



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:35 AM UTC

PDB ID : 4NO1 / pdb_00004no1
Title : yCP in complex with Z-Leu-Leu-Leu-B(OH)₂
Authors : Stein, M.L.; Cui, H.; Beck, P.; Dubiella, C.; Voss, C.; Krueger, A.; Schmidt, B.; Groll, M.
Deposited on : 2013-11-19
Resolution : 2.50 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:

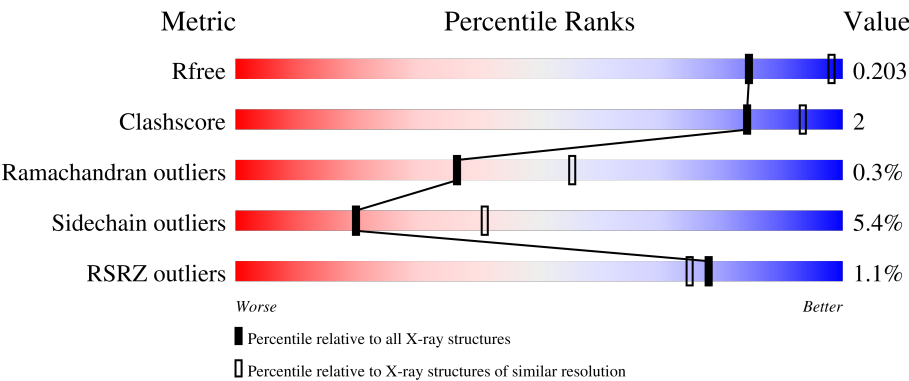
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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% 95% 5% • •
1	O	250	2% 94% 5% •
2	B	258	3% 84% 8% • 5%
2	P	258	4% 84% 8% • 5%
3	C	254	2% 85% 7% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 4% 84% 9% • 6%
4	D	260	 80% 9% • 10%
4	R	260	 80% 10% • 10%
5	E	234	 91% 7% ••
5	S	234	 91% 7% ••
6	F	288	 % 77% 6% • 16%
6	T	288	 2% 77% 7% • 16%
7	G	252	 87% 8% ••
7	U	252	 % 87% 8% ••
8	H	232	 89% 5% ••
8	V	232	 89% 6% ••
9	I	205	 90% 8% •
9	W	205	 90% 8% •
10	J	198	 % 90% 7% •••
10	X	198	 % 90% 7% •••
11	K	212	 88% 10% •
11	Y	212	 % 89% 9% •
12	L	222	 91% 8% •
12	Z	222	 91% 8% •
13	M	246	 87% 7% • 5%
13	a	246	 87% 6% • 5%
14	N	196	 % 92% 7% •
14	b	196	 % 92% 7% •

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50397 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).

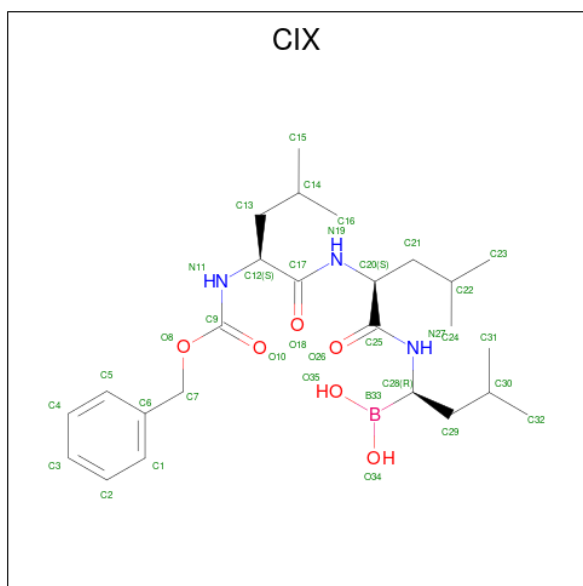
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		

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

- Molecule 16 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(1R)-1-(dihydroxyboranyl)-3-methylbutyl]-L-leucinamide (CCD ID: CIX) (formula: $C_{25}H_{42}BN_3O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total B C N O 35 1 25 3 6	0	0
16	Y	1	Total B C N O 35 1 25 3 6	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	39	Total O 39 39	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	41	Total O 41 41	0	0
17	C	34	Total O 34 34	0	0
17	D	19	Total O 19 19	0	0
17	E	23	Total O 23 23	0	0
17	F	35	Total O 35 35	0	0
17	G	42	Total O 42 42	0	0
17	H	41	Total O 41 41	0	0
17	I	37	Total O 37 37	0	0
17	J	36	Total O 36 36	0	0
17	K	48	Total O 48 48	0	0
17	L	47	Total O 47 47	0	0
17	M	49	Total O 49 49	0	0
17	N	42	Total O 42 42	0	0
17	O	26	Total O 26 26	0	0
17	P	21	Total O 21 21	0	0
17	Q	20	Total O 20 20	0	0
17	R	23	Total O 23 23	0	0
17	S	19	Total O 19 19	0	0
17	T	30	Total O 30 30	0	0
17	U	49	Total O 49 49	0	0
17	V	43	Total O 43 43	0	0

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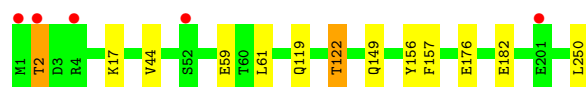
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	33	Total 33	O 33	0	0
17	X	40	Total 40	O 40	0	0
17	Y	34	Total 34	O 34	0	0
17	Z	44	Total 44	O 44	0	0
17	a	55	Total 55	O 55	0	0
17	b	53	Total 53	O 53	0	0

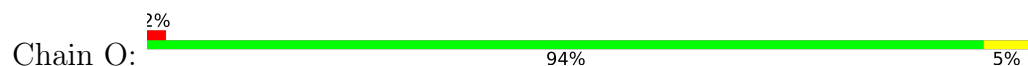
3 Residue-property plots [i](#)

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

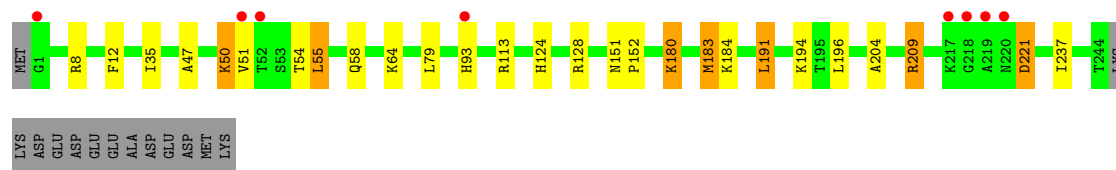
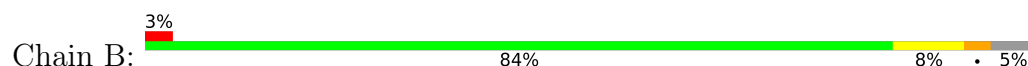
- Molecule 1: Proteasome subunit alpha type-2



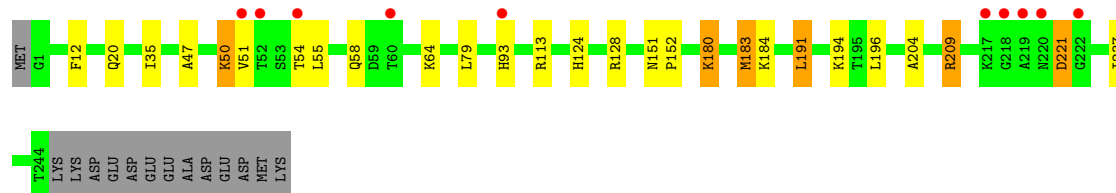
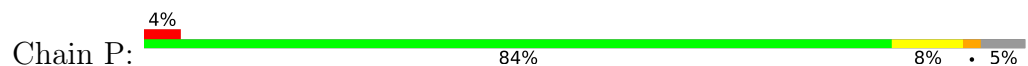
- Molecule 1: Proteasome subunit alpha type-2



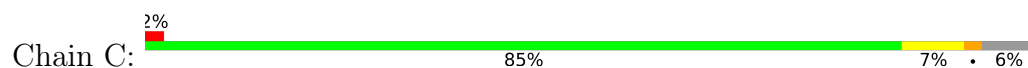
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

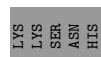
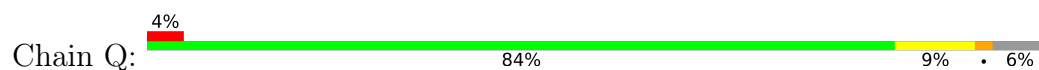


- Molecule 3: Proteasome subunit alpha type-4

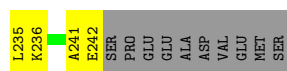
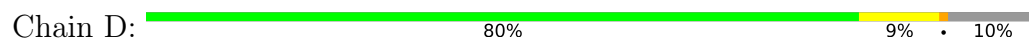




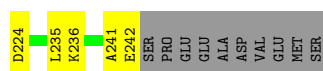
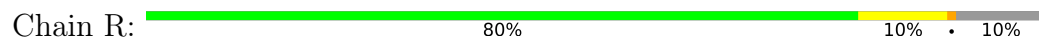
- Molecule 3: Proteasome subunit alpha type-4



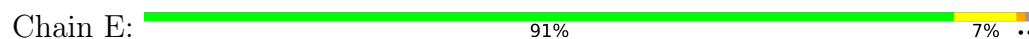
- Molecule 4: Proteasome subunit alpha type-5



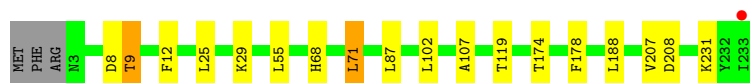
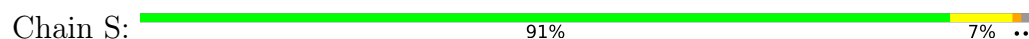
- Molecule 4: Proteasome subunit alpha type-5



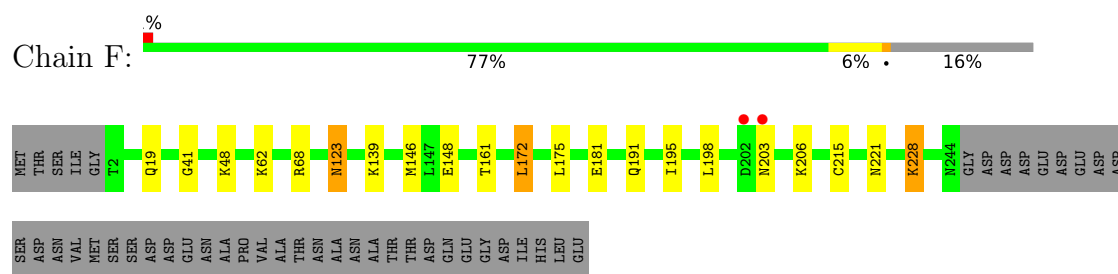
- Molecule 5: Proteasome subunit alpha type-6



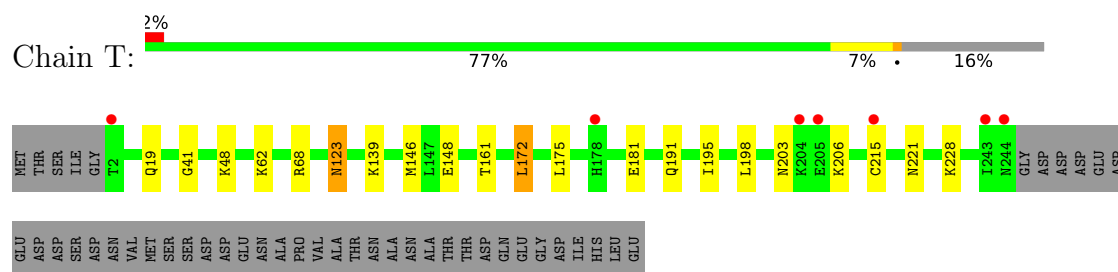
- Molecule 5: Proteasome subunit alpha type-6



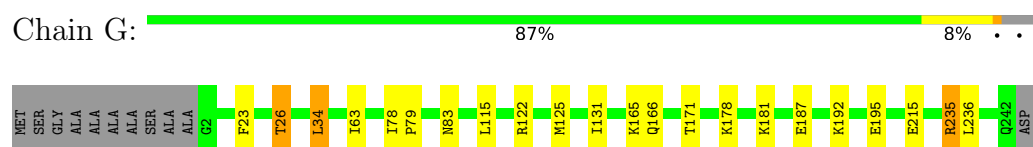
- Molecule 6: Probable proteasome subunit alpha type-7



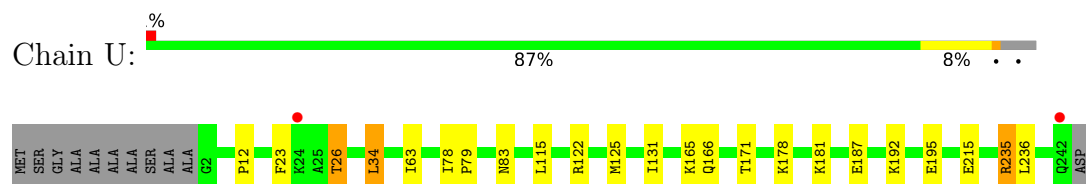
- Molecule 6: Probable proteasome subunit alpha type-7



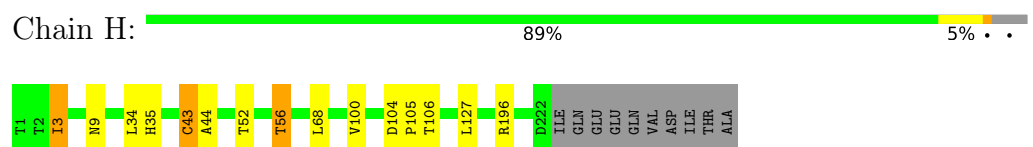
- Molecule 7: Proteasome subunit alpha type-1



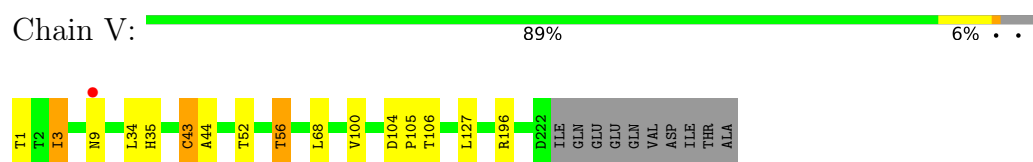
- Molecule 7: Proteasome subunit alpha type-1



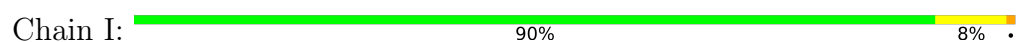
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3

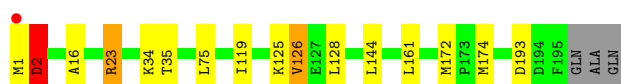
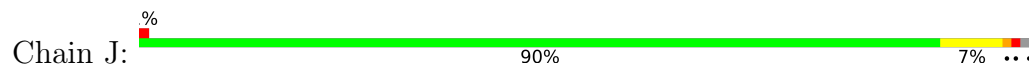




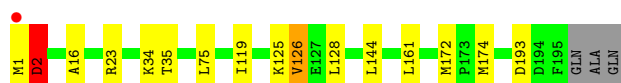
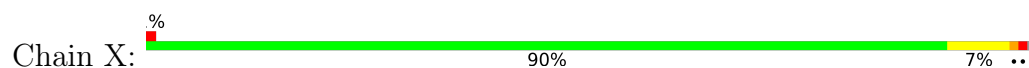
- Molecule 9: Proteasome subunit beta type-3



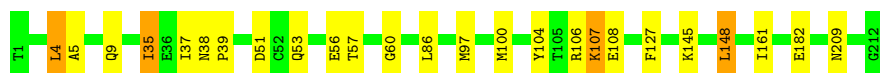
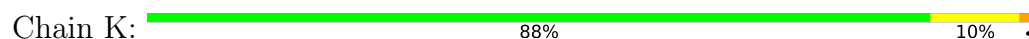
- Molecule 10: Proteasome subunit beta type-4



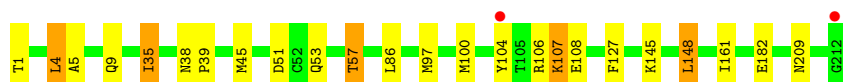
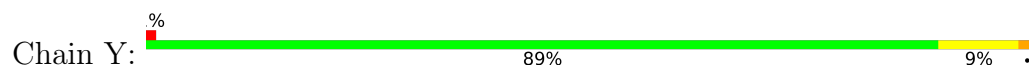
- Molecule 10: Proteasome subunit beta type-4



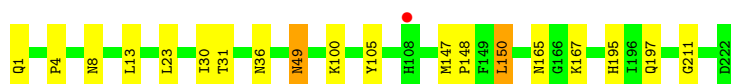
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5

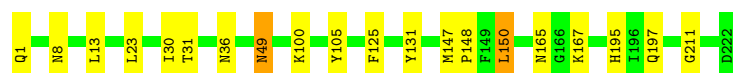


- Molecule 12: Proteasome subunit beta type-6



- Molecule 12: Proteasome subunit beta type-6

Chain Z:  91% 8% .



- Molecule 13: Proteasome subunit beta type-7

Chain M:  87% 7% . 5%



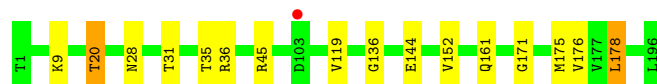
- Molecule 13: Proteasome subunit beta type-7

Chain a:  87% 6% . 5%



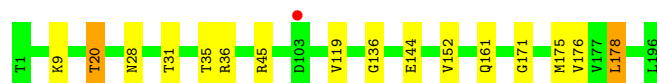
- Molecule 14: Proteasome subunit beta type-1

Chain N:  92% 7% .



- Molecule 14: Proteasome subunit beta type-1

Chain b:  92% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.44Å 301.33Å 144.91Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.50) 98.4 (15.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.214 (Not available) , 0.203	Depositor DCC
R_{free} test set	17905 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50397	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: CIX, MG

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	0.41	0/1952	0.70	0/2642
1	O	0.41	0/1952	0.70	0/2642
2	B	0.41	0/1934	0.72	0/2618
2	P	0.41	0/1934	0.72	0/2618
3	C	0.42	0/1910	0.74	0/2586
3	Q	0.42	0/1910	0.74	0/2586
4	D	0.41	0/1837	0.68	0/2475
4	R	0.41	0/1837	0.68	0/2475
5	E	0.40	0/1800	0.69	0/2433
5	S	0.40	0/1800	0.69	0/2433
6	F	0.41	0/1932	0.72	0/2609
6	T	0.41	0/1932	0.72	0/2609
7	G	0.40	0/1945	0.70	0/2634
7	U	0.40	0/1945	0.70	0/2634
8	H	0.39	0/1715	0.68	0/2326
8	V	0.39	0/1715	0.68	0/2326
9	I	0.38	0/1611	0.70	0/2174
9	W	0.38	0/1611	0.70	0/2174
10	J	0.40	0/1589	0.68	0/2142
10	X	0.39	0/1589	0.68	0/2142
11	K	0.39	0/1681	0.68	0/2274
11	Y	0.39	0/1681	0.68	0/2274
12	L	0.39	0/1795	0.68	0/2420
12	Z	0.39	0/1795	0.68	0/2420
13	M	0.41	0/1855	0.70	0/2514
13	a	0.41	0/1855	0.70	0/2514
14	N	0.38	0/1541	0.69	0/2087
14	b	0.38	0/1541	0.69	0/2087
All	All	0.40	0/50194	0.70	0/67868

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	13	0
3	C	1881	0	1895	13	0
3	Q	1881	0	1895	14	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	9	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	9	0
6	T	1892	0	1883	9	0
7	G	1907	0	1901	8	0
7	U	1907	0	1901	9	0
8	H	1684	0	1688	5	0
8	V	1684	0	1688	7	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	8	0
10	J	1561	0	1569	6	0
10	X	1561	0	1569	5	0
11	K	1644	0	1594	15	0
11	Y	1644	0	1594	15	0
12	L	1757	0	1711	10	0
12	Z	1757	0	1711	11	0
13	M	1824	0	1832	8	0
13	a	1824	0	1832	7	0
14	N	1512	0	1481	10	0
14	b	1512	0	1481	10	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	K	35	0	42	0	0
16	Y	35	0	42	1	0
17	A	39	0	0	0	0
17	B	41	0	0	0	0
17	C	34	0	0	0	0
17	D	19	0	0	0	0
17	E	23	0	0	0	0
17	F	35	0	0	1	0
17	G	42	0	0	0	0
17	H	41	0	0	0	0
17	I	37	0	0	0	0
17	J	36	0	0	0	0
17	K	48	0	0	1	0
17	L	47	0	0	0	0
17	M	49	0	0	0	0
17	N	42	0	0	1	0
17	O	26	0	0	0	0
17	P	21	0	0	0	0
17	Q	20	0	0	1	0
17	R	23	0	0	0	0
17	S	19	0	0	0	0
17	T	30	0	0	1	0
17	U	49	0	0	0	0
17	V	43	0	0	0	0
17	W	33	0	0	0	0
17	X	40	0	0	0	0
17	Y	34	0	0	0	0
17	Z	44	0	0	0	0
17	a	55	0	0	0	0
17	b	53	0	0	1	0
All	All	50397	0	49150	231	0

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

All (231) 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:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.51	0.93
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.52	0.92
3:C:202:GLN:HG3	3:C:203:THR:H	1.35	0.89
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.35	0.89
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.68	0.74
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.69	0.74
4:R:241:ALA:O	4:R:242:GLU:HB2	1.88	0.73
8:H:3:ILE:HG12	8:H:44:ALA:HB1	1.71	0.73
4:D:241:ALA:O	4:D:242:GLU:HB2	1.88	0.72
8:V:3:ILE:HG12	8:V:44:ALA:HB1	1.72	0.71
2:P:50:LYS:HE3	2:P:50:LYS:HA	1.72	0.71
2:B:50:LYS:HE3	2:B:50:LYS:HA	1.72	0.70
11:K:53:GLN:O	11:K:57:THR:HG23	1.92	0.69
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.93	0.68
14:b:152:VAL:HA	14:b:175:MET:HE1	1.75	0.68
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.75	0.67
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.76	0.67
14:N:152:VAL:HA	14:N:175:MET:HE1	1.75	0.66
3:C:51:LYS:O	3:C:52:LEU:HB2	1.98	0.63
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.97	0.63
14:N:20:THR:HG22	14:N:31:THR:OG1	2.01	0.61
7:G:23:PHE:O	7:G:26:THR:HB	2.01	0.60
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.65	0.60
14:b:35:THR:HG21	14:b:45:ARG:HE	1.66	0.60
10:X:1:MET:O	10:X:2:ASP:HB2	2.01	0.60
14:N:35:THR:HG21	14:N:45:ARG:HE	1.67	0.60
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.65	0.59
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.84	0.59
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.65	0.59
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.84	0.59
14:b:20:THR:HG22	14:b:31:THR:OG1	2.01	0.59
7:U:23:PHE:O	7:U:26:THR:HB	2.02	0.59
3:C:201:VAL:O	3:C:202:GLN:HB2	2.04	0.58
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.66	0.58
10:J:1:MET:O	10:J:2:ASP:HB2	2.02	0.58
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.86	0.57
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.04	0.57
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.35	0.57
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.87	0.57
6:T:146:MET:HE3	6:T:161:THR:HB	1.87	0.56
6:F:146:MET:HE3	6:F:161:THR:HB	1.87	0.56
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.87	0.55
14:b:35:THR:HG22	17:b:201:HOH:O	2.07	0.55
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.89	0.55
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.89	0.55
14:b:20:THR:HG23	14:b:28:ASN:HB3	1.89	0.54
14:N:35:THR:HG22	17:N:302:HOH:O	2.08	0.54
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.90	0.54
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.89	0.54
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.72	0.54
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.90	0.54
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.89	0.54
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.73	0.53
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.73	0.53
2:B:12:PHE:H	3:C:17:GLN:HE22	1.55	0.53
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.90	0.53
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.35	0.53
5:E:12:PHE:H	6:F:19:GLN:HE22	1.55	0.53
9:I:98:ARG:O	9:I:126:ILE:HD11	2.09	0.53
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.90	0.53
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.74	0.53
13:a:128:ARG:HH11	13:a:138:SER:HB2	1.74	0.53
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.73	0.52
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.75	0.52
4:D:91:HIS:CG	4:D:99:ILE:HB	2.44	0.52
5:E:9:THR:HG21	5:E:119:THR:HA	1.91	0.52
5:S:9:THR:HG21	5:S:119:THR:HA	1.91	0.52
9:W:98:ARG:O	9:W:126:ILE:HD11	2.10	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.92	0.51
5:E:71:LEU:C	5:E:71:LEU:HD23	2.35	0.51
13:M:128:ARG:HH11	13:M:138:SER:HB2	1.75	0.51
5:S:12:PHE:H	6:T:19:GLN:HE22	1.57	0.51
4:R:91:HIS:CG	4:R:99:ILE:HB	2.45	0.51
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.76	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.51
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.76	0.51
5:S:71:LEU:C	5:S:71:LEU:HD23	2.36	0.51
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.92	0.51
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.93	0.51
9:I:37:ASN:ND2	11:Y:209:ASN:O	2.44	0.50
11:Y:1:THR:HB	16:Y:301:CIX:O35	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:209:ASN:O	9:W:37:ASN:ND2	2.45	0.50
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.50
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.94	0.50
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.94	0.50
2:B:180:LYS:O	2:B:183:MET:HB2	2.12	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.93	0.49
14:b:35:THR:CG2	14:b:45:ARG:HE	2.26	0.49
12:L:165:ASN:CG	12:L:165:ASN:O	2.55	0.49
6:F:123:ASN:C	6:F:123:ASN:HD22	2.20	0.49
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.95	0.49
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.95	0.49
12:Z:165:ASN:CG	12:Z:165:ASN:O	2.55	0.49
3:C:202:GLN:HG3	3:C:203:THR:N	2.16	0.48
2:P:180:LYS:O	2:P:183:MET:HB2	2.12	0.48
12:L:8:ASN:HA	12:L:30:ILE:O	2.14	0.48
14:N:35:THR:CG2	14:N:45:ARG:HE	2.26	0.48
2:B:204:ALA:O	2:B:209:ARG:NH2	2.47	0.48
6:T:123:ASN:C	6:T:123:ASN:HD22	2.21	0.48
2:P:204:ALA:O	2:P:209:ARG:NH2	2.48	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.49	0.47
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.97	0.47
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.96	0.47
6:F:228:LYS:HB2	6:F:228:LYS:HE3	1.71	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.47
11:Y:104:TYR:CD1	11:Y:182:GLU:HA	2.49	0.47
11:K:104:TYR:CD1	11:K:182:GLU:HA	2.49	0.47
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.50	0.47
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.47
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.16	0.46
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.46
6:F:19:GLN:NE2	17:F:323:HOH:O	2.49	0.46
11:K:5:ALA:HB3	11:K:100:MET:CE	2.46	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.46	0.45
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.47	0.45
6:T:19:GLN:NE2	17:T:327:HOH:O	2.47	0.45
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.47	0.45
6:F:175:LEU:HD21	6:F:191:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:27:LEU:HB2	13:a:192:SER:HB3	1.99	0.45
1:O:119:GLN:O	1:O:122:THR:HB	2.17	0.45
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.98	0.45
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.64	0.45
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.99	0.45
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.99	0.44
6:T:175:LEU:HD21	6:T:191:GLN:NE2	2.32	0.44
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.47	0.44
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.98	0.44
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.99	0.44
3:C:168:THR:O	3:C:171:GLU:HB3	2.18	0.44
1:A:149:GLN:O	1:A:156:TYR:HA	2.18	0.44
12:L:195:HIS:HD2	12:L:197:GLN:H	1.65	0.44
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.18	0.44
7:U:63:ILE:HD12	7:U:215:GLU:HG2	2.00	0.44
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.53	0.44
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.00	0.44
7:G:34:LEU:C	7:G:34:LEU:HD23	2.42	0.44
12:L:4:PRO:O	13:M:104:ARG:NH1	2.47	0.44
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.98	0.44
11:K:51:ASP:HB3	11:K:97:MET:HE2	1.99	0.44
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.33	0.44
1:A:119:GLN:O	1:A:122:THR:HB	2.17	0.43
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.00	0.43
4:R:138:GLY:HA2	4:R:214:ILE:HG12	2.01	0.43
3:C:201:VAL:HG13	3:C:202:GLN:N	2.33	0.43
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.99	0.43
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.01	0.43
7:U:34:LEU:C	7:U:34:LEU:HD23	2.42	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.43
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.48	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
6:T:41:GLY:HA3	6:T:215:CYS:O	2.19	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.43
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.00	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.01	0.43
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.48	0.43
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.54	0.43
1:O:149:GLN:O	1:O:156:TYR:HA	2.18	0.43
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.43
10:X:1:MET:HA	10:X:34:LYS:CE	2.49	0.43
7:G:63:ILE:HD12	7:G:215:GLU:HG2	2.01	0.43
9:I:65:MET:HE1	9:I:93:SER:HB3	1.99	0.43
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.66	0.43
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.01	0.43
4:D:138:GLY:HA2	4:D:214:ILE:HG12	2.01	0.42
11:K:104:TYR:CD1	11:K:104:TYR:C	2.97	0.42
9:W:65:MET:HE1	9:W:93:SER:HB3	2.00	0.42
2:B:183:MET:HE1	2:B:191:LEU:HD12	2.01	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
6:F:48:LYS:HG2	6:F:62:LYS:HD2	2.02	0.42
5:E:68:HIS:HE1	5:E:102:LEU:O	2.01	0.42
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.00	0.42
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.01	0.42
11:Y:51:ASP:HB3	11:Y:97:MET:HE2	1.99	0.42
11:Y:104:TYR:CD1	11:Y:104:TYR:C	2.96	0.42
6:F:41:GLY:HA3	6:F:215:CYS:O	2.19	0.42
2:P:183:MET:HE1	2:P:191:LEU:HD12	2.02	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.01	0.42
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.34	0.42
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.68	0.42
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.02	0.41
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.68	0.41
8:H:35:HIS:HB3	8:H:56:THR:HG21	2.02	0.41
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.85	0.41
4:R:99:ILE:HD11	4:R:104:LEU:CB	2.45	0.41
10:J:1:MET:HA	10:J:34:LYS:CE	2.49	0.41
3:C:161:THR:HG21	3:C:169:VAL:HG22	2.03	0.41
8:H:43:CYS:SG	8:H:100:VAL:HG22	2.60	0.41
11:K:86:LEU:HD13	11:K:86:LEU:C	2.45	0.41
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.46	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.55	0.41
3:Q:120:GLN:NE2	17:Q:305:HOH:O	2.53	0.41
8:V:43:CYS:SG	8:V:100:VAL:HG22	2.60	0.41
10:X:119:ILE:HG12	10:X:125:LYS:HG3	2.02	0.41
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.02	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.03	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.55	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.41
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:PHE:CD1	5:E:178:PHE:C	2.99	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.56	0.41
3:Q:161:THR:HG21	3:Q:169:VAL:HG22	2.03	0.41
8:V:52:THR:O	8:V:56:THR:HB	2.20	0.41
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.85	0.41
8:H:52:THR:O	8:H:56:THR:HB	2.20	0.41
11:K:35:ILE:HG21	11:K:56:GLU:HB3	2.03	0.41
13:M:43:ILE:O	13:M:43:ILE:HG12	2.20	0.41
1:O:12:PHE:H	2:P:20:GLN:HE22	1.67	0.40
5:S:178:PHE:CD1	5:S:178:PHE:C	2.99	0.40
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.36	0.40
10:J:23:ARG:HD3	17:K:405:HOH:O	2.20	0.40
12:L:147:MET:N	12:L:148:PRO:HD2	2.36	0.40
6:T:146:MET:CE	6:T:161:THR:HB	2.51	0.40
8:V:1:THR:CG2	8:V:3:ILE:HD12	2.51	0.40
10:J:119:ILE:HG12	10:J:125:LYS:HG3	2.03	0.40
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.04	0.40
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.52	0.40
13:a:43:ILE:O	13:a:43:ILE:HG12	2.20	0.40
6:T:48:LYS:HG2	6:T:62:LYS:HD2	2.03	0.40
11:Y:35:ILE:HB	11:Y:45:MET:HE3	2.04	0.40
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	2.04	0.40
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.57	0.40
13:a:48:ASN:H	13:a:48:ASN:HD22	1.70	0.40
13:a:97:ALA:HA	13:a:130:VAL:HG21	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%)	240 (97%)	7 (3%)	1 (0%)	30 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	49
2	B	242/258 (94%)	233 (96%)	6 (2%)	3 (1%)	10	20
2	P	242/258 (94%)	233 (96%)	6 (2%)	3 (1%)	10	20
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	31
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	31
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%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	220/232 (95%)	212 (96%)	7 (3%)	1 (0%)	24	43
8	V	220/232 (95%)	212 (96%)	7 (3%)	1 (0%)	24	43
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	43
10	X	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	24	43
11	K	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
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%)	6101 (97%)	159 (2%)	16 (0%)	36	55

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL

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Mol	Chain	Res	Type
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
1	A	2	THR
3	C	205	ALA
1	O	2	THR
3	Q	205	ALA
8	H	9	ASN
8	V	9	ASN
2	B	221	ASP
2	P	221	ASP
2	B	183	MET
2	P	183	MET

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	51
1	O	209/209 (100%)	200 (96%)	9 (4%)	26	51
2	B	203/216 (94%)	191 (94%)	12 (6%)	18	37
2	P	203/216 (94%)	191 (94%)	12 (6%)	18	37
3	C	212/226 (94%)	197 (93%)	15 (7%)	13	29
3	Q	212/226 (94%)	197 (93%)	15 (7%)	13	29
4	D	194/215 (90%)	176 (91%)	18 (9%)	8	18
4	R	194/215 (90%)	176 (91%)	18 (9%)	8	18
5	E	190/193 (98%)	179 (94%)	11 (6%)	18	38
5	S	190/193 (98%)	179 (94%)	11 (6%)	18	38
6	F	201/239 (84%)	190 (94%)	11 (6%)	19	40
6	T	201/239 (84%)	190 (94%)	11 (6%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	206/210 (98%)	193 (94%)	13 (6%)	16	34
7	U	206/210 (98%)	193 (94%)	13 (6%)	16	34
8	H	181/190 (95%)	173 (96%)	8 (4%)	25	50
8	V	181/190 (95%)	173 (96%)	8 (4%)	25	50
9	I	172/173 (99%)	164 (95%)	8 (5%)	23	47
9	W	172/173 (99%)	164 (95%)	8 (5%)	23	47
10	J	173/175 (99%)	164 (95%)	9 (5%)	21	42
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	42
11	K	169/169 (100%)	163 (96%)	6 (4%)	31	58
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	53
12	L	185/185 (100%)	180 (97%)	5 (3%)	39	67
12	Z	185/185 (100%)	180 (97%)	5 (3%)	39	67
13	M	199/208 (96%)	187 (94%)	12 (6%)	17	36
13	a	199/208 (96%)	187 (94%)	12 (6%)	17	36
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	57
14	b	162/162 (100%)	156 (96%)	6 (4%)	30	57
All	All	5312/5540 (96%)	5025 (95%)	287 (5%)	20	41

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	44	VAL
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	182	GLU
1	A	250	LEU
2	B	50	LYS
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	180	LYS

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Mol	Chain	Res	Type
2	B	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	209	ARG
2	B	221	ASP
2	B	237	ILE
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	52	LEU
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	200	VAL
3	C	213	VAL
3	C	239	GLN
4	D	1	ASP
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	102	GLU
4	D	117	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	224	ASP
4	D	235	LEU
4	D	236	LYS
5	E	8	ASP
5	E	9	THR
5	E	25	LEU

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Mol	Chain	Res	Type
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	174	THR
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	231	LYS
6	F	68	ARG
6	F	123	ASN
6	F	139	LYS
6	F	148	GLU
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	228	LYS
7	G	26	THR
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	165	LYS
7	G	166	GLN
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	3	ILE
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	106	THR
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE

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Mol	Chain	Res	Type
9	I	133	LYS
9	I	170	LEU
9	I	171	LEU
9	I	182	TRP
9	I	191	LYS
9	I	192	ASP
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	126	VAL
10	J	144	LEU
10	J	172	MET
10	J	174	MET
10	J	193	ASP
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
11	K	107	LYS
11	K	148	LEU
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	138	SER
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	36	ARG
14	N	119	VAL

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Mol	Chain	Res	Type
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	17	LYS
1	O	44	VAL
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	182	GLU
1	O	250	LEU
2	P	50	LYS
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	209	ARG
2	P	221	ASP
2	P	237	ILE
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	52	LEU
3	Q	61	LYS
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	200	VAL
3	Q	213	VAL
3	Q	239	GLN
4	R	1	ASP
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	102	GLU
4	R	117	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	224	ASP
4	R	235	LEU
4	R	236	LYS
5	S	8	ASP
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	174	THR
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	231	LYS
6	T	68	ARG
6	T	123	ASN
6	T	139	LYS
6	T	148	GLU
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	228	LYS
7	U	26	THR
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET

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Mol	Chain	Res	Type
7	U	165	LYS
7	U	166	GLN
7	U	171	THR
7	U	178	LYS
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	3	ILE
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	106	THR
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	133	LYS
9	W	170	LEU
9	W	171	LEU
9	W	182	TRP
9	W	191	LYS
9	W	192	ASP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	126	VAL
10	X	144	LEU
10	X	172	MET
10	X	174	MET
10	X	193	ASP
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	106	ARG
11	Y	107	LYS
11	Y	148	LEU
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	138	SER
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	36	ARG
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 (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	226	GLN
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	228	ASN
3	C	233	GLN

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Mol	Chain	Res	Type
4	D	15	GLN
4	D	100	ASN
4	D	106	GLN
4	D	160	ASN
4	D	217	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
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
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	175	ASN
7	G	186	ASN
8	H	57	GLN
8	H	66	HIS
8	H	86	HIS
8	H	194	ASN
9	I	37	ASN
10	J	55	GLN
10	J	61	GLN
10	J	63	ASN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	1	GLN

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Mol	Chain	Res	Type
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	80	ASN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	48	ASN
13	M	108	ASN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	226	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	228	ASN
3	Q	233	GLN
4	R	15	GLN
4	R	100	ASN
4	R	106	GLN
4	R	160	ASN
4	R	217	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN

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Mol	Chain	Res	Type
5	S	116	GLN
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	27	ASN
7	U	30	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	175	ASN
7	U	186	ASN
7	U	212	ASN
8	V	57	GLN
8	V	66	HIS
8	V	141	HIS
9	W	37	ASN
10	X	55	GLN
10	X	63	ASN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	94	GLN
12	Z	158	ASN
12	Z	165	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	102	GLN

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Mol	Chain	Res	Type
13	a	108	ASN
14	b	38	HIS
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	CIX	Y	301	11	31,35,35	1.01	1 (3%)	41,46,46	1.20	5 (12%)
16	CIX	K	301	11	31,35,35	0.99	1 (3%)	41,46,46	1.21	5 (12%)

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	CIX	Y	301	11	-	4/36/41/41	0/1/1/1
16	CIX	K	301	11	-	4/36/41/41	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	CIX	C7-C6	-4.16	1.40	1.50
16	K	301	CIX	C7-C6	-4.08	1.41	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	CIX	O8-C9-N11	4.38	119.82	110.45
16	K	301	CIX	O8-C9-N11	4.37	119.80	110.45
16	Y	301	CIX	O10-C9-N11	-3.04	119.88	124.86
16	K	301	CIX	O10-C9-N11	-2.98	119.97	124.86
16	Y	301	CIX	C21-C20-C25	-2.40	104.90	110.59
16	K	301	CIX	C21-C20-C25	-2.33	105.06	110.59
16	K	301	CIX	C13-C12-C17	-2.14	105.51	110.59
16	K	301	CIX	O8-C9-O10	-2.10	120.23	124.26
16	Y	301	CIX	O8-C9-O10	-2.06	120.31	124.26
16	Y	301	CIX	C13-C12-C17	-2.05	105.73	110.59

There are no chirality outliers.

All (8) torsion outliers are listed below:

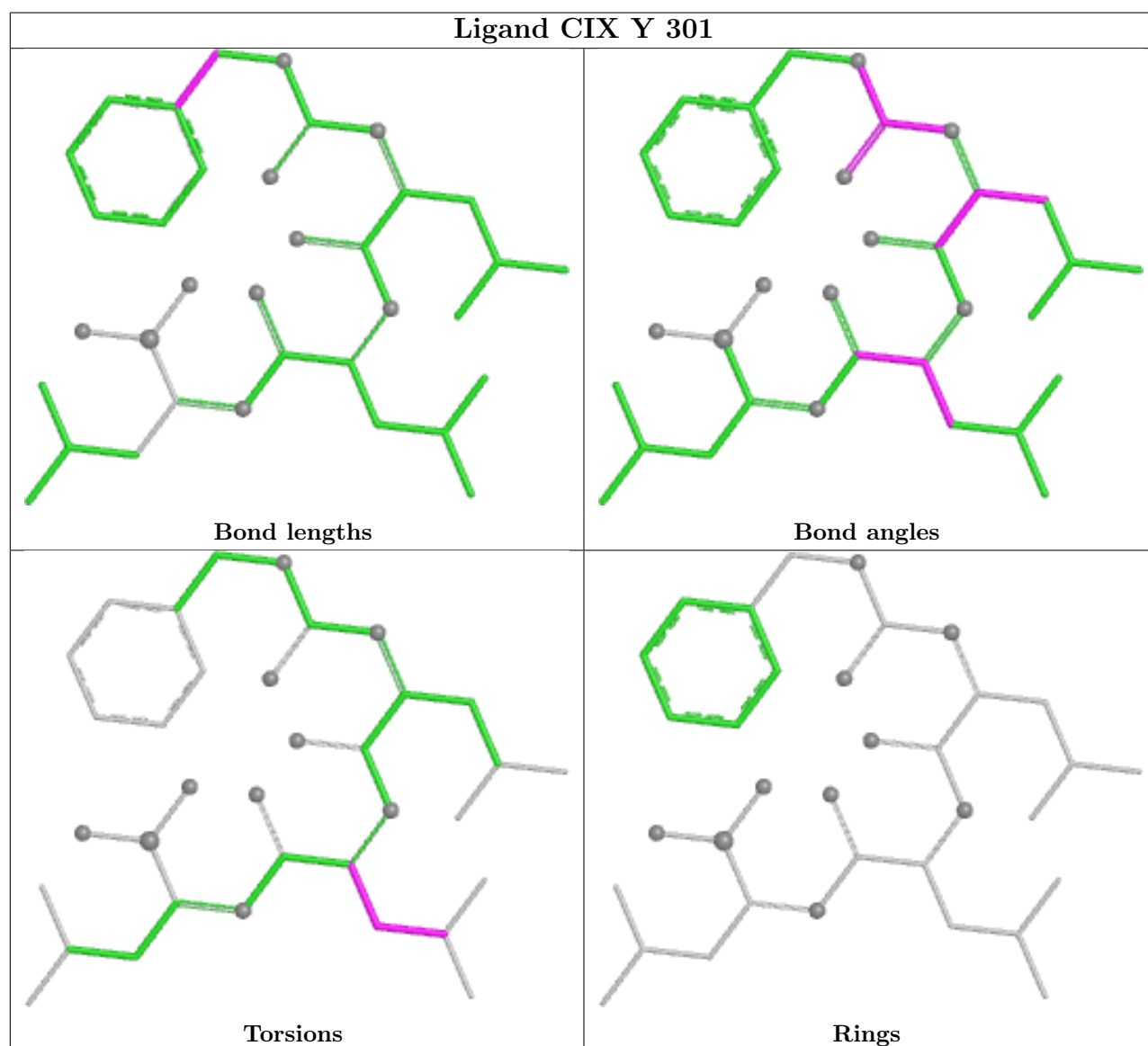
Mol	Chain	Res	Type	Atoms
16	K	301	CIX	C20-C21-C22-C23
16	Y	301	CIX	C20-C21-C22-C23
16	K	301	CIX	C20-C21-C22-C24
16	Y	301	CIX	C20-C21-C22-C24
16	Y	301	CIX	N19-C20-C21-C22
16	K	301	CIX	N19-C20-C21-C22
16	Y	301	CIX	C25-C20-C21-C22
16	K	301	CIX	C25-C20-C21-C22

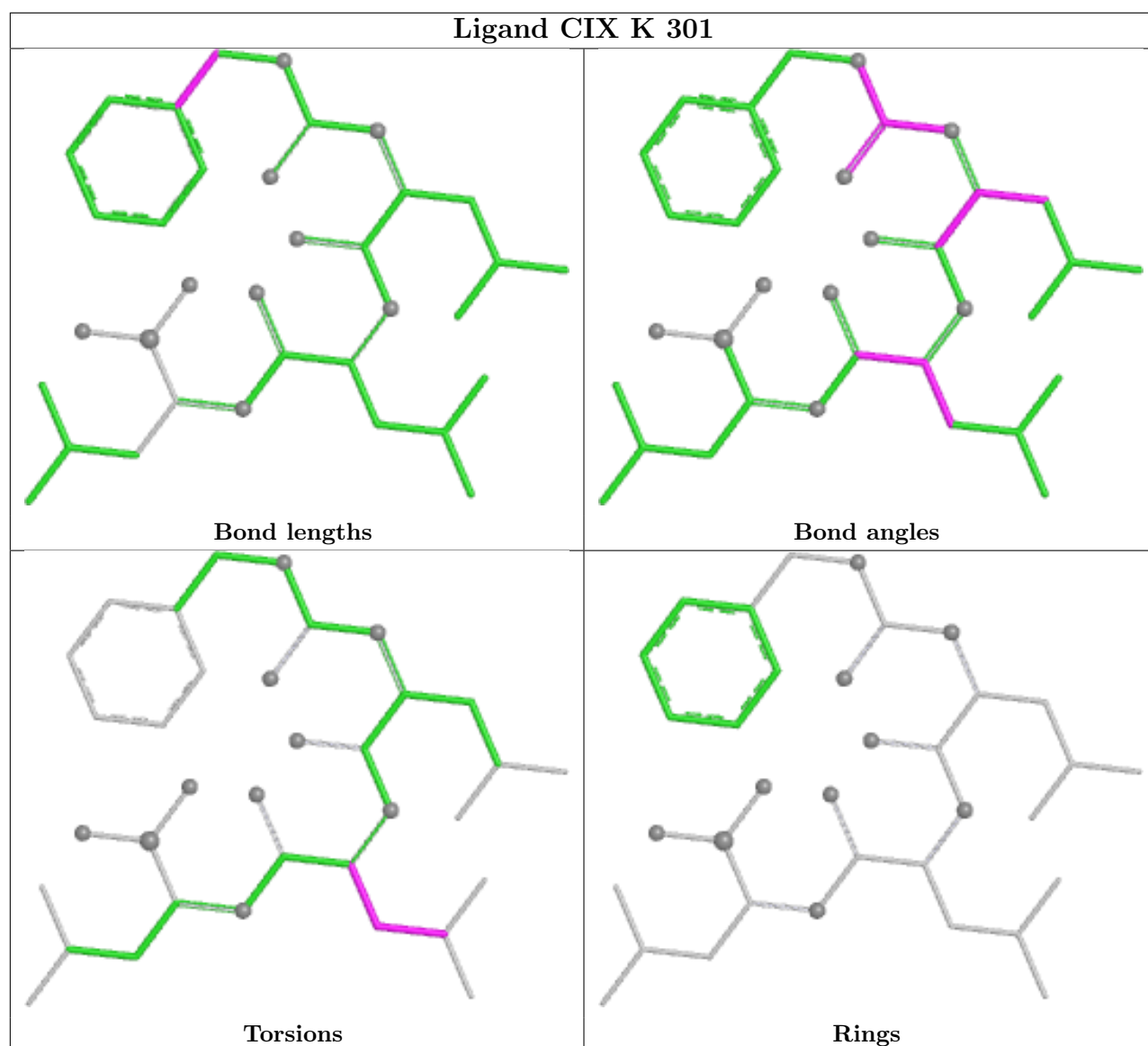
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	301	CIX	1	0

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





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%)	-0.31	5 (2%) 65 61	29, 44, 78, 117	0
1	O	250/250 (100%)	-0.27	4 (1%) 70 67	34, 48, 89, 115	0
2	B	244/258 (94%)	-0.15	8 (3%) 49 45	31, 47, 90, 141	0
2	P	244/258 (94%)	-0.13	10 (4%) 41 37	30, 50, 96, 150	0
3	C	240/254 (94%)	-0.13	5 (2%) 63 59	28, 50, 111, 135	0
3	Q	240/254 (94%)	-0.05	10 (4%) 40 36	30, 55, 119, 157	0
4	D	235/260 (90%)	-0.29	0 100 100	32, 49, 78, 118	0
4	R	235/260 (90%)	-0.29	0 100 100	37, 52, 79, 117	0
5	E	231/234 (98%)	-0.25	1 (0%) 88 86	29, 51, 79, 122	0
5	S	231/234 (98%)	-0.22	1 (0%) 88 86	36, 52, 81, 108	0
6	F	243/288 (84%)	-0.32	2 (0%) 82 80	30, 46, 87, 122	0
6	T	243/288 (84%)	-0.27	7 (2%) 53 49	31, 49, 87, 116	0
7	G	241/252 (95%)	-0.32	0 100 100	28, 43, 78, 133	0
7	U	241/252 (95%)	-0.33	2 (0%) 82 80	33, 45, 74, 110	0
8	H	222/232 (95%)	-0.41	0 100 100	29, 42, 68, 97	0
8	V	222/232 (95%)	-0.44	1 (0%) 87 85	32, 44, 66, 107	0
9	I	204/205 (99%)	-0.54	1 (0%) 87 85	28, 41, 65, 99	0
9	W	204/205 (99%)	-0.50	1 (0%) 87 85	28, 42, 69, 109	0
10	J	195/198 (98%)	-0.48	1 (0%) 87 85	30, 42, 67, 118	0
10	X	195/198 (98%)	-0.48	1 (0%) 87 85	30, 43, 66, 125	0
11	K	212/212 (100%)	-0.40	0 100 100	30, 43, 72, 96	0
11	Y	212/212 (100%)	-0.38	2 (0%) 81 78	28, 44, 74, 96	0
12	L	222/222 (100%)	-0.52	1 (0%) 87 85	30, 43, 65, 86	0
12	Z	222/222 (100%)	-0.48	0 100 100	28, 43, 68, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.54	1 (0%) 88 86	27, 41, 58, 69	0
13	a	233/246 (94%)	-0.55	1 (0%) 88 86	27, 41, 58, 70	0
14	N	196/196 (100%)	-0.53	1 (0%) 87 85	30, 38, 61, 90	0
14	b	196/196 (100%)	-0.54	1 (0%) 87 85	28, 39, 62, 86	0
All	All	6336/6614 (95%)	-0.35	67 (1%) 78 75	27, 45, 80, 157	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	4.8
10	X	1	MET	4.7
2	B	219	ALA	4.6
2	P	218	GLY	4.5
10	J	1	MET	4.3
3	C	206	LYS	4.3
3	Q	205	ALA	4.2
2	B	218	GLY	4.1
1	A	1	MET	3.8
3	Q	50	LEU	3.7
6	T	205	GLU	3.6
3	C	205	ALA	3.6
13	a	1	THR	3.6
2	P	51	VAL	3.5
7	U	242	GLN	3.4
13	M	1	THR	3.4
6	F	202	ASP	3.3
2	B	220	ASN	3.3
1	O	1	MET	3.3
9	W	1	SER	3.2
2	P	93	HIS	3.2
2	B	93	HIS	3.1
1	A	2	THR	3.1
6	T	243	ILE	3.1
2	B	52	THR	3.0
1	O	2	THR	2.9
14	b	103	ASP	2.9
3	Q	240	GLU	2.9
2	P	52	THR	2.9
9	I	1	SER	2.8
2	B	51	VAL	2.8
3	Q	51	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
7	U	24	LYS	2.7
1	O	53	SER	2.6
3	Q	201	VAL	2.6
1	O	4	ARG	2.5
3	Q	204	GLY	2.5
1	A	52	SER	2.5
3	C	203	THR	2.5
1	A	201	GLU	2.5
12	L	108	HIS	2.5
2	P	220	ASN	2.4
3	Q	203	THR	2.4
2	B	1	GLY	2.4
8	V	9	ASN	2.3
11	Y	212	GLY	2.2
14	N	103	ASP	2.2
2	P	217	LYS	2.2
1	A	4	ARG	2.2
2	B	217	LYS	2.2
3	C	48	SER	2.2
3	C	240	GLU	2.2
2	P	222	GLY	2.2
11	Y	104	TYR	2.2
3	Q	239	GLN	2.1
6	T	244	ASN	2.1
6	T	2	THR	2.1
2	P	60	THR	2.1
6	T	215	CYS	2.1
5	E	209	ASN	2.1
2	P	54	THR	2.1
5	S	233	ILE	2.1
6	F	203	ASN	2.0
6	T	178	HIS	2.0
3	Q	236	GLN	2.0
3	Q	206	LYS	2.0
6	T	204	LYS	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

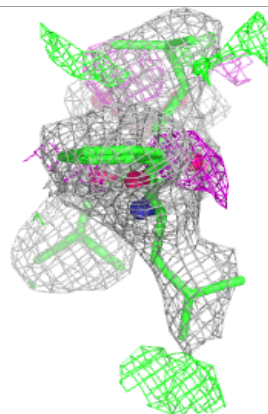
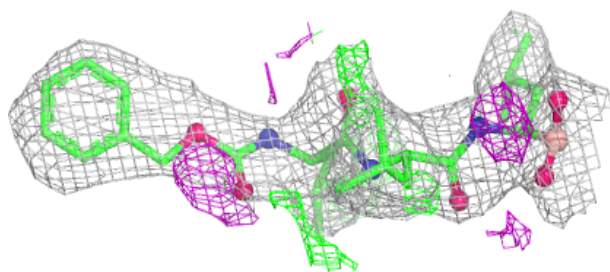
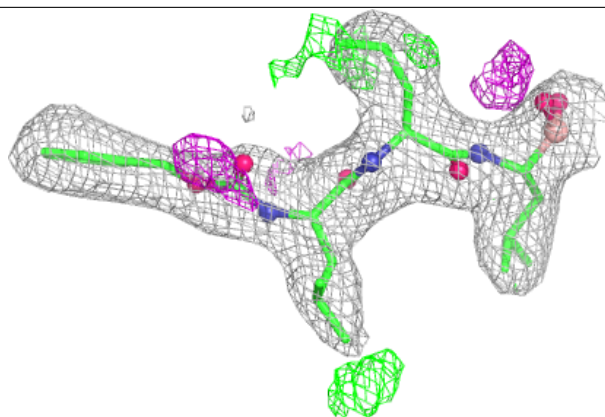
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	CIX	Y	301	35/35	0.85	0.14	55,70,88,90	0
16	CIX	K	301	35/35	0.86	0.14	34,69,95,98	0
15	MG	Z	301	1/1	0.91	0.08	68,68,68,68	0
15	MG	I	301	1/1	0.93	0.18	65,65,65,65	0
15	MG	H	301	1/1	0.96	0.08	60,60,60,60	0
15	MG	N	201	1/1	0.97	0.04	42,42,42,42	0
15	MG	Y	302	1/1	0.98	0.10	42,42,42,42	0
15	MG	K	302	1/1	0.98	0.07	42,42,42,42	0
15	MG	G	301	1/1	0.99	0.04	44,44,44,44	0
15	MG	V	301	1/1	1.00	0.04	48,48,48,48	0

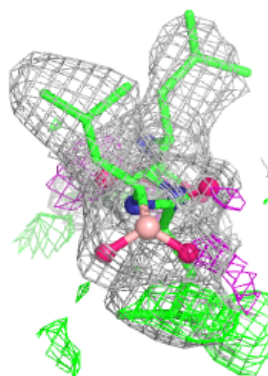
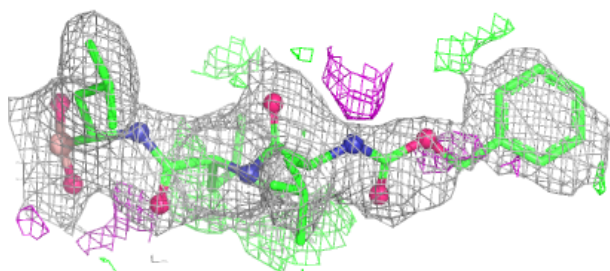
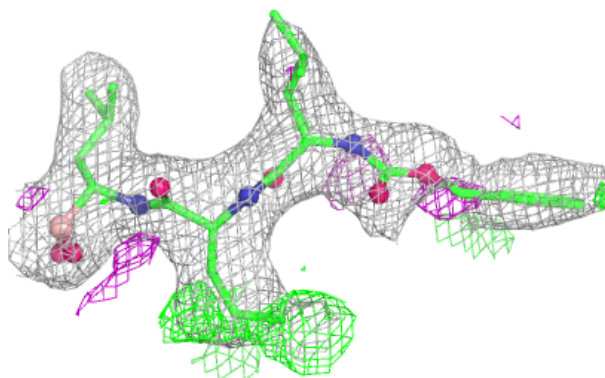
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CIX Y 301:

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

**Electron density around CIX K 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.