Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:50 PM UTC

PDB ID	:	4NO9 / pdb_00004no9
Title	:	yCP in complex with Z-Leu-Leu-Leu-epoxyketone
Authors	:	Stein, M.L.; Cui, H.; Beck, P.; Dubiella, C.; Voss, C.; Krueger, A.; Schmidt, B.; Groll, M.
Deposited on	:	2013-11-19
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

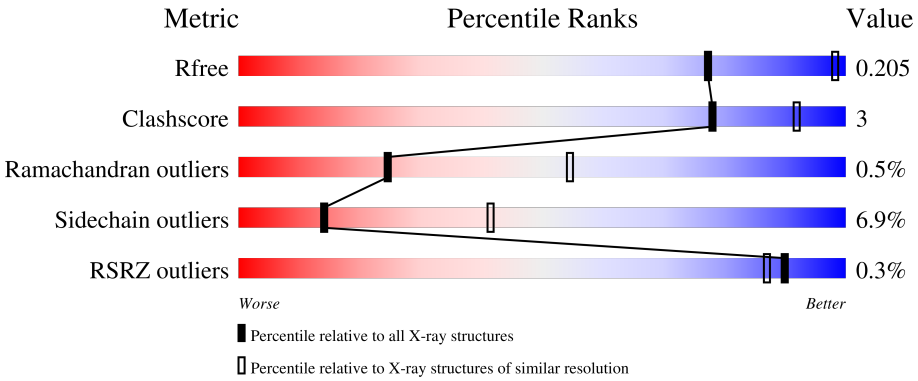
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 13% • 5%
2	P	258	81% 11% • 5%
3	C	254	81% 9% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	2% 81% 9% 6%
4	D	260	76% 13% 10%
4	R	260	75% 14% 10%
5	E	234	84% 13%
5	S	234	84% 13%
6	F	288	76% 7% 16%
6	T	288	75% 8% 16%
7	G	252	86% 8%
7	U	252	85% 9%
8	H	232	85% 9%
8	V	232	84% 10%
9	I	205	90% 9%
9	W	205	90% 10%
10	J	198	% 89% 7%
10	X	198	% 90% 7%
11	K	212	87% 13%
11	Y	212	87% 12%
12	L	222	91% 8%
12	Z	222	90% 9%
13	M	246	86% 7% 5%
13	a	246	85% 9% 5%
14	N	196	90% 10%
14	b	196	90% 10%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49622 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
			1642	1044	280	311	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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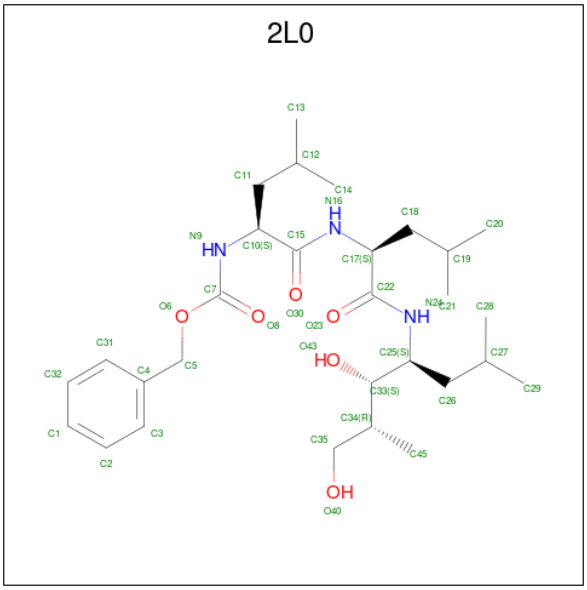
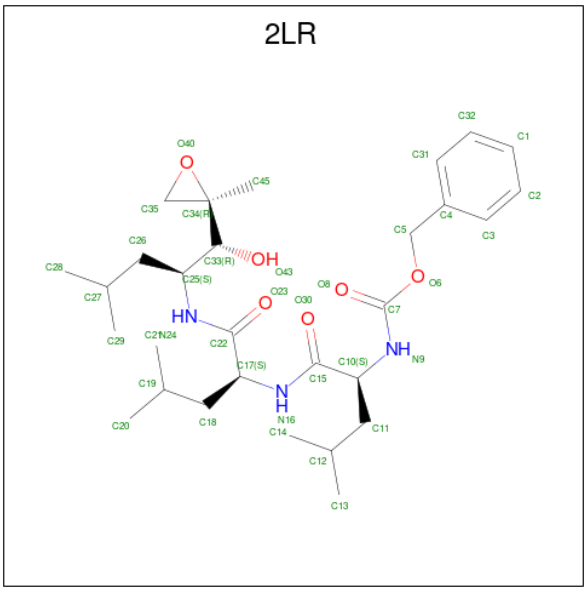
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	I	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-leucinamide (CCD ID: 2L0) (formula: $C_{29}H_{49}N_3O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	H	1	Total C N O 38 29 3 6	0	0
16	K	1	Total C N O 38 29 3 6	0	0
16	Y	1	Total C N O 38 29 3 6	0	0

- Molecule 17 is N-[(benzyloxy)carbonyl]-L-leucyl-N-{(1R,2S)-1-hydroxy-4-methyl-1-[(2R)-2-methyloxiran-2-yl]pentan-2-yl}-L-leucinamide (CCD ID: 2LR) (formula: $C_{29}H_{47}N_3O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	V	1	Total C N O 38 29 3 6	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	3	Total O 3 3	0	0
18	B	4	Total O 4 4	0	0
18	C	1	Total O 1 1	0	0
18	D	4	Total O 4 4	0	0
18	E	2	Total O 2 2	0	0
18	F	6	Total O 6 6	0	0
18	G	6	Total O 6 6	0	0
18	H	7	Total O 7 7	0	0
18	I	5	Total O 5 5	0	0
18	J	10	Total O 10 10	0	0
18	K	12	Total O 12 12	0	0

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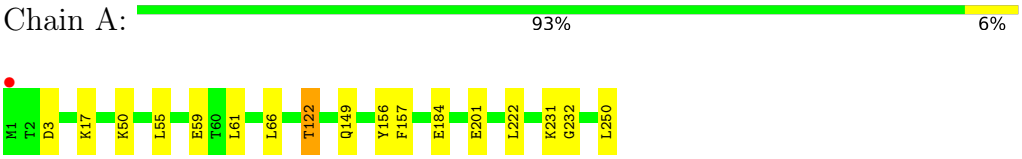
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	L	11	Total O 11 11	0	0
18	M	13	Total O 13 13	0	0
18	N	7	Total O 7 7	0	0
18	O	4	Total O 4 4	0	0
18	P	1	Total O 1 1	0	0
18	Q	1	Total O 1 1	0	0
18	R	4	Total O 4 4	0	0
18	S	2	Total O 2 2	0	0
18	T	6	Total O 6 6	0	0
18	U	11	Total O 11 11	0	0
18	V	7	Total O 7 7	0	0
18	W	3	Total O 3 3	0	0
18	X	9	Total O 9 9	0	0
18	Y	10	Total O 10 10	0	0
18	Z	2	Total O 2 2	0	0
18	a	8	Total O 8 8	0	0
18	b	9	Total O 9 9	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.

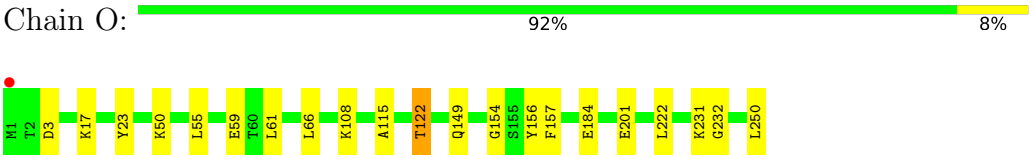
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



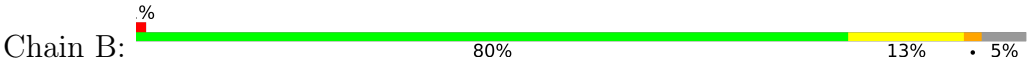
• Molecule 1: Proteasome subunit alpha type-2

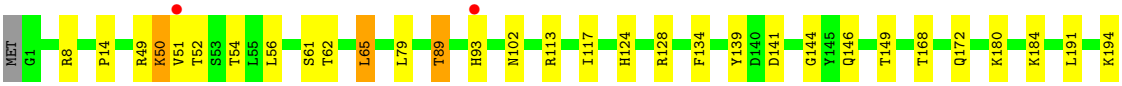
Chain O:



• Molecule 2: Proteasome subunit alpha type-3

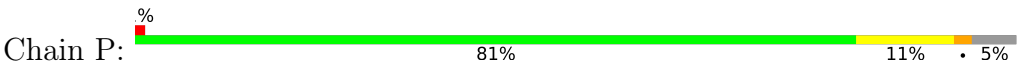
Chain B:

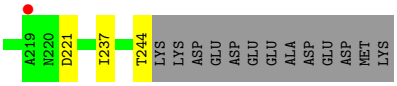




• Molecule 2: Proteasome subunit alpha type-3

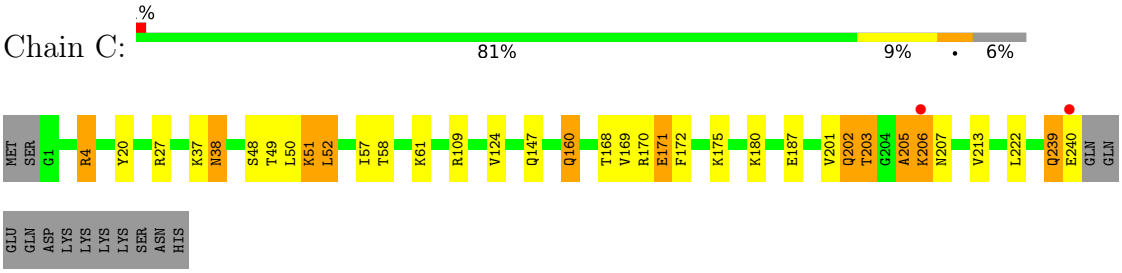
Chain P:





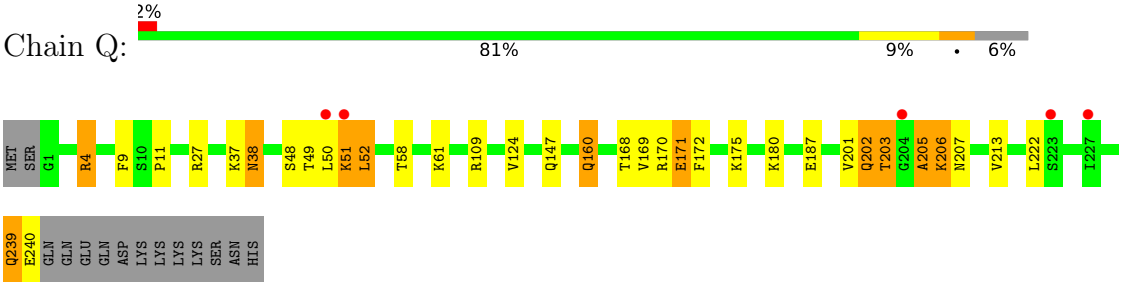
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



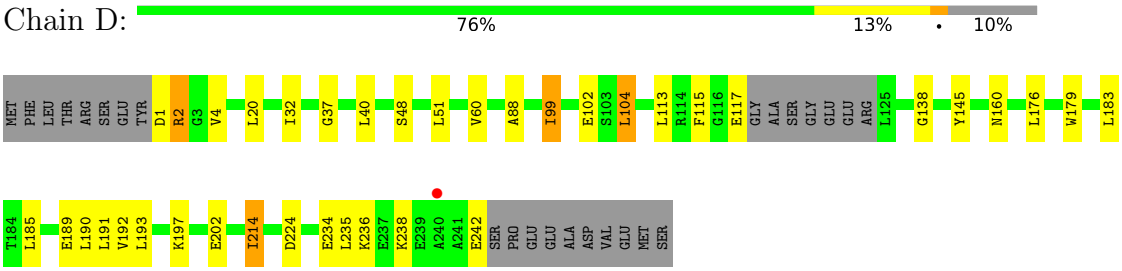
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



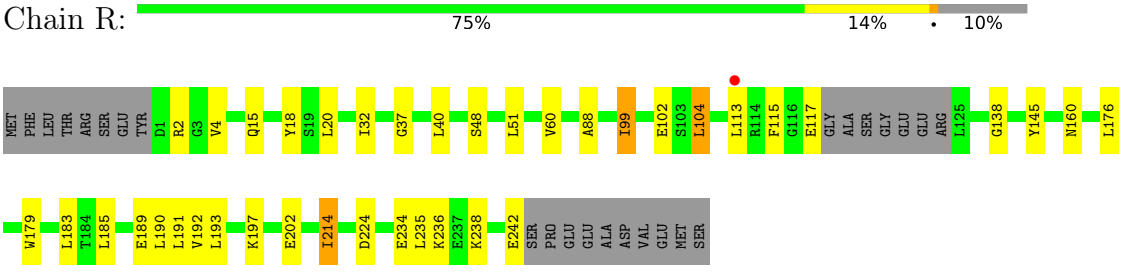
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



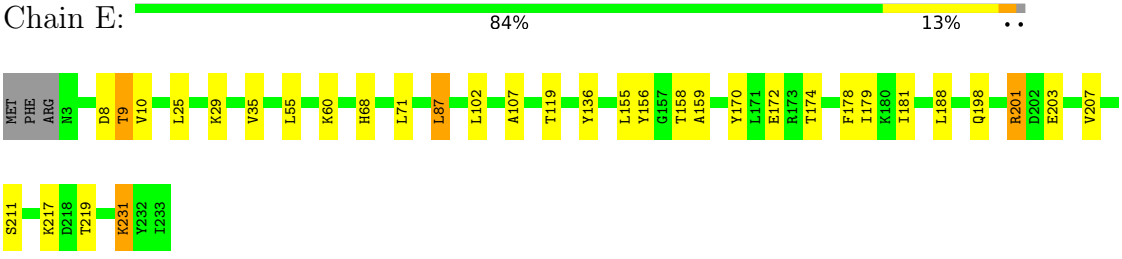
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



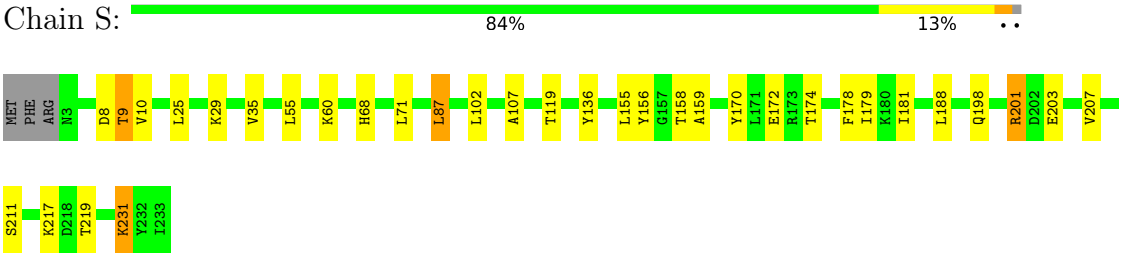
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



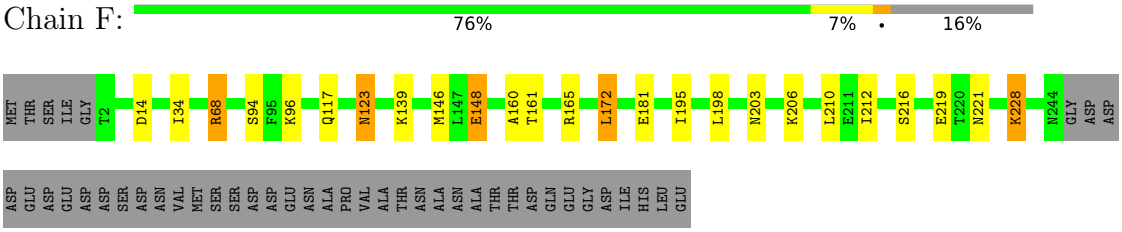
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



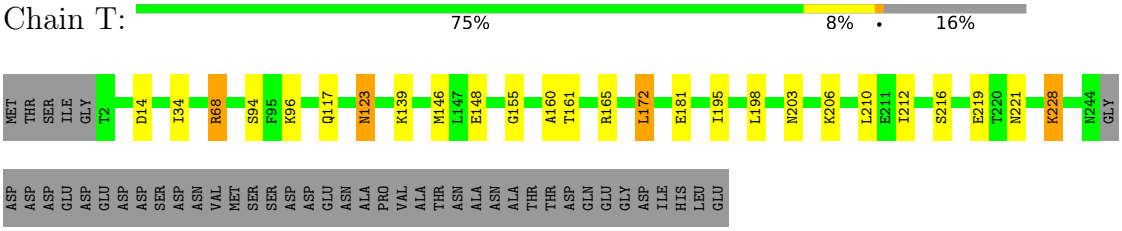
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



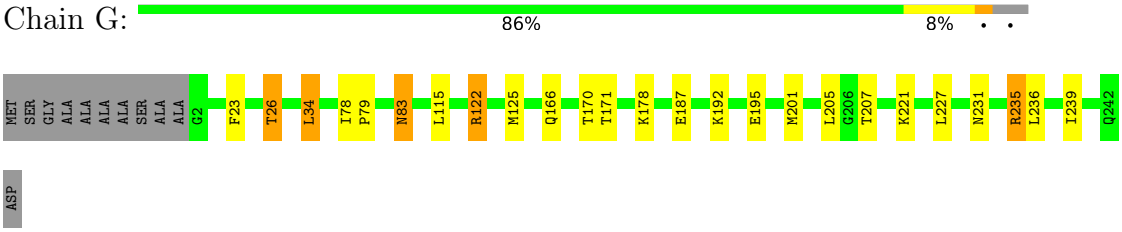
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



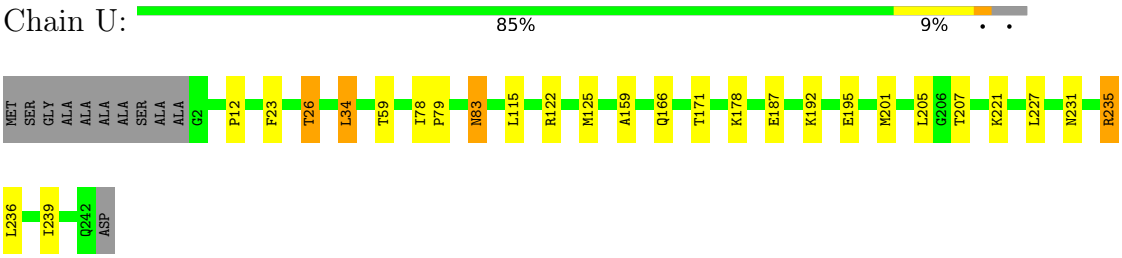
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



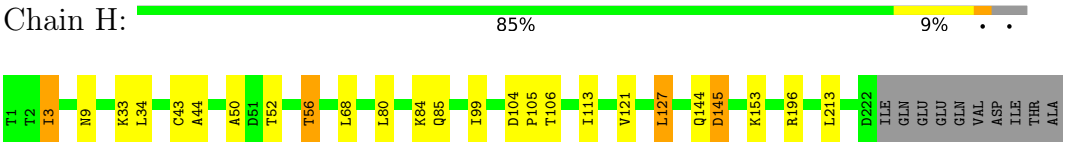
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



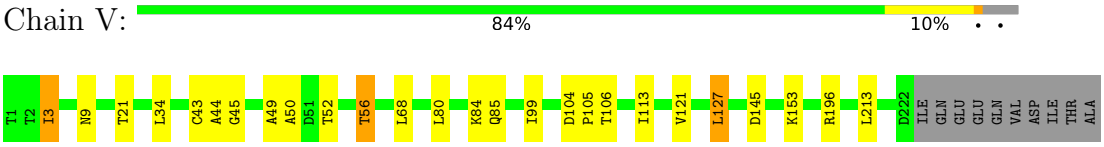
• Molecule 8: Proteasome subunit beta type-2

Chain H:



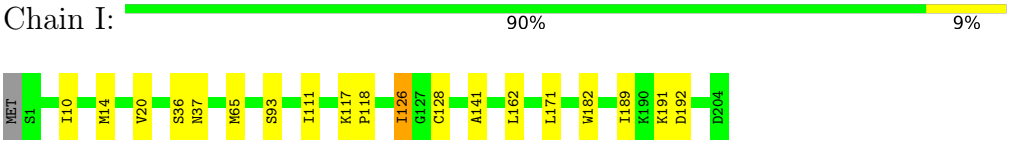
• Molecule 8: Proteasome subunit beta type-2

Chain V:



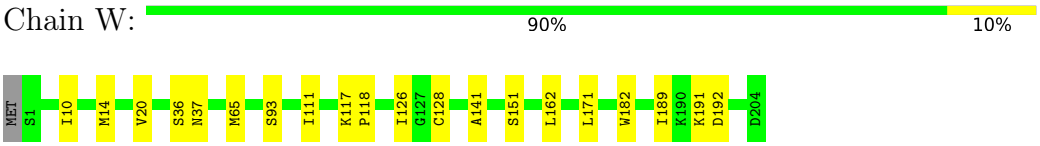
• Molecule 9: Proteasome subunit beta type-3

Chain I:



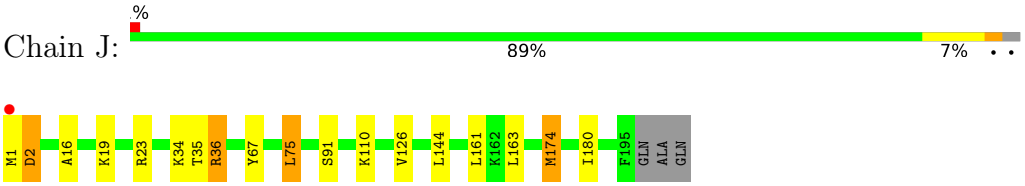
• Molecule 9: Proteasome subunit beta type-3

Chain W:



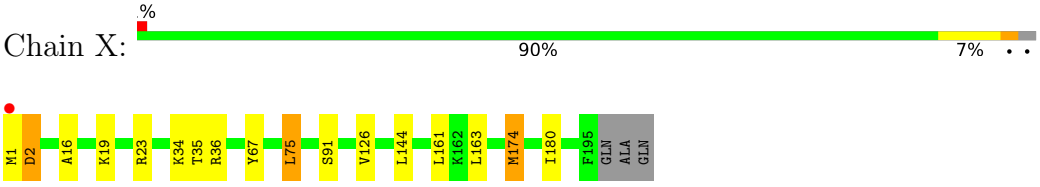
• Molecule 10: Proteasome subunit beta type-4

Chain J:



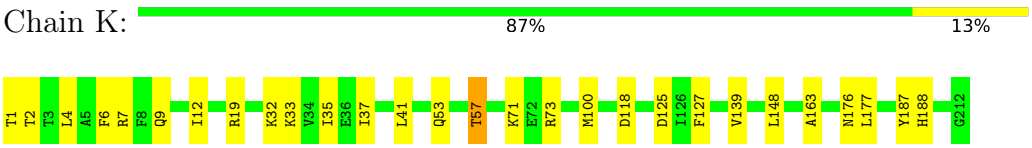
• Molecule 10: Proteasome subunit beta type-4

Chain X:



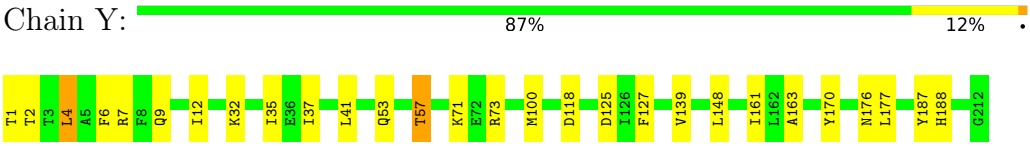
• Molecule 11: Proteasome subunit beta type-5

Chain K:



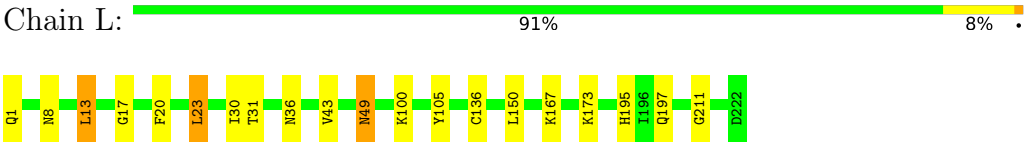
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



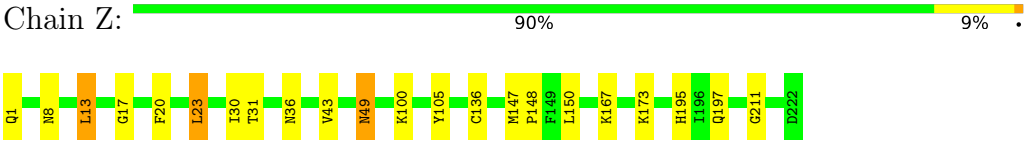
• Molecule 12: Proteasome subunit beta type-6

Chain L:



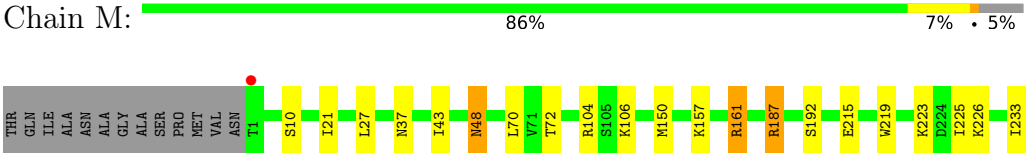
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



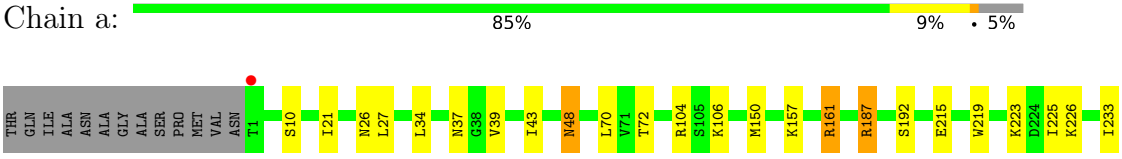
• Molecule 13: Proteasome subunit beta type-7

Chain M:



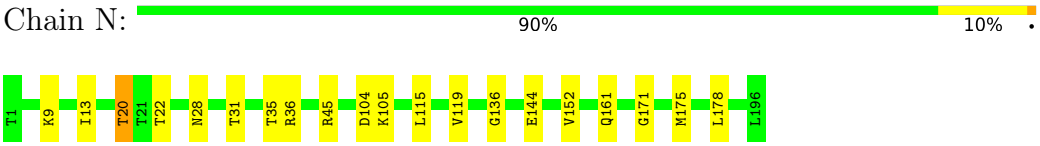
• Molecule 13: Proteasome subunit beta type-7

Chain a:



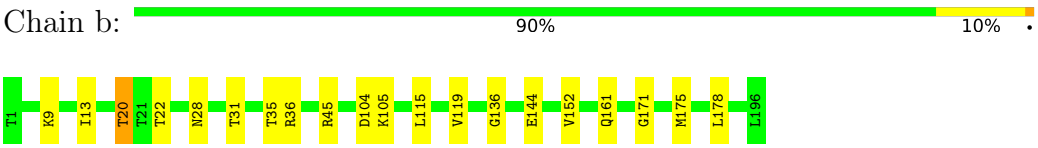
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.49Å 301.49Å 144.39Å 90.00° 114.15° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-2.90) 98.2 (15.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.203 0.181 , 0.205	Depositor DCC
R_{free} test set	11515 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49622	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2LR, MG, 2L0

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	0.74	0/2642
1	O	0.42	0/1952	0.75	0/2642
2	B	0.41	0/1934	0.76	0/2618
2	P	0.42	0/1934	0.76	0/2618
3	C	0.43	0/1910	0.78	0/2586
3	Q	0.43	0/1910	0.78	0/2586
4	D	0.42	0/1837	0.75	0/2475
4	R	0.42	0/1837	0.75	0/2475
5	E	0.40	0/1800	0.72	0/2433
5	S	0.40	0/1800	0.72	0/2433
6	F	0.41	0/1932	0.74	0/2609
6	T	0.41	0/1932	0.74	0/2609
7	G	0.41	0/1945	0.74	0/2634
7	U	0.41	0/1945	0.74	0/2634
8	H	0.39	0/1715	0.72	0/2326
8	V	0.39	0/1715	0.71	0/2326
9	I	0.40	0/1611	0.73	0/2174
9	W	0.40	0/1611	0.73	0/2174
10	J	0.40	0/1589	0.72	0/2142
10	X	0.39	0/1589	0.72	0/2142
11	K	0.39	0/1681	0.70	0/2274
11	Y	0.39	0/1678	0.70	0/2268
12	L	0.39	0/1795	0.71	0/2420
12	Z	0.39	0/1795	0.71	0/2420
13	M	0.41	0/1855	0.74	0/2514
13	a	0.41	0/1855	0.74	0/2514
14	N	0.39	0/1541	0.71	0/2087
14	b	0.39	0/1541	0.71	0/2087
All	All	0.40	0/50191	0.73	0/67862

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	6	0
1	O	1915	0	1929	9	0
2	B	1904	0	1904	17	0
2	P	1904	0	1904	14	0
3	C	1881	0	1895	19	0
3	Q	1881	0	1895	19	0
4	D	1813	0	1797	10	0
4	R	1813	0	1797	11	0
5	E	1773	0	1775	10	0
5	S	1773	0	1775	10	0
6	F	1892	0	1883	11	0
6	T	1892	0	1883	11	0
7	G	1907	0	1901	11	0
7	U	1907	0	1901	12	0
8	H	1684	0	1685	13	0
8	V	1684	0	1687	11	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	7	0
11	K	1644	0	1593	18	0
11	Y	1642	0	1589	13	0
12	L	1757	0	1711	9	0
12	Z	1757	0	1711	10	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	8	0
14	N	1512	0	1481	9	0
14	b	1512	0	1481	9	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	H	38	0	47	4	0
16	K	38	0	47	8	0
16	Y	38	0	47	1	0
17	V	38	0	46	3	0
18	A	3	0	0	1	0
18	B	4	0	0	0	0
18	C	1	0	0	0	0
18	D	4	0	0	0	0
18	E	2	0	0	0	0
18	F	6	0	0	0	0
18	G	6	0	0	0	0
18	H	7	0	0	0	0
18	I	5	0	0	0	0
18	J	10	0	0	0	0
18	K	12	0	0	0	0
18	L	11	0	0	0	0
18	M	13	0	0	0	0
18	N	7	0	0	0	0
18	O	4	0	0	1	0
18	P	1	0	0	0	0
18	Q	1	0	0	0	0
18	R	4	0	0	0	0
18	S	2	0	0	0	0
18	T	6	0	0	0	0
18	U	11	0	0	0	0
18	V	7	0	0	0	0
18	W	3	0	0	0	0
18	X	9	0	0	0	0
18	Y	10	0	0	0	0
18	Z	2	0	0	0	0
18	a	8	0	0	0	0
18	b	9	0	0	0	0
All	All	49622	0	49243	280	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 (280) 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:170:TYR:O	16:Y:301:2L0:H44	1.63	0.99
11:K:33:LYS:NZ	16:K:301:2L0:H45	1.80	0.96
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.53	0.88
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.53	0.88
11:K:33:LYS:HZ3	16:K:301:2L0:H45	1.38	0.86
11:Y:1:THR:CA	11:Y:2:THR:N	2.43	0.81
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.46	0.81
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.46	0.80
11:K:53:GLN:O	11:K:57:THR:HG23	1.84	0.77
14:b:152:VAL:HA	14:b:175:MET:HE1	1.66	0.77
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.84	0.76
14:N:152:VAL:HA	14:N:175:MET:HE1	1.66	0.75
7:G:23:PHE:O	7:G:26:THR:HB	1.91	0.71
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.19	0.71
11:K:100:MET:CE	11:K:127:PHE:HB2	2.20	0.71
8:H:33:LYS:NZ	16:H:301:2L0:H45	2.05	0.71
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.91	0.70
7:U:23:PHE:O	7:U:26:THR:HB	1.90	0.70
2:B:50:LYS:HE3	2:B:50:LYS:HA	1.74	0.70
3:C:51:LYS:O	3:C:52:LEU:HB2	1.91	0.69
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.58	0.69
3:C:202:GLN:HG3	3:C:203:THR:H	1.58	0.69
2:P:50:LYS:HE3	2:P:50:LYS:HA	1.74	0.69
10:J:19:LYS:HD3	10:J:180:ILE:HG13	1.77	0.66
8:H:33:LYS:HZ3	16:H:301:2L0:H45	1.62	0.65
10:X:19:LYS:HD3	10:X:180:ILE:HG13	1.78	0.64
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.26	0.62
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.64	0.62
11:K:33:LYS:HZ1	16:K:301:2L0:H45	1.64	0.61
8:V:3:ILE:HG12	8:V:44:ALA:HB1	1.82	0.61
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.66	0.61
11:K:100:MET:HE3	11:K:127:PHE:CB	2.26	0.61
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.65	0.60
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.82	0.60
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.82	0.60
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.66	0.60
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.84	0.60
8:H:3:ILE:HG12	8:H:44:ALA:HB1	1.83	0.59
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.50	0.59
13:a:161:ARG:HG3	13:a:161:ARG:HH11	1.66	0.59
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.85	0.59
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.85	0.58
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.85	0.58
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.34	0.58
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.85	0.58
6:F:146:MET:HE3	6:F:161:THR:HB	1.86	0.57
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.70	0.57
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.50	0.57
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.04	0.57
3:Q:202:GLN:CG	3:Q:203:THR:H	2.18	0.57
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.70	0.57
3:C:201:VAL:O	3:C:202:GLN:HB2	2.04	0.57
6:T:146:MET:HE3	6:T:161:THR:HB	1.86	0.57
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.33	0.57
3:C:202:GLN:CG	3:C:203:THR:H	2.18	0.56
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.87	0.56
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.70	0.56
8:H:52:THR:O	8:H:56:THR:HB	2.06	0.56
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.88	0.56
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.71	0.55
3:Q:205:ALA:C	3:Q:207:ASN:H	2.14	0.55
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.71	0.55
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.88	0.55
3:C:48:SER:HB2	3:C:207:ASN:OD1	2.07	0.55
14:b:20:THR:HG22	14:b:31:THR:OG1	2.07	0.55
14:b:20:THR:HG23	14:b:28:ASN:HB3	1.89	0.55
14:N:20:THR:HG22	14:N:31:THR:OG1	2.07	0.55
2:P:65:LEU:HD22	2:P:211:GLU:HB3	1.89	0.54
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.88	0.54
8:V:52:THR:O	8:V:56:THR:HB	2.07	0.54
3:C:205:ALA:C	3:C:207:ASN:H	2.15	0.54
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.41	0.54
2:B:50:LYS:HA	2:B:50:LYS:CE	2.36	0.54
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.88	0.54
3:Q:48:SER:HB2	3:Q:207:ASN:OD1	2.08	0.54
7:U:83:ASN:C	7:U:83:ASN:HD22	2.17	0.53
2:B:65:LEU:HD22	2:B:211:GLU:HB3	1.89	0.53
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.89	0.53
2:P:50:LYS:HA	2:P:50:LYS:CE	2.36	0.53
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.91	0.53
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.90	0.53
7:G:83:ASN:C	7:G:83:ASN:HD22	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:33:LYS:NZ	16:K:301:2L0:C45	2.66	0.53
6:T:68:ARG:NH1	13:a:72:THR:OG1	2.42	0.53
13:M:150:MET:HE1	13:M:187:ARG:HG2	1.91	0.52
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.91	0.52
14:N:20:THR:CG2	14:N:31:THR:OG1	2.58	0.52
10:J:1:MET:HA	10:J:34:LYS:CE	2.40	0.52
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.25	0.52
8:V:49:ALA:HB2	17:V:301:2LR:H17	1.91	0.52
10:X:1:MET:HA	10:X:34:LYS:CE	2.40	0.52
4:R:234:GLU:O	4:R:238:LYS:HG3	2.10	0.51
14:b:20:THR:CG2	14:b:31:THR:OG1	2.58	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.92	0.51
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.91	0.51
5:E:68:HIS:HE1	5:E:102:LEU:O	1.94	0.51
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.92	0.51
11:K:19:ARG:O	16:K:301:2L0:C45	2.59	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.50
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.41	0.50
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.42	0.50
4:D:234:GLU:O	4:D:238:LYS:HG3	2.11	0.50
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.92	0.50
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.58	0.50
10:J:1:MET:HA	10:J:34:LYS:HE3	1.94	0.50
12:L:195:HIS:HD2	12:L:197:GLN:H	1.58	0.49
5:S:68:HIS:HE1	5:S:102:LEU:O	1.94	0.49
6:F:146:MET:CE	6:F:161:THR:HB	2.42	0.49
7:G:34:LEU:C	7:G:34:LEU:HD23	2.37	0.49
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.47	0.49
6:T:146:MET:CE	6:T:161:THR:HB	2.42	0.49
10:X:1:MET:HA	10:X:34:LYS:HE3	1.95	0.49
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.47	0.49
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.47	0.49
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.47	0.49
2:B:49:ARG:HH22	2:B:61:SER:HB3	1.78	0.49
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.28	0.49
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.48	0.49
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.47	0.49
10:J:174:MET:HA	10:X:174:MET:HA	1.94	0.48
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.48	0.48
11:K:33:LYS:HZ1	16:K:301:2L0:C45	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:49:ARG:HH22	2:P:61:SER:HB3	1.77	0.48
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.96	0.48
16:H:301:2L0:H36	16:H:301:2L0:H46	1.40	0.48
7:U:34:LEU:C	7:U:34:LEU:HD23	2.38	0.48
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.49	0.48
11:K:19:ARG:O	16:K:301:2L0:H46	2.15	0.47
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.50	0.47
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.97	0.47
8:V:45:GLY:O	17:V:301:2LR:H29	2.13	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.47
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.50	0.47
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.49	0.47
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.96	0.47
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.96	0.47
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.96	0.47
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.62	0.47
6:T:228:LYS:HB2	6:T:228:LYS:HE3	1.70	0.47
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.96	0.47
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.96	0.47
5:S:9:THR:HG21	5:S:119:THR:HA	1.97	0.47
9:W:14:MET:HB3	9:W:162:LEU:HD11	1.96	0.47
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.96	0.47
6:T:123:ASN:C	6:T:123:ASN:HD22	2.23	0.47
2:B:141:ASP:O	10:J:110:LYS:NZ	2.48	0.46
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.50	0.46
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.96	0.46
5:S:155:LEU:HD13	5:S:158:THR:HB	1.98	0.46
3:C:48:SER:C	3:C:50:LEU:H	2.22	0.46
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.97	0.46
8:V:99:ILE:HG13	8:V:127:LEU:HD22	1.97	0.46
6:F:123:ASN:C	6:F:123:ASN:HD22	2.24	0.46
5:E:9:THR:HG21	5:E:119:THR:HA	1.97	0.46
5:E:155:LEU:HD13	5:E:158:THR:HB	1.98	0.46
3:Q:48:SER:C	3:Q:50:LEU:H	2.22	0.46
7:U:83:ASN:C	7:U:83:ASN:ND2	2.74	0.46
8:V:21:THR:OG1	17:V:301:2LR:H20	2.15	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.31	0.45
3:Q:205:ALA:C	3:Q:207:ASN:N	2.74	0.45
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.99	0.45
3:C:205:ALA:C	3:C:207:ASN:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.51	0.45
5:S:170:TYR:HB2	5:S:198:GLN:HG3	1.99	0.45
5:E:170:TYR:HB2	5:E:198:GLN:HG3	1.99	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.99	0.45
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.50	0.45
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.47	0.45
4:D:113:LEU:HD23	4:D:115:PHE:HE1	1.81	0.45
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.99	0.45
4:R:113:LEU:HD23	4:R:115:PHE:HE1	1.81	0.45
11:Y:7:ARG:HG3	11:Y:12:ILE:HG12	1.99	0.45
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.99	0.45
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.99	0.45
7:G:83:ASN:C	7:G:83:ASN:ND2	2.75	0.45
8:H:99:ILE:HG13	8:H:127:LEU:HD22	1.99	0.45
11:K:7:ARG:HG3	11:K:12:ILE:HG12	1.99	0.45
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.99	0.45
7:U:195:GLU:HG2	7:U:239:ILE:HG13	1.99	0.44
14:b:13:ILE:HG21	14:b:175:MET:HE2	2.00	0.44
7:U:227:LEU:HB3	7:U:231:ASN:HB2	2.00	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.47	0.44
13:a:27:LEU:HB2	13:a:192:SER:HB3	1.98	0.44
8:H:84:LYS:HG3	8:H:85:GLN:N	2.32	0.44
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.99	0.44
13:a:48:ASN:H	13:a:48:ASN:HD22	1.65	0.44
3:C:201:VAL:HG13	3:C:202:GLN:N	2.32	0.44
1:O:66:LEU:HD23	1:O:66:LEU:C	2.43	0.44
1:A:66:LEU:C	1:A:66:LEU:HD23	2.42	0.44
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.99	0.44
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.00	0.44
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.48	0.44
11:K:6:PHE:HA	11:K:125:ASP:O	2.18	0.44
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.44
8:V:84:LYS:HG3	8:V:85:GLN:N	2.32	0.43
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.31	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.99	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.43
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.51	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:65:MET:HE1	9:I:93:SER:HB3	2.00	0.43
7:G:195:GLU:HG2	7:G:239:ILE:HG13	2.00	0.43
8:H:33:LYS:HZ1	16:H:301:2L0:H45	1.79	0.43
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.49	0.43
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.18	0.43
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.48	0.43
4:D:185:LEU:O	4:D:189:GLU:HG3	2.19	0.43
6:F:228:LYS:HB2	6:F:228:LYS:HE3	1.71	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.19	0.43
1:O:108:LYS:HG2	18:O:302:HOH:O	2.18	0.42
13:M:48:ASN:H	13:M:48:ASN:HD22	1.66	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
2:P:134:PHE:O	2:P:149:THR:HA	2.20	0.42
3:C:168:THR:O	3:C:171:GLU:HB3	2.19	0.42
5:E:201:ARG:C	5:E:203:GLU:H	2.27	0.42
4:R:185:LEU:O	4:R:189:GLU:HG3	2.20	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.42
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.02	0.42
9:W:65:MET:HE1	9:W:93:SER:HB3	2.00	0.42
1:A:149:GLN:O	1:A:156:TYR:HA	2.20	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.55	0.42
8:H:104:ASP:OD1	8:H:106:THR:HB	2.20	0.42
3:Q:172:PHE:CD1	3:Q:172:PHE:C	2.97	0.42
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.01	0.42
5:S:201:ARG:C	5:S:203:GLU:H	2.27	0.42
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.02	0.42
10:J:36:ARG:HA	10:J:36:ARG:HD3	1.90	0.42
3:Q:27:ARG:CZ	3:Q:27:ARG:HB2	2.50	0.42
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.02	0.42
11:Y:177:LEU:HB3	11:Y:188:HIS:HB2	2.02	0.42
2:B:134:PHE:O	2:B:149:THR:HA	2.20	0.42
5:E:156:TYR:CD1	5:E:179:ILE:HD13	2.55	0.42
16:K:301:2L0:H46	16:K:301:2L0:H36	1.41	0.42
14:b:35:THR:CG2	14:b:45:ARG:HE	2.33	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.42
2:P:204:ALA:O	2:P:209:ARG:NH2	2.53	0.42
5:S:156:TYR:CD1	5:S:179:ILE:HD13	2.55	0.42
3:C:172:PHE:CD1	3:C:172:PHE:C	2.97	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:THR:O	2:B:172:GLN:HB2	2.20	0.41
2:B:204:ALA:O	2:B:209:ARG:NH2	2.53	0.41
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.02	0.41
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.01	0.41
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.56	0.41
5:E:35:VAL:HG22	5:E:159:ALA:HB2	2.03	0.41
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.56	0.41
8:H:144:GLN:O	8:H:145:ASP:HB2	2.21	0.41
11:K:177:LEU:HB3	11:K:188:HIS:HB2	2.02	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.41
8:V:104:ASP:OD1	8:V:106:THR:HB	2.21	0.41
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.02	0.41
11:K:139:VAL:HG21	11:K:163:ALA:CB	2.51	0.41
5:S:35:VAL:HG22	5:S:159:ALA:HB2	2.02	0.41
6:F:146:MET:HE2	6:F:148:GLU:OE2	2.21	0.41
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.02	0.41
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.03	0.41
9:I:111:ILE:HD12	9:I:189:ILE:HG22	2.03	0.41
1:O:115:ALA:HB1	1:O:154:GLY:O	2.21	0.41
2:P:180:LYS:O	2:P:183:MET:HB2	2.21	0.41
11:Y:139:VAL:HG21	11:Y:163:ALA:CB	2.51	0.41
3:C:27:ARG:HB2	3:C:27:ARG:CZ	2.50	0.41
11:K:1:THR:HG22	11:K:2:THR:N	2.36	0.41
9:W:111:ILE:HD12	9:W:189:ILE:HG22	2.03	0.41
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.86	0.40
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.86	0.40
18:A:301:HOH:O	7:G:122:ARG:HD2	2.20	0.40
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.56	0.40
4:D:1:ASP:O	4:D:2:ARG:HB2	2.21	0.40
14:N:35:THR:CG2	14:N:45:ARG:HE	2.34	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.84	0.40
13:a:26:ASN:HA	13:a:39:VAL:O	2.22	0.40
13:a:27:LEU:HD21	13:a:34:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	59
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	59
2	B	242/258 (94%)	229 (95%)	10 (4%)	3 (1%)	10	34
2	P	242/258 (94%)	230 (95%)	9 (4%)	3 (1%)	10	34
3	C	238/254 (94%)	227 (95%)	4 (2%)	7 (3%)	3	15
3	Q	238/254 (94%)	227 (95%)	4 (2%)	7 (3%)	3	15
4	D	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	30	59
4	R	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	30	59
5	E	229/234 (98%)	220 (96%)	8 (4%)	1 (0%)	30	59
5	S	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	30	59
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	4 (2%)	2 (1%)	14	41
8	V	220/232 (95%)	214 (97%)	4 (2%)	2 (1%)	14	41
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	54
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	24	54
11	K	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	54
11	Y	209/212 (99%)	202 (97%)	6 (3%)	1 (0%)	24	54
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6275/6614 (95%)	6068 (97%)	173 (3%)	34 (0%)	24	54

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	62	THR
3	C	38	ASN
3	C	202	GLN
3	C	206	LYS
2	P	62	THR
3	Q	38	ASN
3	Q	202	GLN
2	B	51	VAL
3	C	205	ALA
4	D	2	ARG
5	E	231	LYS
8	H	9	ASN
2	P	51	VAL
3	Q	205	ALA
3	Q	206	LYS
4	R	2	ARG
5	S	231	LYS
8	V	9	ASN
2	B	221	ASP
3	C	239	GLN
10	J	2	ASP
2	P	221	ASP
3	Q	239	GLN
10	X	2	ASP
3	C	49	THR
8	H	145	ASP
3	Q	49	THR
8	V	145	ASP
1	A	3	ASP
11	K	9	GLN
1	O	3	ASP
3	Q	52	LEU
3	C	52	LEU

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Mol	Chain	Res	Type
11	Y	9	GLN

5.3.2 Protein sidechains (i)

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%)	199 (95%)	10 (5%)	23	55
1	O	209/209 (100%)	199 (95%)	10 (5%)	23	55
2	B	203/216 (94%)	187 (92%)	16 (8%)	11	34
2	P	203/216 (94%)	187 (92%)	16 (8%)	11	34
3	C	212/226 (94%)	192 (91%)	20 (9%)	8	26
3	Q	212/226 (94%)	192 (91%)	20 (9%)	8	26
4	D	194/215 (90%)	172 (89%)	22 (11%)	5	19
4	R	194/215 (90%)	172 (89%)	22 (11%)	5	19
5	E	190/193 (98%)	173 (91%)	17 (9%)	9	28
5	S	190/193 (98%)	173 (91%)	17 (9%)	9	28
6	F	201/239 (84%)	185 (92%)	16 (8%)	11	34
6	T	201/239 (84%)	185 (92%)	16 (8%)	11	34
7	G	206/210 (98%)	191 (93%)	15 (7%)	13	38
7	U	206/210 (98%)	191 (93%)	15 (7%)	13	38
8	H	181/190 (95%)	171 (94%)	10 (6%)	19	50
8	V	181/190 (95%)	171 (94%)	10 (6%)	19	50
9	I	172/173 (99%)	165 (96%)	7 (4%)	27	61
9	W	172/173 (99%)	164 (95%)	8 (5%)	23	56
10	J	173/175 (99%)	164 (95%)	9 (5%)	21	52
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	52
11	K	169/169 (100%)	161 (95%)	8 (5%)	23	56
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	56
12	L	185/185 (100%)	178 (96%)	7 (4%)	29	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	Z	185/185 (100%)	178 (96%)	7 (4%)	29 64
13	M	199/208 (96%)	183 (92%)	16 (8%)	11 34
13	a	199/208 (96%)	183 (92%)	16 (8%)	11 34
14	N	162/162 (100%)	152 (94%)	10 (6%)	16 46
14	b	162/162 (100%)	152 (94%)	10 (6%)	16 46
All	All	5312/5540 (96%)	4945 (93%)	367 (7%)	14 41

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	50	LYS
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	184	GLU
1	A	201	GLU
1	A	231	LYS
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	56	LEU
2	B	65	LEU
2	B	79	LEU
2	B	89	THR
2	B	102	ASN
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	202	SER
2	B	209	ARG
2	B	237	ILE
2	B	244	THR
3	C	4	ARG
3	C	37	LYS
3	C	38	ASN
3	C	51	LYS

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Mol	Chain	Res	Type
3	C	58	THR
3	C	61	LYS
3	C	109	ARG
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	206	LYS
3	C	213	VAL
3	C	222	LEU
3	C	239	GLN
3	C	240	GLU
4	D	4	VAL
4	D	20	LEU
4	D	40	LEU
4	D	48	SER
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	102	GLU
4	D	104	LEU
4	D	117	GLU
4	D	176	LEU
4	D	183	LEU
4	D	190	LEU
4	D	191	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
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU

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Mol	Chain	Res	Type
5	E	29	LYS
5	E	55	LEU
5	E	60	LYS
5	E	71	LEU
5	E	87	LEU
5	E	172	GLU
5	E	174	THR
5	E	188	LEU
5	E	201	ARG
5	E	207	VAL
5	E	211	SER
5	E	219	THR
5	E	231	LYS
6	F	14	ASP
6	F	68	ARG
6	F	94	SER
6	F	96	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	148	GLU
6	F	165	ARG
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	166	GLN
7	G	171	THR
7	G	178	LYS
7	G	201	MET
7	G	205	LEU
7	G	207	THR
7	G	221	LYS

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Mol	Chain	Res	Type
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	121	VAL
8	H	127	LEU
8	H	153	LYS
8	H	196	ARG
8	H	213	LEU
9	I	37	ASN
9	I	117	LYS
9	I	126	ILE
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	36	ARG
10	J	75	LEU
10	J	91	SER
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	32	LYS
11	K	35	ILE
11	K	57	THR
11	K	71	LYS
11	K	73	ARG
11	K	118	ASP
11	K	148	LEU
12	L	1	GLN
12	L	13	LEU
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	167	LYS

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Mol	Chain	Res	Type
12	L	173	LYS
13	M	10	SER
13	M	21	ILE
13	M	37	ASN
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	106	LYS
13	M	157	LYS
13	M	161	ARG
13	M	187	ARG
13	M	215	GLU
13	M	223	LYS
13	M	225	ILE
13	M	226	LYS
13	M	233	ILE
14	N	9	LYS
14	N	20	THR
14	N	22	THR
14	N	36	ARG
14	N	104	ASP
14	N	105	LYS
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	17	LYS
1	O	50	LYS
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	184	GLU
1	O	201	GLU
1	O	231	LYS
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	54	THR
2	P	56	LEU
2	P	65	LEU

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Mol	Chain	Res	Type
2	P	79	LEU
2	P	89	THR
2	P	102	ASN
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	202	SER
2	P	209	ARG
2	P	237	ILE
2	P	244	THR
3	Q	4	ARG
3	Q	37	LYS
3	Q	38	ASN
3	Q	51	LYS
3	Q	58	THR
3	Q	61	LYS
3	Q	109	ARG
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	203	THR
3	Q	206	LYS
3	Q	213	VAL
3	Q	222	LEU
3	Q	239	GLN
3	Q	240	GLU
4	R	4	VAL
4	R	20	LEU
4	R	40	LEU
4	R	48	SER
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	102	GLU
4	R	104	LEU
4	R	117	GLU
4	R	176	LEU

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Mol	Chain	Res	Type
4	R	183	LEU
4	R	190	LEU
4	R	191	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
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	60	LYS
5	S	71	LEU
5	S	87	LEU
5	S	172	GLU
5	S	174	THR
5	S	188	LEU
5	S	201	ARG
5	S	207	VAL
5	S	211	SER
5	S	219	THR
5	S	231	LYS
6	T	14	ASP
6	T	68	ARG
6	T	94	SER
6	T	96	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	148	GLU
6	T	165	ARG
6	T	172	LEU
6	T	181	GLU
6	T	198	LEU
6	T	203	ASN
6	T	206	LYS

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Mol	Chain	Res	Type
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
7	U	166	GLN
7	U	171	THR
7	U	178	LYS
7	U	201	MET
7	U	205	LEU
7	U	207	THR
7	U	221	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	121	VAL
8	V	127	LEU
8	V	153	LYS
8	V	196	ARG
8	V	213	LEU
9	W	37	ASN
9	W	117	LYS
9	W	126	ILE
9	W	151	SER
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	36	ARG
10	X	75	LEU
10	X	91	SER
10	X	144	LEU

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Mol	Chain	Res	Type
10	X	163	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	32	LYS
11	Y	35	ILE
11	Y	57	THR
11	Y	71	LYS
11	Y	73	ARG
11	Y	118	ASP
11	Y	148	LEU
12	Z	1	GLN
12	Z	13	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
12	Z	173	LYS
13	a	10	SER
13	a	21	ILE
13	a	37	ASN
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	106	LYS
13	a	157	LYS
13	a	161	ARG
13	a	187	ARG
13	a	215	GLU
13	a	223	LYS
13	a	225	ILE
13	a	226	LYS
13	a	233	ILE
14	b	9	LYS
14	b	20	THR
14	b	22	THR
14	b	36	ARG
14	b	104	ASP
14	b	105	LYS
14	b	115	LEU
14	b	119	VAL
14	b	144	GLU

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Mol	Chain	Res	Type
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	149	GLN
2	B	20	GLN
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	172	GLN
2	B	176	GLN
2	B	226	GLN
2	B	232	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	236	GLN
4	D	15	GLN
4	D	100	ASN
4	D	149	HIS
4	D	198	GLN
4	D	217	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	39	ASN
6	F	58	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN

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Mol	Chain	Res	Type
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	175	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	109	HIS
8	H	172	ASN
8	H	189	ASN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	112	ASN
10	J	146	HIS
11	K	9	GLN
11	K	85	ASN
11	K	143	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	152	ASN
12	L	153	GLN
12	L	155	ASN
12	L	158	ASN
12	L	197	GLN
13	M	48	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS

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Mol	Chain	Res	Type
1	O	149	GLN
2	P	20	GLN
2	P	58	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	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	149	HIS
4	R	198	GLN
4	R	217	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	39	ASN
6	T	58	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
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	30	ASN
8	V	57	GLN
8	V	109	HIS

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Mol	Chain	Res	Type
8	V	172	ASN
8	V	189	ASN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	146	HIS
10	X	147	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	152	ASN
12	Z	153	GLN
12	Z	158	ASN
12	Z	197	GLN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
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 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	$\#\|Z\| > 2$
16	2L0	K	301	11	38,38,38	1.03	2 (5%)	47,50,50	1.65	4 (8%)
16	2L0	Y	301	11	38,38,38	1.52	3 (7%)	47,50,50	2.72	6 (12%)
17	2LR	V	301	8	38,39,39	1.68	4 (10%)	50,54,54	2.60	8 (16%)
16	2L0	H	301	8	38,38,38	1.28	2 (5%)	47,50,50	1.64	6 (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	2L0	K	301	11	-	8/47/47/47	0/1/1/1
16	2L0	Y	301	11	-	6/47/47/47	0/1/1/1
17	2LR	V	301	8	-	6/47/51/51	0/2/2/2
16	2L0	H	301	8	-	7/47/47/47	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	301	2LR	C45-C34	-7.36	1.36	1.52
16	Y	301	2L0	C45-C34	7.17	1.71	1.53
16	H	301	2L0	C45-C34	-4.86	1.40	1.53
16	H	301	2L0	C5-C4	-4.42	1.40	1.50
16	K	301	2L0	C5-C4	-4.37	1.40	1.50
17	V	301	2LR	C5-C4	-4.15	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	2L0	C5-C4	-4.15	1.40	1.50
17	V	301	2LR	C35-C34	2.81	1.53	1.46
16	K	301	2L0	C34-C33	2.26	1.57	1.53
17	V	301	2LR	O40-C35	-2.13	1.39	1.44
16	Y	301	2L0	C34-C33	2.03	1.57	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	301	2L0	C45-C34-C35	-15.00	90.68	109.76
17	V	301	2LR	C45-C34-C35	-11.00	97.95	119.50
17	V	301	2LR	O40-C34-C45	-10.50	94.42	113.82
16	K	301	2L0	C45-C34-C33	-8.66	95.75	111.45
16	Y	301	2L0	C45-C34-C33	8.12	126.18	111.45
16	H	301	2L0	C26-C25-N24	-6.05	102.43	110.20
17	V	301	2LR	C35-O40-C34	5.37	65.86	60.53
16	H	301	2L0	C45-C34-C33	-5.24	101.95	111.45
17	V	301	2LR	C34-C33-C25	-4.53	105.33	115.71
17	V	301	2LR	O6-C7-N9	4.21	119.45	110.45
16	Y	301	2L0	O6-C7-N9	4.16	119.34	110.45
16	H	301	2L0	O6-C7-N9	4.15	119.32	110.45
16	K	301	2L0	O6-C7-N9	4.06	119.14	110.45
16	H	301	2L0	C45-C34-C35	-3.96	104.72	109.76
16	H	301	2L0	O8-C7-N9	-3.00	119.95	124.86
17	V	301	2LR	O8-C7-N9	-2.98	119.97	124.86
16	Y	301	2L0	C26-C25-C33	-2.79	107.71	112.18
16	K	301	2L0	O8-C7-N9	-2.76	120.33	124.86
16	Y	301	2L0	O8-C7-N9	-2.74	120.37	124.86
16	K	301	2L0	C26-C25-C33	-2.29	108.51	112.18
17	V	301	2LR	C12-C11-C10	-2.10	109.76	115.40
16	Y	301	2L0	O6-C7-O8	-2.08	120.28	124.26
16	H	301	2L0	C19-C18-C17	-2.06	109.87	115.40
17	V	301	2LR	O40-C34-C35	-2.06	56.12	59.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	H	301	2L0	N24-C25-C26-C27
16	H	301	2L0	C33-C25-C26-C27
16	K	301	2L0	N24-C25-C33-C34
16	K	301	2L0	N24-C25-C33-O43

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Mol	Chain	Res	Type	Atoms
16	K	301	2L0	C26-C25-C33-C34
16	K	301	2L0	C26-C25-C33-O43
16	K	301	2L0	C33-C34-C35-O40
16	K	301	2L0	C45-C34-C35-O40
16	Y	301	2L0	N24-C25-C33-C34
16	Y	301	2L0	N24-C25-C33-O43
16	Y	301	2L0	C26-C25-C33-C34
16	Y	301	2L0	C26-C25-C33-O43
17	V	301	2LR	C33-C25-C26-C27
16	Y	301	2L0	O8-C7-O6-C5
16	Y	301	2L0	N9-C7-O6-C5
17	V	301	2LR	N16-C17-C18-C19
17	V	301	2LR	C22-C17-C18-C19
16	H	301	2L0	N16-C17-C18-C19
16	H	301	2L0	C22-C17-C18-C19
17	V	301	2LR	N24-C25-C26-C27
16	K	301	2L0	O8-C7-O6-C5
16	K	301	2L0	N9-C7-O6-C5
17	V	301	2LR	C25-C33-C34-O40
16	H	301	2L0	N16-C17-C22-O23
16	H	301	2L0	N16-C17-C22-N24
16	H	301	2L0	N24-C25-C33-O43
17	V	301	2LR	C25-C26-C27-C28

There are no ring outliers.

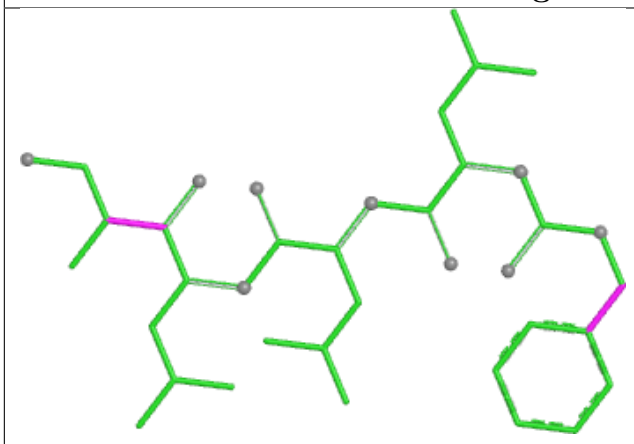
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	301	2L0	8	0
16	Y	301	2L0	1	0
17	V	301	2LR	3	0
16	H	301	2L0	4	0

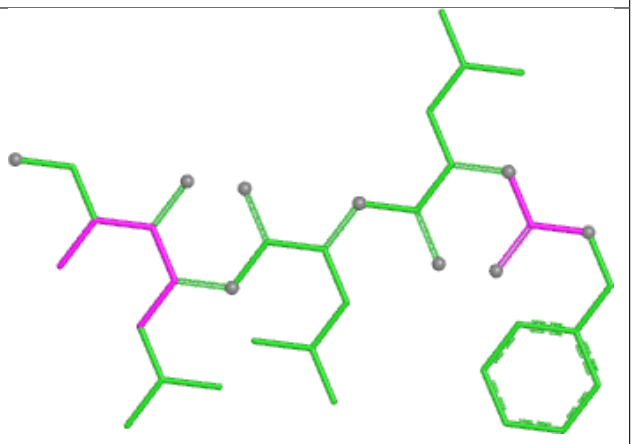
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

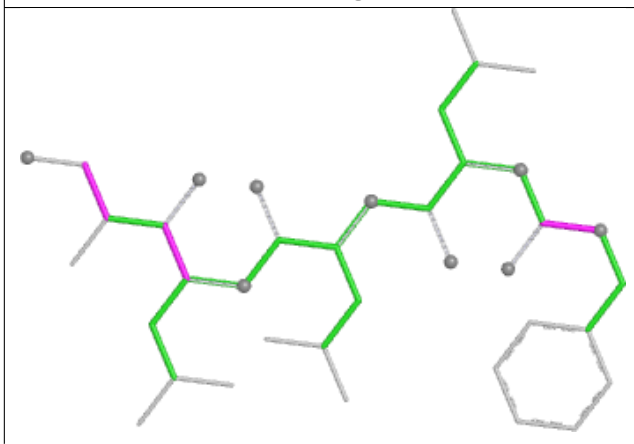
Ligand 2L0 K 301



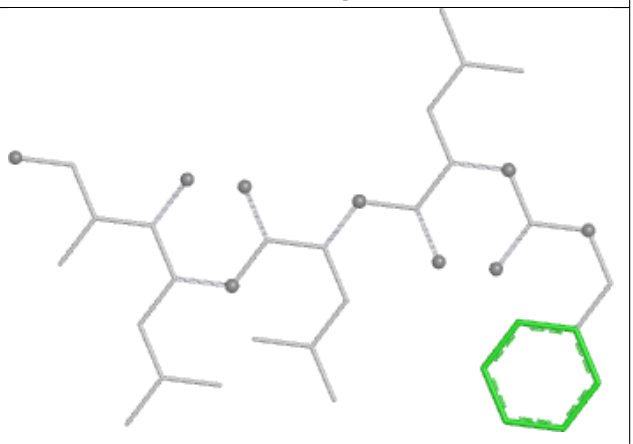
Bond lengths



Bond angles

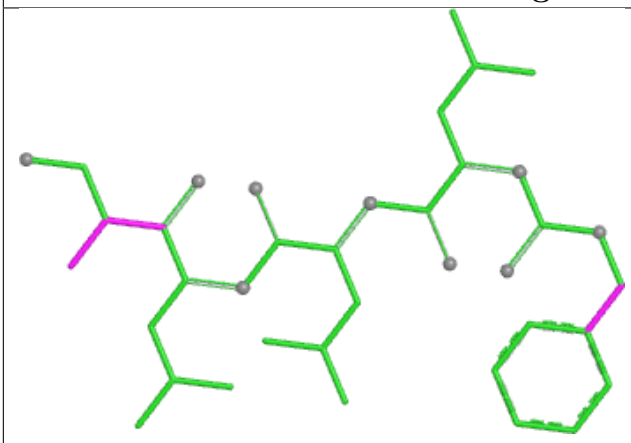


Torsions

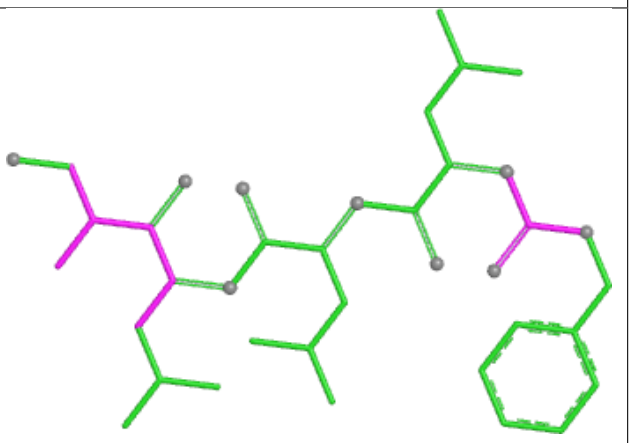


Rings

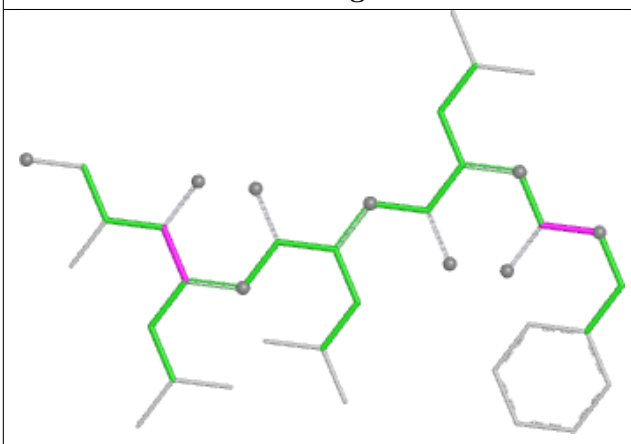
Ligand 2L0 Y 301



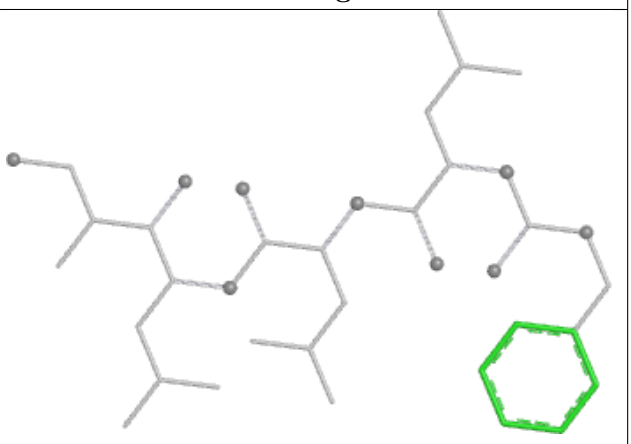
Bond lengths



Bond angles

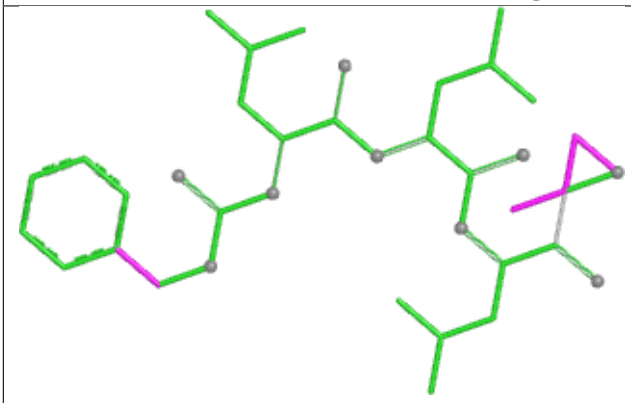


Torsions

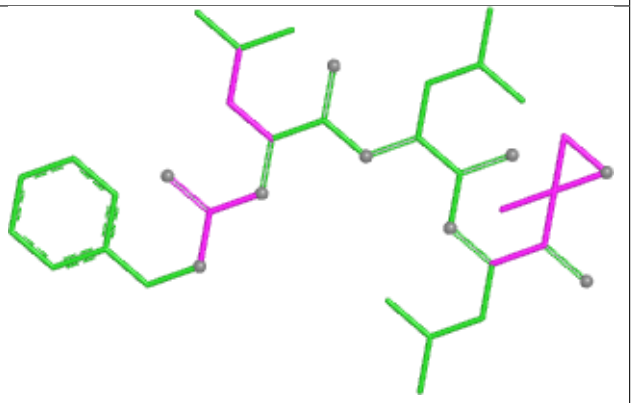


Rings

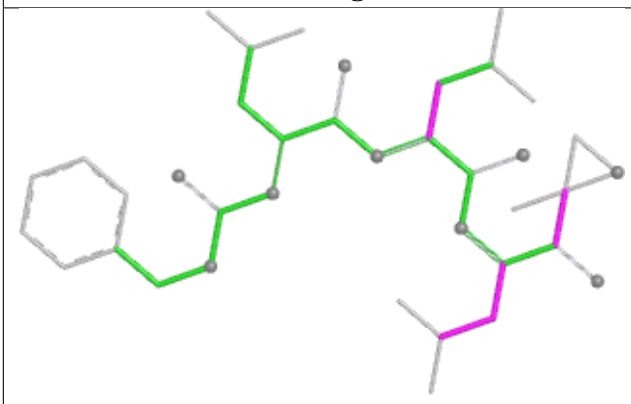
Ligand 2LR V 301



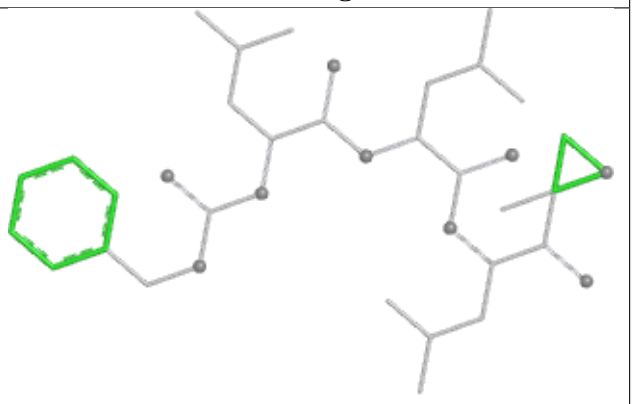
Bond lengths



Bond angles

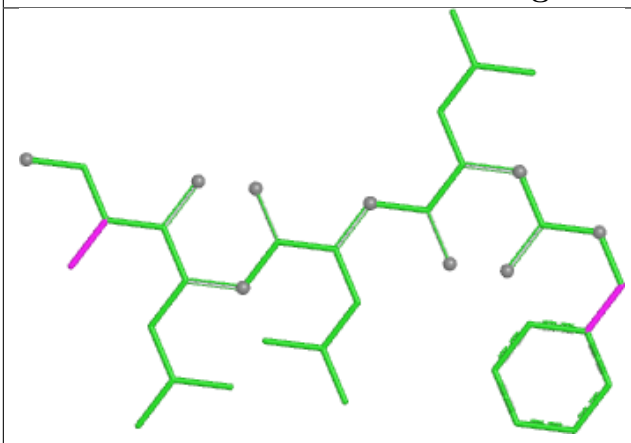


Torsions

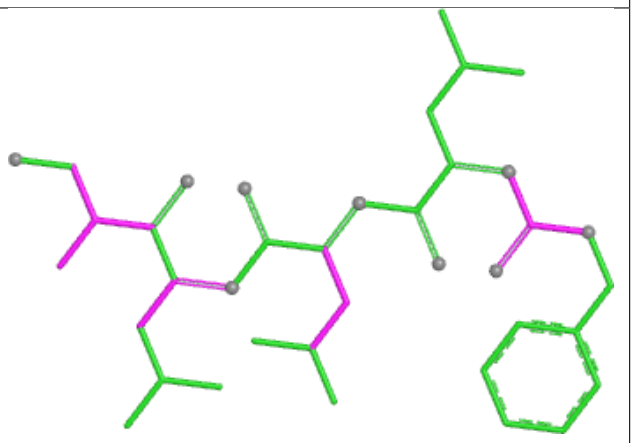


Rings

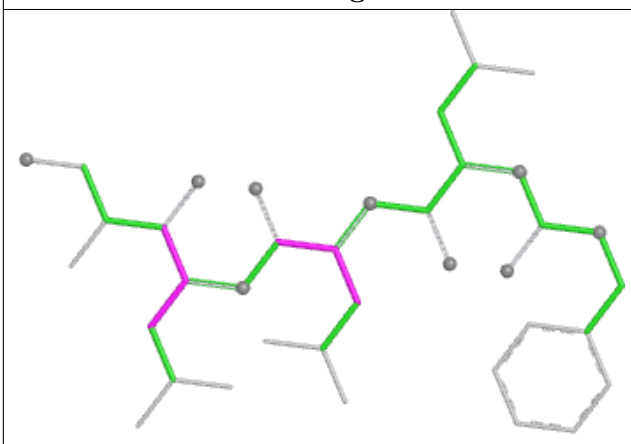
Ligand 2L0 H 301



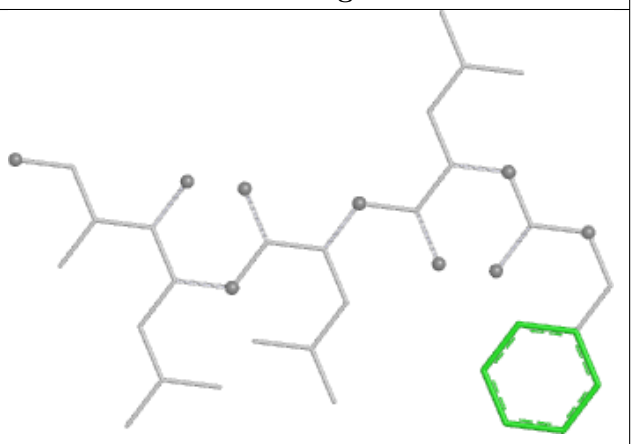
Bond lengths



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, 95^{th} 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%)	-0.58	1 (0%)	88	85	33, 52, 88, 132	0
1	O	250/250 (100%)	-0.50	1 (0%)	88	85	40, 59, 98, 123	0
2	B	244/258 (94%)	-0.36	3 (1%)	76	69	37, 59, 111, 142	0
2	P	244/258 (94%)	-0.28	3 (1%)	76	69	39, 61, 112, 150	0
3	C	240/254 (94%)	-0.37	2 (0%)	82	77	35, 59, 117, 138	0
3	Q	240/254 (94%)	-0.21	5 (2%)	63	54	41, 72, 135, 151	0
4	D	235/260 (90%)	-0.50	1 (0%)	88	85	36, 59, 90, 116	0
4	R	235/260 (90%)	-0.43	1 (0%)	88	85	41, 65, 95, 124	0
5	E	231/234 (98%)	-0.52	0	100	100	38, 61, 88, 116	0
5	S	231/234 (98%)	-0.48	0	100	100	38, 62, 91, 117	0
6	F	243/288 (84%)	-0.54	0	100	100	36, 54, 97, 122	0
6	T	243/288 (84%)	-0.51	0	100	100	36, 55, 91, 120	0
7	G	241/252 (95%)	-0.56	0	100	100	30, 51, 88, 126	0
7	U	241/252 (95%)	-0.57	0	100	100	31, 52, 82, 120	0
8	H	222/232 (95%)	-0.63	0	100	100	33, 49, 74, 116	0
8	V	222/232 (95%)	-0.66	0	100	100	34, 51, 79, 119	0
9	I	204/205 (99%)	-0.73	0	100	100	33, 47, 69, 101	0
9	W	204/205 (99%)	-0.73	0	100	100	32, 50, 74, 107	0
10	J	195/198 (98%)	-0.70	1 (0%)	87	83	32, 50, 75, 123	0
10	X	195/198 (98%)	-0.70	1 (0%)	87	83	36, 52, 77, 135	0
11	K	212/212 (100%)	-0.68	0	100	100	30, 49, 72, 104	0
11	Y	212/212 (100%)	-0.65	0	100	100	34, 51, 77, 103	0
12	L	222/222 (100%)	-0.70	0	100	100	32, 49, 70, 96	0
12	Z	222/222 (100%)	-0.73	0	100	100	32, 48, 71, 102	0

Continued on next page...

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.73	1 (0%) 88 85	33, 47, 67, 77	0
13	a	233/246 (94%)	-0.74	1 (0%) 88 85	31, 46, 66, 80	0
14	N	196/196 (100%)	-0.70	0 100 100	29, 45, 66, 88	0
14	b	196/196 (100%)	-0.71	0 100 100	30, 46, 70, 90	0
All	All	6336/6614 (95%)	-0.57	21 (0%) 90 87	29, 53, 92, 151	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	4.5
3	Q	50	LEU	4.4
2	P	219	ALA	3.7
1	O	1	MET	3.5
13	a	1	THR	3.4
2	P	51	VAL	3.3
2	B	219	ALA	3.2
10	J	1	MET	3.0
1	A	1	MET	2.8
3	Q	223	SER	2.6
13	M	1	THR	2.5
4	D	240	ALA	2.3
3	Q	204	GLY	2.3
2	P	60	THR	2.3
4	R	113	LEU	2.2
3	Q	227	ILE	2.1
2	B	51	VAL	2.1
3	Q	51	LYS	2.1
2	B	93	HIS	2.1
3	C	206	LYS	2.1
3	C	240	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

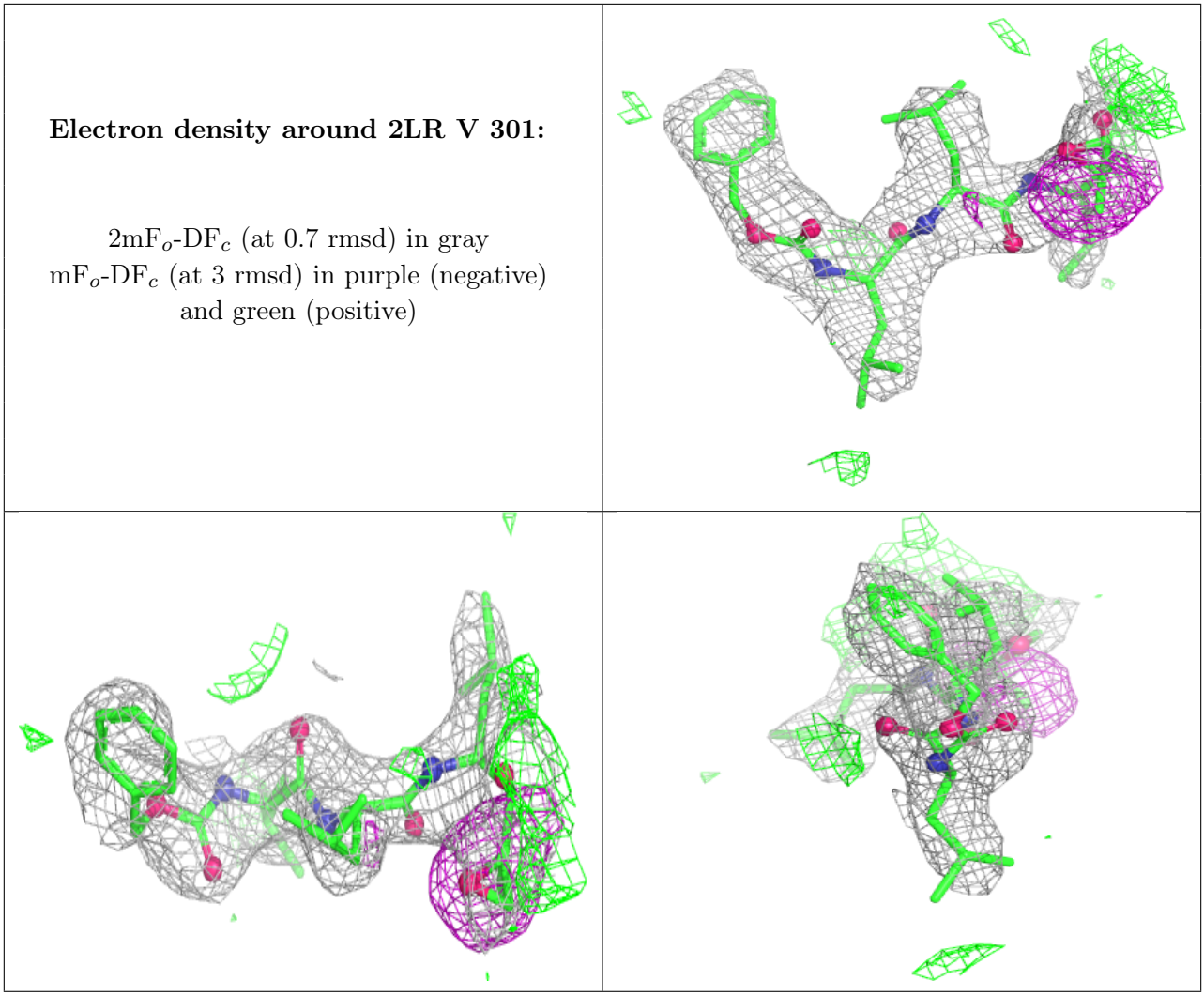
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
17	2LR	V	301	38/38	0.84	0.17	32,83,104,107	0
16	2L0	H	301	38/38	0.89	0.15	63,87,110,111	0
16	2L0	Y	301	38/38	0.90	0.10	36,44,56,56	0
15	MG	I	301	1/1	0.94	0.11	60,60,60,60	0
16	2L0	K	301	38/38	0.94	0.10	44,58,76,76	0
15	MG	K	302	1/1	0.97	0.03	50,50,50,50	0
15	MG	Y	302	1/1	0.98	0.07	51,51,51,51	0
15	MG	G	301	1/1	0.98	0.05	58,58,58,58	0
15	MG	H	302	1/1	0.98	0.16	44,44,44,44	0
15	MG	N	201	1/1	0.98	0.03	38,38,38,38	0
15	MG	V	302	1/1	0.98	0.10	59,59,59,59	0
15	MG	Z	301	1/1	0.99	0.05	45,45,45,45	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.

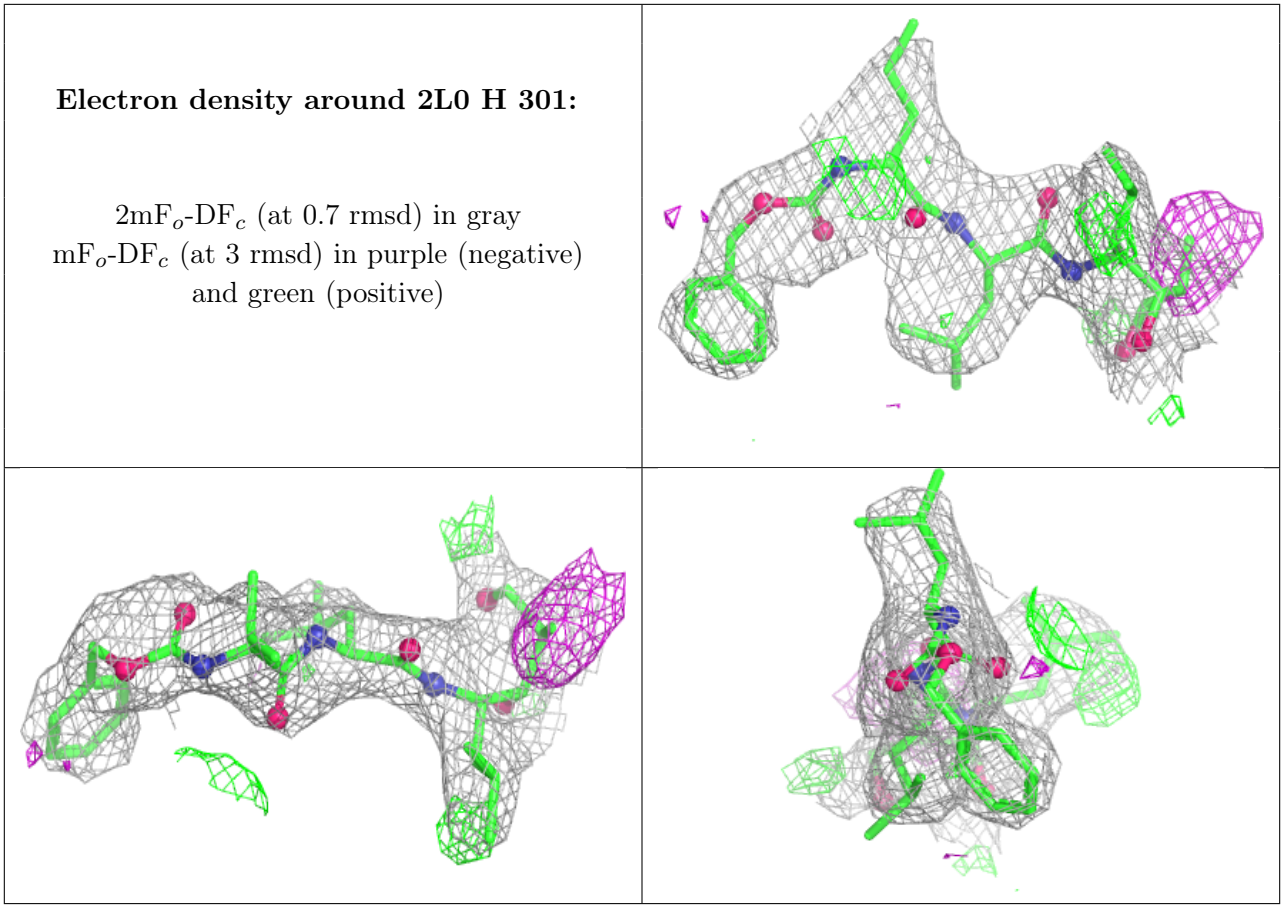
Electron density around 2LR V 301:

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



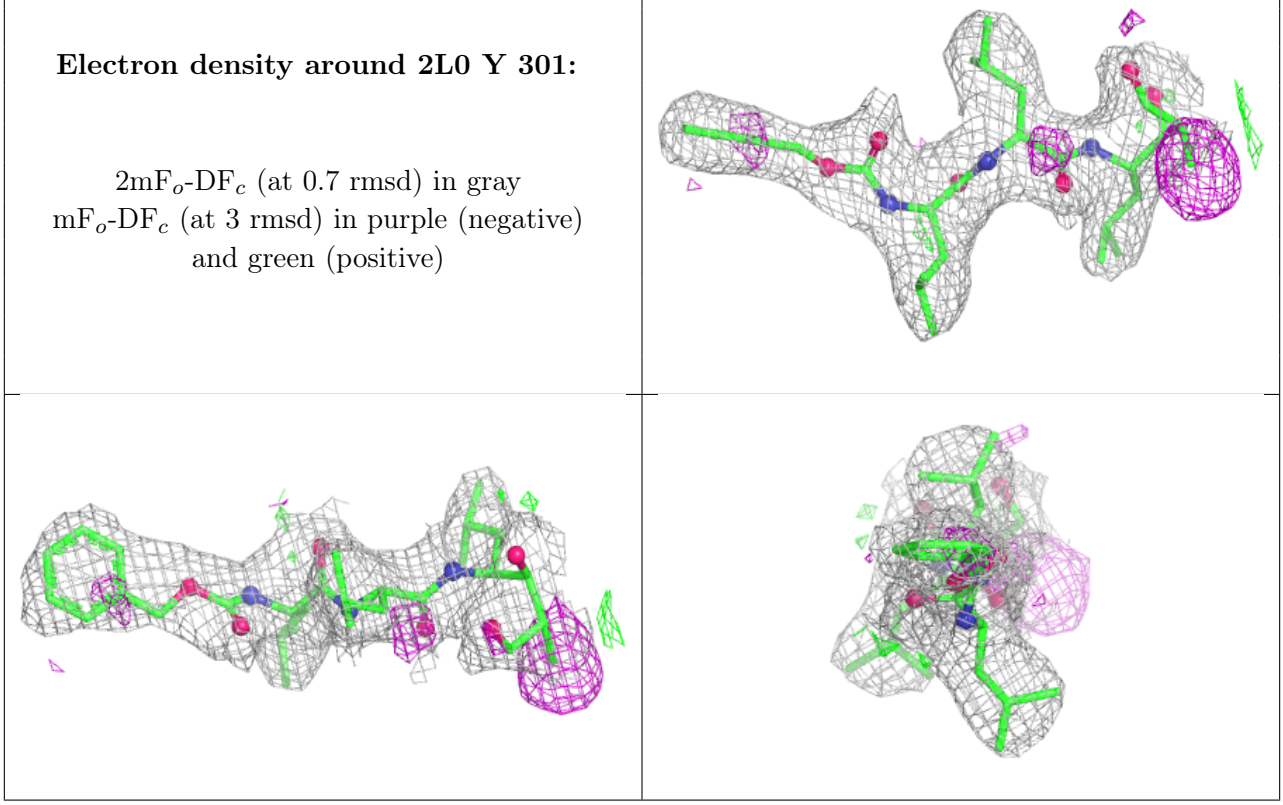
Electron density around 2L0 H 301:

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



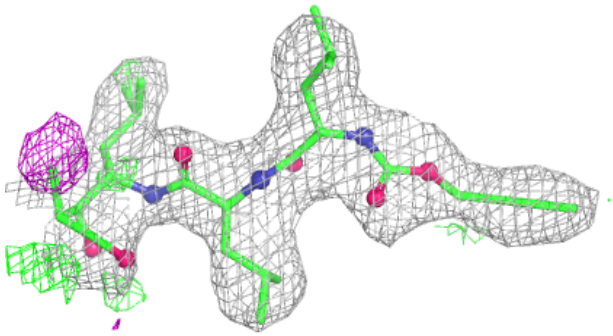
Electron density around 2L0 Y 301:

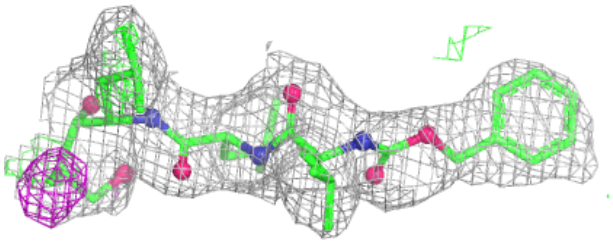
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 2L0 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

There are no such residues in this entry.