ASN

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Mol	Chain	Res	Type
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	175	ASN
8	V	9	ASN
8	V	30	ASN
8	V	57	GLN
8	V	66	HIS
8	V	172	ASN
8	V	189	ASN
9	W	31	GLN
9	W	37	ASN
9	W	63	ASN
9	W	88	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	86	GLN
10	X	112	ASN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	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	80	ASN
12	Z	153	GLN
12	Z	155	ASN
13	a	18	ASN
13	a	26	ASN
13	a	48	ASN
13	a	102	GLN
14	b	38	HIS
14	b	69	GLN

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Mol	Chain	Res	Type
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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$
17	39V	K	303	-	48,50,50	3.83	17 (35%)	61,70,70	1.77	14 (22%)
17	39V	Y	303	-	48,50,50	3.92	16 (33%)	61,70,70	1.88	13 (21%)
16	MES	K	302	-	12,12,12	2.33	1 (8%)	15,16,16	1.22	1 (6%)
16	MES	Y	302	-	12,12,12	2.25	1 (8%)	15,16,16	1.16	1 (6%)

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
17	39V	K	303	-	-	11/42/54/54	0/5/5/5
17	39V	Y	303	-	-	8/42/54/54	0/5/5/5
16	MES	K	302	-	-	0/6/14/14	0/1/1/1
16	MES	Y	302	-	-	0/6/14/14	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	303	39V	C51-C50	-11.61	1.36	1.51
17	K	303	39V	C51-C50	-11.55	1.36	1.51
17	K	303	39V	C67-C68	-8.83	1.30	1.41
17	Y	303	39V	C67-C66	-8.34	1.30	1.44
17	Y	303	39V	C67-C68	-8.31	1.31	1.41
17	K	303	39V	C67-C66	-8.24	1.30	1.44
17	Y	303	39V	O32-C31	7.92	1.33	1.21
16	K	302	MES	C8-S	-7.74	1.66	1.77
16	Y	302	MES	C8-S	-7.49	1.67	1.77
17	Y	303	39V	C57-C58	-7.37	1.30	1.44
17	Y	303	39V	C51-C52	-7.24	1.37	1.50
17	K	303	39V	C63-C67	-7.00	1.29	1.39
17	Y	303	39V	C57-C52	-6.96	1.30	1.39
17	K	303	39V	C51-C52	-6.96	1.38	1.50
17	K	303	39V	C57-C58	-6.90	1.31	1.44
17	K	303	39V	C57-C52	-6.57	1.30	1.39
17	Y	303	39V	C63-C67	-6.52	1.30	1.39
17	K	303	39V	O32-C31	6.33	1.31	1.21
17	Y	303	39V	C30-C41	-6.28	1.36	1.51
17	Y	303	39V	C56-C57	-5.82	1.31	1.39
17	Y	303	39V	C60-C68	-5.78	1.30	1.39
17	K	303	39V	C60-C68	-5.76	1.30	1.39
17	K	303	39V	C30-C41	-5.21	1.39	1.51
17	Y	303	39V	C53-C52	-5.19	1.31	1.39
17	K	303	39V	C56-C57	-5.16	1.32	1.39
17	K	303	39V	C68-N69	-4.62	1.30	1.37
17	K	303	39V	C53-C52	-4.61	1.32	1.39
17	K	303	39V	C65-C66	-4.20	1.30	1.36
17	Y	303	39V	C68-N69	-3.93	1.31	1.37
17	K	303	39V	C65-N69	-3.72	1.31	1.37
17	Y	303	39V	C65-C66	-3.36	1.31	1.36
17	Y	303	39V	C65-N69	-3.16	1.32	1.37
17	Y	303	39V	C50-C58	-2.48	1.31	1.36
17	K	303	39V	C50-C58	-2.39	1.31	1.36
17	K	303	39V	C61-C60	-2.06	1.35	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	303	39V	O32-C31-C37	-7.45	107.83	121.30
17	K	303	39V	O32-C31-C37	-6.50	109.55	121.30
17	Y	303	39V	C11-N1-C2	3.79	127.65	121.27
17	K	303	39V	C16-C17-C66	-3.63	106.58	113.44
17	K	303	39V	C30-C29-N28	-3.59	103.40	110.83
17	Y	303	39V	C66-C65-N69	-3.57	106.39	110.31
17	Y	303	39V	C57-C58-C50	3.51	111.32	109.11
17	Y	303	39V	C16-C17-C66	-3.50	106.82	113.44
17	Y	303	39V	C67-C66-C65	3.45	109.69	106.16
17	K	303	39V	C57-C58-C50	3.08	111.05	109.11
17	K	303	39V	C52-C51-C50	3.03	105.14	102.72
17	Y	303	39V	C30-C29-N28	-2.97	104.69	110.83
17	Y	303	39V	C52-C51-C50	2.96	105.09	102.72
17	Y	303	39V	C63-C67-C68	2.95	121.90	118.84
17	Y	303	39V	C54-C55-C56	-2.94	116.61	120.24
17	K	303	39V	C66-C65-N69	-2.75	107.29	110.31
17	K	303	39V	C11-N1-C2	2.71	125.84	121.27
17	K	303	39V	C54-C55-C56	-2.61	117.02	120.24
17	K	303	39V	C67-C66-C65	2.45	108.67	106.16
17	K	303	39V	C62-C61-C60	-2.45	117.22	120.24
17	Y	303	39V	C30-C41-C46	-2.29	116.64	120.90
17	K	303	39V	C41-C30-C29	2.26	119.37	113.36
17	K	303	39V	C55-C54-C53	-2.17	117.56	120.24
17	K	303	39V	C52-C57-C58	-2.12	107.59	109.46
17	Y	303	39V	C52-C57-C58	-2.12	107.60	109.46
16	Y	302	MES	O2S-S-C8	2.09	109.89	106.73
16	K	302	MES	O3S-S-C8	2.08	110.07	106.00
17	K	303	39V	C17-C66-C65	-2.02	123.03	126.97
17	Y	303	39V	C63-C67-C66	-2.01	130.85	133.85

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	303	39V	C31-C37-C39-O40
17	K	303	39V	C12-C11-C13-O14
17	Y	303	39V	C12-C11-C13-O14
17	K	303	39V	C12-C11-C13-N15
17	Y	303	39V	C12-C11-C13-N15
17	Y	303	39V	C12-C11-N1-C2
17	K	303	39V	C12-C11-N1-C2

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Mol	Chain	Res	Type	Atoms
17	K	303	39V	C29-C30-C41-C42
17	K	303	39V	C29-C30-C41-C46
17	Y	303	39V	C29-C30-C41-C42
17	Y	303	39V	C29-C30-C41-C46
17	K	303	39V	C38-C37-C39-O40
17	K	303	39V	O32-C31-C37-C38
17	Y	303	39V	O32-C31-C37-C38
17	K	303	39V	N28-C29-C31-C37
17	Y	303	39V	N28-C29-C31-C37
17	K	303	39V	C29-C31-C37-C38
17	K	303	39V	C30-C29-C31-O32
17	Y	303	39V	C30-C29-C31-O32

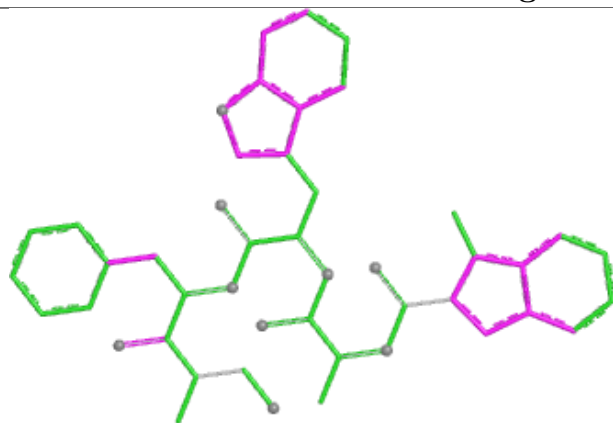
There are no ring outliers.

2 monomers are involved in 15 short contacts:

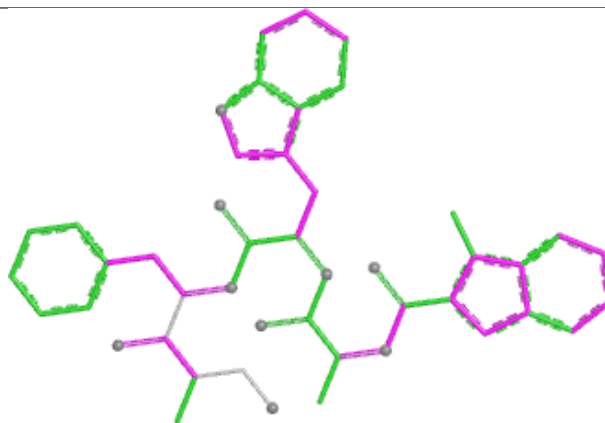
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	303	39V	5	0
17	Y	303	39V	10	0

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.

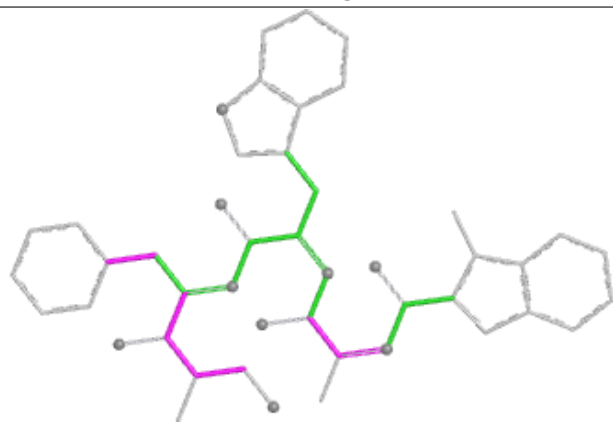
Ligand 39V K 303



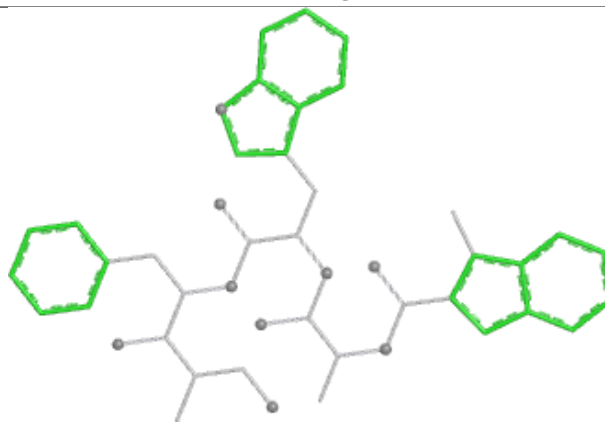
Bond lengths



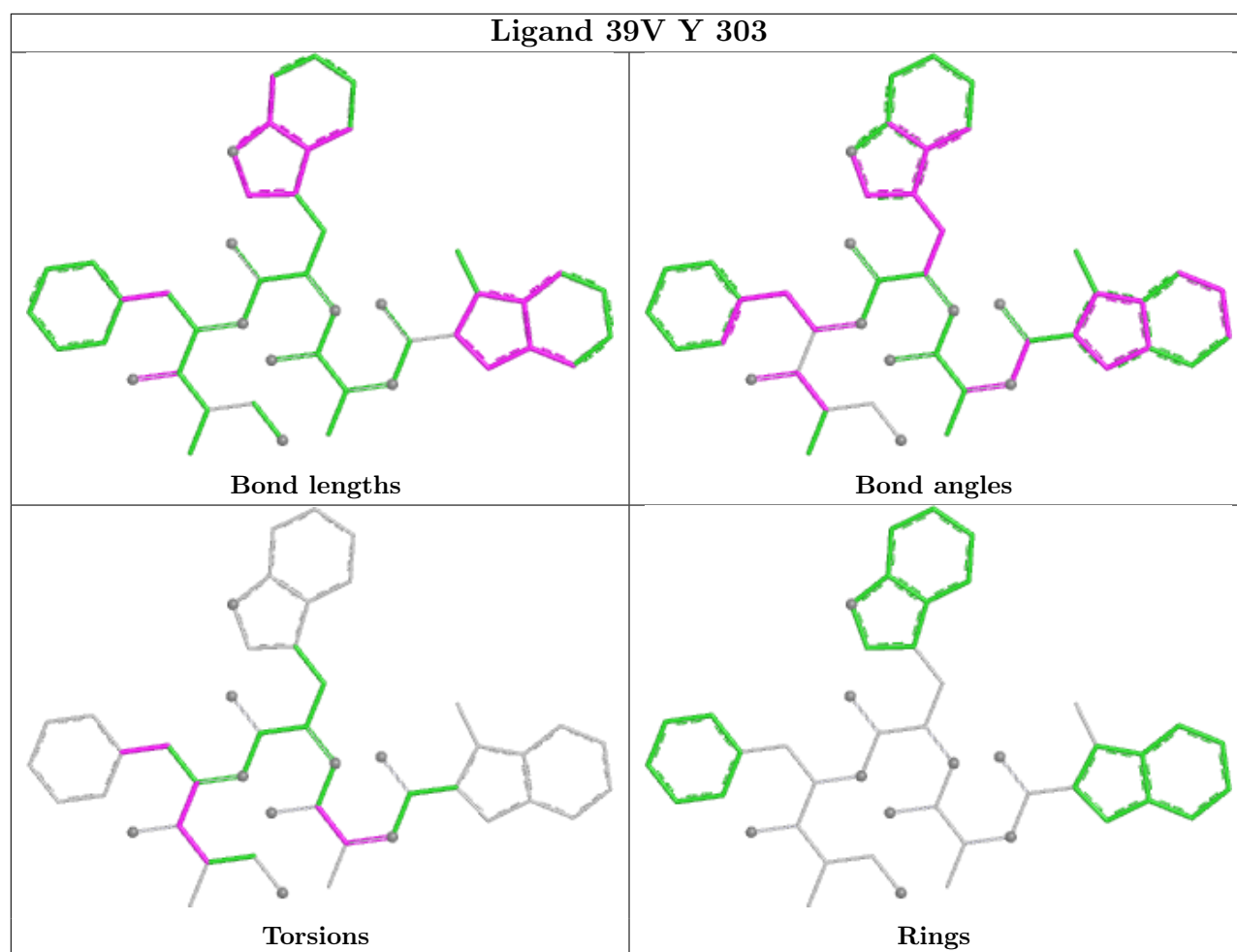
Bond angles



Torsions



Rings



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%)	-0.59	1 (0%) 88 84	40, 55, 90, 123	0
1	O	250/250 (100%)	-0.54	1 (0%) 88 84	41, 60, 97, 126	0
2	B	244/258 (94%)	-0.48	3 (1%) 76 68	39, 58, 103, 159	0
2	P	244/258 (94%)	-0.41	3 (1%) 76 68	40, 61, 114, 162	0
3	C	240/254 (94%)	-0.42	2 (0%) 82 75	42, 63, 123, 147	0
3	Q	240/254 (94%)	-0.28	3 (1%) 75 66	45, 72, 141, 154	0
4	D	235/260 (90%)	-0.47	0 100 100	44, 65, 96, 131	0
4	R	235/260 (90%)	-0.49	0 100 100	44, 67, 98, 143	0
5	E	231/234 (98%)	-0.42	0 100 100	45, 70, 100, 141	0
5	S	231/234 (98%)	-0.34	1 (0%) 88 84	41, 74, 108, 138	0
6	F	243/288 (84%)	-0.47	1 (0%) 88 84	42, 62, 105, 139	0
6	T	243/288 (84%)	-0.45	0 100 100	38, 64, 109, 133	0
7	G	241/252 (95%)	-0.55	0 100 100	34, 56, 93, 129	0
7	U	241/252 (95%)	-0.51	1 (0%) 88 84	39, 57, 89, 121	0
8	H	222/232 (95%)	-0.60	0 100 100	38, 54, 80, 124	0
8	V	222/232 (95%)	-0.60	0 100 100	41, 58, 82, 123	0
9	I	204/205 (99%)	-0.81	0 100 100	34, 49, 78, 112	0
9	W	204/205 (99%)	-0.72	0 100 100	36, 52, 77, 107	0
10	J	195/198 (98%)	-0.71	1 (0%) 87 82	36, 50, 77, 121	0
10	X	195/198 (98%)	-0.69	1 (0%) 87 82	37, 53, 79, 147	0
11	K	212/212 (100%)	-0.74	0 100 100	38, 52, 76, 102	0
11	Y	212/212 (100%)	-0.72	0 100 100	29, 53, 75, 104	0
12	L	222/222 (100%)	-0.67	0 100 100	37, 55, 83, 99	0
12	Z	222/222 (100%)	-0.67	0 100 100	37, 54, 77, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.68	2 (0%) 81 74	36, 54, 77, 109	0
13	a	233/246 (94%)	-0.69	2 (0%) 81 74	36, 52, 76, 108	0
14	N	196/196 (100%)	-0.73	0 100 100	38, 51, 76, 99	0
14	b	196/196 (100%)	-0.72	0 100 100	36, 51, 78, 103	0
All	All	6336/6614 (95%)	-0.57	22 (0%) 90 86	29, 58, 98, 162	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	4.8
2	P	219	ALA	3.9
3	Q	49	THR	3.6
1	A	1	MET	3.5
10	X	1	MET	3.4
3	Q	50	LEU	3.3
3	C	51	LYS	3.3
10	J	1	MET	3.2
1	O	1	MET	2.9
13	M	233	ILE	2.8
2	P	51	VAL	2.6
6	F	203	ASN	2.5
2	B	51	VAL	2.3
5	S	209	ASN	2.3
2	B	93	HIS	2.3
7	U	242	GLN	2.3
13	a	233	ILE	2.3
3	C	203	THR	2.3
13	M	1	THR	2.3
2	P	52	THR	2.2
3	Q	223	SER	2.2
13	a	1	THR	2.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

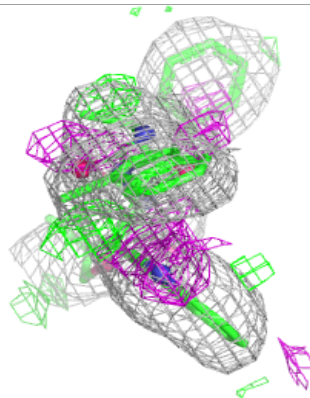
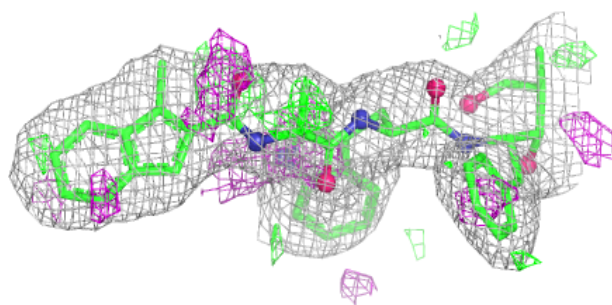
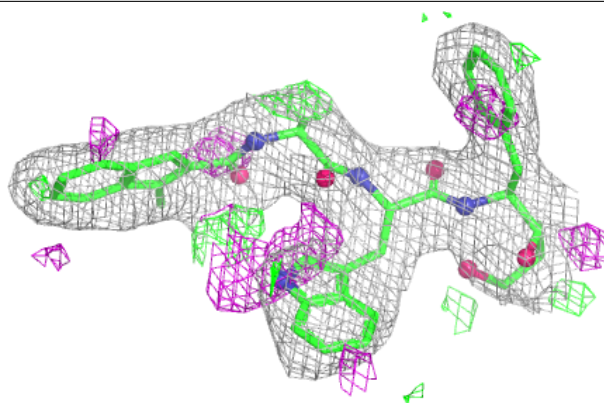
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	N	202	1/1	0.87	0.17	66,66,66,66	0
17	39V	K	303	46/46	0.91	0.10	37,48,65,67	0
17	39V	Y	303	46/46	0.92	0.10	39,50,70,74	0
16	MES	Y	302	12/12	0.95	0.10	66,70,73,75	0
16	MES	K	302	12/12	0.96	0.12	62,64,68,69	0
15	MG	V	301	1/1	0.97	0.06	67,67,67,67	0
15	MG	Z	301	1/1	0.98	0.03	58,58,58,58	0
15	MG	N	201	1/1	0.99	0.03	55,55,55,55	0
15	MG	G	301	1/1	0.99	0.04	52,52,52,52	0
15	MG	I	301	1/1	0.99	0.04	60,60,60,60	0
15	MG	K	301	1/1	0.99	0.04	64,64,64,64	0
15	MG	Y	301	1/1	1.00	0.04	48,48,48,48	0

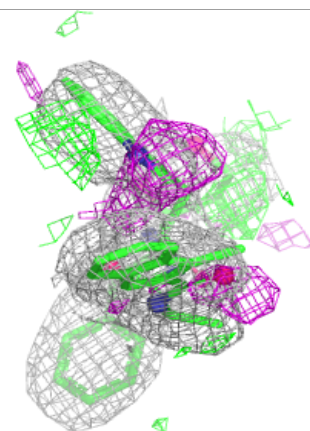
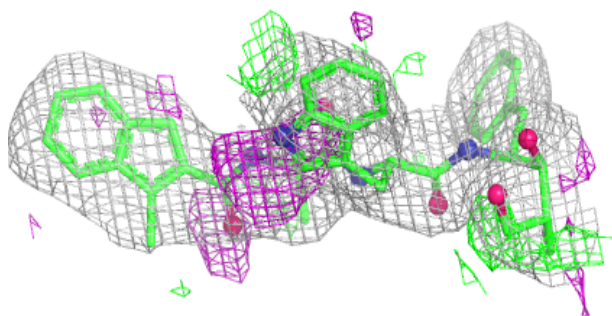
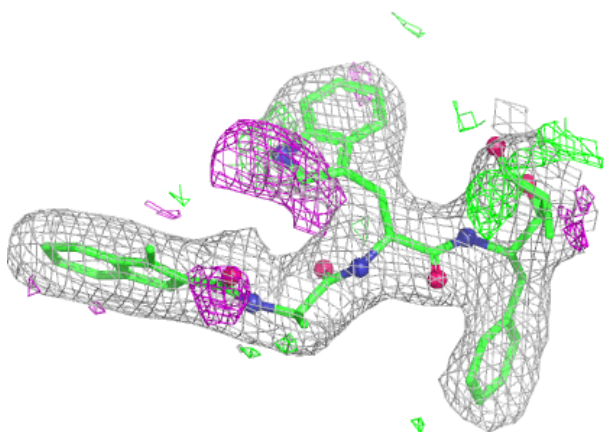
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 39V 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 39V 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.