Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 05:10 am GMT

PDB ID	:	5AHJ
Title	:	Yeast 20S proteasome in complex with Macyranone A
Authors	:	Etzbach, L.; Plaza, A.; Dubiella, C.; Groll, M.; Kaiser, M.; Mueller, R.
Deposited on	:	2015-02-06
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

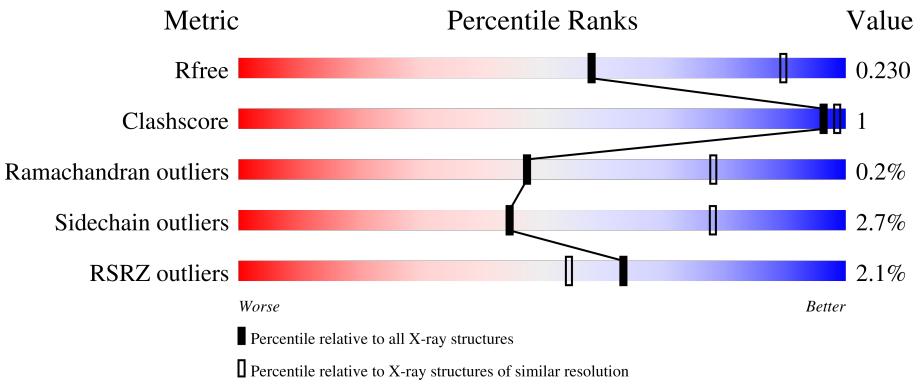
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	4% 99% •
1	O	250	2% 99% •
2	B	258	4% 90% • • 5%
2	P	258	3% 90% • • 5%
3	C	254	4% 91% • • 5%

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Mol	Chain	Length	Quality of chain
3	Q	254	7% 91% 5%
4	D	260	2% 86% 5% 9%
4	R	260	3% 86% 5% 9%
5	E	234	2% 94% 5%
5	S	234	6% 93% 6%
6	F	288	2% 81% 15%
6	T	288	2% 81% 15%
7	G	252	2% 91% 5%
7	U	252	2% 91% 5%
8	H	232	% 93%
8	V	232	% 94%
9	I	205	94% 5%
9	W	205	% 95% 5%
10	J	198	2% 93%
10	X	198	2% 93%
11	K	212	95% 5%
11	Y	212	95% 5%
12	L	222	95% 5%
12	Z	222	% 94% 6%
13	M	233	% 96%
13	a	233	97%
14	N	196	% 97%
14	b	196	% 99%

2 Entry composition (i)

There are 19 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
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	1904	1201	321	379	3	0	0	0
2	P	244	1904	1201	321	379	3	0	0	0

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	1882	1176	330	372	4	0	0	1
3	Q	241	1882	1176	330	372	4	0	0	1

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	236	1814	1136	305	366	7	0	0	1
4	R	236	1814	1136	305	366	7	0	0	1

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	231	1773	1114	307	348	4	0	0	0
5	S	231	1773	1114	307	348	4	0	0	0

- Molecule 6 is a protein called PROBABLE PROTEASOME SUBUNIT ALPHA TYPE-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	244	1893	1203	330	356	4	0	0	1
6	T	244	1893	1203	330	356	4	0	0	1

- Molecule 7 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	242	1908	1214	321	365	8	0	0	1
7	U	242	1907	1214	321	364	8	0	0	1

- Molecule 8 is a protein called PROTEASOME SUBUNIT BETA TYPE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	222	1684	1061	293	323	7	0	0	0
8	V	222	1684	1061	293	323	7	0	0	0

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1581	1010	258	305	8	0	0	0
9	W	204	1581	1010	258	305	8	0	0	0

- Molecule 10 is a protein called PROTEASOME SUBUNIT BETA TYPE-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	195	1561	992	264	299	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	195	1561	992	264	299	6	0	0	0

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

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

- Molecule 12 is a protein called PROTEASOME SUBUNIT BETA TYPE-6.

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

- Molecule 13 is a protein called PROTEASOME SUBUNIT BETA TYPE-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	233	1824	1154	312	351	7	0	0	0
			Total	C	N	O	S			
13	a	233	1824	1154	312	351	7	0	0	0

- Molecule 14 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	196	1512	955	250	300	7	0	0	0
			Total	C	N	O	S			
14	b	196	1512	955	250	300	7	0	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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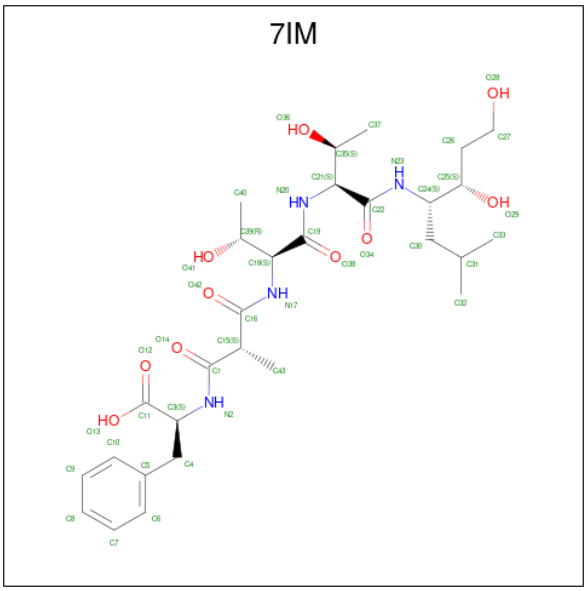
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

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

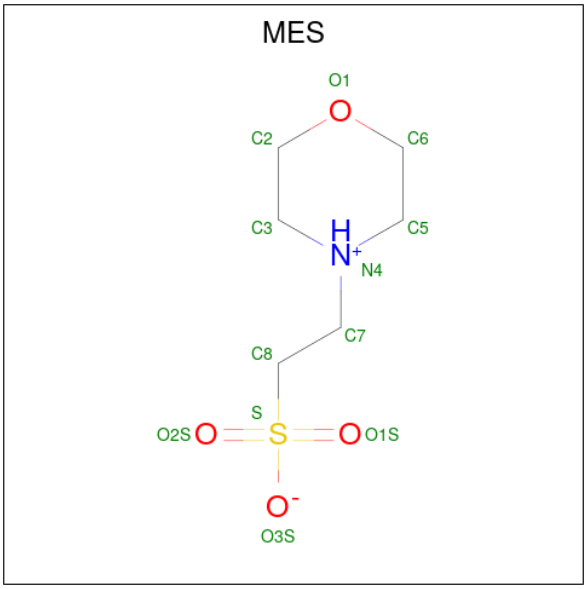
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0
16	b	1	Total Cl 1 1	0	0

- Molecule 17 is N-[(2S)-3-{[(1S)-1-carboxy-2-phenylethyl]amino}-2-methyl-3-oxopropanoyl]-L-threonyl-N-[(3S,4S)-1,3-dihydroxy-6-methylheptan-4-yl]-L-allothreoninamide (three-letter code: 7IM) (formula: $C_{29}H_{46}N_4O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
17	H	1	43	29	4	10	0	0
17	K	1	43	29	4	10	0	0
17	N	1	43	29	4	10	0	0
17	V	1	43	29	4	10	0	0
17	Y	1	43	29	4	10	0	0
17	b	1	43	29	4	10	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	A	24	24	24	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	B	26	26	26	0	0
			Total	O		
19	C	8	8	8	0	0
			Total	O		
19	D	10	10	10	0	0
			Total	O		
19	E	7	7	7	0	0
			Total	O		
19	F	8	8	8	0	0
			Total	O		
19	G	16	16	16	0	0
			Total	O		
19	H	17	17	17	0	0
			Total	O		
19	I	8	8	8	0	0
			Total	O		
19	J	18	18	18	0	0
			Total	O		
19	K	14	14	14	0	0
			Total	O		
19	L	21	21	21	0	0
			Total	O		
19	M	19	19	19	0	0
			Total	O		
19	N	13	13	13	0	0
			Total	O		
19	O	5	5	5	0	0
			Total	O		
19	P	9	9	9	0	0
			Total	O		
19	Q	3	3	3	0	0
			Total	O		
19	R	8	8	8	0	0
			Total	O		
19	S	6	6	6	0	0
			Total	O		
19	T	10	10	10	0	0
			Total	O		
19	U	15	15	15	0	0
			Total	O		
19	V	17	17	17	0	0

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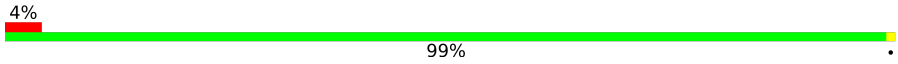
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
19	W	9	9	9	0	0
			Total	O		
19	X	22	22	22	0	0
			Total	O		
19	Y	8	8	8	0	0
			Total	O		
19	Z	12	12	12	0	0

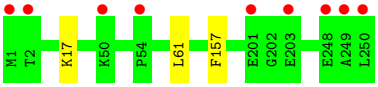
3 Residue-property plots (i)

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

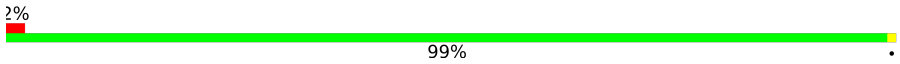
Chain A:

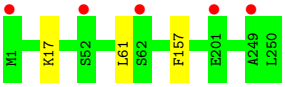




• Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-2

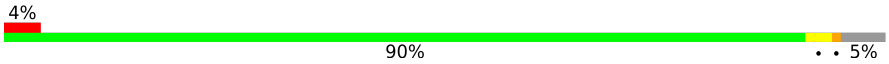
Chain O:

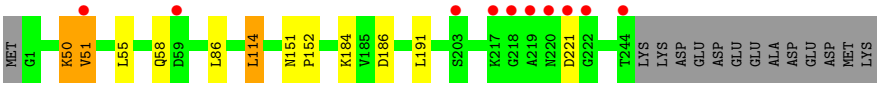




• Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-3

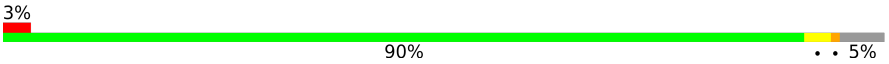
Chain B:

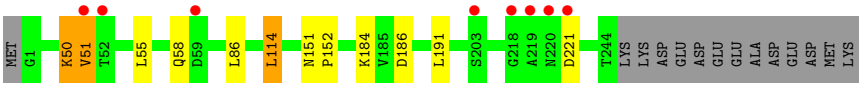




• Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-3

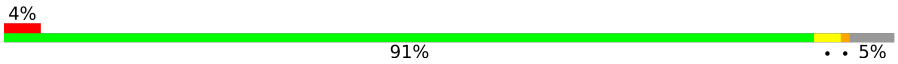
Chain P:

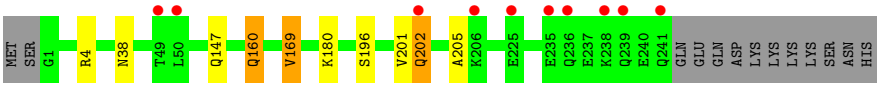




• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

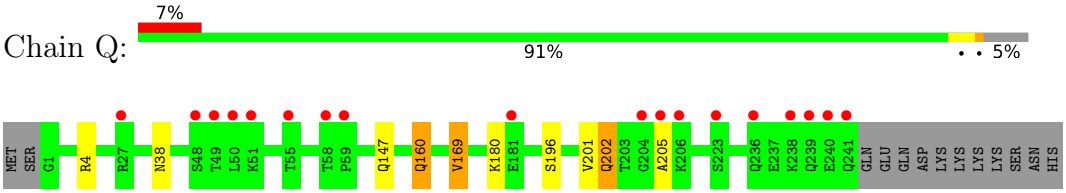
Chain C:





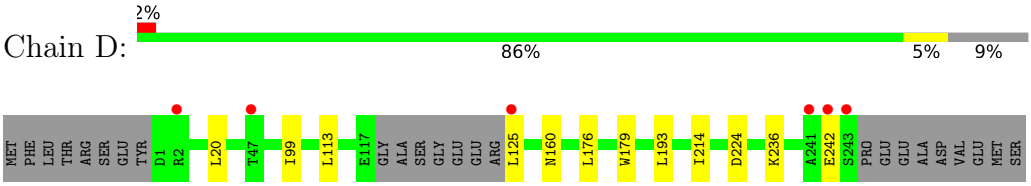
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

Chain Q:



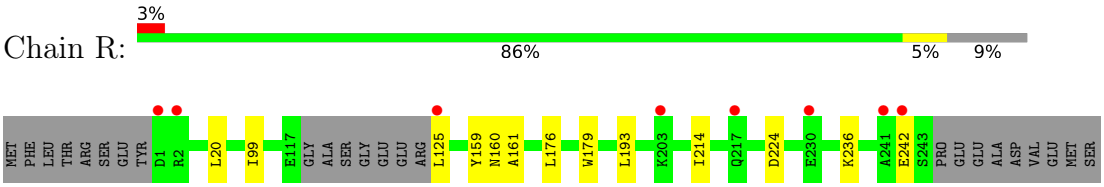
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5

Chain D:



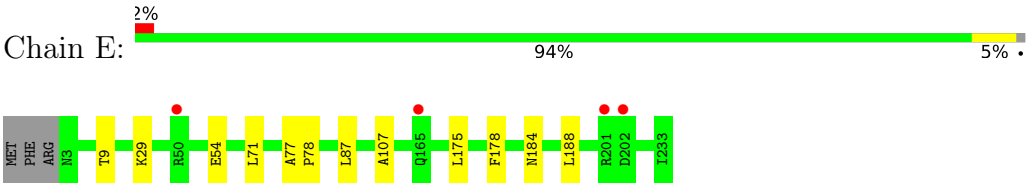
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5

Chain R:



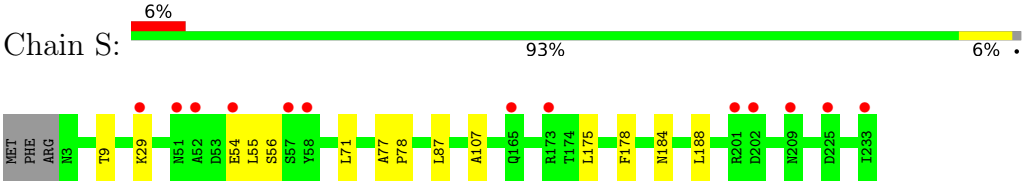
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6

Chain E:



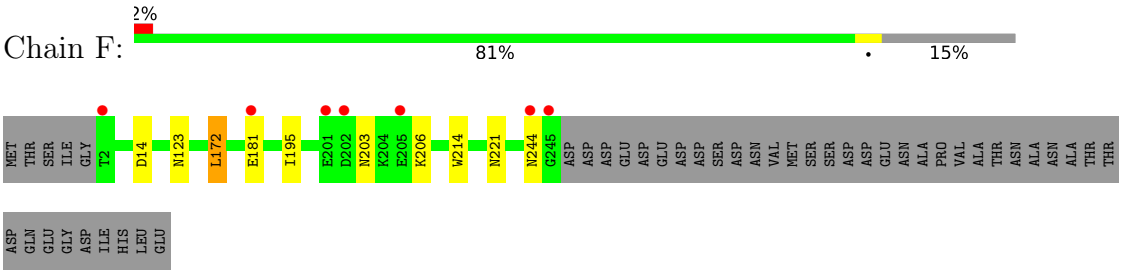
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6

Chain S:



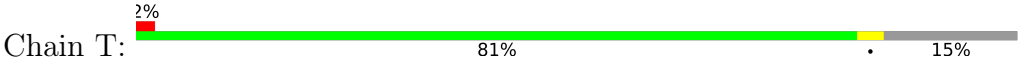
• Molecule 6: PROBABLE PROTEASOME SUBUNIT ALPHA TYPE-7

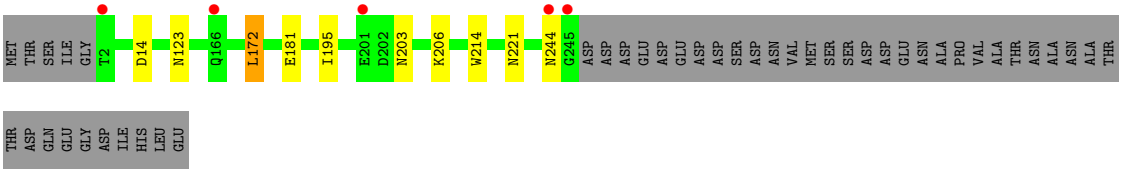
Chain F:



• Molecule 6: PROBABLE PROTEASOME SUBUNIT ALPHA TYPE-7

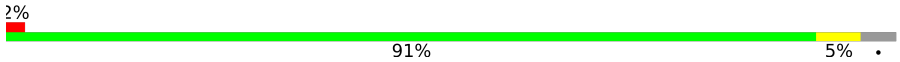
Chain T:

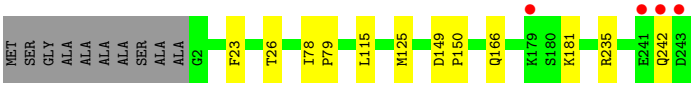




• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1

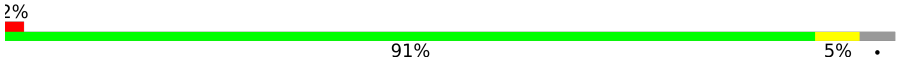
Chain G:

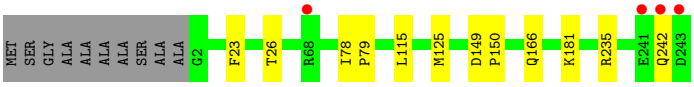




• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1

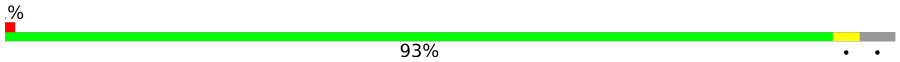
Chain U:

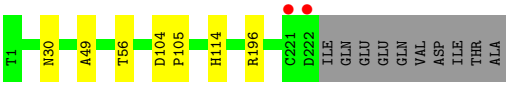




• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-2

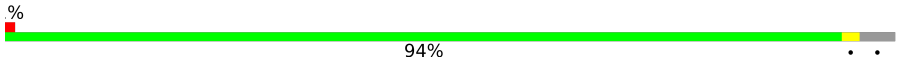
Chain H:

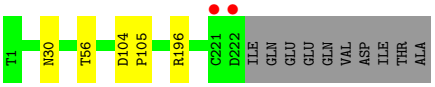




• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-2

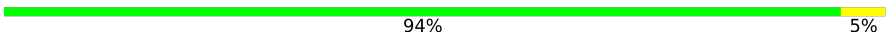
Chain V:





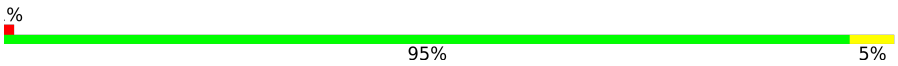
• Molecule 9: PROTEASOME SUBUNIT BETA TYPE-3

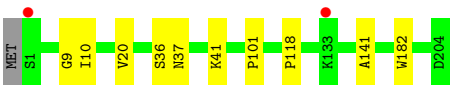
Chain I:



• Molecule 9: PROTEASOME SUBUNIT BETA TYPE-3

Chain W:





• Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4

Chain J: 2% 93%

M1 D2 A16 R23 Y67 L75 Q78 V126 L144 L161 M174 D193 D194 F195 GLN ALA GLN

• Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4

Chain X: 2% 93%

M1 D2 A16 R23 Y67 D72 L75 Q78 V126 L144 L161 M174 D194 F195 GLN ALA GLN

• Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain K: 95% 5%

T1 T2 T3 L4 A5 Q9 I35 R73 M100 R106 F127 G212

• Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain Y: 95% 5%

T1 T2 T3 L4 A5 Q9 I35 R73 M100 R106 F127 G212

• Molecule 12: PROTEASOME SUBUNIT BETA TYPE-6

Chain L: 95% 5%

Q1 N8 L13 L23 I30 T31 N49 C136 M147 P148 F149 L150 K167 D222

• Molecule 12: PROTEASOME SUBUNIT BETA TYPE-6

Chain Z: % 94% 6%

Q1 N8 L13 L23 I30 T31 N49 H108 P127 C136 M147 P148 F149 L150 N165 G166 K167 D210 D222

• Molecule 13: PROTEASOME SUBUNIT BETA TYPE-7

Chain M: % 96%

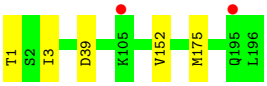
T1 I43 D47 N48 L70 R104 L127 L142 R161 I165 P166 R187 I233

• Molecule 13: PROTEASOME SUBUNIT BETA TYPE-7

Chain a: 97%

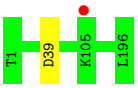
• Molecule 14: 20S PROTEASOME

Chain N: 97%



• Molecule 14: 20S PROTEASOME

Chain b: 99%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.67Å 300.70Å 143.99Å 90.00° 112.52° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-2.80) 97.6 (14.99-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.194 , 0.219 0.204 , 0.230	Depositor DCC
R_{free} test set	12444 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.1	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	0.94	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 2.34% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 7IM, MG, CL

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	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.26	0/1934	0.48	0/2618
2	P	0.26	0/1934	0.48	0/2618
3	C	0.29	0/1911	0.51	0/2588
3	Q	0.29	0/1911	0.50	0/2588
4	D	0.28	0/1838	0.47	0/2477
4	R	0.29	0/1838	0.46	0/2477
5	E	0.27	0/1800	0.46	0/2433
5	S	0.26	0/1800	0.46	0/2433
6	F	0.30	1/1933 (0.1%)	0.46	0/2611
6	T	0.29	1/1933 (0.1%)	0.45	0/2611
7	G	0.29	0/1946	0.47	0/2636
7	U	0.29	0/1945	0.47	0/2634
8	H	0.26	0/1715	0.46	0/2326
8	V	0.26	0/1715	0.46	0/2326
9	I	0.28	0/1611	0.48	0/2174
9	W	0.27	0/1611	0.48	0/2174
10	J	0.26	0/1589	0.49	0/2142
10	X	0.26	0/1589	0.48	0/2142
11	K	0.26	0/1681	0.48	0/2274
11	Y	0.28	0/1681	0.48	0/2274
12	L	0.28	0/1795	0.48	0/2420
12	Z	0.27	0/1795	0.47	0/2420
13	M	0.27	0/1855	0.50	0/2514
13	a	0.27	0/1855	0.50	0/2514
14	N	0.26	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.27	2/50201 (0.0%)	0.47	0/67882

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	244	ASN	C-N	-5.31	1.23	1.33
6	T	244	ASN	C-N	-5.26	1.23	1.33

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	0	0
1	O	1915	0	1929	0	0
2	B	1904	0	1904	3	0
2	P	1904	0	1904	3	0
3	C	1882	0	1895	4	0
3	Q	1882	0	1895	4	0
4	D	1814	0	1797	2	0
4	R	1814	0	1797	3	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	5	0
6	F	1893	0	1883	1	0
6	T	1893	0	1883	1	0
7	G	1908	0	1901	3	0
7	U	1907	0	1901	3	0
8	H	1684	0	1686	3	0
8	V	1684	0	1686	1	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	4	0
11	K	1644	0	1593	5	0
11	Y	1644	0	1592	5	0
12	L	1757	0	1711	4	0
12	Z	1757	0	1711	5	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0
14	N	1512	0	1479	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1512	0	1479	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	43	0	43	1	0
17	K	43	0	42	4	0
17	N	43	0	42	8	0
17	V	43	0	42	5	0
17	Y	43	0	43	4	0
17	b	43	0	43	0	0
18	K	12	0	13	0	0
18	Y	12	0	13	0	0
19	A	24	0	0	0	0
19	B	26	0	0	0	0
19	C	8	0	0	0	0
19	D	10	0	0	0	0
19	E	7	0	0	0	0
19	F	8	0	0	0	0
19	G	16	0	0	0	0
19	H	17	0	0	1	0
19	I	8	0	0	0	0
19	J	18	0	0	0	0
19	K	14	0	0	0	0
19	L	21	0	0	0	0
19	M	19	0	0	0	0
19	N	13	0	0	3	0
19	O	5	0	0	0	0
19	P	9	0	0	0	0
19	Q	3	0	0	0	0
19	R	8	0	0	0	0
19	S	6	0	0	0	0
19	T	10	0	0	0	0
19	U	15	0	0	0	0
19	V	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	W	9	0	0	0	0
19	X	22	0	0	0	0
19	Y	8	0	0	0	0
19	Z	12	0	0	0	0
All	All	49929	0	49336	92	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 1.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:1198:7IM:C43	19:N:2005:HOH:O	2.22	0.87
17:V:1224:7IM:H10	17:V:1224:7IM:O13	1.79	0.82
17:V:1224:7IM:H10	17:V:1224:7IM:C11	2.14	0.76
17:N:1198:7IM:H43B	19:N:2005:HOH:O	1.85	0.71
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.80	0.64
17:Y:1215:7IM:O29	17:Y:1215:7IM:O28	2.14	0.63
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.81	0.61
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.81	0.61
17:Y:1215:7IM:H8	12:Z:108:HIS:ND1	2.16	0.61
14:N:152:VAL:HA	14:N:175:MET:HE1	1.85	0.58
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.87	0.57
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.86	0.57
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.40	0.57
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.40	0.56
17:Y:1215:7IM:O14	12:Z:127:PRO:HD2	2.07	0.55
19:H:2011:HOH:O	17:N:1198:7IM:H43	2.06	0.55
8:H:49:ALA:HA	17:H:1223:7IM:H33B	1.89	0.55
14:N:1:THR:CG2	14:N:3:ILE:HG23	2.37	0.55
17:N:1198:7IM:H43	19:N:2005:HOH:O	1.98	0.54
17:Y:1215:7IM:O14	17:Y:1215:7IM:H10	2.07	0.54
3:C:201:VAL:O	3:C:202:GLN:CB	2.57	0.53
11:K:1:THR:CG2	11:K:3:THR:HG23	2.38	0.53
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.90	0.53
17:N:1198:7IM:H32B	17:N:1198:7IM:O34	2.09	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.57	0.52
17:K:1215:7IM:C11	17:K:1215:7IM:C10	2.87	0.51
17:N:1198:7IM:C6	17:N:1198:7IM:N2	2.72	0.51
11:Y:1:THR:CG2	11:Y:3:THR:HG23	2.40	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.94	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.12	0.49
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.94	0.49
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.48	0.48
17:N:1198:7IM:O29	17:N:1198:7IM:O28	2.27	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.95	0.47
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.45	0.46
10:J:174:MET:HA	10:X:174:MET:HA	1.97	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.46
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.45	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.98	0.46
2:B:86:LEU:HB3	2:B:114:LEU:HD21	1.98	0.45
11:K:100:MET:CE	11:K:127:PHE:HB2	2.47	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.98	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.44
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.47	0.44
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.53	0.44
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.43
17:K:1215:7IM:O34	17:K:1215:7IM:H33A	2.18	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
17:K:1215:7IM:H10	17:K:1215:7IM:O13	2.18	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.43
2:P:86:LEU:HB3	2:P:114:LEU:HD21	2.00	0.43
17:V:1224:7IM:N23	17:V:1224:7IM:H27A	2.34	0.43
8:H:114:HIS:ND1	17:N:1198:7IM:H7	2.34	0.42
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.00	0.42
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.83	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.42
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.84	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
17:V:1224:7IM:H7	9:W:101:PRO:HG3	2.02	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.35	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.01	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.35	0.41
11:K:1:THR:HG22	11:K:3:THR:HG23	2.02	0.41
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.50	0.41
4:R:161:ALA:HB3	5:S:55:LEU:HD23	2.03	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
3:C:201:VAL:HG13	3:C:202:GLN:N	2.35	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
17:K:1215:7IM:H10	17:K:1215:7IM:N2	2.35	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.48	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.40
9:I:65:MET:O	9:I:68:TYR:HB3	2.22	0.40
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.36	0.40
17:V:1224:7IM:C11	17:V:1224:7IM:C10	2.86	0.40
4:D:113:LEU:HD12	5:E:78:PRO:HB2	2.04	0.40
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	49
3	C	239/254 (94%)	231 (97%)	6 (2%)	2 (1%)	19	49
3	Q	239/254 (94%)	231 (97%)	6 (2%)	2 (1%)	19	49
4	D	232/260 (89%)	227 (98%)	5 (2%)	0	100	100
4	R	232/260 (89%)	227 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
6	T	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
7	G	240/252 (95%)	233 (97%)	6 (2%)	1 (0%)	34	66
7	U	240/252 (95%)	233 (97%)	6 (2%)	1 (0%)	34	66
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	214 (97%)	6 (3%)	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	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
10	X	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29	61
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	M	231/233 (99%)	220 (95%)	11 (5%)	0	100	100
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6284/6588 (95%)	6094 (97%)	178 (3%)	12 (0%)	47	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL

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Mol	Chain	Res	Type
3	Q	202	GLN
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
7	G	242	GLN
2	P	221	ASP
7	U	242	GLN
10	J	2	ASP
10	X	2	ASP

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%)	206 (99%)	3 (1%)	67	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	90
2	B	203/216 (94%)	196 (97%)	7 (3%)	37	71
2	P	203/216 (94%)	196 (97%)	7 (3%)	37	71
3	C	212/226 (94%)	206 (97%)	6 (3%)	43	77
3	Q	212/226 (94%)	206 (97%)	6 (3%)	43	77
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	60
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	60
5	E	190/193 (98%)	184 (97%)	6 (3%)	39	73
5	S	190/193 (98%)	184 (97%)	6 (3%)	39	73
6	F	201/239 (84%)	193 (96%)	8 (4%)	31	65
6	T	201/239 (84%)	193 (96%)	8 (4%)	31	65
7	G	206/210 (98%)	201 (98%)	5 (2%)	49	81
7	U	206/210 (98%)	201 (98%)	5 (2%)	49	81
8	H	181/190 (95%)	178 (98%)	3 (2%)	60	87
8	V	181/190 (95%)	178 (98%)	3 (2%)	60	87
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	92
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	75
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	75
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	73
13	M	199/199 (100%)	193 (97%)	6 (3%)	41	75
13	a	199/199 (100%)	193 (97%)	6 (3%)	41	75
14	N	162/162 (100%)	161 (99%)	1 (1%)	86	96
14	b	162/162 (100%)	161 (99%)	1 (1%)	86	96
All	All	5312/5522 (96%)	5168 (97%)	144 (3%)	44	78

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	55	LEU
2	B	58	GLN
2	B	114	LEU
2	B	184	LYS
2	B	186	ASP
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
4	D	20	LEU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE

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Mol	Chain	Res	Type
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
6	F	14	ASP
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
8	H	30	ASN
8	H	56	THR
8	H	196	ARG
9	I	37	ASN
9	I	182	TRP
10	J	23	ARG
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	73	ARG
11	K	106	ARG
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	136	CYS

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Mol	Chain	Res	Type
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	39	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	55	LEU
2	P	58	GLN
2	P	114	LEU
2	P	184	LYS
2	P	186	ASP
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
4	R	20	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
6	T	14	ASP
6	T	123	ASN
6	T	172	LEU

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Mol	Chain	Res	Type
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
8	V	30	ASN
8	V	56	THR
8	V	196	ARG
9	W	37	ASN
9	W	182	TRP
10	X	23	ARG
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	73	ARG
11	Y	106	ARG
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	136	CYS
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	119	GLN
2	B	123	GLN
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
4	D	146	GLN
5	E	68	HIS
5	E	92	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	86	ASN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	117	GLN
7	G	121	GLN
8	H	66	HIS
10	J	55	GLN
10	J	146	HIS
10	J	147	HIS
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	146	GLN
5	S	68	HIS
5	S	92	ASN

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Mol	Chain	Res	Type
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	86	ASN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	117	GLN
7	U	121	GLN
10	X	55	GLN
10	X	146	HIS
10	X	147	HIS
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	7IM	Y	1215	11	43,43,43	1.49	4 (9%)	56,58,58	1.48	8 (14%)
17	7IM	V	1224	8	43,43,43	1.38	3 (6%)	56,58,58	1.17	3 (5%)
17	7IM	K	1215	11	43,43,43	1.37	4 (9%)	56,58,58	1.28	6 (10%)
17	7IM	N	1198	14	43,43,43	1.37	4 (9%)	56,58,58	1.76	8 (14%)
17	7IM	H	1223	8	43,43,43	1.27	4 (9%)	56,58,58	1.68	8 (14%)
17	7IM	b	1197	14	43,43,43	1.12	2 (4%)	56,58,58	1.58	6 (10%)
18	MES	K	1213	-	12,12,12	2.19	1 (8%)	14,16,16	1.58	3 (21%)
18	MES	Y	1213	-	12,12,12	2.20	1 (8%)	14,16,16	1.32	2 (14%)

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	7IM	Y	1215	11	-	11/59/59/59	0/1/1/1
17	7IM	V	1224	8	-	17/59/59/59	0/1/1/1
17	7IM	K	1215	11	-	12/59/59/59	0/1/1/1
17	7IM	N	1198	14	-	20/59/59/59	0/1/1/1
17	7IM	H	1223	8	-	23/59/59/59	0/1/1/1
17	7IM	b	1197	14	-	25/59/59/59	0/1/1/1
18	MES	K	1213	-	-	0/6/14/14	0/1/1/1
18	MES	Y	1213	-	-	0/6/14/14	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	1213	MES	C8-S	-7.28	1.67	1.77
18	K	1213	MES	C8-S	-7.17	1.67	1.77
17	Y	1215	7IM	C4-C5	-6.48	1.35	1.51
17	V	1224	7IM	C4-C5	-5.90	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	1223	7IM	C4-C5	-5.83	1.37	1.51
17	N	1198	7IM	C4-C5	-5.40	1.38	1.51
17	b	1197	7IM	C4-C5	-4.96	1.39	1.51
17	K	1215	7IM	C4-C5	-4.61	1.40	1.51
17	V	1224	7IM	O29-C25	-4.21	1.34	1.43
17	Y	1215	7IM	C15-C1	-3.97	1.48	1.52
17	N	1198	7IM	O29-C25	-3.64	1.35	1.43
17	K	1215	7IM	O29-C25	-3.62	1.35	1.43
17	K	1215	7IM	C15-C16	-3.14	1.49	1.52
17	b	1197	7IM	O29-C25	-3.06	1.36	1.43
17	Y	1215	7IM	C15-C16	-2.96	1.49	1.52
17	N	1198	7IM	C39-C18	-2.81	1.45	1.53
17	H	1223	7IM	O29-C25	-2.78	1.37	1.43
17	Y	1215	7IM	C26-C25	2.40	1.56	1.52
17	H	1223	7IM	C26-C25	2.36	1.56	1.52
17	N	1198	7IM	C15-C16	-2.31	1.50	1.52
17	K	1215	7IM	C15-C1	-2.29	1.50	1.52
17	V	1224	7IM	C15-C16	-2.25	1.50	1.52
17	H	1223	7IM	C15-C1	2.18	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	1223	7IM	C30-C24-N23	-7.96	99.88	110.18
17	N	1198	7IM	O41-C39-C18	-6.28	96.53	109.13
17	b	1197	7IM	C30-C24-N23	-6.26	102.08	110.18
17	N	1198	7IM	C39-C18-N17	-5.78	96.93	111.72
17	N	1198	7IM	C30-C24-N23	-5.00	103.72	110.18
17	V	1224	7IM	C30-C24-N23	-4.96	103.77	110.18
17	K	1215	7IM	C30-C24-N23	-4.19	104.77	110.18
17	Y	1215	7IM	C35-C21-N20	-4.12	101.17	111.72
17	b	1197	7IM	O41-C39-C18	-4.08	100.95	109.13
17	b	1197	7IM	C39-C18-N17	-4.00	101.48	111.72
17	Y	1215	7IM	C5-C4-C3	-3.77	102.98	113.39
17	N	1198	7IM	C27-C26-C25	-3.53	106.33	113.07
17	H	1223	7IM	C35-C21-C22	3.32	118.61	111.28
17	Y	1215	7IM	C30-C24-N23	-3.15	106.11	110.18
18	Y	1213	MES	O2S-S-C8	3.12	110.67	106.92
18	K	1213	MES	O2S-S-C8	3.07	110.62	106.92
17	Y	1215	7IM	C27-C26-C25	-2.93	107.46	113.07
17	b	1197	7IM	C35-C21-C22	-2.88	104.93	111.28
17	H	1223	7IM	C25-C24-N23	2.85	115.41	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	1223	7IM	C27-C26-C25	-2.71	107.89	113.07
17	H	1223	7IM	C30-C24-C25	-2.71	108.46	112.55
17	K	1215	7IM	C27-C26-C25	-2.70	107.90	113.07
17	V	1224	7IM	C27-C26-C25	-2.67	107.96	113.07
17	K	1215	7IM	C35-C21-N20	-2.65	104.93	111.72
17	N	1198	7IM	C15-C16-N17	-2.65	112.53	116.09
17	K	1215	7IM	C37-C35-C21	-2.65	106.95	112.29
17	b	1197	7IM	C27-C26-C25	-2.44	108.40	113.07
18	K	1213	MES	C2-C3-N4	2.38	113.71	110.10
17	H	1223	7IM	C4-C3-N2	2.38	115.80	110.79
17	Y	1215	7IM	C25-C24-N23	2.35	114.44	109.92
17	N	1198	7IM	O28-C27-C26	-2.35	103.09	111.31
17	K	1215	7IM	C40-C39-C18	-2.34	107.56	112.29
17	Y	1215	7IM	C19-C18-N17	-2.30	104.12	110.36
17	Y	1215	7IM	C37-C35-C21	-2.27	107.70	112.29
17	K	1215	7IM	O28-C27-C26	-2.27	103.36	111.31
17	N	1198	7IM	O42-C16-N17	2.24	127.08	122.93
18	Y	1213	MES	O3S-S-C8	2.22	109.36	105.77
17	Y	1215	7IM	C31-C30-C24	-2.18	111.50	115.84
17	b	1197	7IM	C4-C5-C10	-2.16	116.62	120.91
17	H	1223	7IM	O36-C35-C21	2.12	113.39	109.13
18	K	1213	MES	O3S-S-C8	2.11	109.18	105.77
17	N	1198	7IM	C31-C30-C24	-2.09	111.69	115.84
17	H	1223	7IM	C4-C3-C11	-2.04	105.50	110.42
17	V	1224	7IM	C39-C18-C19	2.04	115.78	111.28

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	1223	7IM	N2-C1-C15-C16
17	H	1223	7IM	O14-C1-C15-C16
17	H	1223	7IM	N2-C3-C4-C5
17	H	1223	7IM	C11-C3-C4-C5
17	H	1223	7IM	C43-C15-C16-N17
17	H	1223	7IM	C43-C15-C16-O42
17	H	1223	7IM	N17-C18-C39-C40
17	H	1223	7IM	N17-C18-C39-O41
17	H	1223	7IM	C19-C18-C39-C40
17	H	1223	7IM	C19-C18-C39-O41
17	H	1223	7IM	N20-C21-C35-O36
17	H	1223	7IM	N20-C21-C35-C37

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Mol	Chain	Res	Type	Atoms
17	H	1223	7IM	C22-C21-C35-O36
17	H	1223	7IM	C22-C21-C35-C37
17	H	1223	7IM	C25-C24-C30-C31
17	H	1223	7IM	C24-C25-C26-C27
17	K	1215	7IM	N2-C1-C15-C16
17	K	1215	7IM	O14-C1-C15-C16
17	K	1215	7IM	N23-C24-C25-O29
17	K	1215	7IM	C30-C24-C25-C26
17	K	1215	7IM	C30-C24-C25-O29
17	N	1198	7IM	C1-C15-C16-N17
17	N	1198	7IM	C1-C15-C16-O42
17	N	1198	7IM	N17-C18-C39-O41
17	N	1198	7IM	N23-C24-C25-O29
17	N	1198	7IM	N23-C24-C30-C31
17	N	1198	7IM	C25-C24-C30-C31
17	V	1224	7IM	N2-C1-C15-C16
17	V	1224	7IM	O14-C1-C15-C16
17	V	1224	7IM	N17-C18-C39-C40
17	V	1224	7IM	N17-C18-C39-O41
17	V	1224	7IM	C19-C18-C39-C40
17	V	1224	7IM	C19-C18-C39-O41
17	V	1224	7IM	N23-C24-C25-O29
17	V	1224	7IM	C25-C24-C30-C31
17	V	1224	7IM	C25-C26-C27-O28
17	Y	1215	7IM	N2-C1-C15-C43
17	Y	1215	7IM	O14-C1-C15-C43
17	Y	1215	7IM	N2-C3-C4-C5
17	Y	1215	7IM	C11-C3-C4-C5
17	Y	1215	7IM	N23-C24-C25-O29
17	Y	1215	7IM	C30-C24-C25-C26
17	Y	1215	7IM	C30-C24-C25-O29
17	Y	1215	7IM	C24-C25-C26-C27
17	b	1197	7IM	C1-C15-C16-N17
17	b	1197	7IM	C1-C15-C16-O42
17	b	1197	7IM	C43-C15-C16-O42
17	b	1197	7IM	N17-C18-C39-C40
17	b	1197	7IM	N17-C18-C39-O41
17	b	1197	7IM	C19-C18-C39-C40
17	b	1197	7IM	C19-C18-C39-O41
17	b	1197	7IM	N20-C21-C35-O36
17	b	1197	7IM	N20-C21-C35-C37
17	b	1197	7IM	C22-C21-C35-O36

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Mol	Chain	Res	Type	Atoms
17	b	1197	7IM	C22-C21-C35-C37
17	b	1197	7IM	N23-C24-C25-O29
17	b	1197	7IM	C25-C24-C30-C31
17	b	1197	7IM	C25-C26-C27-O28
17	b	1197	7IM	C11-C3-C4-C5
17	H	1223	7IM	O14-C1-C15-C43
17	V	1224	7IM	O14-C1-C15-C43
17	V	1224	7IM	C43-C15-C16-O42
17	H	1223	7IM	N2-C1-C15-C43
17	N	1198	7IM	C43-C15-C16-N17
17	V	1224	7IM	N2-C1-C15-C43
17	V	1224	7IM	C43-C15-C16-N17
17	b	1197	7IM	N2-C1-C15-C43
17	b	1197	7IM	C43-C15-C16-N17
17	b	1197	7IM	N2-C3-C4-C5
17	Y	1215	7IM	O29-C25-C26-C27
17	N	1198	7IM	N17-C18-C39-C40
17	b	1197	7IM	O14-C1-C15-C43
17	K	1215	7IM	C3-C4-C5-C6
17	K	1215	7IM	C3-C4-C5-C10
17	H	1223	7IM	N23-C24-C30-C31
17	V	1224	7IM	N23-C24-C30-C31
17	b	1197	7IM	N23-C24-C30-C31
17	H	1223	7IM	O29-C25-C26-C27
17	H	1223	7IM	C1-C15-C16-O42
17	V	1224	7IM	C3-C4-C5-C6
17	V	1224	7IM	C3-C4-C5-C10
17	H	1223	7IM	N23-C24-C25-O29
17	N	1198	7IM	C43-C15-C16-O42
17	K	1215	7IM	N23-C24-C25-C26
17	Y	1215	7IM	N23-C24-C25-C26
17	N	1198	7IM	O13-C11-C3-C4
17	b	1197	7IM	O12-C11-C3-C4
17	K	1215	7IM	C24-C25-C26-C27
17	b	1197	7IM	C3-C4-C5-C10
17	b	1197	7IM	C24-C25-C26-C27
17	N	1198	7IM	C19-C18-C39-O41
17	N	1198	7IM	C22-C21-C35-O36
17	N	1198	7IM	C22-C21-C35-C37
17	N	1198	7IM	O12-C11-C3-C4
17	b	1197	7IM	O13-C11-C3-C4
17	H	1223	7IM	C24-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
17	b	1197	7IM	C3-C4-C5-C6
17	K	1215	7IM	O14-C1-C15-C43
17	N	1198	7IM	N20-C21-C35-O36
17	K	1215	7IM	O29-C25-C26-C27
17	K	1215	7IM	C11-C3-C4-C5
17	N	1198	7IM	N2-C1-C15-C16
17	N	1198	7IM	O14-C1-C15-C16
17	Y	1215	7IM	O14-C1-C15-C16
17	N	1198	7IM	N2-C1-C15-C43
17	N	1198	7IM	O14-C1-C15-C43
17	N	1198	7IM	N23-C24-C25-C26
17	V	1224	7IM	N23-C24-C25-C26

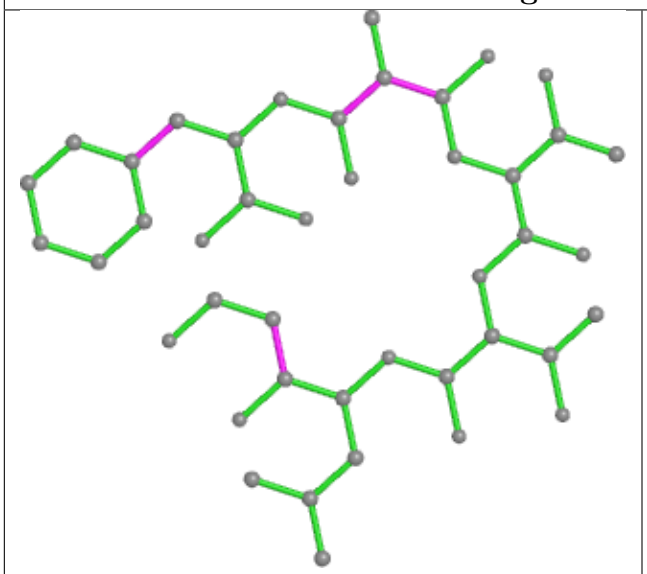
There are no ring outliers.

5 monomers are involved in 22 short contacts:

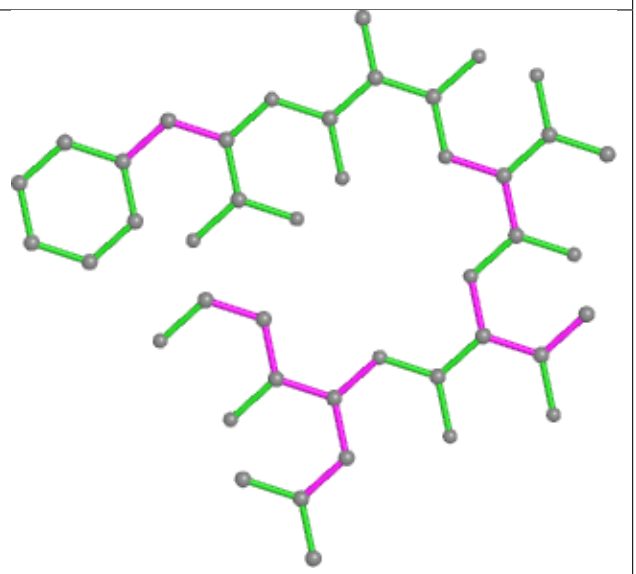
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	1215	7IM	4	0
17	V	1224	7IM	5	0
17	K	1215	7IM	4	0
17	N	1198	7IM	8	0
17	H	1223	7IM	1	0

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

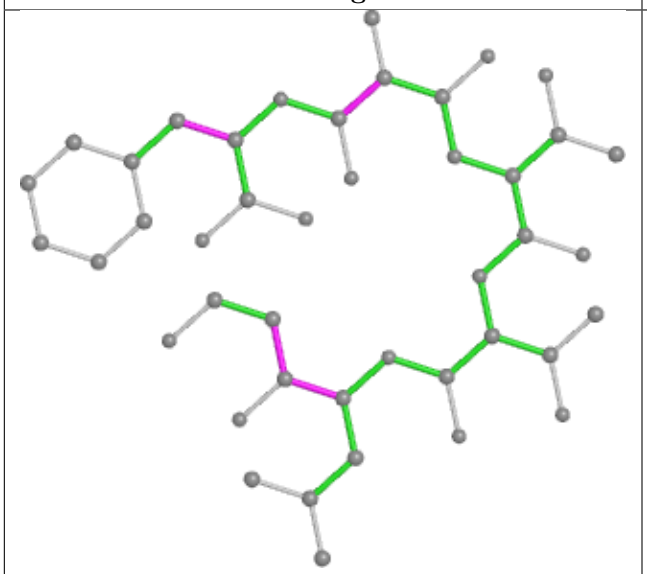
Ligand 7IM Y 1215



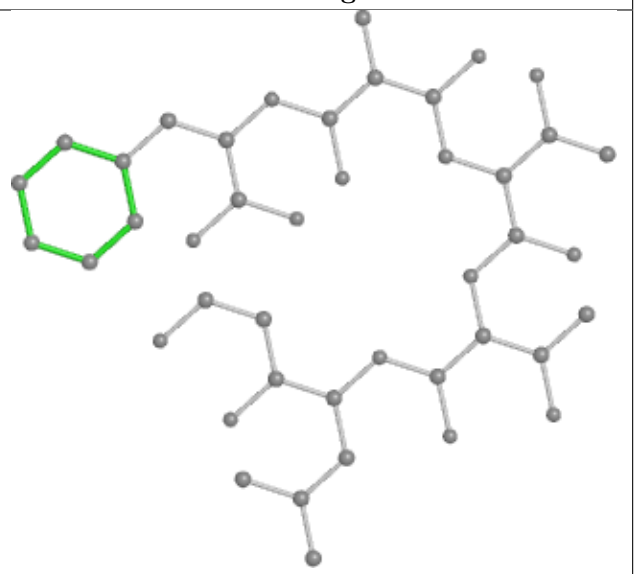
Bond lengths



Bond angles

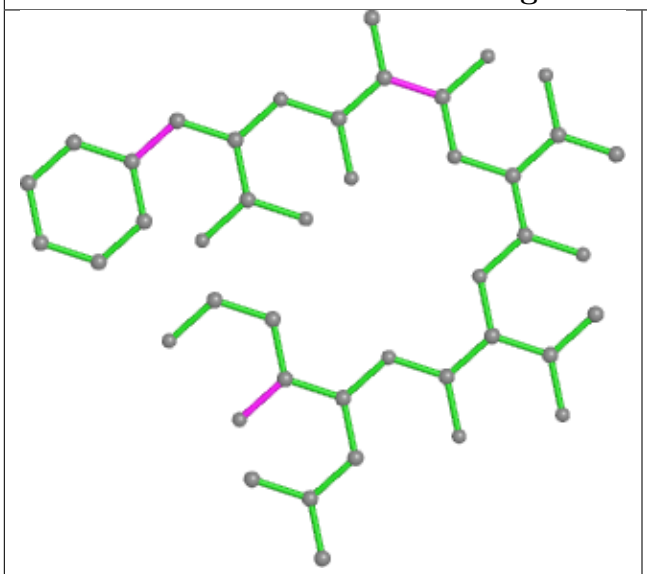


Torsions

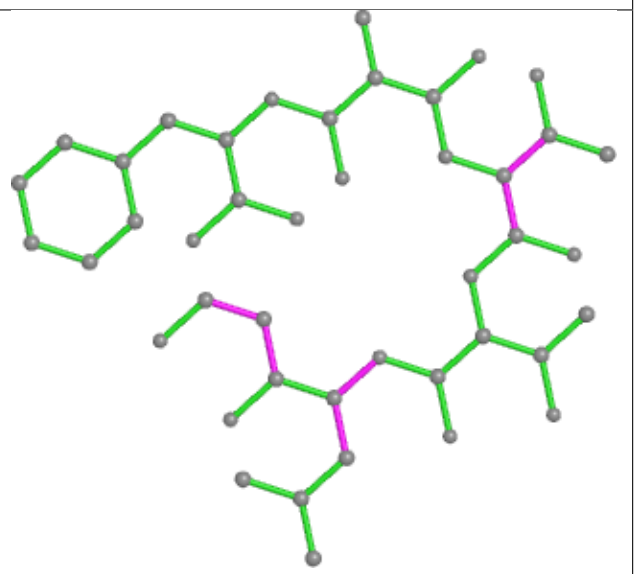


Rings

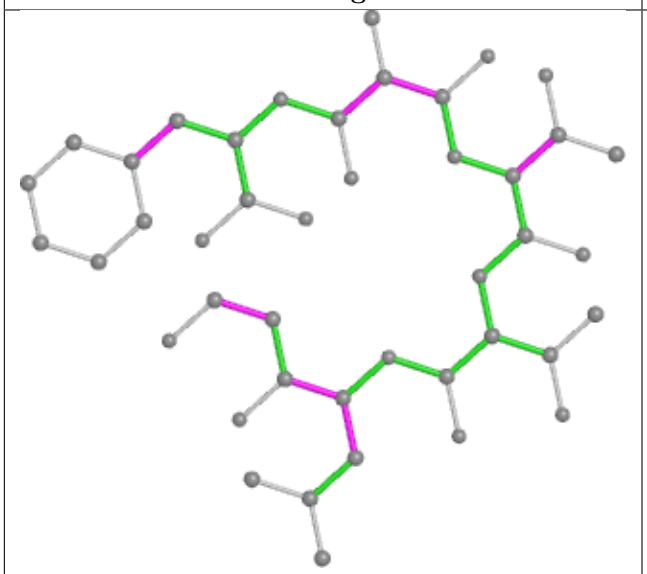
Ligand 7IM V 1224



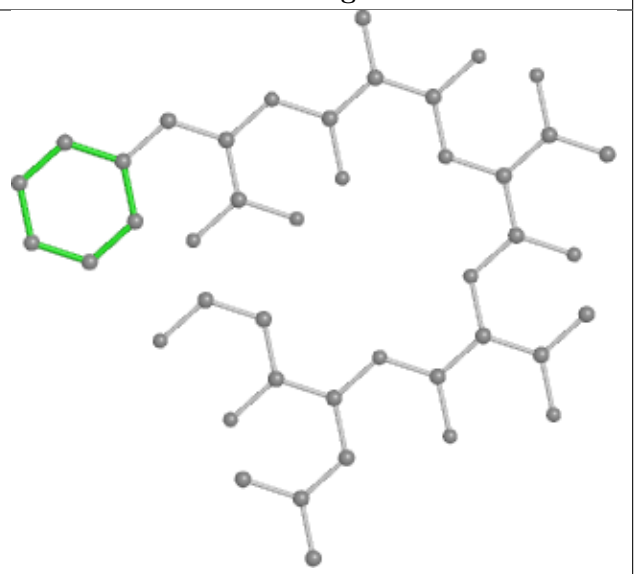
Bond lengths



Bond angles

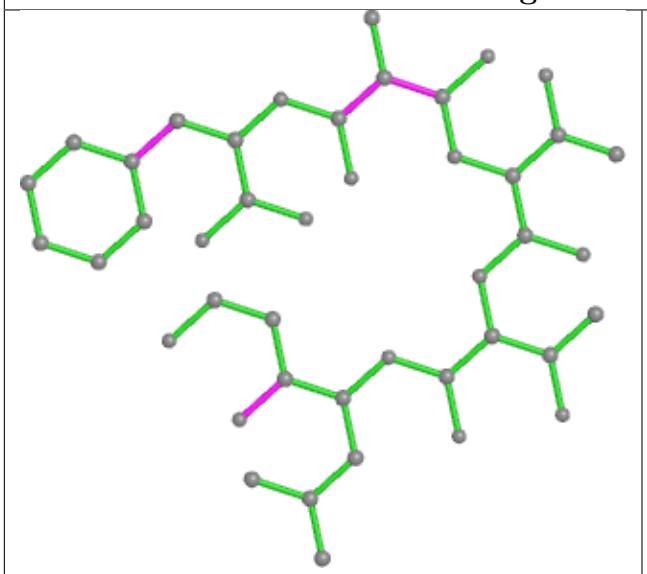


Torsions

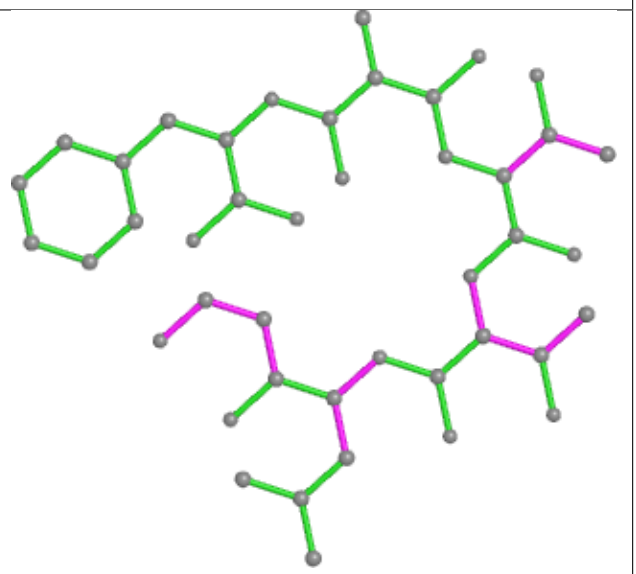


Rings

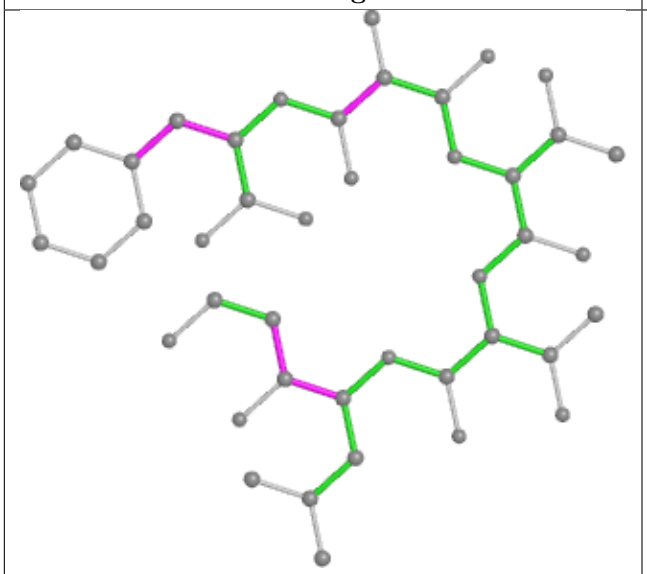
Ligand 7IM K 1215



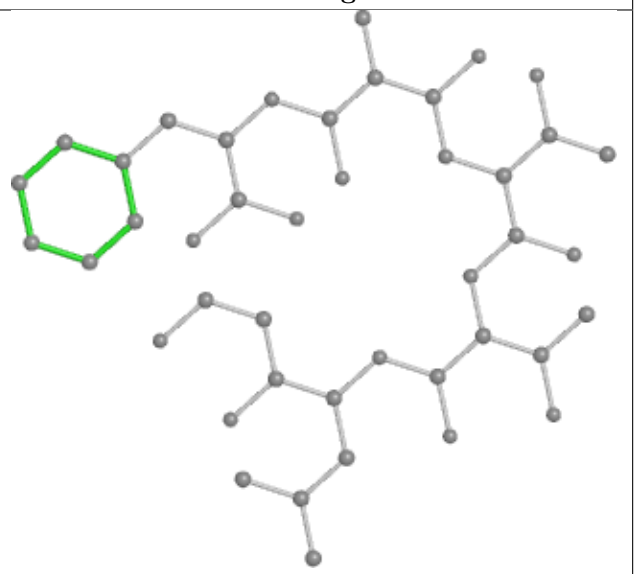
Bond lengths



Bond angles

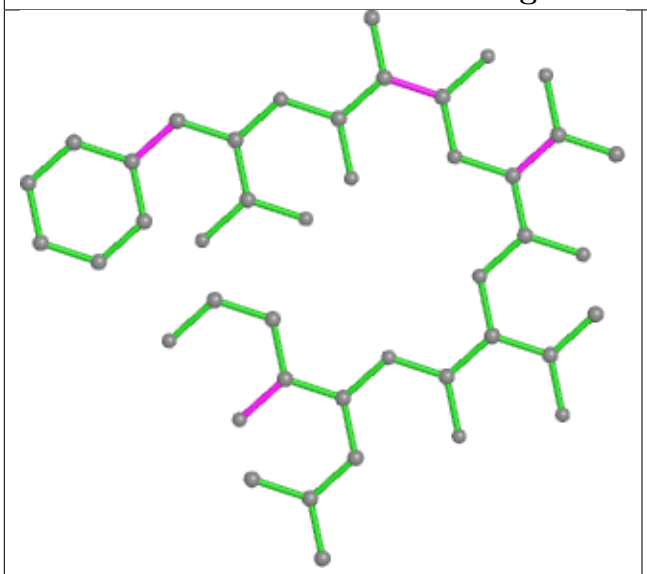


Torsions

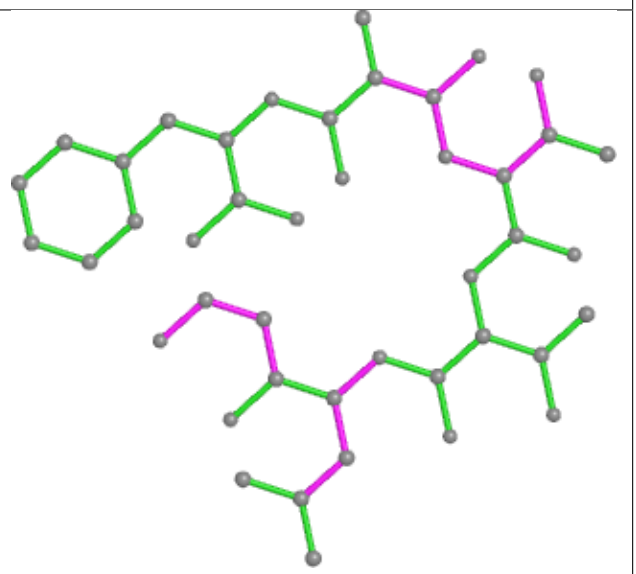


Rings

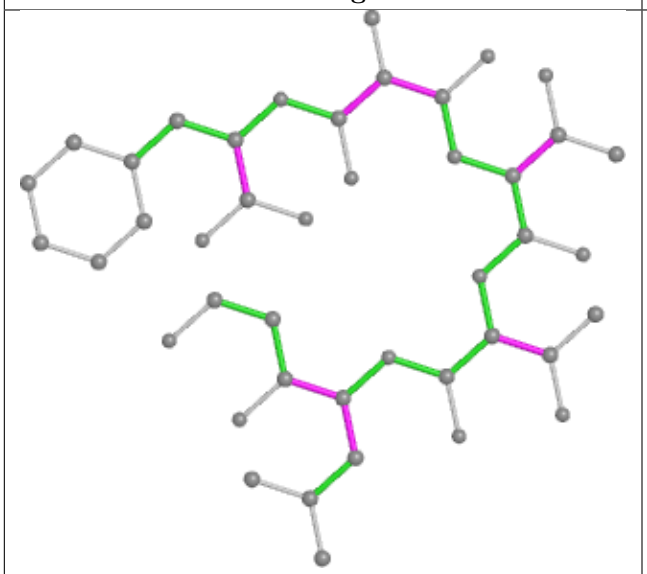
Ligand 7IM N 1198



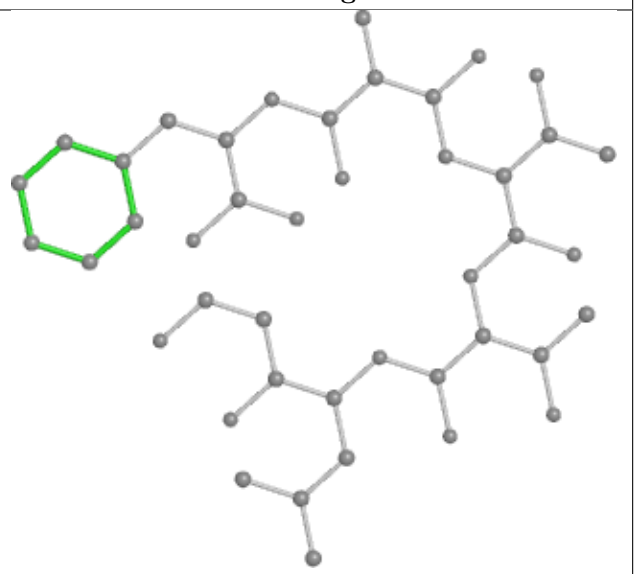
Bond lengths



Bond angles

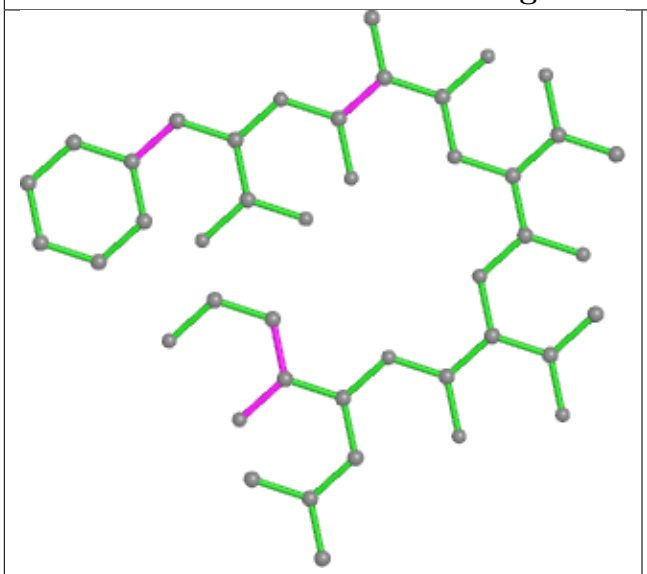


Torsions

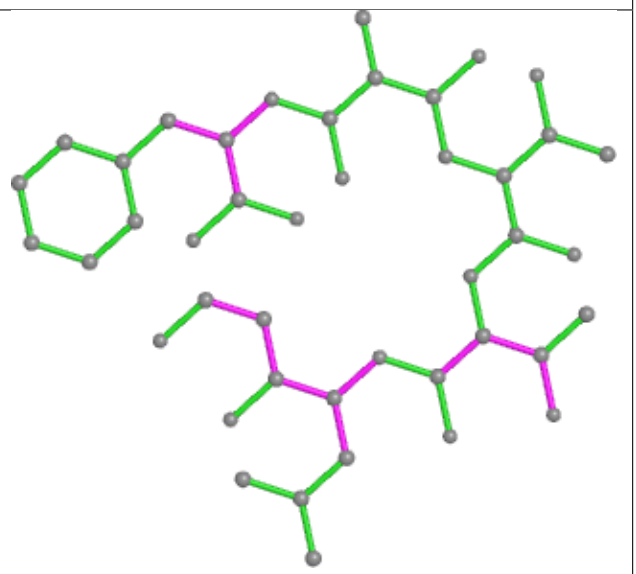


Rings

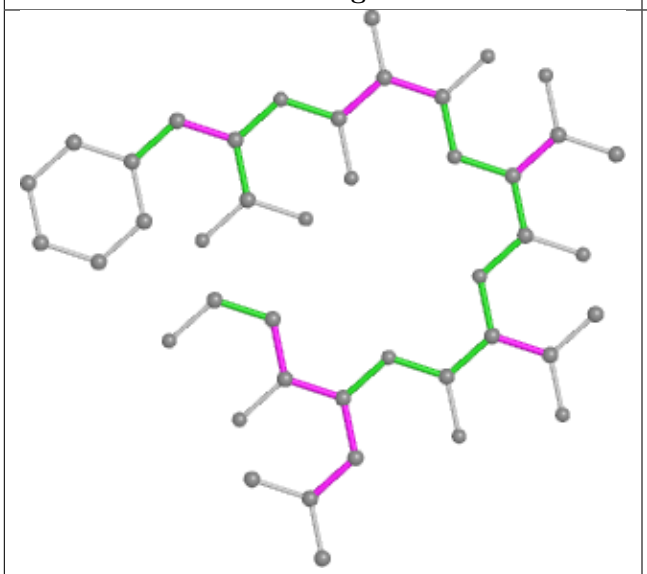
Ligand 7IM H 1223



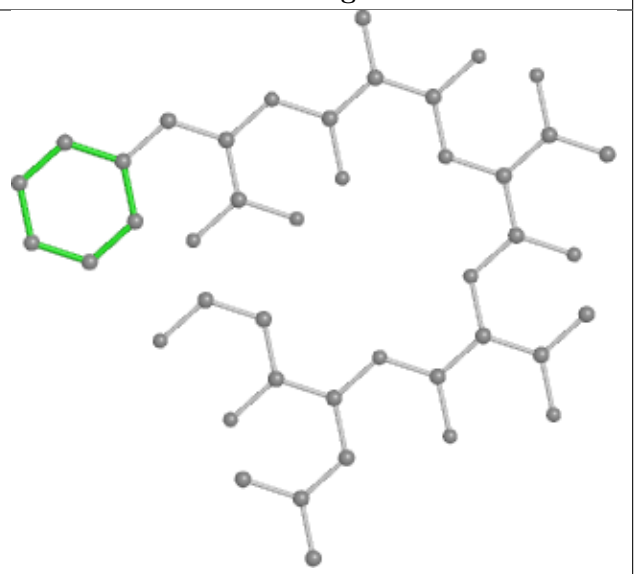
Bond lengths



Bond angles

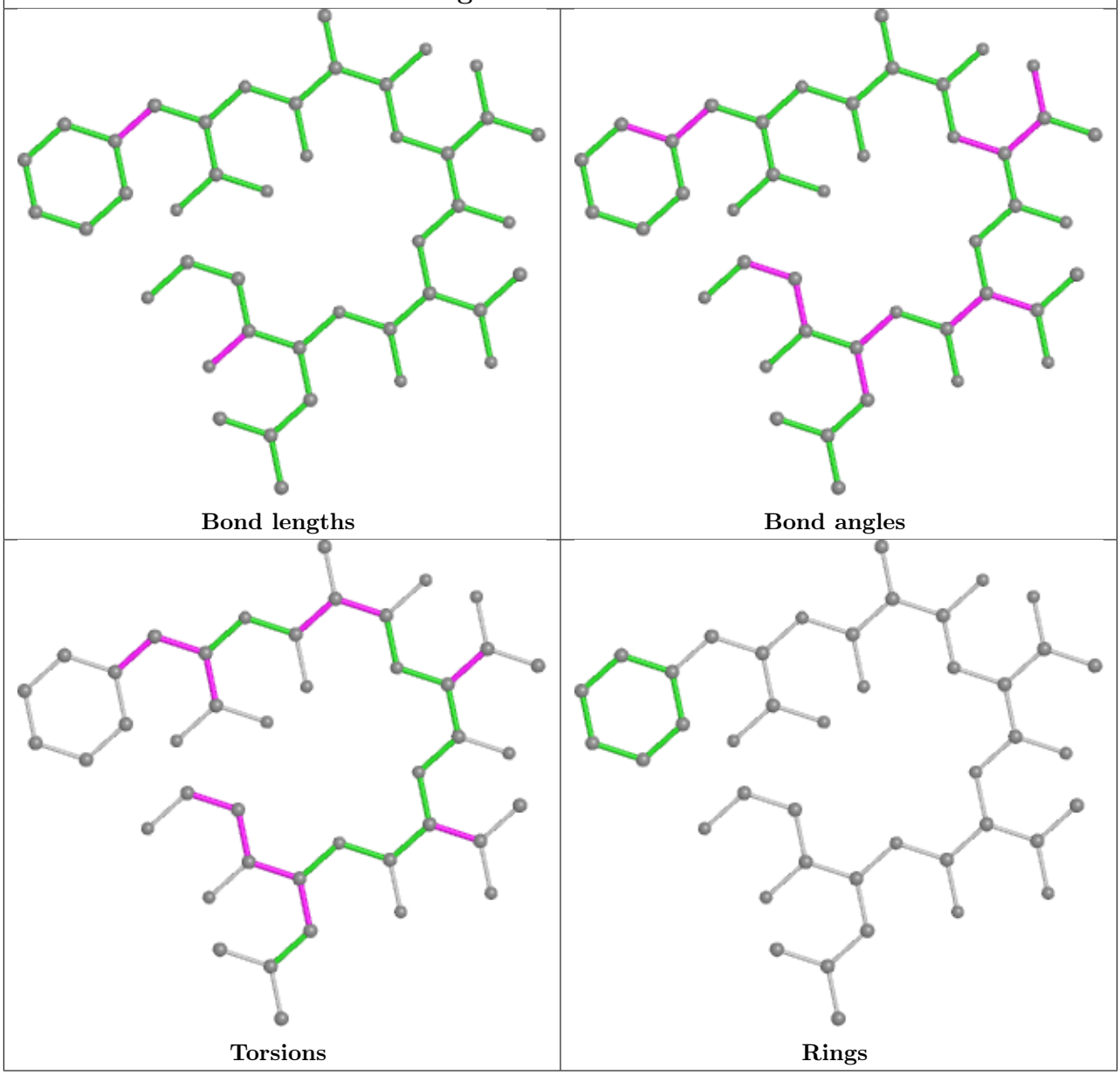


Torsions



Rings

Ligand 7IM b 1197



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.29	9 (3%)	42	32	44, 64, 111, 160	0
1	O	250/250 (100%)	-0.28	5 (2%)	65	56	50, 71, 117, 160	0
2	B	244/258 (94%)	-0.17	10 (4%)	37	27	44, 74, 125, 179	0
2	P	244/258 (94%)	-0.25	8 (3%)	46	36	51, 73, 115, 168	0
3	C	241/254 (94%)	-0.16	10 (4%)	37	27	44, 71, 136, 167	0
3	Q	241/254 (94%)	0.19	18 (7%)	14	8	58, 95, 177, 211	0
4	D	236/260 (90%)	-0.32	6 (2%)	57	47	52, 74, 105, 147	0
4	R	236/260 (90%)	-0.19	8 (3%)	45	35	55, 83, 127, 173	0
5	E	231/234 (98%)	-0.21	4 (1%)	70	63	51, 78, 122, 156	0
5	S	231/234 (98%)	0.05	13 (5%)	24	16	53, 87, 151, 187	0
6	F	244/288 (84%)	-0.38	7 (2%)	51	41	44, 75, 126, 157	0
6	T	244/288 (84%)	-0.25	5 (2%)	65	56	51, 84, 143, 178	0
7	G	242/252 (96%)	-0.41	4 (1%)	70	63	47, 68, 105, 144	0
7	U	242/252 (96%)	-0.37	4 (1%)	70	63	44, 68, 105, 151	0
8	H	222/232 (95%)	-0.55	2 (0%)	84	80	41, 58, 95, 131	0
8	V	222/232 (95%)	-0.52	2 (0%)	84	80	39, 60, 95, 141	0
9	I	204/205 (99%)	-0.62	1 (0%)	91	88	41, 59, 92, 123	0
9	W	204/205 (99%)	-0.60	2 (0%)	82	77	35, 57, 87, 115	0
10	J	195/198 (98%)	-0.56	3 (1%)	73	68	39, 57, 90, 128	0
10	X	195/198 (98%)	-0.54	3 (1%)	73	68	42, 59, 90, 139	0
11	K	212/212 (100%)	-0.55	0	100	100	38, 58, 88, 113	0
11	Y	212/212 (100%)	-0.54	1 (0%)	91	88	42, 62, 97, 121	0
12	L	222/222 (100%)	-0.58	0	100	100	37, 59, 96, 121	0
12	Z	222/222 (100%)	-0.55	2 (0%)	84	80	40, 62, 95, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	-0.55	2 (0%)	84	80	38, 61, 89, 101	0
13	a	233/233 (100%)	-0.56	1 (0%)	92	91	37, 60, 86, 100	0
14	N	196/196 (100%)	-0.63	2 (1%)	82	77	37, 54, 84, 114	0
14	b	196/196 (100%)	-0.60	1 (0%)	91	88	39, 56, 91, 119	0
All	All	6344/6588 (96%)	-0.38	133 (2%)	63	54	35, 67, 120, 211	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	7.8
3	Q	241	GLN	7.6
5	S	202	ASP	7.1
8	V	222	ASP	7.1
2	P	219	ALA	7.0
1	A	1	MET	6.8
3	Q	49	THR	6.8
3	Q	206	LYS	6.5
2	B	219	ALA	6.1
2	B	220	ASN	6.1
2	B	221	ASP	5.5
3	C	206	LYS	5.3
8	H	222	ASP	5.1
5	E	202	ASP	5.1
6	T	245	GLY	5.0
2	P	220	ASN	5.0
2	B	51	VAL	4.9
2	P	51	VAL	4.9
3	C	241	GLN	4.7
8	H	221	CYS	4.6
4	R	241	ALA	4.5
5	S	54	GLU	4.5
1	O	1	MET	4.3
10	J	1	MET	4.3
5	S	51	ASN	4.1
11	Y	212	GLY	3.9
8	V	221	CYS	3.8
3	Q	239	GLN	3.8
3	C	238	LYS	3.8
3	Q	204	GLY	3.8
10	X	1	MET	3.8
6	F	181	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
2	P	221	ASP	3.7
5	S	52	ALA	3.7
13	a	1	THR	3.7
3	Q	238	LYS	3.6
6	T	201	GLU	3.6
7	G	243	ASP	3.6
1	O	52	SER	3.6
3	Q	48	SER	3.5
7	U	241	GLU	3.5
2	P	218	GLY	3.5
3	Q	240	GLU	3.5
7	G	179	LYS	3.4
1	O	249	ALA	3.3
5	S	173	ARG	3.3
6	T	2	THR	3.3
4	D	242	GLU	3.3
7	U	242	GLN	3.3
2	B	218	GLY	3.3
6	F	245	GLY	3.2
3	Q	223	SER	3.2
2	P	59	ASP	3.2
3	C	239	GLN	3.2
3	C	202	GLN	3.2
3	Q	205	ALA	3.1
10	J	194	ASP	3.1
4	R	203	LYS	3.1
3	C	49	THR	3.1
10	X	194	ASP	3.1
5	S	58	TYR	3.1
1	A	2	THR	3.0
3	Q	236	GLN	3.0
1	O	201	GLU	2.9
5	S	209	ASN	2.9
4	D	241	ALA	2.9
6	F	205	GLU	2.8
3	Q	51	LYS	2.8
10	X	72	ASP	2.8
3	C	235	GLU	2.8
4	R	230	GLU	2.8
3	Q	55	THR	2.8
6	T	244	ASN	2.7
6	F	201	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	62	SER	2.6
13	M	47	ASP	2.6
6	F	202	ASP	2.6
1	A	250	LEU	2.6
2	B	222	GLY	2.6
7	U	243	ASP	2.5
5	E	165	GLN	2.5
9	I	131	GLU	2.5
2	B	203	SER	2.5
5	S	29	LYS	2.5
5	E	201	ARG	2.4
5	S	233	ILE	2.4
4	R	2	ARG	2.4
4	D	243	SER	2.4
9	W	1	SER	2.4
4	R	242	GLU	2.3
1	A	248	GLU	2.3
2	P	52	THR	2.3
2	B	217	LYS	2.3
5	E	50	ARG	2.3
1	A	201	GLU	2.3
7	G	241	GLU	2.3
13	M	1	THR	2.3
3	C	50	LEU	2.3
2	P	203	SER	2.2
3	Q	181	GLU	2.2
3	Q	58	THR	2.2
6	T	166	GLN	2.2
14	N	195	GLN	2.2
9	W	133	LYS	2.2
5	S	225	ASP	2.2
3	Q	59	PRO	2.2
4	R	217	GLN	2.2
5	S	201	ARG	2.1
4	R	1	ASP	2.1
2	B	244	THR	2.1
3	C	236	GLN	2.1
7	G	242	GLN	2.1
1	A	50	LYS	2.1
3	C	225	GLU	2.1
2	B	59	ASP	2.1
10	J	193	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
12	Z	210	ASP	2.1
5	S	57	SER	2.1
12	Z	165	ASN	2.1
4	D	47	THR	2.1
14	N	105	LYS	2.1
4	R	125	LEU	2.0
6	F	2	THR	2.0
7	U	68	ARG	2.0
6	F	244	ASN	2.0
1	A	203	GLU	2.0
14	b	105	LYS	2.0
1	A	54	PRO	2.0
3	Q	27	ARG	2.0
1	A	249	ALA	2.0
4	D	2	ARG	2.0
4	D	125	LEU	2.0
5	S	165	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	7IM	b	1197	43/43	0.79	0.29	55,65,98,108	0
17	7IM	N	1198	43/43	0.82	0.26	54,66,101,106	0
17	7IM	K	1215	43/43	0.83	0.24	54,61,99,102	0
17	7IM	Y	1215	43/43	0.88	0.21	57,67,103,107	0
17	7IM	H	1223	43/43	0.89	0.23	54,62,78,82	0
17	7IM	V	1224	43/43	0.90	0.24	53,65,79,89	0

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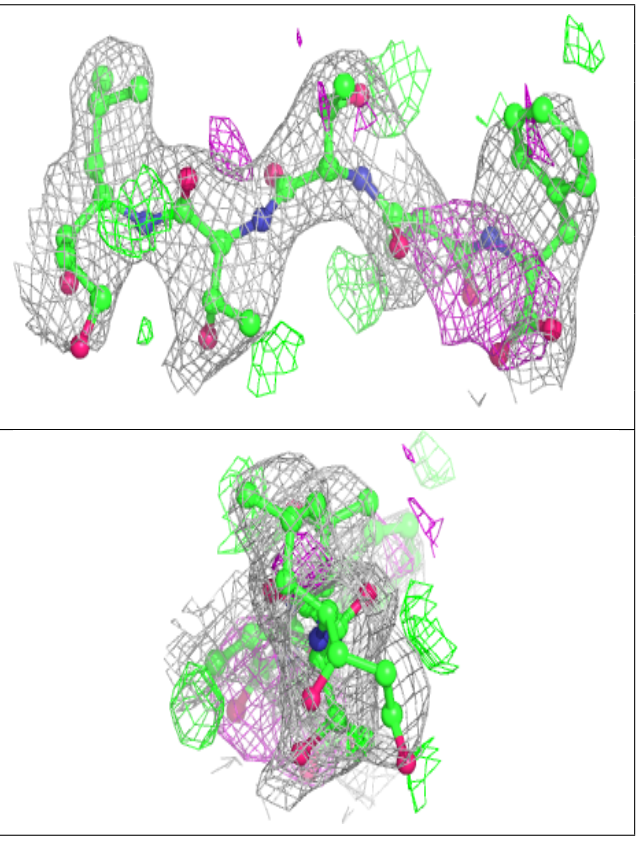
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	MES	K	1213	12/12	0.93	0.39	41,48,85,101	0
18	MES	Y	1213	12/12	0.93	0.41	46,51,89,111	0
15	MG	G	1243	1/1	0.95	0.08	55,55,55,55	0
16	CL	b	1198	1/1	0.95	0.09	56,56,56,56	0
15	MG	Z	1223	1/1	0.96	0.44	74,74,74,74	0
15	MG	V	1223	1/1	0.96	0.09	70,70,70,70	0
15	MG	K	1214	1/1	0.98	0.07	50,50,50,50	0
15	MG	N	1197	1/1	0.98	0.07	48,48,48,48	0
16	CL	G	1244	1/1	0.98	0.11	47,47,47,47	0
15	MG	Y	1214	1/1	0.99	0.03	53,53,53,53	0
16	CL	N	1199	1/1	0.99	0.06	47,47,47,47	0
16	CL	U	1243	1/1	0.99	0.21	46,46,46,46	0
15	MG	I	1205	1/1	0.99	0.09	54,54,54,54	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.

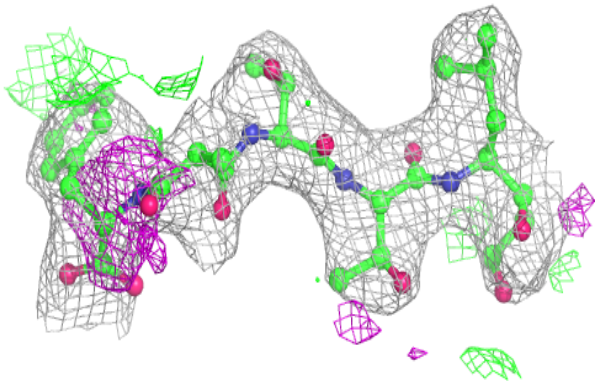
Electron density around 7IM b 1197:

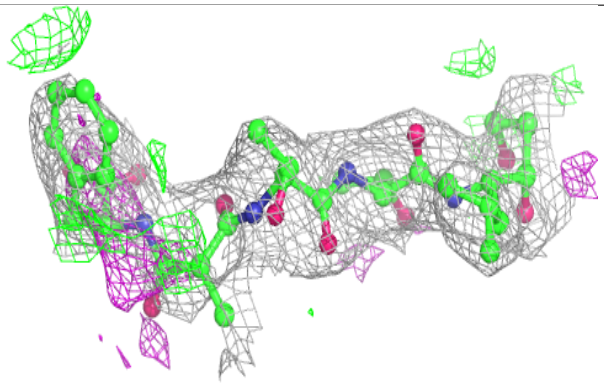
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

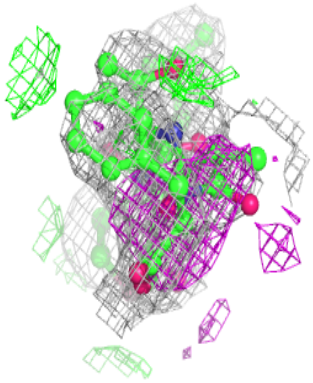


Electron density around 7IM N 1198:

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

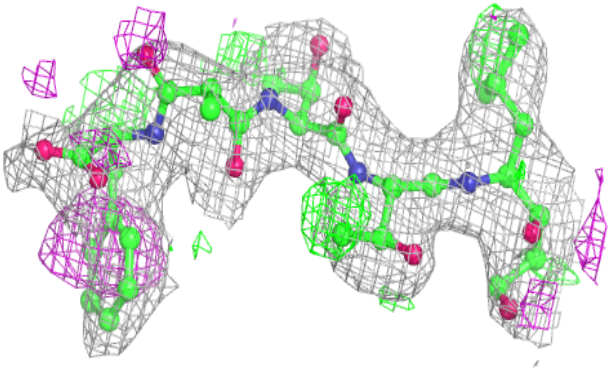


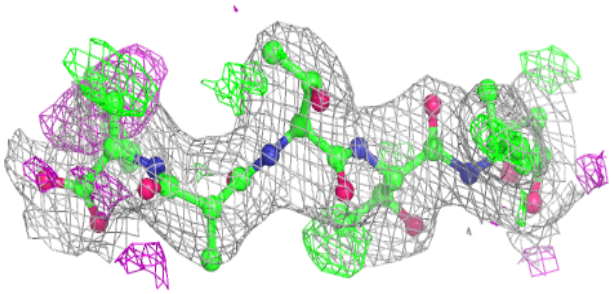


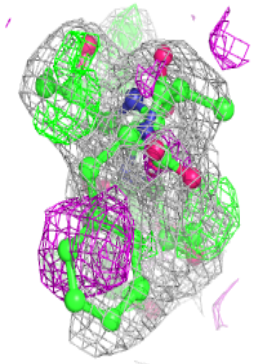


Electron density around 7IM K 1215:

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

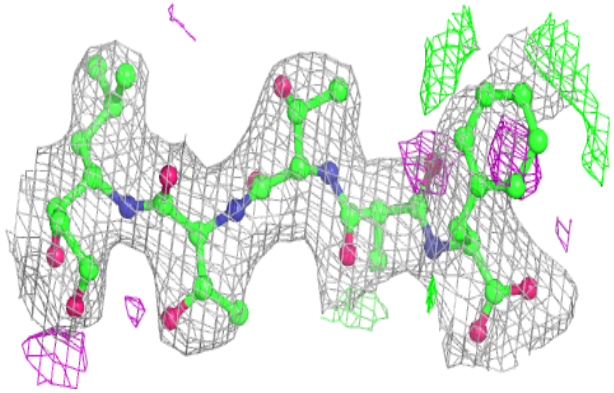


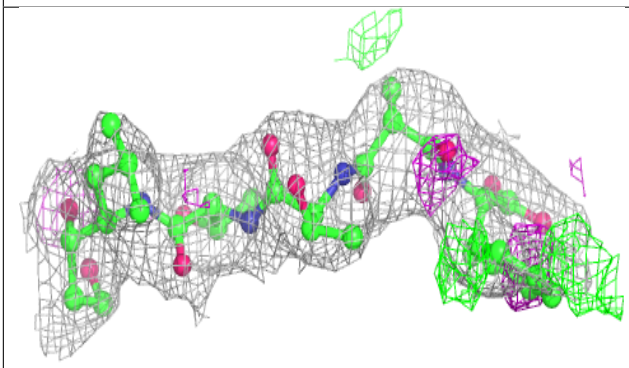


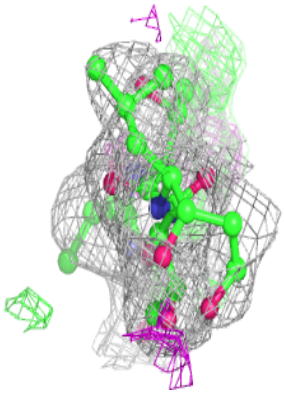


Electron density around 7IM Y 1215:

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

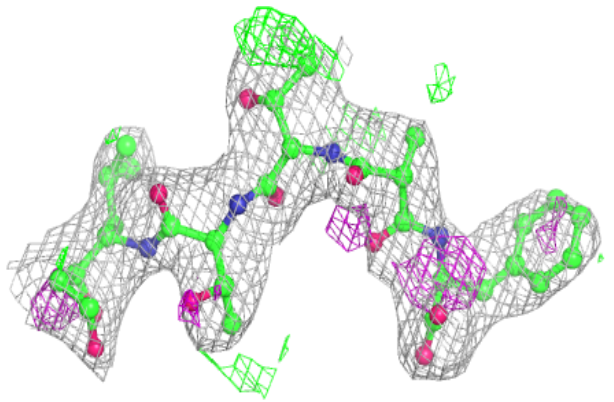


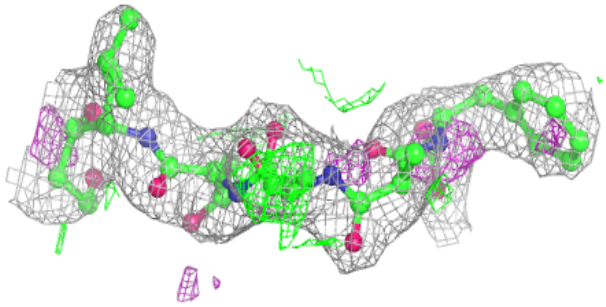


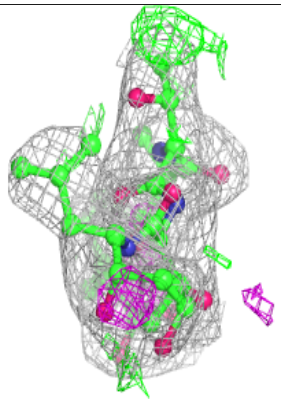


Electron density around 7IM H 1223:

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

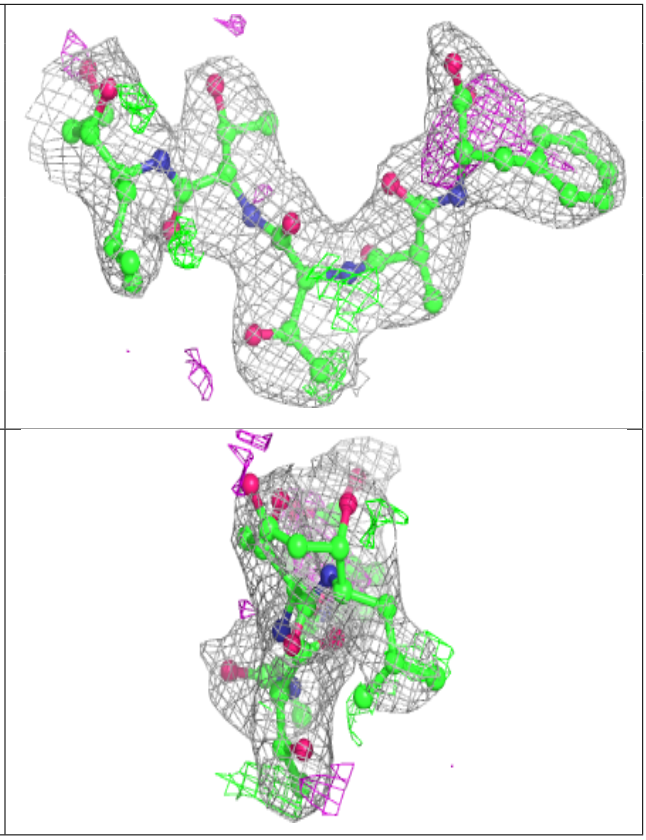






Electron density around 7IM V 1224:

$2mF_o$-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.