Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 10:12 AM EDT

PDB ID	:	8GBU
Title	:	Hepatitis B capsid Y132A mutant with compound AB-506
Authors	:	Horanyi, P.S.; Mayclin, S.J.
Deposited on	:	2023-02-28
Resolution	:	2.50 Å(reported)

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

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

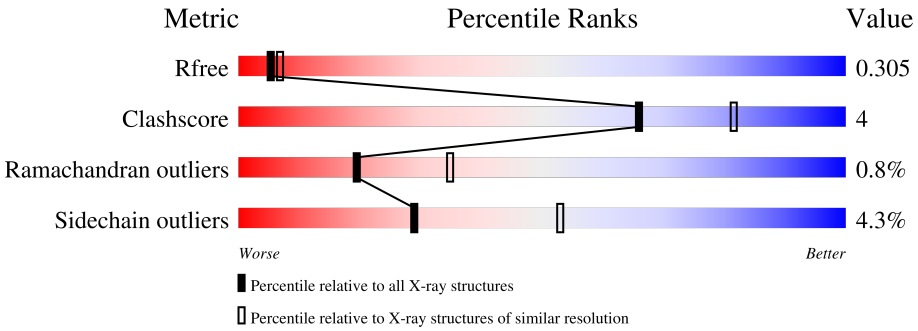
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	167	69% 16% • 14%
1	B	167	75% 7% 18%
1	C	167	72% 11% • 17%
1	D	167	81% • • 14%
1	E	167	71% 14% • 14%
1	F	167	72% 13% • 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6984 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1119	725	187	202	5			
1	B	137	Total	C	N	O	S	0	3	0
			1094	710	178	201	5			
1	C	139	Total	C	N	O	S	0	1	0
			1085	707	177	196	5			
1	D	143	Total	C	N	O	S	0	2	0
			1130	729	189	207	5			
1	E	143	Total	C	N	O	S	0	0	0
			1105	720	182	198	5			
1	F	143	Total	C	N	O	S	0	0	0
			1121	728	186	202	5			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP L7R9I1
A	-1	GLY	-	expression tag	UNP L7R9I1
A	0	SER	-	expression tag	UNP L7R9I1
A	132	ALA	TYR	engineered mutation	UNP L7R9I1
A	150	LYS	-	expression tag	UNP L7R9I1
A	151	LEU	-	expression tag	UNP L7R9I1
A	152	GLU	-	expression tag	UNP L7R9I1
A	153	ASN	-	expression tag	UNP L7R9I1
A	154	LEU	-	expression tag	UNP L7R9I1
A	155	TYR	-	expression tag	UNP L7R9I1
A	156	PHE	-	expression tag	UNP L7R9I1
A	157	GLN	-	expression tag	UNP L7R9I1
A	158	GLY	-	expression tag	UNP L7R9I1
A	159	HIS	-	expression tag	UNP L7R9I1
A	160	HIS	-	expression tag	UNP L7R9I1
A	161	HIS	-	expression tag	UNP L7R9I1
A	162	HIS	-	expression tag	UNP L7R9I1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	163	HIS	-	expression tag	UNP L7R9I1
A	164	HIS	-	expression tag	UNP L7R9I1
B	-2	MET	-	initiating methionine	UNP L7R9I1
B	-1	GLY	-	expression tag	UNP L7R9I1
B	0	SER	-	expression tag	UNP L7R9I1
B	132	ALA	TYR	engineered mutation	UNP L7R9I1
B	150	LYS	-	expression tag	UNP L7R9I1
B	151	LEU	-	expression tag	UNP L7R9I1
B	152	GLU	-	expression tag	UNP L7R9I1
B	153	ASN	-	expression tag	UNP L7R9I1
B	154	LEU	-	expression tag	UNP L7R9I1
B	155	TYR	-	expression tag	UNP L7R9I1
B	156	PHE	-	expression tag	UNP L7R9I1
B	157	GLN	-	expression tag	UNP L7R9I1
B	158	GLY	-	expression tag	UNP L7R9I1
B	159	HIS	-	expression tag	UNP L7R9I1
B	160	HIS	-	expression tag	UNP L7R9I1
B	161	HIS	-	expression tag	UNP L7R9I1
B	162	HIS	-	expression tag	UNP L7R9I1
B	163	HIS	-	expression tag	UNP L7R9I1
B	164	HIS	-	expression tag	UNP L7R9I1
C	-2	MET	-	initiating methionine	UNP L7R9I1
C	-1	GLY	-	expression tag	UNP L7R9I1
C	0	SER	-	expression tag	UNP L7R9I1
C	132	ALA	TYR	engineered mutation	UNP L7R9I1
C	150	LYS	-	expression tag	UNP L7R9I1
C	151	LEU	-	expression tag	UNP L7R9I1
C	152	GLU	-	expression tag	UNP L7R9I1
C	153	ASN	-	expression tag	UNP L7R9I1
C	154	LEU	-	expression tag	UNP L7R9I1
C	155	TYR	-	expression tag	UNP L7R9I1
C	156	PHE	-	expression tag	UNP L7R9I1
C	157	GLN	-	expression tag	UNP L7R9I1
C	158	GLY	-	expression tag	UNP L7R9I1
C	159	HIS	-	expression tag	UNP L7R9I1
C	160	HIS	-	expression tag	UNP L7R9I1
C	161	HIS	-	expression tag	UNP L7R9I1
C	162	HIS	-	expression tag	UNP L7R9I1
C	163	HIS	-	expression tag	UNP L7R9I1
C	164	HIS	-	expression tag	UNP L7R9I1
D	-2	MET	-	initiating methionine	UNP L7R9I1
D	-1	GLY	-	expression tag	UNP L7R9I1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP L7R9I1
D	132	ALA	TYR	engineered mutation	UNP L7R9I1
D	150	LYS	-	expression tag	UNP L7R9I1
D	151	LEU	-	expression tag	UNP L7R9I1
D	152	GLU	-	expression tag	UNP L7R9I1
D	153	ASN	-	expression tag	UNP L7R9I1
D	154	LEU	-	expression tag	UNP L7R9I1
D	155	TYR	-	expression tag	UNP L7R9I1
D	156	PHE	-	expression tag	UNP L7R9I1
D	157	GLN	-	expression tag	UNP L7R9I1
D	158	GLY	-	expression tag	UNP L7R9I1
D	159	HIS	-	expression tag	UNP L7R9I1
D	160	HIS	-	expression tag	UNP L7R9I1
D	161	HIS	-	expression tag	UNP L7R9I1
D	162	HIS	-	expression tag	UNP L7R9I1
D	163	HIS	-	expression tag	UNP L7R9I1
D	164	HIS	-	expression tag	UNP L7R9I1
E	-2	MET	-	initiating methionine	UNP L7R9I1
E	-1	GLY	-	expression tag	UNP L7R9I1
E	0	SER	-	expression tag	UNP L7R9I1
E	132	ALA	TYR	engineered mutation	UNP L7R9I1
E	150	LYS	-	expression tag	UNP L7R9I1
E	151	LEU	-	expression tag	UNP L7R9I1
E	152	GLU	-	expression tag	UNP L7R9I1
E	153	ASN	-	expression tag	UNP L7R9I1
E	154	LEU	-	expression tag	UNP L7R9I1
E	155	TYR	-	expression tag	UNP L7R9I1
E	156	PHE	-	expression tag	UNP L7R9I1
E	157	GLN	-	expression tag	UNP L7R9I1
E	158	GLY	-	expression tag	UNP L7R9I1
E	159	HIS	-	expression tag	UNP L7R9I1
E	160	HIS	-	expression tag	UNP L7R9I1
E	161	HIS	-	expression tag	UNP L7R9I1
E	162	HIS	-	expression tag	UNP L7R9I1
E	163	HIS	-	expression tag	UNP L7R9I1
E	164	HIS	-	expression tag	UNP L7R9I1
F	-2	MET	-	initiating methionine	UNP L7R9I1
F	-1	GLY	-	expression tag	UNP L7R9I1
F	0	SER	-	expression tag	UNP L7R9I1
F	132	ALA	TYR	engineered mutation	UNP L7R9I1
F	150	LYS	-	expression tag	UNP L7R9I1
F	151	LEU	-	expression tag	UNP L7R9I1

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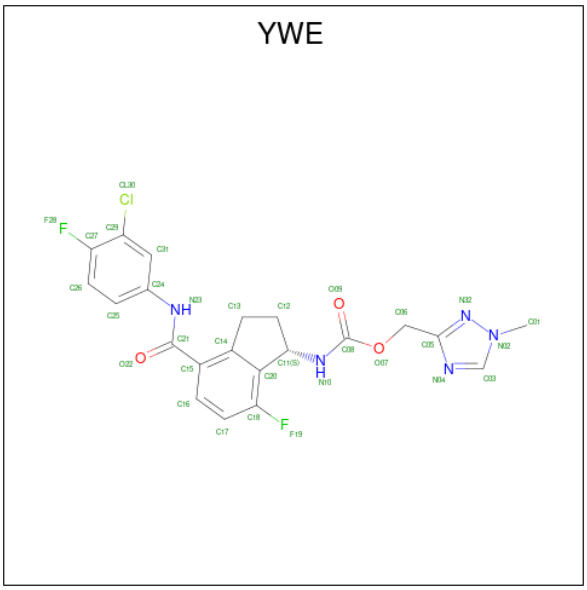
Chain	Residue	Modelled	Actual	Comment	Reference
F	152	GLU	-	expression tag	UNP L7R9I1
F	153	ASN	-	expression tag	UNP L7R9I1
F	154	LEU	-	expression tag	UNP L7R9I1
F	155	TYR	-	expression tag	UNP L7R9I1
F	156	PHE	-	expression tag	UNP L7R9I1
F	157	GLN	-	expression tag	UNP L7R9I1
F	158	GLY	-	expression tag	UNP L7R9I1
F	159	HIS	-	expression tag	UNP L7R9I1
F	160	HIS	-	expression tag	UNP L7R9I1
F	161	HIS	-	expression tag	UNP L7R9I1
F	162	HIS	-	expression tag	UNP L7R9I1
F	163	HIS	-	expression tag	UNP L7R9I1
F	164	HIS	-	expression tag	UNP L7R9I1

- Molecule 2 is (1-methyl-1H-1,2,4-triazol-3-yl)methyl {(1S)-4-[(3-chloro-4-fluorophenyl)carbamoyl]-7-fluoro-2,3-dihydro-1H-inden-1-yl}carbamate (three-letter code: YWE) (formula: $C_{21}H_{18}ClF_2N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	1
			64	42	2	4	10	6		
2	A	1	Total	C	Cl	F	N	O	0	0
			32	21	1	2	5	3		
2	B	1	Total	C	Cl	F	N	O	0	0
			32	21	1	2	5	3		
2	C	1	Total	C	Cl	F	N	O	0	0
			32	21	1	2	5	3		

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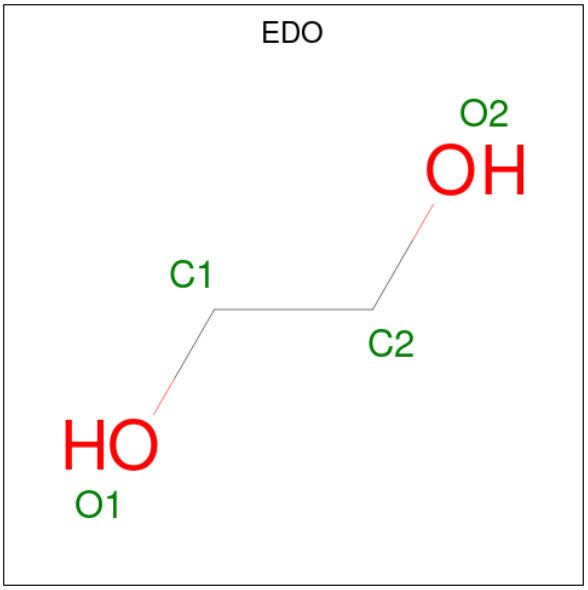
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	Cl	F	N	O	0	0
			32	21	1	2	5	3		
2	E	1	Total	C	Cl	F	N	O	0	0
			32	21	1	2	5	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

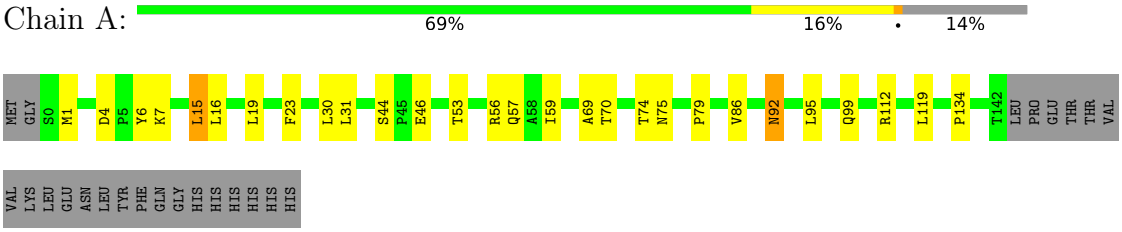
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	10	Total O 10 10	0	0
4	C	17	Total O 17 17	0	0
4	D	13	Total O 13 13	0	0
4	E	10	Total O 10 10	0	0
4	F	11	Total O 11 11	0	0

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. 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. 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.

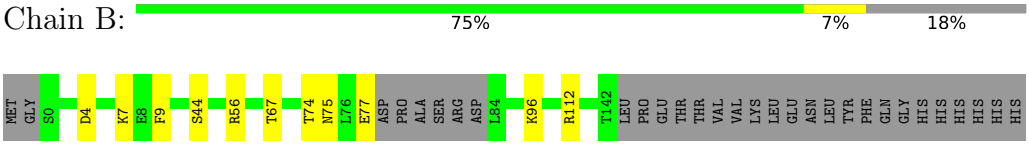
- Molecule 1: Capsid protein

Chain A:



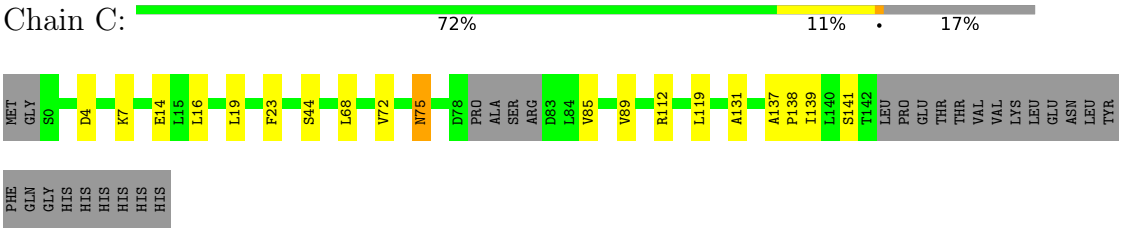
- Molecule 1: Capsid protein

Chain B:



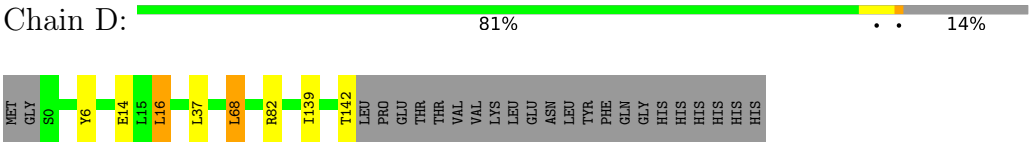
- Molecule 1: Capsid protein

Chain C:



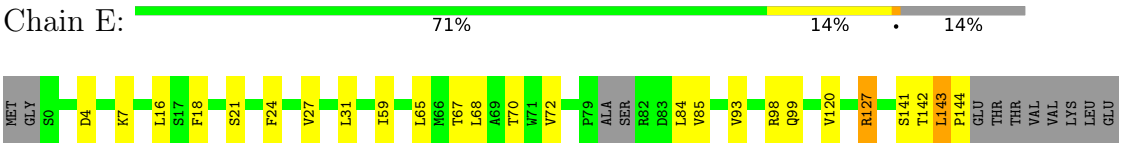
- Molecule 1: Capsid protein

Chain D:



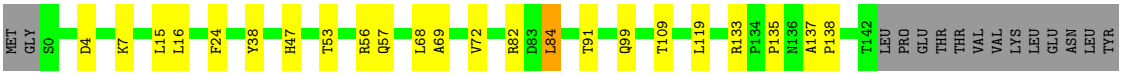
- Molecule 1: Capsid protein

Chain E:



• Molecule 1: Capsid protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.94Å 87.88Å 100.83Å 90.00° 104.12° 90.00°	Depositor
Resolution (Å)	97.78 – 2.50 43.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (97.78-2.50) 99.1 (43.94-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.84 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.233 , 0.285 0.268 , 0.305	Depositor DCC
R_{free} test set	2177 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6984	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% 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: YWE, EDO

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	0.53	0/1153	0.76	1/1581 (0.1%)
1	B	0.53	0/1126	0.71	1/1543 (0.1%)
1	C	0.57	0/1117	0.76	0/1532
1	D	0.54	0/1164	0.73	0/1596
1	E	0.53	0/1138	0.79	2/1561 (0.1%)
1	F	0.54	0/1155	0.76	2/1584 (0.1%)
All	All	0.54	0/6853	0.75	6/9397 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	127	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	B	56	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	F	133	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	E	144	PRO	N-CA-CB	5.26	109.62	103.30
1	F	84	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	56	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	141	SER	Peptide

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	1119	0	1090	15	0
1	B	1094	0	1060	3	0
1	C	1085	0	1048	11	0
1	D	1130	0	1094	5	0
1	E	1105	0	1066	13	0
1	F	1121	0	1100	10	0
2	A	96	0	0	2	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	E	64	0	0	1	0
3	A	4	0	6	0	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0
3	E	8	0	12	0	0
3	F	8	0	12	0	0
4	A	13	0	0	0	0
4	B	10	0	0	0	0
4	C	17	0	0	0	0
4	D	13	0	0	0	0
4	E	10	0	0	0	0
4	F	11	0	0	0	0
All	All	6984	0	6506	53	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 4.

All (53) 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)
1:A:6:TYR:CZ	1:A:16:LEU:HD22	2.15	0.81
1:C:19:LEU:HD11	1:C:119:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ASP:HB3	1:C:7:LYS:HB2	1.87	0.56
1:A:16:LEU:HD23	1:A:99:GLN:HB3	1.86	0.56
1:E:72:VAL:HG21	1:E:85:VAL:CG1	2.36	0.56
1:C:137:ALA:HB1	1:C:138:PRO:HD2	1.88	0.55
1:F:38:TYR:OH	1:F:109:THR:HG22	2.07	0.54
1:E:72:VAL:HG21	1:E:85:VAL:HG11	1.89	0.54
1:C:75:ASN:HD22	1:C:75:ASN:N	2.06	0.54
1:F:137:ALA:HB1	1:F:138:PRO:HD2	1.90	0.54
1:A:53:THR:O	1:A:57:GLN:HG2	2.08	0.53
2:A:501[B]:YWE:N23	2:A:501[B]:YWE:C13	2.70	0.53
1:A:6:TYR:CE1	1:A:16:LEU:HD22	2.44	0.53
1:E:68:LEU:CD1	1:F:68:LEU:HD22	2.39	0.53
1:C:72:VAL:HG11	1:C:85:VAL:HG11	1.91	0.52
1:F:53:THR:O	1:F:57:GLN:HG2	2.10	0.52
1:F:15:LEU:O	1:F:119:LEU:HD11	2.09	0.52
1:C:89:VAL:HG12	1:D:68:LEU:HD11	1.90	0.52
1:D:6:TYR:CZ	1:D:16:LEU:HD22	2.45	0.52
1:E:18:PHE:O	1:E:127:ARG:NH1	2.43	0.51
1:F:24:PHE:CZ	1:F:99:GLN:HG2	2.46	0.51
1:A:69:ALA:HB1	1:A:86:VAL:HG13	1.92	0.51
1:F:47:HIS:O	1:F:56:ARG:NH2	2.44	0.51
1:B:74:THR:HG23	1:B:75:ASN:HD22	1.75	0.50
1:A:95:LEU:HD11	1:A:99:GLN:HE21	1.77	0.50
1:A:15:LEU:CD2	1:A:119:LEU:HD22	2.42	0.50
1:E:143:LEU:HD22	2:E:502:YWE:C06	2.42	0.49
1:C:68:LEU:O	1:C:72:VAL:HG23	2.12	0.49
1:A:23:PHE:CD1	1:A:23:PHE:C	2.85	0.49
1:B:9:PHE:O	1:B:112:ARG:HD3	2.13	0.49
1:E:24:PHE:CZ	1:E:99:GLN:HG2	2.50	0.47
1:A:95:LEU:O	1:A:95:LEU:HD12	2.14	0.46
1:C:137:ALA:HB1	1:C:138:PRO:CD	2.44	0.46
1:D:37:LEU:HD11	1:E:120:VAL:HG13	1.97	0.46
1:C:139:ILE:HD12	1:C:139:ILE:O	2.16	0.46
1:F:4:ASP:HB3	1:F:7:LYS:HB2	1.98	0.46
1:A:92:ASN:OD1	1:A:92:ASN:N	2.50	0.45
1:A:4:ASP:HB3	1:A:7:LYS:HB2	1.99	0.44
1:A:31:LEU:HD22	1:A:59:ILE:HG23	1.99	0.43
1:E:18:PHE:CD1	1:E:127:ARG:NH1	2.87	0.43
1:E:68:LEU:HD11	1:F:68:LEU:HD22	2.01	0.43
1:D:139:ILE:HD12	1:D:139:ILE:O	2.19	0.43
1:A:70:THR:O	1:A:74:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:SER:O	1:E:98:ARG:NH2	2.52	0.42
1:A:30:LEU:HD23	2:A:501[A]:YWE:F28	2.09	0.42
1:C:23:PHE:CD1	1:C:23:PHE:C	2.92	0.42
1:A:74:THR:HG23	1:A:75:ASN:HD22	1.84	0.41
1:E:4:ASP:HB3	1:E:7:LYS:HB2	2.01	0.41
1:E:31:LEU:HD22	1:E:59:ILE:HG23	2.03	0.41
1:E:27:VAL:HG22	1:E:98:ARG:HG3	2.03	0.41
1:F:69:ALA:O	1:F:72:VAL:HG22	2.20	0.41
1:B:4:ASP:HB3	1:B:7:LYS:HB2	2.02	0.40
1:C:89:VAL:HG12	1:D:68:LEU:CD1	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	141/167 (84%)	134 (95%)	5 (4%)	2 (1%)	11	20
1	B	136/167 (81%)	134 (98%)	2 (2%)	0	100	100
1	C	136/167 (81%)	126 (93%)	9 (7%)	1 (1%)	22	39
1	D	143/167 (86%)	132 (92%)	11 (8%)	0	100	100
1	E	139/167 (83%)	129 (93%)	8 (6%)	2 (1%)	11	20
1	F	141/167 (84%)	132 (94%)	7 (5%)	2 (1%)	11	20
All	All	836/1002 (83%)	787 (94%)	42 (5%)	7 (1%)	19	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	PRO
1	F	84	LEU

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Mol	Chain	Res	Type
1	C	131	ALA
1	E	142	THR
1	E	143	LEU
1	F	135	PRO
1	A	134	PRO

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	121/147 (82%)	114 (94%)	7 (6%)	20	38
1	B	120/147 (82%)	116 (97%)	4 (3%)	38	64
1	C	116/147 (79%)	110 (95%)	6 (5%)	23	44
1	D	123/147 (84%)	118 (96%)	5 (4%)	30	55
1	E	117/147 (80%)	111 (95%)	6 (5%)	24	45
1	F	122/147 (83%)	119 (98%)	3 (2%)	47	73
All	All	719/882 (82%)	688 (96%)	31 (4%)	29	53

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	LEU
1	A	19	LEU
1	A	44	SER
1	A	46	GLU
1	A	92	ASN
1	A	112	ARG
1	B	44	SER
1	B	67	THR
1	B	77	GLU
1	B	96	LYS
1	C	14	GLU
1	C	16	LEU

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Mol	Chain	Res	Type
1	C	44	SER
1	C	75	ASN
1	C	112	ARG
1	C	141	SER
1	D	14	GLU
1	D	16	LEU
1	D	68	LEU
1	D	82	ARG
1	D	142	THR
1	E	16	LEU
1	E	65	LEU
1	E	67	THR
1	E	70	THR
1	E	84	LEU
1	E	93	VAL
1	F	16	LEU
1	F	82	ARG
1	F	91	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	99	GLN
1	B	75	ASN
1	C	75	ASN
1	C	99	GLN
1	F	99	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 (i)

15 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	YWE	B	501	-	31,35,35	0.98	0	41,50,50	2.05	13 (31%)
3	EDO	E	503	-	3,3,3	0.66	0	2,2,2	0.10	0
2	YWE	C	501	-	31,35,35	1.01	2 (6%)	41,50,50	1.89	13 (31%)
2	YWE	A	501[A]	-	31,35,35	0.89	1 (3%)	41,50,50	1.25	7 (17%)
3	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.34	0
2	YWE	E	501	-	31,35,35	1.11	1 (3%)	41,50,50	2.08	12 (29%)
3	EDO	F	202	-	3,3,3	0.55	0	2,2,2	0.41	0
3	EDO	E	504	-	3,3,3	0.64	0	2,2,2	0.33	0
2	YWE	A	501[B]	-	31,35,35	0.86	1 (3%)	41,50,50	1.73	9 (21%)
2	YWE	E	502	-	31,35,35	0.96	0	41,50,50	1.87	11 (26%)
3	EDO	C	503	-	3,3,3	0.59	0	2,2,2	0.14	0
3	EDO	C	502	-	3,3,3	0.50	0	2,2,2	0.19	0
3	EDO	D	201	-	3,3,3	0.50	0	2,2,2	0.36	0
2	YWE	A	502	-	31,35,35	0.85	0	41,50,50	2.22	14 (34%)
3	EDO	F	201	-	3,3,3	0.69	0	2,2,2	0.22	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
2	YWE	B	501	-	-	4/15/26/26	0/4/4/4
3	EDO	E	503	-	-	1/1/1/1	-
2	YWE	C	501	-	-	5/15/26/26	0/4/4/4
2	YWE	A	501[A]	-	-	3/15/26/26	0/4/4/4
3	EDO	A	503	-	-	1/1/1/1	-
2	YWE	E	501	-	-	4/15/26/26	0/4/4/4
3	EDO	F	202	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	504	-	-	1/1/1/1	-
2	YWE	A	501[B]	-	-	6/15/26/26	0/4/4/4
2	YWE	E	502	-	-	4/15/26/26	0/4/4/4
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	D	201	-	-	1/1/1/1	-
2	YWE	A	502	-	-	4/15/26/26	0/4/4/4
3	EDO	F	201	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	YWE	C29-CL30	2.74	1.80	1.73
2	A	501[B]	YWE	C29-CL30	2.51	1.79	1.73
2	C	501	YWE	C15-C14	2.13	1.43	1.40
2	C	501	YWE	C29-CL30	2.13	1.78	1.73
2	E	501	YWE	C15-C14	2.01	1.43	1.40

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	YWE	F28-C27-C29	6.68	125.14	118.98
2	B	501	YWE	C31-C29-C27	6.42	126.16	119.77
2	A	502	YWE	C12-C11-C20	-5.58	98.86	103.04
2	A	501[B]	YWE	C12-C11-C20	-5.48	98.94	103.04
2	E	501	YWE	C12-C11-C20	-5.39	99.00	103.04
2	E	501	YWE	C31-C29-C27	5.32	125.06	119.77
2	C	501	YWE	C12-C11-C20	-5.07	99.24	103.04
2	E	502	YWE	C12-C11-C20	-4.89	99.37	103.04
2	E	502	YWE	C31-C29-C27	4.70	124.44	119.77
2	C	501	YWE	C31-C29-C27	4.43	124.18	119.77
2	A	502	YWE	C31-C29-C27	4.19	123.94	119.77
2	A	502	YWE	C06-O07-C08	4.10	125.08	115.93
2	B	501	YWE	C27-C29-CL30	-4.09	114.83	119.78
2	B	501	YWE	C12-C11-C20	-4.02	100.03	103.04
2	A	501[B]	YWE	F19-C18-C20	3.93	121.97	118.13
2	E	501	YWE	F19-C18-C20	3.76	121.81	118.13
2	E	502	YWE	C17-C18-C20	-3.76	120.01	123.98
2	B	501	YWE	F19-C18-C20	3.67	121.72	118.13
2	A	502	YWE	C13-C12-C11	-3.63	99.71	105.54
2	A	502	YWE	C17-C18-C20	-3.37	120.42	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501[B]	YWE	C17-C18-C20	-3.25	120.55	123.98
2	E	502	YWE	C27-C29-CL30	-3.22	115.88	119.78
2	A	501[A]	YWE	F28-C27-C29	3.19	121.92	118.98
2	C	501	YWE	F28-C27-C29	3.08	121.82	118.98
2	B	501	YWE	C24-C31-C29	-3.06	115.74	119.53
2	E	501	YWE	C16-C15-C14	-3.04	116.19	119.78
2	A	502	YWE	C31-C29-CL30	-3.03	113.59	118.49
2	E	501	YWE	C06-O07-C08	3.02	122.66	115.93
2	A	502	YWE	C26-C27-C29	-2.96	118.64	121.32
2	A	501[A]	YWE	C17-C18-C20	-2.96	120.86	123.98
2	B	501	YWE	C17-C18-C20	-2.96	120.86	123.98
2	E	501	YWE	C24-C31-C29	-2.92	115.91	119.53
2	B	501	YWE	F28-C27-C29	2.85	121.61	118.98
2	E	502	YWE	C24-C31-C29	-2.83	116.03	119.53
2	E	501	YWE	C14-C15-C21	2.82	126.10	121.34
2	A	501[A]	YWE	F19-C18-C20	2.79	120.86	118.13
2	A	501[B]	YWE	C31-C29-C27	2.76	122.52	119.77
2	B	501	YWE	C26-C25-C24	2.73	123.45	120.30
2	C	501	YWE	C17-C18-C20	-2.72	121.11	123.98
2	E	502	YWE	C16-C15-C14	-2.68	116.62	119.78
2	C	501	YWE	C27-C29-CL30	-2.64	116.58	119.78
2	E	501	YWE	C24-N23-C21	2.64	133.43	126.58
2	C	501	YWE	C13-C14-C15	2.62	133.16	129.71
2	E	501	YWE	C13-C14-C15	2.62	133.16	129.71
2	C	501	YWE	C24-C31-C29	-2.58	116.34	119.53
2	B	501	YWE	C13-C12-C11	-2.57	101.41	105.54
2	C	501	YWE	C16-C15-C14	-2.57	116.75	119.78
2	A	501[B]	YWE	C12-C13-C14	-2.51	100.73	103.30
2	A	502	YWE	C12-C13-C14	-2.51	100.73	103.30
2	E	502	YWE	C13-C12-C11	-2.50	101.52	105.54
2	B	501	YWE	C26-C27-C29	-2.49	119.07	121.32
2	C	501	YWE	C26-C25-C24	2.48	123.17	120.30
2	C	501	YWE	C31-C24-N23	2.47	128.26	120.18
2	A	501[B]	YWE	C06-O07-C08	2.40	121.29	115.93
2	C	501	YWE	C13-C12-C11	-2.40	101.69	105.54
2	B	501	YWE	C13-C14-C15	2.40	132.87	129.71
2	A	501[B]	YWE	C26-C27-C29	-2.38	119.16	121.32
2	C	501	YWE	C25-C24-N23	-2.38	112.39	120.40
2	E	501	YWE	O22-C21-N23	-2.34	118.36	123.71
2	B	501	YWE	C16-C15-C14	-2.34	117.02	119.78
2	A	501[A]	YWE	C26-C27-C29	-2.33	119.22	121.32
2	A	501[B]	YWE	C27-C29-CL30	-2.31	116.99	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	YWE	C17-C18-C20	-2.30	121.55	123.98
2	E	502	YWE	C13-C14-C15	2.28	132.72	129.71
2	A	501[A]	YWE	C14-C15-C21	-2.25	117.54	121.34
2	E	502	YWE	C26-C25-C24	2.23	122.88	120.30
2	A	502	YWE	F19-C18-C20	2.22	120.30	118.13
2	A	502	YWE	C27-C29-CL30	2.22	122.47	119.78
2	A	502	YWE	C16-C15-C14	-2.20	117.19	119.78
2	B	501	YWE	C24-N23-C21	2.17	132.21	126.58
2	E	501	YWE	O22-C21-C15	2.15	124.95	121.01
2	A	501[B]	YWE	C24-N23-C21	2.10	132.03	126.58
2	A	502	YWE	C24-N23-C21	2.09	132.00	126.58
2	E	502	YWE	C24-N23-C21	2.08	131.99	126.58
2	A	501[A]	YWE	C31-C29-C27	2.07	121.83	119.77
2	C	501	YWE	C24-N23-C21	2.06	131.92	126.58
2	A	502	YWE	C13-C14-C15	2.05	132.42	129.71
2	A	501[A]	YWE	C16-C15-C21	2.05	123.91	118.43
2	E	502	YWE	C25-C26-C27	-2.04	116.58	119.05

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[B]	YWE	O09-C08-O07-C06
2	A	501[B]	YWE	N10-C08-O07-C06
2	E	502	YWE	O09-C08-O07-C06
2	E	502	YWE	N10-C08-O07-C06
2	A	502	YWE	O09-C08-O07-C06
2	A	502	YWE	N10-C08-O07-C06
2	A	501[B]	YWE	C14-C15-C21-N23
2	A	501[A]	YWE	O07-C08-N10-C11
2	A	501[B]	YWE	C25-C24-N23-C21
2	A	501[B]	YWE	C14-C15-C21-O22
2	A	501[B]	YWE	C31-C24-N23-C21
2	E	501	YWE	C14-C15-C21-N23
2	A	501[A]	YWE	O09-C08-N10-C11
2	C	501	YWE	C14-C15-C21-N23
3	D	201	EDO	O1-C1-C2-O2
3	E	503	EDO	O1-C1-C2-O2
2	E	501	YWE	C14-C15-C21-O22
2	B	501	YWE	O07-C08-N10-C11
2	E	502	YWE	C14-C15-C21-N23
2	B	501	YWE	O09-C08-N10-C11

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Mol	Chain	Res	Type	Atoms
2	E	501	YWE	C25-C24-N23-C21
2	C	501	YWE	C14-C15-C21-O22
2	B	501	YWE	C14-C15-C21-N23
2	A	501[A]	YWE	C12-C11-N10-C08
2	C	501	YWE	O07-C08-N10-C11
2	E	502	YWE	C14-C15-C21-O22
3	A	503	EDO	O1-C1-C2-O2
3	E	504	EDO	O1-C1-C2-O2
2	A	502	YWE	C14-C15-C21-N23
2	C	501	YWE	O09-C08-N10-C11
2	C	501	YWE	C25-C24-N23-C21
2	E	501	YWE	C31-C24-N23-C21
3	C	502	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	F	201	EDO	O1-C1-C2-O2
3	F	202	EDO	O1-C1-C2-O2
2	A	502	YWE	C14-C15-C21-O22
2	B	501	YWE	C14-C15-C21-O22

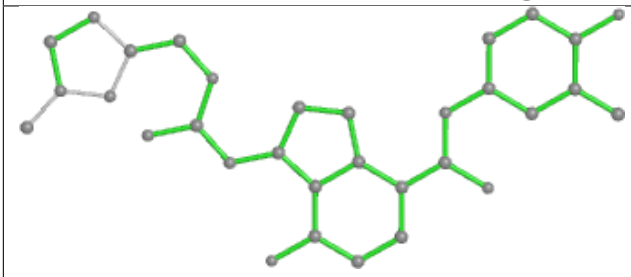
There are no ring outliers.

3 monomers are involved in 3 short contacts:

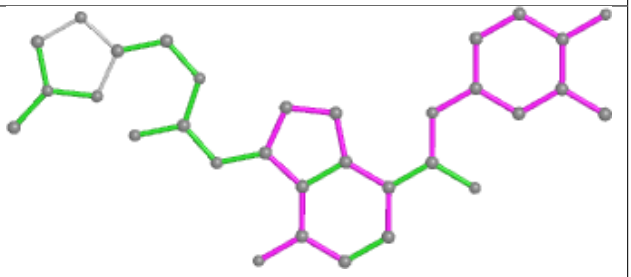
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[A]	YWE	1	0
2	A	501[B]	YWE	1	0
2	E	502	YWE	1	0

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.

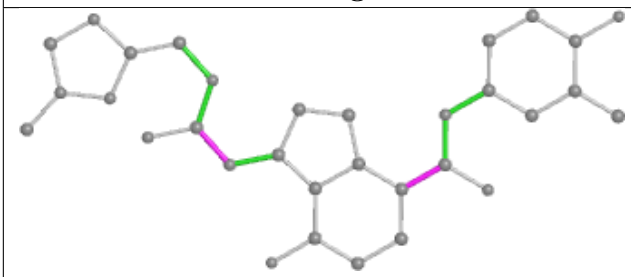
Ligand YWE B 501



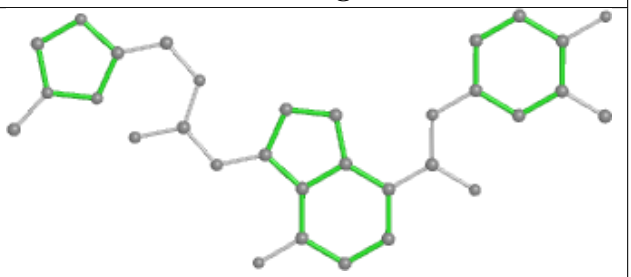
Bond lengths



Bond angles

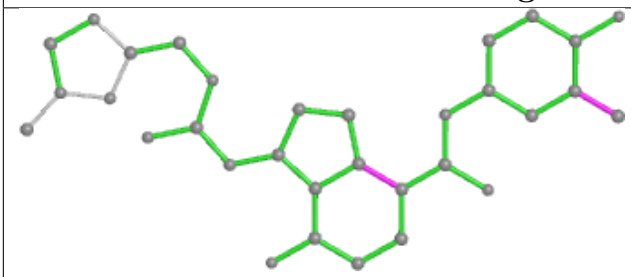


Torsions

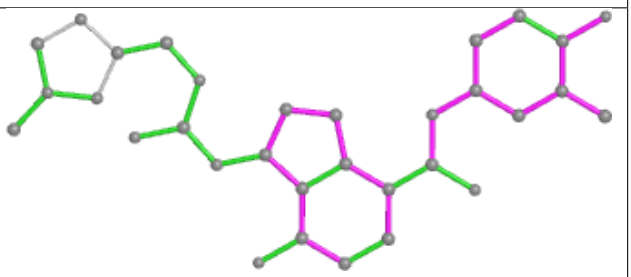


Rings

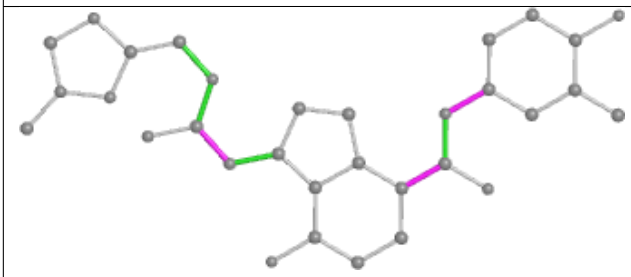
Ligand YWE C 501



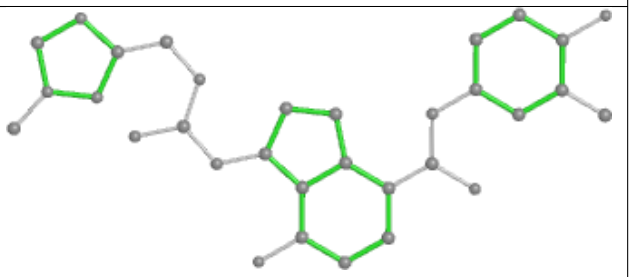
Bond lengths



Bond angles

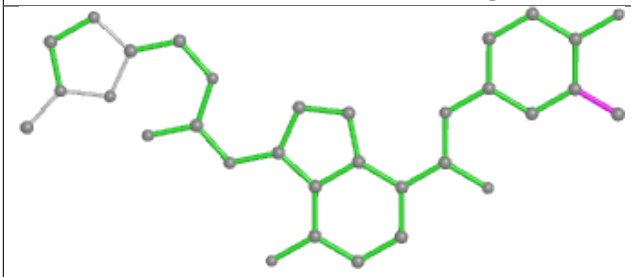


Torsions

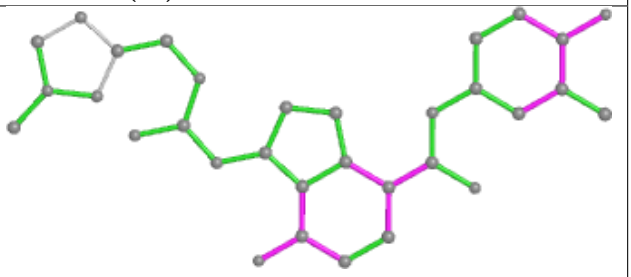


Rings

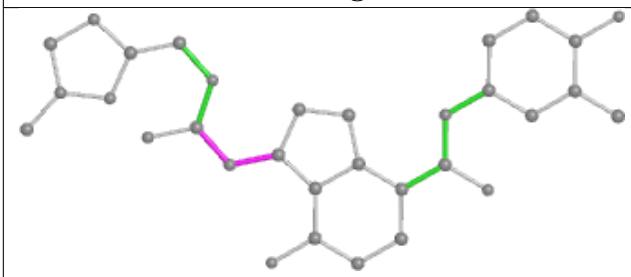
Ligand YWE A 501 (A)



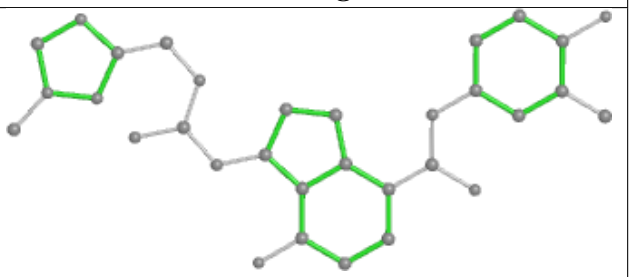
Bond lengths



Bond angles

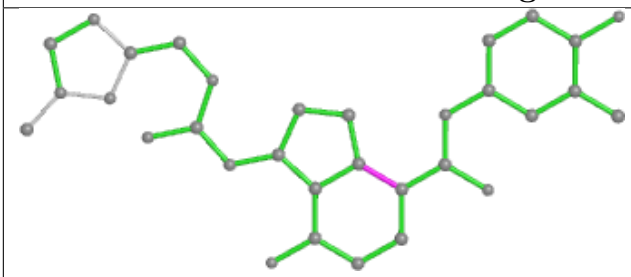


Torsions

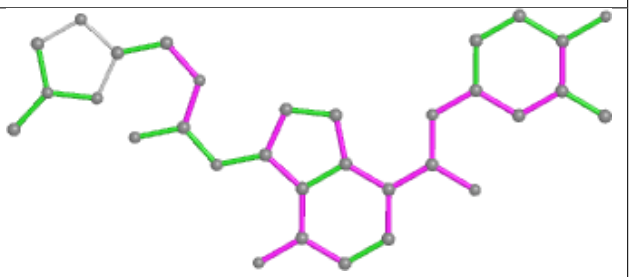


Rings

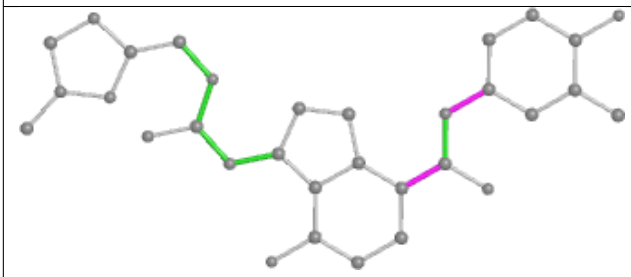
Ligand YWE E 501



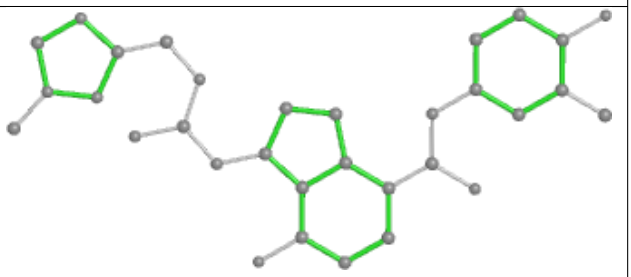
Bond lengths



Bond angles

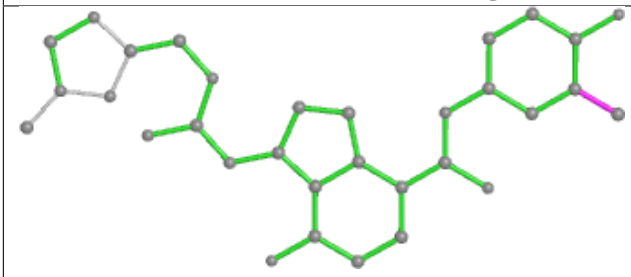


Torsions

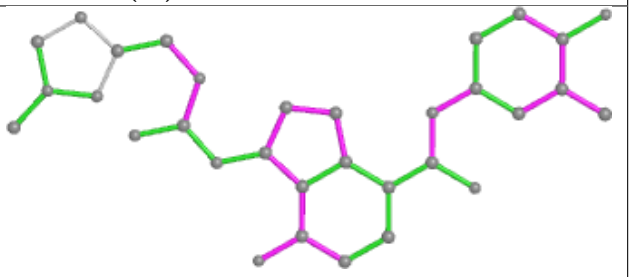


Rings

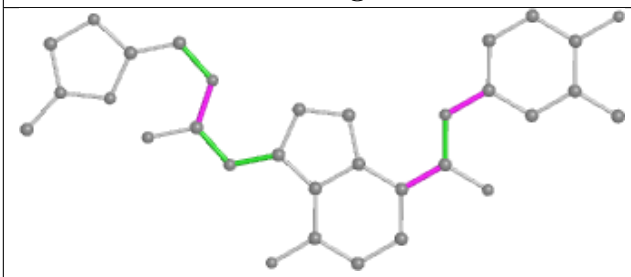
Ligand YWE A 501 (B)



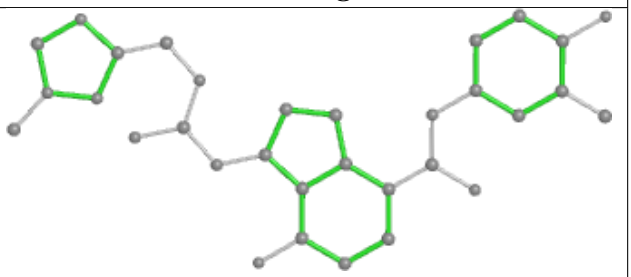
Bond lengths



Bond angles

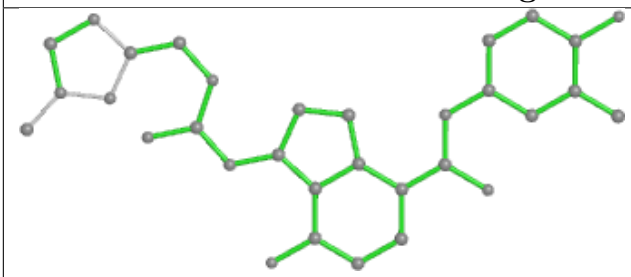


Torsions

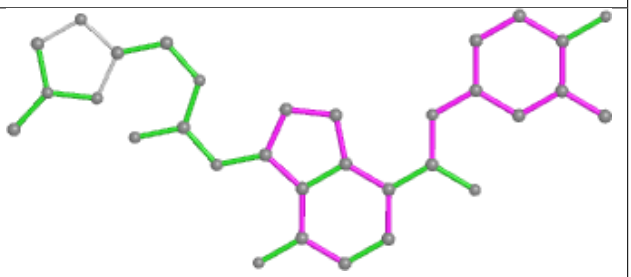


Rings

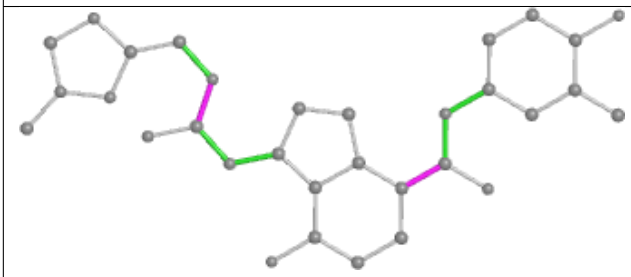
Ligand YWE E 502



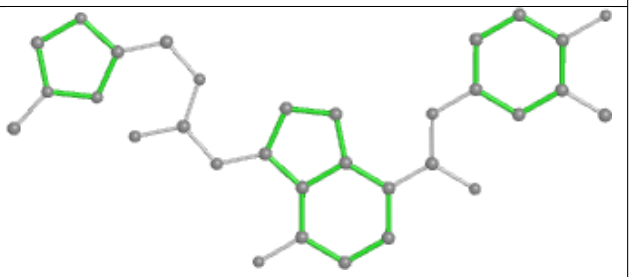
Bond lengths



Bond angles

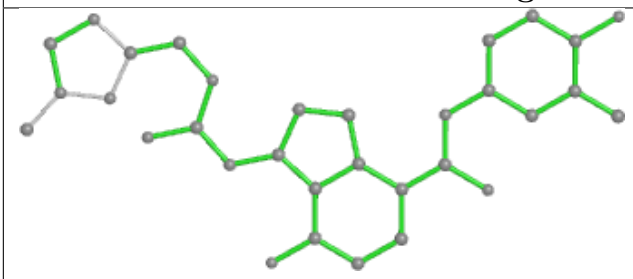


Torsions

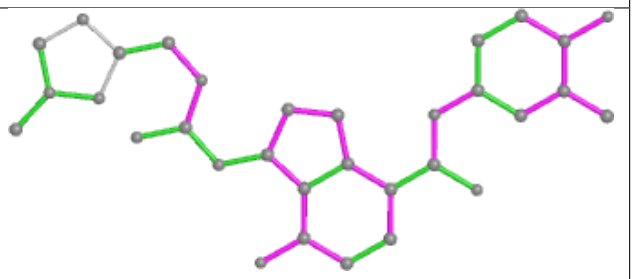


Rings

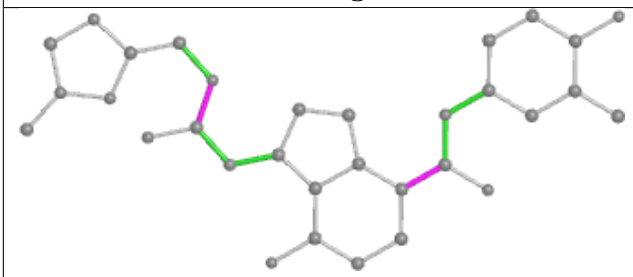
Ligand YWE A 502



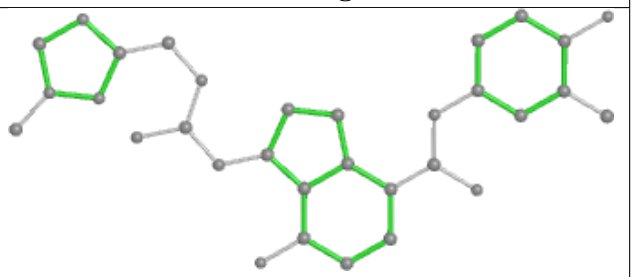
Bond lengths



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

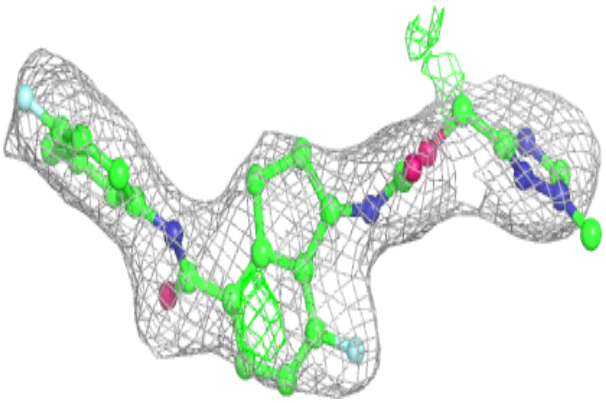
6.4 Ligands

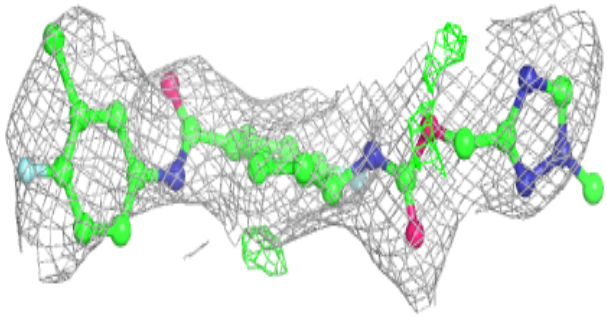
Unable to reproduce the depositors R factor - this section is therefore empty.

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 YWE A 501 (A):

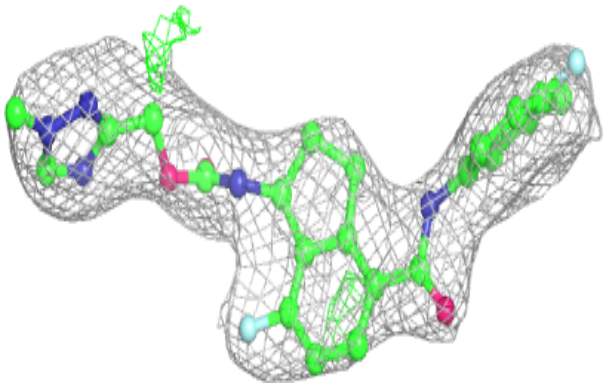
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

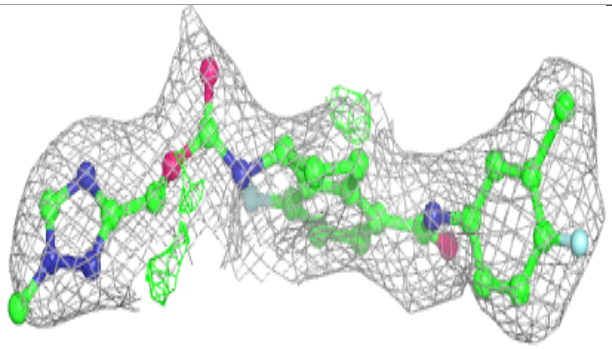


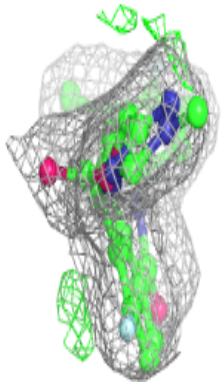


Electron density around YWE A 501 (B):

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

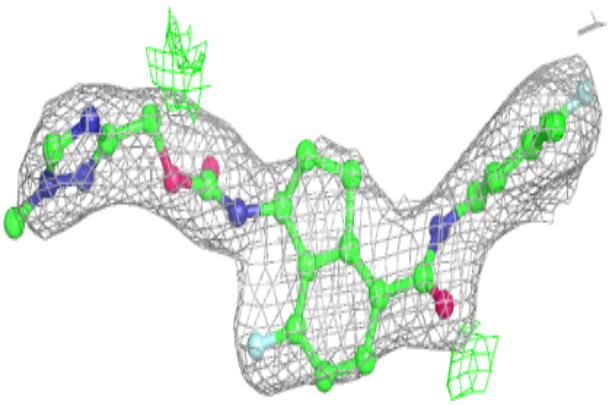


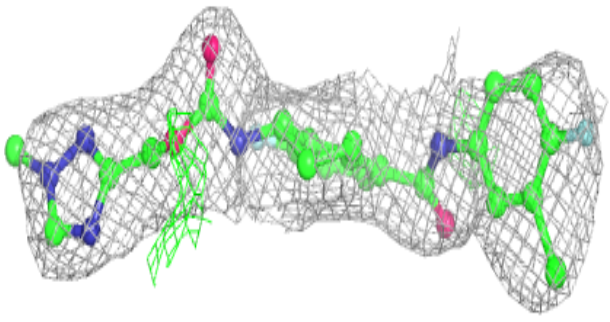


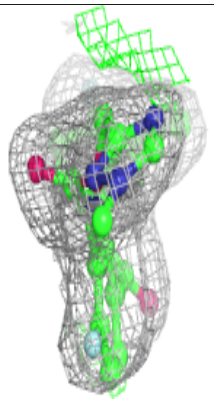


Electron density around YWE A 502:

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

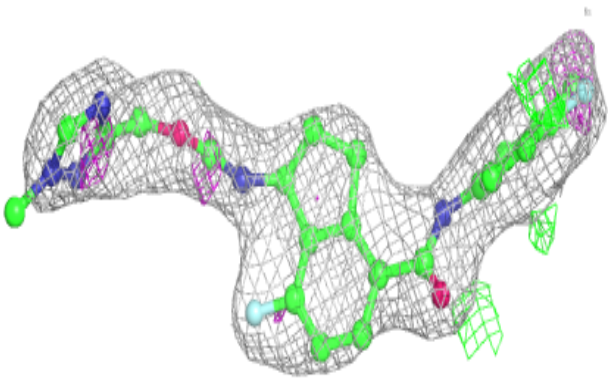


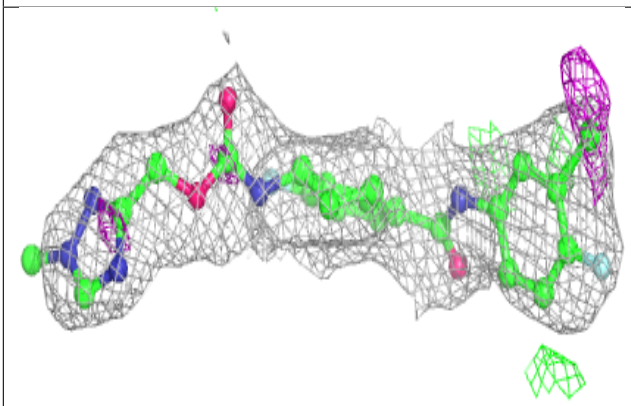


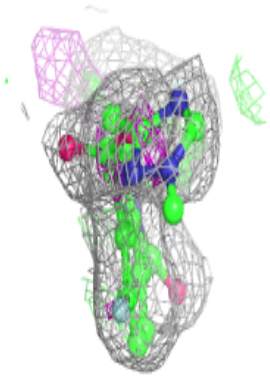


Electron density around YWE B 501:

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

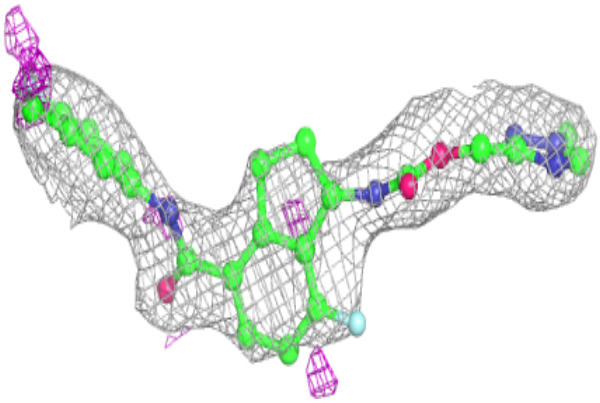


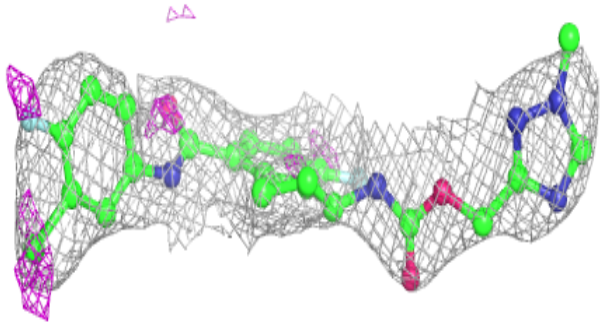


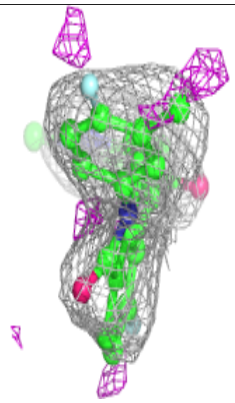


Electron density around YWE C 501:

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

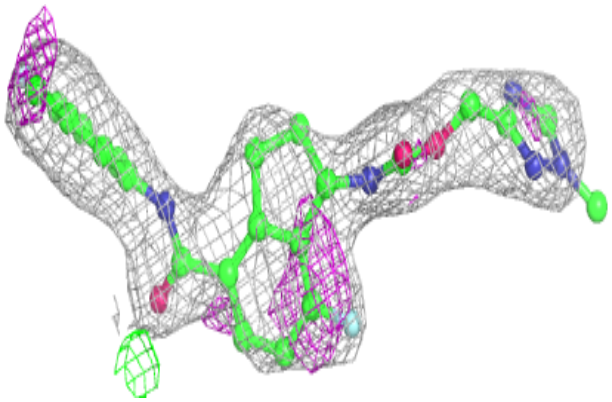


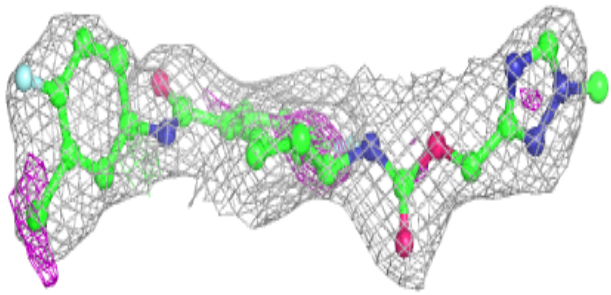


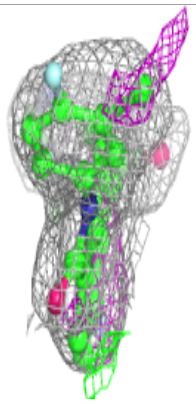


Electron density around YWE E 501:

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

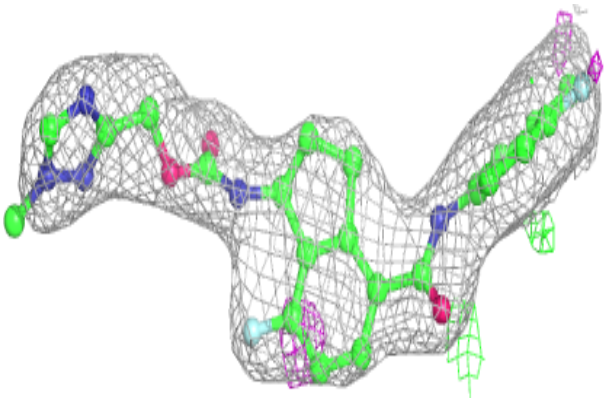


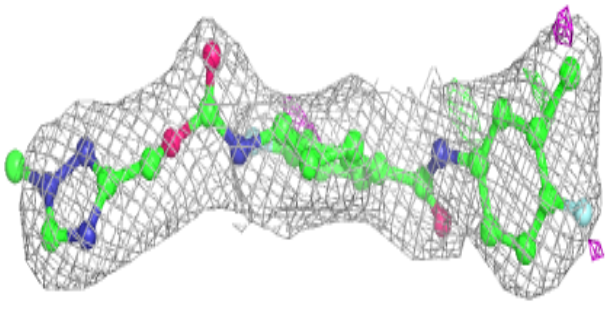


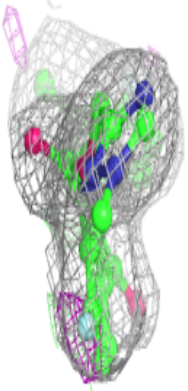


Electron density around YWE E 502:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.