



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:35 AM UTC

PDB ID : 4D0Z / pdb_00004d0z
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

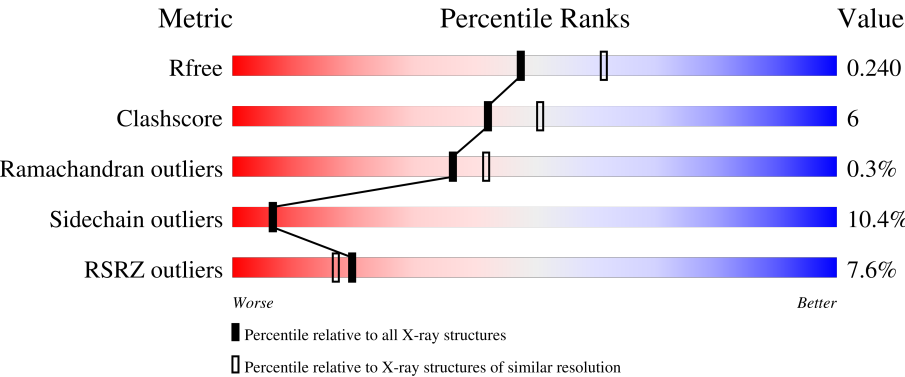
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 ≥ 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	
1	B	571	
1	C	571	
1	D	571	
1	E	571	

Continued on next page...

Continued from previous page...

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

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-ACETYL GALACTOSAMINYLTRANSFERASE 2.

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

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

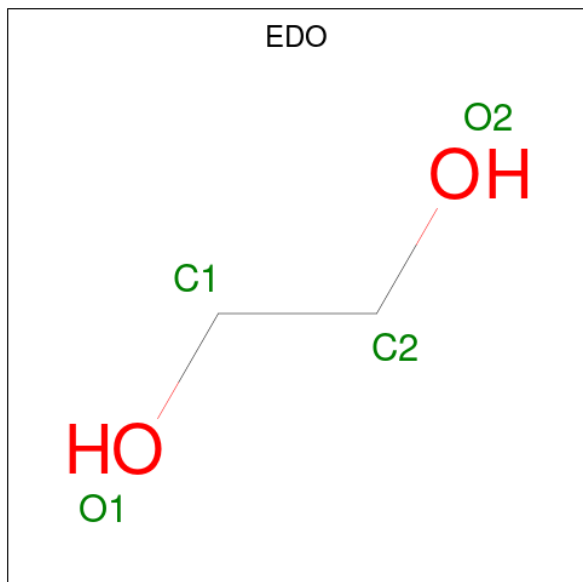
- Molecule 2 is a protein called PEPTIDE.

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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

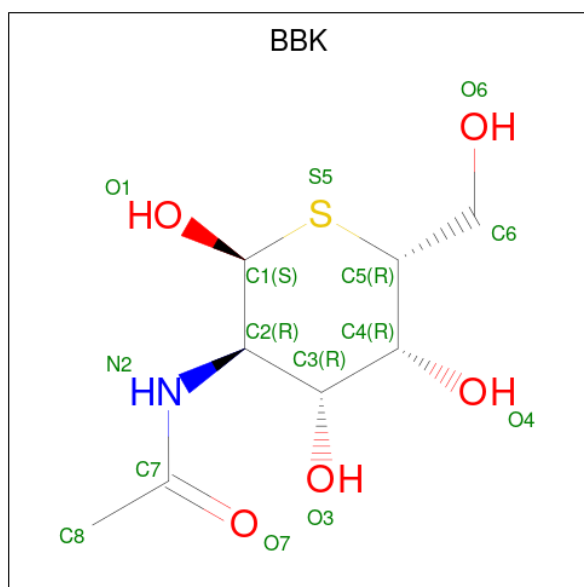
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

Continued on next page...

Continued from previous page...

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 (CCD ID: BBK) (formula: C₈H₁₅NO₅S).



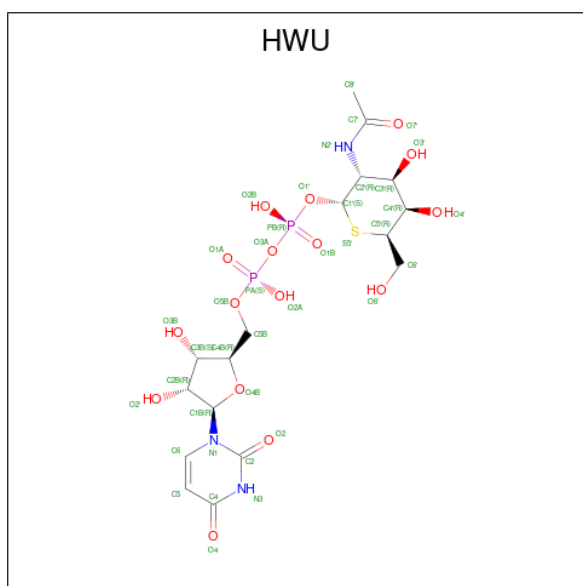
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

Continued on next page...

Continued from previous page...

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 (CCD ID: HWU) (formula: C₁₇H₂₇N₃O₁₆P₂S).



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

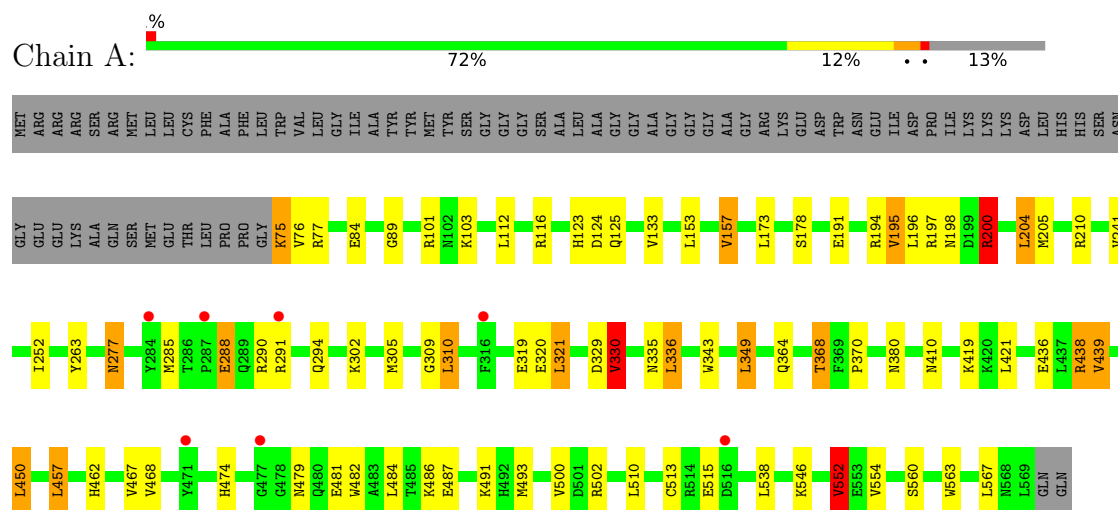
- Molecule 7 is water.

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

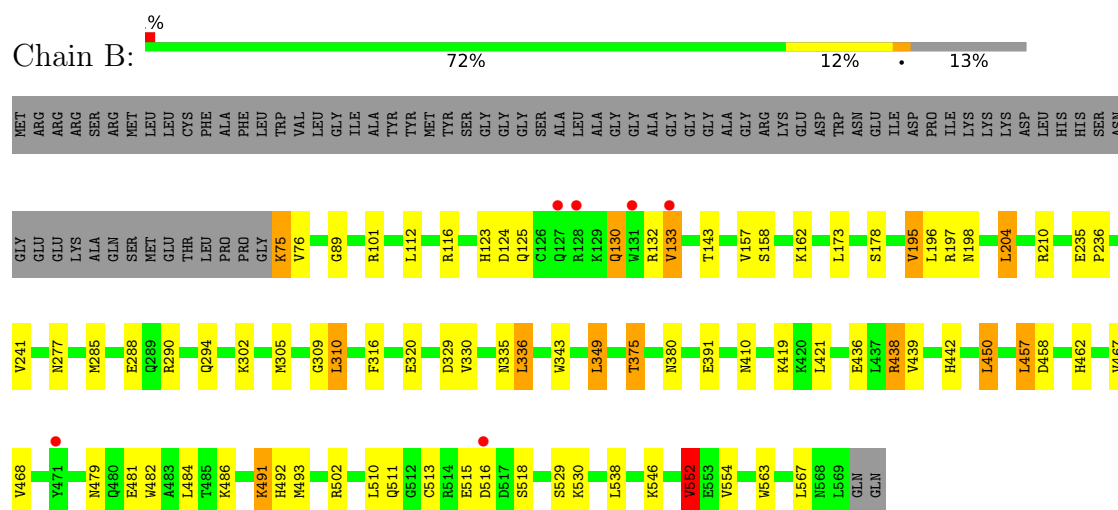
3 Residue-property plots

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.

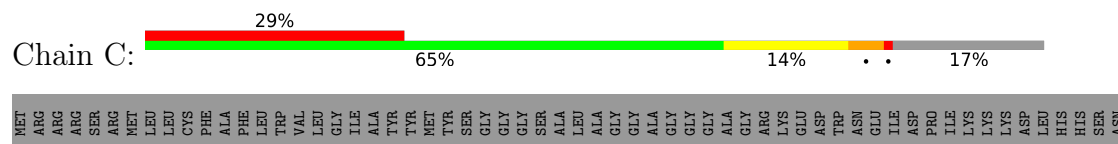
• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

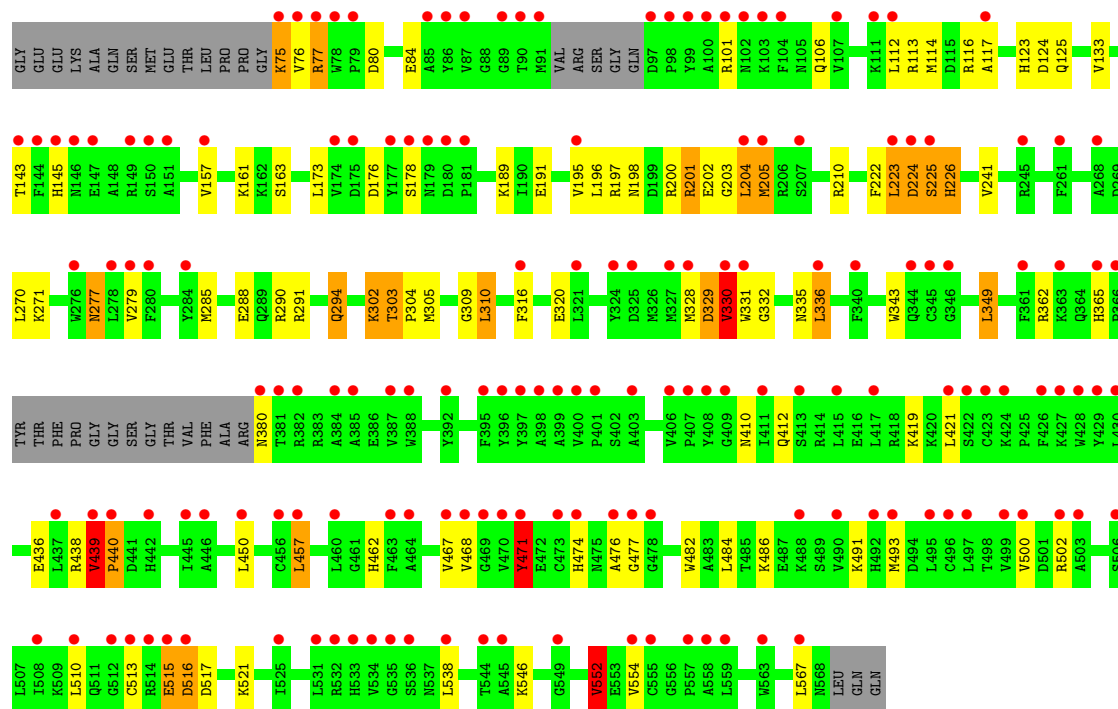


• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

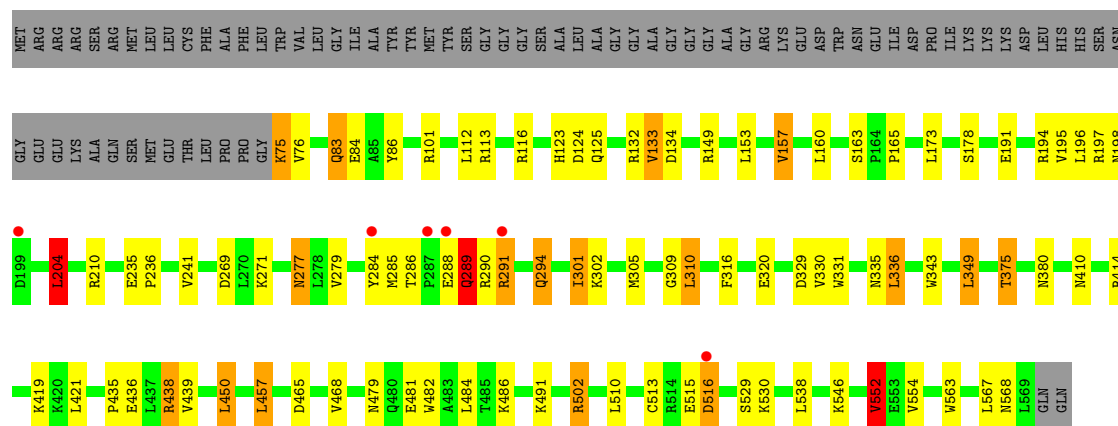


• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

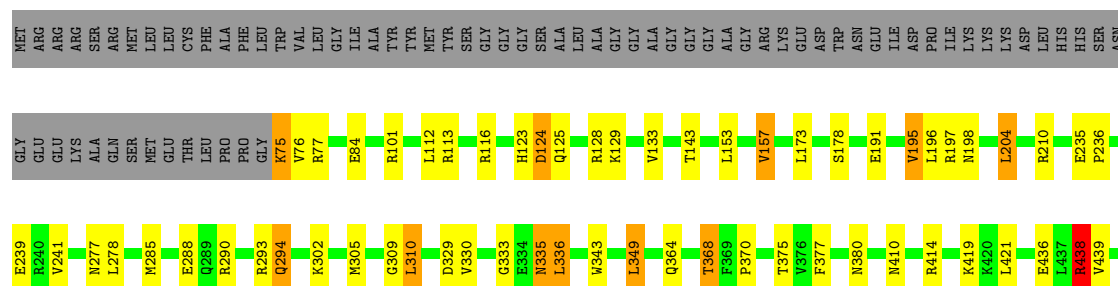


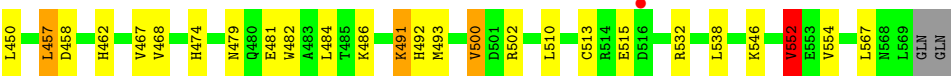


• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

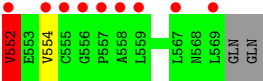
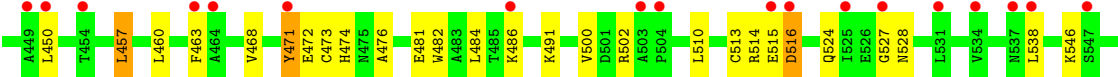
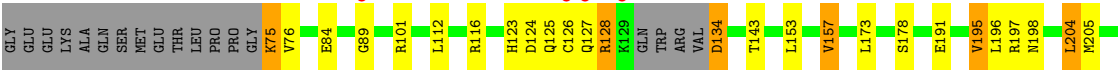
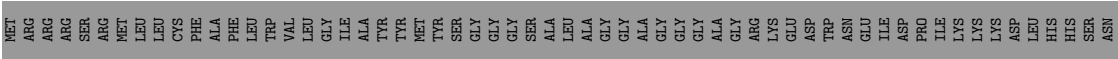


• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2





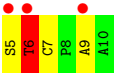
● Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2



● Molecule 2: PEPTIDE



● Molecule 2: PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.48Å 121.14Å 249.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.39 – 2.20 124.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (249.39-2.20) 99.7 (124.69-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.196 , 0.234 0.204 , 0.240	Depositor DCC
R_{free} test set	4937 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24773	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, HWU, MN, BBK

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	1.03	4/4070 (0.1%)	1.08	13/5503 (0.2%)
1	B	1.00	3/4059 (0.1%)	1.01	13/5489 (0.2%)
1	C	1.18	9/3912 (0.2%)	1.11	30/5287 (0.6%)
1	D	1.16	2/4059 (0.0%)	1.03	10/5489 (0.2%)
1	E	1.08	3/4059 (0.1%)	1.06	12/5489 (0.2%)
1	F	0.96	3/4015 (0.1%)	1.00	10/5427 (0.2%)
2	X	1.63	0/32	1.39	0/44
2	Y	2.23	2/32 (6.2%)	1.97	1/44 (2.3%)
All	All	1.07	26/24238 (0.1%)	1.05	89/32772 (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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	224	ASP	C-N	-34.89	0.87	1.33
1	D	75	LYS	CB-CG	-30.37	0.61	1.52
1	C	225	SER	C-N	-24.23	0.99	1.33
1	D	486	LYS	CB-CG	-22.79	0.84	1.52
1	F	75	LYS	CB-CG	-22.46	0.85	1.52
1	C	222	PHE	C-N	22.21	1.63	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	486	LYS	CB-CG	-18.53	0.96	1.52
1	C	84	GLU	CB-CG	-16.82	1.01	1.52
1	E	84	GLU	CB-CG	-15.15	1.06	1.52
1	F	84	GLU	CB-CG	-14.70	1.08	1.52
1	A	75	LYS	CB-CG	-13.39	1.12	1.52
1	E	75	LYS	CB-CG	-12.76	1.14	1.52
1	C	223	LEU	C-N	11.73	1.50	1.33
1	B	75	LYS	CB-CG	-11.46	1.18	1.52
1	A	84	GLU	CB-CG	-10.45	1.21	1.52
1	A	486	LYS	CB-CG	-9.79	1.23	1.52
1	C	486	LYS	CB-CG	-9.39	1.24	1.52
1	C	330	VAL	N-CA	8.10	1.55	1.46
1	C	226	HIS	N-CA	6.63	1.54	1.46
2	Y	9	ALA	C-O	6.30	1.36	1.23
1	B	515	GLU	CB-CG	-6.20	1.33	1.52
1	C	75	LYS	CB-CG	-6.18	1.33	1.52
1	B	294	GLN	CB-CG	5.80	1.69	1.52
1	E	532	ARG	CD-NE	-5.23	1.39	1.46
2	Y	6	THR	N-CA	5.10	1.52	1.46
1	A	294	GLN	CB-CG	5.10	1.67	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	LYS	CA-CB-CG	23.05	160.19	114.10
1	E	75	LYS	CA-CB-CG	17.73	149.55	114.10
1	F	75	LYS	CA-CB-CG	16.66	147.41	114.10
1	A	321	LEU	N-CA-C	-16.28	90.00	110.19
1	D	75	LYS	CB-CG-CD	15.37	146.66	111.30
1	C	225	SER	N-CA-C	-14.61	89.90	110.50
1	E	486	LYS	CB-CG-CD	-14.39	78.21	111.30
1	C	225	SER	O-C-N	-14.36	105.92	122.86
1	C	75	LYS	CA-CB-CG	13.69	141.48	114.10
1	B	486	LYS	CB-CG-CD	-13.08	81.22	111.30
1	C	294	GLN	CB-CG-CD	12.53	133.90	112.60
1	F	84	GLU	CA-CB-CG	11.87	137.83	114.10
1	D	75	LYS	CA-CB-CG	11.66	137.41	114.10
1	E	84	GLU	CA-CB-CG	10.89	135.89	114.10
1	B	486	LYS	CA-CB-CG	-10.49	93.12	114.10
1	C	223	LEU	CA-C-N	10.39	137.46	122.09
1	C	223	LEU	C-N-CA	10.39	137.46	122.09
1	E	486	LYS	CA-CB-CG	-10.35	93.40	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	527	GLY	N-CA-C	-10.30	95.89	111.24
1	A	486	LYS	CB-CG-CD	-10.14	87.98	111.30
1	D	294	GLN	CB-CG-CD	10.09	129.75	112.60
1	C	225	SER	CA-C-N	9.87	140.40	121.54
1	C	225	SER	C-N-CA	9.87	140.40	121.54
1	C	223	LEU	O-C-N	-9.55	109.28	122.94
1	E	84	GLU	CB-CG-CD	9.49	128.74	112.60
1	E	294	GLN	CB-CG-CD	9.22	128.28	112.60
1	B	133	VAL	CB-CA-C	-9.11	102.79	111.44
1	A	294	GLN	CA-CB-CG	-9.07	95.96	114.10
1	A	84	GLU	CA-CB-CG	8.96	132.02	114.10
1	D	194	ARG	NE-CZ-NH2	-8.60	111.46	119.20
1	C	84	GLU	CA-CB-CG	8.58	131.27	114.10
1	C	471	TYR	CA-CB-CG	8.37	128.96	113.90
1	C	302	LYS	N-CA-C	8.12	128.09	110.80
1	F	84	GLU	CB-CG-CD	7.74	125.75	112.60
1	F	294	GLN	CA-CB-CG	-7.50	99.10	114.10
1	A	294	GLN	CB-CG-CD	-7.03	100.66	112.60
1	A	486	LYS	CA-CB-CG	-6.94	100.22	114.10
1	C	439	VAL	CB-CA-C	6.79	123.71	111.36
1	C	294	GLN	CA-CB-CG	-6.67	100.75	114.10
1	C	303	THR	N-CA-C	6.57	124.33	109.81
1	E	195	VAL	N-CA-C	6.54	117.27	108.11
1	C	222	PHE	CA-C-N	-6.48	111.43	123.03
1	C	222	PHE	C-N-CA	-6.48	111.43	123.03
1	B	132	ARG	CA-C-N	6.48	129.62	123.08
1	B	132	ARG	C-N-CA	6.48	129.62	123.08
1	F	552	VAL	CB-CA-C	6.15	120.00	110.83
1	B	552	VAL	CB-CA-C	6.11	119.94	110.83
1	A	84	GLU	CB-CG-CD	6.07	122.92	112.60
1	E	438	ARG	CB-CG-CD	6.07	125.25	111.30
1	A	330	VAL	N-CA-C	6.06	121.94	109.34
1	E	552	VAL	CB-CA-C	6.03	119.48	110.98
1	C	224	ASP	CA-C-N	-6.03	111.48	120.94
1	C	224	ASP	C-N-CA	-6.03	111.48	120.94
1	A	200	ARG	CD-NE-CZ	5.95	132.73	124.40
1	D	552	VAL	CB-CA-C	5.95	119.70	110.83
1	B	195	VAL	N-CA-C	5.92	116.39	108.11
1	D	204	LEU	CA-CB-CG	5.88	136.88	116.30
1	B	493	MET	CB-CA-C	-5.86	109.80	116.54
1	B	294	GLN	CA-CB-CG	-5.81	102.47	114.10
1	A	195	VAL	N-CA-C	5.80	116.23	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	491	LYS	N-CA-C	5.78	118.64	109.50
2	Y	6	THR	N-CA-CB	5.75	118.43	109.97
1	C	329	ASP	CA-C-N	-5.75	112.56	120.49
1	C	329	ASP	C-N-CA	-5.75	112.56	120.49
1	B	75	LYS	CA-CB-CG	5.70	125.49	114.10
1	C	567	LEU	CA-CB-CG	5.69	136.22	116.30
1	A	552	VAL	CB-CA-C	5.63	119.36	110.81
1	C	226	HIS	N-CA-C	5.61	122.74	110.80
1	C	163	SER	CA-C-N	-5.57	114.65	120.38
1	C	163	SER	C-N-CA	-5.57	114.65	120.38
1	D	113	ARG	N-CA-CB	-5.49	101.54	109.83
1	C	477	GLY	N-CA-C	5.49	126.18	113.18
1	F	486	LYS	CA-CB-CG	5.46	125.02	114.10
1	F	195	VAL	N-CA-C	5.41	115.69	108.11
1	C	552	VAL	CB-CA-C	5.39	118.87	110.83
1	D	375	THR	N-CA-CB	5.24	118.01	110.20
1	B	204	LEU	CA-CB-CG	5.21	134.54	116.30
1	E	129	LYS	CD-CE-NZ	5.20	128.55	111.90
1	D	289	GLN	N-CA-CB	5.19	117.74	110.12
1	A	321	LEU	CA-C-O	-5.17	116.59	122.01
1	B	552	VAL	N-CA-CB	-5.10	104.32	111.25
1	F	75	LYS	CB-CG-CD	5.08	122.98	111.30
1	C	362	ARG	CG-CD-NE	5.05	123.11	112.00
1	C	222	PHE	O-C-N	5.03	128.96	123.22
1	D	133	VAL	N-CA-CB	-5.02	102.95	111.23
1	E	204	LEU	CA-CB-CG	5.02	133.86	116.30
1	F	320	GLU	CB-CA-C	-5.01	102.47	110.79
1	C	330	VAL	CA-CB-CG2	-5.01	101.89	110.40
1	B	491	LYS	N-CA-C	5.00	117.41	109.50

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 ⓘ

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	52	0
1	B	3967	0	3890	31	0
1	C	3826	0	3748	78	0
1	D	3967	0	3890	58	0
1	E	3967	0	3890	49	0
1	F	3926	0	3849	35	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
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	10	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	300	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.

All (300) 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
1:C:203:GLY:HA2	1:C:330:VAL:HG21	1.33	1.08
1:C:203:GLY:CA	1:C:330:VAL:HG22	1.88	1.01
1:C:203:GLY:CA	1:C:330:VAL:HG21	1.92	0.98
1:D:479:ASN:HB2	5:D:1572:BBK:H4	1.44	0.98
1:D:271:LYS:HG2	1:D:301:ILE:HD11	1.46	0.96
1:C:330:VAL:HG11	6:C:1569:HWU:C5	1.99	0.92
1:C:145:HIS:CD2	1:C:201:ARG:HH21	1.91	0.89
1:A:479:ASN:HB2	5:A:1581:BBK:H4	1.54	0.88
1:E:479:ASN:HD22	5:E:1584:BBK:H3	1.39	0.86
1:A:291:ARG:CZ	1:D:435:PRO:CB	2.54	0.85
1:C:205:MET:HE3	1:C:328:MET:O	1.77	0.84
1:E:479:ASN:HB2	5:E:1584:BBK:H4	1.56	0.84
1:A:479:ASN:HD22	5:A:1581:BBK:H3	1.45	0.81
1:C:203:GLY:HA2	1:C:330:VAL:CG2	2.03	0.80
1:F:134:ASP:OD1	1:F:134:ASP:O	2.00	0.80
1:B:479:ASN:HB2	5:B:1580:BBK:H4	1.65	0.80
1:F:438:ARG:HG2	1:F:481:GLU:OE2	1.82	0.79
1:F:524:GLN:HG2	1:F:528:ASN:HA	1.63	0.78
1:F:474:HIS:HD2	1:F:476:ALA:H	1.30	0.78
1:C:114:MET:HA	7:C:2004:HOH:O	1.84	0.78
1:D:123:HIS:HD2	1:D:125:GLN:H	1.32	0.77
1:D:438:ARG:HG2	1:D:481:GLU:OE2	1.83	0.77
1:C:474:HIS:HD2	1:C:476:ALA:H	1.30	0.77
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.20	0.77
1:A:438:ARG:HG2	1:A:481:GLU:OE2	1.86	0.76
1:C:305:MET:HE1	1:C:336:LEU:CD2	2.15	0.76
1:A:305:MET:HE1	1:A:336:LEU:CD2	2.16	0.76
1:A:439:VAL:H	1:D:291:ARG:NH2	1.84	0.75
1:E:305:MET:HE1	1:E:336:LEU:CD2	2.16	0.75
1:C:305:MET:HE1	1:C:336:LEU:HD23	1.68	0.75
1:B:305:MET:HE1	1:B:336:LEU:CD2	2.17	0.75
1:F:123:HIS:HD2	1:F:125:GLN:H	1.33	0.74
1:A:305:MET:HE1	1:A:336:LEU:HD23	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ARG:HG2	1:B:481:GLU:OE2	1.88	0.74
1:D:165:PRO:HA	4:D:1576:EDO:H22	1.69	0.74
1:D:479:ASN:HD22	5:D:1572:BBK:H3	1.52	0.74
1:C:123:HIS:HD2	1:C:125:GLN:H	1.36	0.74
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.22	0.73
1:D:305:MET:HE1	1:D:336:LEU:CD2	2.17	0.73
1:E:305:MET:HE1	1:E:336:LEU:HD23	1.71	0.73
6:B:1571:HWU:H1'	2:X:6:THR:OG1	1.88	0.73
1:D:305:MET:HE1	1:D:336:LEU:HD23	1.70	0.73
1:B:305:MET:HE1	1:B:336:LEU:HD23	1.71	0.72
1:C:439:VAL:C	1:C:440:PRO:O	2.30	0.72
1:E:123:HIS:HD2	1:E:125:GLN:H	1.33	0.72
1:D:516:ASP:OD1	1:D:516:ASP:N	2.22	0.72
1:A:123:HIS:HD2	1:A:125:GLN:H	1.36	0.72
1:B:123:HIS:HD2	1:B:125:GLN:H	1.37	0.72
1:A:291:ARG:NH1	1:D:435:PRO:HB2	2.05	0.71
1:C:457:LEU:HD13	1:C:482:TRP:CE2	2.25	0.71
6:C:1569:HWU:O3A	6:C:1569:HWU:H5'	1.91	0.70
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.25	0.70
1:D:277:ASN:ND2	1:D:279:VAL:HG12	2.06	0.70
1:D:457:LEU:HD13	1:D:482:TRP:CE2	2.26	0.70
1:F:457:LEU:HD13	1:F:482:TRP:CE2	2.25	0.70
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.57	0.69
1:E:438:ARG:HG2	1:E:481:GLU:OE2	1.93	0.69
1:C:277:ASN:ND2	1:C:279:VAL:HG12	2.08	0.69
4:B:1573:EDO:H12	7:B:2011:HOH:O	1.92	0.68
1:C:439:VAL:O	1:C:440:PRO:C	2.37	0.68
1:F:316:PHE:CE2	1:F:320:GLU:OE2	2.47	0.68
1:C:145:HIS:CE1	1:C:201:ARG:HE	2.12	0.67
1:C:439:VAL:O	1:C:440:PRO:O	2.12	0.66
1:D:286:THR:OG1	1:D:289:GLN:HG2	1.95	0.66
1:D:329:ASP:H	1:D:380:ASN:HD21	1.41	0.66
1:E:458:ASP:OD1	5:E:1584:BBK:O3	2.14	0.66
1:B:479:ASN:HD22	5:B:1580:BBK:H3	1.60	0.65
1:C:204:LEU:H	1:C:330:VAL:HG13	1.62	0.65
1:D:285:MET:HE2	1:D:301:ILE:CD1	2.27	0.65
1:C:329:ASP:H	1:C:380:ASN:HD21	1.45	0.65
1:C:205:MET:HE2	1:C:205:MET:H	1.61	0.65
1:C:225:SER:O	1:C:226:HIS:CG	2.51	0.64
6:E:1585:HWU:H1'	2:Y:6:THR:HB	1.80	0.63
1:A:320:GLU:C	1:A:321:LEU:O	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ASP:OD1	5:B:1580:BBK:O3	2.17	0.62
1:F:368:THR:HG22	1:F:370:PRO:HD3	1.82	0.62
1:A:263:TYR:H	4:A:1580:EDO:H21	1.65	0.62
6:C:1569:HWU:O3A	6:C:1569:HWU:O6'	2.18	0.62
1:A:194[B]:ARG:HG2	1:A:194[B]:ARG:HH11	1.65	0.62
1:F:329:ASP:H	1:F:380:ASN:HD21	1.48	0.62
1:A:368:THR:HG22	1:A:370:PRO:HD3	1.82	0.62
1:B:316:PHE:CE2	1:B:320:GLU:OE2	2.53	0.62
1:B:162:LYS:HE3	4:B:1573:EDO:O2	1.99	0.61
1:F:460:LEU:CD2	1:F:471:TYR:CE2	2.84	0.61
1:D:285:MET:HE2	1:D:301:ILE:HD13	1.83	0.61
1:E:329:ASP:H	1:E:380:ASN:HD21	1.48	0.61
1:E:368:THR:HG22	1:E:370:PRO:HD3	1.83	0.60
1:B:329:ASP:H	1:B:380:ASN:HD21	1.48	0.60
1:C:316:PHE:CE2	1:C:320:GLU:OE2	2.55	0.60
1:D:160:LEU:HA	4:D:1576:EDO:H12	1.83	0.60
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.49	0.60
1:A:329:ASP:H	1:A:380:ASN:HD21	1.50	0.59
1:C:145:HIS:CD2	1:C:201:ARG:NH2	2.67	0.59
1:D:277:ASN:HD21	1:D:279:VAL:HG12	1.66	0.59
1:D:414:ARG:HD3	7:D:2082:HOH:O	2.01	0.59
1:D:316:PHE:CE2	1:D:320:GLU:OE2	2.56	0.58
1:E:278:LEU:O	4:E:1572:EDO:C1	2.51	0.58
1:C:176:ASP:OD2	1:C:203:GLY:N	2.34	0.58
7:C:2001:HOH:O	1:E:113:ARG:NH2	2.34	0.58
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.52	0.58
1:A:474:HIS:HB2	5:D:1572:BBK:H8A	1.86	0.57
1:A:560:SER:HB3	4:A:1579:EDO:H12	1.86	0.57
1:C:277:ASN:HD21	1:C:279:VAL:HG12	1.68	0.57
1:F:460:LEU:HD22	1:F:471:TYR:CE2	2.39	0.57
6:B:1571:HWU:C1'	2:X:6:THR:OG1	2.52	0.57
1:C:77:ARG:CG	1:C:80:ASP:OD2	2.53	0.57
1:C:517:ASP:O	1:C:521:LYS:HE2	2.04	0.56
1:E:479:ASN:HD22	5:E:1584:BBK:C3	2.14	0.56
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.54	0.56
1:F:127:GLN:C	1:F:128:ARG:HD3	2.31	0.56
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.54	0.56
1:E:333:GLY:N	4:E:1572:EDO:H21	2.21	0.56
1:E:438:ARG:CG	1:E:481:GLU:OE2	2.54	0.56
1:D:271:LYS:CG	1:D:301:ILE:HD11	2.29	0.55
1:C:198:ASN:HD22	1:C:210:ARG:HH11	1.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1585:HWU:O1B	2:Y:5:SER:N	2.38	0.55
1:E:333:GLY:H	4:E:1572:EDO:H21	1.72	0.55
1:A:277:ASN:O	4:A:1575:EDO:O1	2.20	0.55
5:B:1580:BBK:H8A	1:E:474:HIS:HB2	1.89	0.54
1:C:329:ASP:O	1:C:330:VAL:C	2.46	0.54
1:E:479:ASN:ND2	5:E:1584:BBK:H3	2.14	0.54
1:E:414:ARG:HD3	7:E:2102:HOH:O	2.05	0.54
1:C:471:TYR:CD1	1:F:472:GLU:OE1	2.60	0.54
6:C:1569:HWU:PA	6:C:1569:HWU:H6'	2.30	0.54
1:E:492:HIS:HA	4:E:1582:EDO:H11	1.90	0.53
1:C:331:TRP:HE1	1:C:365:HIS:CE1	2.26	0.53
1:B:516:ASP:OD1	1:C:117:ALA:HB3	2.09	0.53
1:C:471:TYR:OH	1:F:473:CYS:O	2.26	0.53
1:B:492:HIS:HA	4:B:1577:EDO:H21	1.91	0.52
1:A:479:ASN:ND2	5:A:1581:BBK:H3	2.21	0.52
1:B:462:HIS:HD2	1:B:467:VAL:O	1.92	0.52
1:E:124:ASP:HB3	1:E:128:ARG:NH2	2.25	0.52
1:C:270:LEU:HD21	1:F:463:PHE:CE1	2.45	0.52
1:D:479:ASN:ND2	5:D:1572:BBK:H3	2.24	0.52
1:A:364:GLN:HE21	4:A:1572:EDO:C1	2.22	0.52
1:D:163:SER:O	4:D:1576:EDO:O1	2.28	0.52
1:C:77:ARG:CD	1:C:77:ARG:H	2.22	0.52
1:E:462:HIS:HD2	1:E:467:VAL:O	1.93	0.52
1:E:364:GLN:HE21	4:E:1573:EDO:H22	1.75	0.51
1:D:286:THR:OG1	1:D:289:GLN:CG	2.59	0.51
6:C:1569:HWU:O6'	6:C:1569:HWU:PA	2.68	0.51
1:C:471:TYR:CE2	1:F:472:GLU:HB3	2.46	0.51
1:E:333:GLY:HA2	4:E:1572:EDO:C2	2.40	0.51
1:D:285:MET:HE2	1:D:301:ILE:HD12	1.93	0.50
1:A:309:GLY:C	1:A:310:LEU:HD23	2.36	0.50
1:D:414:ARG:CD	7:D:2082:HOH:O	2.57	0.50
1:F:309:GLY:C	1:F:310:LEU:HD23	2.36	0.50
1:A:291:ARG:NH2	1:D:435:PRO:CB	2.73	0.50
1:E:500:VAL:O	4:E:1580:EDO:H22	2.12	0.50
1:A:493:MET:HB3	1:D:269:ASP:OD2	2.12	0.49
1:B:158:SER:HB3	4:B:1573:EDO:H11	1.94	0.49
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.59	0.49
1:C:515:GLU:O	1:C:521:LYS:NZ	2.36	0.49
1:E:333:GLY:H	4:E:1572:EDO:C2	2.25	0.49
1:E:343:TRP:CD1	1:E:349:LEU:HD22	2.47	0.49
1:E:309:GLY:C	1:E:310:LEU:HD23	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LYS:HE2	1:A:513:CYS:SG	2.52	0.49
1:B:491:LYS:HE2	1:B:513:CYS:SG	2.52	0.49
1:C:462:HIS:HD2	1:C:467:VAL:O	1.95	0.48
1:E:293:ARG:HD2	4:E:1570:EDO:H22	1.95	0.48
1:C:412:GLN:HB3	7:C:2013:HOH:O	2.13	0.48
1:D:235:GLU:N	1:D:236:PRO:CD	2.77	0.48
1:A:364:GLN:HE21	4:A:1572:EDO:H12	1.79	0.48
1:C:412:GLN:CB	7:C:2013:HOH:O	2.62	0.48
1:A:200:ARG:HG2	1:A:200:ARG:NH1	2.26	0.47
1:A:343:TRP:CD1	1:A:349:LEU:HD22	2.49	0.47
1:A:462:HIS:HD2	1:A:467:VAL:O	1.96	0.47
1:F:491:LYS:HE2	1:F:513:CYS:SG	2.54	0.47
1:F:538:LEU:HB3	1:F:552:VAL:HG22	1.96	0.47
1:E:239:GLU:OE2	7:E:2030:HOH:O	2.20	0.47
1:B:309:GLY:C	1:B:310:LEU:HD23	2.39	0.47
1:B:343:TRP:CD1	1:B:349:LEU:HD22	2.49	0.47
1:C:491:LYS:HE2	1:C:513:CYS:SG	2.54	0.47
1:C:204:LEU:HD12	1:C:205:MET:N	2.29	0.47
1:C:205:MET:HE1	1:C:330:VAL:N	2.28	0.47
1:F:204:LEU:HD12	1:F:205:MET:N	2.29	0.47
1:C:309:GLY:C	1:C:310:LEU:HD23	2.39	0.47
1:C:331:TRP:CZ2	1:C:365:HIS:CG	3.02	0.47
1:E:278:LEU:O	4:E:1572:EDO:H12	2.14	0.47
1:C:77:ARG:NE	1:C:80:ASP:OD2	2.46	0.47
1:A:288:GLU:HA	1:A:291:ARG:NH1	2.30	0.47
1:F:343:TRP:CD1	1:F:349:LEU:HD22	2.50	0.47
1:B:178:SER:O	1:B:197:ARG:NH2	2.42	0.47
1:E:333:GLY:HA2	4:E:1572:EDO:H22	1.97	0.47
1:E:491:LYS:HE2	1:E:513:CYS:SG	2.54	0.47
1:C:538:LEU:HB3	1:C:552:VAL:HG22	1.96	0.46
1:E:305:MET:HE1	1:E:336:LEU:HD22	1.98	0.46
1:A:538:LEU:HB3	1:A:552:VAL:HG22	1.98	0.46
1:D:165:PRO:CA	4:D:1576:EDO:H22	2.44	0.46
1:D:491:LYS:HE2	1:D:513:CYS:SG	2.55	0.46
1:F:514:ARG:C	1:F:516:ASP:H	2.24	0.46
1:A:291:ARG:NH2	1:D:435:PRO:HB2	2.27	0.46
1:A:439:VAL:H	1:D:291:ARG:HH21	1.59	0.46
1:A:305:MET:CE	1:A:336:LEU:HD23	2.43	0.46
1:F:178:SER:O	1:F:197:ARG:NH2	2.43	0.46
1:C:343:TRP:CD1	1:C:349:LEU:HD22	2.51	0.46
1:D:309:GLY:C	1:D:310:LEU:HD23	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:SER:O	1:E:197:ARG:NH2	2.42	0.46
1:A:191:GLU:HG3	1:A:191:GLU:O	2.16	0.45
1:A:319:GLU:O	1:A:321:LEU:O	2.34	0.45
1:E:493:MET:H	4:E:1582:EDO:H22	1.80	0.45
1:C:178:SER:O	1:C:197:ARG:NH2	2.40	0.45
1:E:414:ARG:CD	7:E:2102:HOH:O	2.63	0.45
1:C:204:LEU:HG	1:C:330:VAL:HG13	1.97	0.45
1:C:493:MET:HE1	1:F:290:ARG:NH2	2.31	0.45
1:D:465:ASP:OD1	4:D:1573:EDO:H11	2.17	0.44
1:C:189:LYS:NZ	7:C:2008:HOH:O	2.49	0.44
1:E:191:GLU:O	1:E:191:GLU:HG3	2.17	0.44
1:F:235:GLU:N	1:F:236:PRO:CD	2.80	0.44
1:C:303:THR:HA	1:C:304:PRO:HD3	1.96	0.44
1:D:285:MET:O	1:D:290:ARG:NH1	2.51	0.44
1:D:331:TRP:NE1	6:D:1571:HWU:H5'	2.33	0.44
1:A:103:LYS:HD2	4:A:1572:EDO:H12	1.98	0.44
1:A:178:SER:O	1:A:197:ARG:NH2	2.42	0.44
1:A:204:LEU:HD12	1:A:205:MET:N	2.32	0.44
1:B:518:SER:HB3	1:C:161:LYS:NZ	2.32	0.44
1:C:106:GLN:HB2	7:C:2003:HOH:O	2.17	0.44
1:A:252:ILE:HG23	4:A:1578:EDO:H11	2.00	0.44
1:A:263:TYR:N	4:A:1580:EDO:H21	2.31	0.44
1:B:235:GLU:N	1:B:236:PRO:CD	2.81	0.44
1:E:305:MET:CE	1:E:336:LEU:HD23	2.45	0.44
1:E:335:ASN:HD21	4:E:1572:EDO:C2	2.31	0.44
1:C:515:GLU:C	1:C:517:ASP:H	2.26	0.43
1:D:132:ARG:HB2	1:D:134:ASP:OD1	2.18	0.43
1:D:305:MET:CE	1:D:336:LEU:HD23	2.44	0.43
1:D:538:LEU:HB3	1:D:552:VAL:HG22	1.98	0.43
1:B:538:LEU:HB3	1:B:552:VAL:HG22	2.00	0.43
1:B:391:GLU:H	1:B:391:GLU:CD	2.26	0.43
1:C:77:ARG:H	1:C:77:ARG:HD3	1.81	0.43
1:C:176:ASP:OD1	1:C:202:GLU:N	2.38	0.43
1:C:200:ARG:O	1:C:202:GLU:HG2	2.19	0.43
1:D:153:LEU:O	1:D:157:VAL:HG13	2.19	0.43
1:E:335:ASN:N	1:E:335:ASN:HD22	2.16	0.43
1:C:143:THR:OG1	6:C:1569:HWU:H1B	2.18	0.43
6:C:1569:HWU:O3A	6:C:1569:HWU:C5'	2.62	0.43
1:D:343:TRP:CD1	1:D:349:LEU:HD22	2.53	0.43
1:E:235:GLU:N	1:E:236:PRO:CD	2.81	0.43
1:B:375:THR:HG23	7:B:2079:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:MET:O	1:C:290:ARG:NH1	2.52	0.42
1:D:178:SER:O	1:D:197:ARG:NH2	2.40	0.42
1:D:529:SER:C	1:D:530:LYS:HG2	2.43	0.42
1:F:191:GLU:HG3	1:F:191:GLU:O	2.18	0.42
1:C:305:MET:HB2	1:C:305:MET:HE3	1.75	0.42
1:A:291:ARG:NE	1:D:435:PRO:CB	2.82	0.42
4:B:1573:EDO:C1	7:B:2011:HOH:O	2.59	0.42
1:D:204:LEU:HD13	1:D:331:TRP:HA	2.02	0.42
6:D:1571:HWU:C5B	6:D:1571:HWU:H6	2.49	0.42
6:D:1571:HWU:H6	6:D:1571:HWU:H5B1	1.99	0.42
6:D:1571:HWU:HA	6:D:1571:HWU:H5B2	1.84	0.42
1:E:538:LEU:HB3	1:E:552:VAL:HG22	2.01	0.42
1:A:364:GLN:NE2	4:A:1572:EDO:H12	2.34	0.42
1:E:153:LEU:O	1:E:157:VAL:HG13	2.19	0.42
1:E:285:MET:O	1:E:290:ARG:NH1	2.52	0.42
1:E:377:PHE:CE2	4:E:1579:EDO:H21	2.54	0.42
1:F:309:GLY:CA	6:F:1571:HWU:O3'	2.67	0.42
6:F:1571:HWU:H6	6:F:1571:HWU:H5B2	2.02	0.42
1:A:439:VAL:HG13	1:D:291:ARG:NH2	2.35	0.42
1:C:191:GLU:O	1:C:191:GLU:HG3	2.19	0.42
1:C:331:TRP:NE1	1:C:365:HIS:CE1	2.88	0.42
1:C:330:VAL:HG11	6:C:1569:HWU:H5	1.93	0.42
1:A:153:LEU:O	1:A:157:VAL:HG13	2.20	0.42
1:D:86:TYR:CE2	1:D:149:ARG:HB3	2.55	0.42
1:E:305:MET:HE3	1:E:305:MET:HB2	1.71	0.42
1:A:285:MET:O	1:A:290:ARG:NH1	2.53	0.42
1:C:224:ASP:OD2	6:C:1569:HWU:O2B	2.37	0.42
1:D:502:ARG:HD2	7:D:2111:HOH:O	2.18	0.42
1:D:450:LEU:HD13	1:D:563:TRP:CE3	2.55	0.42
1:F:285:MET:O	1:F:290:ARG:NH1	2.53	0.42
2:X:7:CYS:HA	2:X:8:PRO:HD3	1.89	0.42
1:C:291:ARG:NE	1:F:435:PRO:HB2	2.34	0.41
1:C:224:ASP:O	1:C:225:SER:C	2.47	0.41
1:C:330:VAL:HG11	6:C:1569:HWU:C4	2.48	0.41
1:B:130:GLN:HE21	1:B:130:GLN:HB3	1.67	0.41
1:B:285:MET:O	1:B:290:ARG:NH1	2.53	0.41
1:B:305:MET:HE1	1:B:336:LEU:HD22	1.99	0.41
1:D:305:MET:HE3	1:D:305:MET:HB2	1.71	0.41
1:F:153:LEU:O	1:F:157:VAL:HG13	2.19	0.41
1:A:439:VAL:H	1:D:291:ARG:HH22	1.64	0.41
1:C:225:SER:O	1:C:226:HIS:ND1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:HD13	1:B:563:TRP:CE3	2.55	0.41
1:C:204:LEU:N	1:C:330:VAL:HG13	2.31	0.41
1:F:204:LEU:HD12	1:F:204:LEU:C	2.45	0.41
1:F:126:CYS:C	1:F:128:ARG:N	2.79	0.41
1:A:457:LEU:HD13	1:A:482:TRP:CZ2	2.56	0.41
1:B:511:GLN:NE2	4:B:1572:EDO:H21	2.36	0.41
1:E:377:PHE:CE2	4:E:1579:EDO:C2	3.04	0.41
1:F:460:LEU:HD23	1:F:471:TYR:CE2	2.56	0.41
1:A:450:LEU:HD13	1:A:563:TRP:CE3	2.56	0.41
1:C:515:GLU:O	1:C:517:ASP:N	2.54	0.41
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.17	0.40
1:D:191:GLU:O	1:D:191:GLU:HG3	2.20	0.40
1:D:83:GLN:HG2	1:D:84:GLU:N	2.35	0.40
1:C:271:LYS:HB2	1:C:271:LYS:HE3	1.94	0.40
1:B:529:SER:C	1:B:530:LYS:HG2	2.46	0.40
1:F:391:GLU:H	1:F:391:GLU:CD	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	43	51
1	B	493/571 (86%)	476 (97%)	16 (3%)	1 (0%)	43	51
1	C	470/571 (82%)	451 (96%)	16 (3%)	3 (1%)	21	23
1	D	493/571 (86%)	478 (97%)	14 (3%)	1 (0%)	43	51
1	E	493/571 (86%)	479 (97%)	13 (3%)	1 (0%)	43	51
1	F	487/571 (85%)	473 (97%)	13 (3%)	1 (0%)	43	51
2	X	4/6 (67%)	3 (75%)	1 (25%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	2938/3438 (86%)	2842 (97%)	88 (3%)	8 (0%)	36	42

All (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
1	D	330	VAL
1	F	330	VAL
1	E	330	VAL

5.3.2 Protein sidechains ⓘ

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%)	386 (90%)	43 (10%)	7	7
1	B	428/485 (88%)	388 (91%)	40 (9%)	8	9
1	C	414/485 (85%)	369 (89%)	45 (11%)	6	6
1	D	428/485 (88%)	382 (89%)	46 (11%)	6	6
1	E	428/485 (88%)	385 (90%)	43 (10%)	7	7
1	F	424/485 (87%)	379 (89%)	45 (11%)	6	6
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%)	2294 (90%)	265 (10%)	7	7

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	76	VAL
1	A	77	ARG
1	A	101	ARG
1	A	112	LEU
1	A	116	ARG
1	A	124	ASP
1	A	133	VAL
1	A	157	VAL
1	A	173	LEU
1	A	195	VAL
1	A	196	LEU
1	A	200	ARG
1	A	204	LEU
1	A	241	VAL
1	A	277	ASN
1	A	288	GLU
1	A	302	LYS
1	A	310	LEU
1	A	330	VAL
1	A	335	ASN
1	A	336	LEU
1	A	349	LEU
1	A	368	THR
1	A	410	ASN
1	A	419	LYS
1	A	421	LEU
1	A	436	GLU
1	A	438	ARG
1	A	439	VAL
1	A	450	LEU
1	A	457	LEU
1	A	468	VAL
1	A	484	LEU
1	A	487	GLU
1	A	500	VAL
1	A	502	ARG
1	A	510	LEU
1	A	515	GLU
1	A	546	LYS
1	A	552	VAL
1	A	554	VAL
1	A	567	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	75	LYS
1	B	76	VAL
1	B	101	ARG
1	B	112	LEU
1	B	116	ARG
1	B	124	ASP
1	B	130	GLN
1	B	133	VAL
1	B	143	THR
1	B	157	VAL
1	B	173	LEU
1	B	195	VAL
1	B	196	LEU
1	B	204	LEU
1	B	241	VAL
1	B	277	ASN
1	B	288	GLU
1	B	302	LYS
1	B	310	LEU
1	B	335	ASN
1	B	336	LEU
1	B	349	LEU
1	B	375	THR
1	B	410	ASN
1	B	419	LYS
1	B	421	LEU
1	B	436	GLU
1	B	438	ARG
1	B	439	VAL
1	B	442	HIS
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	484	LEU
1	B	502	ARG
1	B	510	LEU
1	B	546	LYS
1	B	552	VAL
1	B	554	VAL
1	B	567	LEU
1	C	75	LYS
1	C	76	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	77	ARG
1	C	101	ARG
1	C	112	LEU
1	C	113	ARG
1	C	116	ARG
1	C	124	ASP
1	C	133	VAL
1	C	157	VAL
1	C	173	LEU
1	C	195	VAL
1	C	196	LEU
1	C	201	ARG
1	C	204	LEU
1	C	205	MET
1	C	241	VAL
1	C	277	ASN
1	C	288	GLU
1	C	294	GLN
1	C	302	LYS
1	C	310	LEU
1	C	330	VAL
1	C	335	ASN
1	C	336	LEU
1	C	349	LEU
1	C	410	ASN
1	C	419	LYS
1	C	421	LEU
1	C	436	GLU
1	C	438	ARG
1	C	439	VAL
1	C	450	LEU
1	C	457	LEU
1	C	468	VAL
1	C	471	TYR
1	C	484	LEU
1	C	500	VAL
1	C	502	ARG
1	C	510	LEU
1	C	515	GLU
1	C	516	ASP
1	C	546	LYS
1	C	552	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	554	VAL
1	D	75	LYS
1	D	76	VAL
1	D	83	GLN
1	D	101	ARG
1	D	112	LEU
1	D	116	ARG
1	D	124	ASP
1	D	133	VAL
1	D	157	VAL
1	D	173	LEU
1	D	195	VAL
1	D	196	LEU
1	D	204	LEU
1	D	241	VAL
1	D	277	ASN
1	D	284	TYR
1	D	288	GLU
1	D	289	GLN
1	D	291	ARG
1	D	294	GLN
1	D	301	ILE
1	D	302	LYS
1	D	310	LEU
1	D	335	ASN
1	D	336	LEU
1	D	349	LEU
1	D	375	THR
1	D	410	ASN
1	D	419	LYS
1	D	421	LEU
1	D	436	GLU
1	D	438	ARG
1	D	439	VAL
1	D	450	LEU
1	D	457	LEU
1	D	468	VAL
1	D	484	LEU
1	D	502	ARG
1	D	510	LEU
1	D	515	GLU
1	D	516	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	546	LYS
1	D	552	VAL
1	D	554	VAL
1	D	567	LEU
1	D	568	ASN
1	E	75	LYS
1	E	76	VAL
1	E	77	ARG
1	E	101	ARG
1	E	112	LEU
1	E	116	ARG
1	E	124	ASP
1	E	133	VAL
1	E	143	THR
1	E	157	VAL
1	E	173	LEU
1	E	195	VAL
1	E	196	LEU
1	E	204	LEU
1	E	241	VAL
1	E	277	ASN
1	E	288	GLU
1	E	294	GLN
1	E	302	LYS
1	E	310	LEU
1	E	335	ASN
1	E	336	LEU
1	E	349	LEU
1	E	368	THR
1	E	375	THR
1	E	410	ASN
1	E	419	LYS
1	E	421	LEU
1	E	436	GLU
1	E	438	ARG
1	E	439	VAL
1	E	450	LEU
1	E	457	LEU
1	E	468	VAL
1	E	484	LEU
1	E	500	VAL
1	E	502	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	510	LEU
1	E	515	GLU
1	E	546	LYS
1	E	552	VAL
1	E	554	VAL
1	E	567	LEU
1	F	75	LYS
1	F	76	VAL
1	F	101	ARG
1	F	112	LEU
1	F	116	ARG
1	F	124	ASP
1	F	128	ARG
1	F	134	ASP
1	F	143	THR
1	F	157	VAL
1	F	173	LEU
1	F	195	VAL
1	F	196	LEU
1	F	204	LEU
1	F	241	VAL
1	F	277	ASN
1	F	288	GLU
1	F	294	GLN
1	F	302	LYS
1	F	310	LEU
1	F	335	ASN
1	F	336	LEU
1	F	349	LEU
1	F	368	THR
1	F	375	THR
1	F	410	ASN
1	F	419	LYS
1	F	421	LEU
1	F	436	GLU
1	F	438	ARG
1	F	439	VAL
1	F	442	HIS
1	F	450	LEU
1	F	457	LEU
1	F	468	VAL
1	F	471	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	484	LEU
1	F	500	VAL
1	F	502	ARG
1	F	510	LEU
1	F	515	GLU
1	F	516	ASP
1	F	546	LYS
1	F	552	VAL
1	F	554	VAL
2	X	5	SER
2	Y	6	THR
2	Y	7	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	127	GLN
1	A	198	ASN
1	A	216	GLN
1	A	277	ASN
1	A	335	ASN
1	A	344	GLN
1	A	364	GLN
1	A	365	HIS
1	A	380	ASN
1	A	410	ASN
1	A	451	GLN
1	A	452	GLN
1	A	462	HIS
1	A	479	ASN
1	A	537	ASN
1	A	562	GLN
1	B	123	HIS
1	B	125	GLN
1	B	127	GLN
1	B	130	GLN
1	B	198	ASN
1	B	216	GLN
1	B	335	ASN
1	B	344	GLN
1	B	380	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	410	ASN
1	B	451	GLN
1	B	452	GLN
1	B	462	HIS
1	B	479	ASN
1	B	524	GLN
1	B	537	ASN
1	B	562	GLN
1	B	568	ASN
1	C	123	HIS
1	C	127	GLN
1	C	198	ASN
1	C	216	GLN
1	C	277	ASN
1	C	335	ASN
1	C	344	GLN
1	C	365	HIS
1	C	451	GLN
1	C	452	GLN
1	C	462	HIS
1	C	474	HIS
1	C	528	ASN
1	C	537	ASN
1	C	562	GLN
1	D	96	GLN
1	D	102	ASN
1	D	123	HIS
1	D	127	GLN
1	D	198	ASN
1	D	216	GLN
1	D	277	ASN
1	D	335	ASN
1	D	344	GLN
1	D	365	HIS
1	D	380	ASN
1	D	451	GLN
1	D	452	GLN
1	D	479	ASN
1	D	562	GLN
1	E	123	HIS
1	E	125	GLN
1	E	127	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	198	ASN
1	E	216	GLN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	364	GLN
1	E	380	ASN
1	E	410	ASN
1	E	451	GLN
1	E	462	HIS
1	E	479	ASN
1	E	524	GLN
1	E	537	ASN
1	E	562	GLN
1	E	568	ASN
1	F	123	HIS
1	F	125	GLN
1	F	127	GLN
1	F	166	HIS
1	F	198	ASN
1	F	216	GLN
1	F	277	ASN
1	F	335	ASN
1	F	344	GLN
1	F	365	HIS
1	F	380	ASN
1	F	451	GLN
1	F	452	GLN
1	F	474	HIS
1	F	524	GLN
1	F	528	ASN
1	F	537	ASN
1	F	562	GLN
1	F	568	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	D	1576	-	3,3,3	0.57	0	2,2,2	0.55	0
4	EDO	E	1581	-	3,3,3	0.32	0	2,2,2	0.86	0
4	EDO	A	1574	-	3,3,3	0.49	0	2,2,2	0.13	0
4	EDO	A	1576	-	3,3,3	0.27	0	2,2,2	0.75	0
4	EDO	A	1572	-	3,3,3	0.48	0	2,2,2	0.55	0
4	EDO	E	1575	-	3,3,3	0.43	0	2,2,2	0.36	0
6	HWU	A	1582	3	38,41,41	3.59	8 (21%)	52,62,62	1.91	15 (28%)
4	EDO	B	1572	-	3,3,3	0.53	0	2,2,2	0.57	0
4	EDO	E	1570	-	3,3,3	0.74	0	2,2,2	0.35	0
4	EDO	D	1575	-	3,3,3	0.87	0	2,2,2	0.34	0
4	EDO	E	1576	-	3,3,3	0.49	0	2,2,2	0.53	0
4	EDO	B	1574	-	3,3,3	0.59	0	2,2,2	0.34	0
5	BBK	E	1584	-	13,15,15	9.32	2 (15%)	14,21,21	2.00	4 (28%)
4	EDO	E	1583	-	3,3,3	0.54	0	2,2,2	0.15	0
4	EDO	A	1577	-	3,3,3	0.51	0	2,2,2	0.17	0
4	EDO	A	1579	-	3,3,3	0.67	0	2,2,2	0.41	0
4	EDO	B	1577	-	3,3,3	0.25	0	2,2,2	1.09	0
4	EDO	B	1578	-	3,3,3	0.51	0	2,2,2	0.40	0
5	BBK	A	1581	-	13,15,15	9.26	2 (15%)	14,21,21	2.17	4 (28%)
5	BBK	B	1580	-	13,15,15	9.13	2 (15%)	14,21,21	1.72	3 (21%)
6	HWU	B	1571	3	38,41,41	3.69	9 (23%)	52,62,62	2.89	23 (44%)
6	HWU	E	1585	3	38,41,41	3.75	7 (18%)	52,62,62	2.25	17 (32%)
4	EDO	B	1575	-	3,3,3	0.41	0	2,2,2	0.37	0
4	EDO	A	1580	-	3,3,3	0.94	0	2,2,2	1.10	0
6	HWU	C	1569	3	38,41,41	4.73	4 (10%)	52,62,62	2.30	22 (42%)
4	EDO	B	1576	-	3,3,3	0.61	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	1573	-	3,3,3	0.52	0	2,2,2	0.74	0
4	EDO	E	1577	-	3,3,3	0.33	0	2,2,2	0.75	0
4	EDO	A	1571	-	3,3,3	0.84	0	2,2,2	0.25	0
4	EDO	B	1579	-	3,3,3	0.66	0	2,2,2	0.05	0
4	EDO	A	1578	-	3,3,3	0.68	0	2,2,2	0.60	0
4	EDO	E	1572	-	3,3,3	0.36	0	2,2,2	0.40	0
6	HWU	F	1571	3	38,41,41	3.50	3 (7%)	52,62,62	2.10	14 (26%)
4	EDO	E	1579	-	3,3,3	0.43	0	2,2,2	0.60	0
4	EDO	E	1574	-	3,3,3	0.32	0	2,2,2	0.82	0
4	EDO	E	1582	-	3,3,3	0.32	0	2,2,2	0.32	0
4	EDO	B	1573	-	3,3,3	0.27	0	2,2,2	0.33	0
4	EDO	E	1573	-	3,3,3	0.29	0	2,2,2	0.95	0
5	BBK	D	1572	-	13,15,15	9.61	2 (15%)	14,21,21	3.51	5 (35%)
4	EDO	A	1575	-	3,3,3	0.33	0	2,2,2	0.66	0
6	HWU	D	1571	3	38,41,41	4.26	9 (23%)	52,62,62	2.16	18 (34%)
4	EDO	E	1571	-	3,3,3	0.64	0	2,2,2	0.24	0
4	EDO	E	1580	-	3,3,3	0.61	0	2,2,2	0.25	0
4	EDO	D	1577	-	3,3,3	0.40	0	2,2,2	0.68	0
4	EDO	D	1574	-	3,3,3	0.77	0	2,2,2	0.47	0
4	EDO	E	1578	-	3,3,3	0.37	0	2,2,2	0.68	0
4	EDO	A	1573	-	3,3,3	0.79	0	2,2,2	0.04	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	D	1576	-	-	1/1/1/1	-
4	EDO	E	1581	-	-	0/1/1/1	-
4	EDO	A	1574	-	-	1/1/1/1	-
4	EDO	A	1576	-	-	1/1/1/1	-
4	EDO	A	1572	-	-	1/1/1/1	-
4	EDO	E	1575	-	-	1/1/1/1	-
6	HWU	A	1582	3	-	5/25/63/63	0/3/3/3
4	EDO	B	1572	-	-	1/1/1/1	-
4	EDO	E	1570	-	-	1/1/1/1	-
4	EDO	D	1575	-	-	1/1/1/1	-
4	EDO	E	1576	-	-	1/1/1/1	-
4	EDO	B	1574	-	-	1/1/1/1	-
5	BBK	E	1584	-	-	4/6/26/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	1583	-	-	1/1/1/1	-
4	EDO	A	1577	-	-	1/1/1/1	-
4	EDO	A	1579	-	-	0/1/1/1	-
4	EDO	B	1577	-	-	1/1/1/1	-
4	EDO	B	1578	-	-	1/1/1/1	-
5	BBK	A	1581	-	-	5/6/26/26	0/1/1/1
5	BBK	B	1580	-	-	4/6/26/26	0/1/1/1
6	HWU	B	1571	3	-	6/25/63/63	0/3/3/3
6	HWU	E	1585	3	-	7/25/63/63	0/3/3/3
4	EDO	B	1575	-	-	1/1/1/1	-
4	EDO	A	1580	-	-	1/1/1/1	-
6	HWU	C	1569	3	-	6/25/63/63	0/3/3/3
4	EDO	B	1576	-	-	1/1/1/1	-
4	EDO	D	1573	-	-	0/1/1/1	-
4	EDO	E	1577	-	-	1/1/1/1	-
4	EDO	A	1571	-	-	1/1/1/1	-
4	EDO	B	1579	-	-	0/1/1/1	-
4	EDO	A	1578	-	-	0/1/1/1	-
4	EDO	E	1572	-	-	1/1/1/1	-
6	HWU	F	1571	3	-	6/25/63/63	0/3/3/3
4	EDO	E	1579	-	-	1/1/1/1	-
4	EDO	E	1574	-	-	1/1/1/1	-
4	EDO	E	1582	-	-	1/1/1/1	-
4	EDO	B	1573	-	-	1/1/1/1	-
4	EDO	E	1573	-	-	1/1/1/1	-
5	BBK	D	1572	-	-	2/6/26/26	0/1/1/1
4	EDO	A	1575	-	-	1/1/1/1	-
6	HWU	D	1571	3	-	7/25/63/63	0/3/3/3
4	EDO	E	1571	-	-	0/1/1/1	-
4	EDO	E	1580	-	-	0/1/1/1	-
4	EDO	D	1577	-	-	1/1/1/1	-
4	EDO	D	1574	-	-	0/1/1/1	-
4	EDO	E	1578	-	-	0/1/1/1	-
4	EDO	A	1573	-	-	1/1/1/1	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1569	HWU	C5'-S5'	-27.68	1.41	1.82
5	D	1572	BBK	C5-S5	-27.47	1.42	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1584	BBK	C5-S5	-27.08	1.42	1.82
5	B	1580	BBK	C5-S5	-26.38	1.43	1.82
5	A	1581	BBK	C5-S5	-26.21	1.43	1.82
6	D	1571	HWU	C5'-S5'	-23.52	1.47	1.82
6	E	1585	HWU	C5'-S5'	-21.19	1.51	1.82
6	A	1582	HWU	C5'-S5'	-20.84	1.51	1.82
5	D	1572	BBK	C1-S5	-20.83	1.42	1.83
5	A	1581	BBK	C1-S5	-20.60	1.42	1.83
6	F	1571	HWU	C5'-S5'	-20.53	1.52	1.82
6	B	1571	HWU	C5'-S5'	-20.49	1.52	1.82
5	E	1584	BBK	C1-S5	-19.64	1.44	1.83
5	B	1580	BBK	C1-S5	-19.48	1.45	1.83
6	C	1569	HWU	PA-O3A	6.19	1.66	1.59
6	D	1571	HWU	PB-O3A	-5.79	1.53	1.59
6	E	1585	HWU	PB-O3A	5.63	1.65	1.59
6	B	1571	HWU	PB-O3A	5.04	1.64	1.59
6	D	1571	HWU	C4'-C5'	4.74	1.57	1.53
6	D	1571	HWU	PA-O3A	-3.49	1.55	1.59
6	D	1571	HWU	C6'-C5'	3.45	1.55	1.52
6	B	1571	HWU	C4-N3	-3.16	1.33	1.38
6	B	1571	HWU	C6-N1	-3.00	1.30	1.38
6	C	1569	HWU	PB-O3A	2.95	1.62	1.59
6	B	1571	HWU	C4'-C5'	2.73	1.55	1.53
6	B	1571	HWU	O5B-C5B	-2.72	1.34	1.44
6	D	1571	HWU	C6-C5	2.66	1.41	1.35
6	D	1571	HWU	O5B-C5B	-2.64	1.34	1.44
6	D	1571	HWU	C5-C4	-2.64	1.38	1.43
6	F	1571	HWU	C4'-C5'	2.58	1.55	1.53
6	B	1571	HWU	PB-O1'	2.52	1.66	1.59
6	A	1582	HWU	C6'-C5'	2.49	1.54	1.52
6	E	1585	HWU	C4'-C5'	2.49	1.55	1.53
6	B	1571	HWU	PB-O2B	-2.43	1.44	1.55
6	D	1571	HWU	C4-N3	-2.33	1.34	1.38
6	B	1571	HWU	C2-N3	-2.31	1.33	1.38
6	A	1582	HWU	PB-O1B	-2.22	1.43	1.50
6	A	1582	HWU	O2-C2	2.20	1.27	1.23
6	F	1571	HWU	O5B-C5B	-2.19	1.36	1.44
6	A	1582	HWU	C6-C5	2.16	1.40	1.35
6	A	1582	HWU	PA-O3A	-2.15	1.57	1.59
6	A	1582	HWU	PB-O1'	2.14	1.65	1.59
6	A	1582	HWU	C5-C4	-2.12	1.39	1.43
6	E	1585	HWU	C4-N3	-2.12	1.35	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1585	HWU	O4B-C1B	2.12	1.46	1.42
6	C	1569	HWU	PB-O2B	-2.07	1.45	1.55
6	E	1585	HWU	PB-O2B	-2.05	1.45	1.55
6	E	1585	HWU	C5-C4	-2.04	1.39	1.43

All (125) 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
6	B	1571	HWU	C4-N3-C2	-7.87	116.84	126.61
5	D	1572	BBK	O1-C1-C2	-7.78	93.37	109.25
6	B	1571	HWU	N3-C2-N1	7.64	124.83	114.89
6	E	1585	HWU	C4-N3-C2	-6.87	118.08	126.61
6	E	1585	HWU	N3-C2-N1	6.75	123.68	114.89
6	F	1571	HWU	C4-N3-C2	-6.37	118.71	126.61
6	B	1571	HWU	O3A-PB-O1B	-6.26	91.86	110.70
6	B	1571	HWU	O1'-C1'-C2'	5.82	116.37	107.52
6	B	1571	HWU	O5B-PA-O1A	5.48	130.67	108.94
6	D	1571	HWU	O1'-PB-O1B	-5.44	92.43	109.81
6	F	1571	HWU	N3-C2-N1	5.25	121.73	114.89
6	D	1571	HWU	N3-C2-N1	5.14	121.58	114.89
6	A	1582	HWU	C4-N3-C2	-5.01	120.40	126.61
6	C	1569	HWU	C4-N3-C2	-4.96	120.45	126.61
6	B	1571	HWU	PB-O1'-C1'	4.83	140.90	121.21
6	C	1569	HWU	O1'-C1'-C2'	4.82	114.84	107.52
5	A	1581	BBK	C1-C2-N2	4.79	120.31	111.36
6	E	1585	HWU	O3A-PB-O1B	-4.78	96.33	110.70
6	C	1569	HWU	O2A-PA-O3A	4.72	120.04	107.27
5	A	1581	BBK	C2-N2-C7	4.65	134.00	123.11
6	A	1582	HWU	PB-O1'-C1'	4.64	140.12	121.21
6	B	1571	HWU	O1'-PB-O1B	4.64	124.64	109.81
6	D	1571	HWU	O2-C2-N3	-4.61	112.99	121.49
6	B	1571	HWU	O4-C4-C5	-4.40	117.57	125.16
6	A	1582	HWU	C5-C4-N3	4.34	120.88	114.80
6	D	1571	HWU	O3'-C3'-C2'	4.27	118.08	109.58
6	C	1569	HWU	C5-C4-N3	4.20	120.68	114.80
6	F	1571	HWU	C5-C4-N3	4.20	120.68	114.80
6	C	1569	HWU	O6'-C6'-C5'	-4.15	101.31	110.72
6	F	1571	HWU	O2B-PB-O3A	4.11	118.38	107.27
6	A	1582	HWU	N3-C2-N1	4.08	120.20	114.89
5	E	1584	BBK	C3-C2-N2	-4.06	103.13	110.62
6	F	1571	HWU	O4-C4-C5	-4.06	118.16	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1585	HWU	C5-C4-N3	3.94	120.33	114.80
6	D	1571	HWU	O4B-C4B-C5B	-3.88	96.92	109.33
6	B	1571	HWU	O2-C2-N1	-3.84	117.80	122.80
6	C	1569	HWU	O2-C2-N3	-3.67	114.72	121.49
6	C	1569	HWU	C1'-C2'-N2'	-3.66	104.42	111.07
6	B	1571	HWU	C5-C4-N3	3.65	119.91	114.80
6	D	1571	HWU	C6-N1-C2	-3.64	116.56	121.00
6	E	1585	HWU	PB-O1'-C1'	3.62	135.97	121.21
6	D	1571	HWU	C1B-N1-C2	3.57	124.00	117.59
6	B	1571	HWU	O2A-PA-O5B	-3.51	91.68	107.57
6	F	1571	HWU	O3A-PB-O1B	-3.49	100.19	110.70
6	A	1582	HWU	C6'-C5'-C4'	-3.47	99.69	114.44
6	C	1569	HWU	O3A-PA-O1A	-3.41	100.45	110.70
6	C	1569	HWU	N3-C2-N1	3.40	119.32	114.89
6	E	1585	HWU	O2-C2-N3	-3.37	115.27	121.49
6	E	1585	HWU	O1'-C1'-C2'	3.35	112.62	107.52
6	B	1571	HWU	O3A-PA-O1A	-3.35	100.62	110.70
6	F	1571	HWU	O4B-C4B-C5B	-3.35	98.62	109.33
5	B	1580	BBK	C2-N2-C7	3.33	130.90	123.11
6	E	1585	HWU	O4-C4-C5	-3.27	119.52	125.16
6	C	1569	HWU	O3B-C3B-C4B	3.24	120.38	111.08
6	C	1569	HWU	PB-O1'-C1'	3.22	134.32	121.21
5	B	1580	BBK	O4-C4-C5	3.19	115.81	108.90
6	A	1582	HWU	O1'-PB-O1B	-3.18	99.64	109.81
5	E	1584	BBK	O4-C4-C5	3.17	115.75	108.90
5	E	1584	BBK	C2-N2-C7	3.16	130.51	123.11
6	A	1582	HWU	O4-C4-C5	-3.14	119.74	125.16
6	A	1582	HWU	O2B-PB-O1B	3.06	126.70	112.44
6	B	1571	HWU	C4'-C3'-C2'	-3.06	105.94	110.40
6	C	1569	HWU	O4B-C1B-N1	3.04	115.24	108.36
6	D	1571	HWU	C4-N3-C2	-2.98	122.92	126.61
6	D	1571	HWU	C5B-C4B-C3B	-2.97	104.51	115.21
6	F	1571	HWU	PB-O1'-C1'	2.96	133.27	121.21
6	B	1571	HWU	O7'-C7'-N2'	2.95	127.19	121.98
6	E	1585	HWU	O7'-C7'-N2'	2.92	127.13	121.98
6	C	1569	HWU	C4'-C3'-C2'	-2.90	106.18	110.40
6	A	1582	HWU	C2'-N2'-C7'	-2.88	116.36	123.11
6	B	1571	HWU	O4B-C4B-C5B	-2.87	100.14	109.33
6	F	1571	HWU	O5B-PA-O1A	2.82	120.12	108.94
6	C	1569	HWU	O4-C4-C5	-2.72	120.47	125.16
6	E	1585	HWU	O3'-C3'-C2'	2.70	114.96	109.58
6	C	1569	HWU	C1B-N1-C2	2.69	122.42	117.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1572	BBK	C4-C3-C2	2.67	114.30	110.40
6	B	1571	HWU	O2B-PB-O3A	2.66	114.47	107.27
6	A	1582	HWU	O2B-PB-O3A	2.65	114.42	107.27
6	A	1582	HWU	O2-C2-N3	-2.61	116.68	121.49
6	D	1571	HWU	O5B-C5B-C4B	2.55	117.68	108.99
6	D	1571	HWU	O4'-C4'-C3'	-2.54	104.39	110.38
6	B	1571	HWU	O2A-PA-O3A	2.53	114.11	107.27
6	E	1585	HWU	O7'-C7'-C8'	-2.53	117.55	122.05
6	D	1571	HWU	PB-O1'-C1'	2.51	131.44	121.21
6	C	1569	HWU	O4B-C4B-C3B	2.50	110.11	105.15
6	D	1571	HWU	O1'-C1'-C2'	-2.48	103.75	107.52
6	B	1571	HWU	O4'-C4'-C3'	-2.46	104.59	110.38
6	E	1585	HWU	C6-N1-C2	-2.45	118.01	121.00
6	F	1571	HWU	O2-C2-N3	-2.45	116.97	121.49
5	E	1584	BBK	O6-C6-C5	-2.42	105.22	110.72
6	C	1569	HWU	O2-C2-N1	2.41	125.94	122.80
5	D	1572	BBK	O4-C4-C5	2.41	114.12	108.90
6	C	1569	HWU	C1B-N1-C6	-2.38	115.68	120.78
5	A	1581	BBK	C3-C2-N2	-2.37	106.25	110.62
6	F	1571	HWU	O3A-PA-O1A	-2.36	103.59	110.70
6	E	1585	HWU	O2A-PA-O3A	2.36	113.66	107.27
6	A	1582	HWU	C4'-C3'-C2'	-2.34	107.00	110.40
6	C	1569	HWU	O5B-PA-O1A	2.30	118.06	108.94
6	B	1571	HWU	O2A-PA-O1A	2.30	123.15	112.44
6	F	1571	HWU	C4'-C3'-C2'	-2.30	107.05	110.40
5	A	1581	BBK	O3-C3-C4	2.29	115.77	110.38
6	C	1569	HWU	C2B-C1B-N1	-2.27	106.93	113.25
6	B	1571	HWU	O2-C2-N3	-2.25	117.33	121.49
6	B	1571	HWU	C6-N1-C2	-2.25	118.26	121.00
6	B	1571	HWU	O4-C4-N3	2.23	122.51	119.27
6	E	1585	HWU	C1B-N1-C2	2.22	121.58	117.59
6	E	1585	HWU	O1'-PB-O1B	2.21	116.87	109.81
6	D	1571	HWU	O4'-C4'-C5'	2.20	113.67	108.90
6	B	1571	HWU	C6'-C5'-C4'	-2.20	105.08	114.44
6	A	1582	HWU	O7'-C7'-C8'	-2.17	118.19	122.05
6	D	1571	HWU	O2B-PB-O1B	2.17	122.53	112.44
6	D	1571	HWU	C5-C4-N3	2.16	117.83	114.80
6	C	1569	HWU	O7'-C7'-C8'	-2.15	118.22	122.05
5	B	1580	BBK	C3-C2-N2	-2.14	106.67	110.62
6	E	1585	HWU	O3A-PA-O1A	-2.13	104.28	110.70
6	A	1582	HWU	O7'-C7'-N2'	2.13	125.74	121.98
6	A	1582	HWU	O5B-PA-O1A	-2.08	100.71	108.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1569	HWU	C2'-N2'-C7'	-2.07	118.26	123.11
6	F	1571	HWU	O4B-C1B-N1	2.06	113.02	108.36
6	F	1571	HWU	O3'-C3'-C2'	2.03	113.63	109.58
6	D	1571	HWU	O2-C2-N1	2.02	125.43	122.80
6	D	1571	HWU	O3'-C3'-C4'	-2.01	105.64	110.38
6	E	1585	HWU	C4'-C3'-C2'	-2.01	107.47	110.40
5	D	1572	BBK	O3-C3-C4	2.00	115.10	110.38

There are no chirality outliers.

All (80) 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
5	B	1580	BBK	C1-C2-N2-C7
5	B	1580	BBK	O7-C7-N2-C2
5	B	1580	BBK	C8-C7-N2-C2
5	D	1572	BBK	C4-C5-C6-O6
5	D	1572	BBK	S5-C5-C6-O6
5	E	1584	BBK	O7-C7-N2-C2
5	E	1584	BBK	C8-C7-N2-C2
6	B	1571	HWU	C5B-O5B-PA-O1A
6	B	1571	HWU	C5B-O5B-PA-O3A
6	C	1569	HWU	C1'-O1'-PB-O3A
6	C	1569	HWU	C4'-C5'-C6'-O6'
6	C	1569	HWU	S5'-C5'-C6'-O6'
6	F	1571	HWU	C5B-O5B-PA-O2A
6	F	1571	HWU	C5B-O5B-PA-O3A
6	D	1571	HWU	C3B-C4B-C5B-O5B
6	D	1571	HWU	O4B-C4B-C5B-O5B
4	B	1578	EDO	O1-C1-C2-O2
4	E	1575	EDO	O1-C1-C2-O2
4	A	1575	EDO	O1-C1-C2-O2
4	E	1574	EDO	O1-C1-C2-O2
4	E	1576	EDO	O1-C1-C2-O2
4	E	1577	EDO	O1-C1-C2-O2
6	F	1571	HWU	C3B-C4B-C5B-O5B
4	A	1577	EDO	O1-C1-C2-O2
4	A	1580	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	1573	EDO	O1-C1-C2-O2
5	E	1584	BBK	C1-C2-N2-C7
5	B	1580	BBK	C4-C5-C6-O6
6	C	1569	HWU	C1'-O1'-PB-O1B
4	A	1573	EDO	O1-C1-C2-O2
4	B	1576	EDO	O1-C1-C2-O2
4	D	1577	EDO	O1-C1-C2-O2
6	B	1571	HWU	PB-O3A-PA-O2A
4	B	1573	EDO	O1-C1-C2-O2
6	B	1571	HWU	C5B-O5B-PA-O2A
6	D	1571	HWU	C5B-O5B-PA-O2A
6	A	1582	HWU	PB-O3A-PA-O2A
6	D	1571	HWU	PA-O3A-PB-O2B
6	E	1585	HWU	PB-O3A-PA-O2A
6	E	1585	HWU	PA-O3A-PB-O2B
4	B	1575	EDO	O1-C1-C2-O2
4	D	1576	EDO	O1-C1-C2-O2
6	D	1571	HWU	C4B-C5B-O5B-PA
4	E	1579	EDO	O1-C1-C2-O2
4	E	1583	EDO	O1-C1-C2-O2
6	B	1571	HWU	PB-O3A-PA-O1A
6	C	1569	HWU	PB-O3A-PA-O2A
6	D	1571	HWU	PB-O3A-PA-O1A
4	A	1572	EDO	O1-C1-C2-O2
4	A	1576	EDO	O1-C1-C2-O2
4	B	1577	EDO	O1-C1-C2-O2
4	E	1572	EDO	O1-C1-C2-O2
4	E	1582	EDO	O1-C1-C2-O2
6	E	1585	HWU	C4B-C5B-O5B-PA
6	F	1571	HWU	C4B-C5B-O5B-PA
6	E	1585	HWU	C1'-O1'-PB-O1B
6	E	1585	HWU	C4'-C5'-C6'-O6'
6	A	1582	HWU	C4B-C5B-O5B-PA
6	F	1571	HWU	O4B-C4B-C5B-O5B
5	E	1584	BBK	C3-C2-N2-C7
4	A	1571	EDO	O1-C1-C2-O2
4	B	1574	EDO	O1-C1-C2-O2
4	D	1575	EDO	O1-C1-C2-O2
4	E	1570	EDO	O1-C1-C2-O2
6	A	1582	HWU	PB-O3A-PA-O1A
6	A	1582	HWU	PA-O3A-PB-O1B
6	A	1582	HWU	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	1571	HWU	PB-O3A-PA-O2A
6	E	1585	HWU	PB-O3A-PA-O1A
6	F	1571	HWU	PA-O3A-PB-O2B
4	B	1572	EDO	O1-C1-C2-O2
4	A	1574	EDO	O1-C1-C2-O2
6	C	1569	HWU	PB-O3A-PA-O1A
6	E	1585	HWU	PA-O3A-PB-O1B
6	B	1571	HWU	O4B-C4B-C5B-O5B

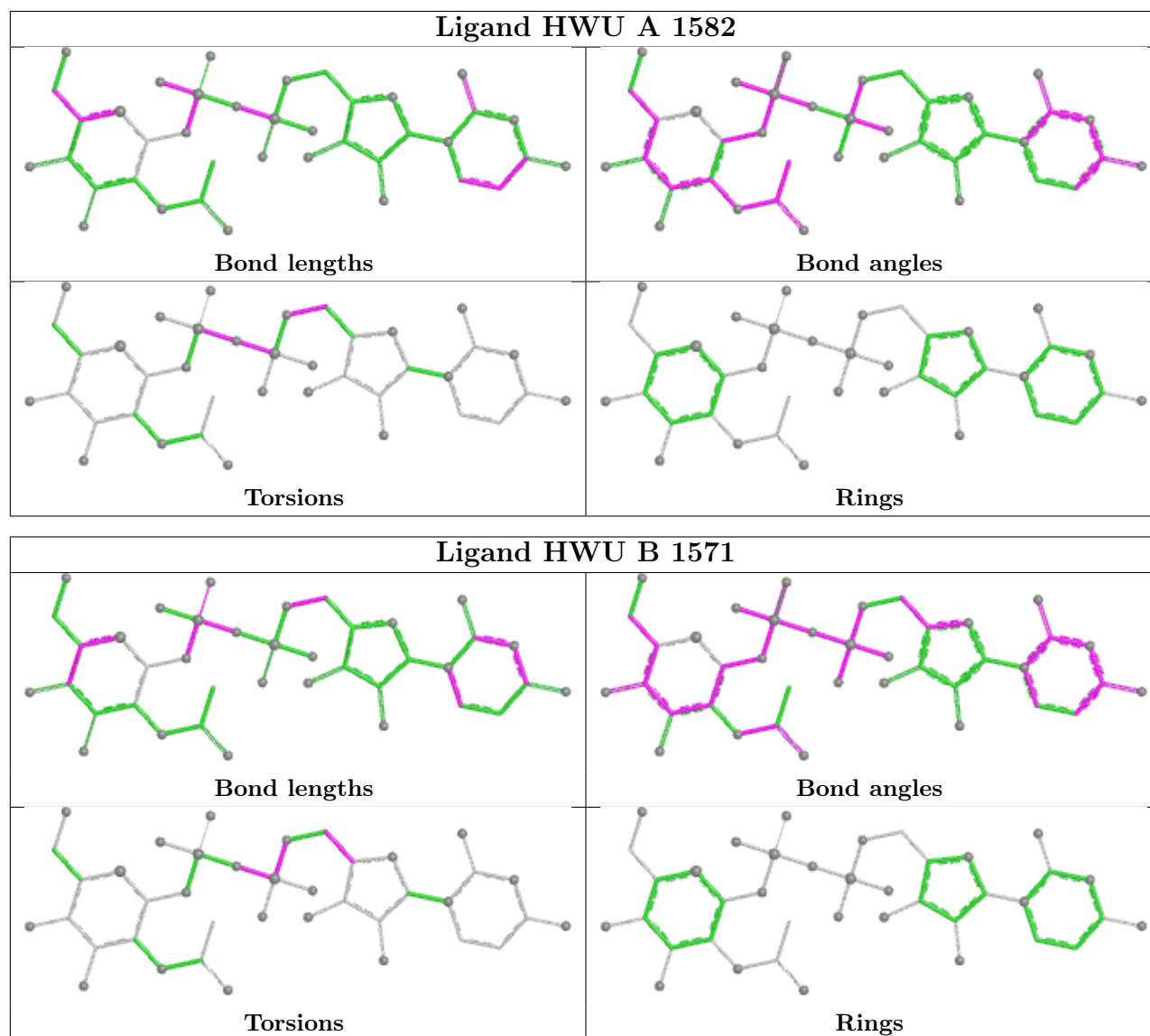
There are no ring outliers.

25 monomers are involved in 71 short contacts:

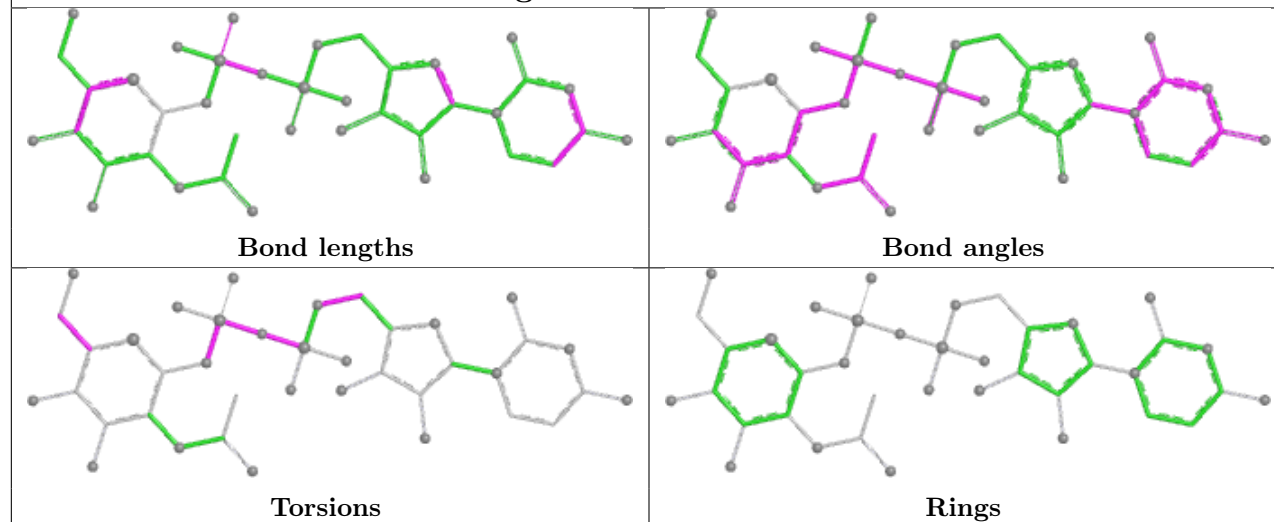
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1576	EDO	4	0
4	A	1572	EDO	4	0
4	B	1572	EDO	1	0
4	E	1570	EDO	1	0
5	E	1584	BBK	5	0
4	A	1579	EDO	1	0
4	B	1577	EDO	1	0
5	A	1581	BBK	3	0
5	B	1580	BBK	4	0
6	B	1571	HWU	2	0
6	E	1585	HWU	2	0
4	A	1580	EDO	2	0
6	C	1569	HWU	10	0
4	D	1573	EDO	1	0
4	A	1578	EDO	1	0
4	E	1572	EDO	8	0
6	F	1571	HWU	2	0
4	E	1579	EDO	2	0
4	E	1582	EDO	2	0
4	B	1573	EDO	4	0
4	E	1573	EDO	1	0
5	D	1572	BBK	4	0
4	A	1575	EDO	1	0
6	D	1571	HWU	4	0
4	E	1580	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

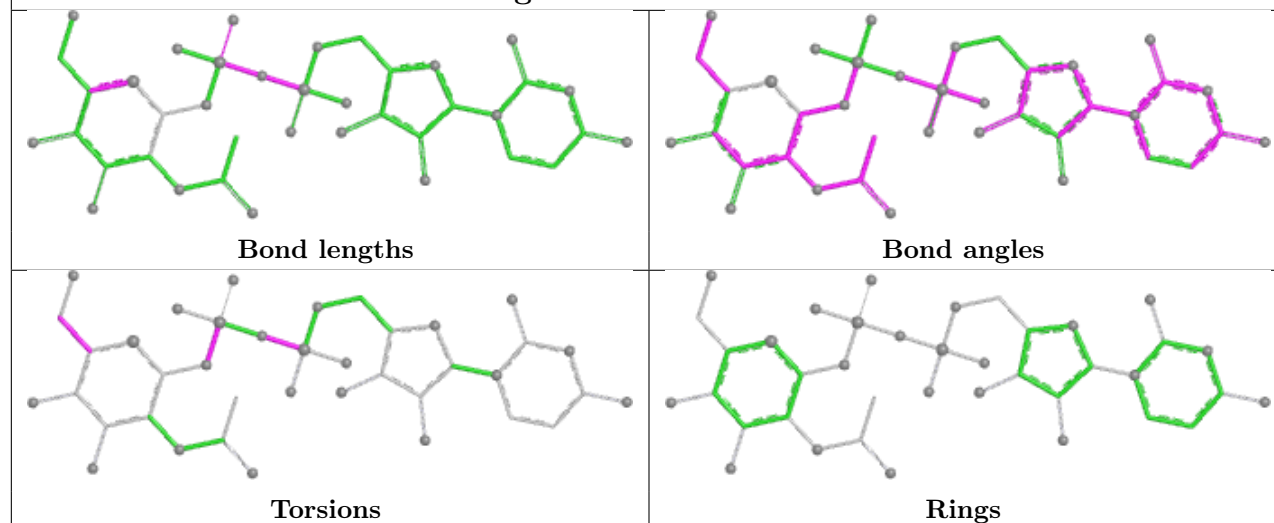
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



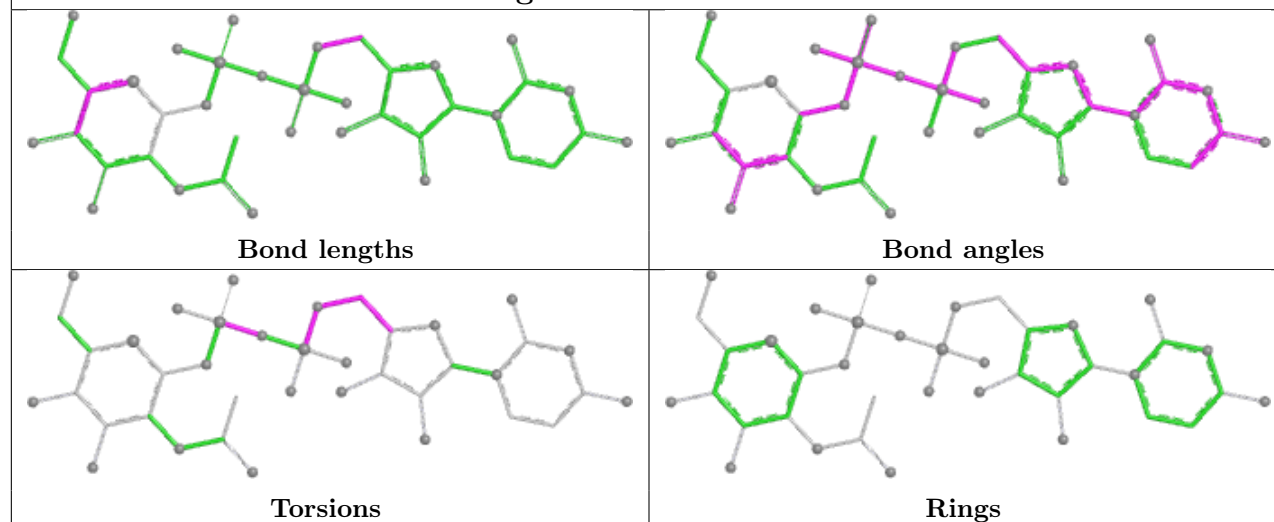
Ligand HWU E 1585

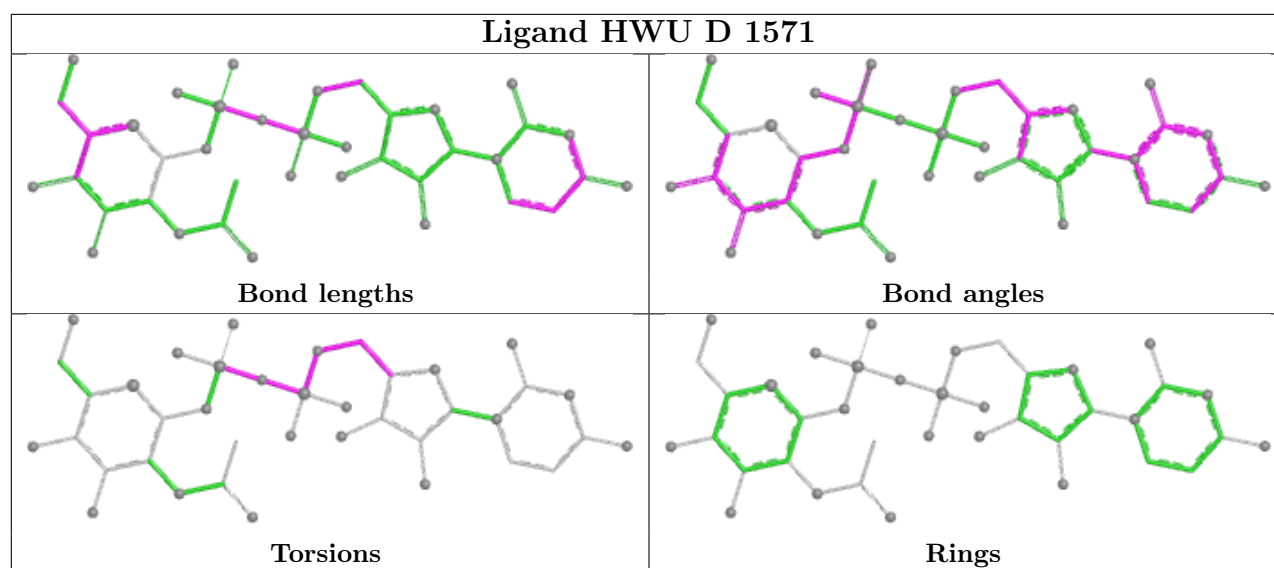


Ligand HWU C 1569



Ligand HWU F 1571





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	495/571 (86%)	-0.16	7 (1%) 73 71	22, 42, 69, 130	6 (1%)
1	B	495/571 (86%)	-0.26	6 (1%) 76 74	23, 40, 66, 106	5 (1%)
1	C	476/571 (83%)	1.66	163 (34%) 1 0	42, 91, 135, 168	5 (1%)
1	D	495/571 (86%)	-0.15	6 (1%) 76 74	25, 41, 66, 142	5 (1%)
1	E	495/571 (86%)	-0.42	1 (0%) 91 90	23, 35, 58, 90	5 (1%)
1	F	491/571 (85%)	0.34	34 (6%) 23 20	28, 57, 111, 140	5 (1%)
2	X	6/6 (100%)	2.43	4 (66%) 0 0	40, 73, 84, 87	0
2	Y	6/6 (100%)	2.23	3 (50%) 0 0	42, 71, 77, 83	0
All	All	2959/3438 (86%)	0.17	224 (7%) 20 17	22, 45, 109, 168	31 (1%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	331	TRP	7.3
1	C	330	VAL	6.1
1	C	534	VAL	5.7
1	C	516	ASP	5.3
1	F	516	ASP	5.1
1	A	516	ASP	5.0
1	C	471	TYR	5.0
1	C	204	LEU	4.6
1	C	89	GLY	4.5
1	C	437	LEU	4.5
1	C	417	LEU	4.4
1	E	516	ASP	4.3
1	C	144	PHE	4.3
1	C	407	PRO	4.2
2	X	6	THR	4.2
1	D	516	ASP	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	143	THR	4.0
1	C	366	PRO	4.0
1	C	559	LEU	4.0
1	C	99	TYR	4.0
1	C	400	VAL	3.9
1	B	131	TRP	3.9
1	C	497	LEU	3.9
1	F	555	CYS	3.8
1	C	181	PRO	3.8
1	C	463	PHE	3.8
2	Y	6	THR	3.8
1	F	515	GLU	3.7
2	Y	5	SER	3.7
1	B	516	ASP	3.7
1	C	147	GLU	3.7
1	F	569	LEU	3.7
1	C	91	MET	3.7
1	D	284	TYR	3.7
1	C	98	PRO	3.7
1	F	89	GLY	3.6
1	F	284	TYR	3.6
1	C	411	ILE	3.6
1	C	406	VAL	3.6
1	C	415	LEU	3.5
1	C	428	TRP	3.5
1	C	177	TYR	3.5
1	C	396	TYR	3.5
1	C	107	VAL	3.5
1	C	284	TYR	3.4
1	D	291	ARG	3.4
2	X	5	SER	3.4
1	C	395	PHE	3.4
1	C	421	LEU	3.3
1	F	559	LEU	3.3
1	C	150	SER	3.3
1	C	422	SER	3.3
1	C	388	TRP	3.3
1	C	476	ALA	3.3
1	F	556	GLY	3.3
1	B	133	VAL	3.3
1	C	558	ALA	3.2
1	C	515	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	423	CYS	3.2
1	C	456	CYS	3.2
1	C	145	HIS	3.1
1	C	470	VAL	3.1
1	C	384	ALA	3.1
1	C	554	VAL	3.1
1	C	531	LEU	3.1
1	C	101	ARG	3.1
1	C	513	CYS	3.1
1	C	468	VAL	3.0
1	A	291	ARG	3.0
1	C	146	ASN	3.0
1	C	380	ASN	3.0
1	C	430	LEU	3.0
1	F	554	VAL	2.9
1	C	151	ALA	2.9
1	C	439	VAL	2.9
1	C	533	HIS	2.9
1	C	340	PHE	2.9
1	C	567	LEU	2.9
1	C	102	ASN	2.9
1	C	178	SER	2.9
1	C	387	VAL	2.9
1	C	225	SER	2.8
1	C	365	HIS	2.8
1	C	76	VAL	2.8
1	C	78	TRP	2.8
1	F	129	LYS	2.8
1	C	77	ARG	2.8
1	C	346	GLY	2.7
1	D	287	PRO	2.7
1	C	328	MET	2.7
1	F	552	VAL	2.7
1	C	79	PRO	2.7
1	C	321	LEU	2.7
1	C	503	ALA	2.7
1	F	503	ALA	2.7
1	C	344	GLN	2.7
1	F	537	ASN	2.7
1	C	440	PRO	2.7
1	C	473	CYS	2.7
1	C	495	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	397	TYR	2.7
1	C	512	GLY	2.7
1	C	557	PRO	2.7
1	C	514	ARG	2.6
1	C	207	SER	2.6
1	C	457	LEU	2.6
1	F	531	LEU	2.6
1	C	325	ASP	2.6
1	C	403	ALA	2.6
1	C	327	MET	2.6
1	C	544	THR	2.6
1	C	401	PRO	2.6
1	C	413	SER	2.6
1	C	382	ARG	2.6
1	C	104	PHE	2.6
1	C	361	PHE	2.6
1	C	392	TYR	2.6
1	C	75	LYS	2.6
1	C	427	LYS	2.6
1	C	97	ASP	2.5
1	C	90	THR	2.5
1	C	477	GLY	2.5
1	C	117	ALA	2.5
1	C	555	CYS	2.5
1	C	536	SER	2.5
1	C	445	ILE	2.5
1	C	525	ILE	2.5
1	C	493	MET	2.5
1	C	149	ARG	2.5
1	C	278	LEU	2.5
1	C	179	ASN	2.5
1	C	474	HIS	2.5
2	X	7	CYS	2.4
1	A	471	TYR	2.4
1	F	486	LYS	2.4
1	C	426	PHE	2.4
1	C	499	VAL	2.4
1	F	525	ILE	2.4
1	C	424	LYS	2.4
1	C	324	TYR	2.4
1	C	492	HIS	2.4
1	C	502	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	385	ALA	2.4
1	C	381	THR	2.4
1	C	488	LYS	2.4
1	F	471	TYR	2.4
1	C	87	VAL	2.4
1	C	279	VAL	2.4
1	C	336	LEU	2.4
1	F	450	LEU	2.4
1	C	563	TRP	2.4
1	C	100	ALA	2.3
1	C	496	CYS	2.3
1	C	442	HIS	2.3
1	C	399	ALA	2.3
1	C	467	VAL	2.3
1	F	504	PRO	2.3
1	C	398	ALA	2.3
1	F	558	ALA	2.3
1	C	157	VAL	2.3
1	C	345	CYS	2.3
1	C	175	ASP	2.3
1	C	478	GLY	2.3
1	C	549	GLY	2.3
1	B	471	TYR	2.3
1	C	86	TYR	2.3
1	A	316	PHE	2.2
1	C	174	VAL	2.3
1	C	205	MET	2.2
1	C	469	GLY	2.2
1	C	532	ARG	2.2
1	F	464	ALA	2.2
2	Y	9	ALA	2.2
1	C	276	TRP	2.2
1	C	111	LYS	2.2
1	C	195	VAL	2.2
1	C	224	ASP	2.2
1	B	128	ARG	2.2
1	C	112	LEU	2.2
1	F	538	LEU	2.2
1	C	490	VAL	2.2
1	F	534	VAL	2.2
1	C	180	ASP	2.2
1	C	409	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	442	HIS	2.2
1	C	545	ALA	2.2
1	C	261	PHE	2.2
1	C	316	PHE	2.2
1	D	288	GLU	2.2
1	F	527	GLY	2.2
1	C	85	ALA	2.2
1	F	449	ALA	2.2
1	A	284	TYR	2.1
1	C	280	PHE	2.1
1	C	535	GLY	2.1
1	C	408	TYR	2.1
1	C	429	TYR	2.1
1	C	450	LEU	2.1
1	C	510	LEU	2.1
1	C	500	VAL	2.1
1	F	463	PHE	2.1
1	A	477	GLY	2.1
1	F	126	CYS	2.1
1	C	103	LYS	2.1
1	C	223	LEU	2.1
1	C	460	LEU	2.1
1	C	508	ILE	2.1
1	F	567	LEU	2.1
1	F	127	GLN	2.1
1	C	506	SER	2.1
1	C	446	ALA	2.1
1	C	245	ARG	2.1
1	F	547	SER	2.0
1	C	268	ALA	2.0
1	B	127	GLN	2.0
1	D	199	ASP	2.0
1	C	363	LYS	2.0
1	F	454	THR	2.0
1	C	464	ALA	2.0
1	F	294	GLN	2.0
1	C	538	LEU	2.0
1	A	287	PRO	2.0
1	F	557	PRO	2.0
2	X	8	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
4	EDO	D	1575	4/4	0.71	0.18	60,63,68,70	0
5	BBK	E	1584	15/15	0.72	0.36	96,105,117,124	0
4	EDO	E	1578	4/4	0.73	0.17	64,64,66,82	0
5	BBK	A	1581	15/15	0.73	0.23	69,86,120,142	0
4	EDO	E	1574	4/4	0.73	0.18	62,68,68,75	0
5	BBK	D	1572	15/15	0.74	0.31	96,105,117,124	0
4	EDO	D	1577	4/4	0.75	0.13	67,68,69,69	0
5	BBK	B	1580	15/15	0.75	0.29	69,86,120,142	0
4	EDO	B	1576	4/4	0.78	0.15	65,69,73,76	0
4	EDO	E	1570	4/4	0.78	0.19	44,48,59,61	0
4	EDO	E	1575	4/4	0.80	0.15	64,69,69,76	0
4	EDO	E	1580	4/4	0.80	0.15	59,70,71,76	0
4	EDO	E	1576	4/4	0.80	0.14	68,68,69,69	0
4	EDO	E	1577	4/4	0.81	0.15	61,61,64,68	0
4	EDO	A	1577	4/4	0.83	0.15	62,68,71,76	0
6	HWU	C	1569	39/39	0.83	0.13	51,76,89,92	0
4	EDO	D	1574	4/4	0.85	0.11	49,50,52,58	0
4	EDO	A	1580	4/4	0.85	0.14	45,52,57,59	0
4	EDO	A	1574	4/4	0.85	0.12	51,52,54,57	0
4	EDO	A	1573	4/4	0.86	0.13	56,68,70,70	0
4	EDO	A	1579	4/4	0.86	0.12	51,52,54,64	0
4	EDO	E	1583	4/4	0.86	0.10	58,61,62,68	0
4	EDO	A	1572	4/4	0.86	0.13	57,66,67,69	0
4	EDO	A	1576	4/4	0.87	0.13	57,62,66,75	0
4	EDO	B	1578	4/4	0.87	0.10	55,58,62,69	0
4	EDO	E	1581	4/4	0.87	0.14	53,56,60,68	0
4	EDO	B	1573	4/4	0.88	0.19	40,41,42,48	0

Continued on next page...

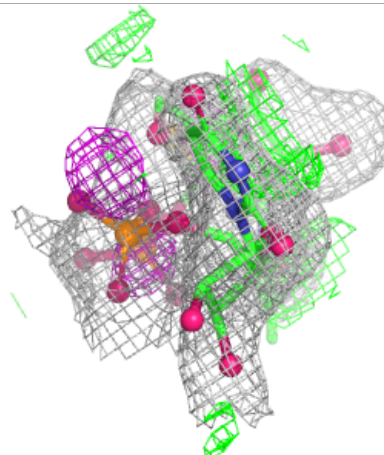
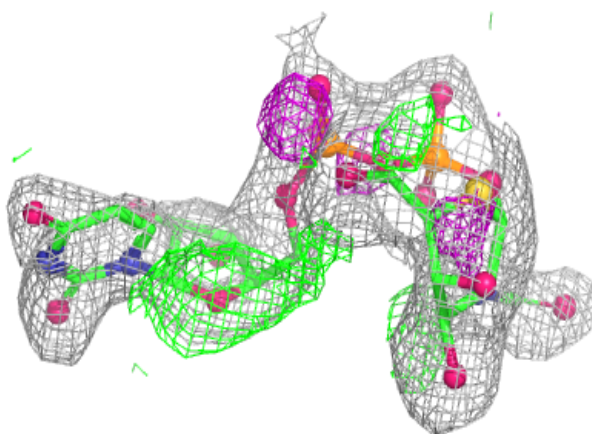
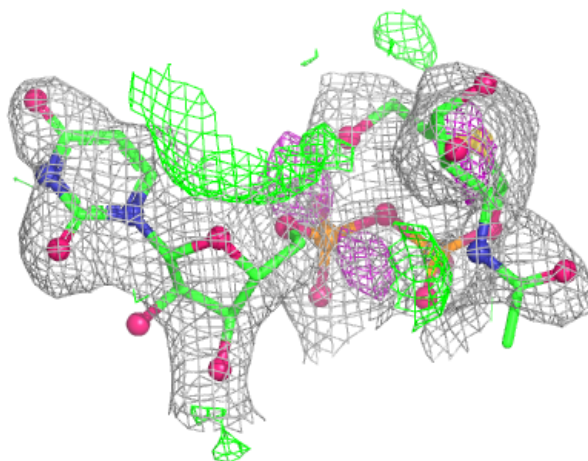
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	1571	4/4	0.88	0.15	43,46,46,52	0
4	EDO	E	1573	4/4	0.88	0.12	49,58,60,71	0
4	EDO	B	1577	4/4	0.88	0.12	42,43,48,57	0
4	EDO	A	1578	4/4	0.89	0.23	38,45,48,63	0
4	EDO	D	1573	4/4	0.89	0.10	38,40,40,45	0
4	EDO	B	1579	4/4	0.91	0.09	41,48,56,56	0
4	EDO	D	1576	4/4	0.92	0.14	39,43,45,49	0
6	HWU	B	1571	39/39	0.93	0.08	30,36,44,49	0
6	HWU	D	1571	39/39	0.93	0.08	24,35,45,46	0
6	HWU	F	1571	39/39	0.93	0.08	38,44,55,60	0
4	EDO	A	1575	4/4	0.94	0.08	53,55,57,59	0
4	EDO	B	1575	4/4	0.94	0.07	66,68,69,69	0
4	EDO	E	1582	4/4	0.94	0.07	47,48,51,56	0
6	HWU	A	1582	39/39	0.95	0.07	26,34,45,48	0
4	EDO	E	1571	4/4	0.95	0.09	38,46,47,50	0
4	EDO	E	1572	4/4	0.95	0.20	38,45,48,51	0
4	EDO	B	1574	4/4	0.95	0.07	40,40,42,45	0
6	HWU	E	1585	39/39	0.95	0.08	26,36,54,58	0
4	EDO	B	1572	4/4	0.95	0.06	34,35,35,42	0
4	EDO	E	1579	4/4	0.96	0.07	43,44,52,53	0
3	MN	C	1570	1/1	0.98	0.06	59,59,59,59	0
3	MN	B	1570	1/1	0.99	0.02	33,33,33,33	0
3	MN	F	1570	1/1	1.00	0.03	42,42,42,42	0
3	MN	A	1570	1/1	1.00	0.01	27,27,27,27	0
3	MN	D	1570	1/1	1.00	0.02	29,29,29,29	0
3	MN	E	1586	1/1	1.00	0.01	26,26,26,26	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.

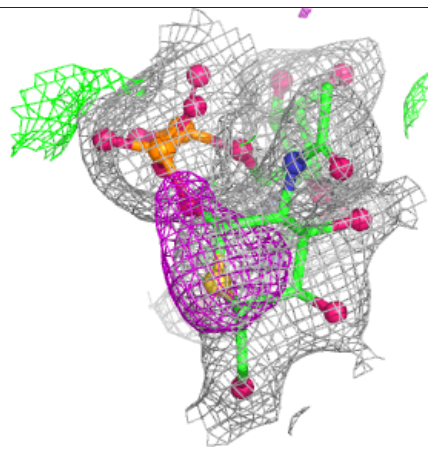
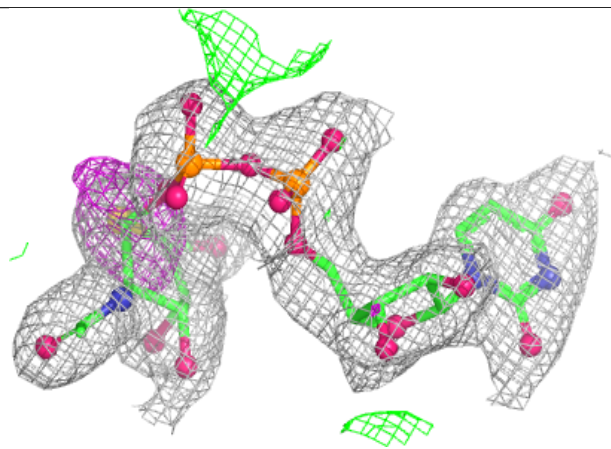
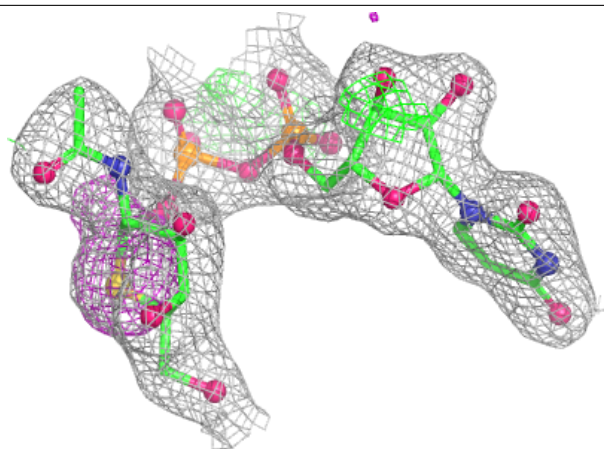
Electron density around HWU C 1569:

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



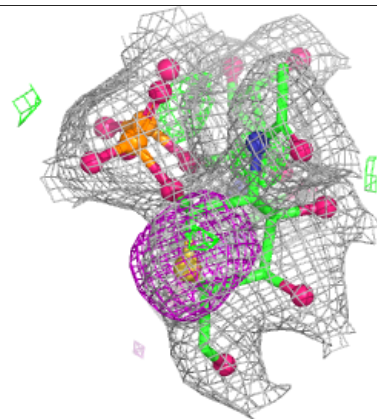
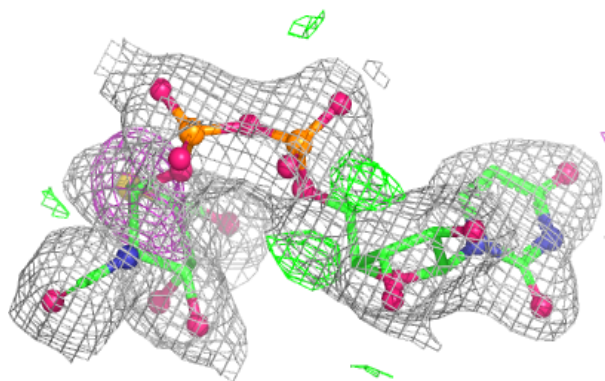
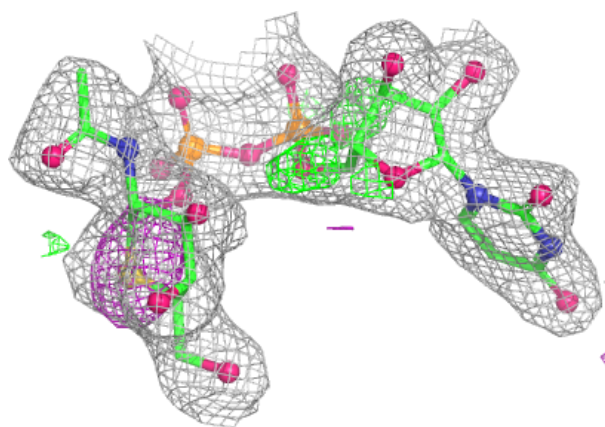
Electron density around HWU B 1571:

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



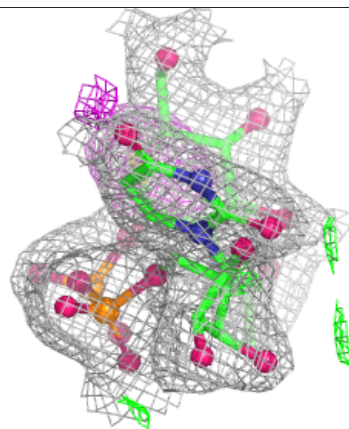
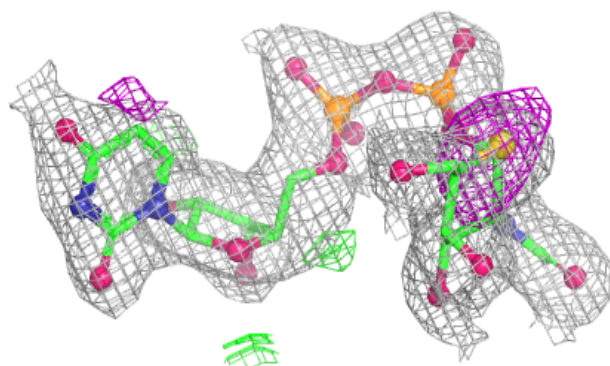
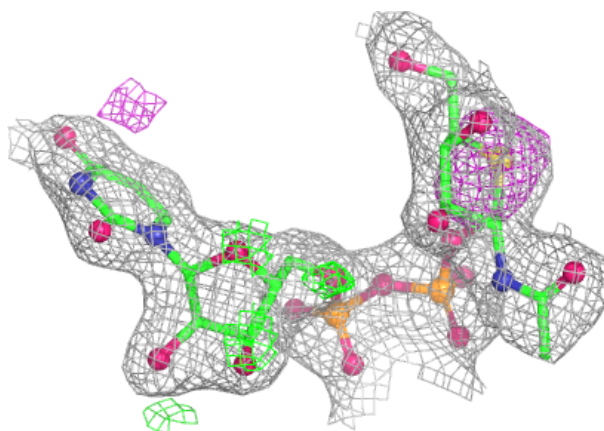
Electron density around HWU D 1571:

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



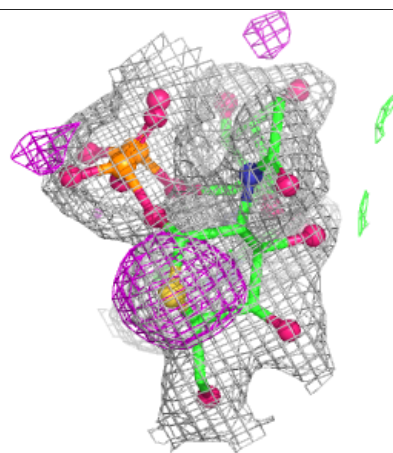
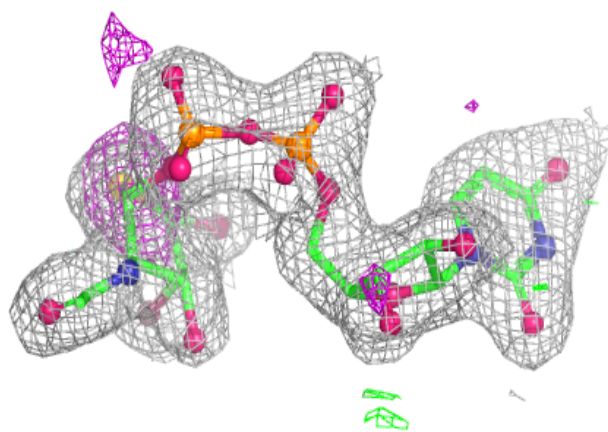
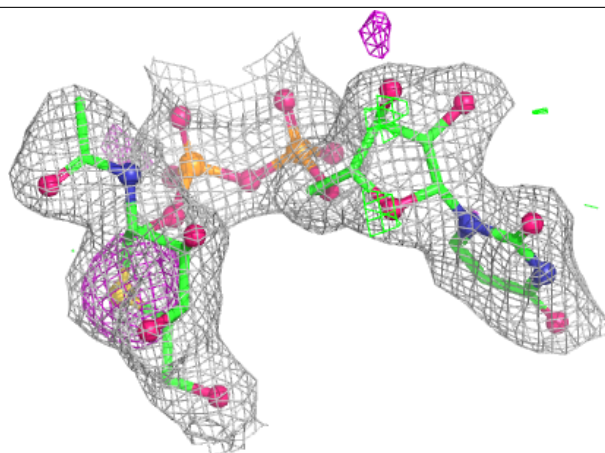
Electron density around HWU F 1571:

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



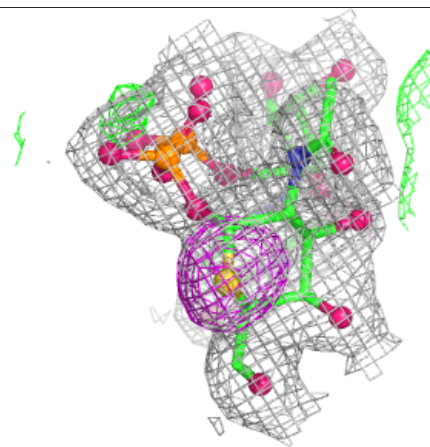
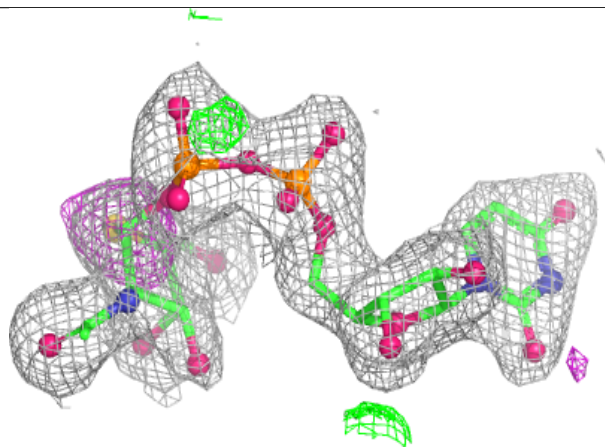
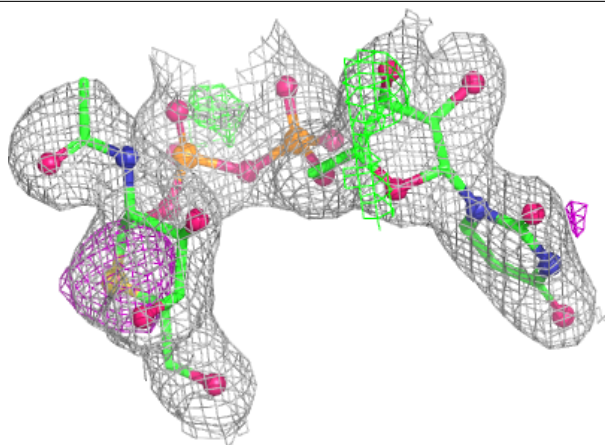
Electron density around HWU A 1582:

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



Electron density around HWU E 1585:

$2mF_o-DF_c$ (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.