



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 05:20 AM EST

PDB ID : 1G1L
Title : THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). TDP-GLUCOSE COMPLEX.
Authors : Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naimsmith, J.H.
Deposited on : 2000-10-12
Resolution : 1.77 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

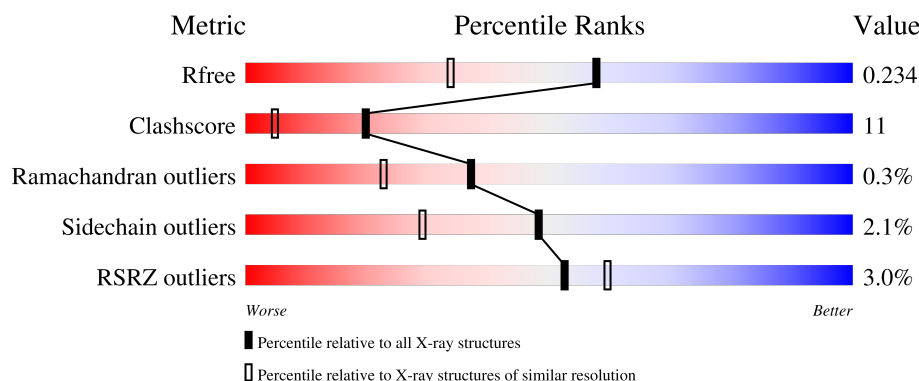
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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	293	<div> <div>5%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	B	293	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	C	293	<div> <div>5%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	D	293	<div> <div>5%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	293	 5% 78% 20%
1	F	293	 4% 81% 19%
1	G	293	 % 84% 16%
1	H	293	 % 81% 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
2	SO4	A	3802	-	-	X	-
2	SO4	A	3818	-	-	X	-
2	SO4	B	3701	-	-	X	-
2	SO4	E	3810	-	-	X	-
2	SO4	G	3702	-	-	X	-
2	SO4	H	3703	-	-	X	-
4	CIT	A	3801	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22376 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	9	0
			2361	1508	398	449	6			
1	B	293	Total	C	N	O	S	0	5	0
			2333	1489	395	442	7			
1	C	292	Total	C	N	O	S	0	6	0
			2335	1492	392	445	6			
1	D	292	Total	C	N	O	S	0	5	0
			2330	1487	397	440	6			
1	E	292	Total	C	N	O	S	0	5	0
			2320	1481	391	442	6			
1	F	293	Total	C	N	O	S	0	9	0
			2362	1508	395	452	7			
1	G	292	Total	C	N	O	S	0	6	0
			2334	1491	393	444	6			
1	H	292	Total	C	N	O	S	0	4	0
			2313	1477	390	440	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



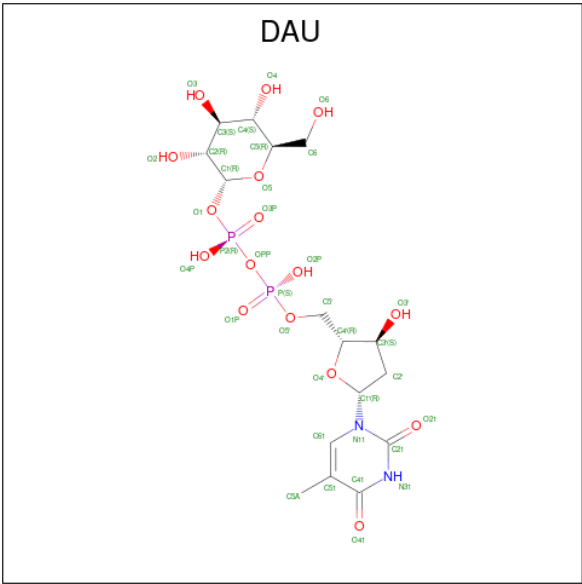
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

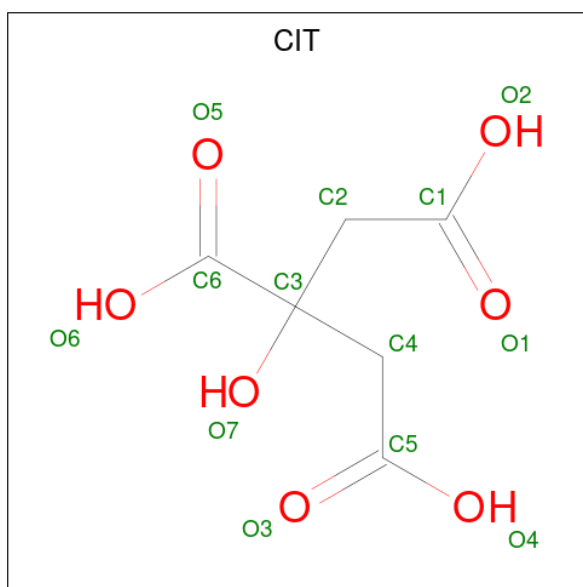
- Molecule 3 is 2'DEOXY-THYMIDINE-5'-DIPHOSPHO-ALPHA-D-GLUCOSE (three-letter code: DAU) (formula: C₁₆H₂₆N₂O₁₆P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	B	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	C	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	C	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	D	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	D	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	E	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	E	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	F	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	F	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	G	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	G	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	H	1	Total	C	N	O	P	0	0
			36	16	2	16	2		
3	H	1	Total	C	N	O	P	0	0
			36	16	2	16	2		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		

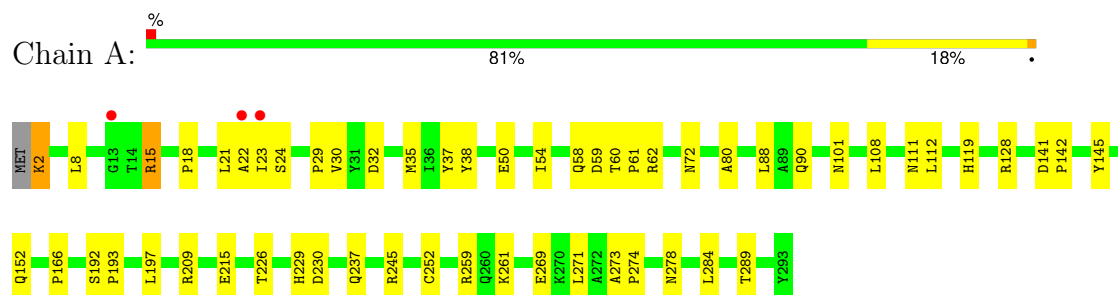
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	406	Total	O	0	0
			406	406		
5	B	414	Total	O	1	0
			414	414		
5	C	358	Total	O	0	0
			358	358		
5	D	309	Total	O	0	0
			309	309		
5	E	324	Total	O	0	0
			324	324		
5	F	325	Total	O	0	0
			325	325		
5	G	420	Total	O	0	0
			420	420		
5	H	415	Total	O	1	0
			415	415		

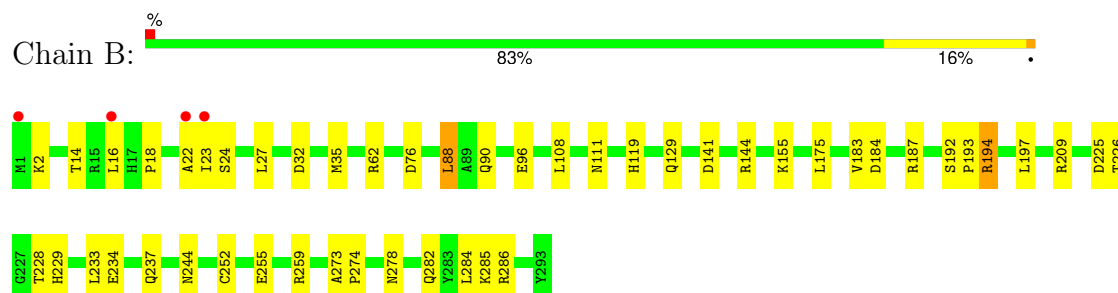
3 Residue-property plots [i](#)

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.

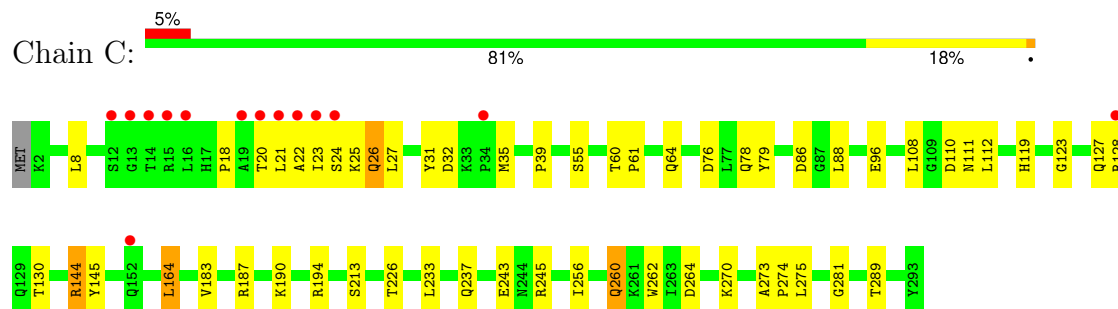
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



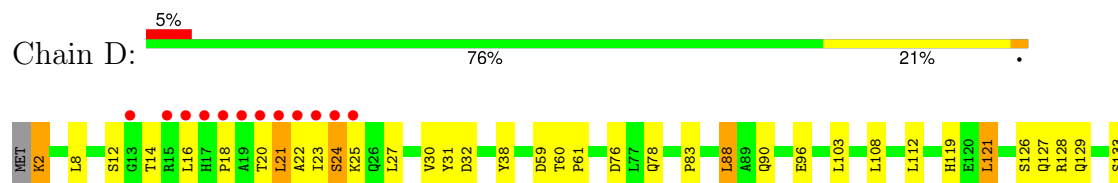
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

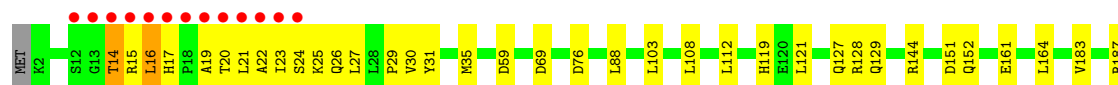
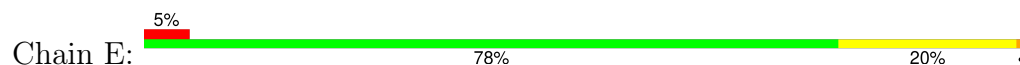


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

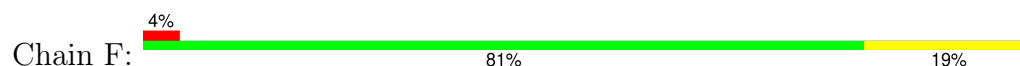




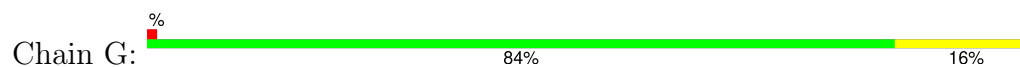
● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



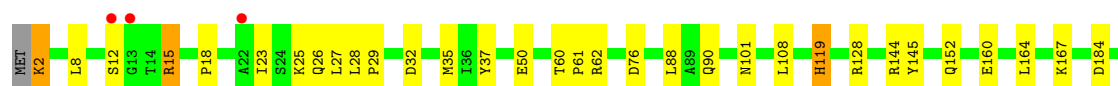
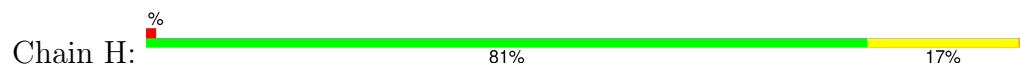
● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.58Å 73.41Å 134.29Å 89.94° 80.61° 80.93°	Depositor
Resolution (Å)	40.64 – 1.77 40.64 – 1.77	Depositor EDS
% Data completeness (in resolution range)	93.3 (40.64-1.77) 93.8 (40.64-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.156 , 0.215 0.182 , 0.234	Depositor DCC
R_{free} test set	12192 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22376	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CIT, DAU

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	1.08	3/2413 (0.1%)	1.05	5/3274 (0.2%)
1	B	1.07	0/2383	1.06	9/3231 (0.3%)
1	C	1.02	1/2386 (0.0%)	1.00	3/3237 (0.1%)
1	D	1.03	1/2380 (0.0%)	1.11	13/3227 (0.4%)
1	E	0.96	0/2370	0.98	5/3215 (0.2%)
1	F	1.05	0/2413	1.05	9/3273 (0.3%)
1	G	1.10	3/2385 (0.1%)	1.05	7/3236 (0.2%)
1	H	1.07	2/2363 (0.1%)	1.05	8/3206 (0.2%)
All	All	1.05	10/19093 (0.1%)	1.04	59/25899 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	37	TYR	CD1-CE1	6.24	1.48	1.39
1	C	55	SER	CB-OG	5.62	1.49	1.42
1	A	37	TYR	CD1-CE1	5.60	1.47	1.39
1	A	215	GLU	CD-OE1	5.36	1.31	1.25
1	A	128	ARG	CB-CG	-5.34	1.38	1.52
1	G	19	ALA	CA-CB	-5.34	1.41	1.52
1	G	128	ARG	CB-CG	-5.33	1.38	1.52
1	G	137	TYR	CG-CD1	5.25	1.46	1.39
1	H	128	ARG	CB-CG	-5.15	1.38	1.52
1	D	78	GLN	CG-CD	-5.08	1.39	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	194	ARG	NE-CZ-NH2	-12.19	114.20	120.30
1	D	259[A]	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	D	259[B]	ARG	NE-CZ-NH1	11.50	126.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	209	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	D	259[A]	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	D	259[B]	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	B	209	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	H	194	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	B	209	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	209	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	A	59	ASP	CB-CG-OD2	8.05	125.54	118.30
1	H	286	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	128	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	F	110	ASP	CB-CG-OD1	7.13	124.72	118.30
1	G	128	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	G	209	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	G	86	ASP	CB-CG-OD2	6.43	124.09	118.30
1	F	86	ASP	CB-CG-OD2	6.23	123.91	118.30
1	H	76	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	88	LEU	CB-CG-CD2	6.12	121.40	111.00
1	F	62	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	F	230	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	76	ASP	CB-CG-OD1	6.08	123.78	118.30
1	B	184	ASP	CB-CG-OD2	5.95	123.66	118.30
1	D	121	LEU	CB-CG-CD1	-5.90	100.98	111.00
1	B	76	ASP	CB-CG-OD1	5.87	123.59	118.30
1	G	110	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	144	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	H	286	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	194	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	209	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	F	76	ASP	CB-CG-OD1	5.61	123.35	118.30
1	E	264	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	76	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	259	ARG	CG-CD-NE	-5.38	100.51	111.80
1	D	88	LEU	CB-CG-CD2	5.38	120.14	111.00
1	B	144	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	H	209	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	E	151	ASP	CB-CG-OD1	5.30	123.07	118.30
1	E	204	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	H	144	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	D	144	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	F	102	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	110	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	194[A]	ARG	NE-CZ-NH2	-5.15	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194[B]	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	F	184	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	69	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	175	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	B	286	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	H	230	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	230	ASP	CB-CG-OD1	5.08	122.88	118.30
1	F	188	ASP	CB-CG-OD2	5.08	122.87	118.30
1	G	128	ARG	CG-CD-NE	-5.05	101.19	111.80
1	E	76	ASP	CB-CG-OD1	5.05	122.84	118.30
1	D	194[A]	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	194[B]	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	188	ASP	CB-CG-OD2	5.02	122.82	118.30
1	G	69	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2361	0	2330	65	0
1	B	2333	0	2320	46	0
1	C	2335	0	2309	61	0
1	D	2330	0	2316	72	0
1	E	2320	0	2300	77	0
1	F	2362	0	2335	45	1
1	G	2334	0	2309	42	0
1	H	2313	0	2294	54	0
2	A	25	0	0	4	0
2	B	10	0	0	2	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	E	20	0	0	3	0
2	F	5	0	0	0	0
2	G	15	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	20	0	0	4	0
3	A	72	0	48	3	0
3	B	72	0	48	2	0
3	C	72	0	48	3	0
3	D	72	0	48	1	0
3	E	72	0	48	3	0
3	F	72	0	48	4	0
3	G	72	0	48	0	0
3	H	72	0	48	2	0
4	A	26	0	10	12	0
5	A	406	0	0	22	1
5	B	414	0	0	18	1
5	C	358	0	0	20	0
5	D	309	0	0	16	2
5	E	324	0	0	26	1
5	F	325	0	0	11	0
5	G	420	0	0	13	1
5	H	415	0	0	9	1
All	All	22376	0	18907	432	4

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 11.

All (432) 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)
4:A:3801:CIT:H22	5:A:4214:HOH:O	1.33	1.26
1:A:119[B]:HIS:ND1	5:A:4023:HOH:O	1.65	1.24
1:C:237[B]:GLN:NE2	1:D:237[B]:GLN:OE1	1.70	1.23
1:C:27:LEU:HD12	5:C:4073:HOH:O	1.51	1.10
1:A:101[B]:ASN:OD1	5:A:4055:HOH:O	1.69	1.09
1:E:215:GLU:HG2	5:E:3953:HOH:O	1.55	1.06
1:B:155:LYS:HE3	5:B:4207:HOH:O	1.51	1.06
1:A:141:ASP:HB2	5:A:4040:HOH:O	1.59	1.02
1:E:25:LYS:HE3	1:E:26:GLN:NE2	1.73	1.02
1:B:237[B]:GLN:NE2	1:D:237[B]:GLN:NE2	2.08	1.01
1:E:269:GLU:OE1	1:E:288:LEU:CD1	2.08	1.01
3:F:3510:DAU:HC22	5:F:3990:HOH:O	1.61	1.00
1:H:62:ARG:NE	2:H:3814:SO4:O3	1.96	0.98
1:G:234:GLU:HA	1:G:237[B]:GLN:HE21	1.30	0.97
1:B:197:LEU:HB3	5:B:4088:HOH:O	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119[B]:HIS:CE1	5:A:4023:HOH:O	2.13	0.94
1:D:264:ASP:OD1	1:D:267:GLN:HG3	1.69	0.93
1:C:237[B]:GLN:HE21	1:D:237[B]:GLN:CD	1.73	0.92
1:E:190:LYS:HD2	1:E:191:PRO:HD2	1.52	0.92
1:B:141:ASP:HB2	5:B:3936:HOH:O	1.70	0.91
1:A:152:GLN:HG2	5:A:3874:HOH:O	1.71	0.90
3:F:3510:DAU:O3P	5:F:4118:HOH:O	1.90	0.89
1:E:23:ILE:HG21	1:F:23:ILE:HD11	1.54	0.88
1:G:237[B]:GLN:OE1	1:H:237:GLN:NE2	2.07	0.87
1:D:259[A]:ARG:HH22	1:D:292:VAL:HB	1.39	0.87
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.39	0.87
1:A:35[B]:MET:HE3	1:A:112[B]:LEU:HD21	1.56	0.87
1:E:269:GLU:OE1	1:E:288:LEU:HD11	1.74	0.87
1:H:15:ARG:HG3	1:H:15:ARG:HH11	1.40	0.87
1:E:190:LYS:NZ	1:E:191:PRO:O	2.08	0.85
2:A:3818:SO4:O2	5:A:3921:HOH:O	1.95	0.85
1:D:24:SER:CB	1:D:59:ASP:OD2	2.25	0.85
1:G:119:HIS:NE2	5:G:4077:HOH:O	2.09	0.84
1:C:23:ILE:HD11	1:D:23:ILE:HG21	1.58	0.84
1:H:101[B]:ASN:OD1	5:H:4130:HOH:O	1.96	0.84
1:G:234:GLU:HA	1:G:237[B]:GLN:NE2	1.94	0.82
1:A:2:LYS:NZ	1:A:50:GLU:OE1	2.12	0.82
1:C:23:ILE:CD1	1:D:23:ILE:HG21	2.10	0.81
1:A:229:HIS:CD2	4:A:3801:CIT:O3	2.33	0.81
1:D:23:ILE:HG13	5:D:4039:HOH:O	1.80	0.81
1:F:144:ARG:NH1	1:F:145[B]:TYR:OH	2.13	0.81
1:B:237[B]:GLN:HE22	1:D:237[B]:GLN:NE2	1.78	0.81
1:H:184:ASP:OD1	1:H:187:ARG:NH1	2.14	0.80
1:B:278:ASN:HB2	5:B:3890:HOH:O	1.80	0.80
1:D:161:GLU:O	1:D:194[B]:ARG:NH2	2.13	0.80
1:A:35[B]:MET:CE	1:A:112[B]:LEU:HD21	2.12	0.79
1:D:24:SER:HB2	1:D:59:ASP:OD2	1.83	0.79
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.65	0.78
1:C:123:GLY:O	1:C:127:GLN:HG2	1.82	0.78
1:E:23:ILE:HG21	1:F:23:ILE:CD1	2.13	0.78
1:G:60:THR:HG23	5:G:3892:HOH:O	1.83	0.78
1:G:15:ARG:NH1	2:G:3702:SO4:O4	2.16	0.78
1:F:144:ARG:HG2	5:F:3985:HOH:O	1.85	0.77
2:B:3701:SO4:O3	5:B:4205:HOH:O	2.02	0.76
1:H:23:ILE:HD11	1:H:27:LEU:CD1	2.15	0.76
1:A:62:ARG:NE	2:A:3802:SO4:O4	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:LYS:NZ	1:F:50:GLU:OE1	2.14	0.76
4:A:3801:CIT:O3	5:A:4216:HOH:O	2.04	0.76
1:A:21:LEU:HA	5:A:4058:HOH:O	1.86	0.75
2:E:3810:SO4:O1	5:E:3990:HOH:O	2.05	0.74
1:F:273:ALA:HB3	1:F:274:PRO:HD3	1.68	0.74
1:A:261:LYS:NZ	5:A:3969:HOH:O	2.20	0.74
2:E:3820:SO4:O2	5:E:4034:HOH:O	2.05	0.74
5:E:4003:HOH:O	1:H:145:TYR:HE1	1.70	0.74
1:C:256:ILE:O	1:C:260:GLN:HG3	1.88	0.73
1:G:27:LEU:HD12	5:G:4176:HOH:O	1.89	0.73
1:E:215:GLU:HG3	5:E:4054:HOH:O	1.87	0.73
1:F:25:LYS:HE2	5:F:3981:HOH:O	1.88	0.73
1:B:197:LEU:HD13	5:B:4088:HOH:O	1.88	0.72
1:C:24:SER:HB2	5:C:4073:HOH:O	1.88	0.72
1:B:237[B]:GLN:CD	5:B:3900:HOH:O	2.27	0.71
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.72	0.71
1:E:282:GLN:OE1	5:E:4036:HOH:O	2.08	0.71
1:A:22:ALA:C	1:A:23:ILE:HG13	2.11	0.71
1:C:86:ASP:OD2	5:C:4159:HOH:O	2.09	0.71
1:H:289:THR:OG1	5:H:4230:HOH:O	2.09	0.71
1:A:237[A]:GLN:HG2	1:C:237[A]:GLN:HG2	1.72	0.70
1:A:229:HIS:HD2	4:A:3801:CIT:O3	1.73	0.70
1:H:194:ARG:HG3	5:H:4169:HOH:O	1.91	0.69
1:A:90:GLN:HG2	1:A:197:LEU:HD12	1.75	0.69
1:H:273:ALA:HB3	1:H:274:PRO:HD3	1.75	0.69
1:H:15:ARG:NH1	2:H:3703:SO4:O4	2.26	0.69
1:B:237[B]:GLN:HE22	1:D:237[B]:GLN:HE22	1.41	0.69
1:D:234:GLU:HA	1:D:237[B]:GLN:HE21	1.58	0.69
1:A:88:LEU:HD13	1:A:108:LEU:HD21	1.74	0.68
1:D:128:ARG:NE	5:D:3874:HOH:O	2.27	0.68
1:G:237[B]:GLN:CD	1:H:237:GLN:HE21	1.96	0.68
1:E:190:LYS:HZ2	1:E:191:PRO:C	1.96	0.68
1:G:15:ARG:NH1	2:G:3702:SO4:S	2.67	0.68
1:H:23:ILE:HD11	1:H:27:LEU:HD13	1.75	0.68
1:G:289:THR:OG1	5:G:4203:HOH:O	2.10	0.68
1:G:64:GLN:HB3	5:G:4038:HOH:O	1.91	0.68
1:G:15:ARG:NH1	2:G:3702:SO4:O2	2.27	0.68
1:E:190:LYS:NZ	1:E:191:PRO:HB2	2.08	0.68
1:A:23:ILE:HD13	1:B:23:ILE:HD13	1.74	0.68
1:E:23:ILE:CG2	1:F:23:ILE:HD11	2.22	0.67
1:A:38:TYR:CB	1:A:112[B]:LEU:CD2	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:CB	5:B:4088:HOH:O	2.35	0.67
1:E:192:SER:HB2	1:E:193:PRO:HD2	1.75	0.67
4:A:3800:CIT:O3	1:B:229:HIS:ND1	2.26	0.66
1:A:35[B]:MET:CE	1:A:112[B]:LEU:CD2	2.73	0.66
1:E:260:GLN:CD	5:E:4017:HOH:O	2.34	0.66
1:C:119:HIS:HD2	5:C:4123:HOH:O	1.79	0.66
2:A:3802:SO4:O3	1:B:62:ARG:NE	2.26	0.65
1:E:234:GLU:OE2	5:E:4074:HOH:O	2.14	0.65
3:B:3502:DAU:HC52	5:B:4201:HOH:O	1.96	0.65
1:A:35[B]:MET:HE3	1:A:112[B]:LEU:CD2	2.27	0.65
4:A:3801:CIT:O2	5:A:4215:HOH:O	2.13	0.65
1:D:23:ILE:CG2	1:D:27:LEU:HB2	2.27	0.65
1:E:22:ALA:C	1:E:23:ILE:HG13	2.17	0.65
1:E:256:ILE:O	1:E:260:GLN:HG3	1.96	0.65
1:D:167:LYS:HE2	5:D:4035:HOH:O	1.96	0.65
1:F:282:GLN:O	1:F:286:ARG:HG3	1.97	0.65
1:B:237[B]:GLN:HE21	1:D:237[B]:GLN:NE2	1.94	0.65
3:C:3504:DAU:O2P	5:C:4149:HOH:O	2.13	0.64
1:G:237[B]:GLN:HG2	1:H:237:GLN:NE2	2.12	0.64
1:A:278:ASN:HB2	5:A:3896:HOH:O	1.98	0.64
1:D:259[A]:ARG:NH2	1:D:292:VAL:HB	2.12	0.64
1:E:16:LEU:HD22	1:E:229:HIS:CE1	2.33	0.64
1:H:23:ILE:HD11	1:H:27:LEU:HD12	1.80	0.64
1:F:16:LEU:HD22	5:F:4058:HOH:O	1.98	0.63
1:G:18:PRO:HD2	1:H:32:ASP:O	1.99	0.62
1:F:2:LYS:HE2	1:F:4:LYS:HE3	1.81	0.62
1:E:103:LEU:HD11	1:E:129:GLN:HG2	1.81	0.62
1:H:101[A]:ASN:ND2	5:H:4160:HOH:O	2.32	0.62
1:A:32:ASP:O	1:B:18:PRO:HD2	2.00	0.61
1:C:96:GLU:OE1	1:C:187:ARG:NH1	2.33	0.61
1:D:278:ASN:OD1	1:D:280:TYR:N	2.32	0.61
1:A:23:ILE:HG21	1:B:23:ILE:HD11	1.83	0.61
1:A:23:ILE:HG22	1:A:24:SER:O	2.01	0.61
1:A:38:TYR:CB	1:A:112[B]:LEU:HD22	2.30	0.61
1:B:234:GLU:HA	1:B:237[A]:GLN:HE21	1.66	0.61
4:A:3801:CIT:H21	5:A:4063:HOH:O	2.01	0.60
1:E:127:GLN:HG2	5:E:3975:HOH:O	2.00	0.60
1:D:2:LYS:O	5:D:4119:HOH:O	2.16	0.60
1:C:237[B]:GLN:NE2	1:D:237[B]:GLN:HG2	2.16	0.60
1:D:96:GLU:OE1	1:D:187:ARG:NH1	2.34	0.60
1:B:237[B]:GLN:NE2	1:D:237[B]:GLN:CD	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ILE:N	5:E:3882:HOH:O	2.34	0.60
1:H:119:HIS:HD2	3:H:3513:DAU:O1P	1.85	0.60
1:F:35[A]:MET:SD	1:F:226:THR:OG1	2.60	0.60
1:E:23:ILE:HD11	1:F:23:ILE:HG21	1.84	0.59
1:G:88:LEU:HD13	1:G:108:LEU:HD21	1.85	0.59
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.83	0.59
1:E:25:LYS:HE3	1:E:26:GLN:HE22	1.60	0.58
1:E:282:GLN:OE1	5:E:4140:HOH:O	2.17	0.58
4:A:3800:CIT:O7	5:A:4206:HOH:O	2.17	0.58
1:E:128:ARG:NH2	5:E:4054:HOH:O	2.22	0.58
1:A:2:LYS:HA	5:A:4083:HOH:O	2.03	0.58
1:A:35[B]:MET:HE1	1:A:112[B]:LEU:HG	1.84	0.58
1:C:26:GLN:NE2	5:C:3904:HOH:O	2.34	0.58
1:G:270:LYS:NZ	5:G:4025:HOH:O	2.37	0.57
1:E:23:ILE:HG22	1:E:24:SER:O	2.04	0.57
1:C:289:THR:OG1	5:C:4163:HOH:O	2.16	0.57
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.34	0.57
5:E:4003:HOH:O	1:H:145:TYR:CE1	2.53	0.57
1:C:128:ARG:NH1	1:C:213:SER:HB2	2.20	0.57
3:E:3508:DAU:O2P	5:E:4128:HOH:O	2.17	0.57
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.69	0.57
1:A:35[B]:MET:SD	1:A:226:THR:HG21	2.45	0.56
1:D:193:PRO:HD2	5:D:4014:HOH:O	2.04	0.56
1:E:152:GLN:HG3	2:E:3810:SO4:O2	2.06	0.56
1:A:38:TYR:HB2	1:A:112[B]:LEU:CD2	2.36	0.56
1:B:35[B]:MET:SD	1:B:226:THR:HG21	2.45	0.56
1:C:130:THR:HG23	2:C:3806:SO4:O1	2.06	0.56
1:D:141:ASP:HB3	5:D:4100:HOH:O	2.04	0.56
1:E:269:GLU:OE1	1:E:288:LEU:HD12	2.02	0.56
1:A:38:TYR:CG	1:A:112[B]:LEU:HD22	2.41	0.56
1:C:23:ILE:HD13	1:D:23:ILE:HG12	1.87	0.55
1:E:237[B]:GLN:CD	1:F:237:GLN:HE21	2.09	0.55
1:A:23:ILE:CA	5:A:4039:HOH:O	2.54	0.55
1:C:88:LEU:HD13	1:C:108:LEU:HD21	1.87	0.55
1:E:23:ILE:CD1	1:F:23:ILE:HG21	2.37	0.55
1:H:192:SER:HB2	1:H:193:PRO:CD	2.37	0.55
1:H:252[A]:CYS:SG	1:H:284:LEU:HD21	2.47	0.55
1:F:60:THR:HB	1:F:61:PRO:HD3	1.89	0.55
1:B:14:THR:N	2:B:3701:SO4:O1	2.40	0.55
1:C:22:ALA:O	5:C:4156:HOH:O	2.18	0.55
1:C:23:ILE:HD13	1:D:23:ILE:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:VAL:O	1:C:187:ARG:HG3	2.07	0.55
1:E:30:VAL:HG21	1:E:35[B]:MET:SD	2.47	0.54
1:F:215:GLU:HG3	5:F:3951:HOH:O	2.06	0.54
1:E:121:LEU:HD12	5:E:3922:HOH:O	2.05	0.54
1:C:8:LEU:HD23	1:C:88:LEU:HD22	1.89	0.54
1:G:273:ALA:HB3	1:G:274:PRO:HD3	1.88	0.54
1:E:17:HIS:HD2	1:E:20:THR:OG1	1.91	0.54
1:G:16:LEU:HA	1:G:229:HIS:CE1	2.43	0.54
1:E:190:LYS:HD2	1:E:191:PRO:CD	2.32	0.54
1:E:278:ASN:ND2	1:F:14:THR:O	2.35	0.54
1:C:60:THR:CG2	5:C:4104:HOH:O	2.56	0.54
1:C:237[B]:GLN:NE2	1:D:237[B]:GLN:CG	2.70	0.54
3:C:3504:DAU:O6	5:C:4154:HOH:O	2.19	0.54
1:E:245:ARG:NH1	5:E:4003:HOH:O	2.41	0.54
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.89	0.53
1:B:252[B]:CYS:SG	1:B:284:LEU:HD21	2.48	0.53
1:F:16:LEU:O	1:F:19:ALA:HB3	2.09	0.53
1:A:35[B]:MET:HE1	1:A:112[B]:LEU:CD2	2.37	0.53
1:B:88:LEU:HD13	1:B:108:LEU:HD21	1.91	0.53
1:C:20:THR:HA	1:C:23:ILE:O	2.09	0.53
1:D:128:ARG:HG3	1:D:128:ARG:O	2.08	0.53
1:E:237[B]:GLN:HG2	1:F:237:GLN:NE2	2.24	0.53
1:E:24:SER:HB2	1:E:59:ASP:CG	2.29	0.53
1:E:35[B]:MET:SD	1:E:226:THR:HG21	2.49	0.53
1:G:18:PRO:HD3	1:H:280:TYR:CD1	2.44	0.53
1:A:145[A]:TYR:OH	1:C:245:ARG:NH1	2.42	0.53
1:A:15:ARG:HG3	1:A:15:ARG:NH1	2.16	0.53
1:B:197:LEU:CG	5:B:4088:HOH:O	2.56	0.53
1:E:25:LYS:CE	1:E:26:GLN:NE2	2.61	0.52
1:F:144:ARG:HG2	1:F:144:ARG:O	2.09	0.52
1:D:90:GLN:HG2	1:D:197:LEU:HD12	1.92	0.52
1:D:16:LEU:HD22	1:D:229:HIS:CE1	2.44	0.52
1:E:16:LEU:HB3	1:E:20:THR:HG23	1.92	0.52
1:A:60:THR:HB	1:A:61:PRO:HD3	1.91	0.52
1:B:282:GLN:HG2	5:B:3990:HOH:O	2.09	0.52
1:E:190:LYS:HZ3	1:E:191:PRO:HB2	1.72	0.52
1:F:8:LEU:HD23	1:F:88:LEU:HD22	1.92	0.52
1:G:28:LEU:HD22	1:H:29:PRO:CG	2.39	0.52
1:C:18:PRO:O	1:C:21:LEU:HB2	2.10	0.52
1:E:23:ILE:HG12	1:F:23:ILE:HG12	1.92	0.52
1:H:15:ARG:HH11	1:H:15:ARG:CG	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:SER:HB2	1:D:193:PRO:HD2	1.92	0.52
1:C:233:LEU:HD11	1:D:237[B]:GLN:HG3	1.92	0.51
1:H:286:ARG:HD2	5:H:4129:HOH:O	2.09	0.51
1:A:22:ALA:O	1:A:23:ILE:HG13	2.10	0.51
1:C:60:THR:HG22	1:C:64:GLN:HE21	1.74	0.51
1:G:64:GLN:NE2	5:G:4215:HOH:O	2.30	0.51
1:B:16:LEU:HD21	1:B:228:THR:C	2.30	0.51
1:F:88:LEU:HD13	1:F:108:LEU:HD21	1.92	0.51
1:E:237[B]:GLN:HG3	1:F:233:LEU:HD11	1.92	0.51
1:H:192:SER:HB2	1:H:193:PRO:HD2	1.93	0.51
1:A:8:LEU:HG	3:A:3500:DAU:O21	2.11	0.51
1:F:141:ASP:OD2	1:F:144:ARG:NH2	2.43	0.51
1:C:22:ALA:HB3	5:C:4128:HOH:O	2.11	0.51
1:F:4:LYS:NZ	1:F:102:ASP:OD2	2.39	0.51
1:F:112:LEU:C	1:F:112:LEU:HD23	2.31	0.51
1:E:252[A]:CYS:SG	1:E:284:LEU:HD21	2.51	0.50
2:G:3702:SO4:O3	5:G:4204:HOH:O	2.18	0.50
1:D:126:SER:HB2	5:D:4104:HOH:O	2.10	0.50
1:D:267:GLN:HB3	5:D:3870:HOH:O	2.11	0.50
1:E:183:VAL:O	1:E:187:ARG:HG3	2.12	0.50
1:D:18:PRO:O	1:D:21:LEU:HB2	2.12	0.50
1:E:23:ILE:CA	5:E:3882:HOH:O	2.60	0.50
1:C:78:GLN:OE1	5:C:4095:HOH:O	2.20	0.50
1:B:197:LEU:CD1	5:B:4088:HOH:O	2.55	0.50
3:E:3508:DAU:HC52	5:E:4126:HOH:O	2.10	0.50
1:D:20:THR:HB	1:D:23:ILE:O	2.12	0.50
1:C:237[B]:GLN:NE2	1:D:237[B]:GLN:CD	2.48	0.49
1:D:23:ILE:HG22	1:D:24:SER:O	2.11	0.49
1:A:269:GLU:HG3	5:A:4078:HOH:O	2.11	0.49
3:B:3502:DAU:O3P	5:B:4199:HOH:O	2.20	0.49
1:D:32:ASP:OD2	1:D:243:GLU:OE1	2.31	0.49
1:E:234:GLU:HA	1:E:237[B]:GLN:NE2	2.26	0.49
1:B:282:GLN:CG	5:B:3990:HOH:O	2.60	0.49
1:D:155:LYS:HG2	5:D:4098:HOH:O	2.12	0.49
1:C:27:LEU:HB2	5:C:4073:HOH:O	2.12	0.49
1:B:23:ILE:CG2	1:B:27:LEU:HB2	2.42	0.49
1:E:128:ARG:NH1	5:E:4054:HOH:O	2.40	0.49
1:F:141:ASP:OD1	5:F:4127:HOH:O	2.19	0.49
1:D:25:LYS:HE2	1:D:25:LYS:HB3	1.61	0.48
1:A:60:THR:N	1:A:61:PRO:CD	2.76	0.48
1:H:192:SER:OG	1:H:194:ARG:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:SER:HB2	1:B:193:PRO:CD	2.43	0.48
1:E:23:ILE:HD13	1:F:23:ILE:HD13	1.96	0.48
1:B:22:ALA:O	5:B:4059:HOH:O	2.19	0.48
1:B:23:ILE:HG22	1:B:24:SER:O	2.12	0.48
1:C:144:ARG:NH2	1:C:145[B]:TYR:OH	2.47	0.48
1:E:23:ILE:CG2	1:E:27:LEU:HB2	2.44	0.48
1:A:38:TYR:HB3	1:A:112[B]:LEU:HD22	1.96	0.48
1:D:112:LEU:C	1:D:112:LEU:HD23	2.34	0.48
1:D:234:GLU:HA	1:D:237[B]:GLN:NE2	2.27	0.48
1:H:90:GLN:HG2	1:H:197:LEU:HD12	1.95	0.48
1:E:17:HIS:CE1	1:E:21:LEU:HD23	2.48	0.48
1:G:139:VAL:HG21	1:G:145[A]:TYR:CE1	2.48	0.48
1:C:26:GLN:CG	5:C:4049:HOH:O	2.61	0.48
1:D:121:LEU:HD12	5:D:4027:HOH:O	2.13	0.48
1:H:12:SER:OG	2:H:3703:SO4:O1	2.31	0.48
1:D:8:LEU:HG	3:D:3506:DAU:O21	2.14	0.48
1:D:103:LEU:HD11	1:D:129:GLN:HG2	1.95	0.47
1:G:23:ILE:HG22	1:G:27:LEU:HB2	1.96	0.47
1:H:164:LEU:HD21	5:H:4132:HOH:O	2.14	0.47
1:C:25:LYS:HE2	5:C:4152:HOH:O	2.14	0.47
1:C:237[B]:GLN:HG3	1:D:233:LEU:HD11	1.95	0.47
1:E:25:LYS:CE	1:E:26:GLN:HE22	2.26	0.47
1:F:57:PRO:HG3	1:F:81[A]:VAL:HG11	1.95	0.47
1:D:128:ARG:HD2	1:D:133:SER:OG	2.14	0.47
1:E:30:VAL:CG2	1:E:35[B]:MET:SD	3.02	0.47
1:H:88:LEU:HD13	1:H:108:LEU:HD21	1.96	0.47
1:F:121:LEU:HD12	5:F:3903:HOH:O	2.14	0.47
1:A:245:ARG:NH1	1:C:145[B]:TYR:OH	2.46	0.47
1:E:237[B]:GLN:OE1	1:F:237:GLN:NE2	2.34	0.47
1:H:194:ARG:N	5:H:4169:HOH:O	2.46	0.46
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.96	0.46
1:E:161:GLU:O	1:E:194:ARG:NH2	2.48	0.46
1:E:190:LYS:HZ3	1:E:191:PRO:CB	2.29	0.46
1:A:35[B]:MET:HE1	1:A:112[B]:LEU:CG	2.45	0.46
1:E:23:ILE:C	5:E:3882:HOH:O	2.54	0.46
1:G:143:GLU:OE2	5:G:4219:HOH:O	2.21	0.46
1:H:2:LYS:HB2	1:H:2:LYS:HE3	1.55	0.46
1:D:183:VAL:O	1:D:187:ARG:HG3	2.16	0.46
1:H:25:LYS:HE3	1:H:26:GLN:NE2	2.31	0.46
4:A:3801:CIT:C5	5:A:4216:HOH:O	2.62	0.45
1:B:90:GLN:HG2	1:B:197:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35[A]:MET:SD	1:C:226:THR:OG1	2.69	0.45
1:E:29:PRO:CD	5:E:4068:HOH:O	2.63	0.45
1:E:20:THR:O	1:E:21:LEU:C	2.54	0.45
1:B:278:ASN:CB	5:B:3890:HOH:O	2.54	0.45
1:C:190:LYS:HE3	5:C:4131:HOH:O	2.15	0.45
5:G:4211:HOH:O	1:H:229:HIS:HD2	1.99	0.45
1:D:16:LEU:HD13	5:D:4063:HOH:O	2.16	0.45
1:D:23:ILE:HG22	1:D:27:LEU:HB2	1.96	0.45
1:E:215:GLU:CG	5:E:3953:HOH:O	2.34	0.45
1:F:256:ILE:O	1:F:260:GLN:HG2	2.16	0.45
1:G:16:LEU:O	1:G:229:HIS:HE1	1.99	0.45
1:C:112:LEU:C	1:C:112:LEU:HD23	2.37	0.45
1:H:60:THR:N	1:H:61:PRO:CD	2.79	0.45
1:B:244:ASN:HB3	5:B:4000:HOH:O	2.16	0.45
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.46	0.45
1:D:25:LYS:HB2	5:D:3989:HOH:O	2.17	0.45
1:E:128:ARG:CZ	5:E:4054:HOH:O	2.64	0.45
1:A:259:ARG:HD3	3:A:3501:DAU:H5A1	1.98	0.45
1:B:96:GLU:OE1	1:B:187:ARG:NH1	2.48	0.45
1:C:270:LYS:HG2	5:C:4038:HOH:O	2.17	0.45
1:B:285:LYS:NZ	5:B:4165:HOH:O	2.34	0.45
1:F:11:GLY:HA2	1:F:85:PRO:HB3	1.98	0.44
1:H:35[A]:MET:SD	1:H:226:THR:OG1	2.75	0.44
1:H:60:THR:HB	1:H:61:PRO:HD3	1.98	0.44
4:A:3800:CIT:C5	1:B:229:HIS:HD1	2.26	0.44
1:G:237[B]:GLN:CG	1:H:237:GLN:NE2	2.78	0.44
1:A:252[A]:CYS:SG	1:A:284:LEU:HD21	2.57	0.44
1:B:255:GLU:O	1:B:259[B]:ARG:HG3	2.17	0.44
1:D:251:ALA:O	1:D:253:PRO:HD3	2.16	0.44
1:E:29:PRO:HD3	5:E:4068:HOH:O	2.18	0.44
1:A:54:ILE:HA	1:A:80:ALA:O	2.16	0.44
1:A:237[B]:GLN:HG3	1:B:233:LEU:HD11	1.98	0.44
3:C:3504:DAU:HC52	5:C:4154:HOH:O	2.17	0.44
1:H:286:ARG:HG3	5:H:4129:HOH:O	2.17	0.44
1:A:18:PRO:HD2	1:B:32:ASP:O	2.18	0.44
1:F:273:ALA:HB3	1:F:274:PRO:CD	2.43	0.44
1:H:249:LYS:HB2	1:H:252[B]:CYS:SG	2.57	0.44
1:E:190:LYS:NZ	1:E:191:PRO:CB	2.80	0.44
1:F:51:ILE:HB	1:F:77:LEU:HD23	2.00	0.44
1:H:25:LYS:HE3	1:H:26:GLN:HE22	1.82	0.44
1:H:160:GLU:OE2	1:H:167:LYS:NZ	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:HB3	1:A:112[B]:LEU:CD2	2.47	0.44
1:G:192:SER:HB2	1:G:193:PRO:CD	2.48	0.44
1:C:164:LEU:HD22	1:C:164:LEU:HA	1.83	0.43
1:G:29:PRO:HD3	1:H:28:LEU:HD22	1.99	0.43
1:D:127:GLN:HG3	5:D:4121:HOH:O	2.17	0.43
1:E:271:LEU:O	1:E:274:PRO:HD2	2.18	0.43
1:C:275:LEU:O	1:C:281:GLY:HA3	2.19	0.43
1:G:22:ALA:O	1:G:23:ILE:HG12	2.19	0.43
1:A:142:PRO:HG2	1:A:166:PRO:HG2	2.00	0.43
1:E:26:GLN:NE2	3:E:3508:DAU:O3'	2.51	0.43
1:G:282:GLN:HG2	5:G:4062:HOH:O	2.18	0.43
1:A:23:ILE:HA	5:A:4039:HOH:O	2.17	0.43
1:G:27:LEU:HD23	1:G:27:LEU:HA	1.75	0.43
1:C:25:LYS:HE2	1:C:25:LYS:HB3	1.78	0.43
1:F:260:GLN:O	1:F:261:LYS:HB2	2.18	0.43
1:B:183:VAL:O	1:B:187:ARG:HG3	2.18	0.43
1:F:144:ARG:CG	5:F:3985:HOH:O	2.58	0.43
1:D:183:VAL:HG23	5:D:3884:HOH:O	2.18	0.43
1:D:278:ASN:OD1	1:D:278:ASN:C	2.57	0.43
1:E:112:LEU:C	1:E:112:LEU:HD23	2.38	0.43
1:E:127:GLN:CG	5:E:3975:HOH:O	2.64	0.43
1:C:260:GLN:CD	5:C:4125:HOH:O	2.57	0.43
1:D:162:LYS:N	1:D:163:PRO:CD	2.82	0.43
1:F:264:ASP:N	1:F:267:GLN:OE1	2.41	0.43
1:D:60:THR:HB	1:D:61:PRO:HD3	2.00	0.42
1:E:164:LEU:HD23	1:E:164:LEU:HA	1.83	0.42
1:F:16:LEU:HD12	1:F:25:LYS:HD3	2.01	0.42
1:G:237[B]:GLN:HG3	1:H:233:LEU:HD11	2.01	0.42
1:H:15:ARG:HG3	1:H:15:ARG:NH1	2.18	0.42
1:C:26:GLN:HE21	1:C:26:GLN:HB2	1.49	0.42
1:D:194[B]:ARG:HG3	5:D:4014:HOH:O	2.19	0.42
1:F:152:GLN:NE2	5:F:4002:HOH:O	2.52	0.42
1:E:233:LEU:HD21	1:F:237:GLN:HA	2.00	0.42
1:H:194:ARG:HD3	1:H:198:GLU:OE2	2.19	0.42
1:H:8:LEU:HG	3:H:3512:DAU:O21	2.19	0.42
1:H:188:ASP:HB3	5:H:4183:HOH:O	2.19	0.42
1:A:23:ILE:HD11	1:B:23:ILE:HG21	2.00	0.42
1:A:30:VAL:HB	1:A:38:TYR:CE1	2.55	0.42
1:C:237[B]:GLN:HE22	1:D:237[B]:GLN:HG2	1.83	0.42
1:E:16:LEU:O	1:E:19:ALA:HB3	2.18	0.42
1:G:64:GLN:HG2	1:G:79:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:PRO:HG2	1:G:166:PRO:HG2	2.02	0.42
1:D:255:GLU:O	1:D:259[B]:ARG:HG3	2.19	0.42
1:E:144:ARG:NH2	1:E:225:ASP:OD2	2.52	0.42
1:H:15:ARG:NH1	2:H:3703:SO4:S	2.93	0.42
3:F:3510:DAU:O6	5:F:4119:HOH:O	2.17	0.42
1:A:229:HIS:HD2	4:A:3801:CIT:C5	2.31	0.42
1:D:264:ASP:OD1	1:D:267:GLN:CG	2.52	0.42
1:E:194:ARG:HD3	5:E:3928:HOH:O	2.20	0.42
1:G:62:ARG:HD3	5:G:4180:HOH:O	2.18	0.42
1:C:60:THR:N	1:C:61:PRO:CD	2.83	0.41
1:A:289:THR:OG1	5:A:4220:HOH:O	2.22	0.41
1:C:260:GLN:NE2	1:C:262:TRP:CH2	2.89	0.41
1:D:88:LEU:HD13	1:D:108:LEU:HD21	2.02	0.41
1:H:23:ILE:CD1	1:H:27:LEU:HD12	2.50	0.41
1:F:8:LEU:HG	3:F:3510:DAU:O21	2.20	0.41
1:A:72:ASN:HB3	1:A:271:LEU:HD21	2.02	0.41
1:A:237[A]:GLN:HA	1:B:233:LEU:HD21	2.03	0.41
1:F:27:LEU:HD23	1:F:27:LEU:HA	1.84	0.41
1:B:129:GLN:O	1:E:208:GLU:HG2	2.19	0.41
1:C:260:GLN:NE2	1:C:262:TRP:CZ2	2.87	0.41
1:C:264:ASP:HB2	5:C:4100:HOH:O	2.21	0.41
1:D:30:VAL:HB	1:D:38:TYR:CE1	2.54	0.41
1:D:275:LEU:O	1:D:281:GLY:HA3	2.21	0.41
1:G:60:THR:N	1:G:61:PRO:CD	2.83	0.41
1:A:15:ARG:NH1	1:A:15:ARG:CG	2.82	0.41
2:A:3818:SO4:O1	3:A:3501:DAU:O4	2.11	0.41
1:C:18:PRO:HA	1:C:21:LEU:HG	2.02	0.41
1:G:136:ALA:HA	1:G:171:ALA:O	2.21	0.41
1:G:280:TYR:CD1	1:H:18:PRO:HD3	2.56	0.41
1:A:58:GLN:H	1:A:58:GLN:CD	2.24	0.41
1:C:35[B]:MET:SD	1:C:226:THR:HG21	2.61	0.41
1:D:259[A]:ARG:HH22	1:D:292:VAL:CB	2.21	0.41
1:G:35[A]:MET:SD	1:G:226:THR:OG1	2.78	0.41
1:A:23:ILE:N	5:A:4039:HOH:O	2.53	0.40
1:A:229:HIS:HD2	4:A:3801:CIT:H41	1.86	0.40
1:C:35[B]:MET:O	1:C:39:PRO:HD2	2.21	0.40
1:H:2:LYS:NZ	1:H:50:GLU:OE1	2.51	0.40
1:C:32:ASP:OD2	1:C:243:GLU:OE1	2.38	0.40
1:E:88:LEU:HD13	1:E:108:LEU:HD21	2.02	0.40
1:G:2:LYS:HA	5:G:4191:HOH:O	2.20	0.40
1:C:27:LEU:HD22	1:D:22:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLN:HG2	1:C:79:TYR:CE1	2.57	0.40
1:C:264:ASP:C	1:C:264:ASP:OD1	2.58	0.40
1:G:60:THR:HB	1:G:61:PRO:HD3	2.03	0.40
1:A:21:LEU:CA	5:A:4058:HOH:O	2.58	0.40
1:D:83:PRO:HD2	5:D:3850:HOH:O	2.22	0.40
1:E:24:SER:HB3	1:E:27:LEU:HD12	2.04	0.40
1:H:287:LEU:HD23	1:H:287:LEU:HA	1.93	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:3941:HOH:O	5:H:4205:HOH:O[1_565]	2.12	0.08
5:D:4087:HOH:O	5:E:4106:HOH:O[1_655]	2.14	0.06
5:A:4001:HOH:O	5:B:4113:HOH:O[1_565]	2.19	0.01
1:F:64:GLN:OE1	5:G:4216:HOH:O[1_455]	2.19	0.01

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	299/293 (102%)	295 (99%)	4 (1%)	0	100	100
1	B	296/293 (101%)	292 (99%)	4 (1%)	0	100	100
1	C	296/293 (101%)	293 (99%)	2 (1%)	1 (0%)	37	23
1	D	295/293 (101%)	289 (98%)	5 (2%)	1 (0%)	37	23
1	E	295/293 (101%)	290 (98%)	3 (1%)	2 (1%)	19	7
1	F	300/293 (102%)	296 (99%)	3 (1%)	1 (0%)	37	23
1	G	296/293 (101%)	293 (99%)	2 (1%)	1 (0%)	37	23
1	H	294/293 (100%)	291 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2371/2344 (101%)	2339 (99%)	26 (1%)	6 (0%)	37	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	31	TYR
1	D	31	TYR
1	E	14	THR
1	E	31	TYR
1	F	31	TYR
1	G	31	TYR

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	248/240 (103%)	244 (98%)	4 (2%)	58	41
1	B	245/240 (102%)	240 (98%)	5 (2%)	50	32
1	C	245/240 (102%)	240 (98%)	5 (2%)	50	32
1	D	244/240 (102%)	238 (98%)	6 (2%)	42	22
1	E	244/240 (102%)	238 (98%)	6 (2%)	42	22
1	F	249/240 (104%)	243 (98%)	6 (2%)	44	24
1	G	245/240 (102%)	242 (99%)	3 (1%)	67	54
1	H	243/240 (101%)	237 (98%)	6 (2%)	42	22
All	All	1963/1920 (102%)	1922 (98%)	41 (2%)	48	29

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	15	ARG
1	A	29	PRO
1	A	111	ASN

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Mol	Chain	Res	Type
1	B	2	LYS
1	B	111	ASN
1	B	119	HIS
1	B	194	ARG
1	B	225	ASP
1	C	26	GLN
1	C	111	ASN
1	C	164	LEU
1	C	194	ARG
1	C	260	GLN
1	D	2	LYS
1	D	12	SER
1	D	14	THR
1	D	21	LEU
1	D	24	SER
1	D	119	HIS
1	E	14	THR
1	E	15	ARG
1	E	16	LEU
1	E	119	HIS
1	E	225	ASP
1	E	260	GLN
1	F	24[A]	SER
1	F	24[B]	SER
1	F	119	HIS
1	F	126	SER
1	F	155	LYS
1	F	197	LEU
1	G	2	LYS
1	G	194	ARG
1	G	225	ASP
1	H	2	LYS
1	H	15	ARG
1	H	119	HIS
1	H	152	GLN
1	H	225	ASP
1	H	278	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS

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Mol	Chain	Res	Type
1	A	26	GLN
1	A	229	HIS
1	C	26	GLN
1	C	64	GLN
1	C	65	GLN
1	D	65	GLN
1	D	229	HIS
1	E	17	HIS
1	E	26	GLN
1	E	282	GLN
1	F	17	HIS
1	F	65	GLN
1	F	152	GLN
1	F	244	ASN
1	G	17	HIS
1	G	26	GLN
1	G	119	HIS
1	G	229	HIS
1	H	26	GLN
1	H	119	HIS
1	H	229	HIS
1	H	237	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

41 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DAU	C	3505	-	37,38,38	1.95	8 (21%)	55,58,58	1.48	9 (16%)
3	DAU	B	3503	-	37,38,38	1.76	7 (18%)	55,58,58	1.79	9 (16%)
3	DAU	A	3501	-	37,38,38	1.70	4 (10%)	55,58,58	2.00	10 (18%)
4	CIT	A	3800	-	12,12,12	1.03	0	17,17,17	2.12	6 (35%)
3	DAU	E	3509	-	37,38,38	1.73	9 (24%)	55,58,58	1.72	10 (18%)
2	SO4	G	3813	-	4,4,4	0.32	0	6,6,6	0.51	0
2	SO4	C	3806	-	4,4,4	0.26	0	6,6,6	0.39	0
2	SO4	D	3819	-	4,4,4	0.48	0	6,6,6	0.42	0
2	SO4	A	3803	-	4,4,4	0.38	0	6,6,6	0.50	0
3	DAU	F	3510	-	37,38,38	1.97	10 (27%)	55,58,58	2.43	17 (30%)
2	SO4	A	3817	-	4,4,4	0.43	0	6,6,6	0.39	0
3	DAU	G	3515	-	37,38,38	1.65	6 (16%)	55,58,58	2.05	10 (18%)
3	DAU	C	3504	-	37,38,38	1.81	7 (18%)	55,58,58	2.46	21 (38%)
2	SO4	E	3820	-	4,4,4	0.38	0	6,6,6	0.61	0
2	SO4	E	3808	-	4,4,4	0.32	0	6,6,6	0.26	0
2	SO4	H	3814	-	4,4,4	0.31	0	6,6,6	0.40	0
2	SO4	H	3815	-	4,4,4	0.38	0	6,6,6	0.36	0
3	DAU	F	3511	-	37,38,38	1.86	10 (27%)	55,58,58	1.81	10 (18%)
2	SO4	E	3810	-	4,4,4	0.38	0	6,6,6	0.84	0
2	SO4	A	3818	-	4,4,4	0.27	0	6,6,6	0.38	0
2	SO4	H	3703	-	4,4,4	0.24	0	6,6,6	0.28	0
2	SO4	F	3811	-	4,4,4	0.27	0	6,6,6	0.35	0
3	DAU	B	3502	-	37,38,38	1.88	10 (27%)	55,58,58	2.09	12 (21%)
2	SO4	A	3802	-	4,4,4	0.27	0	6,6,6	0.35	0
2	SO4	H	3816	-	4,4,4	0.25	0	6,6,6	0.44	0
3	DAU	E	3508	-	37,38,38	1.90	9 (24%)	55,58,58	2.40	17 (30%)
3	DAU	A	3500	-	37,38,38	1.85	9 (24%)	55,58,58	2.75	19 (34%)
2	SO4	D	3807	-	4,4,4	0.25	0	6,6,6	0.40	0
3	DAU	D	3506	-	37,38,38	1.98	11 (29%)	55,58,58	2.08	15 (27%)
3	DAU	G	3514	-	37,38,38	2.13	9 (24%)	55,58,58	2.73	14 (25%)
3	DAU	H	3512	-	37,38,38	1.91	11 (29%)	55,58,58	2.42	16 (29%)
3	DAU	H	3513	-	37,38,38	1.96	10 (27%)	55,58,58	1.90	9 (16%)
2	SO4	G	3702	-	4,4,4	0.28	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DAU	D	3507	-	37,38,38	1.89	9 (24%)	55,58,58	1.61	10 (18%)
2	SO4	E	3809	-	4,4,4	0.25	0	6,6,6	0.22	0
4	CIT	A	3801	-	12,12,12	1.17	1 (8%)	17,17,17	1.97	5 (29%)
2	SO4	G	3812	-	4,4,4	0.34	0	6,6,6	0.50	0
2	SO4	C	3805	-	4,4,4	0.29	0	6,6,6	0.62	0
2	SO4	B	3701	-	4,4,4	0.23	0	6,6,6	0.46	0
2	SO4	B	3804	-	4,4,4	0.26	0	6,6,6	0.53	0
2	SO4	A	3700	-	4,4,4	0.20	0	6,6,6	0.29	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
3	DAU	C	3504	-	-	1/23/55/55	0/3/3/3
3	DAU	C	3505	-	-	5/23/55/55	0/3/3/3
3	DAU	B	3503	-	-	3/23/55/55	0/3/3/3
3	DAU	E	3508	-	-	0/23/55/55	0/3/3/3
3	DAU	D	3507	-	-	4/23/55/55	0/3/3/3
3	DAU	A	3500	-	-	2/23/55/55	0/3/3/3
3	DAU	A	3501	-	-	3/23/55/55	0/3/3/3
4	CIT	A	3800	-	-	3/16/16/16	-
3	DAU	E	3509	-	-	5/23/55/55	0/3/3/3
3	DAU	F	3511	-	-	4/23/55/55	0/3/3/3
4	CIT	A	3801	-	-	8/16/16/16	-
3	DAU	H	3513	-	-	3/23/55/55	0/3/3/3
3	DAU	G	3514	-	-	0/23/55/55	0/3/3/3
3	DAU	G	3515	-	-	3/23/55/55	0/3/3/3
3	DAU	F	3510	-	-	2/23/55/55	0/3/3/3
3	DAU	D	3506	-	-	0/23/55/55	0/3/3/3
3	DAU	B	3502	-	-	2/23/55/55	0/3/3/3
3	DAU	H	3512	-	-	1/23/55/55	0/3/3/3

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3514	DAU	P2-OPP	-8.63	1.50	1.59
3	C	3505	DAU	O41-C41	6.04	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3507	DAU	P-OPP	5.99	1.66	1.59
3	A	3501	DAU	O21-C21	5.90	1.33	1.23
3	B	3503	DAU	O21-C21	5.82	1.33	1.23
3	F	3511	DAU	P-OPP	5.77	1.65	1.59
3	D	3506	DAU	O21-C21	5.53	1.32	1.23
3	C	3504	DAU	P2-OPP	-5.43	1.53	1.59
3	H	3512	DAU	P2-OPP	-5.21	1.53	1.59
3	G	3515	DAU	O21-C21	5.13	1.32	1.23
3	H	3513	DAU	O21-C21	5.03	1.32	1.23
3	E	3508	DAU	P-OPP	5.01	1.64	1.59
3	C	3505	DAU	O21-C21	5.00	1.31	1.23
3	H	3513	DAU	P-OPP	4.82	1.64	1.59
3	A	3501	DAU	C41-C51	-4.78	1.37	1.44
3	B	3503	DAU	C41-C51	-4.76	1.37	1.44
3	D	3506	DAU	O41-C41	4.71	1.32	1.23
3	E	3509	DAU	O41-C41	4.71	1.32	1.23
3	B	3502	DAU	O41-C41	4.61	1.32	1.23
3	F	3510	DAU	P2-OPP	-4.58	1.54	1.59
3	B	3502	DAU	O21-C21	4.53	1.31	1.23
3	C	3504	DAU	O21-C21	4.52	1.31	1.23
3	A	3500	DAU	O21-C21	4.48	1.31	1.23
3	C	3504	DAU	O41-C41	4.35	1.31	1.23
3	E	3508	DAU	O21-C21	4.33	1.30	1.23
3	F	3510	DAU	O21-C21	4.31	1.30	1.23
3	B	3502	DAU	C41-N31	-4.30	1.30	1.38
3	D	3507	DAU	O21-C21	4.27	1.30	1.23
3	H	3512	DAU	O41-C41	4.24	1.31	1.23
3	F	3511	DAU	C41-C51	-4.20	1.38	1.44
3	E	3509	DAU	O21-C21	4.13	1.30	1.23
3	D	3507	DAU	C41-C51	-4.13	1.38	1.44
3	E	3508	DAU	C41-C51	-4.10	1.38	1.44
3	G	3515	DAU	C41-C51	-4.04	1.38	1.44
3	H	3513	DAU	O41-C41	4.00	1.31	1.23
3	H	3512	DAU	C61-C51	3.99	1.41	1.34
3	C	3505	DAU	C41-C51	-3.99	1.38	1.44
3	B	3502	DAU	C61-C51	3.96	1.41	1.34
3	D	3507	DAU	O41-C41	3.96	1.31	1.23
3	H	3513	DAU	C41-C51	-3.92	1.38	1.44
3	H	3513	DAU	P2-OPP	3.91	1.63	1.59
3	F	3510	DAU	C61-N11	-3.83	1.31	1.38
3	E	3508	DAU	O41-C41	3.78	1.30	1.23
3	D	3506	DAU	C41-C51	-3.74	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3514	DAU	C41-N31	-3.71	1.31	1.38
3	E	3509	DAU	P-OPP	3.71	1.63	1.59
3	H	3512	DAU	C41-C51	-3.67	1.38	1.44
3	F	3511	DAU	C41-N31	-3.61	1.32	1.38
3	A	3501	DAU	O41-C41	3.60	1.30	1.23
3	A	3500	DAU	C41-N31	-3.51	1.32	1.38
3	A	3500	DAU	O41-C41	3.51	1.30	1.23
3	A	3500	DAU	P2-OPP	-3.51	1.55	1.59
3	F	3510	DAU	P2-O3P	3.50	1.62	1.50
3	G	3515	DAU	P2-OPP	3.45	1.63	1.59
3	A	3501	DAU	C61-C51	3.45	1.40	1.34
3	G	3514	DAU	P2-O3P	3.43	1.62	1.50
3	G	3514	DAU	C61-C51	3.40	1.40	1.34
3	F	3510	DAU	C41-C51	-3.39	1.39	1.44
3	G	3514	DAU	C61-N11	-3.34	1.32	1.38
3	G	3514	DAU	O21-C21	3.34	1.29	1.23
3	H	3512	DAU	O21-C21	3.33	1.29	1.23
3	E	3509	DAU	C61-C51	3.29	1.40	1.34
3	A	3500	DAU	C21-N11	-3.23	1.33	1.38
3	A	3500	DAU	P2-O3P	3.21	1.61	1.50
3	H	3513	DAU	P2-O3P	3.20	1.61	1.50
3	F	3511	DAU	O21-C21	3.20	1.28	1.23
3	B	3502	DAU	P2-OPP	-3.15	1.56	1.59
3	C	3505	DAU	P-OPP	3.14	1.62	1.59
3	D	3506	DAU	P2-OPP	-3.12	1.56	1.59
3	F	3511	DAU	C21-N31	-3.12	1.32	1.38
3	C	3505	DAU	C21-N31	-3.11	1.32	1.38
3	F	3510	DAU	O41-C41	3.11	1.29	1.23
3	F	3510	DAU	C41-N31	-3.08	1.33	1.38
3	H	3512	DAU	P-O1P	3.05	1.61	1.50
3	E	3508	DAU	C41-N31	-3.04	1.33	1.38
3	A	3500	DAU	P-O1P	3.03	1.61	1.50
3	E	3508	DAU	P2-OPP	-2.97	1.56	1.59
3	A	3500	DAU	C61-C51	2.96	1.39	1.34
3	F	3510	DAU	C21-N31	-2.94	1.32	1.38
3	F	3510	DAU	P-OPP	-2.92	1.56	1.59
3	B	3502	DAU	C21-N11	-2.91	1.33	1.38
3	B	3503	DAU	C61-C51	2.88	1.39	1.34
3	D	3506	DAU	C61-C51	2.88	1.39	1.34
3	C	3504	DAU	C21-N11	-2.84	1.34	1.38
3	F	3511	DAU	O41-C41	2.84	1.28	1.23
3	E	3509	DAU	C21-N31	-2.83	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3506	DAU	C61-N11	-2.83	1.33	1.38
3	G	3514	DAU	O41-C41	2.82	1.28	1.23
3	A	3500	DAU	C41-C51	-2.81	1.40	1.44
3	D	3507	DAU	C61-C51	2.80	1.39	1.34
3	D	3506	DAU	C41-N31	-2.80	1.33	1.38
3	G	3515	DAU	P2-O3P	2.79	1.60	1.50
3	D	3507	DAU	C41-N31	-2.75	1.33	1.38
3	C	3505	DAU	C61-C51	2.73	1.39	1.34
3	B	3502	DAU	C61-N11	-2.70	1.33	1.38
3	E	3508	DAU	P2-O3P	2.62	1.59	1.50
3	D	3506	DAU	C21-N11	-2.62	1.34	1.38
3	C	3504	DAU	P2-O3P	2.62	1.59	1.50
3	B	3503	DAU	P-OPP	2.62	1.62	1.59
3	E	3508	DAU	C61-C51	2.59	1.38	1.34
3	D	3506	DAU	C21-N31	-2.57	1.33	1.38
3	H	3512	DAU	C21-N31	-2.54	1.33	1.38
3	B	3503	DAU	C41-N31	-2.54	1.34	1.38
3	B	3502	DAU	P-O1P	2.52	1.59	1.50
3	F	3511	DAU	C61-C51	2.51	1.38	1.34
3	C	3504	DAU	C41-C51	-2.51	1.40	1.44
3	G	3515	DAU	P-OPP	2.50	1.62	1.59
3	B	3502	DAU	P2-O3P	2.49	1.59	1.50
3	H	3512	DAU	C61-N11	-2.49	1.33	1.38
3	D	3506	DAU	P2-O3P	2.45	1.59	1.50
3	D	3506	DAU	P-O1P	2.44	1.59	1.50
3	H	3513	DAU	C61-N11	-2.39	1.33	1.38
3	E	3508	DAU	P-O1P	2.35	1.58	1.50
3	F	3511	DAU	C21-N11	-2.33	1.34	1.38
3	H	3512	DAU	P2-O3P	2.30	1.58	1.50
3	F	3510	DAU	C21-N11	-2.30	1.34	1.38
3	F	3511	DAU	P2-O3P	2.29	1.58	1.50
3	G	3514	DAU	P-O1P	2.29	1.58	1.50
3	E	3509	DAU	C41-C51	-2.27	1.41	1.44
3	E	3509	DAU	C41-N31	-2.26	1.34	1.38
3	H	3512	DAU	C41-N31	-2.26	1.34	1.38
3	H	3513	DAU	C21-N31	-2.26	1.34	1.38
3	B	3502	DAU	C41-C51	-2.25	1.41	1.44
3	G	3515	DAU	O41-C41	2.25	1.27	1.23
3	D	3507	DAU	P2-O1	2.20	1.65	1.59
3	H	3513	DAU	C61-C51	2.20	1.38	1.34
3	H	3513	DAU	C41-N31	-2.18	1.34	1.38
3	C	3505	DAU	C61-N11	-2.17	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3503	DAU	O41-C41	2.15	1.27	1.23
3	B	3503	DAU	C61-N11	-2.13	1.34	1.38
3	E	3509	DAU	P2-OPP	2.12	1.61	1.59
4	A	3801	CIT	O2-C1	-2.12	1.23	1.30
3	C	3505	DAU	P-O1P	2.11	1.58	1.50
3	G	3514	DAU	O4'-C1'	2.11	1.47	1.42
3	D	3507	DAU	P-O1P	2.10	1.58	1.50
3	E	3509	DAU	P2-O1	2.09	1.65	1.59
3	H	3512	DAU	C21-N11	-2.06	1.35	1.38
3	D	3507	DAU	C21-N11	-2.02	1.35	1.38
3	C	3504	DAU	P-O1P	2.02	1.57	1.50
3	F	3511	DAU	P2-O1	2.01	1.65	1.59

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3514	DAU	O2P-P-OPP	-9.26	82.24	107.27
3	F	3510	DAU	O5-C1-O1	-8.44	100.33	111.36
3	G	3514	DAU	C41-N31-C21	-7.83	117.08	127.34
3	A	3501	DAU	C51-C41-N31	7.21	121.59	115.32
3	G	3514	DAU	N31-C21-N11	7.10	124.13	114.89
3	G	3515	DAU	C51-C41-N31	7.09	121.49	115.32
3	F	3510	DAU	OPP-P2-O3P	-6.83	90.14	110.70
3	B	3503	DAU	C51-C41-N31	6.76	121.20	115.32
3	A	3500	DAU	C41-N31-C21	-6.71	118.55	127.34
3	G	3515	DAU	C41-N31-C21	-6.69	118.57	127.34
3	G	3514	DAU	C51-C41-N31	6.60	121.06	115.32
3	F	3511	DAU	C51-C41-N31	6.38	120.87	115.32
3	E	3508	DAU	C51-C41-N31	6.34	120.83	115.32
3	E	3508	DAU	C41-N31-C21	-6.24	119.16	127.34
3	A	3501	DAU	C41-N31-C21	-6.23	119.17	127.34
3	A	3500	DAU	C51-C41-N31	6.22	120.73	115.32
3	A	3500	DAU	OPP-P2-O3P	-6.22	92.00	110.70
3	A	3500	DAU	N31-C21-N11	6.21	122.97	114.89
3	H	3512	DAU	N31-C21-N11	6.14	122.88	114.89
3	C	3504	DAU	C41-N31-C21	-6.14	119.29	127.34
3	D	3506	DAU	O5-C1-O1	-5.95	103.58	111.36
3	A	3501	DAU	O41-C41-C51	-5.93	118.13	124.92
3	A	3500	DAU	O2P-P-OPP	-5.91	91.29	107.27
3	C	3504	DAU	O2P-P-OPP	-5.91	91.31	107.27
3	H	3512	DAU	C41-N31-C21	-5.90	119.60	127.34
3	B	3502	DAU	N31-C21-N11	5.87	122.53	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3513	DAU	C41-N31-C21	-5.82	119.71	127.34
3	H	3512	DAU	O2P-P-OPP	-5.72	91.80	107.27
3	E	3508	DAU	N31-C21-N11	5.71	122.33	114.89
3	E	3509	DAU	N31-C21-N11	5.57	122.15	114.89
3	B	3502	DAU	O2P-P-OPP	-5.55	92.27	107.27
3	B	3502	DAU	C41-N31-C21	-5.43	120.22	127.34
3	G	3515	DAU	O41-C41-C51	-5.43	118.71	124.92
3	A	3500	DAU	O41-C41-C51	-5.42	118.72	124.92
3	F	3510	DAU	N31-C21-N11	5.30	121.78	114.89
3	D	3507	DAU	C51-C41-N31	5.28	119.91	115.32
3	C	3504	DAU	N31-C21-N11	5.20	121.65	114.89
3	H	3512	DAU	OPP-P2-O3P	-5.17	95.15	110.70
3	H	3512	DAU	C51-C41-N31	5.10	119.76	115.32
3	A	3500	DAU	C51-C61-N11	-5.07	117.80	123.31
3	F	3510	DAU	C41-N31-C21	-5.07	120.70	127.34
3	C	3504	DAU	C51-C41-N31	5.01	119.68	115.32
3	H	3513	DAU	C51-C41-N31	4.98	119.65	115.32
3	B	3503	DAU	C41-N31-C21	-4.95	120.86	127.34
3	E	3508	DAU	O41-C41-C51	-4.92	119.29	124.92
3	H	3513	DAU	N31-C21-N11	4.91	121.28	114.89
3	E	3509	DAU	C41-N31-C21	-4.89	120.93	127.34
3	D	3506	DAU	C5A-C51-C41	4.88	124.00	118.78
3	E	3508	DAU	OPP-P2-O3P	-4.85	96.10	110.70
4	A	3800	CIT	O7-C3-C6	-4.85	102.08	108.96
3	F	3511	DAU	C41-N31-C21	-4.84	120.99	127.34
3	F	3511	DAU	N31-C21-N11	4.82	121.17	114.89
3	E	3508	DAU	O5-C1-O1	-4.82	105.07	111.36
3	G	3514	DAU	C51-C61-N11	-4.78	118.12	123.31
3	B	3502	DAU	O2P-P-O1P	4.78	134.66	112.44
3	D	3507	DAU	C41-N31-C21	-4.77	121.08	127.34
3	B	3502	DAU	C51-C41-N31	4.73	119.44	115.32
3	C	3504	DAU	O2P-P-O1P	4.68	134.22	112.44
3	H	3512	DAU	O41-C41-C51	-4.65	119.59	124.92
3	G	3514	DAU	O2P-P-O1P	4.62	133.91	112.44
3	E	3508	DAU	O2P-P-OPP	-4.60	94.84	107.27
3	D	3507	DAU	N31-C21-N11	4.57	120.84	114.89
3	D	3506	DAU	O2P-P-OPP	-4.54	94.99	107.27
3	E	3509	DAU	C51-C41-N31	4.53	119.26	115.32
3	A	3500	DAU	O5-C1-O1	-4.53	105.44	111.36
3	A	3500	DAU	O4P-P2-OPP	4.48	119.39	107.27
3	G	3515	DAU	N31-C21-N11	4.44	120.67	114.89
3	B	3502	DAU	C51-C61-N11	-4.39	118.54	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3514	DAU	OPP-P2-O3P	-4.36	97.59	110.70
3	B	3503	DAU	O5-C1-O1	-4.35	105.68	111.36
3	C	3504	DAU	OPP-P2-O3P	-4.30	97.76	110.70
3	H	3513	DAU	O5-C1-O1	-4.28	105.77	111.36
3	C	3504	DAU	O41-C41-C51	-4.26	120.04	124.92
3	C	3505	DAU	C5A-C51-C41	4.25	123.32	118.78
3	H	3512	DAU	O2P-P-O1P	4.24	132.16	112.44
3	F	3510	DAU	O41-C41-C51	-4.16	120.15	124.92
3	A	3500	DAU	O4'-C1'-C2'	-4.16	98.47	106.25
3	F	3511	DAU	O41-C41-C51	-3.99	120.35	124.92
4	A	3801	CIT	O6-C6-C3	3.98	120.78	113.14
3	B	3503	DAU	O41-C41-C51	-3.95	120.40	124.92
3	A	3501	DAU	N31-C21-N11	3.94	120.02	114.89
3	H	3513	DAU	O41-C41-C51	-3.94	120.41	124.92
3	C	3504	DAU	O21-C21-N11	-3.93	117.68	122.80
3	G	3514	DAU	O21-C21-N11	-3.86	117.77	122.80
3	F	3510	DAU	C51-C41-N31	3.85	118.67	115.32
3	H	3513	DAU	C51-C61-N11	-3.84	119.15	123.31
3	F	3510	DAU	O4P-P2-OPP	3.80	117.54	107.27
3	H	3512	DAU	C51-C61-N11	-3.77	119.22	123.31
3	D	3506	DAU	N31-C21-N11	3.76	119.79	114.89
3	D	3506	DAU	O2P-P-O1P	3.76	129.92	112.44
3	A	3500	DAU	O21-C21-N11	-3.74	117.93	122.80
3	D	3506	DAU	OPP-P2-O3P	-3.73	99.50	110.70
4	A	3800	CIT	O4-C5-C4	3.63	125.85	114.35
3	A	3500	DAU	O2P-P-O1P	3.61	129.23	112.44
3	C	3504	DAU	C51-C61-N11	-3.59	119.42	123.31
3	H	3512	DAU	O4'-C1'-N11	-3.55	101.57	107.86
3	D	3506	DAU	C51-C41-N31	3.52	118.38	115.32
3	E	3508	DAU	O2P-P-O1P	3.49	128.68	112.44
3	G	3514	DAU	C5A-C51-C41	3.46	122.48	118.78
3	G	3515	DAU	C5A-C51-C41	3.46	122.48	118.78
4	A	3801	CIT	O7-C3-C6	-3.41	104.12	108.96
3	F	3510	DAU	O5-C1-C2	3.38	117.32	110.37
3	C	3505	DAU	N31-C21-N11	3.36	119.27	114.89
3	H	3512	DAU	O21-C21-N11	-3.32	118.48	122.80
3	B	3503	DAU	N31-C21-N11	3.31	119.20	114.89
3	E	3508	DAU	C51-C61-N11	-3.30	119.73	123.31
3	C	3504	DAU	C5A-C51-C41	3.29	122.30	118.78
3	G	3514	DAU	C5A-C51-C61	-3.29	118.40	122.85
3	C	3505	DAU	C51-C41-N31	3.28	118.17	115.32
3	G	3514	DAU	O41-C41-C51	-3.25	121.20	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3506	DAU	O5-C1-C2	3.25	117.04	110.37
3	H	3512	DAU	O5-C1-O1	-3.22	107.16	111.36
4	A	3801	CIT	O2-C1-O1	-3.17	115.17	123.33
3	D	3506	DAU	C41-N31-C21	-3.15	123.21	127.34
3	C	3504	DAU	C5A-C51-C61	-3.14	118.60	122.85
3	F	3511	DAU	O4P-P2-OPP	3.07	115.58	107.27
3	F	3510	DAU	O2P-P-O1P	3.06	126.70	112.44
3	D	3506	DAU	C5A-C51-C61	-3.03	118.74	122.85
3	F	3511	DAU	O1-P2-O3P	-3.03	100.13	109.81
3	F	3510	DAU	O21-C21-N11	-3.02	118.86	122.80
3	H	3513	DAU	O21-C21-N11	-3.00	118.89	122.80
3	C	3504	DAU	O5-C1-O1	-3.00	107.45	111.36
3	A	3501	DAU	C51-C61-N11	-2.99	120.07	123.31
3	A	3500	DAU	O4'-C1'-N11	-2.98	102.58	107.86
3	A	3500	DAU	C1'-N11-C61	-2.96	115.77	120.74
3	H	3512	DAU	C2'-C1'-N11	2.93	121.15	113.81
3	D	3506	DAU	C1-O5-C5	2.93	119.44	113.72
3	E	3508	DAU	O4'-C1'-C2'	-2.86	100.91	106.25
3	B	3503	DAU	O5-C1-C2	2.85	116.23	110.37
3	E	3509	DAU	C51-C61-N11	-2.84	120.22	123.31
3	D	3506	DAU	O5'-P-O1P	-2.84	97.67	108.94
3	F	3511	DAU	C51-C61-N11	-2.81	120.27	123.31
3	C	3504	DAU	C2'-C1'-N11	2.80	120.80	113.81
3	C	3505	DAU	C41-N31-C21	-2.79	123.68	127.34
3	E	3508	DAU	C2'-C1'-N11	2.78	120.77	113.81
4	A	3800	CIT	O6-C6-C3	2.75	118.42	113.14
3	F	3510	DAU	O3'-C3'-C4'	-2.72	99.74	110.07
3	C	3504	DAU	O5'-P-O1P	-2.72	98.14	108.94
3	C	3504	DAU	O4'-C1'-C2'	-2.72	101.16	106.25
3	G	3515	DAU	C5A-C51-C61	-2.72	119.17	122.85
3	A	3500	DAU	O5-C1-C2	2.71	115.94	110.37
3	D	3506	DAU	O4P-P2-O3P	2.71	125.05	112.44
3	E	3508	DAU	C1-O5-C5	2.70	119.00	113.72
3	B	3502	DAU	O4P-P2-O3P	2.70	125.02	112.44
3	A	3500	DAU	C1'-N11-C21	2.70	122.93	117.66
3	B	3502	DAU	O21-C21-N11	-2.67	119.32	122.80
3	C	3505	DAU	C5A-C51-C61	-2.65	119.26	122.85
3	C	3504	DAU	O1-P2-O3P	-2.65	101.33	109.81
3	D	3506	DAU	C3-C4-C5	2.65	115.03	110.23
3	D	3507	DAU	O4P-P2-O3P	2.65	124.75	112.44
4	A	3801	CIT	O7-C3-C4	2.63	115.37	109.38
3	G	3515	DAU	C51-C61-N11	-2.61	120.48	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3514	DAU	O5-C1-O1	-2.59	107.97	111.36
4	A	3800	CIT	O2-C1-O1	-2.59	116.67	123.33
3	F	3510	DAU	C5A-C51-C41	2.54	121.49	118.78
3	A	3501	DAU	C1'-N11-C21	2.53	122.62	117.66
3	D	3506	DAU	O41-C41-N31	-2.53	115.36	120.11
3	G	3514	DAU	O4P-P2-OPP	2.52	114.09	107.27
3	F	3510	DAU	O4P-P2-O3P	2.48	123.98	112.44
3	A	3501	DAU	O1-P2-O3P	-2.47	101.91	109.81
3	E	3509	DAU	C61-N11-C21	-2.46	118.86	121.30
3	E	3509	DAU	O3-C3-C2	-2.43	104.64	110.38
3	H	3512	DAU	C6-C5-C4	-2.43	107.05	113.02
3	E	3508	DAU	C61-N11-C21	-2.43	118.88	121.30
3	B	3502	DAU	C3-C4-C5	2.43	114.64	110.23
3	F	3510	DAU	C61-N11-C21	-2.42	118.89	121.30
3	B	3502	DAU	OPP-P2-O3P	-2.41	103.45	110.70
3	B	3502	DAU	O41-C41-C51	-2.40	122.17	124.92
3	E	3509	DAU	O21-C21-N11	-2.40	119.68	122.80
3	E	3508	DAU	O21-C21-N31	-2.39	117.09	121.49
3	G	3514	DAU	O5-C1-C2	2.38	115.26	110.37
3	D	3507	DAU	C61-N11-C21	-2.38	118.94	121.30
3	E	3509	DAU	O41-C41-C51	-2.37	122.21	124.92
3	C	3505	DAU	O4P-P2-O3P	2.36	123.44	112.44
3	A	3500	DAU	O4-C4-C3	2.36	115.93	110.38
3	A	3500	DAU	O5-C5-C4	2.34	113.92	109.70
3	E	3508	DAU	O5'-P-O1P	-2.32	99.73	108.94
3	G	3515	DAU	O5-C1-O1	-2.32	108.34	111.36
3	B	3503	DAU	O4P-P2-OPP	2.29	113.47	107.27
3	H	3512	DAU	O5-C1-C2	2.29	115.07	110.37
3	B	3503	DAU	C51-C61-N11	-2.28	120.83	123.31
3	A	3501	DAU	O5-C5-C4	2.28	113.81	109.70
3	C	3504	DAU	O5'-C5'-C4'	2.28	116.75	108.99
3	F	3510	DAU	O4'-C1'-N11	2.27	111.90	107.86
4	A	3800	CIT	O3-C5-C4	-2.26	116.55	122.95
3	H	3512	DAU	OPP-P-O1P	2.25	117.46	110.70
3	G	3515	DAU	O4P-P2-OPP	2.24	113.34	107.27
3	C	3505	DAU	O4P-P2-OPP	2.24	113.32	107.27
3	A	3501	DAU	O4P-P2-O3P	2.24	122.85	112.44
4	A	3800	CIT	O4-C5-O3	-2.23	117.59	123.33
3	A	3501	DAU	O5-C1-O1	-2.23	108.45	111.36
4	A	3801	CIT	O4-C5-C4	2.23	121.40	114.35
3	F	3510	DAU	C3-C4-C5	2.22	114.26	110.23
3	C	3504	DAU	O5-C1-C2	2.21	114.92	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3508	DAU	O1-P2-O3P	-2.21	102.75	109.81
3	H	3513	DAU	C5A-C51-C61	-2.21	119.86	122.85
3	C	3504	DAU	O4'-C4'-C5'	-2.20	102.28	109.33
3	F	3511	DAU	C61-N11-C21	-2.19	119.12	121.30
3	D	3507	DAU	C51-C61-N11	-2.18	120.95	123.31
3	E	3508	DAU	O4'-C1'-N11	-2.18	104.00	107.86
3	C	3504	DAU	C1'-N11-C21	2.18	121.92	117.66
3	E	3509	DAU	C5A-C51-C41	2.17	121.10	118.78
3	B	3502	DAU	O3'-C3'-C4'	-2.15	101.91	110.07
3	D	3507	DAU	O4P-P2-OPP	2.15	113.08	107.27
3	C	3504	DAU	C1'-N11-C61	-2.14	117.14	120.74
3	F	3510	DAU	C5A-C51-C61	-2.14	119.95	122.85
3	C	3505	DAU	O1-P2-O3P	-2.14	102.96	109.81
3	H	3513	DAU	O1-C1-C2	2.14	112.30	108.38
3	E	3509	DAU	O2-C2-C1	2.13	115.16	110.08
3	F	3511	DAU	O21-C21-N31	-2.13	117.56	121.49
3	B	3503	DAU	O21-C21-N11	-2.11	120.05	122.80
3	D	3507	DAU	C2-C3-C4	-2.10	107.15	110.83
3	G	3515	DAU	O5-C1-C2	2.08	114.64	110.37
3	C	3505	DAU	C4'-O4'-C1'	2.08	114.44	109.51
3	D	3507	DAU	O5-C1-O1	-2.06	108.67	111.36
3	F	3511	DAU	C1-C2-C3	-2.05	105.69	110.01
3	H	3512	DAU	C2-C3-C4	-2.04	107.25	110.83
3	D	3507	DAU	O1-P2-O3P	-2.04	103.30	109.81
3	A	3500	DAU	C2'-C1'-N11	2.01	118.83	113.81

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3501	DAU	P2-OPP-P-O5'
3	D	3507	DAU	P2-OPP-P-O5'
3	F	3510	DAU	C1-O1-P2-OPP
3	F	3511	DAU	P2-OPP-P-O5'
3	H	3513	DAU	P2-OPP-P-O5'
4	A	3800	CIT	C1-C2-C3-C4
4	A	3800	CIT	C1-C2-C3-C6
4	A	3801	CIT	O7-C3-C6-O5
4	A	3801	CIT	O7-C3-C6-O6
4	A	3801	CIT	C4-C3-C6-O5
4	A	3801	CIT	C4-C3-C6-O6
4	A	3801	CIT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	A	3801	CIT	C1-C2-C3-C6
4	A	3800	CIT	C1-C2-C3-O7
3	C	3504	DAU	O5-C5-C6-O6
4	A	3801	CIT	C2-C3-C4-C5
3	B	3503	DAU	P2-OPP-P-O5'
3	C	3505	DAU	P2-OPP-P-O5'
3	E	3509	DAU	P2-OPP-P-O5'
3	G	3515	DAU	P2-OPP-P-O5'
4	A	3801	CIT	C6-C3-C4-C5
3	D	3507	DAU	C1-O1-P2-O4P
3	E	3509	DAU	C1-O1-P2-O4P
3	A	3501	DAU	P-OPP-P2-O4P
3	B	3502	DAU	P2-OPP-P-O1P
3	B	3503	DAU	P-OPP-P2-O4P
3	G	3515	DAU	P-OPP-P2-O4P
3	H	3513	DAU	P-OPP-P2-O4P
3	C	3505	DAU	P-OPP-P2-O4P
3	D	3507	DAU	P-OPP-P2-O4P
3	E	3509	DAU	P-OPP-P2-O4P
3	F	3511	DAU	P-OPP-P2-O4P
3	H	3513	DAU	P-OPP-P2-O3P
3	A	3500	DAU	P2-OPP-P-O1P
3	A	3501	DAU	P-OPP-P2-O3P
3	G	3515	DAU	P-OPP-P2-O3P
3	C	3505	DAU	C1-O1-P2-O3P
3	C	3505	DAU	C1-O1-P2-O4P
3	E	3509	DAU	C1-O1-P2-O3P
3	F	3510	DAU	C1-O1-P2-O4P
3	F	3511	DAU	C1-O1-P2-O3P
3	D	3507	DAU	P-OPP-P2-O3P
3	E	3509	DAU	P-OPP-P2-O3P
3	F	3511	DAU	P-OPP-P2-O3P
3	H	3512	DAU	P2-OPP-P-O2P
3	A	3500	DAU	P2-OPP-P-O2P
3	B	3502	DAU	P2-OPP-P-O2P
3	B	3503	DAU	P-OPP-P2-O3P
3	C	3505	DAU	P-OPP-P2-O3P

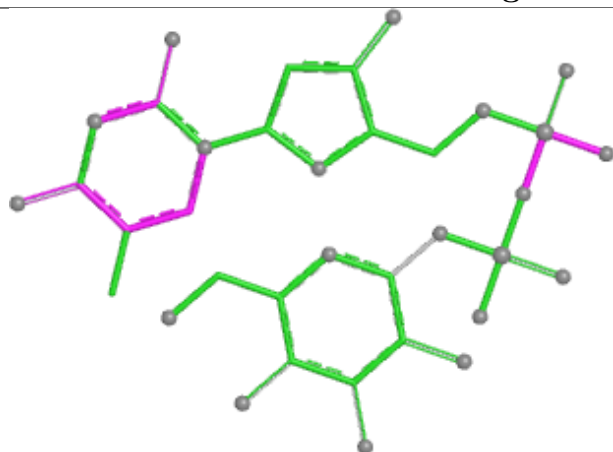
There are no ring outliers.

20 monomers are involved in 47 short contacts:

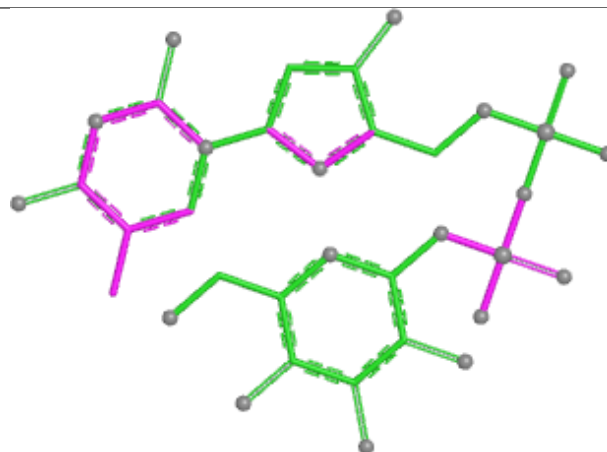
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3501	DAU	2	0
4	A	3800	CIT	3	0
2	C	3806	SO4	1	0
3	F	3510	DAU	4	0
3	C	3504	DAU	3	0
2	E	3820	SO4	1	0
2	H	3814	SO4	1	0
2	E	3810	SO4	2	0
2	A	3818	SO4	2	0
2	H	3703	SO4	3	0
3	B	3502	DAU	2	0
2	A	3802	SO4	2	0
3	E	3508	DAU	3	0
3	A	3500	DAU	1	0
3	D	3506	DAU	1	0
3	H	3512	DAU	1	0
3	H	3513	DAU	1	0
2	G	3702	SO4	4	0
4	A	3801	CIT	9	0
2	B	3701	SO4	2	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.

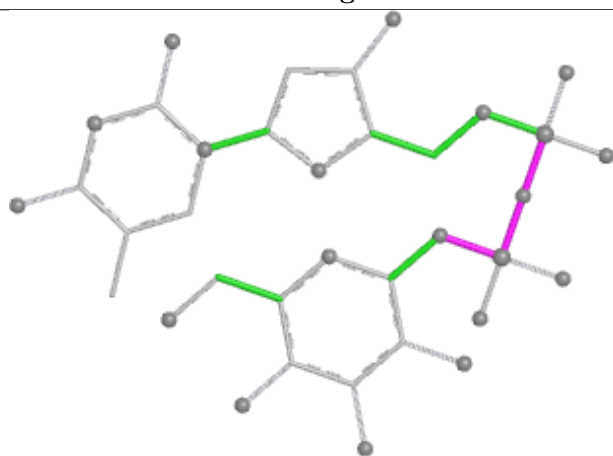
Ligand DAU C 3505



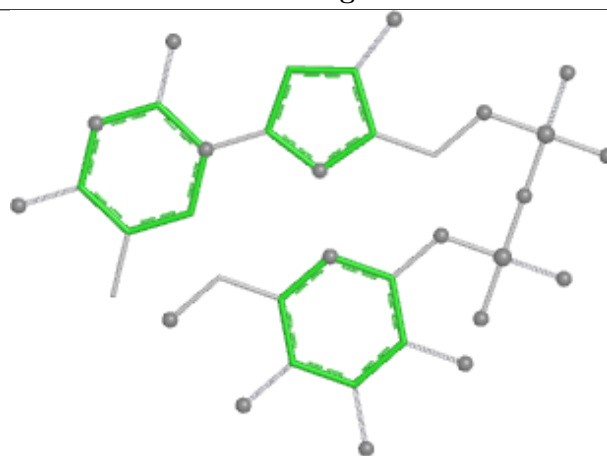
Bond lengths



Bond angles

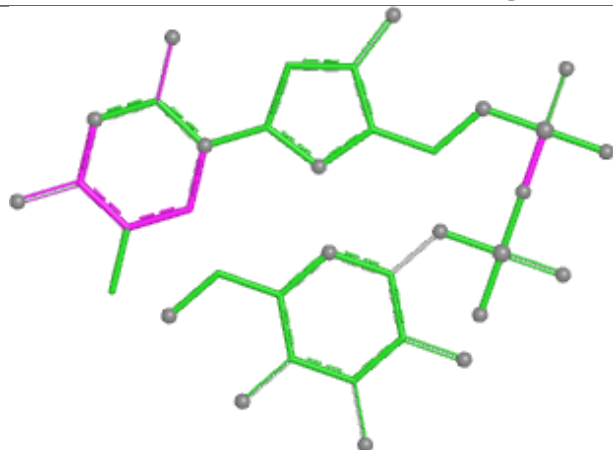


Torsions

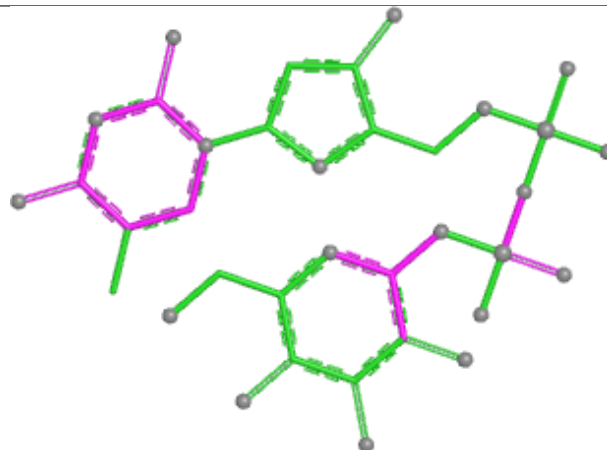


Rings

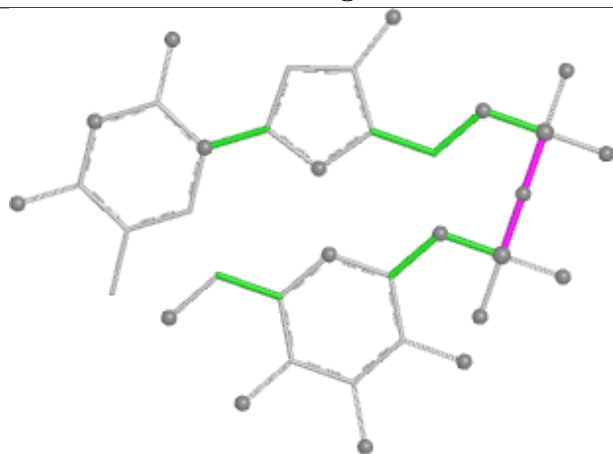
Ligand DAU B 3503



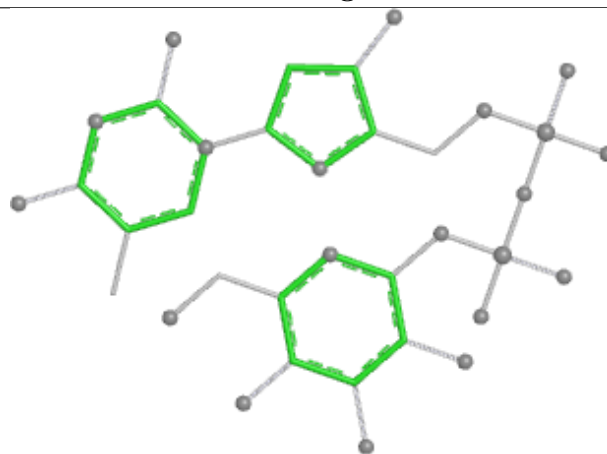
Bond lengths



Bond angles

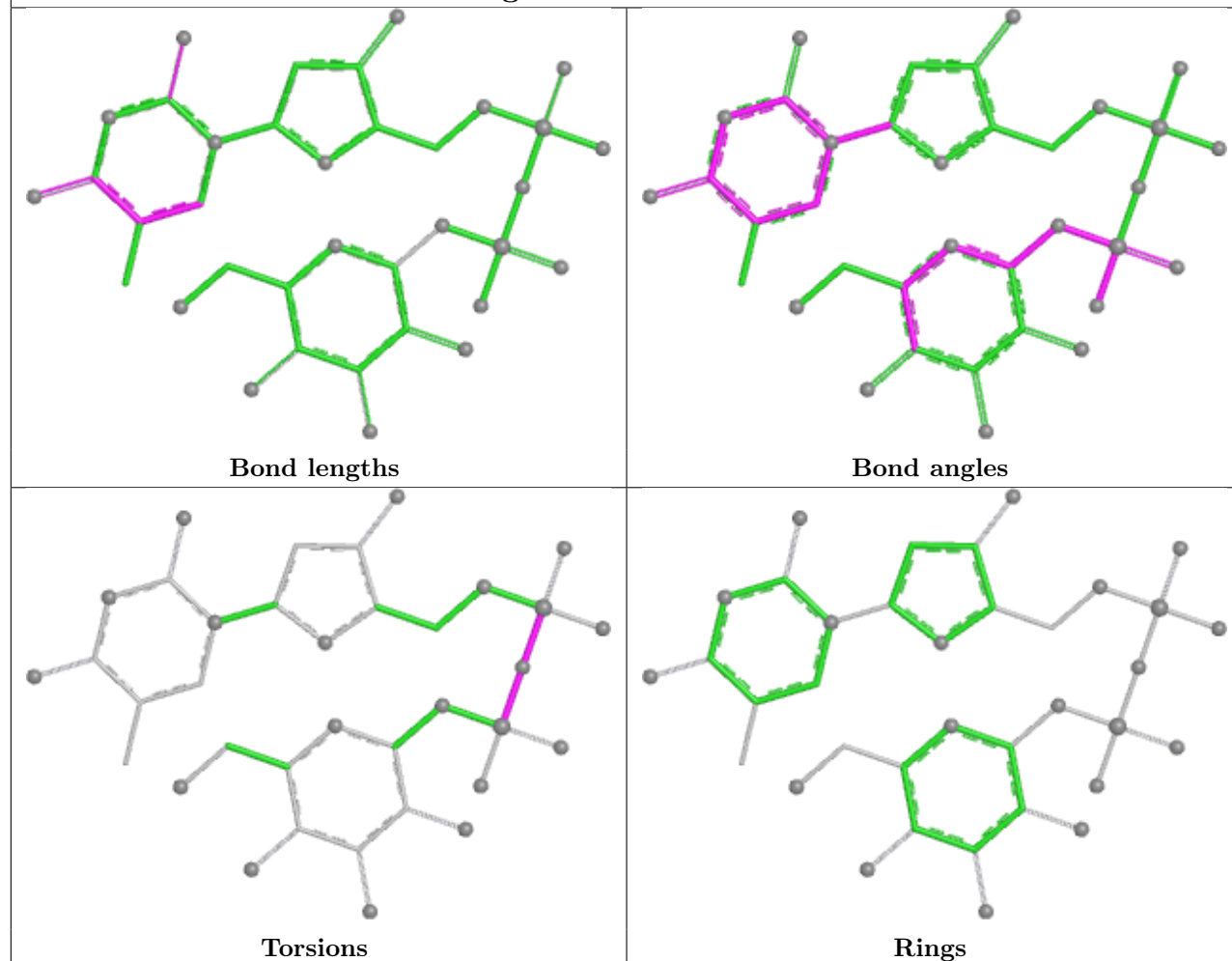


Torsions

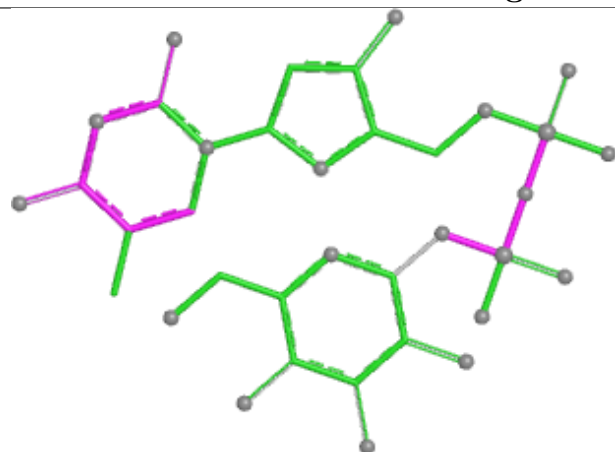


Rings

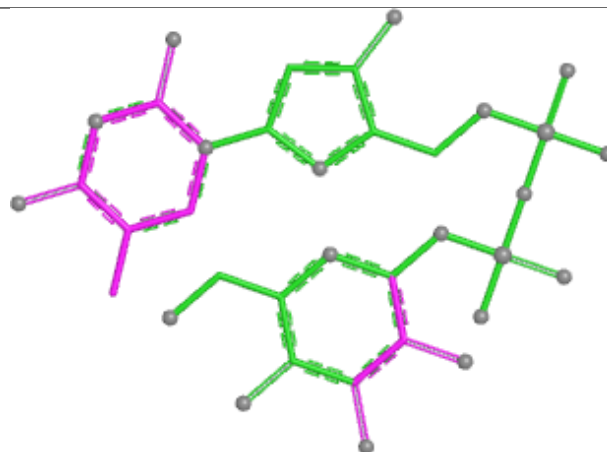
Ligand DAU A 3501



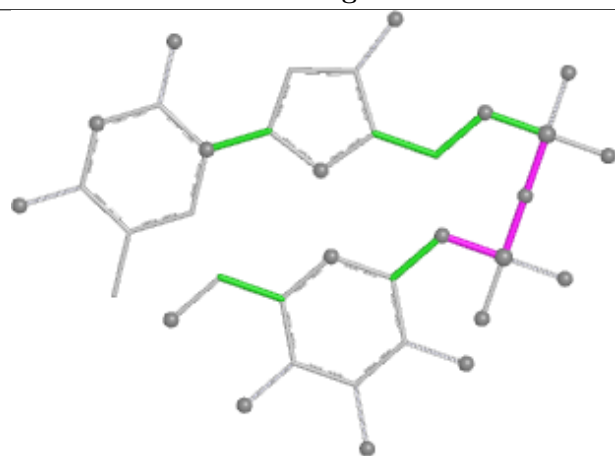
Ligand DAU E 3509



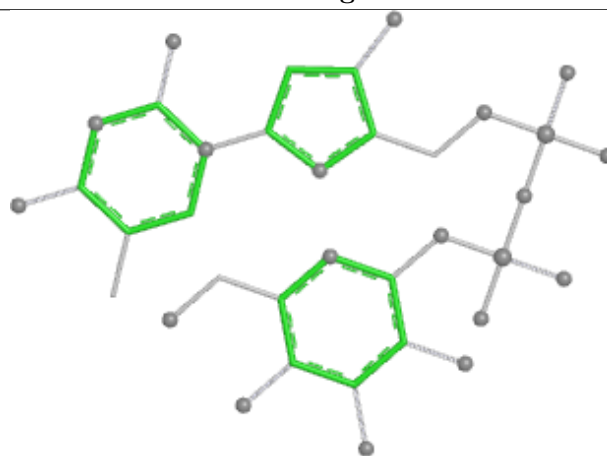
Bond lengths



Bond angles

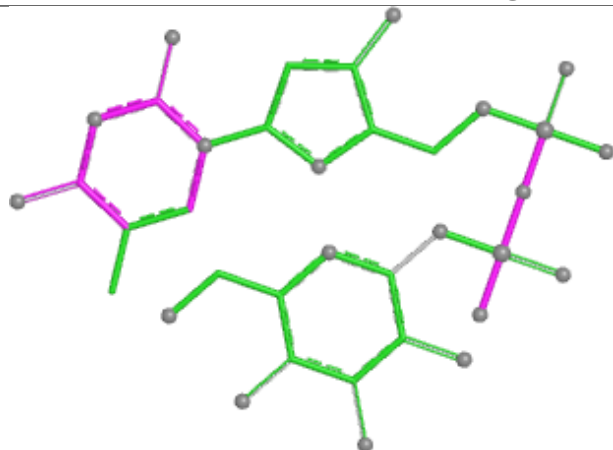


Torsions

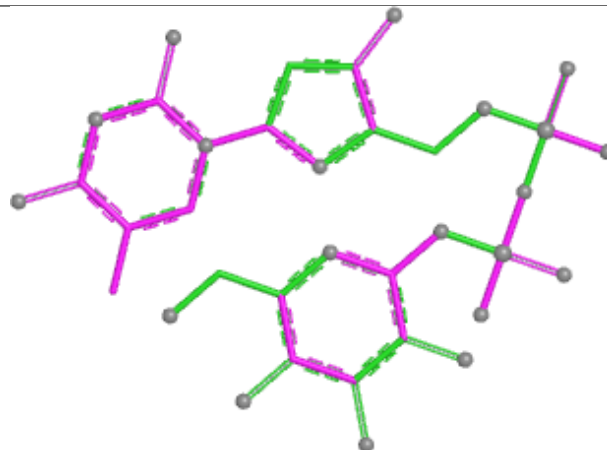


Rings

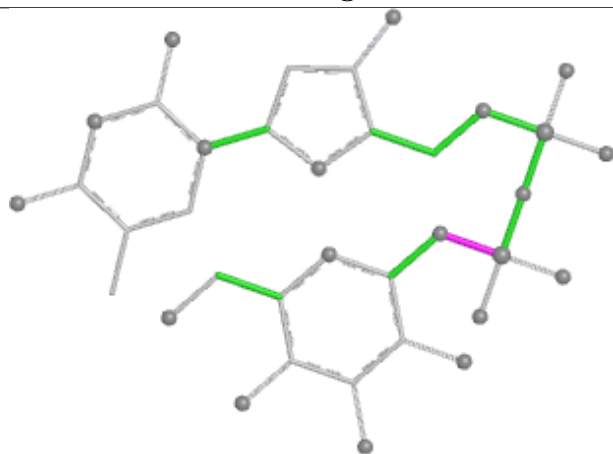
Ligand DAU F 3510



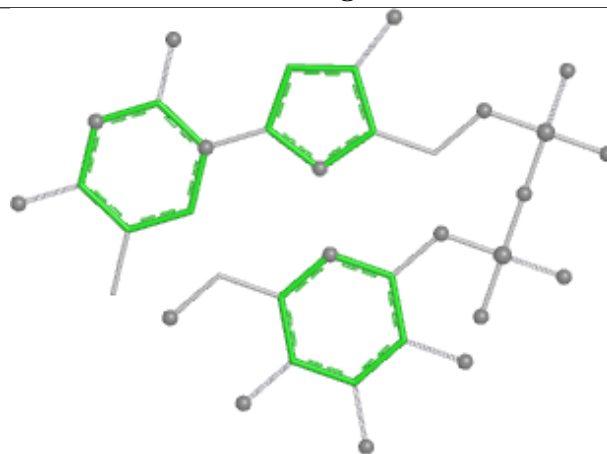
Bond lengths



Bond angles

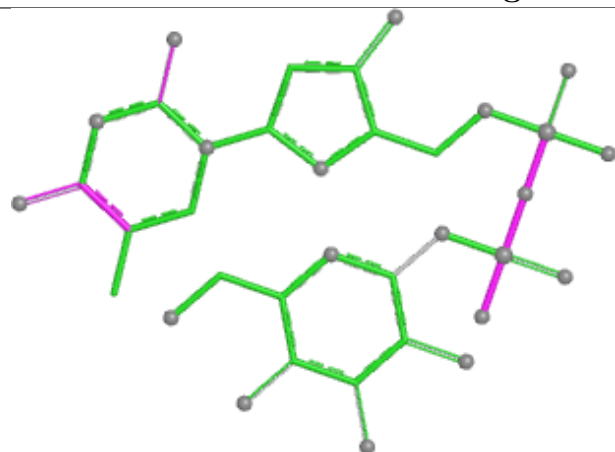


Torsions

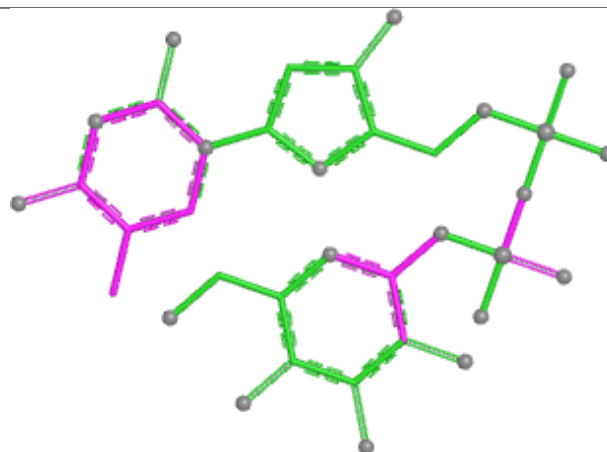


Rings

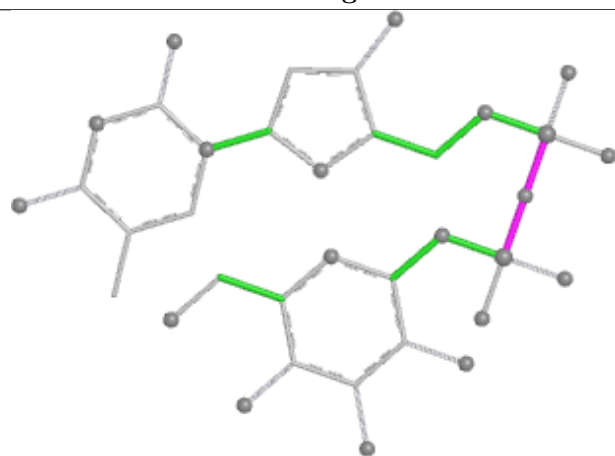
Ligand DAU G 3515



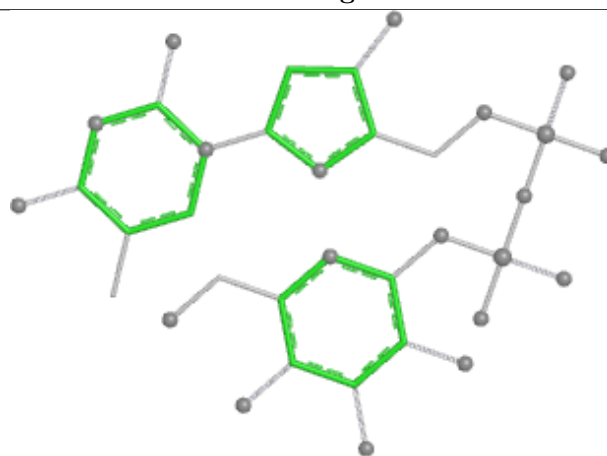
Bond lengths



Bond angles

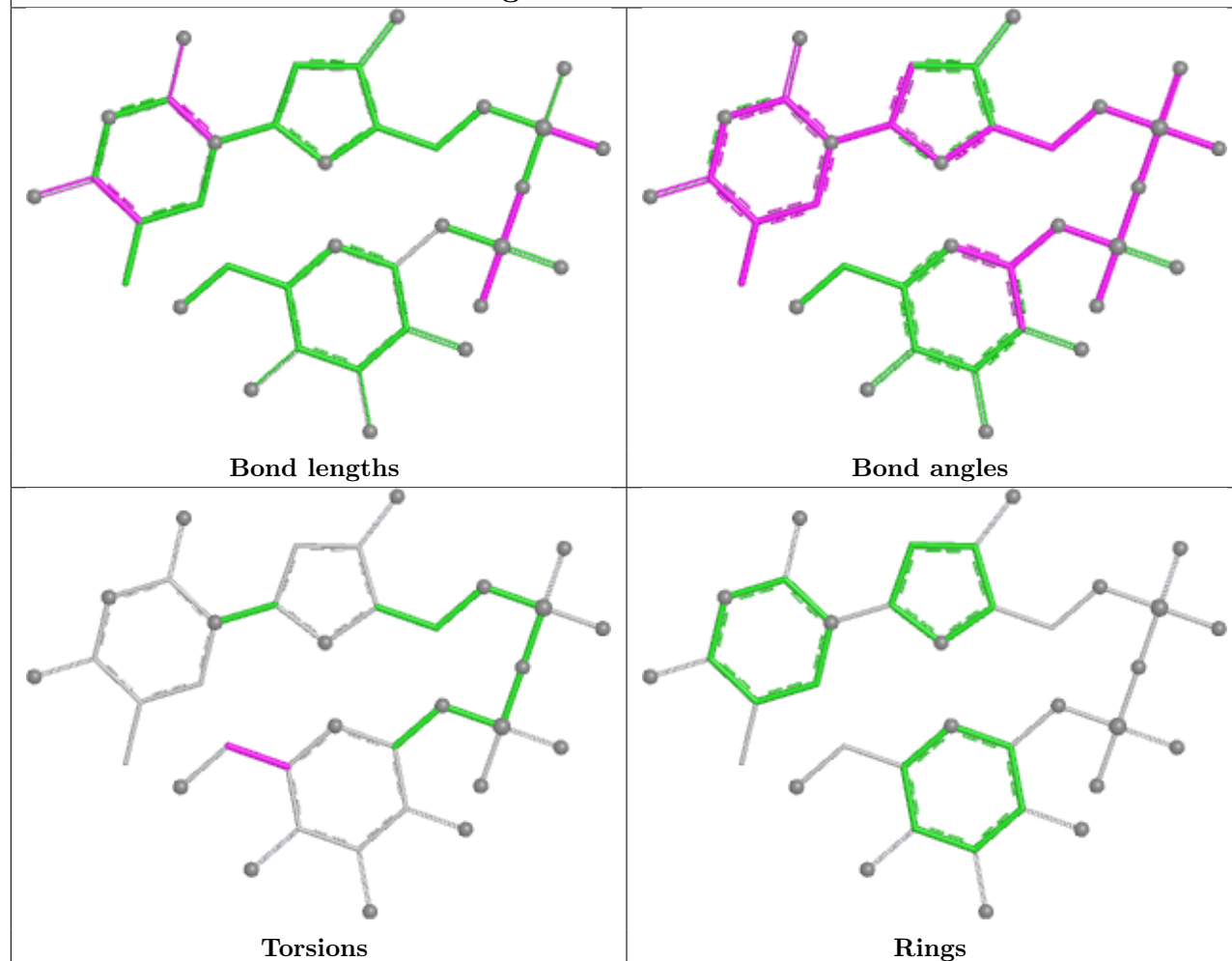


Torsions

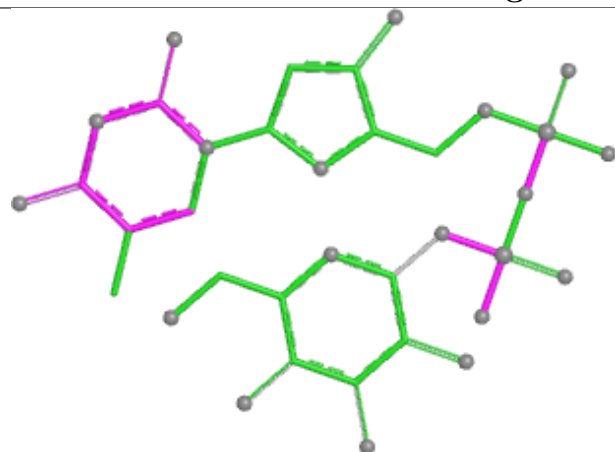


Rings

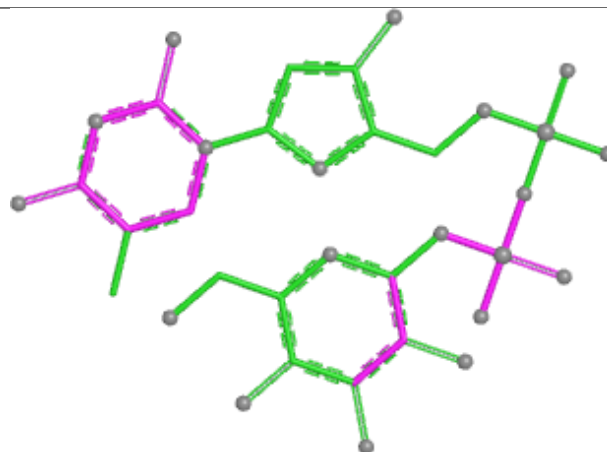
Ligand DAU C 3504



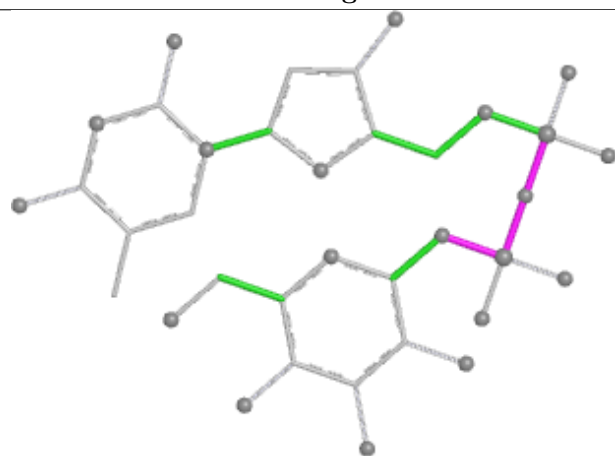
Ligand DAU F 3511



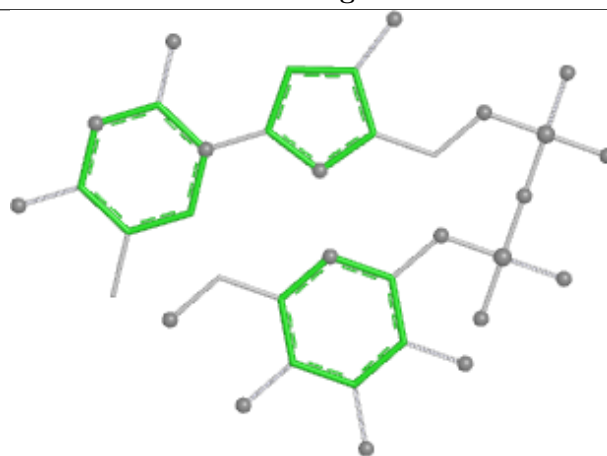
Bond lengths



Bond angles

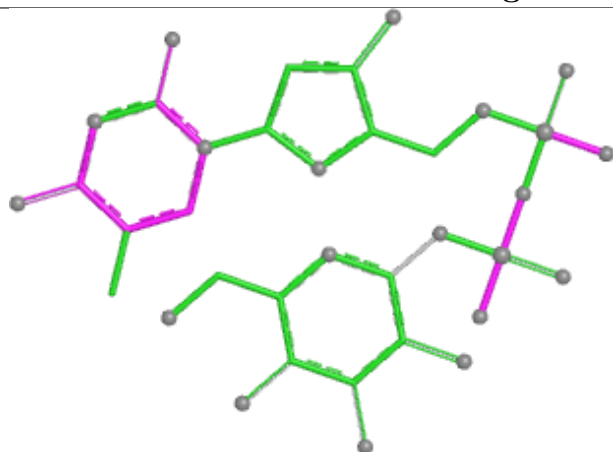


Torsions

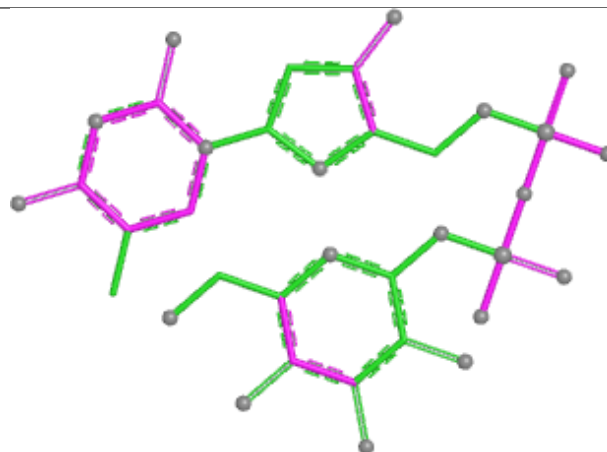


Rings

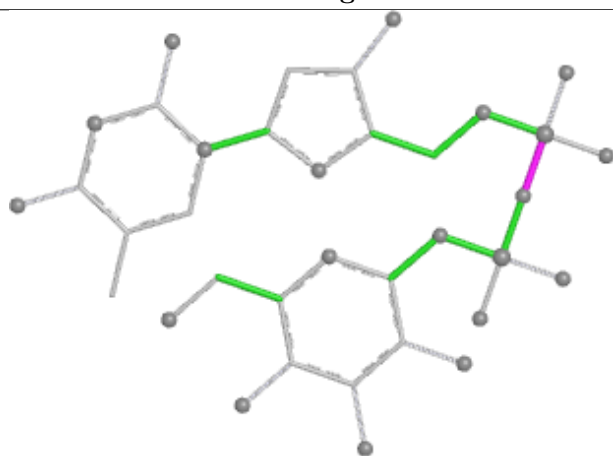
Ligand DAU B 3502



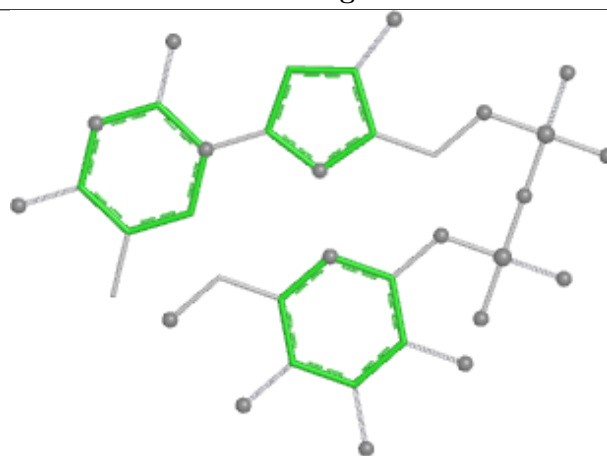
Bond lengths



Bond angles

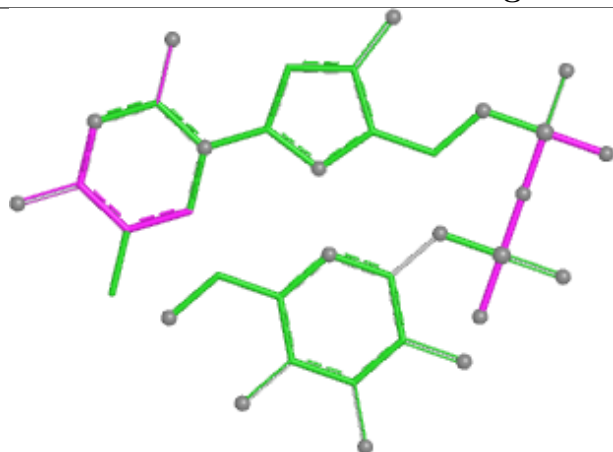


Torsions

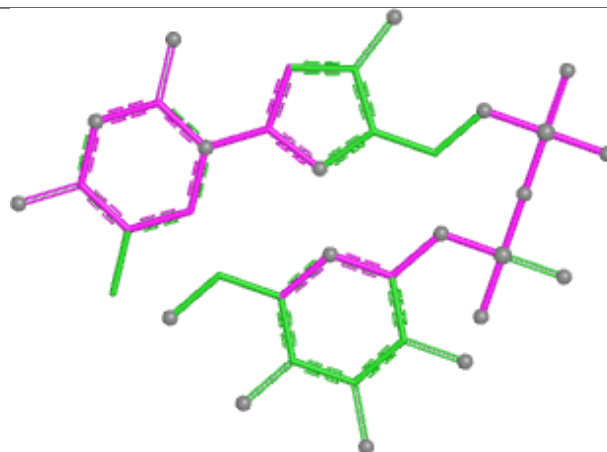


Rings

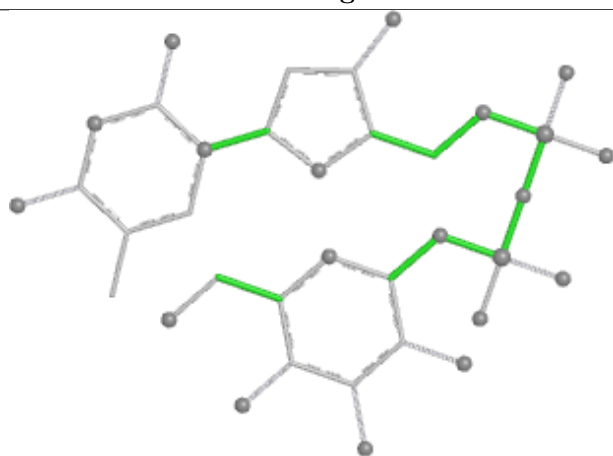
Ligand DAU E 3508



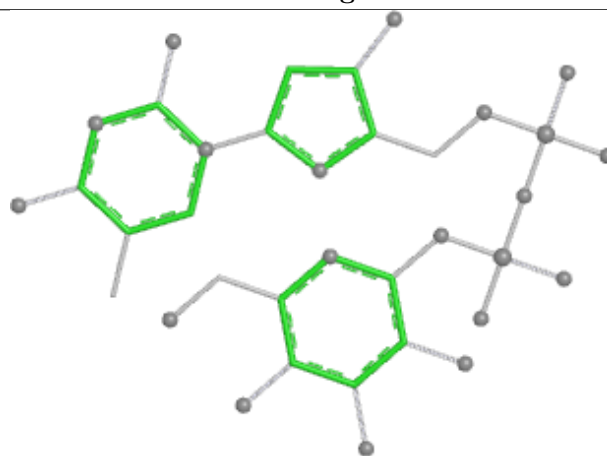
Bond lengths



Bond angles

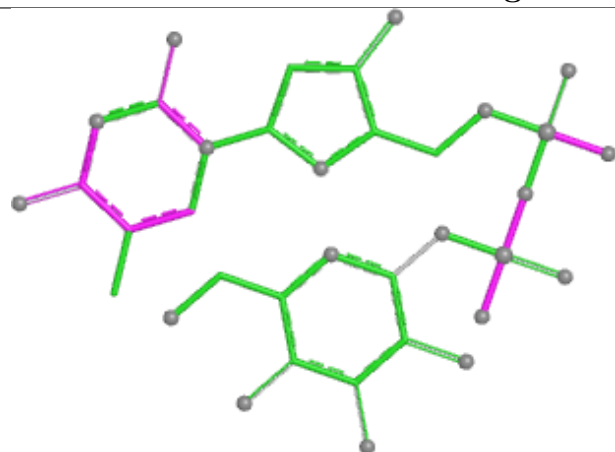


Torsions

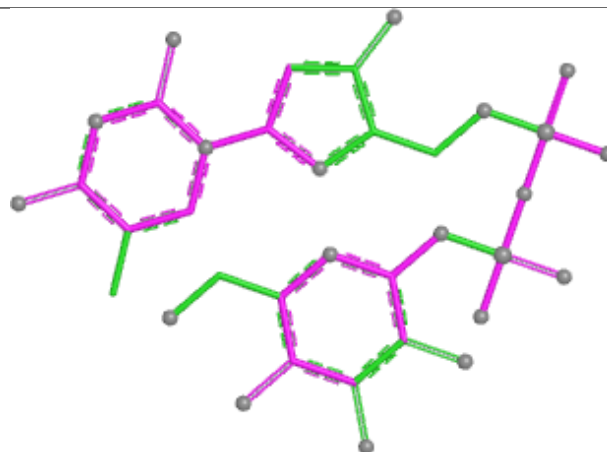


Rings

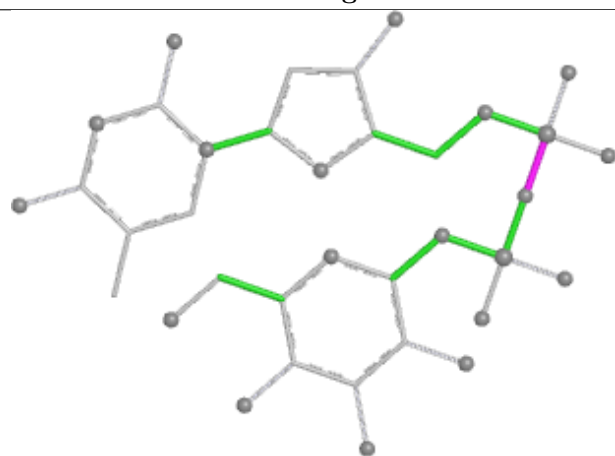
Ligand DAU A 3500



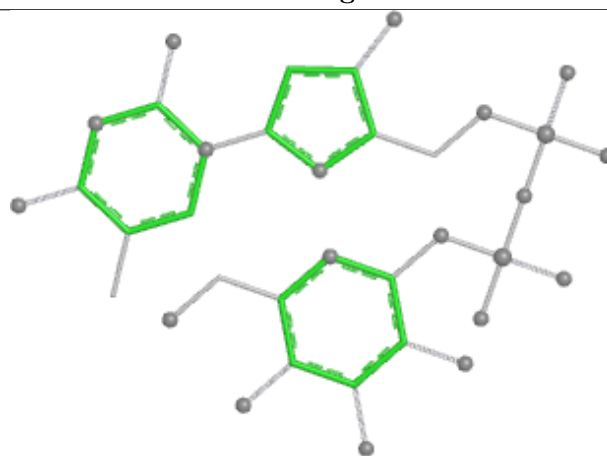
Bond lengths



Bond angles

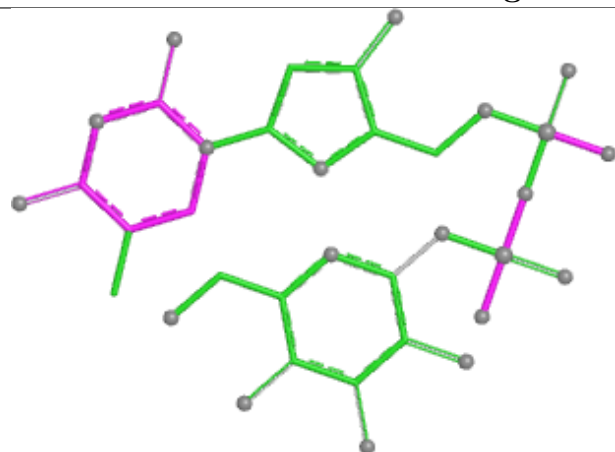


Torsions

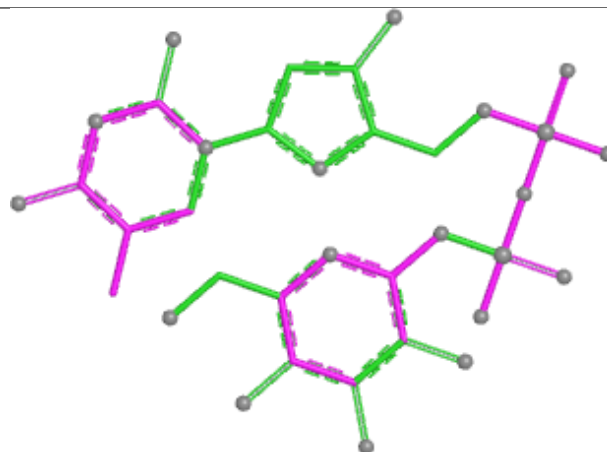


Rings

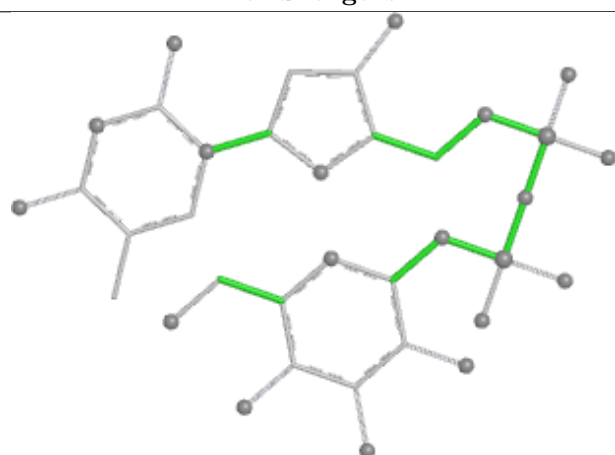
Ligand DAU D 3506



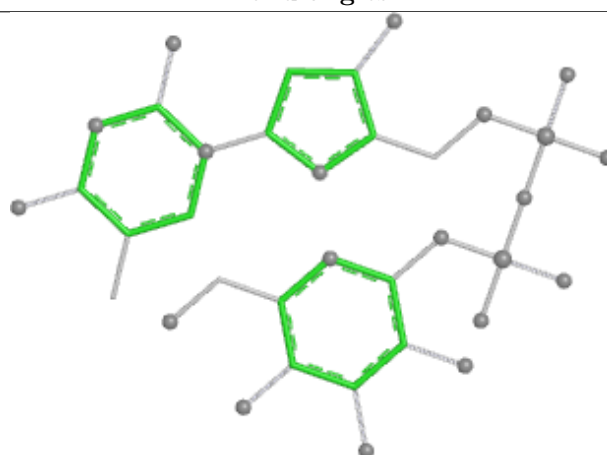
Bond lengths



Bond angles

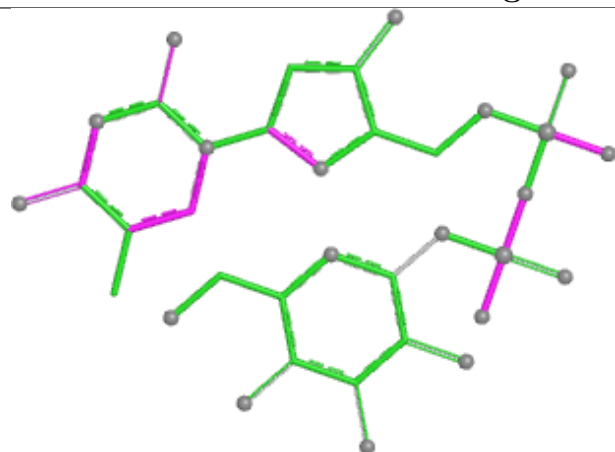


Torsions

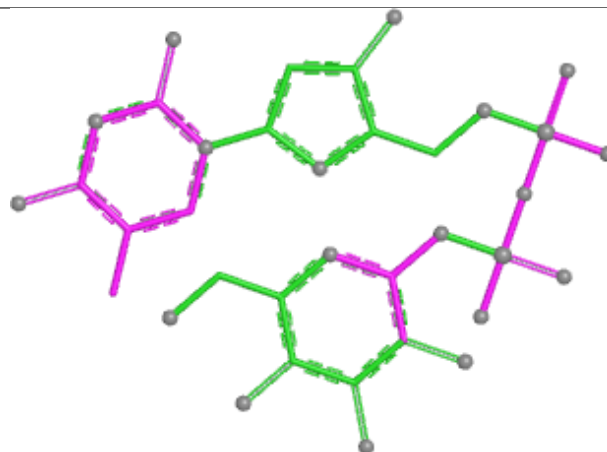


Rings

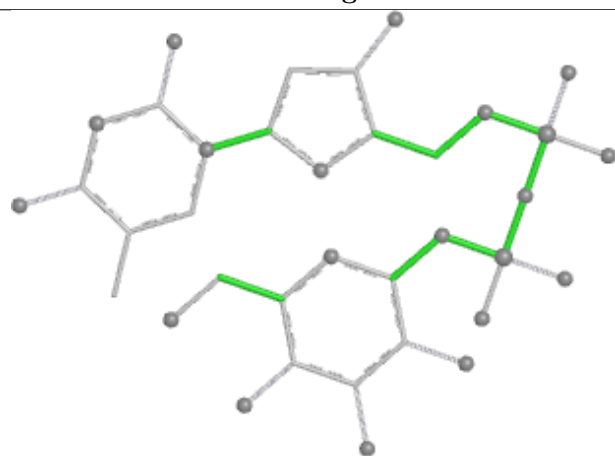
Ligand DAU G 3514



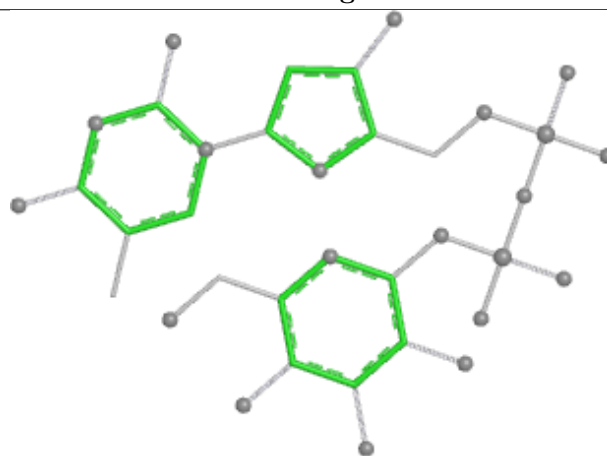
Bond lengths



Bond angles

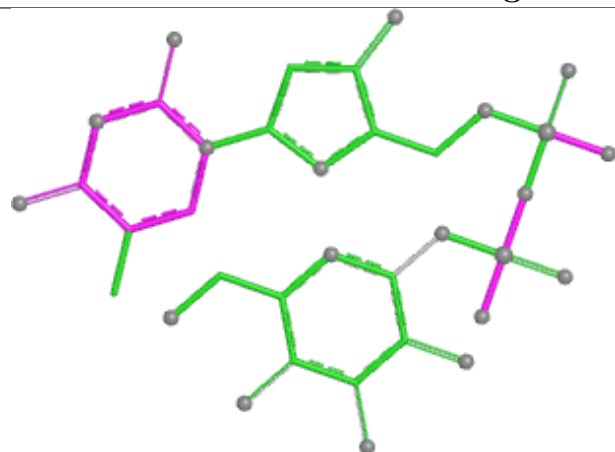


Torsions

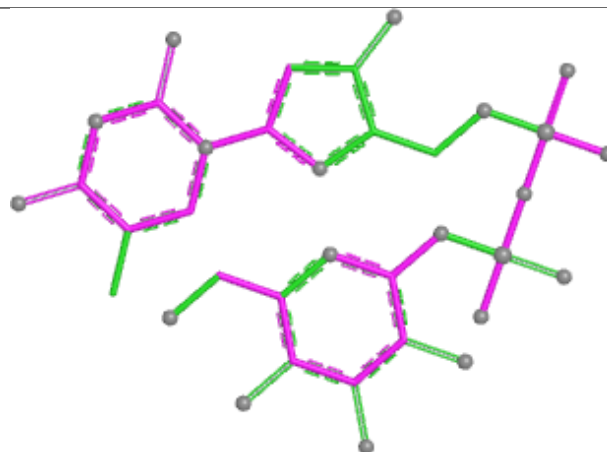


Rings

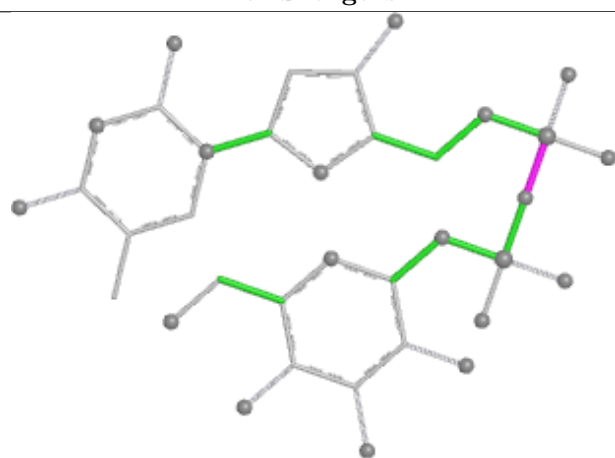
Ligand DAU H 3512



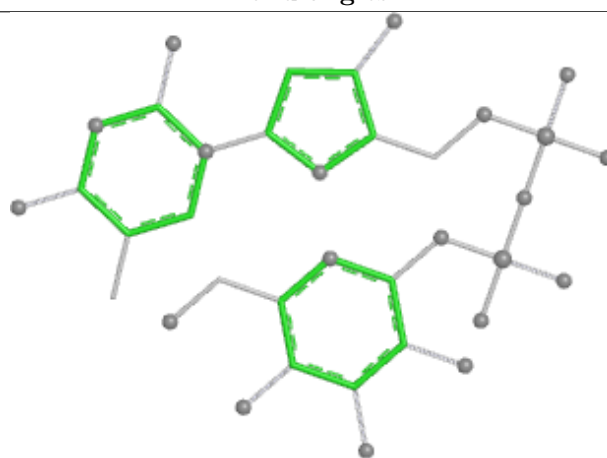
Bond lengths



Bond angles

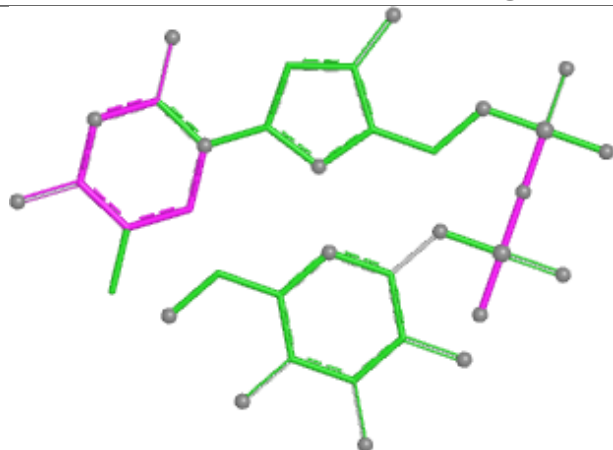


Torsions

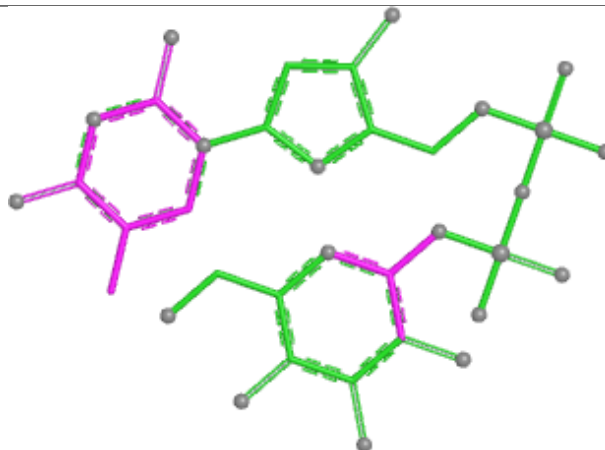


Rings

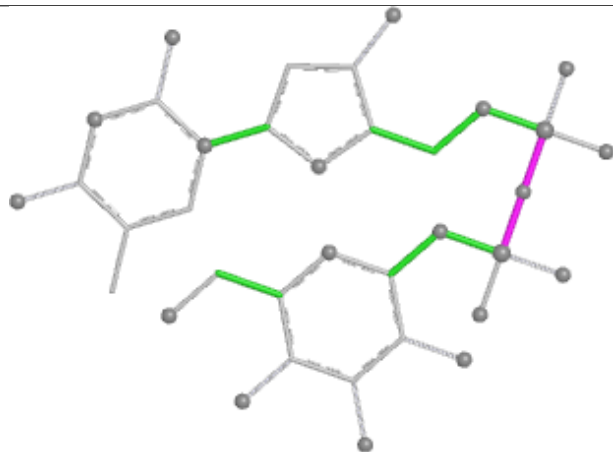
Ligand DAU H 3513



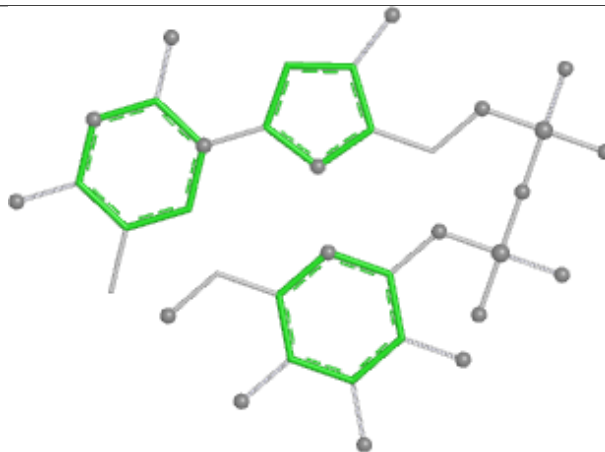
Bond lengths



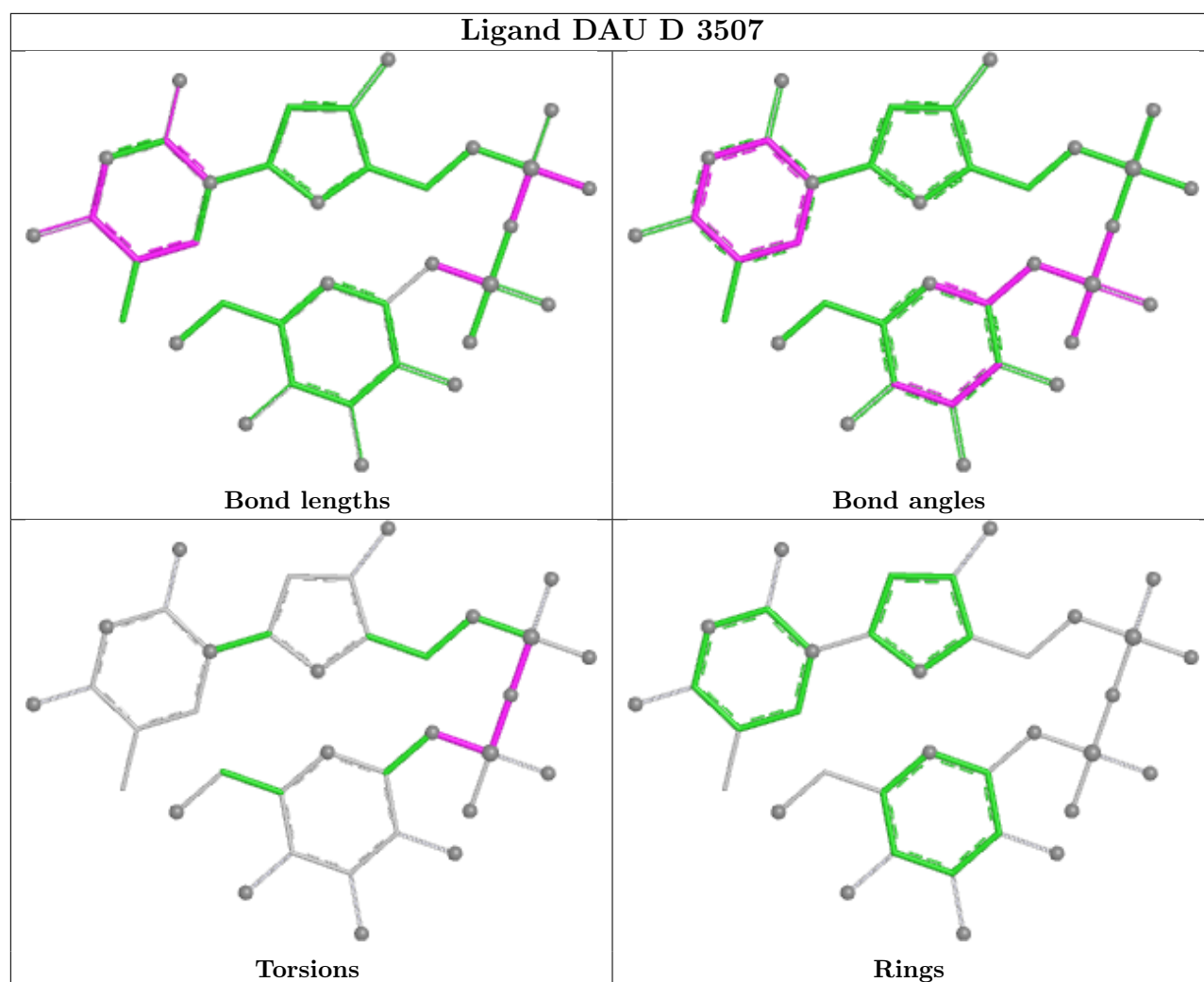
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	292/293 (99%)	-0.28	3 (1%) 79 84	4, 10, 20, 30	9 (3%)
1	B	293/293 (100%)	-0.28	4 (1%) 73 79	3, 9, 20, 34	5 (1%)
1	C	292/293 (99%)	-0.05	14 (4%) 36 42	4, 10, 32, 47	6 (2%)
1	D	292/293 (99%)	0.11	15 (5%) 34 40	4, 11, 36, 49	5 (1%)
1	E	292/293 (99%)	0.17	16 (5%) 32 38	4, 12, 36, 56	5 (1%)
1	F	293/293 (100%)	-0.08	11 (3%) 44 51	4, 10, 29, 48	9 (3%)
1	G	292/293 (99%)	-0.31	3 (1%) 79 84	2, 9, 20, 66	6 (2%)
1	H	292/293 (99%)	-0.21	3 (1%) 79 84	4, 10, 21, 28	4 (1%)
All	All	2338/2344 (99%)	-0.12	69 (2%) 52 59	2, 10, 25, 66	49 (2%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	23	ILE	7.0
1	D	23	ILE	6.3
1	D	22	ALA	5.6
1	E	19	ALA	5.3
1	E	16	LEU	5.0
1	D	20	THR	5.0
1	A	23	ILE	4.8
1	D	19	ALA	4.7
1	B	23	ILE	4.6
1	F	99	ILE	4.3
1	D	194[A]	ARG	4.2
1	B	22	ALA	4.2
1	F	13	GLY	4.0
1	E	14	THR	4.0
1	C	21	LEU	3.9
1	E	20	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	23	ILE	3.8
1	D	24	SER	3.7
1	E	195	GLY	3.7
1	E	15	ARG	3.5
1	E	13	GLY	3.4
1	F	206	TYR	3.4
1	E	22	ALA	3.3
1	C	23	ILE	3.2
1	D	16	LEU	3.2
1	C	14	THR	3.2
1	F	14	THR	3.2
1	C	22	ALA	3.1
1	D	15	ARG	3.1
1	F	12	SER	3.1
1	D	21	LEU	3.1
1	F	100	GLY	3.1
1	F	22	ALA	2.9
1	G	116	HIS	2.8
1	E	17	HIS	2.8
1	B	1	MET	2.8
1	F	15	ARG	2.8
1	F	1	MET	2.8
1	H	13	GLY	2.6
1	E	21	LEU	2.6
1	H	22	ALA	2.6
1	A	22	ALA	2.6
1	E	12	SER	2.5
1	C	16	LEU	2.5
1	H	12	SER	2.5
1	C	12	SER	2.5
1	A	13	GLY	2.5
1	E	194	ARG	2.4
1	C	24	SER	2.4
1	C	20	THR	2.3
1	C	13	GLY	2.3
1	D	276	ALA	2.3
1	C	128	ARG	2.3
1	D	188	ASP	2.3
1	E	24	SER	2.3
1	D	25	LYS	2.2
1	D	17	HIS	2.2
1	C	152	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	18	PRO	2.2
1	E	18	PRO	2.2
1	F	16	LEU	2.2
1	E	193	PRO	2.2
1	B	16	LEU	2.2
1	D	13	GLY	2.2
1	G	12	SER	2.1
1	C	34	PRO	2.1
1	F	17	HIS	2.1
1	C	15	ARG	2.0
1	C	19	ALA	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	CIT	A	3800	13/13	0.71	0.20	47,51,55,57	0
2	SO4	H	3814	5/5	0.72	0.14	57,58,58,58	0
4	CIT	A	3801	13/13	0.72	0.20	55,57,60,61	0
2	SO4	E	3820	5/5	0.78	0.16	48,48,49,51	0
2	SO4	A	3818	5/5	0.78	0.14	46,49,50,52	0
2	SO4	A	3817	5/5	0.81	0.13	38,44,46,47	0
2	SO4	A	3700	5/5	0.82	0.13	55,55,56,59	0
2	SO4	D	3819	5/5	0.83	0.14	44,44,45,49	0
2	SO4	A	3802	5/5	0.84	0.11	62,63,64,65	0
2	SO4	B	3701	5/5	0.85	0.14	53,54,55,57	0
2	SO4	G	3813	5/5	0.87	0.13	38,38,43,45	0
2	SO4	C	3806	5/5	0.87	0.12	42,46,49,49	0

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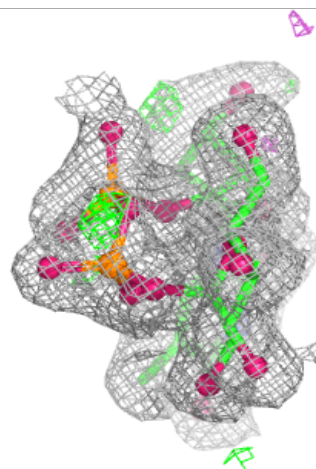
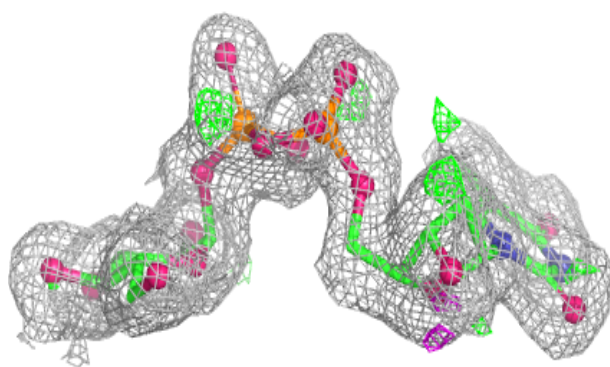
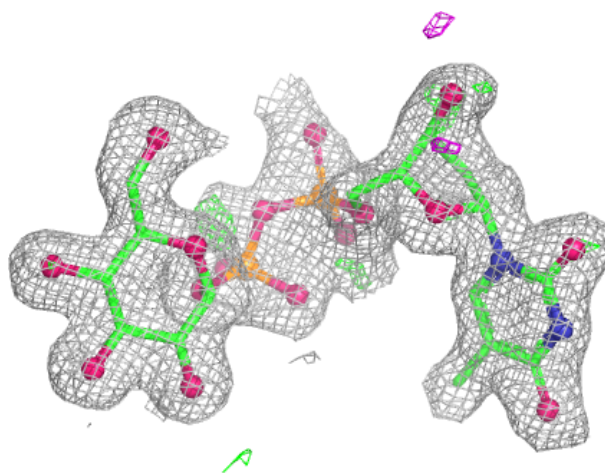
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	3804	5/5	0.88	0.12	45,45,50,52	0
2	SO4	H	3703	5/5	0.89	0.10	49,49,50,52	0
2	SO4	E	3808	5/5	0.90	0.11	47,50,54,54	0
2	SO4	G	3702	5/5	0.90	0.10	39,40,41,44	0
2	SO4	G	3812	5/5	0.90	0.12	41,42,43,48	0
2	SO4	E	3809	5/5	0.90	0.10	46,50,51,53	0
2	SO4	F	3811	5/5	0.91	0.10	43,44,47,49	0
2	SO4	H	3816	5/5	0.91	0.10	39,43,45,46	0
2	SO4	D	3807	5/5	0.92	0.10	45,47,47,47	0
2	SO4	E	3810	5/5	0.92	0.12	35,38,41,44	0
2	SO4	H	3815	5/5	0.93	0.11	38,38,40,43	0
2	SO4	C	3805	5/5	0.94	0.10	38,41,45,46	0
2	SO4	A	3803	5/5	0.94	0.11	37,38,39,44	0
3	DAU	E	3508	36/36	0.95	0.08	11,24,34,36	0
3	DAU	F	3510	36/36	0.95	0.08	12,18,28,34	0
3	DAU	A	3500	36/36	0.95	0.08	10,17,29,30	0
3	DAU	D	3506	36/36	0.95	0.08	12,19,31,32	0
3	DAU	G	3514	36/36	0.96	0.07	9,15,27,30	0
3	DAU	H	3512	36/36	0.96	0.08	10,18,28,31	0
3	DAU	C	3504	36/36	0.96	0.07	11,17,30,31	0
3	DAU	B	3502	36/36	0.96	0.07	8,16,28,30	0
3	DAU	E	3509	36/36	0.97	0.06	11,15,21,22	0
3	DAU	F	3511	36/36	0.98	0.06	10,15,22,23	0
3	DAU	D	3507	36/36	0.98	0.06	9,15,18,19	0
3	DAU	G	3515	36/36	0.98	0.06	8,12,16,16	0
3	DAU	A	3501	36/36	0.98	0.06	8,11,15,16	0
3	DAU	H	3513	36/36	0.98	0.06	10,13,17,17	0
3	DAU	C	3505	36/36	0.98	0.06	10,14,20,22	0
3	DAU	B	3503	36/36	0.98	0.06	10,12,17,18	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.

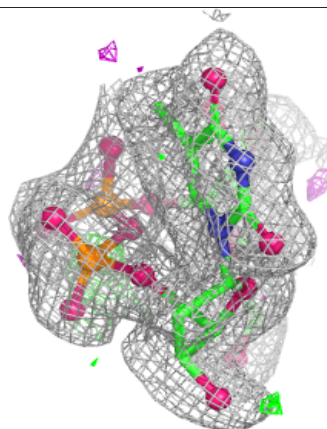
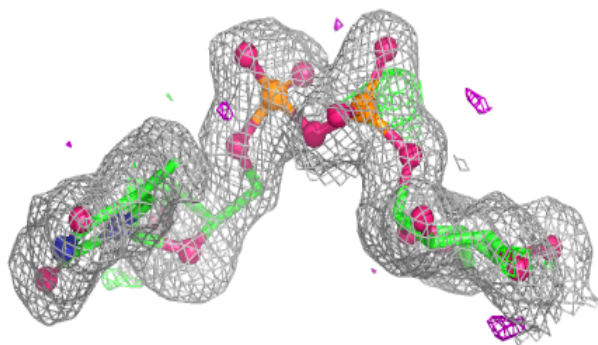
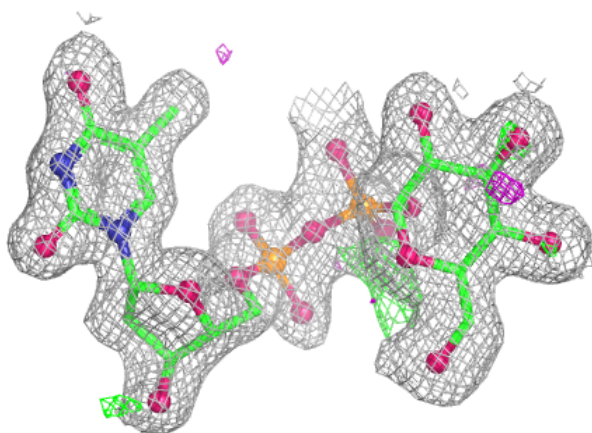
Electron density around DAU E 3508:

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

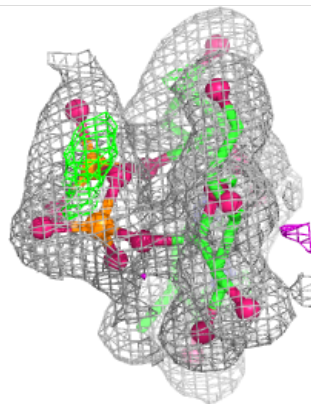
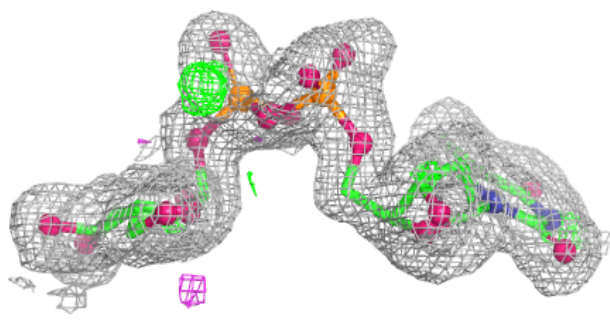
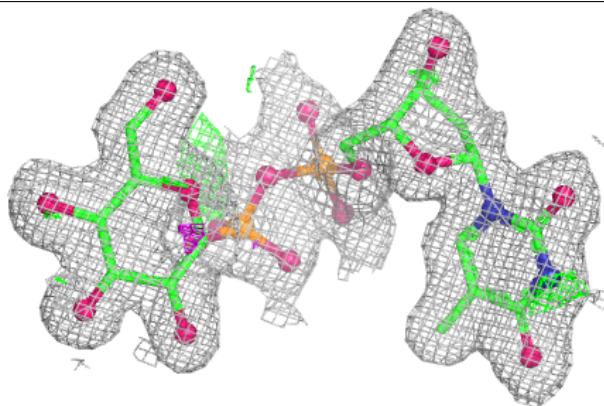


Electron density around DAU F 3510:

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

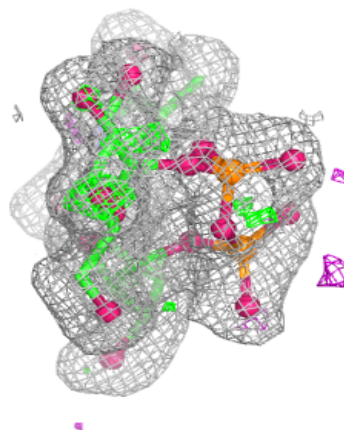
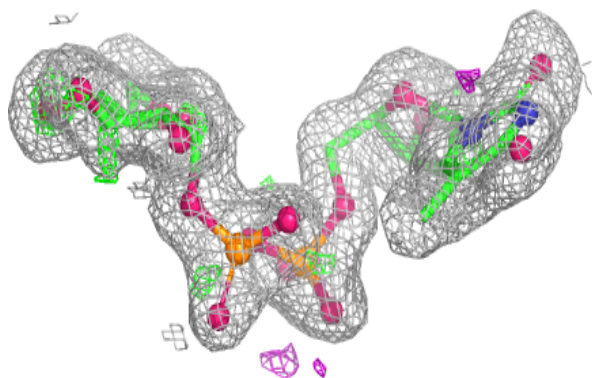
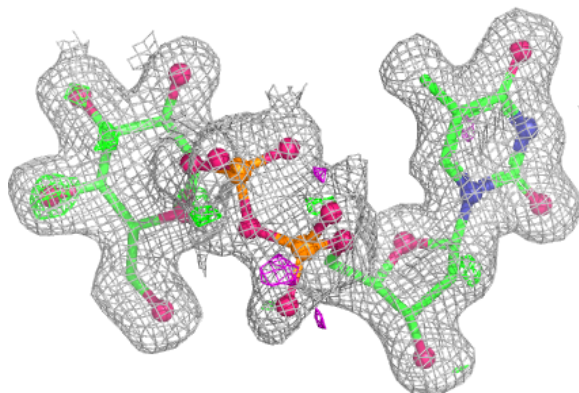
**Electron density around DAU A 3500:**

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



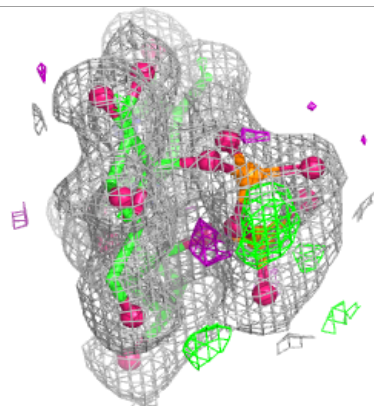
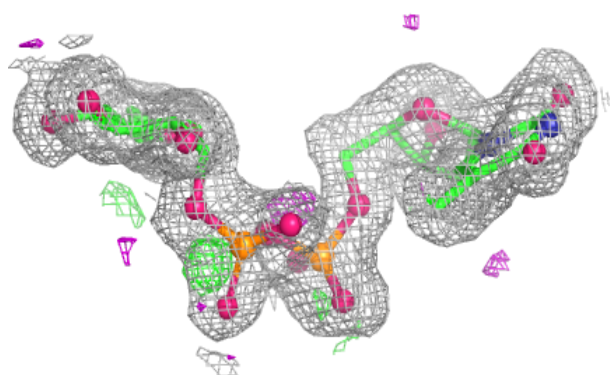
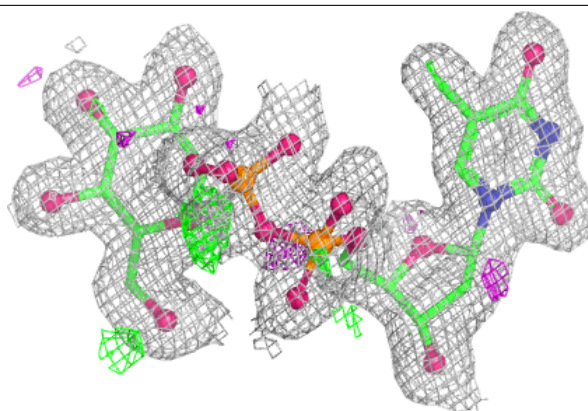
Electron density around DAU D 3506:

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

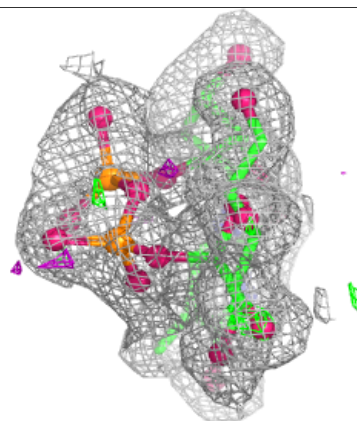
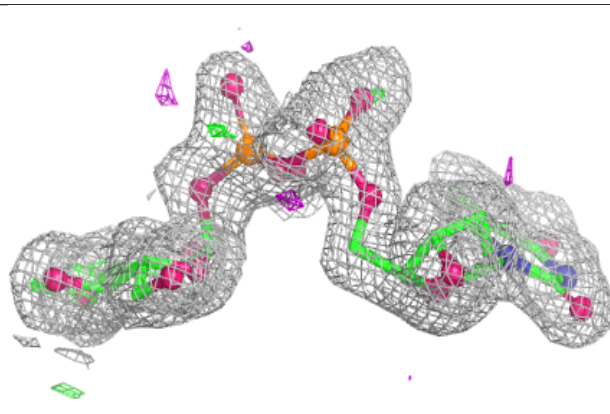
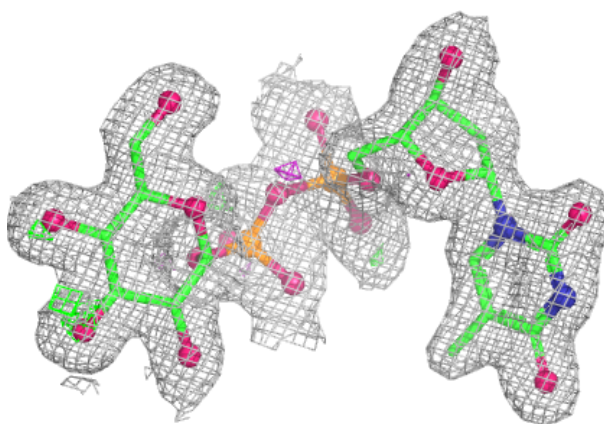


Electron density around DAU G 3514:

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

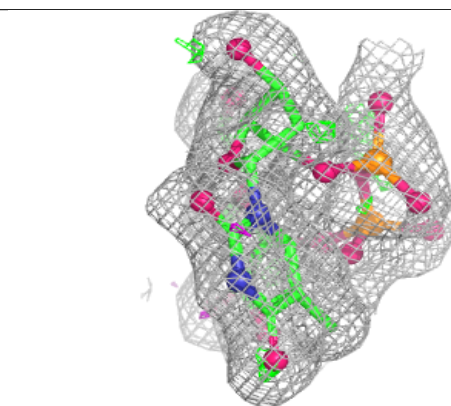
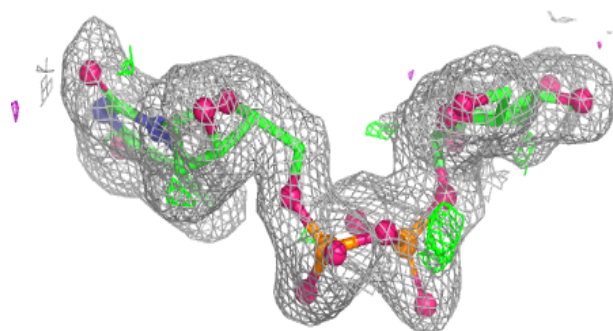
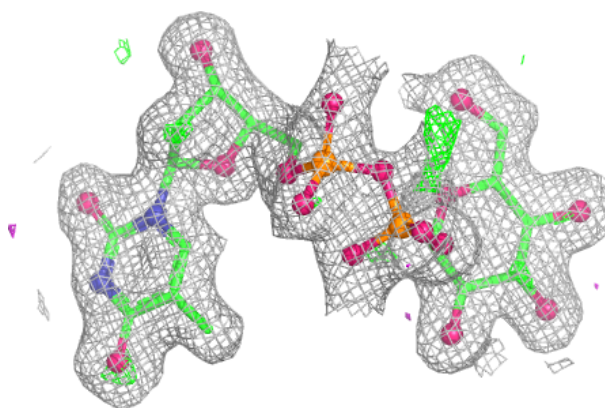
**Electron density around DAU H 3512:**

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

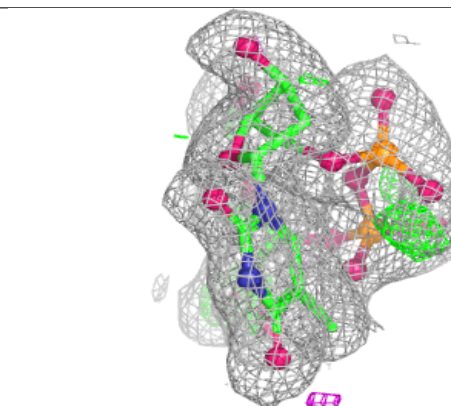
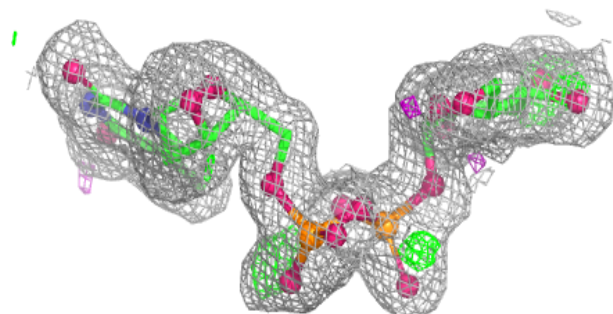
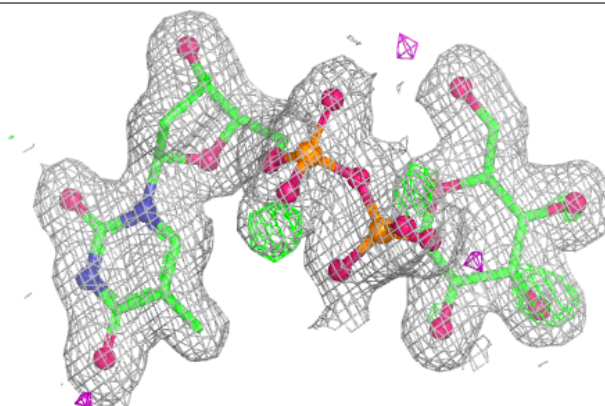


Electron density around DAU C 3504:

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

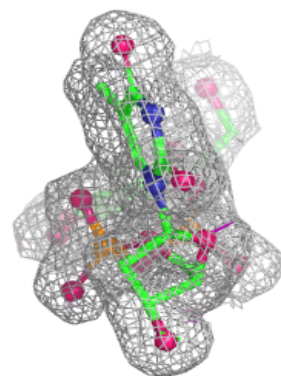
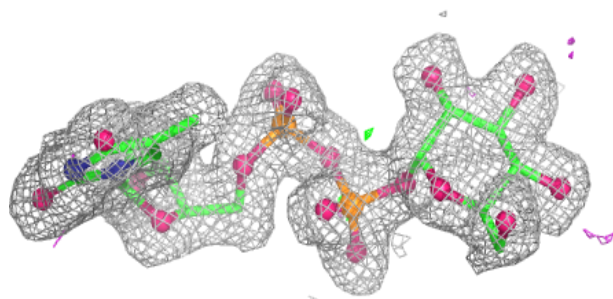
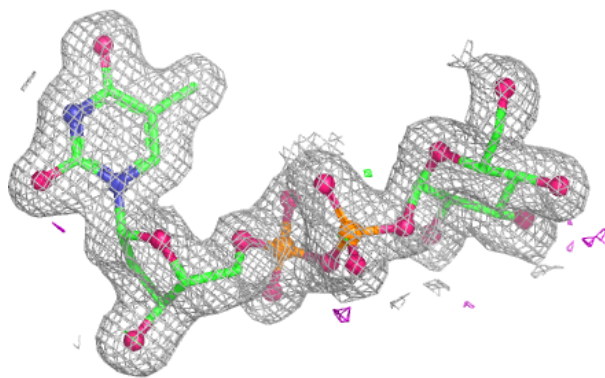
**Electron density around DAU B 3502:**

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

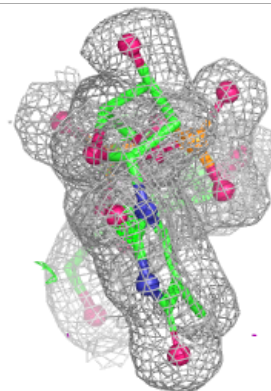
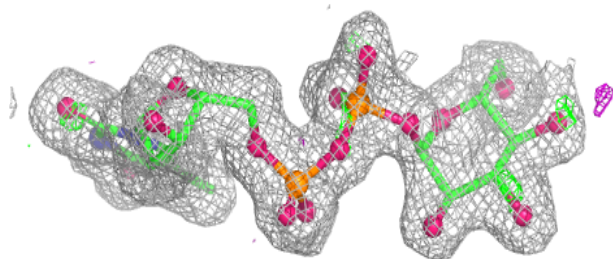
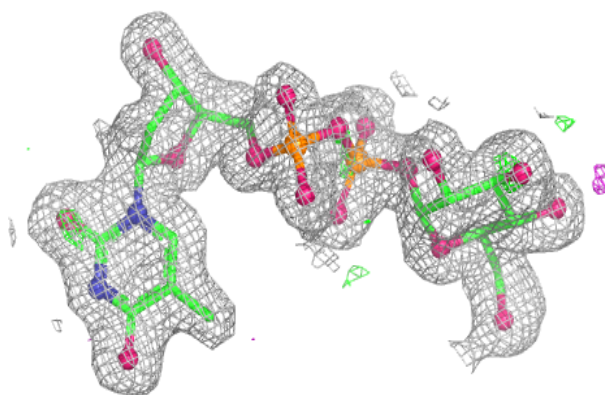


Electron density around DAU E 3509:

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

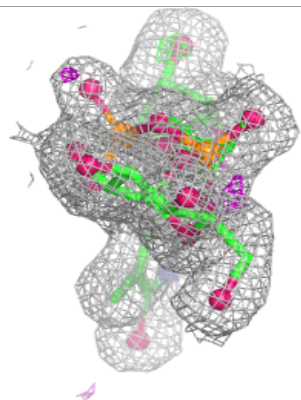
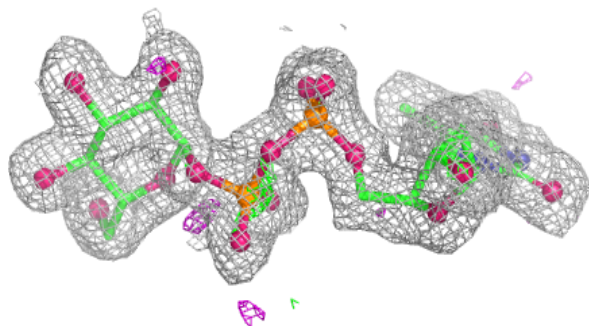
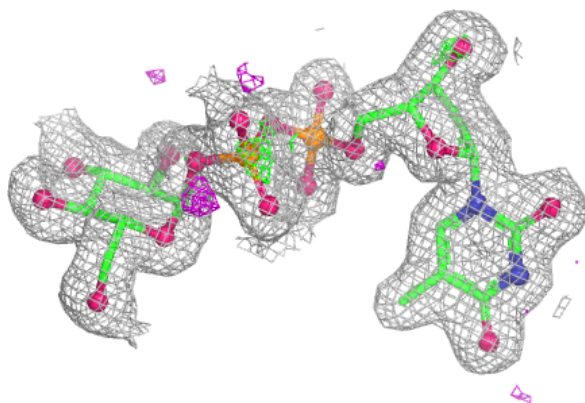
**Electron density around DAU F 3511:**

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

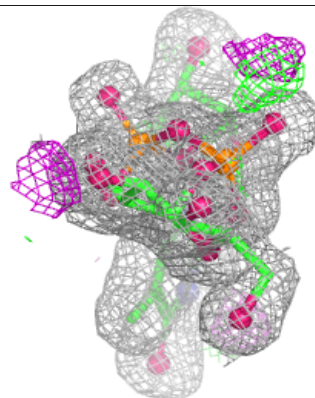
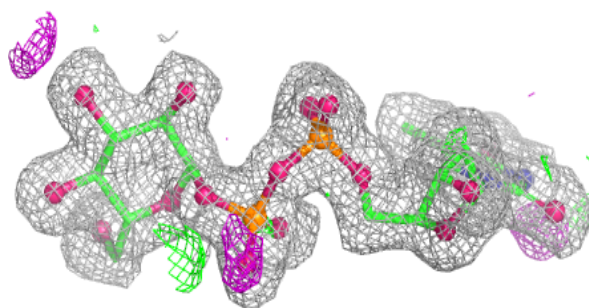
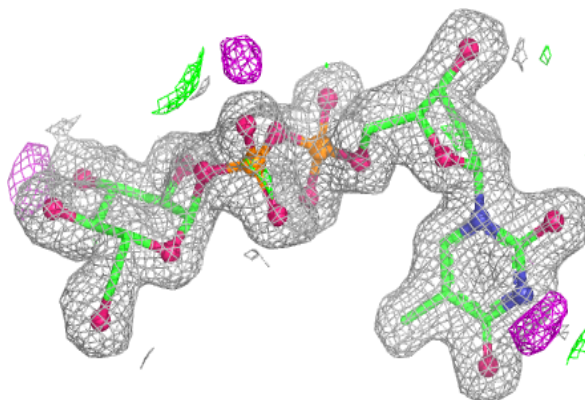


Electron density around DAU D 3507:

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

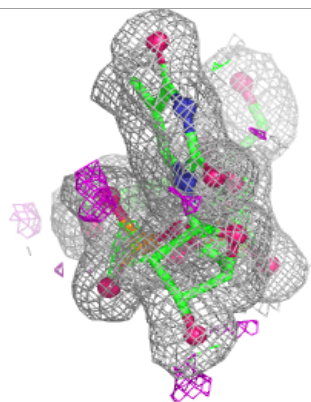
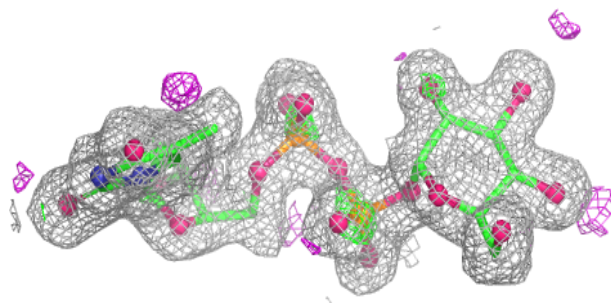
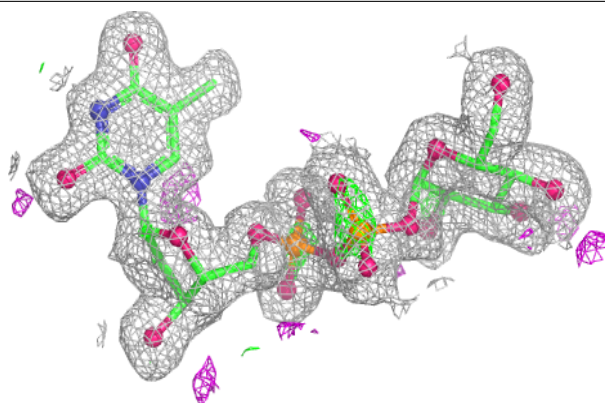
**Electron density around DAU G 3515:**

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

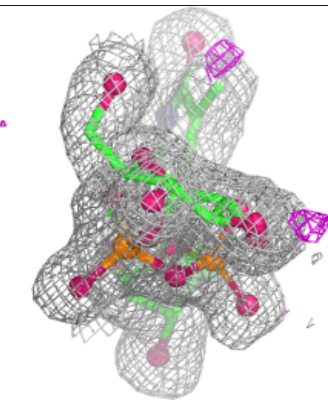
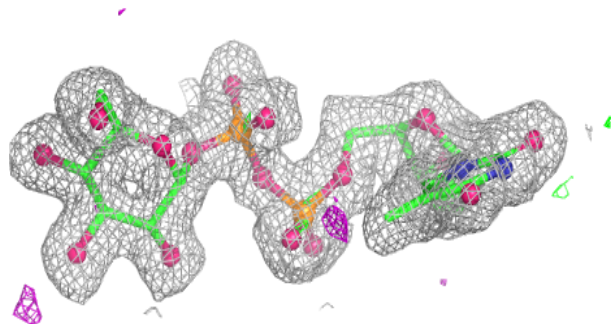
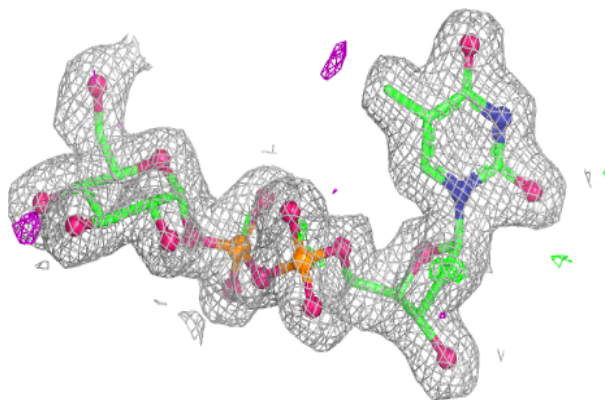


Electron density around DAU A 3501:

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

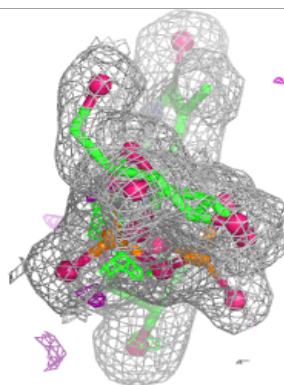
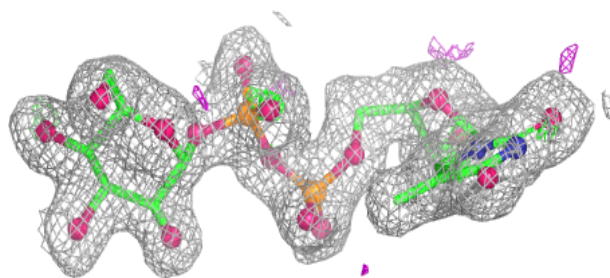
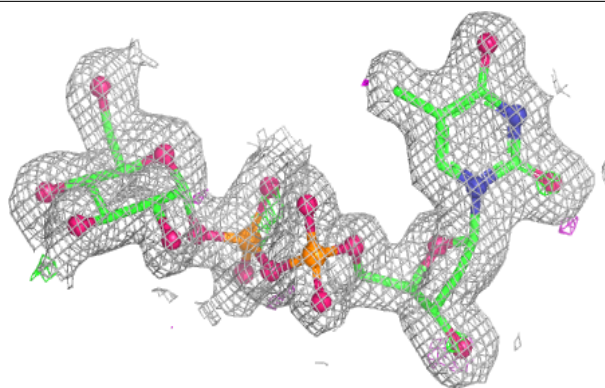
**Electron density around DAU H 3513:**

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

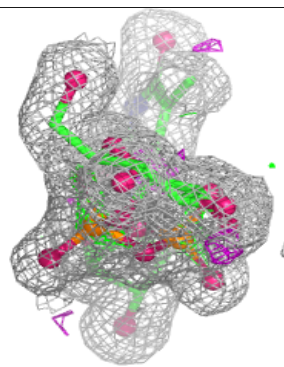
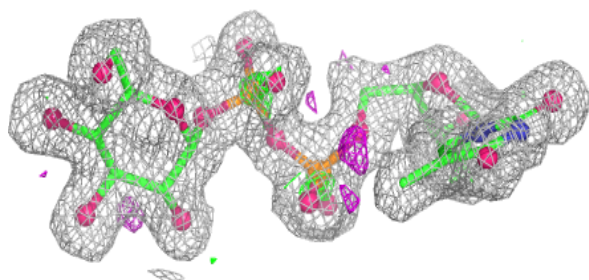
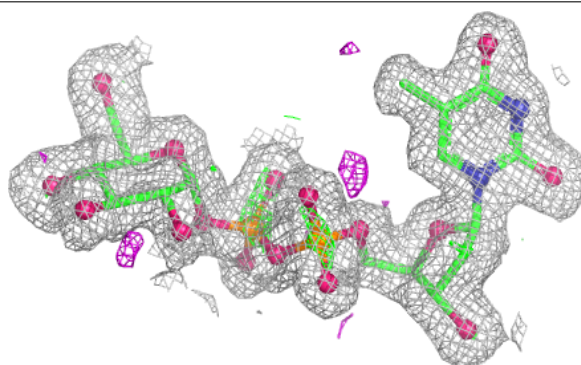


Electron density around DAU C 3505:

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

**Electron density around DAU B 3503:**

$2mF_o-DF_c$ (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.