Full wwPDB X-ray Structure Validation Report (i)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

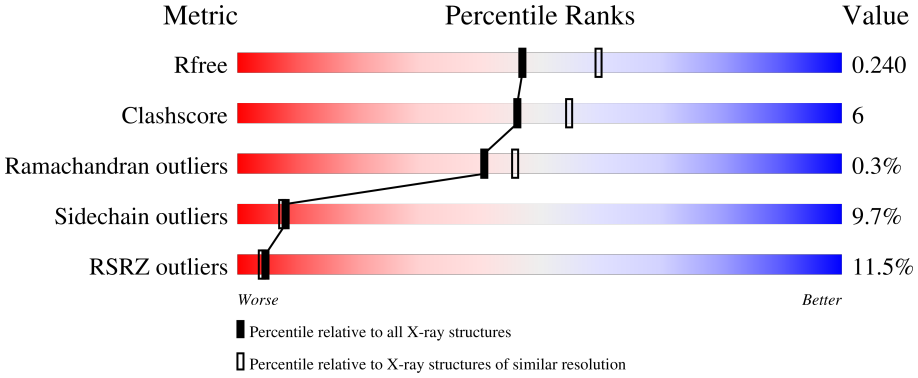
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	571	3% 71% 13% • 13%
1	B	571	2% 73% 12% • 13%
1	C	571	33% 64% 15% • • 17%
1	D	571	4% 70% 14% • 13%
1	E	571	2% 71% 12% • 13%

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Mol	Chain	Length	Quality of chain
1	F	571	15% 71% 13% • 14%
2	X	6	33% 33% 67%
2	Y	6	67% 33% 50% 17%

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	3975	2502	722	727	24	20	1	0
1	B	495	3967	2497	719	727	24	20	0	0
1	C	476	3826	2407	693	702	24	20	0	0
1	D	495	3967	2497	719	727	24	20	0	0
1	E	495	3967	2497	719	727	24	20	0	0
1	F	491	3926	2470	710	722	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

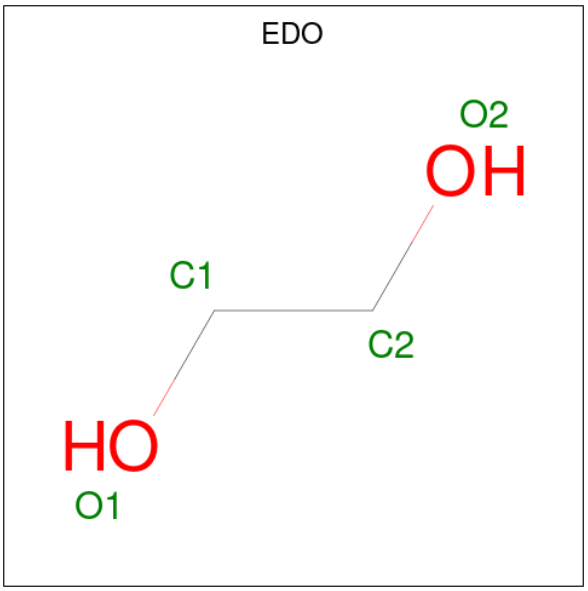
- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	X	6	32	18	6	7	1	0	0	1
2	Y	6	32	18	6	7	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: $C_2H_6O_2$).



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
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	D	1	4	2	2		0	0
			Total	C	O			
4	D	1	4	2	2		0	0
			Total	C	O			
4	D	1	4	2	2		0	0
			Total	C	O			
4	D	1	4	2	2		0	0
			Total	C	O			
4	D	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0

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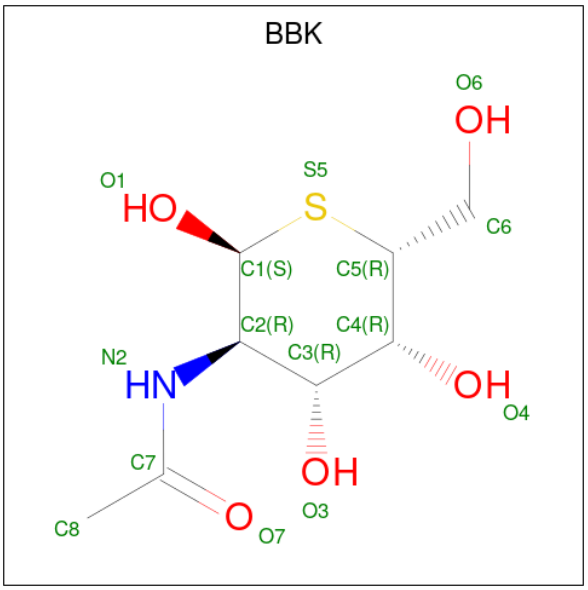
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2	2		0	0
			Total	C	O			
4	E	1	4	2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

- Molecule 5 is 2-acetamido-2-deoxy-5-thio-alpha-D-galactopyranose (three-letter code: BBK) (formula: $C_8H_{15}NO_5S$).



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

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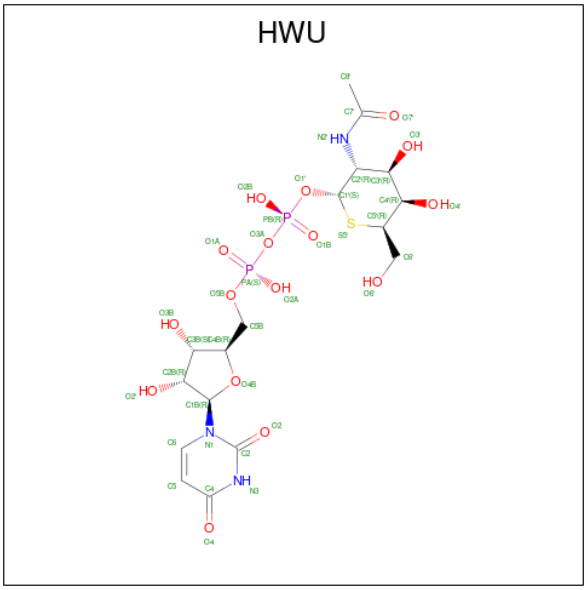
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	15	8	1	5	1	0	0
			Total	C	N	O	S		
5	D	1	15	8	1	5	1	0	0
			Total	C	N	O	S		
5	E	1	15	8	1	5	1	0	0

- 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: $C_{17}H_{27}N_3O_{16}P_2S$).



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

- Molecule 7 is water.

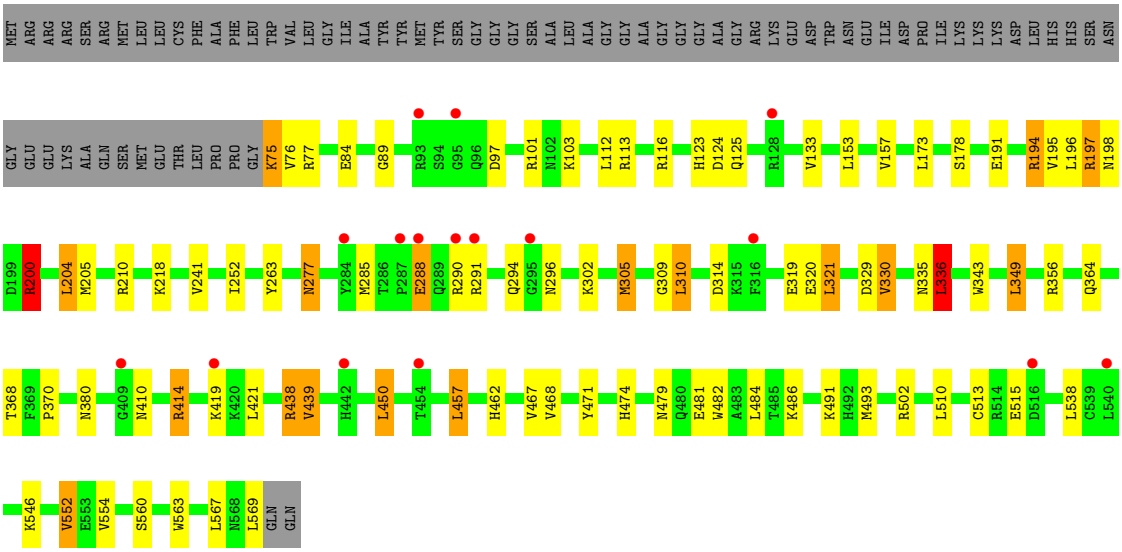
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	144	144	144	0	0
			Total	O		
7	B	125	125	125	0	0
			Total	O		
7	C	13	13	13	0	0
			Total	O		
7	D	122	122	122	0	0
			Total	O		
7	E	168	168	168	0	0
			Total	O		
7	F	61	61	61	0	0

3 Residue-property plots (i)

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

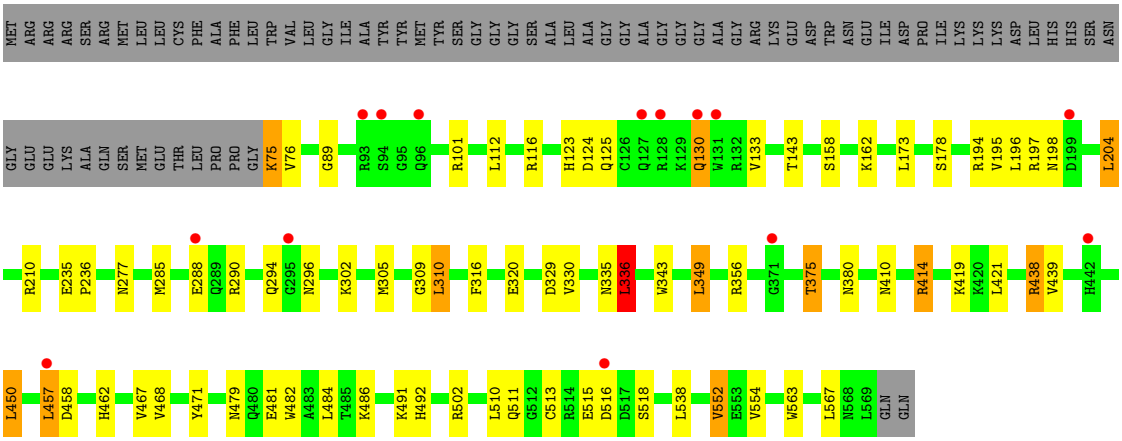
• Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain A:



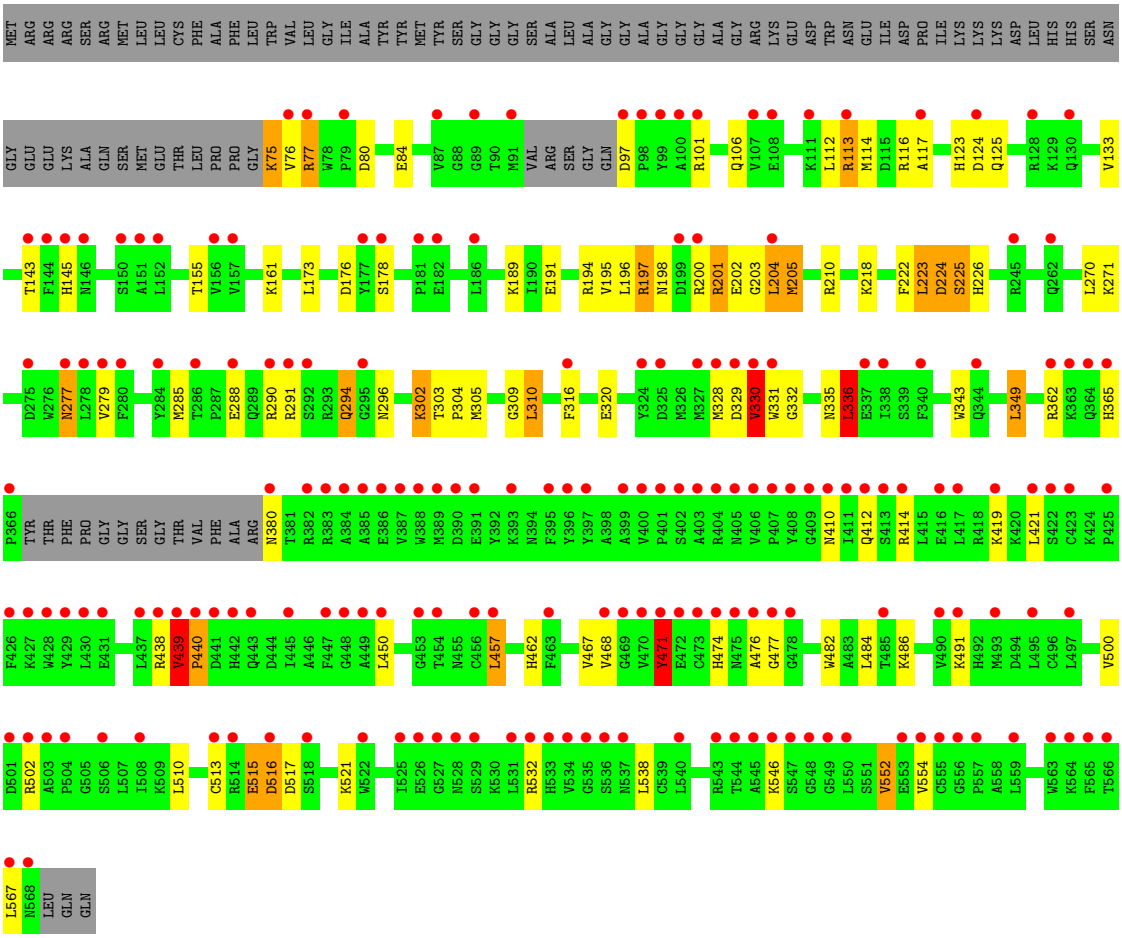
• Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain B:



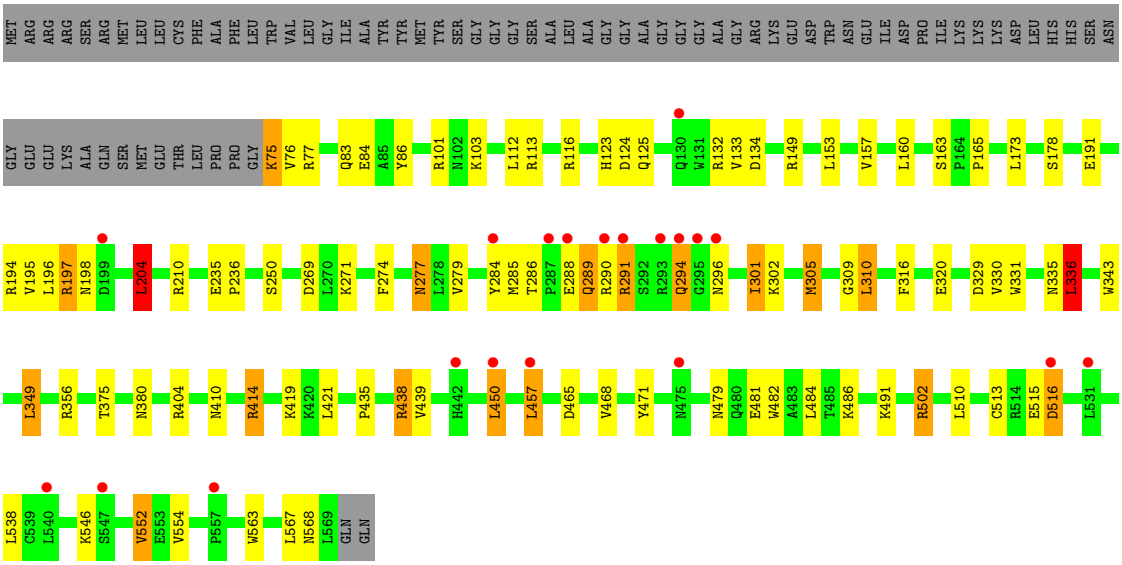
• Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain C:



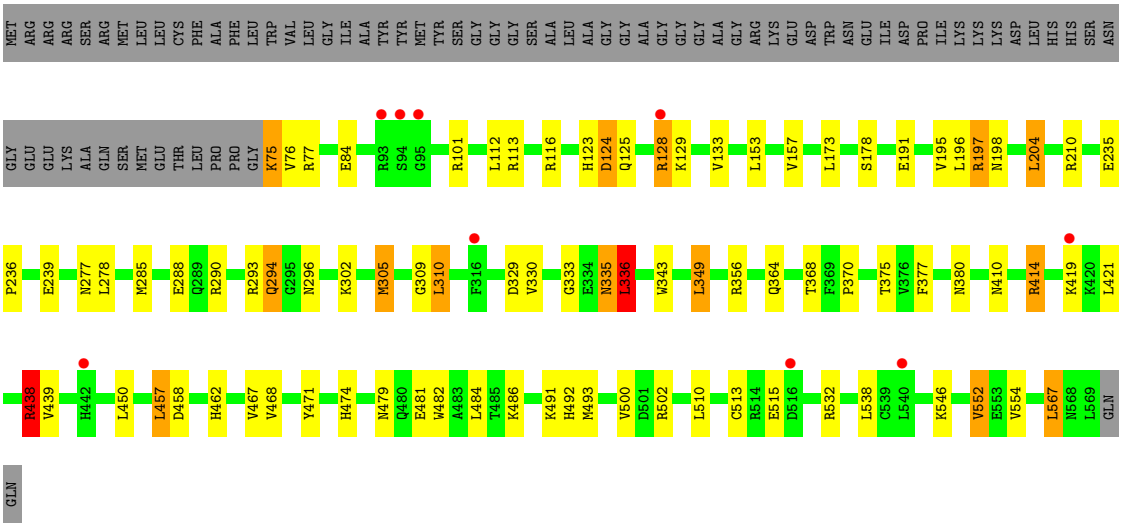
- Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain D:



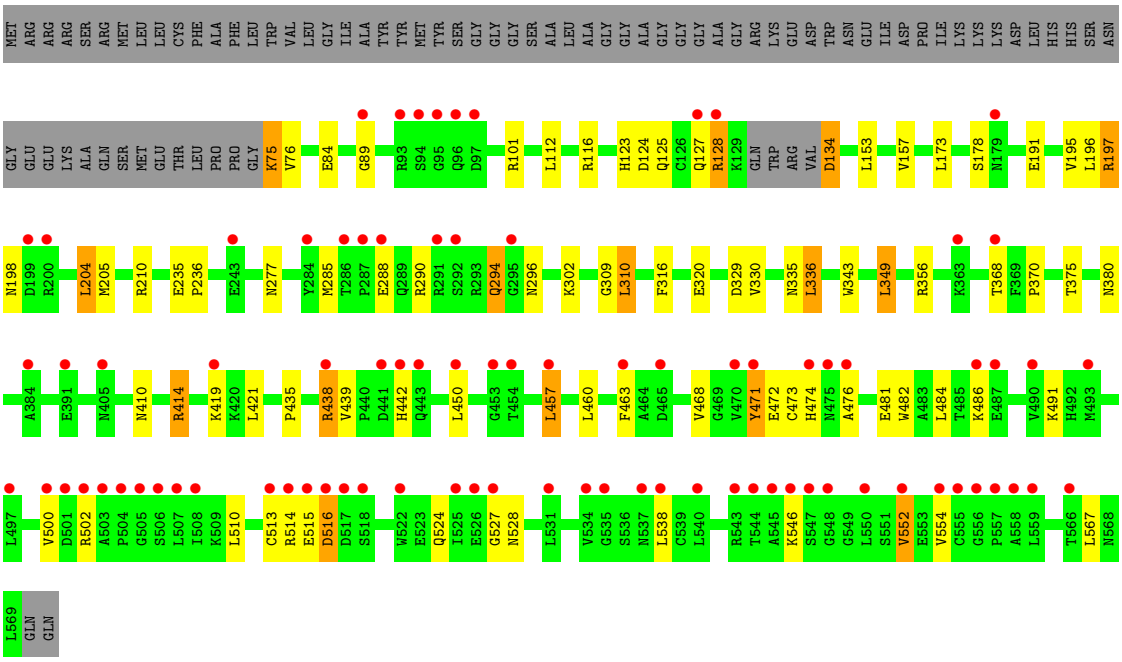
- Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain E:



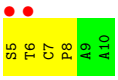
- Molecule 1: POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE 2

Chain F:



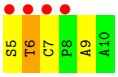
- Molecule 2: PEPTIDE

Chain X:



- Molecule 2: PEPTIDE

Chain Y:


S5
T6
C7
P8
A9
A10

4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [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	4936 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)	0.35 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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

All (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
1	F	84	GLU	CB-CG	-23.05	1.08	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	486	LYS	CB-CG	-20.62	0.96	1.52
1	C	224	ASP	C-N	-20.14	0.87	1.34
1	A	84	GLU	CB-CG	-16.34	1.21	1.52
1	A	75	LYS	CB-CG	-14.91	1.12	1.52
1	C	225	SER	C-N	-14.91	0.99	1.34
1	E	75	LYS	CB-CG	-14.21	1.14	1.52
1	C	222	PHE	C-N	12.92	1.63	1.34
1	B	75	LYS	CB-CG	-12.78	1.18	1.52
1	A	486	LYS	CB-CG	-10.92	1.23	1.52
1	C	486	LYS	CB-CG	-10.47	1.24	1.52
1	B	515	GLU	CB-CG	-9.63	1.33	1.52
1	C	223	LEU	C-N	7.13	1.50	1.34
1	C	75	LYS	CB-CG	-6.90	1.33	1.52
2	Y	9	ALA	C-O	6.73	1.36	1.23
1	B	294	GLN	CB-CG	6.40	1.69	1.52
1	A	294	GLN	CB-CG	5.63	1.67	1.52
1	E	294	GLN	CB-CG	5.50	1.67	1.52
1	D	250	SER	CB-OG	-5.18	1.35	1.42

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	E	486	LYS	CB-CG-CD	-12.84	78.21	111.60
1	C	75	LYS	CA-CB-CG	12.77	141.48	113.40
1	B	486	LYS	CB-CG-CD	-11.69	81.22	111.60
1	F	84	GLU	CA-CB-CG	11.10	137.83	113.40
1	A	200	ARG	NE-CZ-NH1	10.95	125.77	120.30
1	D	75	LYS	CA-CB-CG	10.92	137.41	113.40
1	C	225	SER	O-C-N	-10.49	105.92	122.70
1	D	194	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	E	84	GLU	CA-CB-CG	10.22	135.89	113.40
1	D	204	LEU	CA-CB-CG	9.38	136.88	115.30
1	C	225	SER	CA-C-N	9.35	137.77	117.20
1	B	486	LYS	CA-CB-CG	-9.22	93.12	113.40
1	C	567	LEU	CA-CB-CG	9.10	136.22	115.30
1	E	486	LYS	CA-CB-CG	-9.09	93.40	113.40
1	A	486	LYS	CB-CG-CD	-9.09	87.98	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	294	GLN	CB-CG-CD	8.58	133.90	111.60
1	A	84	GLU	CA-CB-CG	8.46	132.02	113.40
1	C	223	LEU	O-C-N	-8.39	109.28	122.70
1	B	204	LEU	CA-CB-CG	8.37	134.54	115.30
1	C	471	TYR	CA-CB-CG	8.19	128.96	113.40
1	C	84	GLU	CA-CB-CG	8.12	131.27	113.40
1	E	204	LEU	CA-CB-CG	8.07	133.86	115.30
1	D	414	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	294	GLN	CA-CB-CG	-7.93	95.96	113.40
1	C	225	SER	N-CA-C	-7.82	89.90	111.00
1	A	321	LEU	N-CA-C	-7.78	90.00	111.00
1	E	128	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	225	SER	C-N-CA	7.48	140.40	121.70
1	B	414	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	D	404	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	414	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	E	129	LYS	CD-CE-NZ	7.32	128.55	111.70
1	D	414	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	E	414	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	D	294	GLN	CB-CG-CD	6.98	129.75	111.60
1	E	532	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	113	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	F	527	GLY	N-CA-C	-6.88	95.89	113.10
1	A	197	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	414	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	F	414	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	D	567	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	200	ARG	CD-NE-CZ	6.52	132.73	123.60
1	F	294	GLN	CA-CB-CG	-6.50	99.10	113.40
1	C	439	VAL	CB-CA-C	6.48	123.71	111.40
1	B	414	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	E	294	GLN	CB-CG-CD	6.41	128.28	111.60
1	F	356	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	F	414	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	302	LYS	N-CA-C	6.33	128.09	111.00
1	C	223	LEU	C-N-CA	6.30	137.46	121.70
1	A	197	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	194[A]	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	194[B]	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	356	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	194	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	314	ASP	CB-CG-OD2	-6.05	112.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	197	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	330	VAL	CA-CB-CG2	-6.01	101.89	110.90
1	A	486	LYS	CA-CB-CG	-5.99	100.22	113.40
1	E	336	LEU	CA-CB-CG	5.97	129.03	115.30
1	D	103	LYS	CD-CE-NZ	5.91	125.30	111.70
1	E	414	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	E	197	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	336	LEU	CA-CB-CG	5.85	128.75	115.30
1	F	336	LEU	CA-CB-CG	5.84	128.74	115.30
1	E	532	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	F	356	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	C	294	GLN	CA-CB-CG	-5.75	100.75	113.40
1	A	97	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	305	MET	CG-SD-CE	-5.68	91.11	100.20
1	F	567	LEU	CA-CB-CG	5.62	128.23	115.30
1	C	336	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	336	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	321	LEU	CA-C-N	5.57	127.33	116.20
1	E	356	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	414	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	D	404	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	75	LYS	CA-CB-CG	5.50	125.49	113.40
1	D	197	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	336	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	194[A]	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	194[B]	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	77	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	362	ARG	CG-CD-NE	5.38	123.11	111.80
1	E	84	GLU	CB-CG-CD	5.38	128.74	114.20
1	C	97	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	197	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	197	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	F	486	LYS	CA-CB-CG	5.28	125.02	113.40
1	C	532	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	E	567	LEU	CA-CB-CG	5.25	127.38	115.30
1	E	438	ARG	CB-CG-CD	5.25	125.25	111.60
1	E	305	MET	CG-SD-CE	-5.24	91.81	100.20
1	C	477	GLY	N-CA-C	5.23	126.18	113.10
1	D	305	MET	CG-SD-CE	-5.22	91.85	100.20
1	C	218	LYS	CB-CA-C	-5.18	100.03	110.40
1	B	356	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	113	ARG	NE-CZ-NH1	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	194	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	356	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	569	LEU	CB-CG-CD2	5.09	119.66	111.00
1	C	194	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	218	LYS	CB-CA-C	-5.07	100.27	110.40
1	D	113	ARG	N-CA-CB	-5.03	101.54	110.60

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.

All (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
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:E:479:ASN:HB2	5:E:1584:BBK:H4	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:439:VAL:H	1:D:291:ARG:NH2	1.84	0.75
1:F:123:HIS:HD2	1:F:125:GLN:H	1.33	0.74
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
6:B:1571:HWU:H1'	2:X:6:THR:OG1	1.88	0.73
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:C	1:C:440:PRO:O	2.30	0.68
1:F:316:PHE:CE2	1:F:320:GLU:OE2	2.47	0.68
1:A:320:GLU:C	1:A:321:LEU:O	2.28	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:329:ASP:H	1:C:380:ASN:HD21	1.45	0.65
1:C:225:SER:O	1:C:226:HIS:CG	2.51	0.64
1:C:439:VAL:O	1:C:440:PRO:C	2.37	0.63
6:E:1585:HWU:H1'	2:Y:6:THR:HB	1.80	0.63
1:B:458:ASP:OD1	5:B:1580:BBK:O3	2.17	0.62
1:C:205:MET:HE3	1:C:328:MET:O	2.00	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: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:B:305:MET:HE1	1:B:336:LEU:CD2	2.32	0.60
1:D:305:MET:HE1	1:D:336:LEU:CD2	2.32	0.59
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:D:305:MET:HE1	1:D:336:LEU:HD23	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:MET:HE2	1:C:205:MET:H	1.68	0.57
1:B:305:MET:HE1	1:B:336:LEU:HD23	1.86	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:A:305:MET:HE1	1:A:336:LEU:CD2	2.36	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:C:305:MET:HE1	1:C:336:LEU:CD2	2.36	0.55
1:C:305:MET:HE1	1:C:336:LEU:HD23	1.88	0.55
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
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:305:MET:HE1	1:A:336:LEU:HD23	1.90	0.54
5:B:1580:BBK:H8A	1:E:474:HIS:HB2	1.89	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:C:329:ASP:O	1:C:330:VAL:C	2.46	0.51
1:E:364:GLN:HE21	4:E:1573:EDO:H22	1.75	0.51
1:F:127:GLN:C	1:F:128:ARG:HD3	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:414:ARG:CD	7:D:2082:HOH:O	2.57	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: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:A:305:MET:HE3	1:A:305:MET:HB2	1.61	0.48
1:A:305:MET:CE	1:A:336:LEU:HD23	2.43	0.48
1:D:305:MET:CE	1:D:336:LEU:HD23	2.44	0.48
1:C:305:MET:CE	1:C:336:LEU:HD23	2.43	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: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:F:204:LEU:HD12	1:F:205:MET:N	2.29	0.47
1:C:331:TRP:CZ2	1:C:365:HIS:CG	3.02	0.47
1:E:305:MET:HB2	1:E:305:MET:HE3	1.60	0.47
1:E:278:LEU:O	4:E:1572:EDO:H12	2.14	0.47
1:B:305:MET:HE3	1:B:305:MET:HB2	1.69	0.47
1:C:77:ARG:NE	1:C:80:ASP:OD2	2.46	0.47
1:E:305:MET:CE	1:E:336:LEU:HD23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:HA	1:A:291:ARG:NH1	2.30	0.47
1:A:277:ASN:O	4:A:1575:EDO:O1	2.20	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:CD2	2.45	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:C:155:THR:HG1	1:C:226:HIS:N	2.14	0.46
1:D:491:LYS:HE2	1:D:513:CYS:SG	2.55	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: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:E:178:SER:O	1:E:197:ARG:NH2	2.42	0.46
1:F:309:GLY:C	1:F:310:LEU:HD23	2.36	0.46
1:A:191:GLU:HG3	1:A:191:GLU:O	2.16	0.45
1:A:309:GLY:C	1:A:310:LEU:HD23	2.36	0.45
1:A:319:GLU:O	1:A:321:LEU:O	2.34	0.45
1:C:205:MET:CE	1:C:328:MET:O	2.64	0.45
1:C:305:MET:HB2	1:C:305:MET:HE3	1.64	0.45
1:D:274:PHE:CD2	1:D:305:MET:HE1	2.51	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: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:E:309:GLY:C	1:E:310:LEU:HD23	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:305:MET:CE	1:B:336:LEU:HD23	2.47	0.44
1:E:335:ASN:HD21	4:E:1572:EDO:C2	2.31	0.44
1:D:132:ARG:HB2	1:D:134:ASP:OD1	2.18	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:D:305:MET:HE3	1:D:305:MET:HB2	1.62	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:C:205:MET:HE3	1:C:205:MET:HB2	1.86	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:HG1	6:C:1569:HWU:H1B	1.83	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:C:191:GLU:HG3	1:C:191:GLU:O	2.19	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
1:C:205:MET:H	1:C:205:MET:CE	2.32	0.42
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:F:191:GLU:HG3	1:F:191:GLU:O	2.18	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:C:309:GLY:C	1:C:310:LEU:HD23	2.39	0.42
1:D:191:GLU:O	1:D:191:GLU:HG3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLY:C	1:B:310:LEU:HD23	2.39	0.42
1:A:439:VAL:HG13	1:D:291:ARG:NH2	2.35	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:E:305:MET:CE	1:E:336:LEU:CD2	2.98	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: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:E:305:MET:HE1	1:E:336:LEU:HD23	2.00	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:330:VAL:HG11	6:C:1569:HWU:C4	2.48	0.41
1:A:305:MET:CE	1:A:336:LEU:CD2	2.97	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: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
1:C:305:MET:CE	1:C:336:LEU:CD2	2.98	0.41
1:F:514:ARG:C	1:F:516:ASP:H	2.24	0.41
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:A:457:LEU:HD13	1:A:482:TRP:CZ2	2.56	0.41
1:D:309:GLY:C	1:D:310:LEU:HD23	2.41	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: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

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

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 (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
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

All (249) 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	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	296	ASN
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	410	ASN
1	A	414	ARG
1	A	419	LYS
1	A	421	LEU

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Mol	Chain	Res	Type
1	A	438	ARG
1	A	439	VAL
1	A	450	LEU
1	A	457	LEU
1	A	468	VAL
1	A	471	TYR
1	A	484	LEU
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
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	173	LEU
1	B	195	VAL
1	B	196	LEU
1	B	204	LEU
1	B	277	ASN
1	B	288	GLU
1	B	296	ASN
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	414	ARG
1	B	419	LYS
1	B	421	LEU
1	B	438	ARG
1	B	439	VAL

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Mol	Chain	Res	Type
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	471	TYR
1	B	484	LEU
1	B	502	ARG
1	B	510	LEU
1	B	552	VAL
1	B	554	VAL
1	B	567	LEU
1	C	75	LYS
1	C	76	VAL
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	173	LEU
1	C	195	VAL
1	C	196	LEU
1	C	201	ARG
1	C	204	LEU
1	C	205	MET
1	C	277	ASN
1	C	288	GLU
1	C	294	GLN
1	C	296	ASN
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	438	ARG
1	C	439	VAL
1	C	450	LEU
1	C	457	LEU

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Mol	Chain	Res	Type
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
1	C	554	VAL
1	D	75	LYS
1	D	76	VAL
1	D	101	ARG
1	D	112	LEU
1	D	116	ARG
1	D	124	ASP
1	D	133	VAL
1	D	173	LEU
1	D	195	VAL
1	D	196	LEU
1	D	204	LEU
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	296	ASN
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	438	ARG
1	D	439	VAL
1	D	450	LEU

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Mol	Chain	Res	Type
1	D	457	LEU
1	D	468	VAL
1	D	471	TYR
1	D	484	LEU
1	D	502	ARG
1	D	510	LEU
1	D	515	GLU
1	D	516	ASP
1	D	546	LYS
1	D	552	VAL
1	D	554	VAL
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	173	LEU
1	E	195	VAL
1	E	196	LEU
1	E	204	LEU
1	E	277	ASN
1	E	288	GLU
1	E	294	GLN
1	E	296	ASN
1	E	302	LYS
1	E	310	LEU
1	E	335	ASN
1	E	336	LEU
1	E	349	LEU
1	E	375	THR
1	E	410	ASN
1	E	419	LYS
1	E	421	LEU
1	E	438	ARG
1	E	439	VAL
1	E	450	LEU
1	E	457	LEU
1	E	468	VAL

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Mol	Chain	Res	Type
1	E	471	TYR
1	E	484	LEU
1	E	502	ARG
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	173	LEU
1	F	195	VAL
1	F	196	LEU
1	F	204	LEU
1	F	277	ASN
1	F	288	GLU
1	F	294	GLN
1	F	296	ASN
1	F	302	LYS
1	F	310	LEU
1	F	335	ASN
1	F	336	LEU
1	F	349	LEU
1	F	375	THR
1	F	410	ASN
1	F	414	ARG
1	F	419	LYS
1	F	421	LEU
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

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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 (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	123	HIS
1	A	127	GLN
1	A	198	ASN
1	A	277	ASN
1	A	296	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	432	ASN
1	A	452	GLN
1	A	462	HIS
1	A	479	ASN
1	A	537	ASN
1	B	106	GLN
1	B	123	HIS
1	B	127	GLN
1	B	130	GLN
1	B	198	ASN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN

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Mol	Chain	Res	Type
1	B	365	HIS
1	B	380	ASN
1	B	410	ASN
1	B	451	GLN
1	B	452	GLN
1	B	462	HIS
1	B	479	ASN
1	B	537	ASN
1	C	106	GLN
1	C	123	HIS
1	C	127	GLN
1	C	198	ASN
1	C	277	ASN
1	C	296	ASN
1	C	335	ASN
1	C	344	GLN
1	C	365	HIS
1	C	410	ASN
1	C	451	GLN
1	C	452	GLN
1	C	462	HIS
1	C	474	HIS
1	C	537	ASN
1	D	106	GLN
1	D	123	HIS
1	D	127	GLN
1	D	198	ASN
1	D	277	ASN
1	D	296	ASN
1	D	335	ASN
1	D	344	GLN
1	D	365	HIS
1	D	380	ASN
1	D	410	ASN
1	D	432	ASN
1	D	451	GLN
1	D	452	GLN
1	D	479	ASN
1	E	102	ASN
1	E	106	GLN
1	E	123	HIS
1	E	127	GLN

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Mol	Chain	Res	Type
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	364	GLN
1	E	365	HIS
1	E	380	ASN
1	E	410	ASN
1	E	451	GLN
1	E	452	GLN
1	E	462	HIS
1	E	479	ASN
1	E	537	ASN
1	F	106	GLN
1	F	123	HIS
1	F	127	GLN
1	F	198	ASN
1	F	277	ASN
1	F	296	ASN
1	F	335	ASN
1	F	344	GLN
1	F	365	HIS
1	F	380	ASN
1	F	410	ASN
1	F	432	ASN
1	F	451	GLN
1	F	452	GLN
1	F	474	HIS
1	F	537	ASN
1	F	562	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1580	BBK	C5-S5	-25.96	1.43	1.82
5	A	1581	BBK	C5-S5	-25.79	1.43	1.82
6	D	1571	HWU	C5'-S5'	-23.15	1.47	1.82
6	E	1585	HWU	C5'-S5'	-20.86	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	A	1582	HWU	C5'-S5'	-20.51	1.51	1.82
6	F	1571	HWU	C5'-S5'	-20.20	1.52	1.82
6	B	1571	HWU	C5'-S5'	-20.16	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	D	1571	HWU	C4'-C5'	4.68	1.57	1.53
6	D	1571	HWU	C6'-C5'	3.44	1.55	1.52
6	B	1571	HWU	C4-N3	-2.99	1.33	1.38
6	B	1571	HWU	C6-N1	-2.91	1.30	1.38
6	B	1571	HWU	O5B-C5B	-2.72	1.34	1.44
6	D	1571	HWU	C6-C5	2.68	1.41	1.35
6	B	1571	HWU	C4'-C5'	2.68	1.55	1.53
6	D	1571	HWU	O5B-C5B	-2.64	1.34	1.44
6	D	1571	HWU	C5-C4	-2.56	1.38	1.43
6	F	1571	HWU	C4'-C5'	2.53	1.55	1.53
6	A	1582	HWU	C6'-C5'	2.49	1.54	1.52
6	B	1571	HWU	PB-O1'	2.45	1.66	1.60
6	E	1585	HWU	C4'-C5'	2.44	1.55	1.53
6	B	1571	HWU	PB-O2B	-2.40	1.44	1.55
6	B	1571	HWU	C2-N3	-2.26	1.33	1.38
6	F	1571	HWU	O5B-C5B	-2.20	1.36	1.44
6	A	1582	HWU	PB-O1B	-2.20	1.43	1.50
6	D	1571	HWU	C4-N3	-2.20	1.34	1.38
6	A	1582	HWU	C6-C5	2.18	1.40	1.35
6	A	1582	HWU	O2-C2	2.15	1.27	1.23
6	E	1585	HWU	O4B-C1B	2.07	1.46	1.42
6	A	1582	HWU	C5-C4	-2.05	1.39	1.43
6	C	1569	HWU	PB-O2B	-2.04	1.45	1.55
6	E	1585	HWU	PB-O2B	-2.01	1.45	1.55
6	D	1571	HWU	C4'-C3'	2.00	1.57	1.52
6	A	1582	HWU	PB-O1'	2.00	1.65	1.60

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1572	BBK	C1-C2-N2	-9.34	93.88	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1572	BBK	O1-C1-C2	-7.78	93.37	109.25
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
6	E	1585	HWU	C4-N3-C2	-6.44	118.08	126.58
6	F	1571	HWU	C4-N3-C2	-5.97	118.71	126.58
6	B	1571	HWU	O1'-C1'-C2'	5.89	116.37	107.47
6	C	1569	HWU	O3A-PB-O1'	5.62	113.82	102.48
6	B	1571	HWU	O5B-PA-O1A	5.53	130.67	109.07
6	B	1571	HWU	PB-O1'-C1'	5.47	140.90	119.74
6	A	1582	HWU	PB-O1'-C1'	5.27	140.12	119.74
6	F	1571	HWU	N3-C2-N1	5.15	121.73	114.89
6	D	1571	HWU	N3-C2-N1	5.04	121.58	114.89
6	C	1569	HWU	O1'-C1'-C2'	4.88	114.84	107.47
5	A	1581	BBK	C1-C2-N2	4.79	120.31	111.36
6	A	1582	HWU	C4-N3-C2	-4.69	120.40	126.58
6	C	1569	HWU	C4-N3-C2	-4.64	120.45	126.58
6	D	1571	HWU	O2-C2-N3	-4.57	112.99	121.50
6	D	1571	HWU	O1'-PB-O1B	-4.54	92.43	109.47
5	A	1581	BBK	C2-N2-C7	4.45	134.00	123.18
6	C	1569	HWU	PB-O3A-PA	-4.43	117.62	132.83
6	B	1571	HWU	O4-C4-C5	-4.32	117.57	125.16
6	E	1585	HWU	PB-O1'-C1'	4.20	135.97	119.74
6	D	1571	HWU	O3'-C3'-C2'	4.17	118.08	109.66
6	C	1569	HWU	O6'-C6'-C5'	-4.11	101.31	110.73
6	A	1582	HWU	O3A-PB-O1'	-4.08	94.27	102.48
6	B	1571	HWU	O1'-PB-O1B	4.04	124.64	109.47
6	A	1582	HWU	C5-C4-N3	4.04	120.88	114.84
6	B	1571	HWU	O3A-PB-O1'	-4.01	94.40	102.48
6	A	1582	HWU	N3-C2-N1	4.00	120.20	114.89
6	F	1571	HWU	O4-C4-C5	-3.98	118.16	125.16
5	E	1584	BBK	C1-C2-C3	-3.97	103.98	110.27
5	E	1584	BBK	C3-C2-N2	-3.97	103.13	110.62
6	C	1569	HWU	C5-C4-N3	3.91	120.68	114.84
6	F	1571	HWU	C5-C4-N3	3.91	120.68	114.84
5	B	1580	BBK	C1-C2-C3	-3.88	104.13	110.27
6	E	1585	HWU	O3A-PB-O1'	-3.80	94.83	102.48
6	D	1571	HWU	O4B-C4B-C5B	-3.78	96.92	109.37
6	C	1569	HWU	PB-O1'-C1'	3.77	134.32	119.74
6	B	1571	HWU	O2-C2-N1	-3.75	117.80	122.79
6	E	1585	HWU	C5-C4-N3	3.67	120.33	114.84
6	C	1569	HWU	O2-C2-N3	-3.64	114.72	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1569	HWU	C1'-C2'-N2'	-3.63	104.42	111.17
6	D	1571	HWU	C1B-N1-C2	3.55	124.00	117.57
6	F	1571	HWU	PB-O1'-C1'	3.50	133.27	119.74
6	D	1571	HWU	C6-N1-C2	-3.46	116.56	120.99
6	B	1571	HWU	O2A-PA-O5B	-3.46	91.68	107.75
6	E	1585	HWU	O1'-C1'-C2'	3.41	112.62	107.47
6	B	1571	HWU	C5-C4-N3	3.39	119.91	114.84
6	E	1585	HWU	O2-C2-N3	-3.34	115.27	121.50
6	C	1569	HWU	N3-C2-N1	3.34	119.32	114.89
6	F	1571	HWU	O4B-C4B-C5B	-3.27	98.62	109.37
6	C	1569	HWU	O3B-C3B-C4B	3.23	120.38	111.05
5	B	1580	BBK	O4-C4-C5	3.22	115.81	108.82
6	E	1585	HWU	O4-C4-C5	-3.21	119.52	125.16
5	E	1584	BBK	O4-C4-C5	3.19	115.75	108.82
5	B	1580	BBK	C2-N2-C7	3.17	130.90	123.18
6	A	1582	HWU	O4-C4-C5	-3.08	119.74	125.16
6	D	1571	HWU	PB-O1'-C1'	3.03	131.44	119.74
5	E	1584	BBK	C2-N2-C7	3.01	130.51	123.18
6	C	1569	HWU	O4B-C1B-N1	3.01	115.24	108.36
6	B	1571	HWU	C4'-C3'-C2'	-3.01	105.94	110.34
6	A	1582	HWU	O2B-PB-O1B	2.93	126.70	112.24
6	B	1571	HWU	O7'-C7'-N2'	2.85	127.19	121.95
6	D	1571	HWU	C5B-C4B-C3B	-2.85	104.51	115.18
6	C	1569	HWU	C4'-C3'-C2'	-2.84	106.18	110.34
6	F	1571	HWU	O5B-PA-O1A	2.83	120.12	109.07
6	E	1585	HWU	O7'-C7'-N2'	2.82	127.13	121.95
5	A	1581	BBK	C1-C2-C3	-2.81	105.81	110.27
6	B	1571	HWU	O4B-C4B-C5B	-2.81	100.14	109.37
6	A	1582	HWU	C2'-N2'-C7'	-2.81	116.36	123.18
6	D	1571	HWU	C4-N3-C2	-2.78	122.92	126.58
5	D	1572	BBK	C4-C3-C2	2.70	114.30	110.34
6	C	1569	HWU	C1B-N1-C2	2.68	122.42	117.57
6	C	1569	HWU	O4-C4-C5	-2.67	120.47	125.16
6	E	1585	HWU	O3'-C3'-C2'	2.63	114.96	109.66
6	A	1582	HWU	O1'-PB-O1B	-2.62	99.64	109.47
6	A	1582	HWU	O2-C2-N3	-2.59	116.68	121.50
6	D	1571	HWU	O4'-C4'-C3'	-2.58	104.39	110.35
6	D	1571	HWU	O5B-C5B-C4B	2.52	117.68	108.99
6	C	1569	HWU	O4B-C4B-C3B	2.52	110.11	105.11
6	B	1571	HWU	O4'-C4'-C3'	-2.49	104.59	110.35
6	D	1571	HWU	O1'-C1'-C2'	-2.46	103.75	107.47
5	D	1572	BBK	O4-C4-C5	2.44	114.12	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	1571	HWU	O2-C2-N3	-2.43	116.97	121.50
6	E	1585	HWU	O7'-C7'-C8'	-2.43	117.55	122.06
5	E	1584	BBK	O6-C6-C5	-2.40	105.22	110.73
6	C	1569	HWU	O2-C2-N1	2.37	125.94	122.79
6	C	1569	HWU	C1B-N1-C6	-2.37	115.68	120.84
5	A	1581	BBK	O3-C3-C4	2.35	115.77	110.35
6	A	1582	HWU	C6'-C5'-C4'	-2.34	99.69	115.02
6	E	1585	HWU	C6-N1-C2	-2.33	118.01	120.99
5	A	1581	BBK	C3-C2-N2	-2.31	106.25	110.62
6	C	1569	HWU	O5B-PA-O1A	2.30	118.06	109.07
6	D	1571	HWU	O3A-PB-O1'	-2.29	97.87	102.48
6	A	1582	HWU	C4'-C3'-C2'	-2.29	107.00	110.34
6	F	1571	HWU	C4'-C3'-C2'	-2.24	107.05	110.34
6	B	1571	HWU	O2-C2-N3	-2.24	117.33	121.50
6	D	1571	HWU	O4'-C4'-C5'	2.23	113.67	108.82
6	C	1569	HWU	C2B-C1B-N1	-2.22	106.93	113.22
6	E	1585	HWU	C1B-N1-C2	2.22	121.58	117.57
6	B	1571	HWU	O2A-PA-O1A	2.21	123.15	112.24
6	B	1571	HWU	O4-C4-N3	2.18	122.51	119.31
6	A	1582	HWU	O5B-PA-O1A	-2.14	100.71	109.07
6	B	1571	HWU	C6-N1-C2	-2.14	118.26	120.99
6	B	1571	HWU	PB-O3A-PA	-2.13	125.51	132.83
5	B	1580	BBK	C3-C2-N2	-2.09	106.67	110.62
6	D	1571	HWU	O2B-PB-O1B	2.08	122.53	112.24
6	A	1582	HWU	O7'-C7'-C8'	-2.08	118.19	122.06
6	C	1569	HWU	O7'-C7'-C8'	-2.07	118.22	122.06
6	A	1582	HWU	O7'-C7'-N2'	2.06	125.74	121.95
5	D	1572	BBK	O3-C3-C4	2.05	115.10	110.35
6	D	1571	HWU	PB-O3A-PA	2.05	139.86	132.83
6	D	1571	HWU	O3'-C3'-C4'	-2.04	105.64	110.35
6	F	1571	HWU	O4B-C1B-N1	2.04	113.02	108.36
6	C	1569	HWU	C2'-N2'-C7'	-2.02	118.26	123.18

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
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	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
6	F	1571	HWU	C3B-C4B-C5B-O5B
4	A	1575	EDO	O1-C1-C2-O2
4	B	1578	EDO	O1-C1-C2-O2
4	E	1575	EDO	O1-C1-C2-O2
4	E	1576	EDO	O1-C1-C2-O2
4	A	1580	EDO	O1-C1-C2-O2
4	E	1574	EDO	O1-C1-C2-O2
4	E	1577	EDO	O1-C1-C2-O2
6	C	1569	HWU	C1'-O1'-PB-O1B
4	A	1573	EDO	O1-C1-C2-O2
4	A	1577	EDO	O1-C1-C2-O2
4	B	1576	EDO	O1-C1-C2-O2
4	D	1577	EDO	O1-C1-C2-O2
4	E	1573	EDO	O1-C1-C2-O2
5	B	1580	BBK	C4-C5-C6-O6
5	E	1584	BBK	C1-C2-N2-C7
6	B	1571	HWU	C5B-O5B-PA-O3A
6	B	1571	HWU	PB-O3A-PA-O2A
6	B	1571	HWU	C5B-O5B-PA-O2A
6	D	1571	HWU	C5B-O5B-PA-O2A
4	B	1573	EDO	O1-C1-C2-O2
6	D	1571	HWU	C4B-C5B-O5B-PA
4	A	1572	EDO	O1-C1-C2-O2
4	B	1575	EDO	O1-C1-C2-O2
4	E	1579	EDO	O1-C1-C2-O2
4	E	1583	EDO	O1-C1-C2-O2
6	A	1582	HWU	PB-O3A-PA-O2A

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

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

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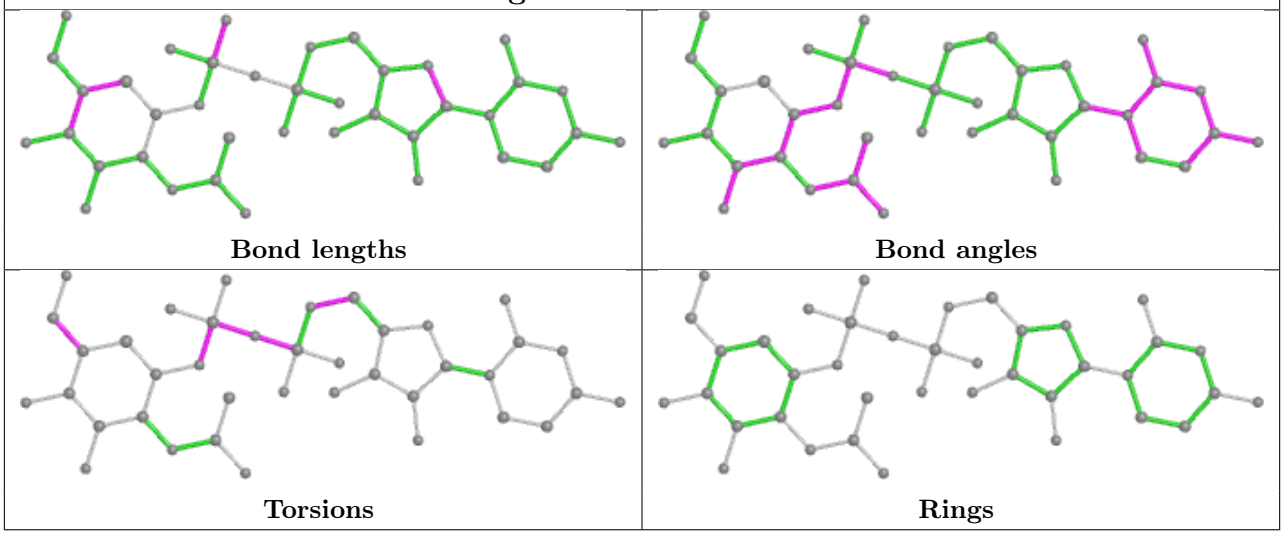
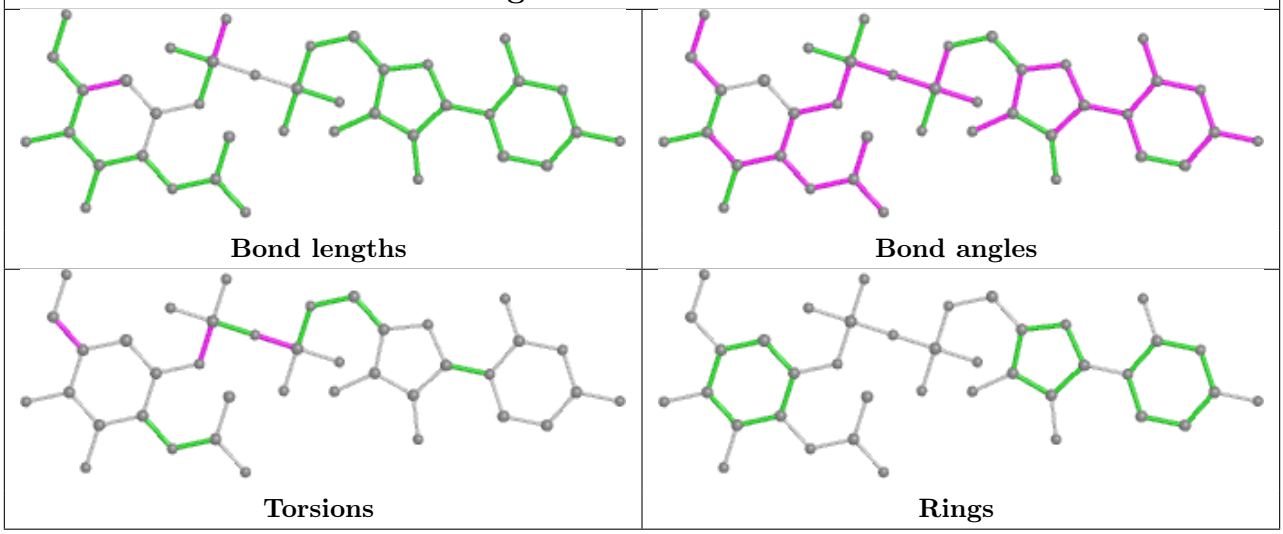
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1577	EDO	1	0
6	C	1569	HWU	11	0
4	A	1572	EDO	4	0
6	B	1571	HWU	2	0
4	A	1579	EDO	1	0
5	D	1572	BBK	4	0
6	F	1571	HWU	2	0
4	E	1570	EDO	1	0
4	D	1576	EDO	4	0
6	D	1571	HWU	4	0
5	E	1584	BBK	5	0
4	E	1579	EDO	2	0
4	E	1580	EDO	1	0
4	E	1572	EDO	8	0
4	B	1572	EDO	1	0
5	A	1581	BBK	3	0
4	B	1573	EDO	4	0
4	E	1573	EDO	1	0
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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

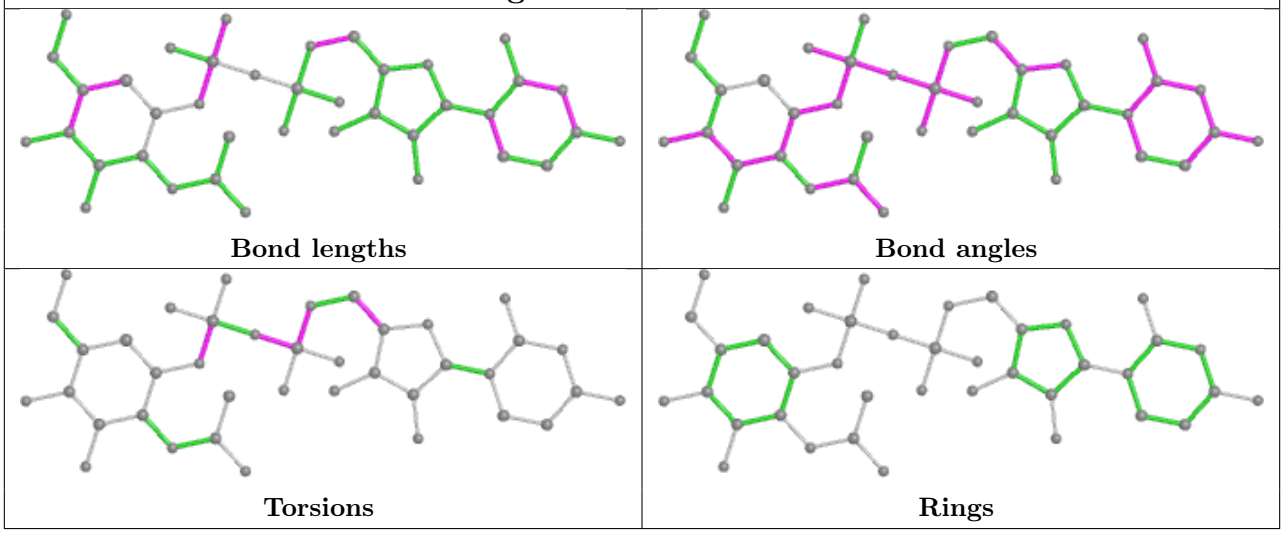
Ligand HWU E 1585



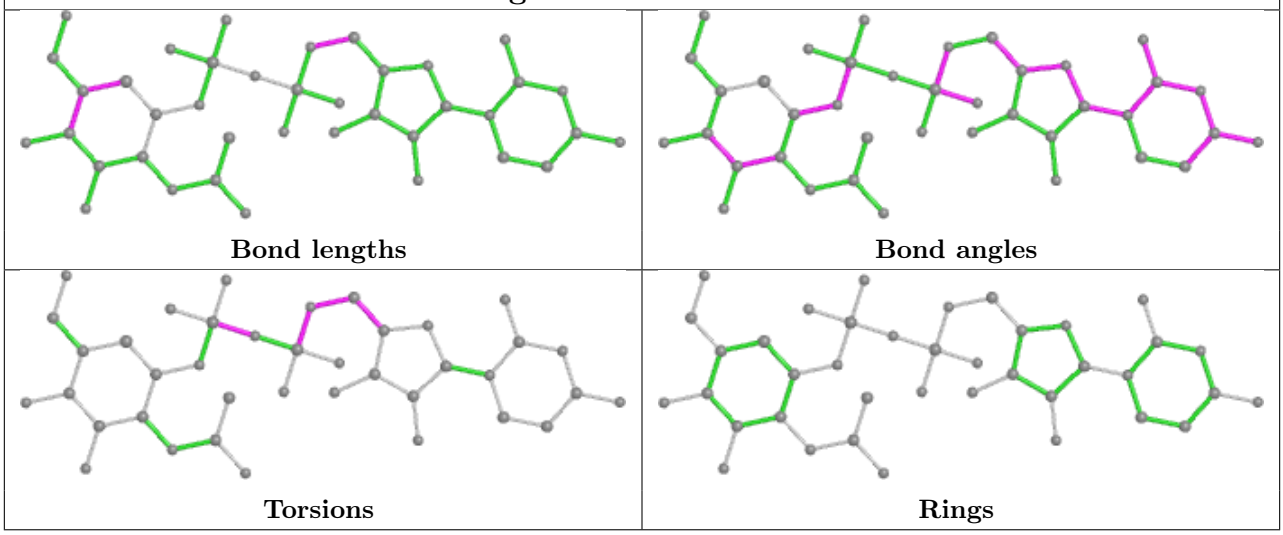
Ligand HWU C 1569



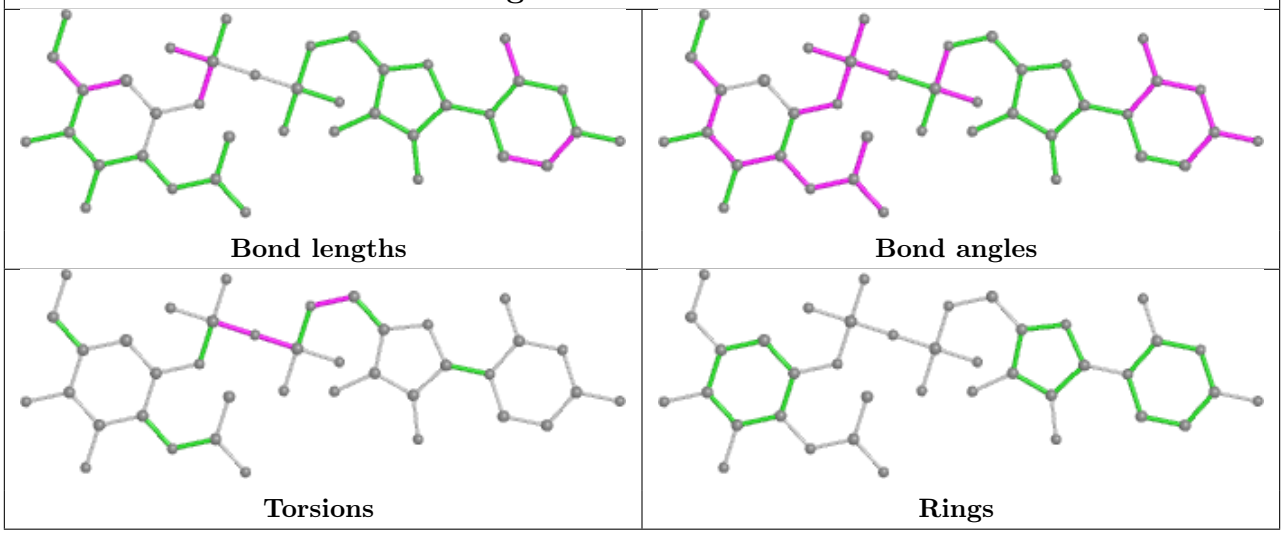
Ligand HWU B 1571



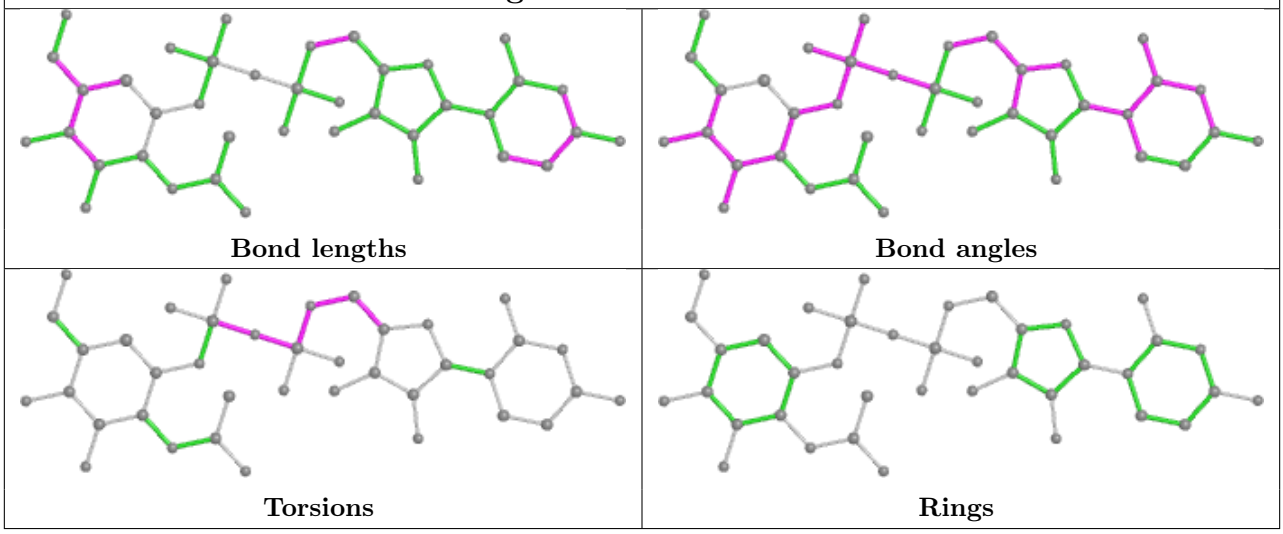
Ligand HWU F 1571



Ligand HWU A 1582



Ligand HWU D 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	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%)

All (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
1	C	400	VAL	8.5
1	F	557	PRO	8.4
1	C	423	CYS	8.3
1	C	475	ASN	8.1
1	C	442	HIS	7.7
1	C	516	ASP	7.5
1	C	497	LEU	7.5
1	F	503	ALA	7.3
1	C	443	GLN	7.2
1	C	471	TYR	7.1
1	F	531	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	284	TYR	6.6
1	C	438	ARG	6.5
1	C	101	ARG	6.4
1	F	552	VAL	6.3
1	F	96	GLN	6.2
1	C	547	SER	6.2
1	C	531	LEU	6.1
1	C	514	ARG	6.0
1	C	410	ASN	6.0
1	A	291	ARG	5.9
1	C	417	LEU	5.9
1	C	405	ASN	5.9
1	C	546	LYS	5.8
1	F	95	GLY	5.8
1	D	284	TYR	5.8
1	C	440	PRO	5.7
1	C	534	VAL	5.7
1	F	559	LEU	5.7
1	F	540	LEU	5.6
1	C	99	TYR	5.6
1	C	408	TYR	5.6
1	D	287	PRO	5.6
1	F	537	ASN	5.5
1	C	403	ALA	5.5
1	C	513	CYS	5.5
1	C	98	PRO	5.5
1	C	406	VAL	5.5
1	C	177	TYR	5.4
1	C	401	PRO	5.2
1	C	502	ARG	5.2
1	F	475	ASN	5.2
1	C	117	ALA	5.2
1	F	516	ASP	5.2
1	C	540	LEU	5.1
1	F	94	SER	5.0
1	C	89	GLY	5.0
1	C	421	LEU	5.0
1	C	399	ALA	5.0
2	Y	7	CYS	4.9
1	D	291	ARG	4.9
1	F	127	GLN	4.9
1	C	445	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	504	PRO	4.8
1	A	516	ASP	4.8
1	C	363	LYS	4.8
1	F	555	CYS	4.8
1	F	525	ILE	4.8
1	C	457	LEU	4.8
1	C	364	GLN	4.8
1	C	456	CYS	4.8
1	C	453	GLY	4.8
1	F	501	ASP	4.7
1	C	439	VAL	4.7
1	C	413	SER	4.7
1	C	493	MET	4.6
1	C	527	GLY	4.6
1	C	107	VAL	4.6
1	F	453	GLY	4.6
1	C	427	LYS	4.6
1	F	128	ARG	4.5
1	E	516	ASP	4.5
1	C	130	GLN	4.5
1	C	437	LEU	4.5
1	F	93	ARG	4.4
1	C	441	ASP	4.4
1	C	366	PRO	4.4
1	C	454	THR	4.4
1	C	477	GLY	4.4
1	C	199	ASP	4.4
1	C	279	VAL	4.4
1	F	522	TRP	4.4
1	C	280	PHE	4.4
1	C	447	PHE	4.3
1	F	89	GLY	4.3
2	X	6	THR	4.2
1	C	128	ARG	4.2
1	C	419	LYS	4.2
1	A	287	PRO	4.2
1	C	473	CYS	4.2
1	F	543	ARG	4.2
1	C	554	VAL	4.1
1	C	204	LEU	4.1
1	C	151	ALA	4.0
1	F	442	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	143	THR	4.0
1	C	522	TRP	4.0
1	C	383	ARG	4.0
1	C	504	PRO	4.0
1	C	97	ASP	4.0
1	C	548	GLY	4.0
1	F	535	GLY	3.9
1	F	497	LEU	3.9
1	F	554	VAL	3.9
1	C	182	GLU	3.9
1	D	557	PRO	3.9
1	C	544	THR	3.9
1	F	287	PRO	3.9
1	C	100	ALA	3.9
1	C	495	LEU	3.9
1	C	329	ASP	3.8
2	Y	6	THR	3.8
1	F	515	GLU	3.8
1	C	384	ALA	3.8
1	C	566	THR	3.7
1	A	295	GLY	3.7
1	C	463	PHE	3.7
1	C	113	ARG	3.7
1	C	412	GLN	3.7
1	F	544	THR	3.7
1	C	411	ILE	3.7
1	C	144	PHE	3.7
1	F	405	ASN	3.6
1	B	93	ARG	3.6
1	C	533	HIS	3.6
1	F	546	LYS	3.6
1	C	200	ARG	3.6
1	C	396	TYR	3.5
1	A	288	GLU	3.5
1	C	152	LEU	3.5
1	C	468	VAL	3.5
1	C	555	CYS	3.5
1	C	407	PRO	3.5
1	F	514	ARG	3.5
1	F	508	ILE	3.4
1	C	508	ILE	3.4
1	C	528	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	79	PRO	3.4
1	C	365	HIS	3.4
1	F	454	THR	3.4
1	B	516	ASP	3.4
1	C	327	MET	3.4
1	C	559	LEU	3.4
1	C	567	LEU	3.4
1	C	77	ARG	3.4
1	C	340	PHE	3.4
1	F	438	ARG	3.4
1	C	490	VAL	3.3
1	F	534	VAL	3.3
1	B	371	GLY	3.3
1	D	516	ASP	3.3
1	F	527	GLY	3.3
1	C	111	LYS	3.3
1	C	474	HIS	3.3
1	F	506	SER	3.3
1	C	430	LEU	3.3
1	C	146	ASN	3.3
1	F	474	HIS	3.2
1	C	150	SER	3.2
1	C	550	LEU	3.2
1	F	292	SER	3.2
1	F	558	ALA	3.2
1	C	532	ARG	3.2
1	C	316	PHE	3.2
1	A	442	HIS	3.2
1	D	295	GLY	3.2
1	C	422	SER	3.2
1	C	536	SER	3.2
1	F	476	ALA	3.2
1	C	568	ASN	3.2
1	F	443	GLN	3.1
1	B	199	ASP	3.1
1	C	391	GLU	3.1
1	C	485	THR	3.1
1	C	506	SER	3.1
1	C	503	ALA	3.1
1	C	385	ALA	3.1
1	C	288	GLU	3.0
1	F	548	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	128	ARG	3.0
1	F	465	ASP	3.0
1	A	540	LEU	3.0
1	F	493	MET	3.0
1	C	181	PRO	3.0
1	B	94	SER	3.0
1	C	186	LEU	3.0
1	C	472	GLU	3.0
1	C	525	ILE	3.0
1	C	537	ASN	3.0
1	F	513	CYS	2.9
1	C	292	SER	2.9
1	C	262	GLN	2.9
1	D	130	GLN	2.9
1	E	93	ARG	2.9
1	B	131	TRP	2.9
1	C	328	MET	2.9
1	C	557	PRO	2.9
1	F	284	TYR	2.9
1	C	124	ASP	2.9
1	C	145	HIS	2.9
1	B	96	GLN	2.8
1	F	288	GLU	2.8
1	B	127	GLN	2.8
1	A	95	GLY	2.8
1	C	390	ASP	2.8
1	C	397	TYR	2.8
1	C	91	MET	2.8
1	C	518	SER	2.8
1	F	286	THR	2.8
1	F	526	GLU	2.8
1	F	545	ALA	2.8
1	C	543	ARG	2.8
1	F	457	LEU	2.8
1	D	450	LEU	2.7
1	C	286	THR	2.7
1	C	108	GLU	2.7
1	C	416	GLU	2.7
1	D	540	LEU	2.7
1	A	93	ARG	2.7
1	C	501	ASP	2.7
1	F	97	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	277	ASN	2.7
1	F	486	LYS	2.7
1	F	441	ASP	2.7
1	C	290	ARG	2.7
1	A	284	TYR	2.7
1	C	278	LEU	2.7
1	A	409	GLY	2.7
1	C	275	ASP	2.7
1	C	449	ALA	2.7
1	C	386	GLU	2.7
1	C	549	GLY	2.7
1	C	291	ARG	2.6
1	B	457	LEU	2.6
1	D	290	ARG	2.6
1	F	550	LEU	2.6
1	A	419	LYS	2.6
1	C	526	GLU	2.6
1	C	426	PHE	2.6
1	C	402	SER	2.6
1	C	404	ARG	2.6
1	E	442	HIS	2.6
1	F	487	GLU	2.6
1	C	535	GLY	2.6
1	C	380	ASN	2.6
1	D	457	LEU	2.6
1	F	391	GLU	2.6
1	C	425	PRO	2.6
1	D	296	ASN	2.6
1	D	531	LEU	2.5
1	F	450	LEU	2.5
1	C	362	ARG	2.5
1	C	428	TRP	2.5
1	F	500	VAL	2.5
1	D	288	GLU	2.5
1	F	463	PHE	2.5
1	F	505	GLY	2.5
1	C	387	VAL	2.5
1	C	545	ALA	2.5
1	F	384	ALA	2.5
2	X	5	SER	2.5
1	C	409	GLY	2.5
1	F	363	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	563	TRP	2.5
1	B	442	HIS	2.5
1	F	566	THR	2.4
1	F	199	ASP	2.4
1	F	243	GLU	2.4
1	B	295	GLY	2.4
1	C	388	TRP	2.4
1	C	491	LYS	2.4
1	E	540	LEU	2.4
1	C	295	GLY	2.4
1	C	469	GLY	2.4
1	C	325	ASP	2.4
1	B	128	ARG	2.4
1	C	389	MET	2.4
1	C	431	GLU	2.4
1	F	179	ASN	2.4
1	D	294	GLN	2.4
1	F	291	ARG	2.3
1	D	442	HIS	2.3
1	A	290	ARG	2.3
1	F	295	GLY	2.3
2	Y	5	SER	2.3
1	A	316	PHE	2.3
1	F	419	LYS	2.3
1	C	414	ARG	2.3
1	F	502	ARG	2.3
1	F	471	TYR	2.3
1	D	293	ARG	2.3
1	C	429	TYR	2.2
1	F	517	ASP	2.2
1	C	157	VAL	2.2
1	C	395	PHE	2.2
1	F	518	SER	2.2
1	E	95	GLY	2.2
1	C	564	LYS	2.2
1	F	368	THR	2.2
1	D	199	ASP	2.2
1	B	130	GLN	2.2
1	B	288	GLU	2.2
1	C	344	GLN	2.2
1	C	553	GLU	2.2
1	F	490	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	565	PHE	2.2
1	E	316	PHE	2.1
1	F	538	LEU	2.1
2	Y	8	PRO	2.1
1	C	382	ARG	2.1
1	F	470	VAL	2.1
1	E	419	LYS	2.1
1	F	507	LEU	2.1
1	C	245	ARG	2.1
1	C	478	GLY	2.1
1	C	324	TYR	2.1
1	C	337	GLU	2.1
1	C	76	VAL	2.1
1	E	128	ARG	2.1
1	C	450	LEU	2.1
1	A	454	THR	2.1
1	C	448	GLY	2.1
1	E	94	SER	2.1
1	C	178	SER	2.1
1	D	547	SER	2.1
1	C	338	ILE	2.0
1	D	475	ASN	2.0
1	C	556	GLY	2.0
1	C	87	VAL	2.0
1	C	156	VAL	2.0
1	C	529	SER	2.0
1	F	200	ARG	2.0
1	C	393	LYS	2.0
1	C	470	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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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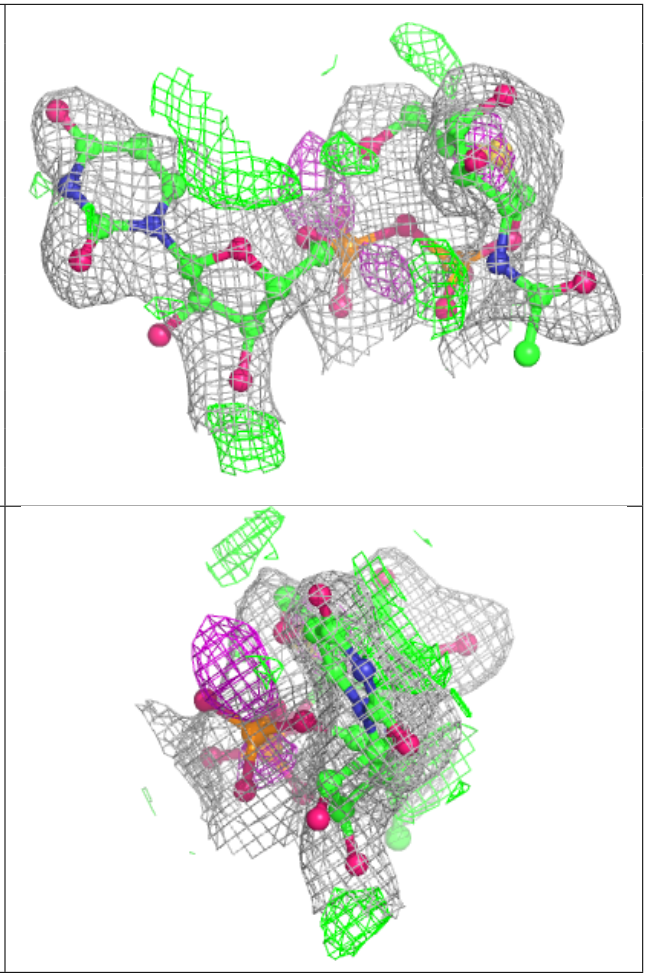
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	E	1577	4/4	0.94	0.21	61,61,64,68	0
4	EDO	D	1576	4/4	0.94	0.15	39,43,45,49	0
4	EDO	B	1577	4/4	0.94	0.20	42,43,48,57	0
4	EDO	A	1571	4/4	0.94	0.20	43,46,46,52	0
4	EDO	B	1572	4/4	0.95	0.10	34,35,35,42	0
4	EDO	A	1575	4/4	0.95	0.11	53,55,57,59	0
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.

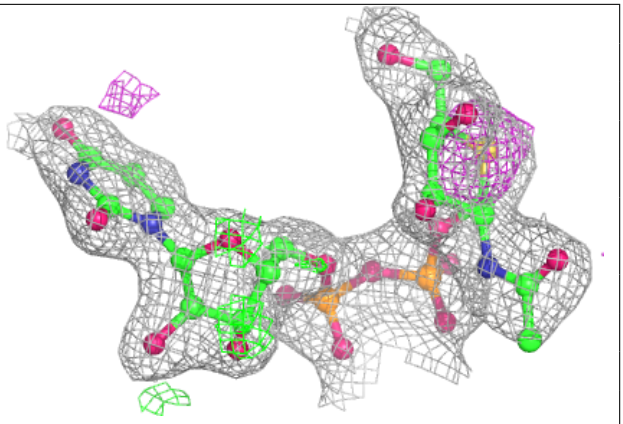
Electron density around HWU C 1569:

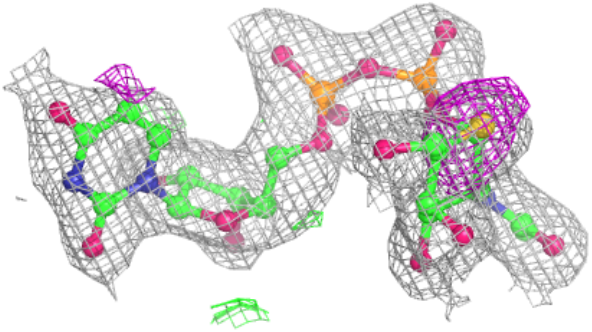
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

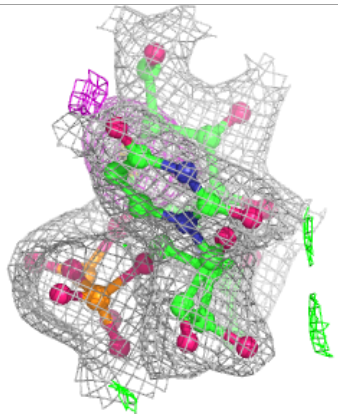


Electron density around HWU F 1571:

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

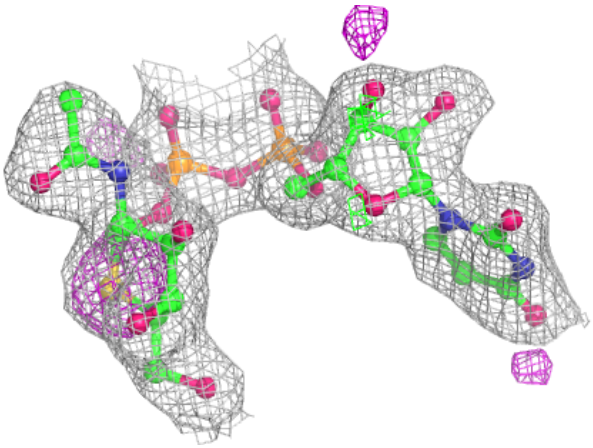


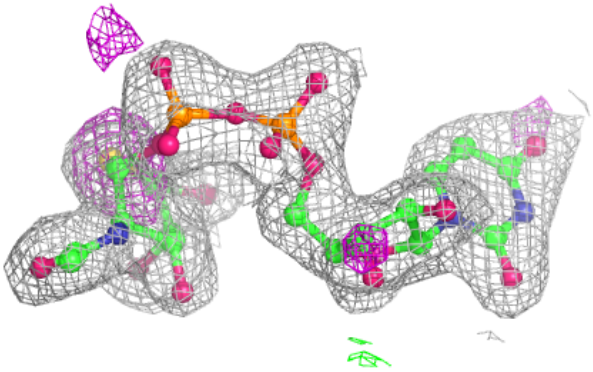


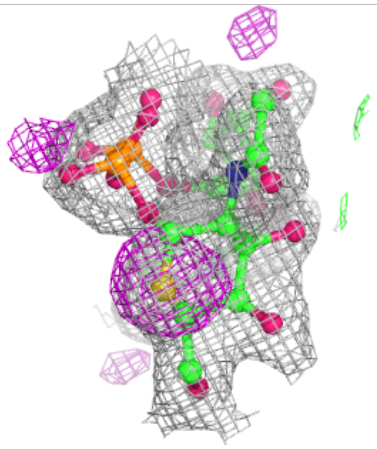


Electron density around HWU A 1582:

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

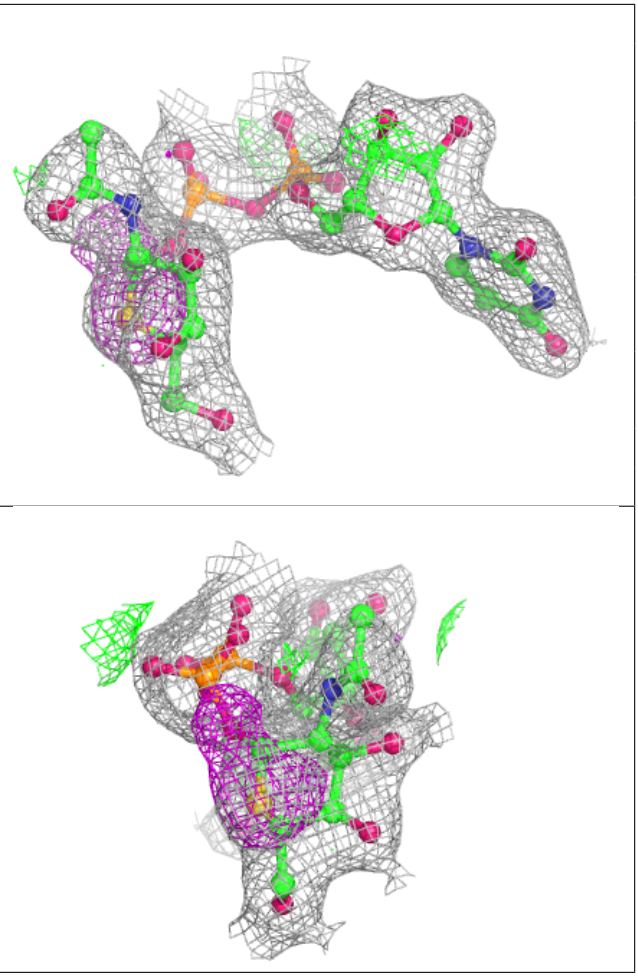






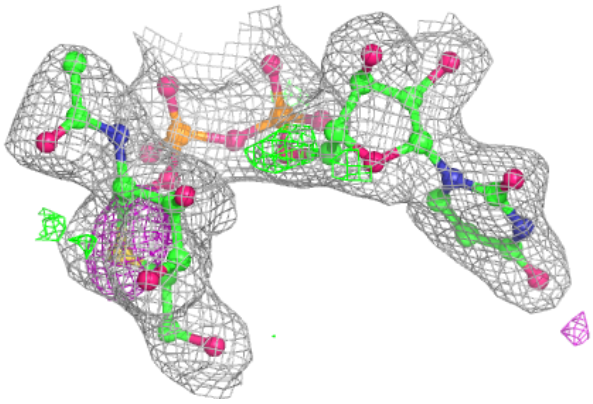
Electron density around HWU B 1571:

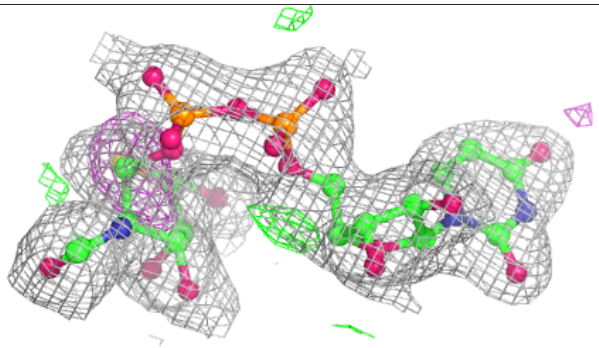
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

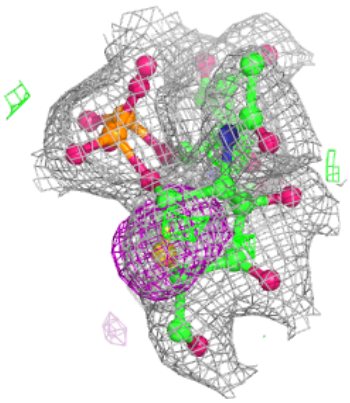


Electron density around HWU D 1571:

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

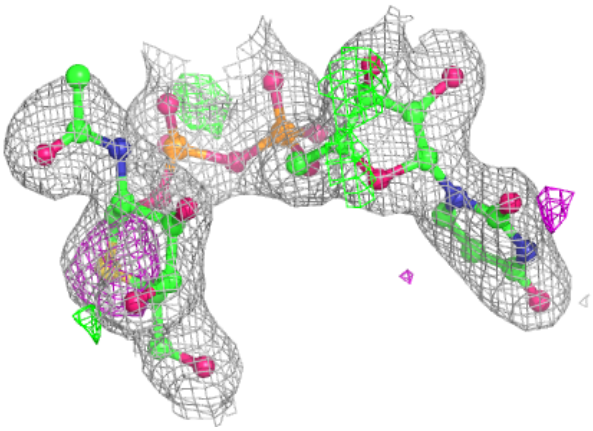


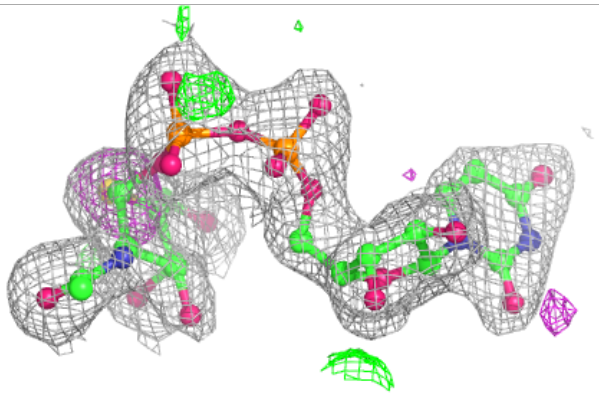




Electron density around HWU E 1585:

$2mF_o$-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.