Full wwPDB X-ray Structure Validation Report ⓘ

Jul 10, 2024 – 02:02 am BST

PDB ID	:	9FT0
Title	:	Yeast 20S proteasome in complex with epoxyketone inhibitor 42
Authors	:	Maurits, E.; Huber, E.M.; Dekker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleeft, H.S.
Deposited on	:	2024-06-23
Resolution	:	2.75 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:

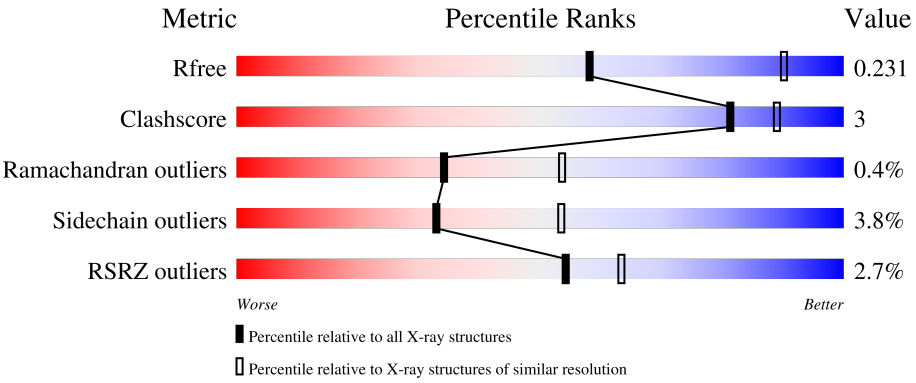
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	2% 94% 6% ·
1	O	250	2% 92% 7%
2	B	258	5% 84% 10% 5%
2	P	258	5% 84% 10% 5%
3	C	254	4% 85% 9% · 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	7% 86% 8% 5%
4	D	260	4% 84% 9% 7%
4	R	260	5% 85% 8% 7%
5	E	234	3% 86% 13%
5	S	234	5% 88% 11%
6	F	288	3% 79% 5% 15%
6	T	288	4% 78% 6% 15%
7	G	252	2% 89% 6%
7	U	252	% 88% 8%
8	H	231	% 90% 6%
8	V	231	2% 90% 5%
9	I	205	92% 7%
9	W	205	92% 7%
10	J	198	3% 87% 11%
10	X	198	3% 91% 7%
11	K	211	2% 85% 13%
11	Y	211	% 87% 11%
12	L	222	91% 8%
12	Z	222	% 91% 8%
13	M	246	% 87% 8% 5%
13	a	246	% 92% 5%
14	N	196	% 94% 6%
14	b	196	% 98%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	Z	301	-	-	-	X
19	SO4	V	302	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 49929 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	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	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	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	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 (three-letter code: MG) (formula: Mg).

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

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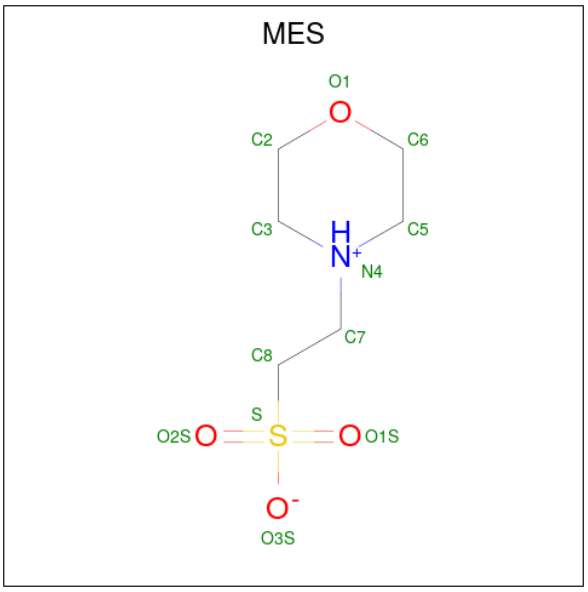
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	X	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

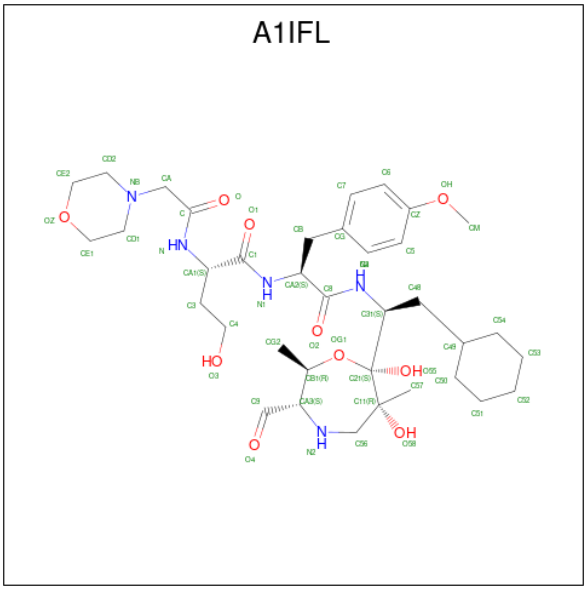
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	N	2	Total Cl 2 2	0	0
16	U	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



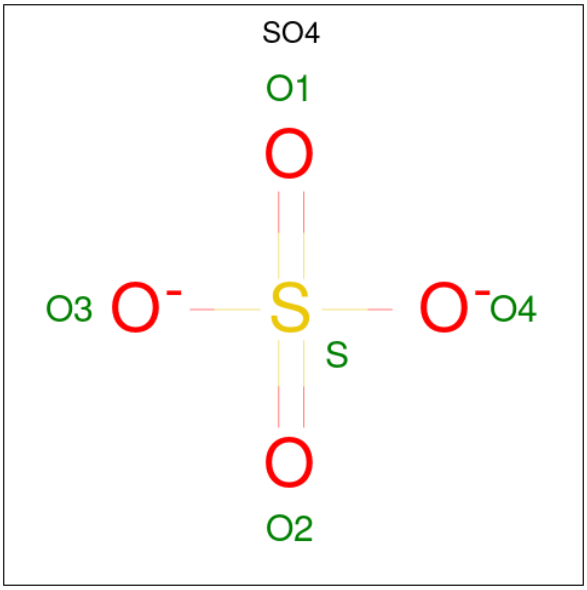
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	1	Total C N O S 12 6 1 4 1	0	0
17	K	1	Total C N O S 12 6 1 4 1	0	0
17	X	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 18 is (2S)-N-[(2S)-1-[[(1S)-2-cyclohexyl-1-[(2R,3S,6R,7S)-3-methanoyl-2,6-dimethyl-6,7-bis(oxidanyl)-1,4-oxazepan-7-yl]ethyl]amino]-3-(4-methoxyphenyl)-1-oxidanylidene-propan-2-yl]-2-(2-morpholin-4-ylethanoylamino)-4-oxidanyl-butanamide (three-letter code: A1IFL) (formula: $C_{36}H_{57}N_5O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	H	1	Total	C	N	O	0	0
			51	36	5	10		
18	K	1	Total	C	N	O	0	0
			51	36	5	10		
18	V	1	Total	C	N	O	0	0
			51	36	5	10		
18	Y	1	Total	C	N	O	0	0
			51	36	5	10		

- Molecule 19 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	K	1	Total	O	S	0	0
			5	4	1		
19	V	1	Total	O	S	0	0
			5	4	1		
19	Y	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	2	Total	O	0	0
			2	2		
20	B	6	Total	O	0	0
			6	6		
20	C	3	Total	O	0	0
			3	3		

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

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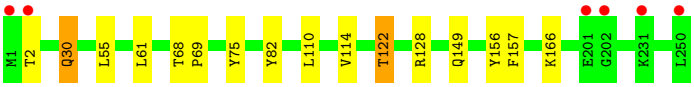
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	Y	7	Total O 7 7	0	0
20	Z	10	Total O 10 10	0	0
20	a	10	Total O 10 10	0	0
20	b	7	Total O 7 7	0	0

3 Residue-property plots (i)

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

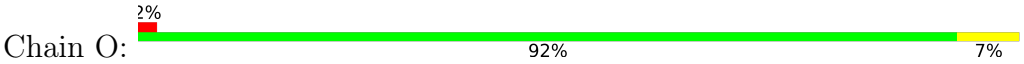
• Molecule 1: Proteasome subunit alpha type-2

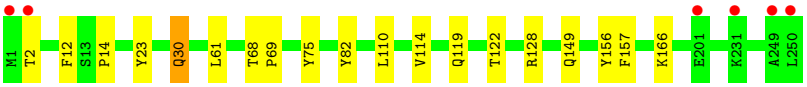
Chain A:



• Molecule 1: Proteasome subunit alpha type-2

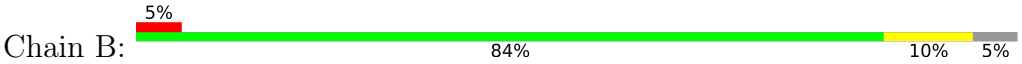
Chain O:

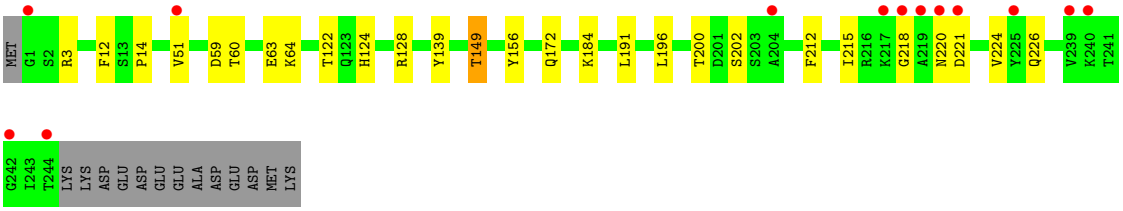




• Molecule 2: Proteasome subunit alpha type-3

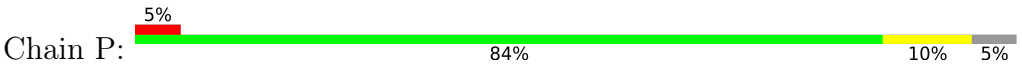
Chain B:

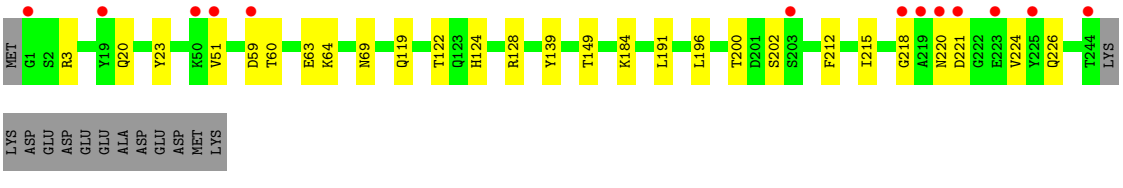




• Molecule 2: Proteasome subunit alpha type-3

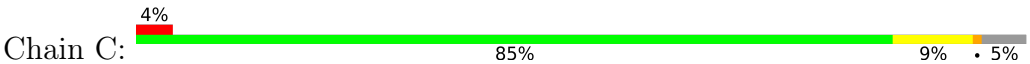
Chain P:

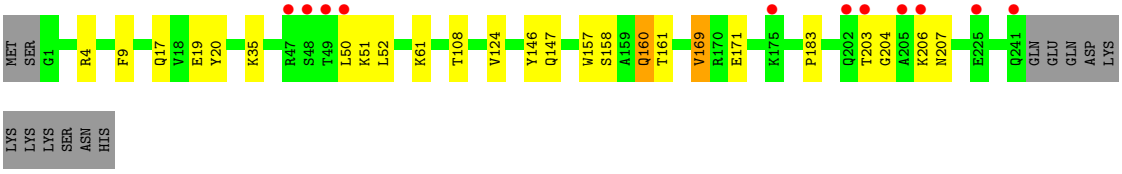




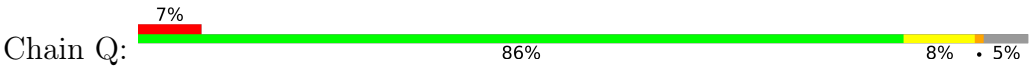
• Molecule 3: Proteasome subunit alpha type-4

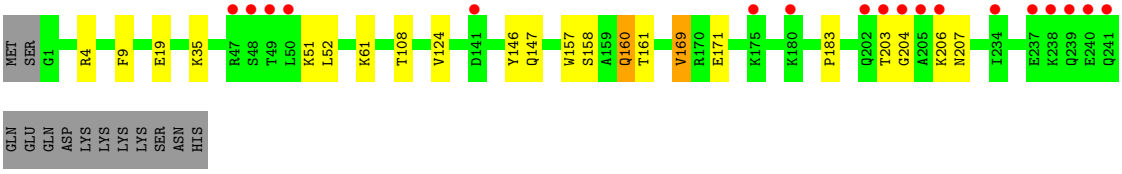
Chain C:



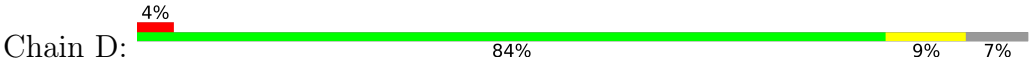


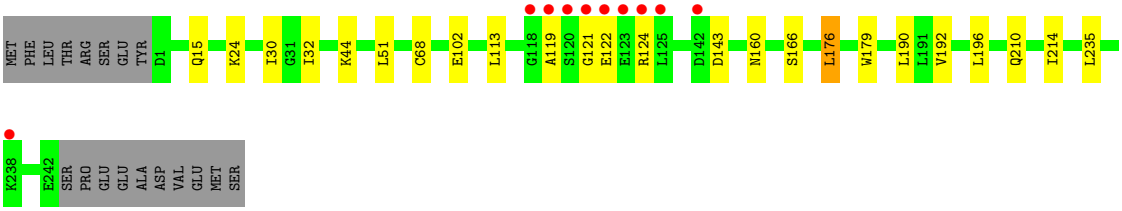
• Molecule 3: Proteasome subunit alpha type-4



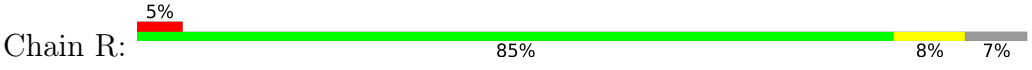


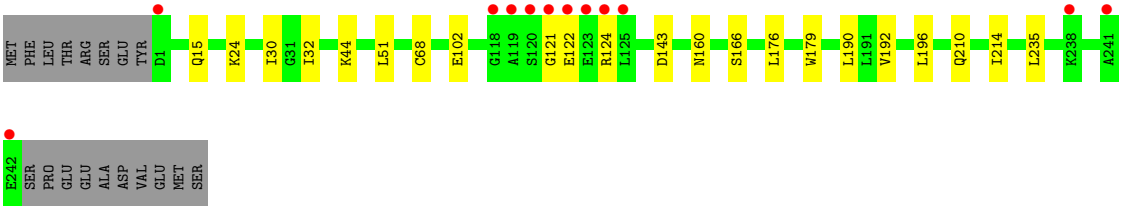
• Molecule 4: Proteasome subunit alpha type-5



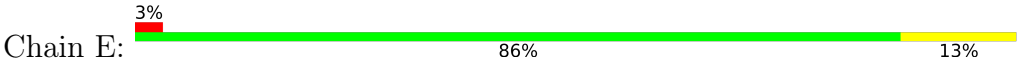


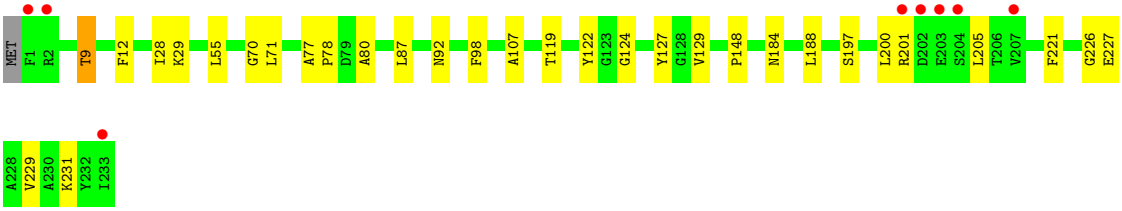
• Molecule 4: Proteasome subunit alpha type-5





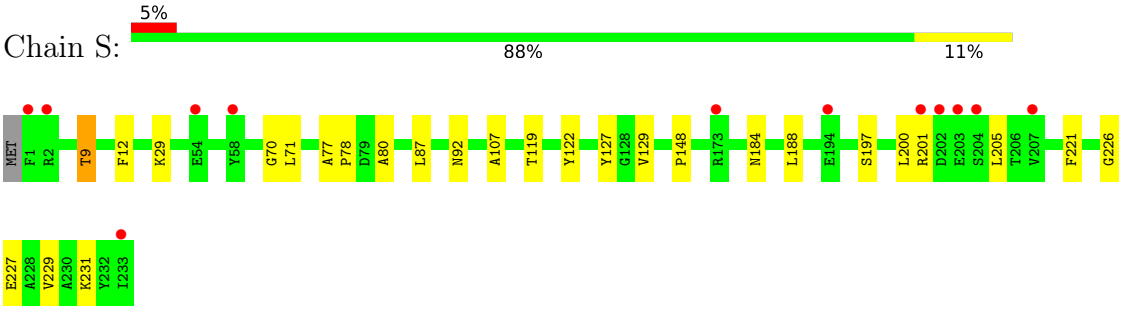
• Molecule 5: Proteasome subunit alpha type-6





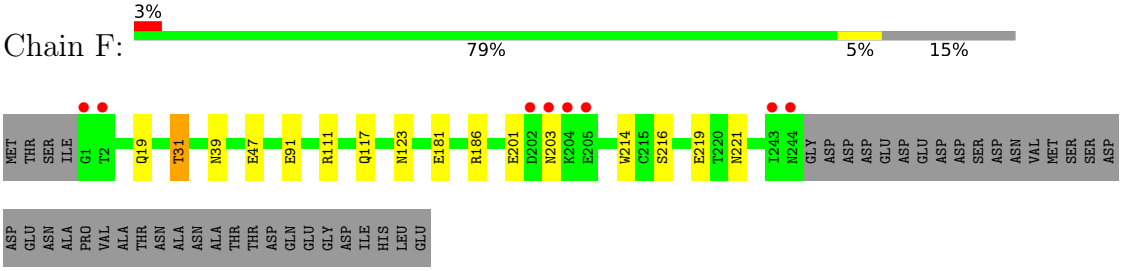
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



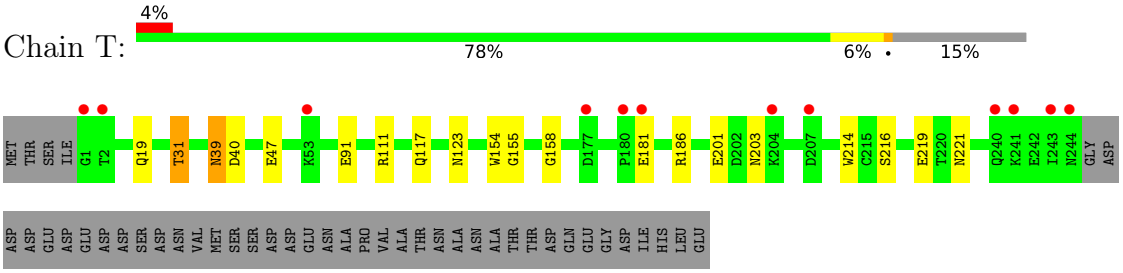
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



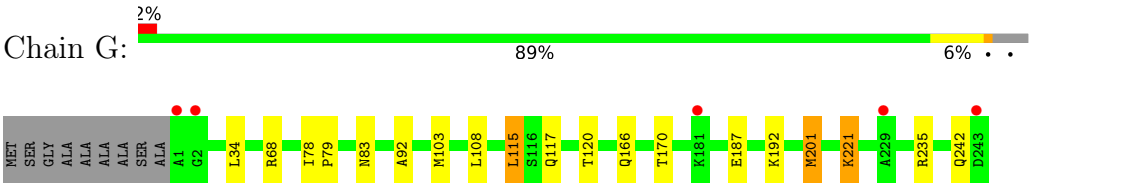
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



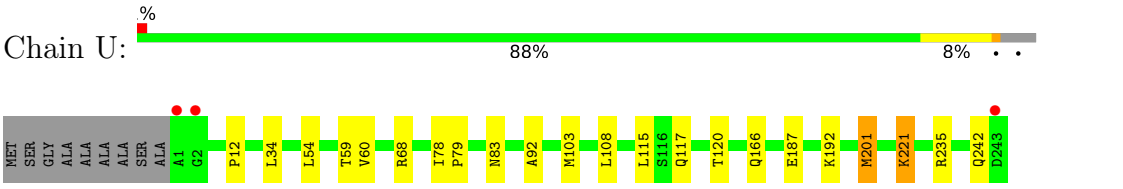
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



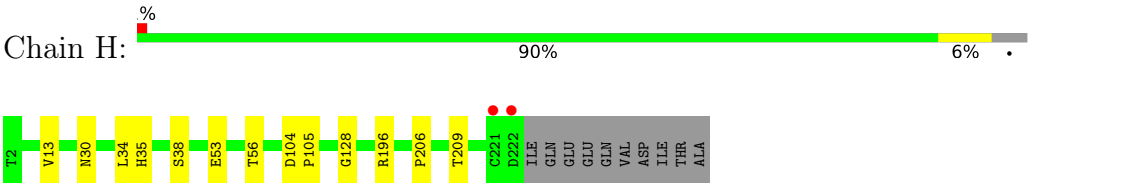
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



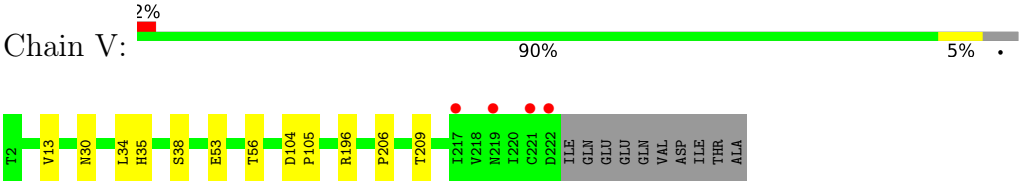
• Molecule 8: Proteasome subunit beta type-2

Chain H:



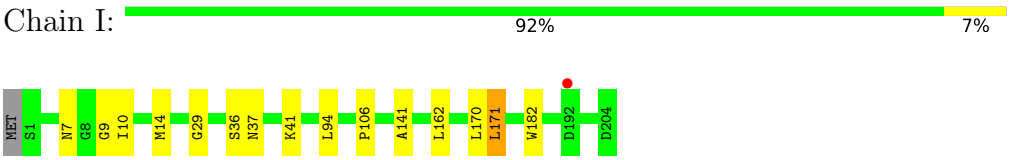
• Molecule 8: Proteasome subunit beta type-2

Chain V:



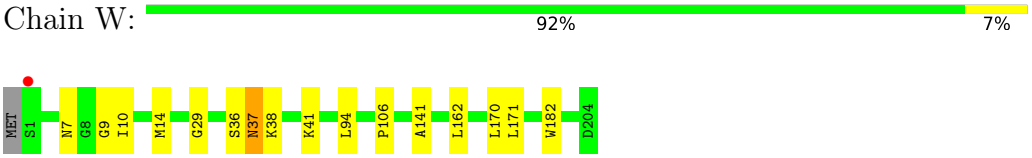
• Molecule 9: Proteasome subunit beta type-3

Chain I:



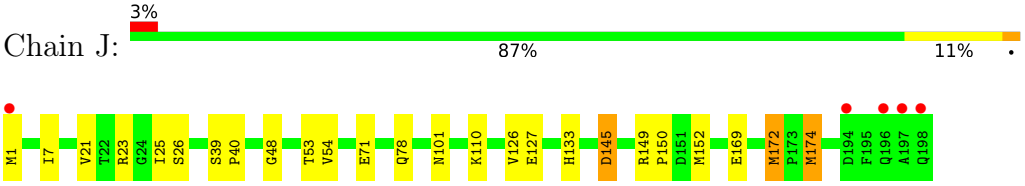
• Molecule 9: Proteasome subunit beta type-3

Chain W:



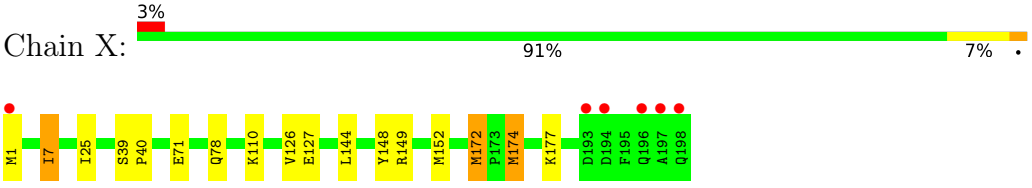
• Molecule 10: Proteasome subunit beta type-4

Chain J:



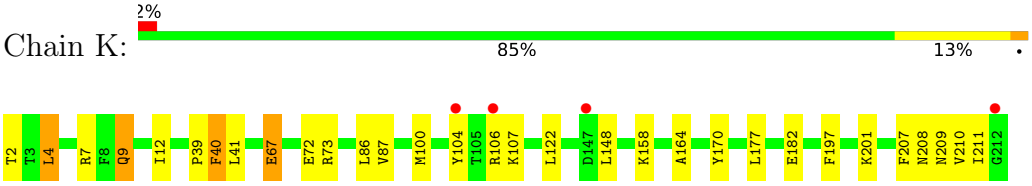
• Molecule 10: Proteasome subunit beta type-4

Chain X:



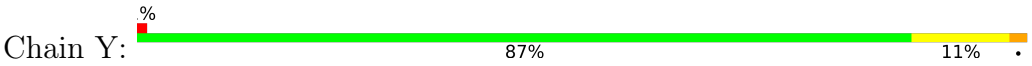
• Molecule 11: Proteasome subunit beta type-5

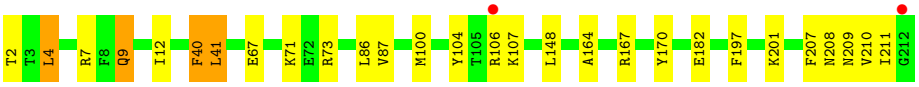
Chain K:



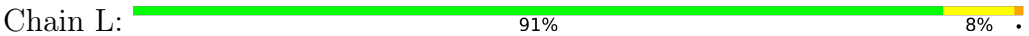
• Molecule 11: Proteasome subunit beta type-5

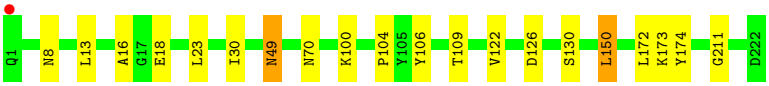
Chain Y:



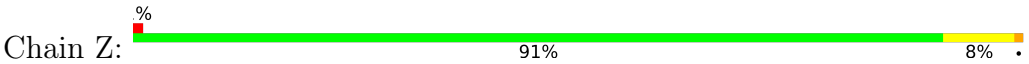


• Molecule 12: Proteasome subunit beta type-6

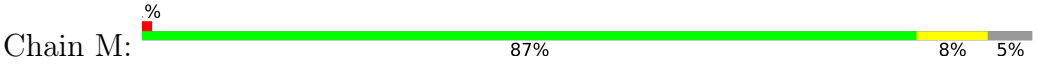


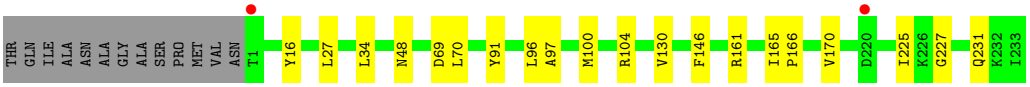


• Molecule 12: Proteasome subunit beta type-6

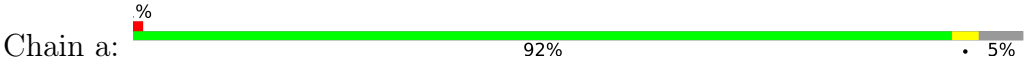


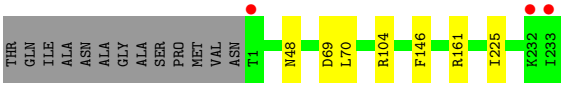
• Molecule 13: Proteasome subunit beta type-7



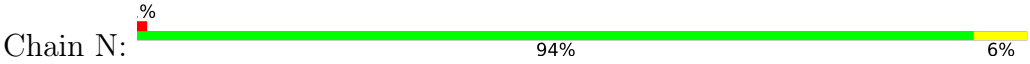


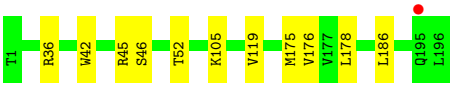
• Molecule 13: Proteasome subunit beta type-7



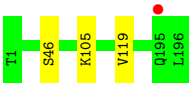


• Molecule 14: Proteasome subunit beta type-1





• Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.52Å 299.48Å 145.00Å 90.00° 112.90° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 29.89 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-2.75) 96.4 (29.89-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.232 0.195 , 0.231	Depositor DCC
R_{free} test set	13235 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 26.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49929	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: A1IFL, CL, MES, SO4, 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	0.66	0/1952	0.71	0/2642
1	O	0.67	0/1952	0.71	0/2642
2	B	0.66	0/1934	0.72	0/2618
2	P	0.66	0/1934	0.72	0/2618
3	C	0.67	0/1919	0.72	0/2598
3	Q	0.67	0/1919	0.72	0/2598
4	D	0.67	0/1886	0.72	0/2541
4	R	0.67	0/1886	0.72	0/2541
5	E	0.67	0/1823	0.72	0/2463
5	S	0.67	0/1823	0.72	0/2463
6	F	0.66	0/1936	0.71	0/2614
6	T	0.66	0/1936	0.71	0/2614
7	G	0.65	0/1959	0.71	0/2652
7	U	0.65	0/1959	0.71	0/2652
8	H	0.67	0/1708	0.72	0/2316
8	V	0.67	0/1708	0.73	0/2316
9	I	0.66	0/1611	0.71	0/2174
9	W	0.66	0/1611	0.71	0/2174
10	J	0.67	0/1613	0.75	0/2173
10	X	0.66	0/1613	0.74	0/2173
11	K	0.66	0/1674	0.77	0/2264
11	Y	0.66	0/1674	0.78	0/2264
12	L	0.66	0/1795	0.72	0/2420
12	Z	0.66	0/1795	0.73	0/2420
13	M	0.66	0/1855	0.72	0/2514
13	a	0.66	0/1855	0.73	0/2514
14	N	0.66	0/1541	0.71	0/2087
14	b	0.66	0/1541	0.71	0/2087
All	All	0.66	0/50412	0.72	0/68152

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	8	0
1	O	1915	0	1929	11	0
2	B	1904	0	1904	12	0
2	P	1904	0	1904	10	0
3	C	1890	0	1903	11	0
3	Q	1890	0	1903	8	0
4	D	1861	0	1839	11	0
4	R	1861	0	1839	8	0
5	E	1795	0	1800	19	0
5	S	1795	0	1800	15	0
6	F	1896	0	1889	4	0
6	T	1896	0	1889	8	0
7	G	1921	0	1913	10	0
7	U	1921	0	1913	12	0
8	H	1677	0	1678	5	0
8	V	1677	0	1678	3	0
9	I	1581	0	1574	8	0
9	W	1581	0	1574	10	0
10	J	1585	0	1590	14	0
10	X	1585	0	1590	13	0
11	K	1637	0	1585	19	0
11	Y	1637	0	1585	20	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	14	0
13	M	1824	0	1832	7	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	2	0	0	1	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	12	0	13	2	0
17	K	12	0	13	0	0
17	X	12	0	13	0	0
18	H	51	0	0	1	0
18	K	51	0	0	2	0
18	V	51	0	0	4	0
18	Y	51	0	0	3	0
19	K	5	0	0	0	0
19	V	5	0	0	2	0
19	Y	5	0	0	0	0
20	A	2	0	0	0	0
20	B	6	0	0	0	0
20	C	3	0	0	0	0
20	D	2	0	0	0	0
20	E	4	0	0	0	0
20	F	5	0	0	0	0
20	G	4	0	0	0	0
20	H	4	0	0	0	0
20	I	3	0	0	0	0
20	J	7	0	0	1	0
20	K	6	0	0	0	0
20	L	5	0	0	0	0
20	M	5	0	0	0	0
20	N	8	0	0	0	0
20	O	2	0	0	0	0
20	P	6	0	0	0	0
20	Q	3	0	0	0	0
20	R	2	0	0	0	0
20	S	4	0	0	0	0
20	T	7	0	0	0	0
20	U	8	0	0	0	0
20	V	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	W	5	0	0	0	0
20	X	11	0	0	0	0
20	Y	7	0	0	0	0
20	Z	10	0	0	0	0
20	a	10	0	0	0	0
20	b	7	0	0	0	0
All	All	49929	0	49295	240	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 (240) 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:104:TYR:CZ	11:Y:182:GLU:HG3	2.07	0.90
11:K:104:TYR:CZ	11:K:182:GLU:HG3	2.08	0.88
19:V:302:SO4:O3	18:V:303:A1IFL:O58	1.92	0.87
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.67	0.76
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.68	0.75
11:K:104:TYR:CE1	11:K:182:GLU:HG3	2.22	0.74
11:K:208:ASN:ND2	10:X:148:TYR:O	2.21	0.73
8:H:128:GLY:H	17:H:301:MES:H31	1.52	0.73
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.54	0.72
11:Y:104:TYR:CE1	11:Y:182:GLU:HG3	2.24	0.71
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.54	0.71
10:J:174:MET:HA	10:X:174:MET:HA	1.73	0.71
12:L:18:GLU:HA	12:L:174:TYR:CE2	2.28	0.69
7:U:92:ALA:HA	7:U:103:MET:HE2	1.75	0.69
11:K:209:ASN:O	9:W:37:ASN:ND2	2.27	0.68
12:Z:18:GLU:HA	12:Z:174:TYR:CE2	2.28	0.68
6:T:31:THR:HG21	6:T:47:GLU:O	1.96	0.66
6:F:31:THR:HG21	6:F:47:GLU:O	1.96	0.64
7:G:92:ALA:HA	7:G:103:MET:HE2	1.79	0.64
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.63	0.63
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.64	0.62
10:X:174:MET:SD	10:X:174:MET:N	2.73	0.62
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.48	0.61
10:X:25:ILE:HG13	10:X:25:ILE:O	2.01	0.61
5:S:12:PHE:H	6:T:19:GLN:HE22	1.49	0.60
7:G:78:ILE:N	7:G:79:PRO:HD2	2.16	0.60
7:U:78:ILE:N	7:U:79:PRO:HD2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:174:MET:SD	10:J:174:MET:N	2.73	0.59
11:Y:167:ARG:HH21	11:Y:209:ASN:ND2	2.02	0.58
11:K:211:ILE:HD11	9:W:38:LYS:HG2	1.86	0.58
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.51	0.56
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.36	0.56
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.88	0.56
10:X:7:ILE:HD11	10:X:144:LEU:HD22	1.87	0.56
11:K:67:GLU:HA	11:K:72:GLU:O	2.07	0.55
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.36	0.55
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.88	0.55
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.28	0.54
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.42	0.54
11:K:4:LEU:HD22	11:K:4:LEU:C	2.28	0.54
18:V:303:A1IFL:C8	18:V:303:A1IFL:C57	2.86	0.53
18:Y:303:A1IFL:C8	18:Y:303:A1IFL:C57	2.85	0.53
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.90	0.53
3:C:35:LYS:HG2	3:C:158:SER:O	2.09	0.53
18:V:303:A1IFL:C57	18:V:303:A1IFL:N4	2.72	0.53
10:J:101:ASN:HB3	10:J:133:HIS:ND1	2.24	0.52
11:K:2:THR:HG21	11:K:164:ALA:CB	2.39	0.52
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.74	0.52
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.91	0.51
2:B:12:PHE:H	3:C:17:GLN:HE22	1.59	0.51
11:K:170:TYR:O	18:K:304:A1IFL:C56	2.59	0.51
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.10	0.51
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.92	0.51
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.46	0.51
5:E:12:PHE:H	6:F:19:GLN:HE22	1.58	0.50
11:Y:40:PHE:HE1	11:Y:182:GLU:O	1.95	0.50
1:O:30:GLN:HA	1:O:30:GLN:HE21	1.76	0.50
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.09	0.50
5:S:127:TYR:O	5:S:148:PRO:HB3	2.10	0.50
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.94	0.50
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.76	0.50
2:B:3:ARG:HB2	5:E:122:TYR:OH	2.11	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.94	0.49
5:E:127:TYR:O	5:E:148:PRO:HB3	2.12	0.49
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.77	0.49
11:Y:2:THR:HG21	11:Y:164:ALA:CB	2.42	0.49
3:C:9:PHE:H	4:D:15:GLN:HE22	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.78	0.48
1:O:12:PHE:H	2:P:20:GLN:HE22	1.61	0.48
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.95	0.48
8:V:206:PRO:O	8:V:209:THR:OG1	2.22	0.48
12:L:8:ASN:HA	12:L:30:ILE:O	2.13	0.48
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.94	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.48
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.95	0.48
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.96	0.48
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.95	0.48
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.49	0.48
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.48
11:K:201:LYS:HG3	11:K:207:PHE:HB2	1.96	0.48
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.96	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.48
11:Y:201:LYS:HG3	11:Y:207:PHE:HB2	1.96	0.48
2:B:196:LEU:O	2:B:200:THR:OG1	2.31	0.47
11:K:197:PHE:HZ	11:K:210:VAL:HG21	1.78	0.47
6:T:158:GLY:O	7:U:54:LEU:HB3	2.14	0.47
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.94	0.47
10:X:172:MET:HB3	10:X:172:MET:HE2	1.65	0.47
8:H:206:PRO:O	8:H:209:THR:OG1	2.22	0.47
2:P:200:THR:HG22	2:P:202:SER:H	1.79	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.49	0.47
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.12	0.47
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.47
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.96	0.47
11:K:40:PHE:HE1	11:K:182:GLU:O	1.98	0.47
11:Y:167:ARG:NH2	11:Y:209:ASN:ND2	2.63	0.47
2:B:172:GLN:HG2	3:C:50:LEU:HD12	1.95	0.47
2:B:200:THR:HG22	2:B:202:SER:H	1.80	0.46
5:S:9:THR:HG21	5:S:119:THR:HA	1.97	0.46
5:E:9:THR:HG21	5:E:119:THR:HA	1.97	0.46
5:E:205:LEU:H	5:E:205:LEU:HD23	1.80	0.46
10:X:1:MET:HB2	10:X:1:MET:HE3	1.50	0.46
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.97	0.46
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.98	0.46
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.50	0.46
5:E:226:GLY:O	5:E:229:VAL:HG22	2.16	0.46
5:S:205:LEU:HD23	5:S:205:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.45
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.97	0.45
18:H:302:A1IFL:C57	18:H:302:A1IFL:N4	2.79	0.45
11:Y:2:THR:HG21	11:Y:164:ALA:HB3	1.98	0.45
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.98	0.45
12:Z:18:GLU:HB2	12:Z:174:TYR:CD2	2.51	0.45
10:J:172:MET:HE2	10:J:172:MET:HB3	1.68	0.45
5:S:226:GLY:O	5:S:229:VAL:HG22	2.17	0.45
7:G:103:MET:HE1	7:G:108:LEU:HD13	1.99	0.45
10:J:150:PRO:HD3	11:Y:208:ASN:HD22	1.81	0.45
2:P:63:GLU:HG3	2:P:64:LYS:HG3	1.99	0.45
11:Y:7:ARG:HG3	11:Y:12:ILE:HG12	1.98	0.45
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.98	0.45
18:K:304:A1IFL:N4	18:K:304:A1IFL:C57	2.80	0.45
2:P:196:LEU:O	2:P:200:THR:OG1	2.31	0.45
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.99	0.45
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.52	0.45
11:Y:170:TYR:O	18:Y:303:A1IFL:C56	2.65	0.45
11:K:7:ARG:HG3	11:K:12:ILE:HG12	1.98	0.44
11:K:9:GLN:NE2	11:K:148:LEU:O	2.50	0.44
11:K:4:LEU:HD22	11:K:4:LEU:O	2.18	0.44
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.52	0.44
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.99	0.44
2:B:63:GLU:HG3	2:B:64:LYS:HG3	1.99	0.44
5:E:98:PHE:O	13:M:91:TYR:HA	2.18	0.44
12:L:18:GLU:HB2	12:L:174:TYR:CD2	2.52	0.44
11:Y:9:GLN:NE2	11:Y:148:LEU:O	2.51	0.44
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.15	0.44
5:E:197:SER:HA	5:E:200:LEU:HG	2.00	0.44
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.00	0.44
7:U:34:LEU:HD23	7:U:201:MET:HE3	1.99	0.44
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.00	0.43
7:G:34:LEU:HD23	7:G:201:MET:HE3	2.00	0.43
13:M:165:ILE:N	13:M:166:PRO:HD2	2.33	0.43
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.00	0.43
10:J:145:ASP:OD1	11:Y:209:ASN:ND2	2.51	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.53	0.43
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.43
10:X:1:MET:N	10:X:1:MET:HE2	2.33	0.43
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.01	0.43
1:O:119:GLN:O	1:O:122:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:302:SO4:S	18:V:303:A1IFL:O58	2.74	0.43
10:X:149:ARG:HB2	10:X:152:MET:HG3	2.00	0.43
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.00	0.43
8:H:35:HIS:HB2	8:H:56:THR:HG21	2.00	0.43
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.54	0.43
14:N:45:ARG:NH2	16:N:203:CL:CL	2.82	0.43
5:S:197:SER:HA	5:S:200:LEU:HG	1.99	0.43
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.43
12:Z:100:LYS:O	12:Z:104:PRO:HA	2.18	0.43
10:J:48:GLY:HA2	20:J:207:HOH:O	2.19	0.43
9:W:10:ILE:HD12	9:W:170:LEU:HD12	2.01	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43
11:Y:197:PHE:HZ	11:Y:210:VAL:HG21	1.83	0.43
9:I:10:ILE:HD12	9:I:170:LEU:HD12	2.01	0.43
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.42
4:D:176:LEU:HD22	5:E:55:LEU:HD13	2.01	0.42
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.01	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
3:C:204:GLY:HA3	3:C:207:ASN:HB2	2.01	0.42
2:P:3:ARG:HB2	5:S:122:TYR:OH	2.19	0.42
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.00	0.42
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.01	0.42
8:V:35:HIS:HB2	8:V:56:THR:HG21	2.00	0.42
9:W:36:SER:CB	10:X:126:VAL:HG21	2.49	0.42
12:Z:126:ASP:C	12:Z:126:ASP:OD2	2.57	0.42
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.02	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG21	2.01	0.42
4:R:24:LYS:O	4:R:166:SER:HA	2.19	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.42
4:D:24:LYS:O	4:D:166:SER:HA	2.20	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
11:Y:211:ILE:HD13	11:Y:211:ILE:HG21	1.63	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CZ2	2.55	0.42
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.42
9:W:14:MET:HB3	9:W:162:LEU:HD11	2.02	0.42
11:Y:4:LEU:HD22	11:Y:4:LEU:O	2.19	0.42
4:R:32:ILE:HD12	4:R:192:VAL:HG23	2.02	0.42
4:R:30:ILE:HD12	4:R:196:LEU:HG	2.01	0.41
12:Z:18:GLU:HA	12:Z:174:TYR:HE2	1.83	0.41
9:I:14:MET:HB3	9:I:162:LEU:HD11	2.02	0.41
10:J:149:ARG:HB2	10:J:152:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	2.01	0.41
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.01	0.41
1:A:110:LEU:O	1:A:114:VAL:HG23	2.20	0.41
4:D:32:ILE:HD12	4:D:192:VAL:HG23	2.03	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CZ2	2.55	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.41
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.88	0.41
12:Z:18:GLU:CB	12:Z:174:TYR:CD2	3.03	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.55	0.41
12:L:18:GLU:CB	12:L:174:TYR:CD2	3.03	0.41
9:W:7:ASN:HA	9:W:29:GLY:O	2.20	0.41
2:B:215:ILE:HG12	2:B:226:GLN:HG2	2.02	0.41
2:P:215:ILE:HG12	2:P:226:GLN:HG2	2.03	0.41
9:I:7:ASN:HA	9:I:29:GLY:O	2.20	0.41
9:I:171:LEU:HD12	9:I:171:LEU:HA	1.92	0.41
7:U:221:LYS:HA	7:U:221:LYS:HE3	2.02	0.41
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.01	0.41
1:A:68:THR:HB	1:A:69:PRO:HD2	2.03	0.41
8:H:128:GLY:N	17:H:301:MES:H31	2.28	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.02	0.41
1:O:110:LEU:O	1:O:114:VAL:HG23	2.20	0.41
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.41	0.41
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.56	0.41
7:G:221:LYS:HE3	7:G:221:LYS:HA	2.02	0.41
1:O:68:THR:HB	1:O:69:PRO:HD2	2.03	0.41
5:S:80:ALA:HB2	5:S:129:VAL:HG21	2.01	0.41
7:U:103:MET:HE1	7:U:108:LEU:HD13	2.01	0.41
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.55	0.41
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.57	0.41
10:J:101:ASN:HB3	10:J:133:HIS:CE1	2.56	0.40
11:K:86:LEU:C	11:K:86:LEU:HD13	2.41	0.40
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.40
6:T:39:ASN:HD22	6:T:40:ASP:N	2.19	0.40
10:J:169:GLU:O	10:X:177:LYS:NZ	2.54	0.40
12:L:100:LYS:O	12:L:104:PRO:HA	2.21	0.40
14:N:45:ARG:NH1	14:N:52:THR:OG1	2.55	0.40
7:U:187:GLU:HG2	7:U:192:LYS:HB2	2.03	0.40
18:Y:303:A1IFL:C57	18:Y:303:A1IFL:N4	2.82	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	0.40
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:115:LEU:HD12	7:G:115:LEU:HA	1.88	0.40
10:J:53:THR:HG23	10:J:54:VAL:HG23	2.04	0.40
11:K:39:PRO:HB2	11:K:40:PHE:CD2	2.56	0.40
11:K:158:LYS:HB2	11:K:177:LEU:HD11	2.04	0.40
2:B:149:THR:O	2:B:156:TYR:HA	2.22	0.40
7:G:187:GLU:HG2	7:G:192:LYS:HB2	2.04	0.40
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.56	0.40
11:Y:211:ILE:O	11:Y:211:ILE:CG2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	19	34
1	O	248/250 (99%)	241 (97%)	5 (2%)	2 (1%)	19	34
2	B	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	13	23
2	P	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	13	23
3	C	239/254 (94%)	227 (95%)	9 (4%)	3 (1%)	12	21
3	Q	239/254 (94%)	228 (95%)	8 (3%)	3 (1%)	12	21
4	D	240/260 (92%)	230 (96%)	8 (3%)	2 (1%)	19	34
4	R	240/260 (92%)	230 (96%)	8 (3%)	2 (1%)	19	34
5	E	231/234 (99%)	218 (94%)	11 (5%)	2 (1%)	17	31
5	S	231/234 (99%)	218 (94%)	11 (5%)	2 (1%)	17	31
6	F	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
7	G	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	34	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	U	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	34 53
8	H	219/231 (95%)	214 (98%)	5 (2%)	0	100 100
8	V	219/231 (95%)	214 (98%)	5 (2%)	0	100 100
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	196/198 (99%)	191 (97%)	5 (3%)	0	100 100
10	X	196/198 (99%)	191 (97%)	5 (3%)	0	100 100
11	K	209/211 (99%)	204 (98%)	5 (2%)	0	100 100
11	Y	209/211 (99%)	205 (98%)	4 (2%)	0	100 100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100 100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100 100
13	M	231/246 (94%)	220 (95%)	11 (5%)	0	100 100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100 100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100 100
14	b	194/196 (99%)	185 (95%)	9 (5%)	0	100 100
All	All	6308/6610 (95%)	6081 (96%)	201 (3%)	26 (0%)	34 53

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LYS
3	C	203	THR
5	E	201	ARG
1	O	166	LYS
3	Q	203	THR
5	S	201	ARG
2	B	51	VAL
2	B	221	ASP
4	D	121	GLY
5	E	227	GLU
2	P	51	VAL
2	P	221	ASP
4	R	121	GLY
5	S	227	GLU
3	C	52	LEU
4	D	122	GLU
3	Q	52	LEU

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Mol	Chain	Res	Type
4	R	122	GLU
1	A	2	THR
3	C	183	PRO
7	G	242	GLN
1	O	2	THR
3	Q	183	PRO
7	U	242	GLN
2	B	218	GLY
2	P	218	GLY

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%)	205 (98%)	4 (2%)	57	73
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	79
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	52
2	P	203/216 (94%)	193 (95%)	10 (5%)	25	43
3	C	213/226 (94%)	204 (96%)	9 (4%)	30	49
3	Q	213/226 (94%)	204 (96%)	9 (4%)	30	49
4	D	198/215 (92%)	190 (96%)	8 (4%)	31	51
4	R	198/215 (92%)	190 (96%)	8 (4%)	31	51
5	E	192/193 (100%)	186 (97%)	6 (3%)	40	60
5	S	192/193 (100%)	186 (97%)	6 (3%)	40	60
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	42
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	42
7	G	207/210 (99%)	199 (96%)	8 (4%)	32	52
7	U	207/210 (99%)	199 (96%)	8 (4%)	32	52
8	H	180/189 (95%)	174 (97%)	6 (3%)	38	58
8	V	180/189 (95%)	174 (97%)	6 (3%)	38	58
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	169 (98%)	3 (2%)	60	76
10	J	175/175 (100%)	163 (93%)	12 (7%)	15	27
10	X	175/175 (100%)	168 (96%)	7 (4%)	31	51
11	K	168/168 (100%)	158 (94%)	10 (6%)	19	33
11	Y	168/168 (100%)	157 (94%)	11 (6%)	17	30
12	L	185/185 (100%)	176 (95%)	9 (5%)	25	43
12	Z	185/185 (100%)	176 (95%)	9 (5%)	25	43
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	56
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	56
14	N	162/162 (100%)	159 (98%)	3 (2%)	57	73
14	b	162/162 (100%)	159 (98%)	3 (2%)	57	73
All	All	5328/5536 (96%)	5125 (96%)	203 (4%)	33	53

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	59	ASP
2	B	60	THR
2	B	122	THR
2	B	149	THR
2	B	184	LYS
2	B	191	LEU
2	B	212	PHE
2	B	220	ASN
3	C	4	ARG
3	C	19	GLU
3	C	51	LYS
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	206	LYS
4	D	68	CYS

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Mol	Chain	Res	Type
4	D	102	GLU
4	D	124	ARG
4	D	143	ASP
4	D	176	LEU
4	D	190	LEU
4	D	214	ILE
4	D	235	LEU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	231	LYS
6	F	31	THR
6	F	39	ASN
6	F	117	GLN
6	F	123	ASN
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	203	ASN
6	F	214	TRP
6	F	221	ASN
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	166	GLN
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	38	SER
8	H	53	GLU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	1	MET
10	J	7	ILE

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Mol	Chain	Res	Type
10	J	23	ARG
10	J	25	ILE
10	J	26	SER
10	J	71	GLU
10	J	78	GLN
10	J	110	LYS
10	J	127	GLU
10	J	145	ASP
10	J	172	MET
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	40	PHE
11	K	41	LEU
11	K	67	GLU
11	K	73	ARG
11	K	87	VAL
11	K	100	MET
11	K	106	ARG
11	K	107	LYS
12	L	23	LEU
12	L	49	ASN
12	L	106	TYR
12	L	109	THR
12	L	126	ASP
12	L	130	SER
12	L	150	LEU
12	L	172	LEU
12	L	173	LYS
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	225	ILE
14	N	46	SER
14	N	105	LYS
14	N	119	VAL
1	O	30	GLN
1	O	61	LEU
1	O	157	PHE

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Mol	Chain	Res	Type
2	P	59	ASP
2	P	60	THR
2	P	69	ASN
2	P	119	GLN
2	P	122	THR
2	P	149	THR
2	P	184	LYS
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
3	Q	4	ARG
3	Q	19	GLU
3	Q	51	LYS
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
3	Q	206	LYS
4	R	68	CYS
4	R	102	GLU
4	R	124	ARG
4	R	143	ASP
4	R	176	LEU
4	R	190	LEU
4	R	214	ILE
4	R	235	LEU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	231	LYS
6	T	31	THR
6	T	39	ASN
6	T	117	GLN
6	T	123	ASN
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	203	ASN
6	T	214	TRP

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Mol	Chain	Res	Type
6	T	221	ASN
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	166	GLN
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	38	SER
8	V	53	GLU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	7	ILE
10	X	71	GLU
10	X	78	GLN
10	X	110	LYS
10	X	127	GLU
10	X	172	MET
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	40	PHE
11	Y	41	LEU
11	Y	67	GLU
11	Y	71	LYS
11	Y	73	ARG
11	Y	87	VAL
11	Y	100	MET
11	Y	106	ARG
11	Y	107	LYS
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	109	THR
12	Z	126	ASP
12	Z	130	SER

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Mol	Chain	Res	Type
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	225	ILE
14	b	46	SER
14	b	105	LYS
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
2	B	20	GLN
2	B	69	ASN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	241	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN

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Mol	Chain	Res	Type
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
5	E	198	GLN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
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	144	GLN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	158	ASN
12	L	165	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	213	GLN
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
2	P	20	GLN
2	P	69	ASN
2	P	95	GLN
2	P	119	GLN

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Mol	Chain	Res	Type
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
3	Q	17	GLN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	198	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	184	ASN
5	S	198	GLN
6	T	19	GLN
6	T	39	ASN
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	186	ASN
8	V	66	HIS
8	V	144	GLN
8	V	172	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN

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Mol	Chain	Res	Type
10	X	147	HIS
11	Y	85	ASN
11	Y	166	HIS
11	Y	176	ASN
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	165	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	213	GLN
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	MES	K	302	-	12,12,12	0.75	0	14,16,16	0.50	0
18	A1IFL	K	304	11	47,54,54	1.77	7 (14%)	52,75,75	1.06	2 (3%)
18	A1IFL	Y	303	11	47,54,54	1.56	6 (12%)	52,75,75	1.05	3 (5%)
18	A1IFL	V	303	8	47,54,54	1.14	3 (6%)	52,75,75	1.07	4 (7%)
19	SO4	V	302	-	4,4,4	0.56	0	6,6,6	0.09	0
17	MES	X	202	-	12,12,12	0.77	0	14,16,16	0.38	0
19	SO4	Y	302	-	4,4,4	0.38	0	6,6,6	0.05	0
19	SO4	K	303	-	4,4,4	0.67	0	6,6,6	0.09	0
18	A1IFL	H	302	8	47,54,54	1.12	2 (4%)	52,75,75	1.24	4 (7%)
17	MES	H	301	-	12,12,12	0.72	0	14,16,16	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	K	302	-	-	4/6/14/14	0/1/1/1
18	A1IFL	K	304	11	-	13/37/85/85	0/3/4/4
18	A1IFL	Y	303	11	-	10/37/85/85	0/3/4/4
18	A1IFL	V	303	8	-	6/37/85/85	0/3/4/4
17	MES	X	202	-	-	2/6/14/14	0/1/1/1
18	A1IFL	H	302	8	-	13/37/85/85	0/3/4/4
17	MES	H	301	-	-	2/6/14/14	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	304	A1IFL	CB-CG	-6.75	1.35	1.51
18	H	302	A1IFL	CB-CG	-6.08	1.36	1.51
18	Y	303	A1IFL	CB-CG	-6.02	1.36	1.51
18	V	303	A1IFL	CB-CG	-5.34	1.38	1.51
18	K	304	A1IFL	O58-C11	-4.97	1.37	1.44
18	Y	303	A1IFL	O58-C11	-4.50	1.38	1.44
18	V	303	A1IFL	OG1-CB1	-3.89	1.38	1.43
18	K	304	A1IFL	OG1-CB1	-3.34	1.39	1.43
18	K	304	A1IFL	OG1-C21	-3.23	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	303	A1IFL	OG1-CB1	-3.20	1.39	1.43
18	K	304	A1IFL	C54-C49	-2.75	1.44	1.52
18	H	302	A1IFL	OG1-CB1	-2.49	1.40	1.43
18	Y	303	A1IFL	OG1-C21	-2.35	1.38	1.43
18	K	304	A1IFL	C53-C54	-2.28	1.47	1.53
18	Y	303	A1IFL	C54-C49	-2.24	1.46	1.52
18	V	303	A1IFL	OG1-C21	-2.20	1.38	1.43
18	Y	303	A1IFL	C57-C11	-2.19	1.49	1.52
18	K	304	A1IFL	CB-CA2	-2.03	1.49	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	302	A1IFL	CM-OH-CZ	-3.82	109.22	117.51
18	V	303	A1IFL	CE2-CD2-NB	3.06	114.74	110.10
18	H	302	A1IFL	CA-NB-CD2	-2.80	106.75	111.09
18	K	304	A1IFL	C53-C54-C49	-2.76	106.93	112.15
18	H	302	A1IFL	C3-CA1-N	-2.65	105.51	110.88
18	K	304	A1IFL	CM-OH-CZ	-2.33	112.44	117.51
18	H	302	A1IFL	C53-C54-C49	-2.29	107.82	112.15
18	Y	303	A1IFL	CM-OH-CZ	-2.22	112.70	117.51
18	V	303	A1IFL	CM-OH-CZ	-2.20	112.73	117.51
18	V	303	A1IFL	CA-NB-CD2	-2.19	107.69	111.09
18	Y	303	A1IFL	C53-C54-C49	-2.19	108.01	112.15
18	V	303	A1IFL	C3-CA1-N	-2.12	106.58	110.88
18	Y	303	A1IFL	C48-C31-N4	-2.12	104.60	109.46

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	302	MES	C7-C8-S-O1S
17	X	202	MES	C8-C7-N4-C3
18	H	302	A1IFL	CA1-C3-C4-O3
18	H	302	A1IFL	C21-C31-C48-C49
18	H	302	A1IFL	C31-C48-C49-C54
18	K	304	A1IFL	C21-C31-C48-C49
18	V	303	A1IFL	CA1-C3-C4-O3
18	V	303	A1IFL	C21-C31-C48-C49
18	V	303	A1IFL	C31-C48-C49-C54
18	Y	303	A1IFL	CA1-C3-C4-O3
18	Y	303	A1IFL	C21-C31-C48-C49

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Mol	Chain	Res	Type	Atoms
18	H	302	A1IFL	N4-C31-C48-C49
18	Y	303	A1IFL	N4-C31-C48-C49
18	H	302	A1IFL	C6-CZ-OH-CM
18	H	302	A1IFL	C5-CZ-OH-CM
18	K	304	A1IFL	N4-C31-C48-C49
18	V	303	A1IFL	N4-C31-C48-C49
17	K	302	MES	C7-C8-S-O3S
18	H	302	A1IFL	C31-C48-C49-C50
18	V	303	A1IFL	C31-C48-C49-C50
18	K	304	A1IFL	N1-CA2-CB-CG
18	H	302	A1IFL	N-C-CA-NB
18	Y	303	A1IFL	N1-CA2-CB-CG
18	H	302	A1IFL	O-C-CA-NB
18	K	304	A1IFL	C4-C3-CA1-N
18	H	302	A1IFL	C4-C3-CA1-C1
18	K	304	A1IFL	C4-C3-CA1-C1
17	K	302	MES	C8-C7-N4-C3
18	K	304	A1IFL	O2-C8-CA2-N1
18	Y	303	A1IFL	C31-C48-C49-C54
18	K	304	A1IFL	N4-C8-CA2-N1
17	K	302	MES	C7-C8-S-O2S
18	H	302	A1IFL	C4-C3-CA1-N
18	Y	303	A1IFL	O1-C1-CA1-N
17	H	301	MES	C8-C7-N4-C5
18	Y	303	A1IFL	N1-C1-CA1-N
18	K	304	A1IFL	C31-C48-C49-C54
18	K	304	A1IFL	C31-C48-C49-C50
18	Y	303	A1IFL	C31-C48-C49-C50
18	K	304	A1IFL	C8-CA2-CB-CG
18	H	302	A1IFL	O2-C8-CA2-N1
18	H	302	A1IFL	N4-C8-CA2-N1
18	V	303	A1IFL	O1-C1-CA1-N
18	K	304	A1IFL	N-C-CA-NB
18	K	304	A1IFL	C6-CZ-OH-CM
18	Y	303	A1IFL	C8-CA2-CB-CG
18	Y	303	A1IFL	O2-C8-CA2-N1
17	X	202	MES	C7-C8-S-O1S
18	K	304	A1IFL	O2-C8-CA2-CB
17	H	301	MES	C8-C7-N4-C3

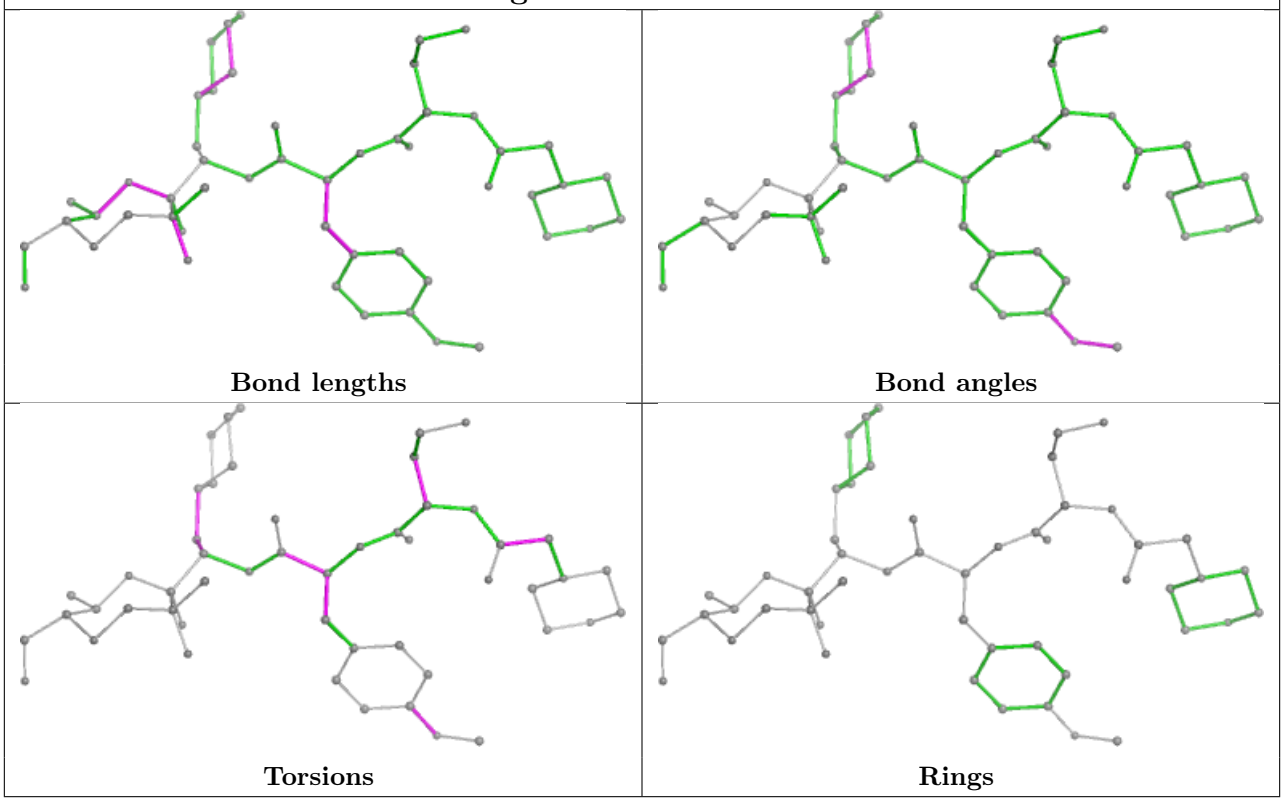
There are no ring outliers.

6 monomers are involved in 12 short contacts:

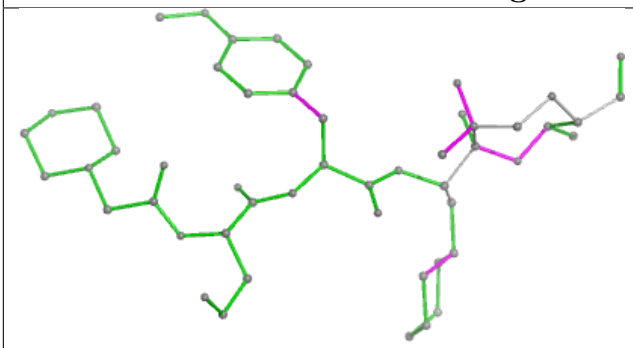
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	304	A1IFL	2	0
18	Y	303	A1IFL	3	0
18	V	303	A1IFL	4	0
19	V	302	SO4	2	0
18	H	302	A1IFL	1	0
17	H	301	MES	2	0

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

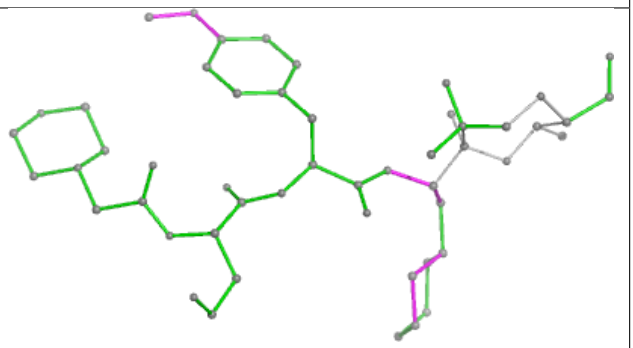
Ligand A1IFL K 304



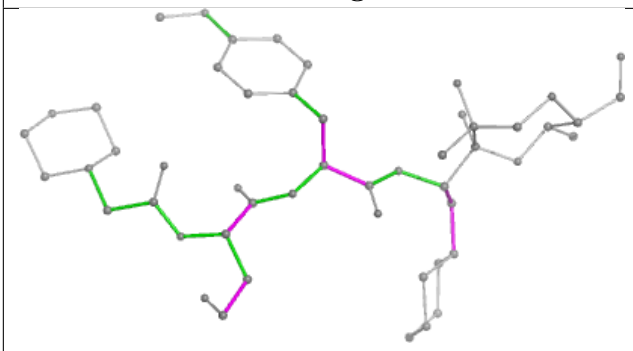
Ligand A1IFL Y 303



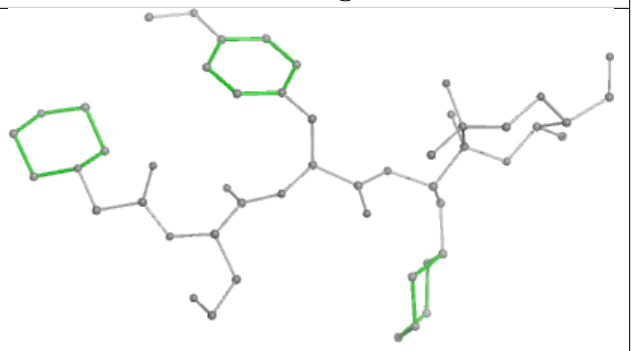
Bond lengths



Bond angles

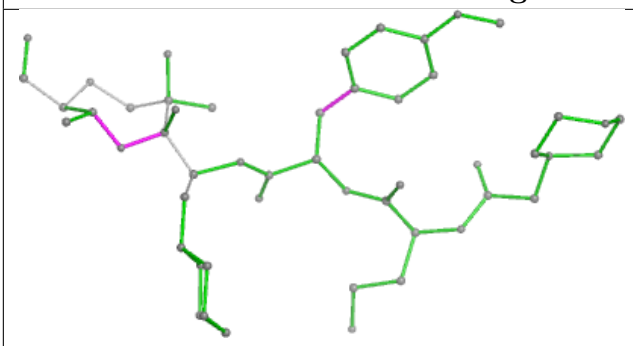


Torsions

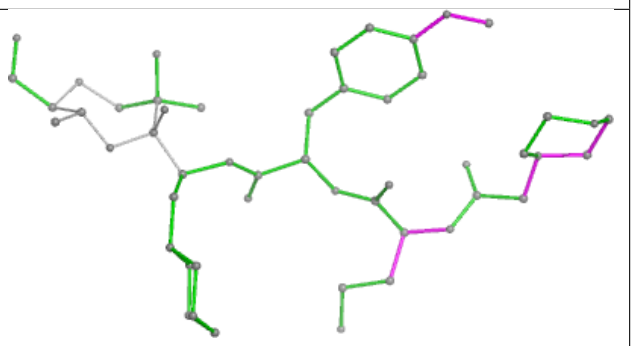


Rings

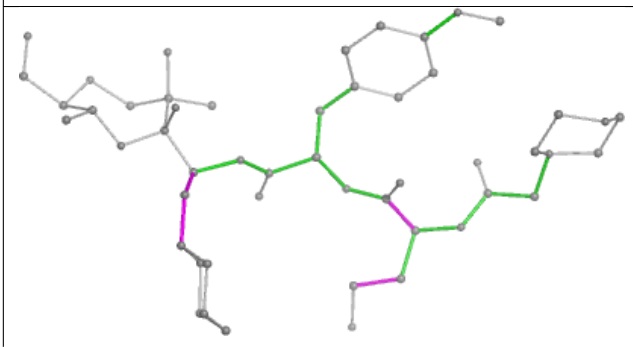
Ligand A1IFL V 303



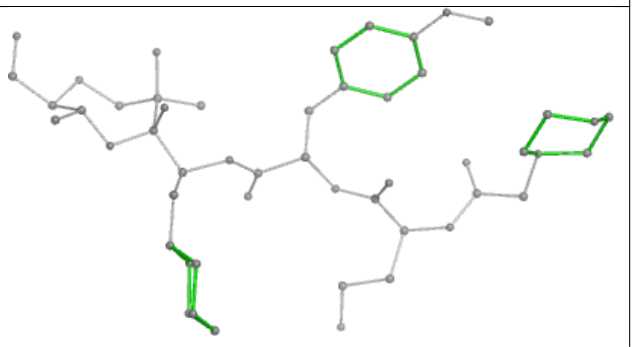
Bond lengths



Bond angles

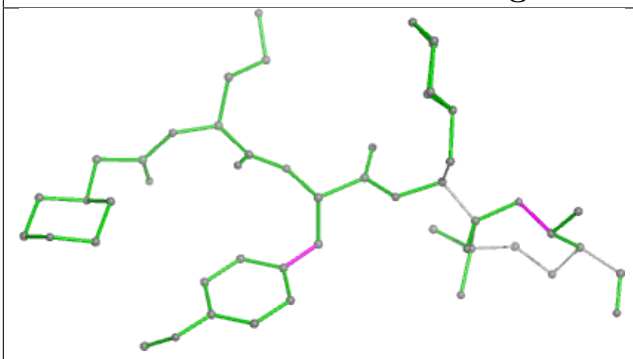


Torsions

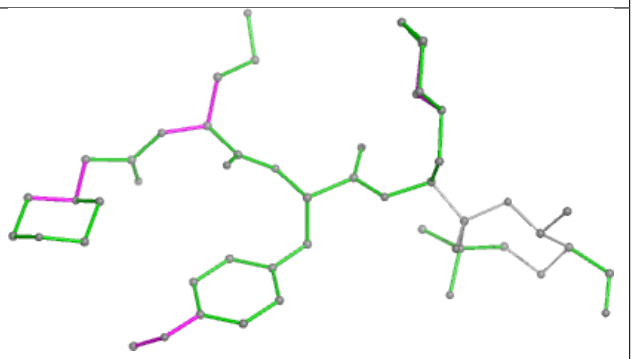


Rings

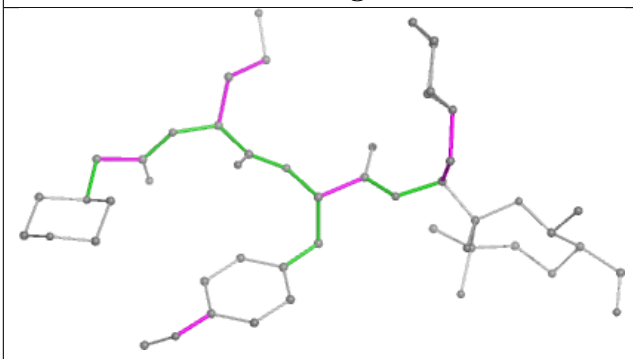
Ligand A1IFL H 302



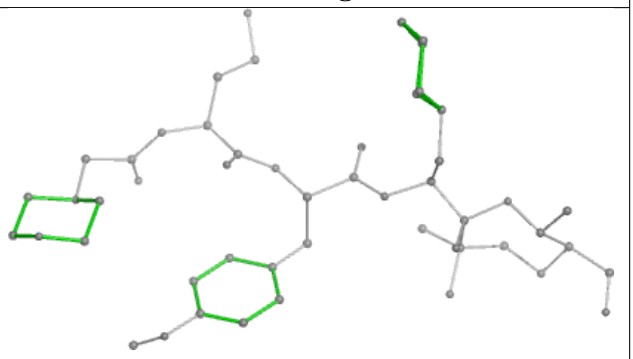
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.18	6 (2%)	59	68	49, 65, 94, 137	0
1	O	250/250 (100%)	-0.14	6 (2%)	59	68	56, 73, 106, 145	0
2	B	244/258 (94%)	0.09	13 (5%)	26	31	53, 72, 114, 147	0
2	P	244/258 (94%)	0.04	13 (5%)	26	31	56, 73, 120, 153	0
3	C	241/254 (94%)	0.01	11 (4%)	32	39	53, 75, 131, 143	0
3	Q	241/254 (94%)	0.21	18 (7%)	14	17	57, 84, 146, 165	0
4	D	242/260 (93%)	0.10	10 (4%)	37	44	55, 76, 114, 153	0
4	R	242/260 (93%)	0.11	12 (4%)	28	35	58, 81, 121, 162	0
5	E	233/234 (99%)	-0.04	8 (3%)	45	53	57, 77, 112, 140	0
5	S	233/234 (99%)	0.08	12 (5%)	27	33	57, 80, 114, 160	0
6	F	244/288 (84%)	-0.15	8 (3%)	46	54	52, 70, 106, 138	0
6	T	244/288 (84%)	0.01	12 (4%)	29	36	55, 73, 112, 138	0
7	G	243/252 (96%)	-0.24	5 (2%)	63	72	50, 65, 96, 148	0
7	U	243/252 (96%)	-0.22	3 (1%)	79	85	53, 66, 93, 148	0
8	H	221/231 (95%)	-0.22	2 (0%)	84	89	51, 62, 86, 141	0
8	V	221/231 (95%)	-0.16	4 (1%)	68	76	53, 66, 92, 136	0
9	I	204/205 (99%)	-0.43	1 (0%)	91	94	48, 61, 84, 112	0
9	W	204/205 (99%)	-0.36	1 (0%)	91	94	46, 64, 85, 102	0
10	J	198/198 (100%)	-0.16	5 (2%)	57	66	48, 64, 90, 148	0
10	X	198/198 (100%)	-0.20	6 (3%)	50	59	51, 66, 90, 149	0
11	K	211/211 (100%)	-0.12	4 (1%)	66	75	48, 63, 90, 111	0
11	Y	211/211 (100%)	-0.24	2 (0%)	84	89	52, 63, 91, 109	0
12	L	222/222 (100%)	-0.35	1 (0%)	91	94	48, 65, 88, 103	0
12	Z	222/222 (100%)	-0.25	3 (1%)	75	82	50, 65, 92, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.37	2 (0%) 84 89	48, 63, 84, 110	0
13	a	233/246 (94%)	-0.29	3 (1%) 77 84	46, 62, 82, 111	0
14	N	196/196 (100%)	-0.34	1 (0%) 91 94	47, 59, 88, 113	0
14	b	196/196 (100%)	-0.35	1 (0%) 91 94	46, 59, 86, 108	0
All	All	6364/6610 (96%)	-0.14	173 (2%) 54 63	46, 68, 108, 165	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	120	SER	11.8
4	D	118	GLY	11.2
4	R	121	GLY	10.9
4	D	119	ALA	9.6
4	D	121	GLY	9.6
7	U	1	ALA	8.9
10	J	197	ALA	8.7
5	S	1	PHE	8.1
3	C	49	THR	8.0
7	G	1	ALA	8.0
7	U	243	ASP	8.0
4	R	119	ALA	7.8
10	J	198	GLN	7.7
10	X	198	GLN	7.5
3	C	50	LEU	7.4
2	B	220	ASN	7.3
4	D	124	ARG	7.1
3	Q	50	LEU	7.0
4	D	120	SER	7.0
2	P	220	ASN	6.7
8	V	222	ASP	6.6
1	A	1	MET	6.5
8	H	222	ASP	6.4
2	B	219	ALA	6.3
3	Q	49	THR	6.1
2	P	219	ALA	5.9
4	R	124	ARG	5.9
10	X	197	ALA	5.7
4	D	125	LEU	5.4
5	E	202	ASP	5.3
5	S	2	ARG	5.3
1	O	1	MET	5.3

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Mol	Chain	Res	Type	RSRZ
4	D	122	GLU	5.2
3	Q	203	THR	5.0
5	S	207	VAL	4.9
5	S	202	ASP	4.9
2	P	1	GLY	4.6
7	G	2	GLY	4.6
3	Q	48	SER	4.5
6	T	2	THR	4.5
5	E	1	PHE	4.4
5	S	233	ILE	4.4
2	P	244	THR	4.3
6	F	1	GLY	4.3
13	M	1	THR	4.3
10	J	196	GLN	4.1
10	X	1	MET	4.1
7	G	243	ASP	4.1
3	Q	241	GLN	4.1
10	X	196	GLN	4.1
8	H	221	CYS	3.9
3	Q	180	LYS	3.8
8	V	221	CYS	3.8
3	Q	238	LYS	3.8
9	W	1	SER	3.8
5	E	233	ILE	3.7
2	B	244	THR	3.6
13	a	1	THR	3.5
3	Q	240	GLU	3.5
4	R	122	GLU	3.5
1	A	250	LEU	3.5
2	B	1	GLY	3.5
1	O	249	ALA	3.4
2	B	221	ASP	3.4
3	Q	47	ARG	3.3
6	F	243	ILE	3.3
10	X	194	ASP	3.3
5	S	204	SER	3.3
4	R	123	GLU	3.3
6	F	202	ASP	3.2
1	A	2	THR	3.2
4	R	241	ALA	3.1
4	R	125	LEU	3.1
3	Q	237	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	123	GLU	3.1
6	T	244	ASN	3.1
3	Q	205	ALA	3.1
11	Y	212	GLY	3.0
5	E	2	ARG	3.0
2	B	218	GLY	3.0
6	F	203	ASN	3.0
5	S	54	GLU	3.0
1	O	2	THR	2.9
6	T	53	LYS	2.9
13	a	233	ILE	2.9
3	Q	234	ILE	2.9
11	K	106	ARG	2.9
3	C	203	THR	2.8
4	R	242	GLU	2.8
8	V	219	ASN	2.8
12	Z	1	GLN	2.8
10	J	194	ASP	2.8
10	J	1	MET	2.8
4	R	118	GLY	2.8
2	B	51	VAL	2.7
2	B	225	TYR	2.7
1	A	202	GLY	2.7
6	T	204	LYS	2.7
5	S	201	ARG	2.7
6	F	204	LYS	2.7
9	I	192	ASP	2.7
6	T	243	ILE	2.6
5	E	201	ARG	2.6
3	Q	141	ASP	2.6
3	Q	239	GLN	2.6
6	F	244	ASN	2.6
7	G	181	LYS	2.6
4	R	1	ASP	2.6
11	K	212	GLY	2.6
14	N	195	GLN	2.5
2	P	221	ASP	2.5
3	C	47	ARG	2.5
5	S	203	GLU	2.5
6	T	241	LYS	2.5
6	F	205	GLU	2.5
14	b	195	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
6	T	207	ASP	2.5
3	C	241	GLN	2.5
3	Q	202	GLN	2.4
2	P	50	LYS	2.4
6	F	2	THR	2.4
2	P	51	VAL	2.4
4	D	238	LYS	2.4
6	T	177	ASP	2.4
6	T	181	GLU	2.4
5	E	204	SER	2.3
2	P	218	GLY	2.3
4	R	238	LYS	2.3
13	a	232	LYS	2.3
12	L	1	GLN	2.3
1	O	250	LEU	2.3
2	B	217	LYS	2.3
3	C	202	GLN	2.3
7	U	2	GLY	2.3
1	O	231	LYS	2.3
3	Q	175	LYS	2.3
13	M	220	ASP	2.3
5	E	203	GLU	2.2
11	Y	106	ARG	2.2
7	G	229	ALA	2.2
2	P	19	TYR	2.2
2	P	225	TYR	2.2
6	T	1	GLY	2.2
6	T	240	GLN	2.2
10	X	193	ASP	2.2
2	P	223	GLU	2.2
3	Q	204	GLY	2.2
12	Z	171	PRO	2.2
2	B	240	LYS	2.2
5	E	207	VAL	2.2
11	K	104	TYR	2.2
2	P	203	SER	2.2
3	C	175	LYS	2.2
2	B	204	ALA	2.2
5	S	58	TYR	2.1
6	T	180	PRO	2.1
11	K	147	ASP	2.1
5	S	173	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	206	LYS	2.1
2	B	242	GLY	2.1
3	C	225	GLU	2.1
2	B	239	VAL	2.1
1	O	201	GLU	2.1
2	P	59	ASP	2.1
3	C	48	SER	2.1
8	V	217	ILE	2.1
1	A	231	LYS	2.1
3	C	205	ALA	2.1
3	C	206	LYS	2.0
5	S	194	GLU	2.0
12	Z	173	LYS	2.0
4	D	142	ASP	2.0
1	A	201	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 monosaccharides 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
15	MG	Z	301	1/1	0.44	0.43	98,98,98,98	0
15	MG	G	301	1/1	0.81	0.26	75,75,75,75	0
18	A1IFL	H	302	51/51	0.87	0.22	50,65,74,76	51
17	MES	H	301	12/12	0.88	0.26	60,64,68,68	12
18	A1IFL	V	303	51/51	0.90	0.23	55,66,83,84	51
15	MG	W	301	1/1	0.91	0.22	78,78,78,78	0
15	MG	V	301	1/1	0.92	0.17	112,112,112,112	0
15	MG	N	201	1/1	0.94	0.21	74,74,74,74	0

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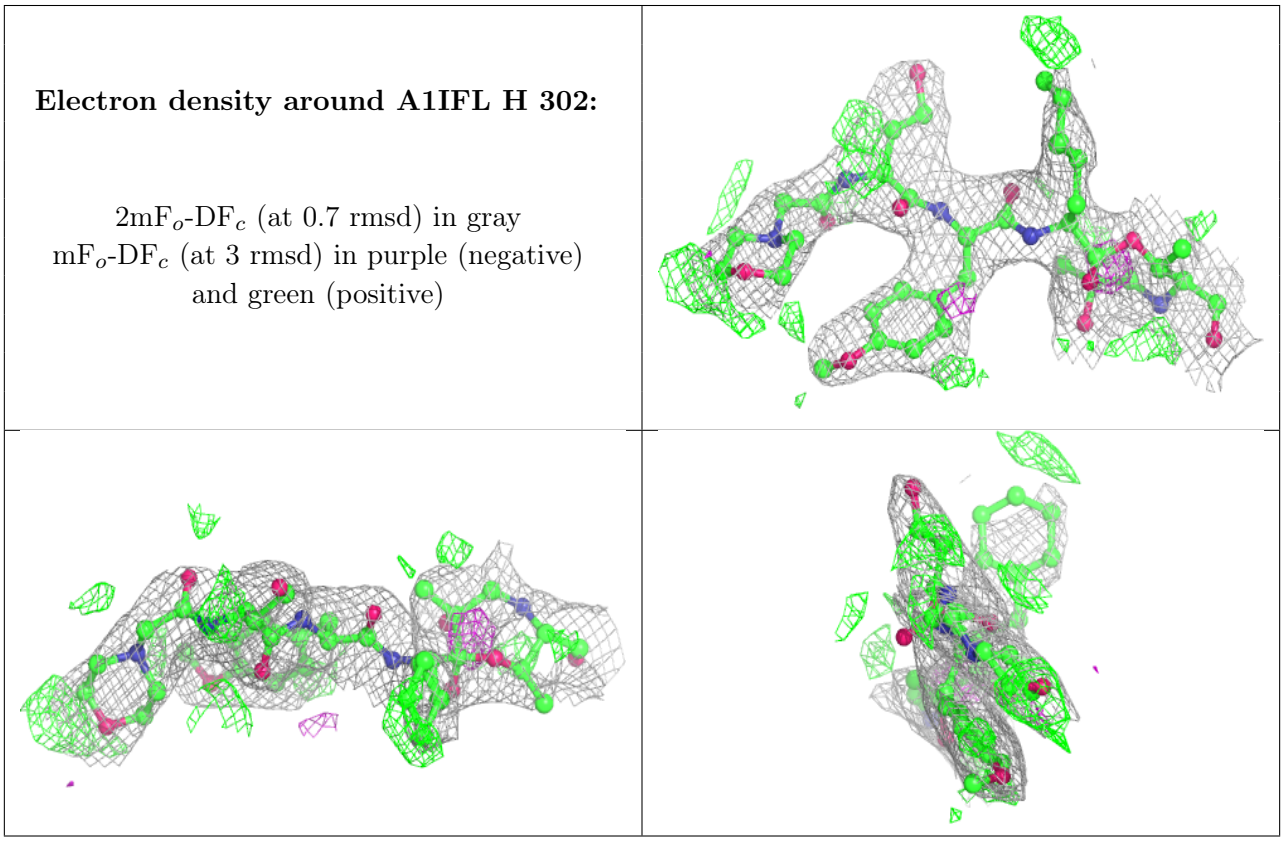
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	CL	N	203	1/1	0.95	0.17	95,95,95,95	0
18	A1IFL	K	304	51/51	0.95	0.15	48,52,76,76	0
15	MG	K	301	1/1	0.95	0.23	89,89,89,89	0
18	A1IFL	Y	303	51/51	0.95	0.16	46,56,72,72	0
19	SO4	K	303	5/5	0.95	0.25	100,107,110,110	0
16	CL	U	301	1/1	0.96	0.07	66,66,66,66	0
16	CL	b	201	1/1	0.96	0.07	70,70,70,70	0
19	SO4	Y	302	5/5	0.96	0.24	70,72,73,76	5
15	MG	I	301	1/1	0.97	0.13	75,75,75,75	0
17	MES	K	302	12/12	0.97	0.17	75,82,86,88	0
19	SO4	V	302	5/5	0.97	0.25	78,83,88,88	5
17	MES	X	202	12/12	0.97	0.13	69,78,84,86	0
16	CL	N	202	1/1	0.98	0.08	70,70,70,70	0
16	CL	G	302	1/1	0.98	0.06	59,59,59,59	0
15	MG	X	201	1/1	0.99	0.32	52,52,52,52	0
15	MG	Y	301	1/1	0.99	0.05	84,84,84,84	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.

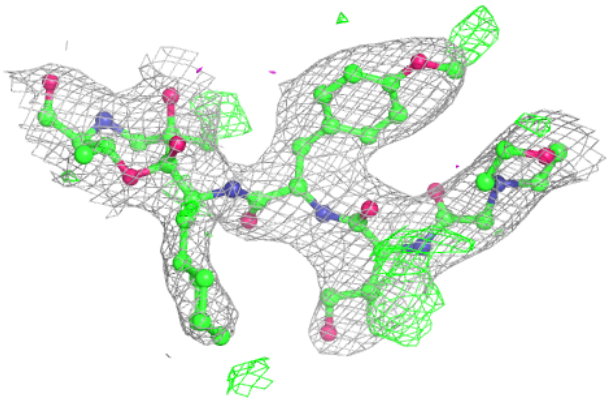
Electron density around A1IFL H 302:

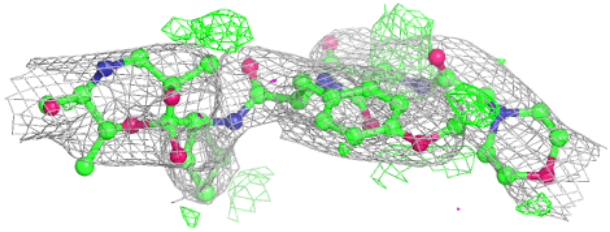
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

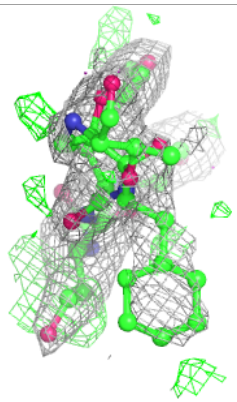


Electron density around A1IFL V 303:

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

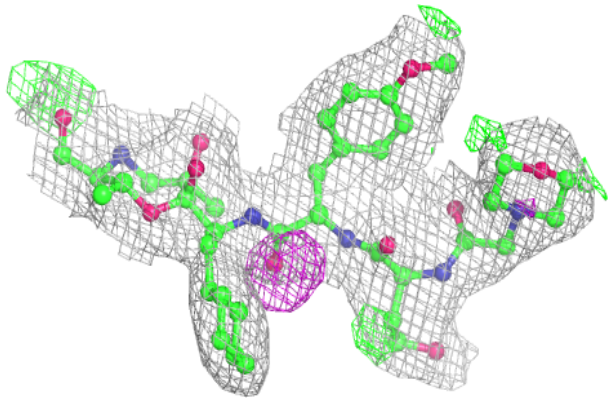


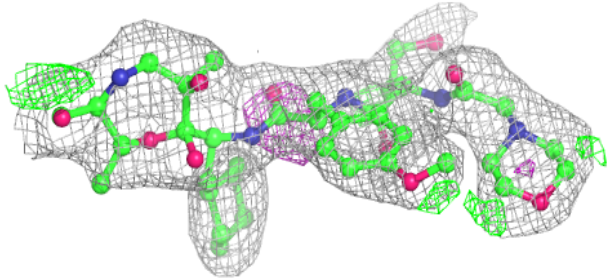


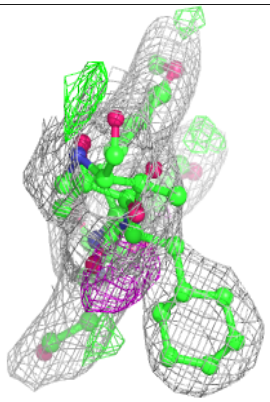


Electron density around A1IFL K 304:

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

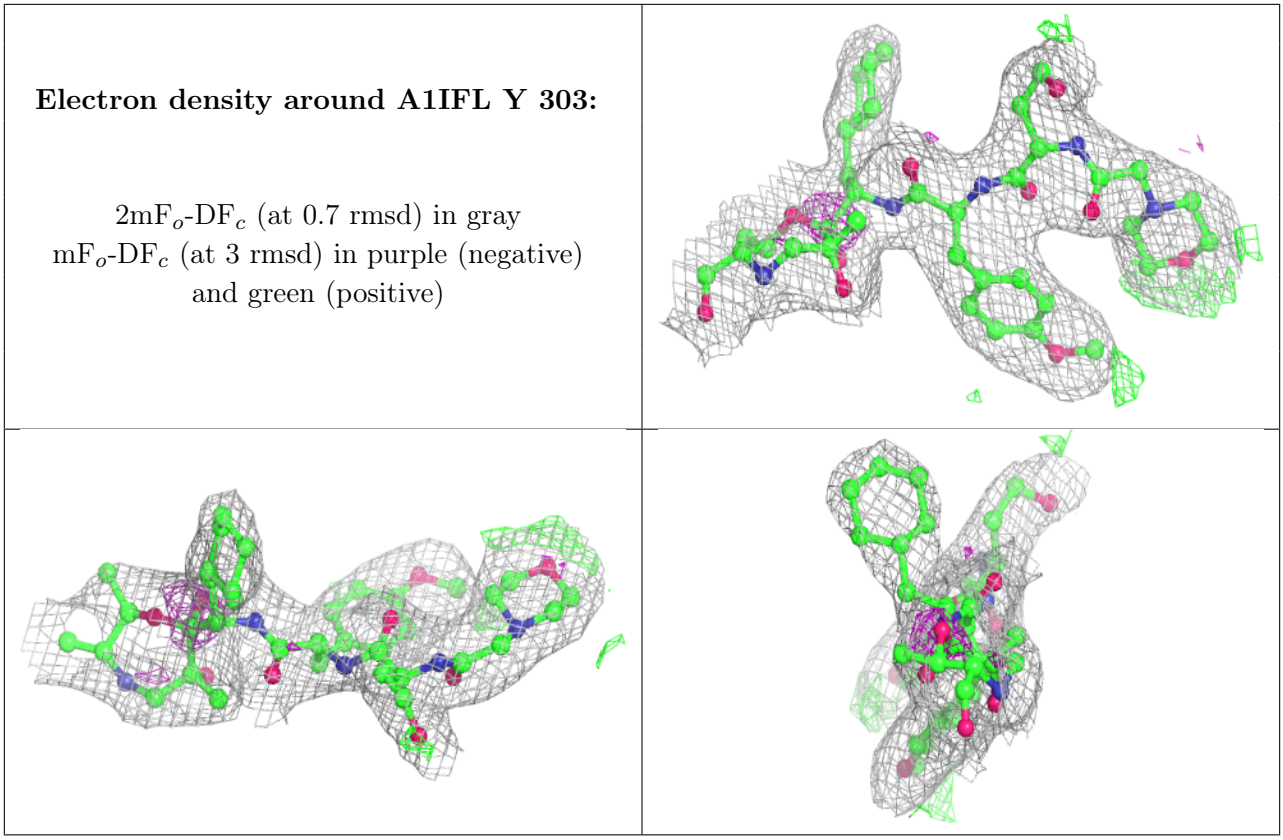






Electron density around A1IFL Y 303:

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



6.5 Other polymers (i)

There are no such residues in this entry.