



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 11:48 pm GMT

PDB ID : 4D0Z  
Title : GalNAc-T2 crystal soaked with UDP-5SGalNAc, mEA2 and manganese (Higher resolution dataset)  
Authors : Lira-Navarrete, E.; Iglesias-Fernandez, J.; Zandberg, W.F.; Companon, I.; Kong, Y.; Corzana, F.; Pinto, B.M.; Clausen, H.; Peregrina, J.M.; Vocadlo, D.; Rovira, C.; Hurtado-Guerrero, R.  
Deposited on : 2014-04-30  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (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

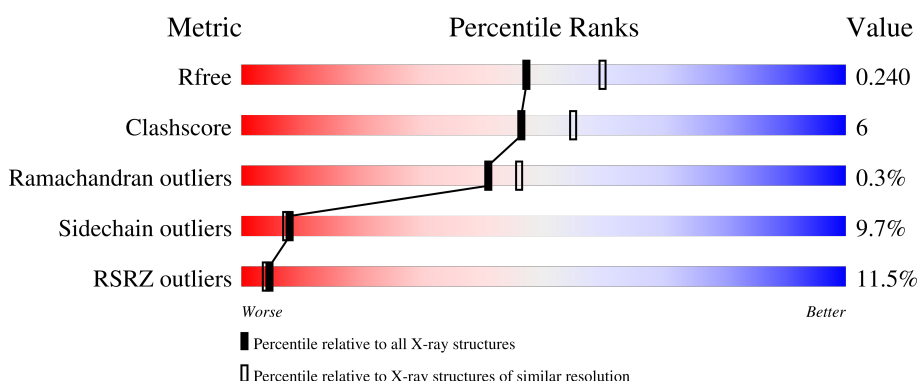
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	571	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3%      71%      13%      •      13%</p>
1	B	571	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      73%      12%      •      13%</p>
1	C	571	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">33%      64%      15%      • •      17%</p>
1	D	571	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      70%      14%      •      13%</p>
1	E	571	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      71%      12%      •      13%</p>

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Mol	Chain	Length	Quality of chain
1	F	571	
2	X	6	
2	Y	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	1572	-	-	X	-
4	EDO	B	1573	-	-	X	-
4	EDO	D	1576	-	-	X	-
4	EDO	E	1572	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 24773 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 POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	495	Total 3975	C 2502	N 722	O 727	S 24	20	1	0
1	B	495	Total 3967	C 2497	N 719	O 727	S 24	20	0	0
1	C	476	Total 3826	C 2407	N 693	O 702	S 24	20	0	0
1	D	495	Total 3967	C 2497	N 719	O 727	S 24	20	0	0
1	E	495	Total 3967	C 2497	N 719	O 727	S 24	20	0	0
1	F	491	Total 3926	C 2470	N 710	O 722	S 24	20	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	engineered mutation	UNP Q10471
B	516	ASP	ASN	engineered mutation	UNP Q10471
C	516	ASP	ASN	engineered mutation	UNP Q10471
D	516	ASP	ASN	engineered mutation	UNP Q10471
E	516	ASP	ASN	engineered mutation	UNP Q10471
F	516	ASP	ASN	engineered mutation	UNP Q10471

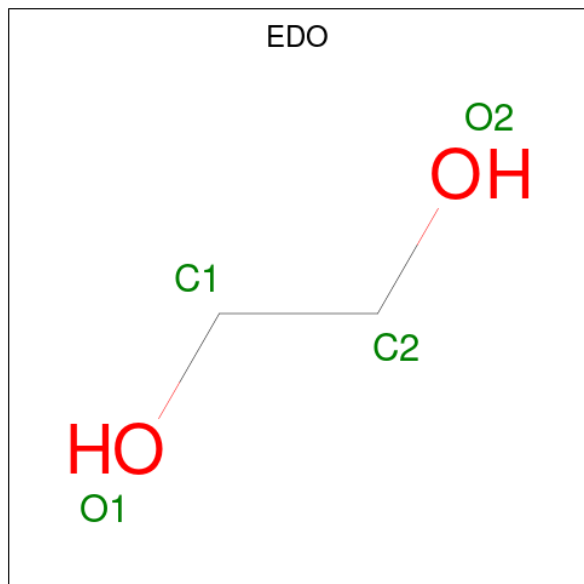
- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	X	6	Total 32	C 18	N 6	O 7	S 1	0	0	1
2	Y	6	Total 32	C 18	N 6	O 7	S 1	0	0	1

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

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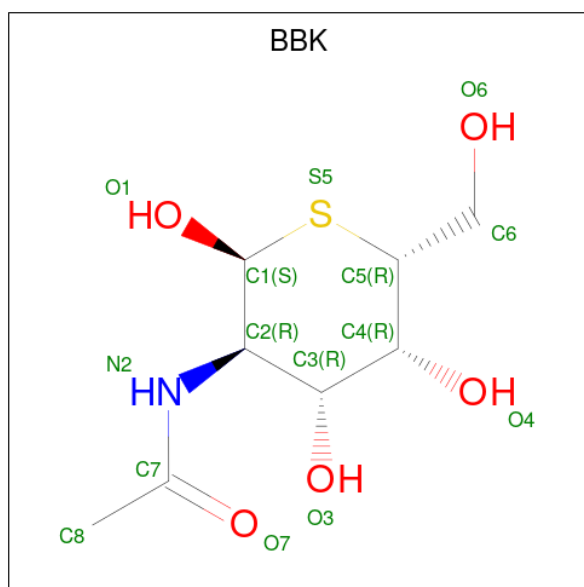
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-acetamido-2-deoxy-5-thio-alpha-D-galactopyranose (three-letter code: BBK) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

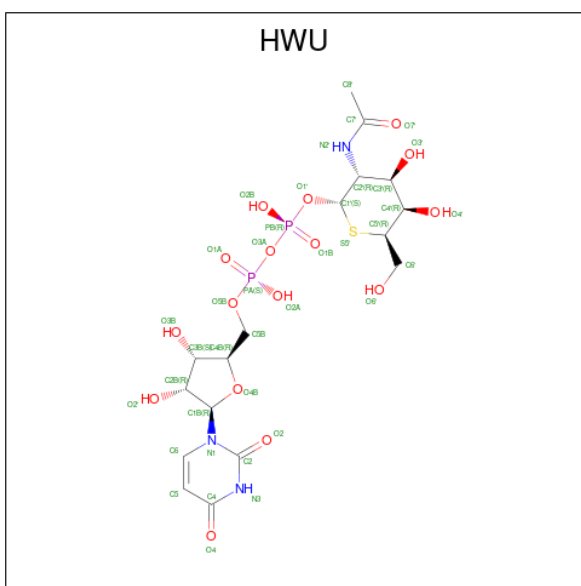
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

- Molecule 6 is (2R,3R,4R,5R,6R)-3-(acetylamino)-4,5-dihydroxy-6-(hydroxymethyl)tetrahydro-2H-thiopyran-2-yl [(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl dihydrogen diphosphate (three-letter code: HWU) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>3</sub>O<sub>16</sub>P<sub>2</sub>S).



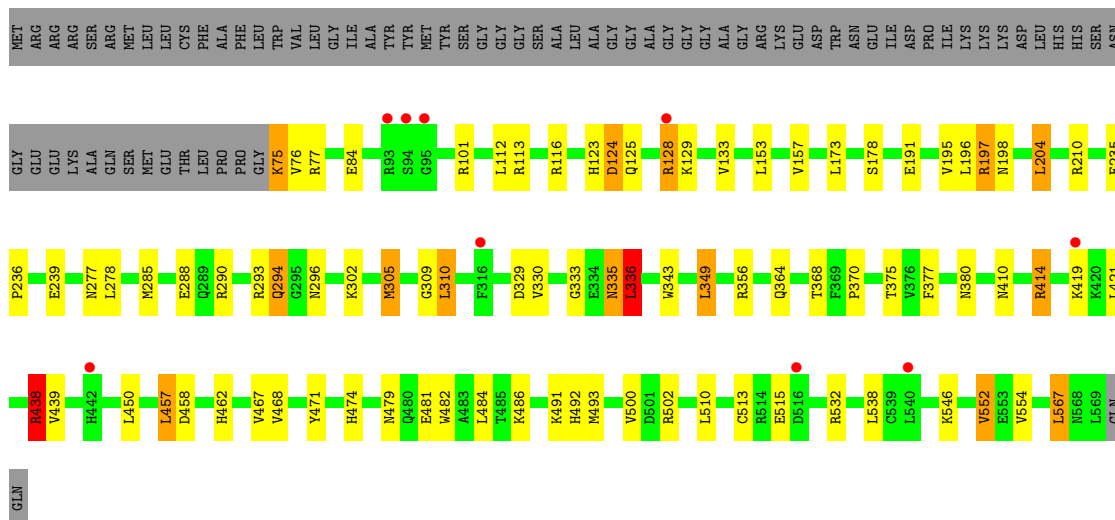
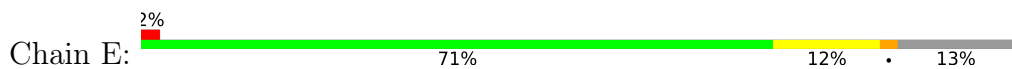
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	B	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	C	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	D	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	E	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
6	F	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

- Molecule 7 is water.

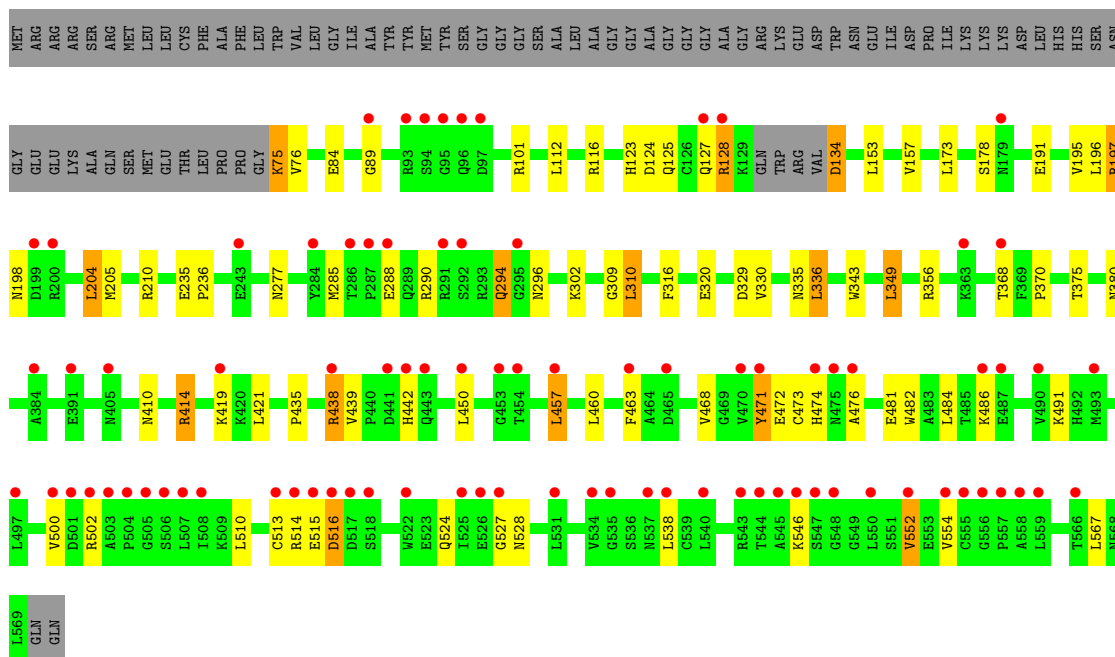
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	144	Total O 144 144	0	0
7	B	125	Total O 125 125	0	0
7	C	13	Total O 13 13	0	0
7	D	122	Total O 122 122	0	0
7	E	168	Total O 168 168	0	0
7	F	61	Total O 61 61	0	0







• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2



• Molecule 2: PEPTIDE



• Molecule 2: PEPTIDE





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.48Å 121.14Å 249.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.39 – 2.20 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (249.39-2.20) 99.8 (19.95-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.196 , 0.234 0.204 , 0.240	Depositor DCC
$R_{free}$ test set	4936 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtrriage
Anisotropy	0.540	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MN, BBK, HWU

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	0.85	4/4070 (0.1%)	0.98	25/5503 (0.5%)
1	B	0.79	3/4059 (0.1%)	0.91	9/5489 (0.2%)
1	C	0.88	7/3912 (0.2%)	0.98	26/5287 (0.5%)
1	D	1.01	3/4059 (0.1%)	0.98	19/5489 (0.3%)
1	E	0.92	3/4059 (0.1%)	0.98	19/5489 (0.3%)
1	F	0.89	3/4015 (0.1%)	0.90	12/5427 (0.2%)
2	X	1.42	0/32	1.09	0/44
2	Y	1.82	1/32 (3.1%)	1.53	0/44
All	All	0.89	24/24238 (0.1%)	0.95	110/32772 (0.3%)

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	A	0	1
1	B	0	1
1	C	0	1
1	F	0	1
All	All	0	4

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	75	LYS	CB-CG	-33.78	0.61	1.52
1	C	84	GLU	CB-CG	-26.41	1.01	1.52
1	D	486	LYS	CB-CG	-25.36	0.84	1.52
1	F	75	LYS	CB-CG	-25.00	0.85	1.52
1	E	84	GLU	CB-CG	-23.77	1.06	1.52



The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	LYS	CA-CB-CG	21.27	160.19	113.40
1	D	194	ARG	NE-CZ-NH2	-17.68	111.46	120.30
1	E	75	LYS	CA-CB-CG	16.43	149.55	113.40
1	F	75	LYS	CA-CB-CG	15.46	147.41	113.40
1	D	75	LYS	CB-CG-CD	13.48	146.66	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	GLY	Peptide
1	B	89	GLY	Peptide
1	C	223	LEU	Mainchain
1	F	89	GLY	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	3975	0	3903	54	0
1	B	3967	0	3890	30	0
1	C	3826	0	3748	81	0
1	D	3967	0	3890	55	0
1	E	3967	0	3890	49	0
1	F	3926	0	3849	31	0
2	X	32	0	28	3	0
2	Y	32	0	28	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	40	0	60	9	0
4	B	32	0	48	6	0
4	D	20	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	56	0	84	15	0
5	A	15	0	15	3	0
5	B	15	0	14	4	0
5	D	15	0	14	4	0
5	E	15	0	13	5	0
6	A	39	0	24	0	0
6	B	39	0	24	2	0
6	C	39	0	25	11	0
6	D	39	0	25	4	0
6	E	39	0	25	2	0
6	F	39	0	24	2	0
7	A	144	0	0	0	0
7	B	125	0	0	3	0
7	C	13	0	0	6	0
7	D	122	0	0	3	0
7	E	168	0	0	3	0
7	F	61	0	0	0	0
All	All	24773	0	23651	298	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 6.

The worst 5 of 298 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:C:203:GLY:HA3	1:C:330:VAL:CG2	1.71	1.19
1:C:203:GLY:CA	1:C:330:VAL:CG2	2.26	1.13
1:A:291:ARG:CZ	1:D:435:PRO:HB2	1.79	1.11
1:C:203:GLY:HA3	1:C:330:VAL:HG22	1.20	1.10
1:C:330:VAL:HG12	1:C:331:TRP:HB3	1.32	1.08

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	494/571 (86%)	479 (97%)	14 (3%)	1 (0%)	47	55
1	B	493/571 (86%)	476 (97%)	16 (3%)	1 (0%)	47	55
1	C	470/571 (82%)	451 (96%)	16 (3%)	3 (1%)	25	26
1	D	493/571 (86%)	478 (97%)	14 (3%)	1 (0%)	47	55
1	E	493/571 (86%)	479 (97%)	13 (3%)	1 (0%)	47	55
1	F	487/571 (85%)	473 (97%)	13 (3%)	1 (0%)	47	55
2	X	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	Y	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	2938/3438 (86%)	2842 (97%)	88 (3%)	8 (0%)	41	46

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	C	440	PRO
1	B	330	VAL
1	C	332	GLY
1	C	516	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	429/485 (88%)	388 (90%)	41 (10%)	8	8
1	B	428/485 (88%)	390 (91%)	38 (9%)	9	9
1	C	414/485 (85%)	371 (90%)	43 (10%)	7	6
1	D	428/485 (88%)	385 (90%)	43 (10%)	7	7
1	E	428/485 (88%)	389 (91%)	39 (9%)	9	9
1	F	424/485 (87%)	382 (90%)	42 (10%)	8	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	4/4 (100%)	3 (75%)	1 (25%)	0	0
2	Y	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	2559/2918 (88%)	2310 (90%)	249 (10%)	8	7

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	502	ARG
1	F	310	LEU
1	D	335	ASN
1	F	296	ASN
1	F	471	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	365	HIS
1	E	335	ASN
1	D	410	ASN
1	E	106	GLN
1	E	380	ASN

### 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 53 ligands modelled in this entry, 6 are monoatomic - leaving 47 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
4	EDO	E	1577	-	3,3,3	0.35	0	2,2,2	0.73	0
6	HWU	E	1585	3	36,41,41	3.66	4 (11%)	50,62,62	2.16	13 (26%)
4	EDO	A	1578	-	3,3,3	0.70	0	2,2,2	0.66	0
4	EDO	A	1575	-	3,3,3	0.36	0	2,2,2	0.63	0
4	EDO	E	1582	-	3,3,3	0.35	0	2,2,2	0.29	0
4	EDO	A	1580	-	3,3,3	0.96	0	2,2,2	1.17	0
4	EDO	B	1577	-	3,3,3	0.27	0	2,2,2	1.09	0
4	EDO	B	1574	-	3,3,3	0.61	0	2,2,2	0.30	0
6	HWU	C	1569	3	36,41,41	4.64	2 (5%)	50,62,62	2.38	22 (44%)
4	EDO	A	1572	-	3,3,3	0.50	0	2,2,2	0.53	0
6	HWU	B	1571	3	36,41,41	3.62	8 (22%)	50,62,62	2.74	20 (40%)
4	EDO	A	1574	-	3,3,3	0.53	0	2,2,2	0.12	0
4	EDO	A	1579	-	3,3,3	0.70	0	2,2,2	0.38	0
4	EDO	D	1575	-	3,3,3	0.91	0	2,2,2	0.42	0
5	BBK	D	1572	-	13,15,15	9.52	2 (15%)	15,21,21	3.40	5 (33%)
4	EDO	A	1573	-	3,3,3	0.82	0	2,2,2	0.03	0
6	HWU	F	1571	3	36,41,41	3.51	3 (8%)	50,62,62	1.92	10 (20%)
4	EDO	E	1570	-	3,3,3	0.76	0	2,2,2	0.32	0
4	EDO	A	1577	-	3,3,3	0.55	0	2,2,2	0.17	0
4	EDO	B	1578	-	3,3,3	0.54	0	2,2,2	0.36	0
4	EDO	D	1576	-	3,3,3	0.59	0	2,2,2	0.64	0
6	HWU	A	1582	3	36,41,41	3.61	7 (19%)	50,62,62	1.91	15 (30%)
4	EDO	E	1578	-	3,3,3	0.39	0	2,2,2	0.65	0
4	EDO	B	1579	-	3,3,3	0.70	0	2,2,2	0.06	0
4	EDO	E	1571	-	3,3,3	0.68	0	2,2,2	0.30	0
6	HWU	D	1571	3	36,41,41	4.16	8 (22%)	50,62,62	2.15	18 (36%)
5	BBK	E	1584	-	13,15,15	9.23	2 (15%)	15,21,21	2.16	5 (33%)
4	EDO	B	1575	-	3,3,3	0.44	0	2,2,2	0.33	0
4	EDO	A	1571	-	3,3,3	0.87	0	2,2,2	0.26	0
4	EDO	E	1579	-	3,3,3	0.46	0	2,2,2	0.70	0
4	EDO	E	1574	-	3,3,3	0.35	0	2,2,2	0.80	0
4	EDO	E	1580	-	3,3,3	0.64	0	2,2,2	0.21	0
4	EDO	E	1572	-	3,3,3	0.40	0	2,2,2	0.39	0
4	EDO	E	1583	-	3,3,3	0.58	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	1572	-	3,3,3	0.53	0	2,2,2	0.65	0
4	EDO	D	1577	-	3,3,3	0.44	0	2,2,2	0.66	0
4	EDO	E	1576	-	3,3,3	0.53	0	2,2,2	0.50	0
4	EDO	E	1581	-	3,3,3	0.35	0	2,2,2	0.84	0
5	BBK	A	1581	-	13,15,15	9.17	2 (15%)	15,21,21	2.19	5 (33%)
4	EDO	B	1573	-	3,3,3	0.27	0	2,2,2	0.40	0
4	EDO	B	1576	-	3,3,3	0.64	0	2,2,2	0.12	0
4	EDO	E	1573	-	3,3,3	0.30	0	2,2,2	0.97	0
4	EDO	E	1575	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	1576	-	3,3,3	0.29	0	2,2,2	0.74	0
5	BBK	B	1580	-	13,15,15	9.03	2 (15%)	15,21,21	1.92	4 (26%)
4	EDO	D	1574	-	3,3,3	0.81	0	2,2,2	0.50	0
4	EDO	D	1573	-	3,3,3	0.52	0	2,2,2	0.74	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
4	EDO	E	1577	-	-	1/1/1/1	-
6	HWU	E	1585	3	-	6/25/63/63	0/3/3/3
4	EDO	A	1578	-	-	0/1/1/1	-
4	EDO	A	1575	-	-	1/1/1/1	-
4	EDO	E	1582	-	-	1/1/1/1	-
4	EDO	A	1580	-	-	1/1/1/1	-
4	EDO	B	1577	-	-	1/1/1/1	-
4	EDO	B	1574	-	-	1/1/1/1	-
6	HWU	C	1569	3	-	6/25/63/63	0/3/3/3
4	EDO	A	1572	-	-	1/1/1/1	-
6	HWU	B	1571	3	-	7/25/63/63	0/3/3/3
4	EDO	A	1574	-	-	0/1/1/1	-
4	EDO	A	1579	-	-	0/1/1/1	-
4	EDO	D	1575	-	-	1/1/1/1	-
5	BBK	D	1572	-	-	2/6/26/26	0/1/1/1
4	EDO	A	1573	-	-	1/1/1/1	-
6	HWU	F	1571	3	-	6/25/63/63	0/3/3/3
4	EDO	E	1570	-	-	1/1/1/1	-
4	EDO	A	1577	-	-	1/1/1/1	-
4	EDO	B	1578	-	-	1/1/1/1	-
4	EDO	D	1576	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HWU	A	1582	3	-	5/25/63/63	0/3/3/3
4	EDO	E	1578	-	-	0/1/1/1	-
4	EDO	B	1579	-	-	0/1/1/1	-
4	EDO	E	1571	-	-	0/1/1/1	-
6	HWU	D	1571	3	-	7/25/63/63	0/3/3/3
5	BBK	E	1584	-	-	4/6/26/26	0/1/1/1
4	EDO	B	1575	-	-	1/1/1/1	-
4	EDO	A	1571	-	-	1/1/1/1	-
4	EDO	E	1579	-	-	1/1/1/1	-
4	EDO	E	1574	-	-	1/1/1/1	-
4	EDO	E	1580	-	-	0/1/1/1	-
4	EDO	E	1572	-	-	1/1/1/1	-
4	EDO	E	1583	-	-	1/1/1/1	-
4	EDO	B	1572	-	-	1/1/1/1	-
4	EDO	D	1577	-	-	1/1/1/1	-
4	EDO	E	1576	-	-	1/1/1/1	-
4	EDO	E	1581	-	-	0/1/1/1	-
5	BBK	A	1581	-	-	5/6/26/26	0/1/1/1
4	EDO	B	1573	-	-	1/1/1/1	-
4	EDO	B	1576	-	-	1/1/1/1	-
4	EDO	E	1573	-	-	1/1/1/1	-
4	EDO	E	1575	-	-	1/1/1/1	-
4	EDO	A	1576	-	-	1/1/1/1	-
5	BBK	B	1580	-	-	4/6/26/26	0/1/1/1
4	EDO	D	1574	-	-	0/1/1/1	-
4	EDO	D	1573	-	-	0/1/1/1	-

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1569	HWU	C5'-S5'	-27.24	1.41	1.82
5	D	1572	BBK	C5-S5	-27.03	1.42	1.82
5	E	1584	BBK	C5-S5	-26.64	1.42	1.82
5	B	1580	BBK	C5-S5	-25.96	1.43	1.82
5	A	1581	BBK	C5-S5	-25.79	1.43	1.82

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1572	BBK	C1-C2-N2	-9.34	93.88	111.36
5	D	1572	BBK	O1-C1-C2	-7.78	93.37	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1571	HWU	N3-C2-N1	7.49	124.83	114.89
6	B	1571	HWU	C4-N3-C2	-7.38	116.84	126.58
6	E	1585	HWU	N3-C2-N1	6.62	123.68	114.89

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1581	BBK	C1-C2-N2-C7
5	A	1581	BBK	O7-C7-N2-C2
5	A	1581	BBK	C8-C7-N2-C2
5	A	1581	BBK	C4-C5-C6-O6
5	A	1581	BBK	S5-C5-C6-O6

There are no ring outliers.

25 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1585	HWU	2	0
4	A	1578	EDO	1	0
4	A	1575	EDO	1	0
4	E	1582	EDO	2	0
4	A	1580	EDO	2	0
4	B	1577	EDO	1	0
6	C	1569	HWU	11	0
4	A	1572	EDO	4	0
6	B	1571	HWU	2	0
4	A	1579	EDO	1	0
5	D	1572	BBK	4	0
6	F	1571	HWU	2	0
4	E	1570	EDO	1	0
4	D	1576	EDO	4	0
6	D	1571	HWU	4	0
5	E	1584	BBK	5	0
4	E	1579	EDO	2	0
4	E	1580	EDO	1	0
4	E	1572	EDO	8	0
4	B	1572	EDO	1	0
5	A	1581	BBK	3	0
4	B	1573	EDO	4	0
4	E	1573	EDO	1	0

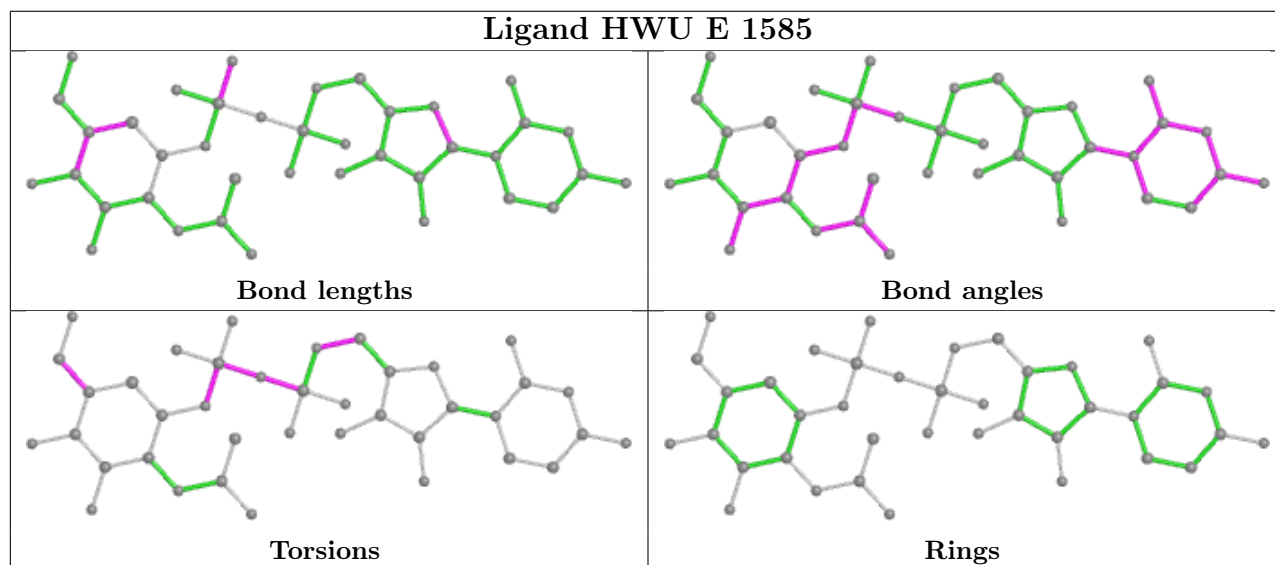
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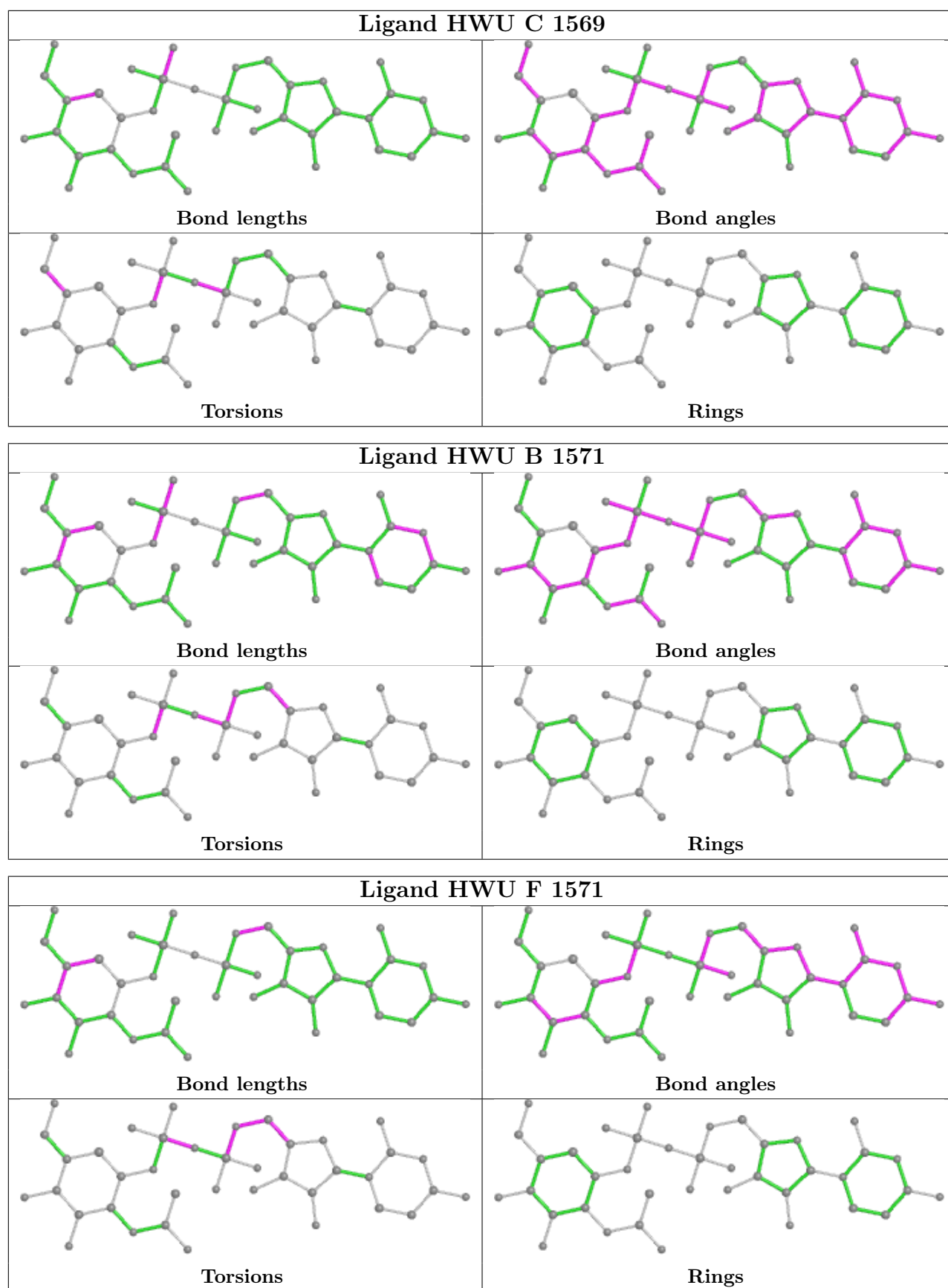


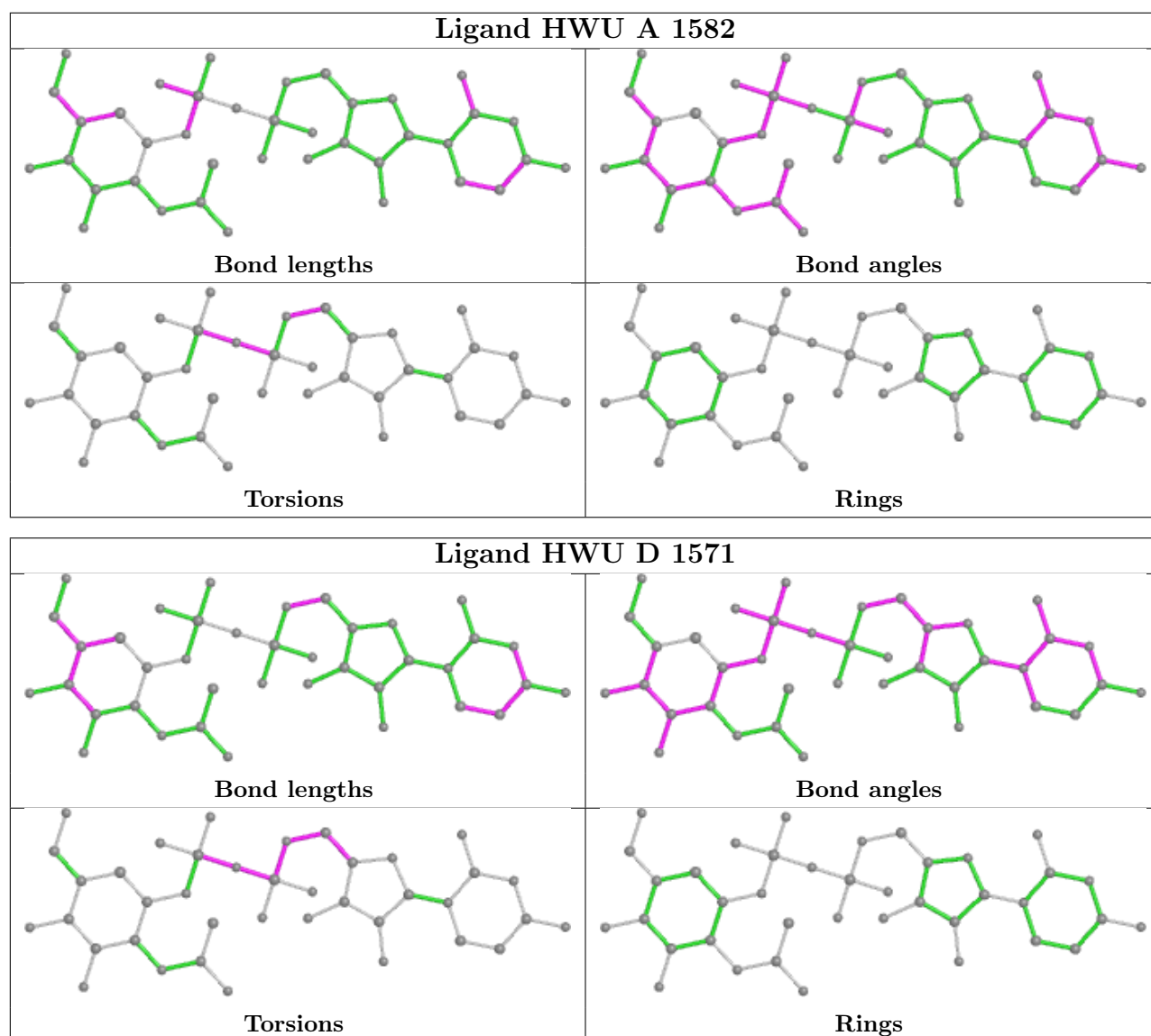
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1580	BBK	4	0
4	D	1573	EDO	1	0

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







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	222:PHE	C	223:LEU	N	1.63
1	C	225:SER	C	226:HIS	N	0.99
1	C	224:ASP	C	225:SER	N	0.87

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	495/571 (86%)	-0.03	16 (3%) 47 45	26, 42, 70, 130	5 (1%)
1	B	495/571 (86%)	-0.10	14 (2%) 53 51	26, 40, 66, 106	5 (1%)
1	C	476/571 (83%)	1.98	189 (39%) 0 0	42, 92, 135, 168	5 (1%)
1	D	495/571 (86%)	-0.04	20 (4%) 38 36	26, 41, 66, 142	5 (1%)
1	E	495/571 (86%)	-0.20	9 (1%) 68 66	23, 36, 58, 90	5 (1%)
1	F	491/571 (85%)	0.65	85 (17%) 1 1	34, 57, 112, 140	5 (1%)
2	X	6/6 (100%)	1.38	2 (33%) 0 0	40, 73, 84, 87	0
2	Y	6/6 (100%)	2.65	4 (66%) 0 0	42, 71, 77, 83	0
All	All	2959/3438 (86%)	0.37	339 (11%) 4 4	23, 45, 109, 168	30 (1%)

The worst 5 of 339 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	330	VAL	14.2
1	C	476	ALA	10.8
1	C	331	TRP	10.8
1	F	547	SER	10.4
1	F	556	GLY	8.7

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	D	1575	4/4	0.64	0.22	60,63,68,70	0
5	BBK	B	1580	15/15	0.64	0.29	69,86,120,142	0
5	BBK	D	1572	15/15	0.65	0.31	96,105,117,124	0
5	BBK	E	1584	15/15	0.70	0.32	96,105,117,124	0
4	EDO	B	1576	4/4	0.73	0.24	65,69,73,76	0
5	BBK	A	1581	15/15	0.77	0.23	69,86,120,142	0
4	EDO	E	1580	4/4	0.78	0.32	59,70,71,76	0
4	EDO	A	1580	4/4	0.80	0.22	45,52,57,59	0
4	EDO	E	1575	4/4	0.81	0.17	64,69,69,76	0
4	EDO	A	1572	4/4	0.81	0.24	57,66,67,69	0
4	EDO	E	1570	4/4	0.82	0.31	44,48,59,61	0
4	EDO	E	1574	4/4	0.82	0.19	62,68,68,75	0
4	EDO	A	1573	4/4	0.84	0.19	56,68,70,70	0
4	EDO	D	1577	4/4	0.85	0.20	67,68,69,69	0
4	EDO	A	1579	4/4	0.85	0.18	51,52,54,64	0
4	EDO	A	1577	4/4	0.85	0.48	62,68,71,76	0
6	HWU	C	1569	39/39	0.86	0.18	51,76,89,92	0
4	EDO	E	1576	4/4	0.87	0.19	68,68,69,69	0
4	EDO	B	1573	4/4	0.88	0.28	40,41,42,48	0
4	EDO	A	1576	4/4	0.88	0.25	57,62,66,75	0
4	EDO	A	1574	4/4	0.89	0.15	51,52,54,57	0
4	EDO	E	1578	4/4	0.89	0.23	64,64,66,82	0
4	EDO	B	1578	4/4	0.90	0.28	55,58,62,69	0
4	EDO	E	1573	4/4	0.90	0.22	49,58,60,71	0
4	EDO	B	1579	4/4	0.90	0.13	41,48,56,56	0
4	EDO	E	1583	4/4	0.91	0.15	58,61,62,68	0
4	EDO	D	1574	4/4	0.91	0.13	49,50,52,58	0
4	EDO	E	1572	4/4	0.91	0.25	38,45,48,51	0
6	HWU	F	1571	39/39	0.91	0.12	38,44,55,60	0
4	EDO	A	1578	4/4	0.92	0.19	38,45,48,63	0
6	HWU	A	1582	39/39	0.92	0.12	26,34,45,48	0
6	HWU	B	1571	39/39	0.92	0.13	30,36,44,49	0
4	EDO	E	1581	4/4	0.92	0.16	53,56,60,68	0
4	EDO	D	1573	4/4	0.92	0.13	38,40,40,45	0
6	HWU	D	1571	39/39	0.93	0.12	24,35,45,46	0
4	EDO	B	1575	4/4	0.93	0.25	66,68,69,69	0
4	EDO	B	1574	4/4	0.94	0.10	40,40,42,45	0

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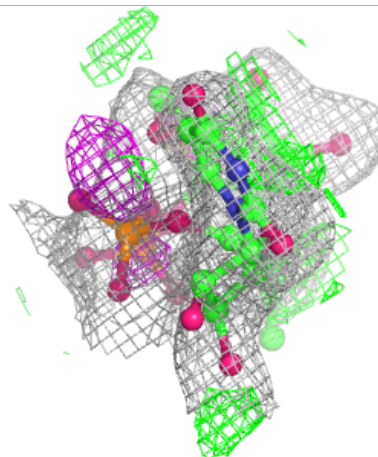
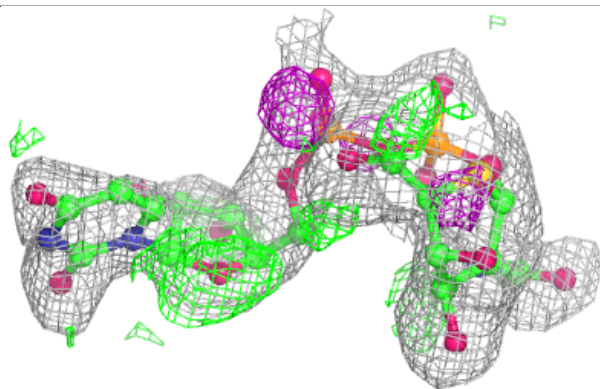
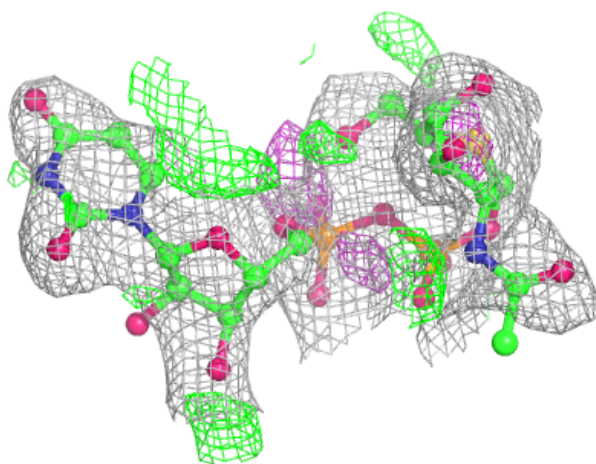
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	E	1577	4/4	0.94	0.21	61,61,64,68	0
4	EDO	D	1576	4/4	0.94	0.15	39,43,45,49	0
4	EDO	B	1577	4/4	0.94	0.20	42,43,48,57	0
4	EDO	A	1571	4/4	0.94	0.20	43,46,46,52	0
4	EDO	B	1572	4/4	0.95	0.10	34,35,35,42	0
4	EDO	A	1575	4/4	0.95	0.11	53,55,57,59	0
6	HWU	E	1585	39/39	0.95	0.12	26,36,54,58	0
3	MN	C	1570	1/1	0.95	0.04	59,59,59,59	0
4	EDO	E	1582	4/4	0.96	0.12	47,48,51,56	0
4	EDO	E	1571	4/4	0.96	0.16	38,46,47,50	0
4	EDO	E	1579	4/4	0.96	0.11	43,44,52,53	0
3	MN	E	1586	1/1	0.99	0.08	26,26,26,26	0
3	MN	F	1570	1/1	1.00	0.03	42,42,42,42	0
3	MN	A	1570	1/1	1.00	0.08	27,27,27,27	0
3	MN	D	1570	1/1	1.00	0.08	29,29,29,29	0
3	MN	B	1570	1/1	1.00	0.09	33,33,33,33	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 HWU C 1569:**

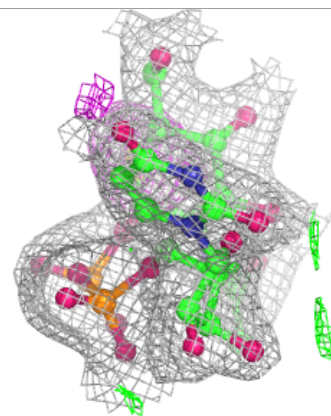
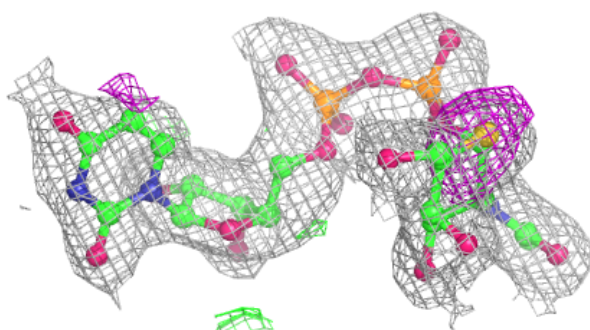
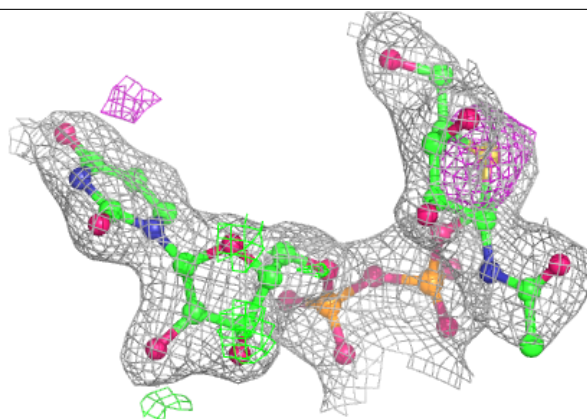
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



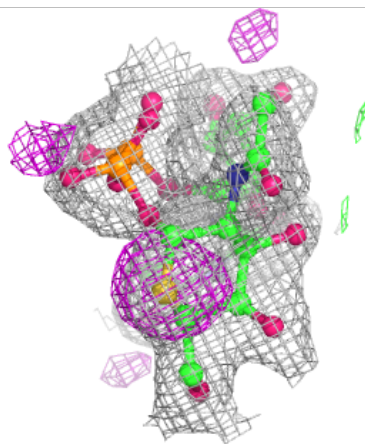
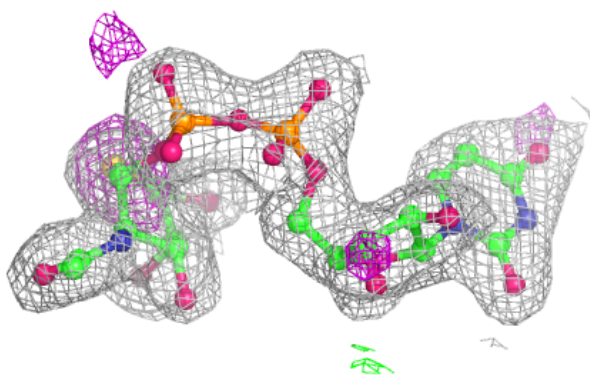
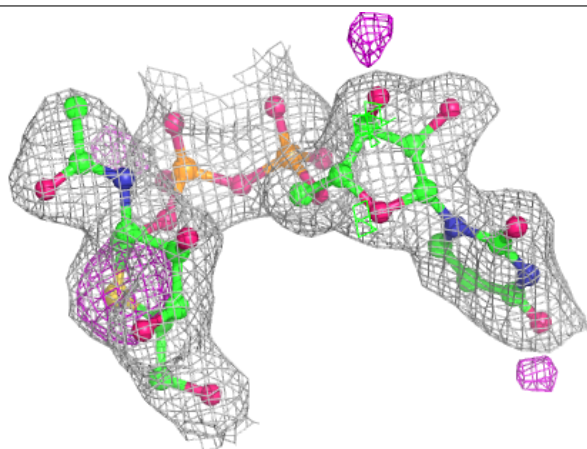


**Electron density around HWU F 1571:**

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

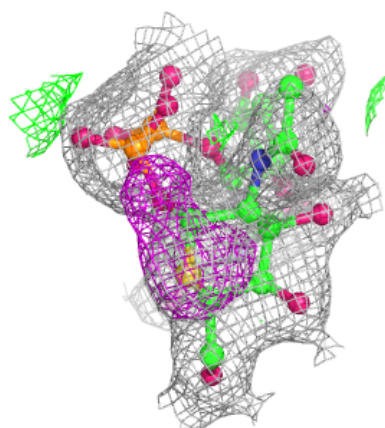
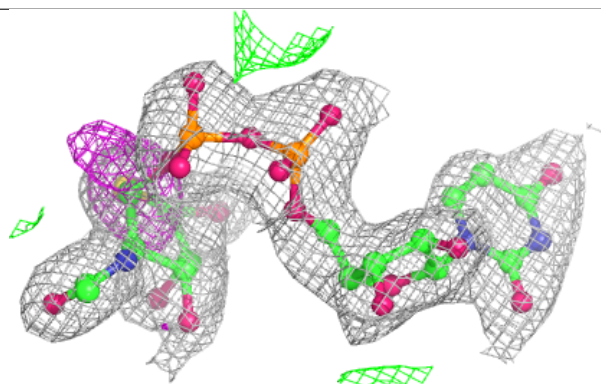
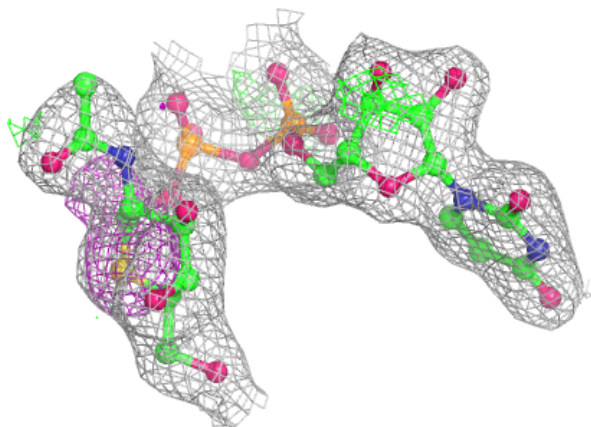
**Electron density around HWU A 1582:**

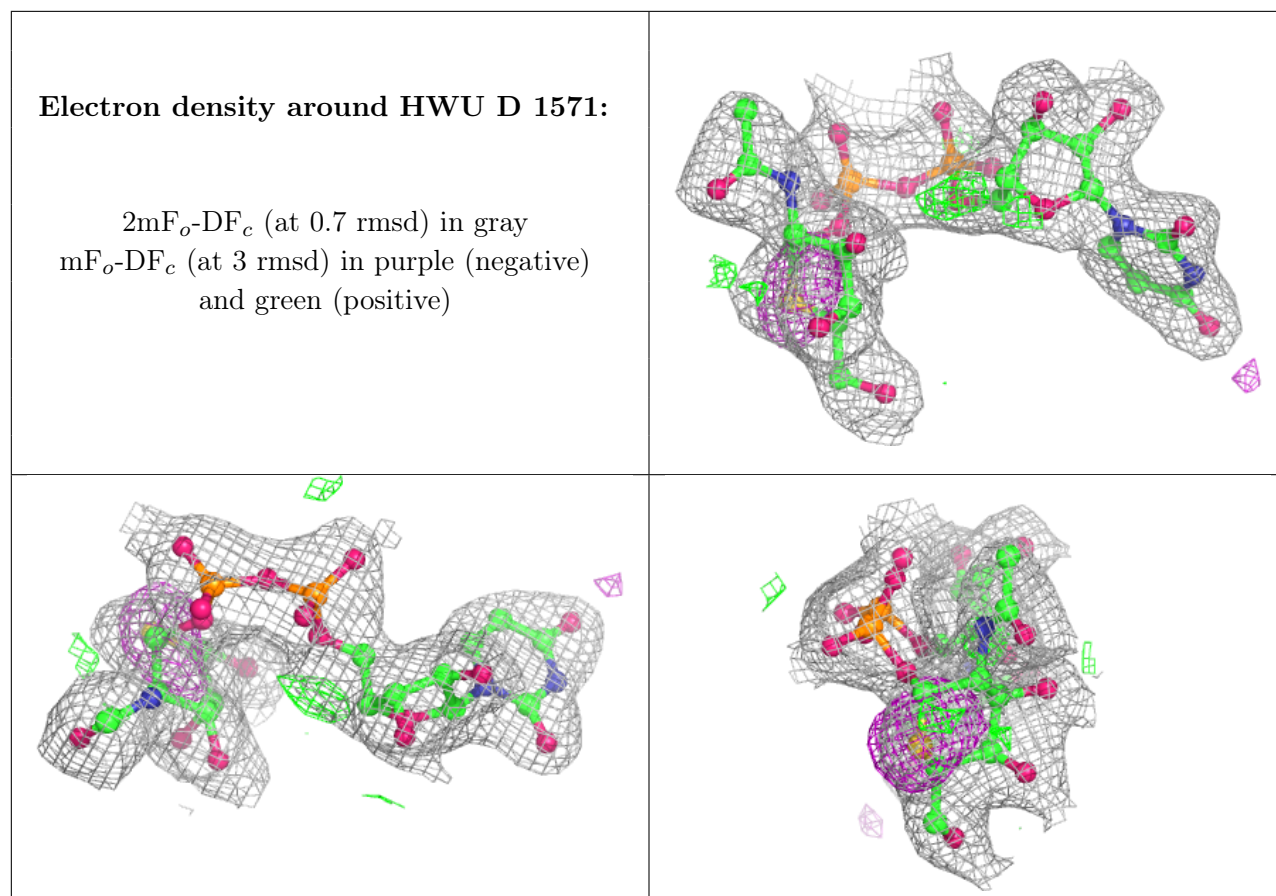
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

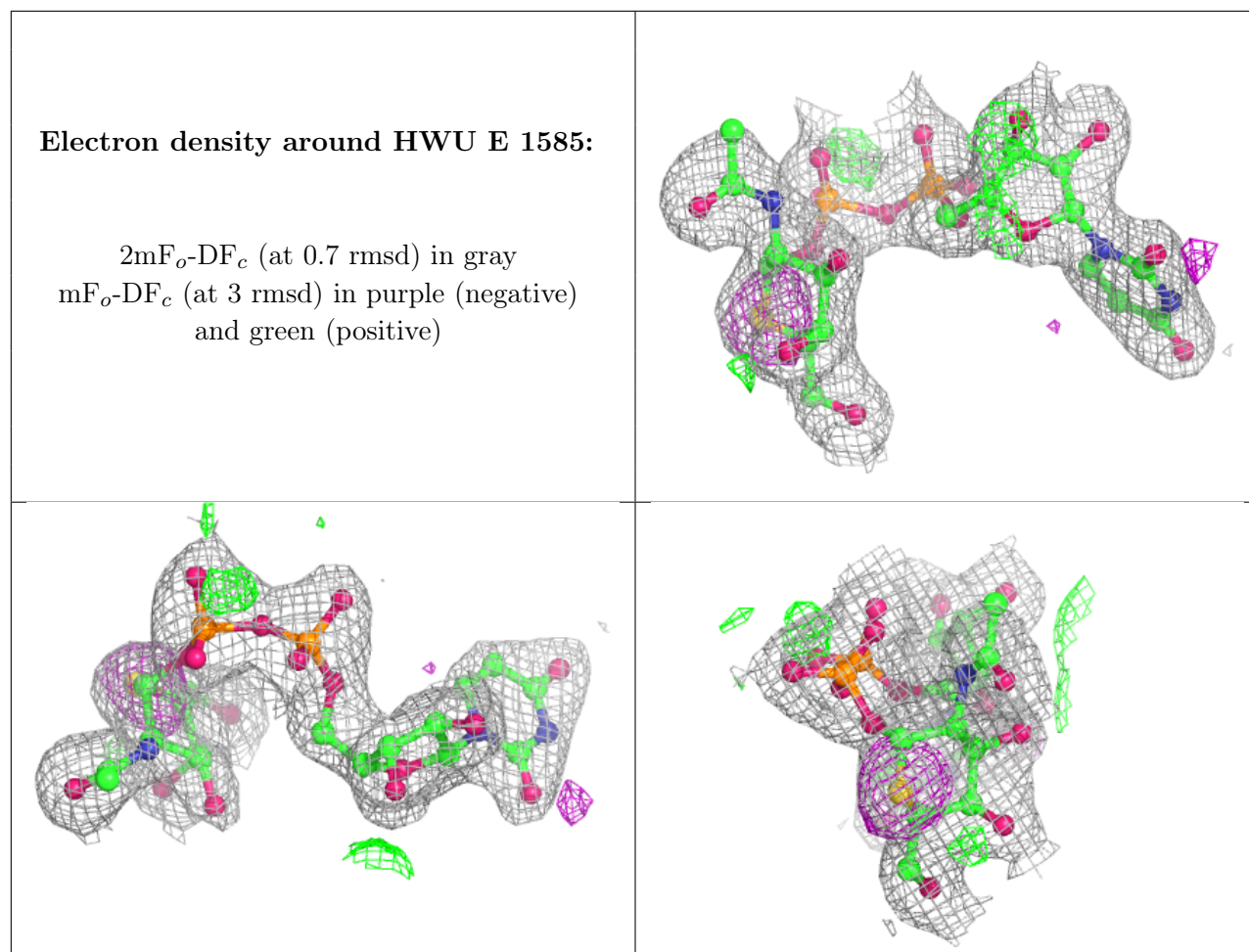


**Electron density around HWU B 1571:**

$2mF_o-DF_c$  (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.