



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:12 PM UTC

PDB ID : 9HIA / pdb_00009hia
Title : K115 acetylated human muscle pyruvate kinase, isoform M2 (PKM2), in complex with FBP
Authors : Pavlenko, D.; Nudelman, H.; Shahar, A.; Arbely, E.
Deposited on : 2024-11-25
Resolution : 2.02 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

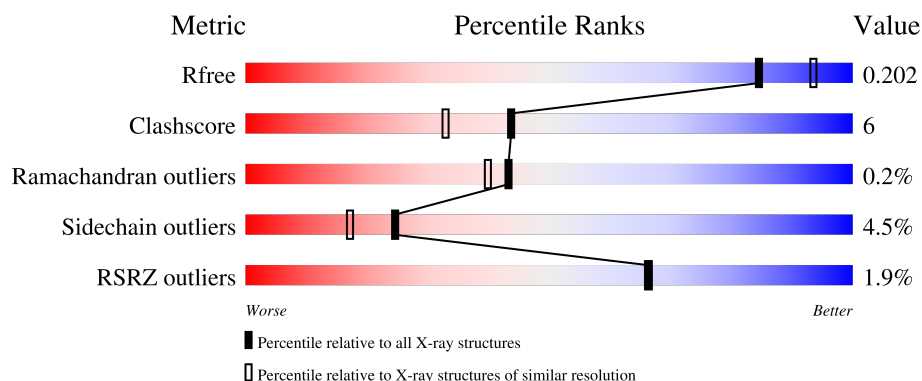
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.02 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	537	
1	B	537	
1	C	537	
1	D	537	

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
3	EDO	A	602	-	X	X	-
4	SIN	A	606	-	X	-	-
4	SIN	B	604	-	X	-	-
5	GOL	C	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17472 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3977	2500	707	745	25			
1	B	519	Total	C	N	O	S	0	0	0
			3977	2500	707	745	25			
1	C	518	Total	C	N	O	S	0	1	0
			3970	2496	704	744	26			
1	D	518	Total	C	N	O	S	0	1	0
			3976	2499	705	747	25			

There are 24 discrepancies between the modelled and reference sequences:

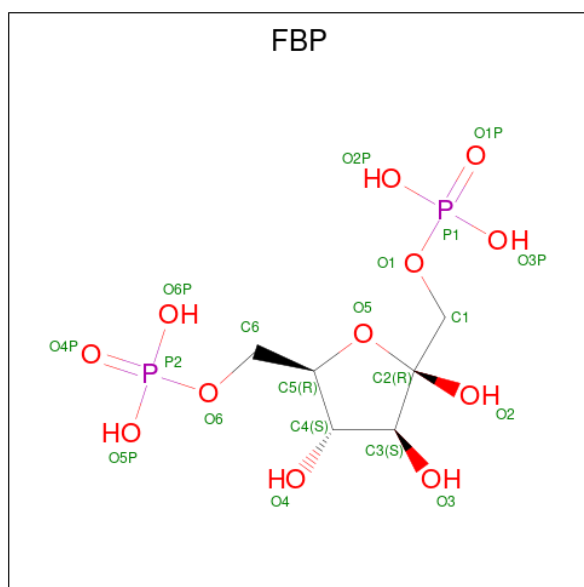
Chain	Residue	Modelled	Actual	Comment	Reference
A	532	HIS	-	expression tag	UNP P14618
A	533	HIS	-	expression tag	UNP P14618
A	534	HIS	-	expression tag	UNP P14618
A	535	HIS	-	expression tag	UNP P14618
A	536	HIS	-	expression tag	UNP P14618
A	537	HIS	-	expression tag	UNP P14618
B	532	HIS	-	expression tag	UNP P14618
B	533	HIS	-	expression tag	UNP P14618
B	534	HIS	-	expression tag	UNP P14618
B	535	HIS	-	expression tag	UNP P14618
B	536	HIS	-	expression tag	UNP P14618
B	537	HIS	-	expression tag	UNP P14618
C	532	HIS	-	expression tag	UNP P14618
C	533	HIS	-	expression tag	UNP P14618
C	534	HIS	-	expression tag	UNP P14618
C	535	HIS	-	expression tag	UNP P14618
C	536	HIS	-	expression tag	UNP P14618
C	537	HIS	-	expression tag	UNP P14618
D	532	HIS	-	expression tag	UNP P14618
D	533	HIS	-	expression tag	UNP P14618
D	534	HIS	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	535	HIS	-	expression tag	UNP P14618
D	536	HIS	-	expression tag	UNP P14618
D	537	HIS	-	expression tag	UNP P14618

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



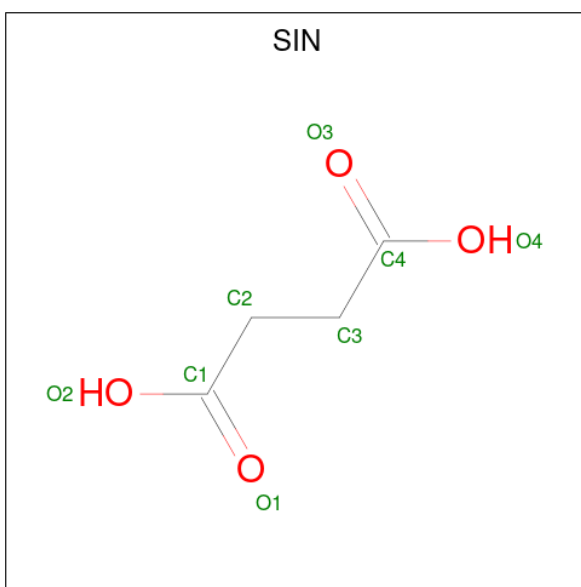
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



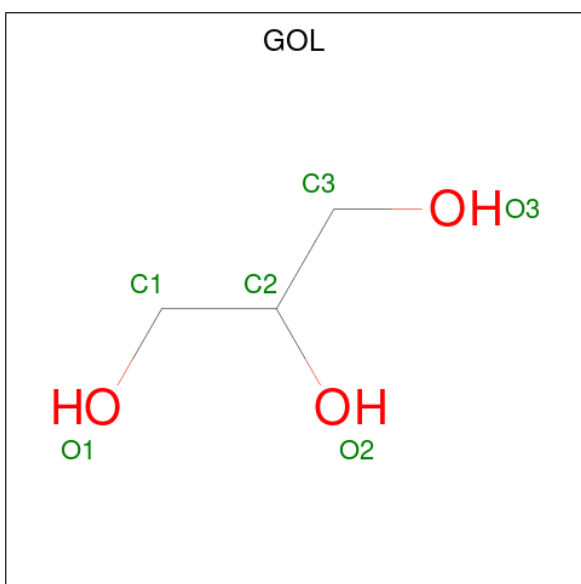
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		
4	B	1	Total	C	O	0	0
			8	4	4		
4	C	1	Total	C	O	0	0
			8	4	4		
4	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	2	Total K 2 2	0	0

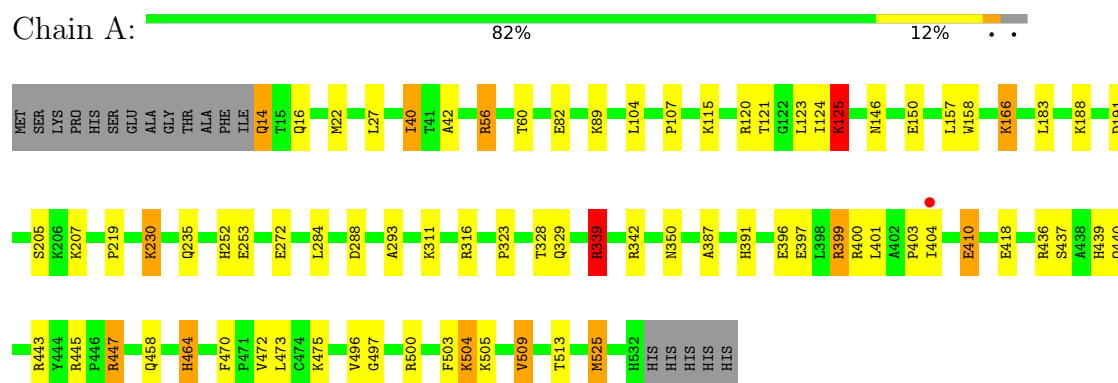
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	440	Total O 440 440	0	0
7	B	439	Total O 439 439	0	0
7	C	291	Total O 291 291	0	0
7	D	248	Total O 248 248	0	0

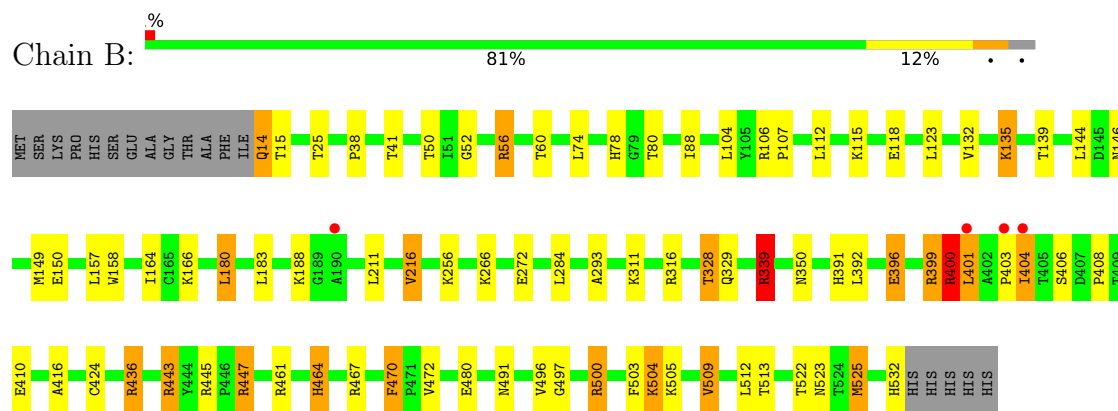
3 Residue-property plots

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

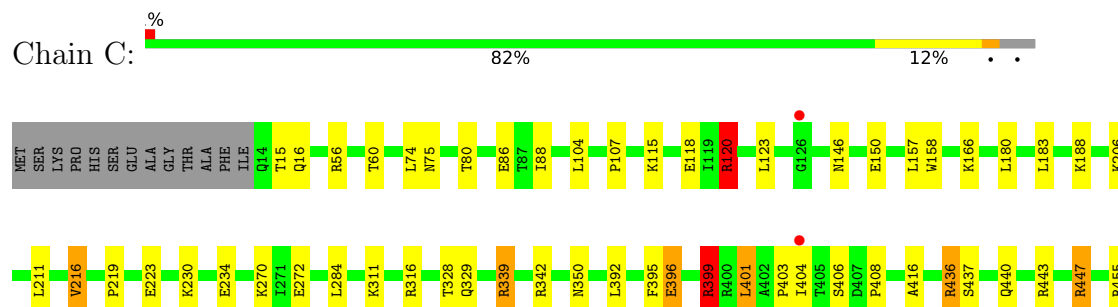
• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM

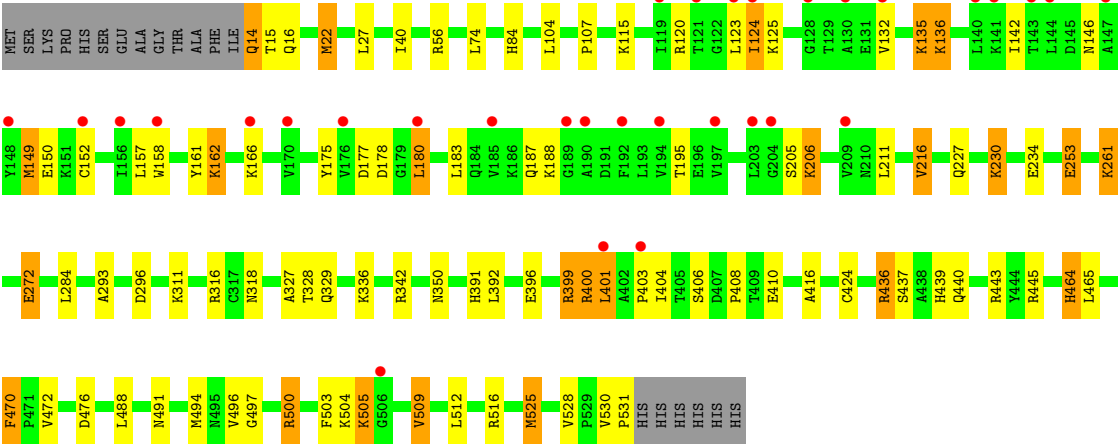
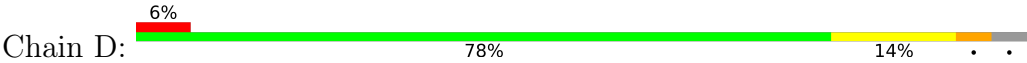


• Molecule 1: Pyruvate kinase PKM





● Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.23Å 155.17Å 101.02Å 90.00° 107.61° 90.00°	Depositor
Resolution (Å)	29.69 – 2.02 29.69 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.69-2.02) 98.1 (29.69-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.160 , 0.200 0.161 , 0.202	Depositor DCC
R_{free} test set	7594 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17472	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: FBP, GOL, ALY, SIN, K, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.99	2/4029 (0.0%)	1.40	37/5442 (0.7%)
1	B	1.01	2/4029 (0.0%)	1.42	45/5442 (0.8%)
1	C	0.82	2/4024 (0.0%)	1.38	34/5435 (0.6%)
1	D	0.81	1/4027 (0.0%)	1.35	36/5439 (0.7%)
All	All	0.91	7/16109 (0.0%)	1.39	152/21758 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
1	C	0	5
1	D	0	6
All	All	0	20

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	ARG	NE-CZ	8.61	1.42	1.33
1	A	447	ARG	NE-CZ	7.72	1.41	1.33
1	B	467	ARG	NE-CZ	7.47	1.41	1.33
1	C	518	GLY	N-CA	6.96	1.53	1.45
1	D	396	GLU	CD-OE1	6.94	1.38	1.25
1	A	410	GLU	CD-OE1	5.75	1.36	1.25
1	C	447	ARG	NE-CZ	5.21	1.38	1.33

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	517	PRO	CA-C-N	-14.09	102.52	121.96
1	C	517	PRO	C-N-CA	-14.09	102.52	121.96
1	D	396	GLU	CB-CG-CD	13.61	135.74	112.60
1	B	504	LYS	CB-CG-CD	11.46	137.67	111.30
1	C	517	PRO	O-C-N	-11.20	107.77	122.22
1	D	470	PHE	CB-CA-C	10.85	120.20	110.44
1	C	470	PHE	CB-CA-C	10.56	119.94	110.44
1	B	509	VAL	N-CA-CB	-10.25	95.22	112.44
1	A	525	MET	CG-SD-CE	10.01	122.92	100.90
1	C	528	VAL	N-CA-CB	-9.95	97.28	111.21
1	A	470	PHE	CB-CA-C	9.78	120.30	110.33
1	D	509	VAL	N-CA-CB	-9.32	95.12	112.36
1	B	56	ARG	CB-CA-C	-9.23	92.48	109.29
1	A	253	GLU	CB-CG-CD	9.01	127.91	112.60
1	B	339	ARG	CB-CG-CD	8.99	131.98	111.30
1	C	509	VAL	N-CA-CB	-8.80	96.08	112.36
1	D	136	LYS	CB-CA-C	8.76	122.98	109.84
1	B	525	MET	CG-SD-CE	8.72	120.08	100.90
1	A	509	VAL	N-CA-CB	-8.64	96.38	112.36
1	D	525	MET	CG-SD-CE	8.62	119.86	100.90
1	A	504	LYS	CB-CG-CD	8.49	130.82	111.30
1	C	396	GLU	N-CA-CB	8.31	122.32	109.94
1	B	445	ARG	NE-CZ-NH1	-8.22	113.28	121.50
1	B	38	PRO	N-CA-CB	7.96	107.36	103.22
1	B	56	ARG	CD-NE-CZ	-7.88	113.36	124.40
1	C	525	MET	CG-SD-CE	7.86	118.20	100.90
1	A	401	LEU	N-CA-CB	7.78	123.48	110.41
1	D	216	VAL	N-CA-CB	7.78	120.92	110.26
1	A	445	ARG	NE-CZ-NH1	-7.75	113.75	121.50
1	B	396	GLU	N-CA-CB	7.63	121.08	110.01
1	B	470	PHE	CB-CA-C	7.50	117.19	110.44
1	C	531	PRO	CA-C-O	-7.39	96.81	119.00
1	B	106	ARG	NE-CZ-NH1	-7.38	114.12	121.50
1	D	396	GLU	N-CA-CB	7.36	120.69	110.01
1	C	56	ARG	N-CA-CB	-7.29	99.81	110.53
1	C	517	PRO	N-CA-C	7.29	123.49	113.65
1	D	166	LYS	CB-CG-CD	7.25	127.98	111.30
1	A	272	GLU	CB-CA-C	-7.24	97.47	110.35
1	C	216	VAL	N-CA-CB	7.22	120.16	110.26
1	A	56	ARG	CD-NE-CZ	-7.04	114.55	124.40
1	B	56	ARG	CG-CD-NE	-6.94	96.73	112.00
1	A	410	GLU	CG-CD-OE2	-6.91	102.52	118.40
1	D	136	LYS	CB-CG-CD	6.88	127.13	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	ARG	CB-CG-CD	6.88	127.12	111.30
1	A	188	LYS	CG-CD-CE	6.86	127.07	111.30
1	B	403	PRO	CB-CA-C	6.83	119.90	110.95
1	A	500	ARG	CA-CB-CG	-6.83	100.44	114.10
1	A	396	GLU	N-CA-CB	6.81	119.88	110.01
1	B	500	ARG	CA-CB-CG	-6.77	100.55	114.10
1	B	216	VAL	N-CA-CB	6.72	119.47	110.26
1	D	136	LYS	CA-CB-CG	6.71	127.52	114.10
1	D	401	LEU	N-CA-CB	6.71	121.34	110.40
1	D	445	ARG	NE-CZ-NH1	-6.57	114.93	121.50
1	A	22	MET	CG-SD-CE	6.54	115.29	100.90
1	D	410	GLU	CG-CD-OE1	6.53	133.42	118.40
1	C	339	ARG	CA-CB-CG	-6.51	101.09	114.10
1	A	403	PRO	CB-CA-C	6.50	119.50	111.12
1	B	491	ASN	CA-CB-CG	-6.47	106.13	112.60
1	B	410	GLU	CG-CD-OE1	-6.45	103.57	118.40
1	C	219	PRO	CB-CA-C	6.33	119.50	111.39
1	C	80	THR	CA-CB-OG1	-6.28	100.17	109.60
1	D	56	ARG	CD-NE-CZ	-6.27	115.63	124.40
1	A	252	HIS	CA-CB-CG	-6.22	107.58	113.80
1	D	403	PRO	CB-CA-C	6.22	119.14	111.12
1	A	219	PRO	CB-CA-C	6.22	119.19	111.23
1	B	339	ARG	CD-NE-CZ	6.19	133.06	124.40
1	A	410	GLU	CG-CD-OE1	6.17	132.59	118.40
1	B	272	GLU	CB-CA-C	-6.17	99.37	110.35
1	B	328	THR	CA-CB-OG1	-6.16	100.36	109.60
1	B	399	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	C	120	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	C	480	GLU	CB-CG-CD	6.12	123.00	112.60
1	D	399	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	D	135	LYS	CA-CB-CG	6.10	126.30	114.10
1	B	339	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	D	177	ASP	CB-CA-C	6.06	122.48	110.42
1	D	528	VAL	N-CA-CB	-6.03	102.77	111.21
1	C	403	PRO	CB-CA-C	6.00	118.87	111.12
1	C	339	ARG	CB-CG-CD	6.00	125.09	111.30
1	D	491	ASN	CA-CB-CG	-5.98	106.62	112.60
1	A	339	ARG	CA-CB-CG	-5.96	102.19	114.10
1	A	339	ARG	CB-CG-CD	5.90	124.86	111.30
1	D	135	LYS	CB-CG-CD	5.88	124.82	111.30
1	B	188	LYS	CB-CA-C	-5.88	99.56	109.72
1	A	230	LYS	CB-CG-CD	5.87	124.81	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	491	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	464	HIS	CB-CG-CD2	-5.85	123.59	131.20
1	B	410	GLU	CB-CA-C	-5.84	101.67	110.90
1	B	135	LYS	CB-CG-CD	5.83	124.72	111.30
1	B	401	LEU	N-CA-CB	5.81	119.86	110.40
1	B	266	LYS	CG-CD-CE	5.78	124.58	111.30
1	A	89	LYS	CD-CE-NZ	-5.76	93.47	111.90
1	C	16	GLN	N-CA-CB	-5.75	103.55	112.30
1	B	41	THR	CA-CB-OG1	-5.75	100.98	109.60
1	C	272	GLU	CB-CA-C	-5.75	100.12	110.35
1	A	191	ASP	N-CA-CB	-5.74	101.74	111.27
1	C	436	ARG	CD-NE-CZ	-5.73	116.38	124.40
1	C	399	ARG	CA-CB-CG	-5.72	102.66	114.10
1	C	188	LYS	CB-CA-C	-5.72	99.83	109.72
1	D	399	ARG	CA-CB-CG	-5.68	102.74	114.10
1	D	401	LEU	N-CA-C	-5.66	105.88	112.89
1	D	188	LYS	CB-CA-C	-5.62	100.00	109.72
1	D	14	GLN	CB-CA-C	5.59	120.72	110.10
1	B	15	THR	CA-CB-OG1	-5.58	101.24	109.60
1	C	15	THR	CA-CB-OG1	-5.57	101.25	109.60
1	D	272	GLU	CB-CA-C	-5.51	100.55	110.35
1	D	15	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	166	LYS	CB-CG-CD	5.48	123.91	111.30
1	B	118	GLU	CB-CA-C	-5.48	98.67	110.45
1	D	410	GLU	CB-CA-C	-5.47	102.25	110.90
1	A	205	SER	N-CA-CB	-5.45	101.74	110.63
1	D	410	GLU	CG-CD-OE2	-5.43	105.90	118.40
1	A	436	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	256	LYS	CG-CD-CE	-5.41	98.86	111.30
1	A	399	ARG	CA-CB-CG	-5.38	103.34	114.10
1	B	410	GLU	CG-CD-OE2	5.38	130.78	118.40
1	D	516	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	C	518	GLY	O-C-N	-5.36	118.20	122.81
1	D	22	MET	CG-SD-CE	5.34	112.64	100.90
1	C	401	LEU	N-CA-CB	5.33	119.09	110.40
1	D	500	ARG	CA-CB-CG	-5.31	103.49	114.10
1	D	336	LYS	CG-CD-CE	5.28	123.45	111.30
1	A	82	GLU	CG-CD-OE1	5.27	130.51	118.40
1	B	445	ARG	NH1-CZ-NH2	5.27	126.14	119.30
1	B	80	THR	CA-CB-OG1	-5.26	101.72	109.60
1	C	399	ARG	CB-CA-C	-5.24	101.94	110.85
1	B	464	HIS	CB-CG-CD2	-5.21	124.43	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	THR	CA-CB-OG1	-5.19	101.81	109.60
1	A	120	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	D	464	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	C	464	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	B	339	ARG	CA-CB-CG	-5.15	103.80	114.10
1	B	505	LYS	CG-CD-CE	5.15	123.14	111.30
1	A	125	LYS	CA-CB-CG	5.14	124.38	114.10
1	B	78	HIS	CA-CB-CG	-5.11	108.69	113.80
1	C	516	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	B	60	THR	CA-CB-OG1	-5.10	101.95	109.60
1	C	56	ARG	CB-CG-CD	-5.09	99.59	111.30
1	A	60	THR	CA-CB-OG1	-5.09	101.97	109.60
1	A	207	LYS	CA-C-N	5.08	125.50	120.31
1	A	207	LYS	C-N-CA	5.08	125.50	120.31
1	A	339	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	B	447	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	B	14	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	139	THR	OG1-CB-CG2	-5.06	99.18	109.30
1	B	399	ARG	CA-CB-CG	-5.05	104.00	114.10
1	A	272	GLU	CB-CG-CD	5.03	121.15	112.60
1	B	522	THR	CA-CB-OG1	-5.02	102.07	109.60
1	D	318	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	329	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	C	528	VAL	CA-CB-CG1	5.00	118.91	110.40
1	D	56	ARG	CB-CG-CD	-5.00	99.80	111.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	ARG	Sidechain
1	A	339	ARG	Sidechain
1	A	400	ARG	Sidechain
1	B	316	ARG	Sidechain
1	B	339	ARG	Sidechain
1	B	400	ARG	Sidechain
1	B	436	ARG	Sidechain
1	B	443	ARG	Sidechain
1	B	461	ARG	Sidechain
1	C	120	ARG	Sidechain
1	C	316	ARG	Sidechain
1	C	399	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	436	ARG	Sidechain
1	C	526	ARG	Sidechain
1	D	120	ARG	Sidechain
1	D	316	ARG	Sidechain
1	D	327	ALA	Peptide
1	D	400	ARG	Sidechain
1	D	436	ARG	Sidechain
1	D	443	ARG	Sidechain

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	3977	0	4057	55	0
1	B	3977	0	4057	44	0
1	C	3970	0	4055	54	0
1	D	3976	0	4055	69	0
2	A	20	0	10	0	0
2	B	20	0	9	0	0
2	C	20	0	10	0	0
2	D	20	0	9	0	0
3	A	16	0	22	15	0
3	B	8	0	12	2	0
3	D	4	0	6	0	0
4	A	8	0	4	3	0
4	B	8	0	4	2	0
4	C	8	0	3	3	0
4	D	8	0	4	2	0
5	C	12	0	16	8	0
6	C	2	0	0	0	0
7	A	440	0	0	14	0
7	B	439	0	0	10	0
7	C	291	0	0	14	0
7	D	248	0	0	15	0
All	All	17472	0	16333	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:CD	3:A:602:EDO:H21	1.67	1.23
1:A:447:ARG:HD3	3:A:602:EDO:H21	1.23	1.17
1:A:447:ARG:NE	3:A:602:EDO:H21	1.65	1.09
1:D:494:MET:HE1	1:D:530:VAL:HG22	1.31	1.05
1:D:505:LYS:HD3	1:D:505:LYS:H	1.23	0.99
1:D:504:LYS:HE3	7:D:707:HOH:O	1.64	0.95
1:C:234:GLU:HG3	7:C:973:HOH:O	1.72	0.89
1:C:443:ARG:HD3	7:C:870:HOH:O	1.73	0.88
1:C:504:LYS:HZ2	1:C:504:LYS:HB3	1.39	0.87
1:D:494:MET:HE2	1:D:530:VAL:HG13	1.58	0.86
1:B:339:ARG:HH11	1:B:339:ARG:HG3	1.41	0.85
1:C:474:CYS:SG	7:C:769:HOH:O	2.35	0.83
1:A:447:ARG:HD3	3:A:602:EDO:C2	2.06	0.82
1:D:505:LYS:H	1:D:505:LYS:CD	1.93	0.82
1:A:447:ARG:HE	3:A:602:EDO:C1	1.93	0.82
1:A:447:ARG:NE	3:A:602:EDO:C2	2.42	0.81
1:A:399:ARG:HH22	1:C:399:ARG:HH22	1.34	0.76
1:A:447:ARG:HE	3:A:602:EDO:C2	1.99	0.75
1:A:399:ARG:NH2	1:C:399:ARG:HH22	1.85	0.75
1:D:123:LEU:HD13	1:D:150:GLU:HG2	1.69	0.74
1:C:342:ARG:H	1:D:329:GLN:HE21	1.34	0.73
1:D:146:ASN:HD22	1:D:158:TRP:HE1	1.37	0.73
1:B:443:ARG:HD3	7:B:718:HOH:O	1.88	0.73
1:D:505:LYS:HD3	1:D:505:LYS:N	2.03	0.72
1:C:146:ASN:HD22	1:C:158:TRP:HE1	1.39	0.71
1:A:40:ILE:HA	7:A:1047:HOH:O	1.92	0.70
1:D:504:LYS:HG2	7:D:707:HOH:O	1.92	0.70
1:D:436:ARG:NH1	7:D:703:HOH:O	2.23	0.69
5:C:602:GOL:H32	7:C:854:HOH:O	1.91	0.69
5:C:602:GOL:O3	7:C:701:HOH:O	2.10	0.69
1:D:399:ARG:NH1	7:D:702:HOH:O	2.14	0.68
1:A:125:LYS:HA	1:A:125:LYS:HE2	1.76	0.67
1:D:494:MET:CE	1:D:530:VAL:HG13	2.24	0.67
1:A:410:GLU:OE2	7:A:701:HOH:O	2.11	0.67
1:B:50:THR:HG21	3:B:603:EDO:H22	1.76	0.67
1:C:118:GLU:OE1	1:C:120:ARG:HD3	1.94	0.67
1:B:339:ARG:NH1	7:B:703:HOH:O	2.29	0.66
1:C:234:GLU:CG	7:C:973:HOH:O	2.37	0.66
1:D:296:ASP:OD2	7:D:701:HOH:O	2.13	0.66
1:A:439:HIS:HD2	7:A:1074:HOH:O	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:CD	3:A:602:EDO:C2	2.61	0.65
1:B:399:ARG:NH1	7:B:701:HOH:O	2.21	0.65
1:B:399:ARG:HH12	1:D:399:ARG:NH2	1.94	0.65
1:A:124:ILE:HG22	1:A:125:LYS:HG2	1.79	0.64
1:C:329:GLN:HE21	1:D:342:ARG:HG2	1.63	0.64
1:D:22:MET:HA	1:D:22:MET:HE3	1.80	0.63
1:A:146:ASN:HD22	1:A:158:TRP:HE1	1.45	0.63
1:C:455:ARG:HB2	5:C:602:GOL:H31	1.80	0.63
1:B:146:ASN:HD22	1:B:158:TRP:HE1	1.45	0.62
1:C:464:HIS:HD2	7:C:949:HOH:O	1.81	0.62
1:C:395:PHE:CZ	1:C:399:ARG:HD2	2.34	0.62
1:A:339:ARG:NH1	7:A:705:HOH:O	2.33	0.62
1:A:311:LYS:NZ	1:B:350:ASN:HD21	1.97	0.61
1:B:513:THR:HB	7:B:992:HOH:O	2.00	0.61
1:D:476:ASP:OD2	1:D:488:LEU:HD21	2.00	0.61
1:C:86:GLU:HG3	7:C:740:HOH:O	2.00	0.61
1:A:513:THR:HB	7:A:840:HOH:O	1.99	0.61
4:D:603:SIN:H32	7:D:710:HOH:O	2.01	0.60
1:C:339:ARG:HH12	1:D:180:LEU:HD22	1.66	0.60
1:D:437:SER:HA	1:D:440:GLN:HE21	1.66	0.60
1:C:342:ARG:H	1:D:329:GLN:NE2	1.97	0.60
5:C:604:GOL:H11	7:C:929:HOH:O	2.01	0.60
5:C:604:GOL:C1	7:C:929:HOH:O	2.49	0.60
1:B:14:GLN:HG3	7:B:1012:HOH:O	2.01	0.59
1:B:400:ARG:HD2	1:D:392:LEU:HD11	1.84	0.59
1:B:464:HIS:HD2	7:B:1039:HOH:O	1.84	0.59
1:D:234:GLU:HG3	7:D:939:HOH:O	2.01	0.59
1:C:437:SER:HA	1:C:440:GLN:HE21	1.66	0.59
1:D:494:MET:CE	1:D:530:VAL:HG22	2.20	0.59
1:A:342:ARG:H	1:B:329:GLN:HE21	1.48	0.58
1:A:342:ARG:H	1:B:329:GLN:NE2	2.02	0.58
1:A:464:HIS:HD2	3:A:603:EDO:O1	1.87	0.58
1:D:142:ILE:HD11	1:D:195:THR:HG21	1.85	0.58
1:A:121:THR:HB	1:A:157:LEU:HD11	1.84	0.57
1:A:447:ARG:HE	3:A:602:EDO:H12	1.68	0.57
1:B:107:PRO:O	1:B:464:HIS:HE1	1.86	0.57
1:C:443:ARG:CD	7:C:870:HOH:O	2.39	0.57
1:B:293:ALA:HB1	4:B:604:SIN:C2	2.34	0.57
1:C:270:LYS:HZ1	4:C:603:SIN:H21	1.68	0.57
1:B:399:ARG:HH22	1:D:399:ARG:HH22	1.51	0.57
1:A:437:SER:HA	1:A:440:GLN:HE21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:HIS:HD2	7:B:993:HOH:O	1.86	0.57
1:C:311:LYS:NZ	1:D:350:ASN:HD21	2.02	0.56
1:A:387:ALA:O	3:A:602:EDO:H11	2.05	0.56
4:A:606:SIN:H32	7:A:704:HOH:O	2.04	0.56
1:B:123:LEU:HD12	1:B:150:GLU:HG2	1.88	0.56
1:D:124:ILE:O	1:D:152:CYS:O	2.23	0.55
1:D:234:GLU:CG	7:D:939:HOH:O	2.55	0.55
1:C:270:LYS:NZ	4:C:603:SIN:H21	2.22	0.55
1:C:504:LYS:HB3	1:C:504:LYS:NZ	2.11	0.54
1:D:391:HIS:HD2	7:D:879:HOH:O	1.90	0.54
1:C:455:ARG:CB	5:C:602:GOL:H31	2.37	0.54
1:C:350:ASN:HD21	1:D:311:LYS:NZ	2.05	0.54
1:A:293:ALA:HB1	4:A:606:SIN:H31	1.90	0.54
1:B:52:GLY:O	1:B:56:ARG:HG3	2.08	0.54
1:C:107:PRO:O	1:C:464:HIS:HE1	1.90	0.53
1:D:464:HIS:HD2	7:D:918:HOH:O	1.90	0.53
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.90	0.53
1:B:293:ALA:HB1	4:B:604:SIN:H22	1.91	0.53
1:C:270:LYS:CE	4:C:603:SIN:H21	2.37	0.53
1:D:107:PRO:O	1:D:464:HIS:HE1	1.92	0.53
1:A:311:LYS:HZ1	1:B:350:ASN:HD21	1.55	0.52
1:C:455:ARG:HB2	5:C:602:GOL:C3	2.39	0.52
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.91	0.52
1:B:339:ARG:HH11	1:B:339:ARG:CG	2.15	0.52
1:C:329:GLN:NE2	1:D:342:ARG:H	2.07	0.52
1:C:447:ARG:NE	7:C:709:HOH:O	2.38	0.52
1:C:392:LEU:O	1:C:396:GLU:HG3	2.08	0.52
1:C:123:LEU:HD12	1:C:150:GLU:HG2	1.92	0.52
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.92	0.52
1:B:146:ASN:HB3	1:B:149:MET:HE3	1.91	0.52
1:D:230:LYS:NZ	1:D:261:LYS:HE3	2.24	0.52
1:D:84:HIS:ND1	7:D:706:HOH:O	2.34	0.51
1:B:399:ARG:NH2	1:D:399:ARG:HH12	2.08	0.51
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.92	0.51
1:A:40:ILE:HG23	1:A:42:ALA:H	1.75	0.51
1:B:392:LEU:HD21	1:D:400:ARG:HE	1.76	0.50
1:B:436:ARG:NH2	7:B:711:HOH:O	2.43	0.50
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.93	0.50
1:A:27:LEU:HD23	1:B:401:LEU:HD22	1.93	0.50
1:C:342:ARG:HG2	1:D:329:GLN:NE2	2.27	0.49
1:A:443:ARG:HD3	7:A:710:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:SER:HB3	1:D:206:LYS:HE2	1.93	0.49
1:A:350:ASN:HD21	1:B:311:LYS:NZ	2.10	0.49
1:B:392:LEU:O	1:B:396:GLU:HG3	2.11	0.49
1:B:470:PHE:CZ	1:B:500:ARG:HD2	2.48	0.49
1:A:473:LEU:CD2	1:A:475:LYS:HE3	2.43	0.49
1:D:230:LYS:HA	1:D:230:LYS:HD2	1.53	0.49
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.95	0.48
1:D:161:TYR:HB2	7:D:818:HOH:O	2.12	0.48
1:A:418:GLU:OE2	7:A:702:HOH:O	2.18	0.48
1:A:387:ALA:HA	3:A:602:EDO:H11	1.95	0.48
1:A:391:HIS:HD2	7:A:910:HOH:O	1.95	0.48
1:C:339:ARG:HH12	1:D:180:LEU:CD2	2.26	0.48
1:C:311:LYS:HZ1	1:D:350:ASN:HD21	1.62	0.47
1:A:439:HIS:CD2	7:A:1074:HOH:O	2.60	0.47
1:D:494:MET:HE3	1:D:503:PHE:CE1	2.50	0.47
1:A:107:PRO:O	1:A:464:HIS:HE1	1.98	0.46
1:A:146:ASN:ND2	1:A:158:TRP:HE1	2.11	0.46
1:A:293:ALA:HB1	4:A:606:SIN:C3	2.45	0.46
1:D:146:ASN:CG	1:D:149:MET:HE3	2.39	0.46
1:D:439:HIS:HD2	7:D:934:HOH:O	1.99	0.46
1:C:339:ARG:NH2	1:D:178:ASP:O	2.49	0.46
3:B:603:EDO:H21	7:B:1037:HOH:O	2.15	0.46
1:B:339:ARG:HG3	1:B:339:ARG:NH1	2.18	0.46
1:D:84:HIS:CE1	7:D:706:HOH:O	2.68	0.45
1:B:144:LEU:HD11	1:B:164:ILE:HG22	1.98	0.45
1:A:14:GLN:CG	7:A:1050:HOH:O	2.65	0.45
1:D:175:TYR:C	7:D:722:HOH:O	2.59	0.45
1:B:399:ARG:NH1	1:D:399:ARG:NH2	2.65	0.45
1:C:339:ARG:HH22	1:D:180:LEU:HD23	1.82	0.45
1:D:142:ILE:CD1	1:D:195:THR:HG21	2.46	0.45
1:C:395:PHE:CE2	1:C:399:ARG:HD2	2.52	0.45
1:A:399:ARG:NH1	1:C:399:ARG:NH2	2.64	0.44
1:C:146:ASN:HD22	1:C:158:TRP:NE1	2.11	0.44
1:C:75:ASN:ND2	5:C:604:GOL:H2	2.31	0.44
1:C:223:GLU:HG2	7:C:983:HOH:O	2.17	0.44
1:C:401:LEU:HD22	1:D:27:LEU:HD23	1.98	0.44
1:D:162:LYS:HE3	1:D:162:LYS:H	1.83	0.44
1:D:494:MET:HE2	1:D:531:PRO:HD2	2.00	0.43
1:A:14:GLN:HG2	7:A:1050:HOH:O	2.18	0.43
1:D:146:ASN:ND2	1:D:158:TRP:HE1	2.10	0.43
1:A:399:ARG:NH2	1:C:399:ARG:NH2	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.53	0.43
1:C:406:SER:O	1:C:408:PRO:HD3	2.18	0.43
1:C:440:GLN:HG2	7:C:705:HOH:O	2.19	0.43
1:C:329:GLN:HE21	1:D:342:ARG:H	1.66	0.43
1:C:516:ARG:HB2	1:C:517:PRO:HD2	2.00	0.43
1:B:112:LEU:HD23	1:B:112:LEU:C	2.44	0.43
1:C:180:LEU:HD23	1:C:180:LEU:HA	1.90	0.43
1:A:458:GLN:NE2	7:A:728:HOH:O	2.53	0.42
1:B:447:ARG:NE	7:B:710:HOH:O	2.42	0.42
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.54	0.42
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.55	0.42
1:A:56:ARG:HH11	1:A:56:ARG:HD3	1.52	0.42
1:B:74:LEU:HD21	1:B:88:ILE:HG13	2.02	0.42
1:C:74:LEU:HD21	1:C:88:ILE:HG13	2.00	0.42
1:D:494:MET:HE1	1:D:530:VAL:CG2	2.23	0.42
1:A:123:LEU:HD12	1:A:150:GLU:HG2	2.01	0.41
1:A:16:GLN:HB3	3:A:602:EDO:O2	2.19	0.41
1:D:293:ALA:HB1	4:D:603:SIN:C2	2.49	0.41
1:B:406:SER:O	1:B:408:PRO:HD3	2.20	0.41
1:A:288:ASP:O	1:A:323:PRO:HD2	2.20	0.41
1:B:180:LEU:HD22	1:B:180:LEU:HA	1.88	0.41
1:D:16:GLN:HG2	1:D:40:ILE:HG23	2.03	0.41
1:D:253[A]:GLU:OE2	1:D:253[A]:GLU:HA	2.21	0.41
1:A:397:GLU:CD	1:B:25:THR:HB	2.45	0.41
1:D:146:ASN:CB	1:D:149:MET:HE3	2.52	0.40
1:A:40:ILE:HG13	7:A:1047:HOH:O	2.21	0.40
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.56	0.40
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.02	0.40
1:D:230:LYS:HZ3	1:D:261:LYS:HE3	1.85	0.40
1:D:406:SER:O	1:D:408:PRO:HD3	2.20	0.40
1:A:235:GLN:HA	3:A:605:EDO:H22	2.04	0.40
1:B:404:ILE:HD12	1:B:404:ILE:HA	1.96	0.40
1:D:470:PHE:CZ	1:D:500:ARG:HD2	2.57	0.40
1:A:16:GLN:O	3:A:602:EDO:H22	2.20	0.40
1:C:470:PHE:CZ	1:C:500:ARG:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	516/537 (96%)	506 (98%)	9 (2%)	1 (0%)	43	40
1	B	516/537 (96%)	506 (98%)	9 (2%)	1 (0%)	43	40
1	C	516/537 (96%)	506 (98%)	9 (2%)	1 (0%)	43	40
1	D	516/537 (96%)	507 (98%)	7 (1%)	2 (0%)	30	22
All	All	2064/2148 (96%)	2025 (98%)	34 (2%)	5 (0%)	43	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	ILE
1	A	328	THR
1	B	328	THR
1	C	328	THR
1	D	328	THR

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	426/441 (97%)	413 (97%)	13 (3%)	35	31
1	B	426/441 (97%)	407 (96%)	19 (4%)	24	17
1	C	426/441 (97%)	410 (96%)	16 (4%)	29	23
1	D	426/441 (97%)	396 (93%)	30 (7%)	14	7
All	All	1704/1764 (97%)	1626 (95%)	78 (5%)	24	17

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	40	ILE
1	A	104	LEU
1	A	125	LYS
1	A	166	LYS
1	A	183	LEU
1	A	230	LYS
1	A	284	LEU
1	A	404	ILE
1	A	504	LYS
1	A	505	LYS
1	A	509	VAL
1	A	525	MET
1	B	104	LEU
1	B	132	VAL
1	B	135	LYS
1	B	157	LEU
1	B	166	LYS
1	B	180	LEU
1	B	183	LEU
1	B	211	LEU
1	B	216	VAL
1	B	284	LEU
1	B	400	ARG
1	B	404	ILE
1	B	424	CYS
1	B	480	GLU
1	B	504	LYS
1	B	509	VAL
1	B	523	ASN
1	B	525	MET
1	B	532	HIS
1	C	104	LEU
1	C	157	LEU
1	C	166	LYS
1	C	183	LEU
1	C	206	LYS
1	C	211	LEU
1	C	216	VAL
1	C	230	LYS
1	C	284	LEU
1	C	404	ILE

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Mol	Chain	Res	Type
1	C	465	LEU
1	C	488	LEU
1	C	505	LYS
1	C	509	VAL
1	C	525	MET
1	C	528	VAL
1	D	14	GLN
1	D	74	LEU
1	D	104	LEU
1	D	125	LYS
1	D	132	VAL
1	D	135	LYS
1	D	136	LYS
1	D	149	MET
1	D	157	LEU
1	D	162	LYS
1	D	180	LEU
1	D	183	LEU
1	D	187	GLN
1	D	206	LYS
1	D	211	LEU
1	D	216	VAL
1	D	227	GLN
1	D	230	LYS
1	D	253[A]	GLU
1	D	253[B]	GLU
1	D	261	LYS
1	D	272	GLU
1	D	284	LEU
1	D	401	LEU
1	D	404	ILE
1	D	424	CYS
1	D	465	LEU
1	D	505	LYS
1	D	509	VAL
1	D	525	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	155	ASN

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Mol	Chain	Res	Type
1	A	252	HIS
1	A	264	ASN
1	A	350	ASN
1	A	378	GLN
1	A	391	HIS
1	A	393	GLN
1	A	439	HIS
1	A	440	GLN
1	A	464	HIS
1	A	491	ASN
1	B	90	ASN
1	B	146	ASN
1	B	199	ASN
1	B	264	ASN
1	B	329	GLN
1	B	350	ASN
1	B	378	GLN
1	B	391	HIS
1	B	393	GLN
1	B	464	HIS
1	B	479	GLN
1	B	495	ASN
1	B	523	ASN
1	C	90	ASN
1	C	146	ASN
1	C	227	GLN
1	C	252	HIS
1	C	264	ASN
1	C	329	GLN
1	C	350	ASN
1	C	378	GLN
1	C	391	HIS
1	C	440	GLN
1	C	464	HIS
1	C	479	GLN
1	C	491	ASN
1	C	495	ASN
1	D	44	ASN
1	D	90	ASN
1	D	146	ASN
1	D	199	ASN
1	D	252	HIS

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Mol	Chain	Res	Type
1	D	264	ASN
1	D	329	GLN
1	D	350	ASN
1	D	391	HIS
1	D	439	HIS
1	D	440	GLN
1	D	464	HIS
1	D	495	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	ALY	C	115	1	10,11,12	0.61	0	7,12,14	1.73	1 (14%)
1	ALY	B	115	1	10,11,12	0.77	0	7,12,14	0.91	1 (14%)
1	ALY	D	115	1	10,11,12	0.61	0	7,12,14	1.28	1 (14%)
1	ALY	A	115	1	10,11,12	0.58	0	7,12,14	2.09	2 (28%)

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
1	ALY	C	115	1	-	1/9/10/12	-
1	ALY	B	115	1	-	1/9/10/12	-
1	ALY	D	115	1	-	1/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	A	115	1	-	2/9/10/12	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ALY	CE-NZ-CH	4.82	129.67	122.56
1	C	115	ALY	CE-NZ-CH	4.41	129.08	122.56
1	D	115	ALY	CE-NZ-CH	3.23	127.33	122.56
1	A	115	ALY	CG-CD-CE	2.42	124.71	113.56
1	B	115	ALY	CE-NZ-CH	2.11	125.67	122.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	115	ALY	OH-CH-NZ-CE
1	A	115	ALY	CH3-CH-NZ-CE
1	C	115	ALY	CE-CD-CG-CB
1	B	115	ALY	CE-CD-CG-CB
1	D	115	ALY	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SIN	C	603	6	7,7,7	0.83	0	8,8,8	1.36	1 (12%)
2	FBP	B	601	-	18,20,20	1.34	3 (16%)	21,32,32	1.50	2 (9%)
4	SIN	B	604	-	7,7,7	1.83	2 (28%)	8,8,8	2.03	2 (25%)
2	FBP	A	601	-	18,20,20	0.74	0	21,32,32	0.96	2 (9%)
5	GOL	C	602	-	5,5,5	0.37	0	5,5,5	0.94	0
4	SIN	A	606	-	7,7,7	1.38	2 (28%)	8,8,8	2.73	4 (50%)
4	SIN	D	603	-	7,7,7	1.09	1 (14%)	8,8,8	1.96	2 (25%)
3	EDO	B	603	-	3,3,3	0.63	0	2,2,2	0.71	0
2	FBP	D	601	-	18,20,20	1.09	2 (11%)	21,32,32	1.53	3 (14%)
3	EDO	A	603	-	3,3,3	1.05	0	2,2,2	0.25	0
3	EDO	B	602	-	3,3,3	0.37	0	2,2,2	0.30	0
3	EDO	A	605	-	3,3,3	0.40	0	2,2,2	0.50	0
3	EDO	D	602	-	3,3,3	0.32	0	2,2,2	0.11	0
5	GOL	C	604	-	5,5,5	0.11	0	5,5,5	0.64	0
3	EDO	A	604	-	3,3,3	0.63	0	2,2,2	0.55	0
2	FBP	C	601	-	18,20,20	0.95	1 (5%)	21,32,32	1.22	2 (9%)
3	EDO	A	602	-	3,3,3	1.49	1 (33%)	2,2,2	2.19	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SIN	C	603	6	-	1/5/5/5	-
2	FBP	B	601	-	-	3/13/32/32	0/1/1/1
4	SIN	B	604	-	-	4/5/5/5	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
5	GOL	C	602	-	-	3/4/4/4	-
4	SIN	A	606	-	-	5/5/5/5	-
4	SIN	D	603	-	-	3/5/5/5	-
3	EDO	B	603	-	-	1/1/1/1	-
2	FBP	D	601	-	-	4/13/32/32	0/1/1/1
3	EDO	A	603	-	-	1/1/1/1	-
3	EDO	B	602	-	-	0/1/1/1	-
3	EDO	A	605	-	-	0/1/1/1	-
3	EDO	D	602	-	-	1/1/1/1	-
5	GOL	C	604	-	-	0/4/4/4	-
3	EDO	A	604	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	EDO	A	602	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	SIN	O2-C1	-3.42	1.19	1.30
2	D	601	FBP	O2-C2	-3.36	1.34	1.40
4	B	604	SIN	C3-C2	-3.21	1.40	1.51
2	B	601	FBP	O2-C2	-3.01	1.35	1.40
2	B	601	FBP	P1-O1P	2.86	1.59	1.50
4	A	606	SIN	C3-C2	-2.52	1.43	1.51
2	B	601	FBP	P1-O1	2.39	1.67	1.60
2	C	601	FBP	P2-O6	2.37	1.67	1.60
4	A	606	SIN	O4-C4	-2.26	1.23	1.30
3	A	602	EDO	O1-C1	-2.19	1.30	1.42
4	D	603	SIN	O2-C1	-2.02	1.24	1.30
2	D	601	FBP	P2-O6	2.00	1.66	1.60

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	SIN	C3-C2-C1	-5.93	97.95	113.67
2	B	601	FBP	O2-C2-O5	-4.66	100.37	109.33
2	D	601	FBP	O2-C2-O5	-4.16	101.34	109.33
4	D	603	SIN	C2-C3-C4	-3.57	104.18	113.67
2	C	601	FBP	O5P-P2-O6	-3.36	97.91	106.67
4	A	606	SIN	O1-C1-C2	-3.31	112.59	123.09
4	B	604	SIN	O3-C4-C3	-3.14	113.13	123.09
4	B	604	SIN	C2-C3-C4	-3.13	105.38	113.67
2	D	601	FBP	O5-C5-C6	-3.03	102.39	109.50
3	A	602	EDO	O1-C1-C2	-2.61	92.55	112.39
4	D	603	SIN	O1-C1-C2	-2.59	114.86	123.09
4	C	603	SIN	O1-C1-C2	-2.54	115.05	123.09
2	C	601	FBP	O6P-P2-O5P	2.41	116.83	107.80
2	D	601	FBP	O3P-P1-O2P	2.26	116.28	107.80
2	B	601	FBP	O3P-P1-O2P	2.25	116.25	107.80
4	A	606	SIN	O3-C4-C3	-2.19	116.15	123.09
2	A	601	FBP	O6P-P2-O4P	2.16	119.25	110.83
4	A	606	SIN	O2-C1-O1	2.03	128.56	123.33
2	A	601	FBP	O1-P1-O1P	-2.01	101.00	106.44

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FBP	O1-C1-C2-O2
2	B	601	FBP	O1-C1-C2-C3
2	B	601	FBP	O1-C1-C2-O5
2	D	601	FBP	O1-C1-C2-O2
2	D	601	FBP	O1-C1-C2-C3
2	D	601	FBP	O1-C1-C2-O5
5	C	602	GOL	O1-C1-C2-O2
2	C	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C4-C5-C6-O6
5	C	602	GOL	O1-C1-C2-C3
4	C	603	SIN	C1-C2-C3-C4
2	C	601	FBP	O5-C5-C6-O6
4	A	606	SIN	C1-C2-C3-C4
2	A	601	FBP	O5-C5-C6-O6
3	A	602	EDO	O1-C1-C2-O2
3	A	603	EDO	O1-C1-C2-O2
3	B	603	EDO	O1-C1-C2-O2
2	D	601	FBP	C4-C5-C6-O6
4	B	604	SIN	O2-C1-C2-C3
4	A	606	SIN	C2-C3-C4-O3
4	A	606	SIN	C2-C3-C4-O4
4	A	606	SIN	O1-C1-C2-C3
4	B	604	SIN	O1-C1-C2-C3
4	D	603	SIN	O2-C1-C2-C3
4	D	603	SIN	O1-C1-C2-C3
3	D	602	EDO	O1-C1-C2-O2
4	B	604	SIN	C2-C3-C4-O3
4	A	606	SIN	O2-C1-C2-C3
4	B	604	SIN	C2-C3-C4-O4
4	D	603	SIN	C2-C3-C4-O3
5	C	602	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 35 short contacts:

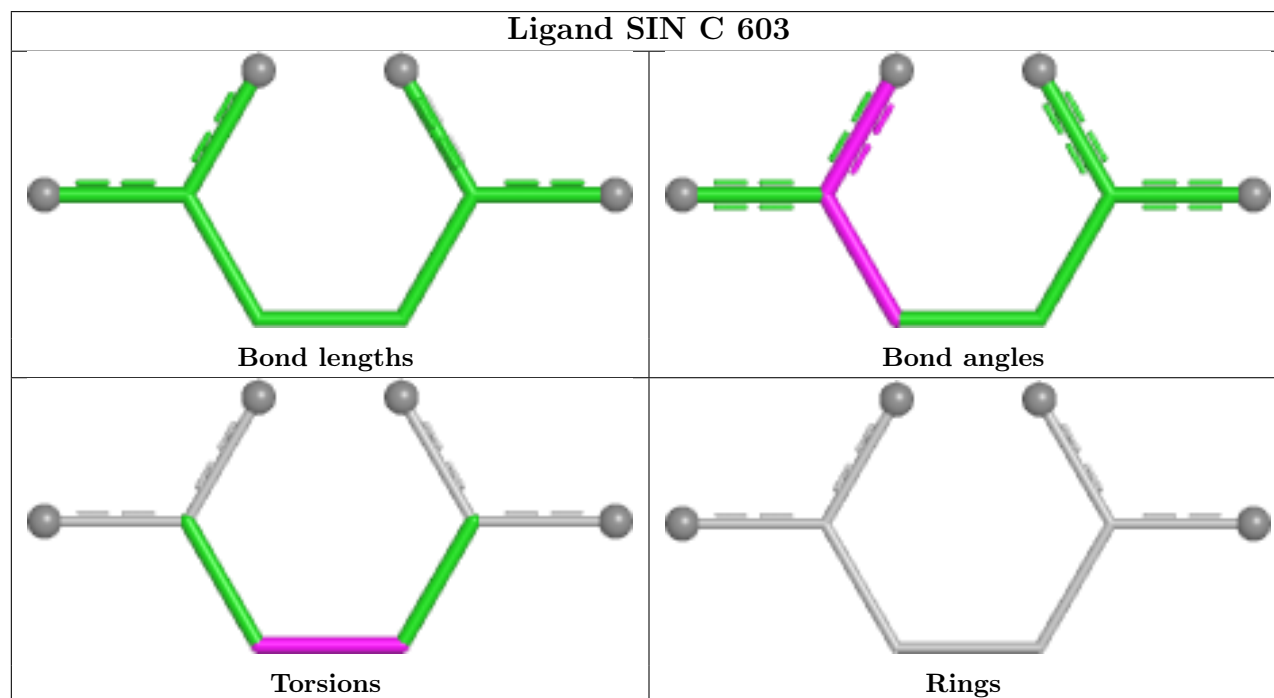
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	SIN	3	0
4	B	604	SIN	2	0
5	C	602	GOL	5	0
4	A	606	SIN	3	0

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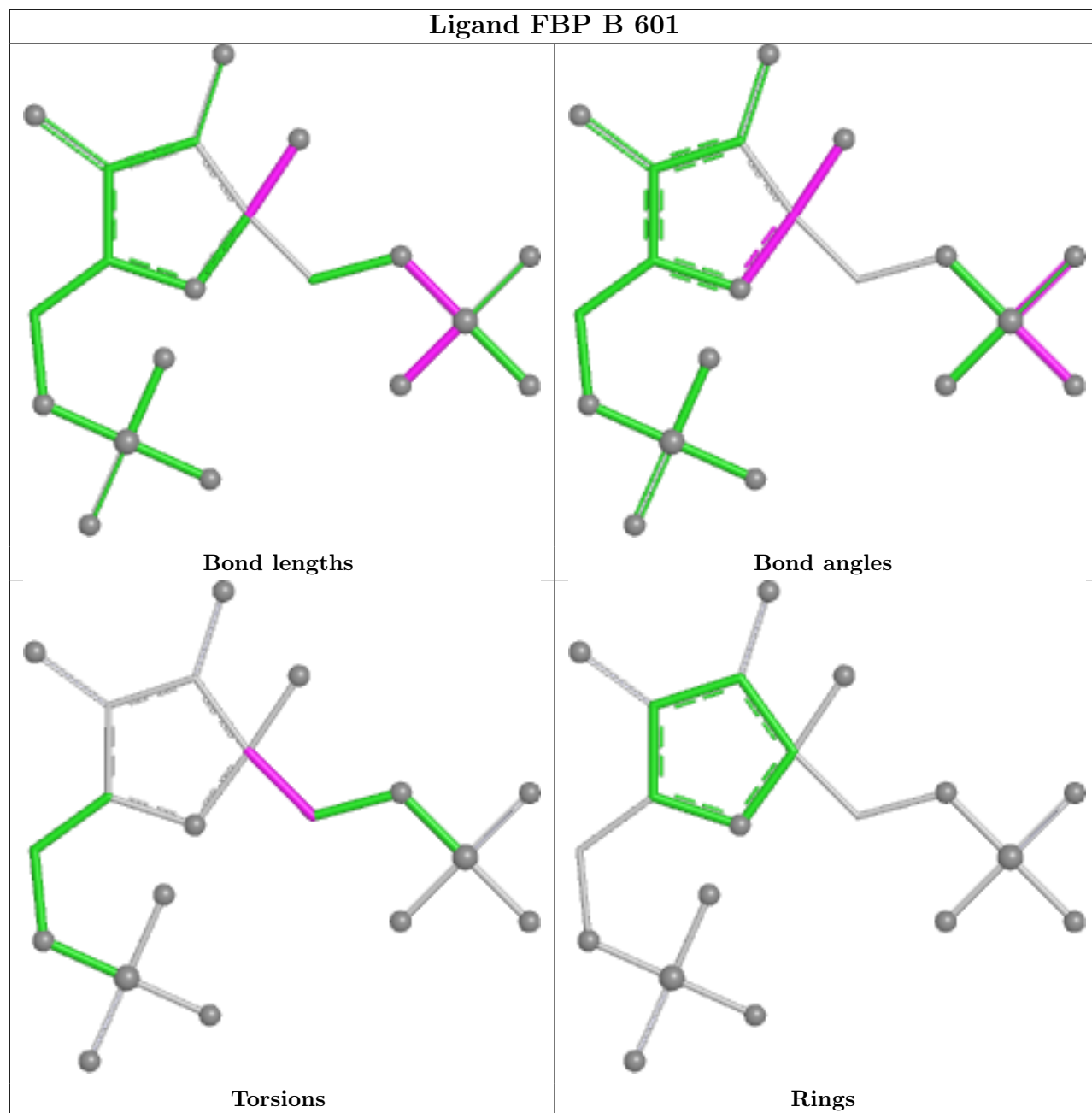
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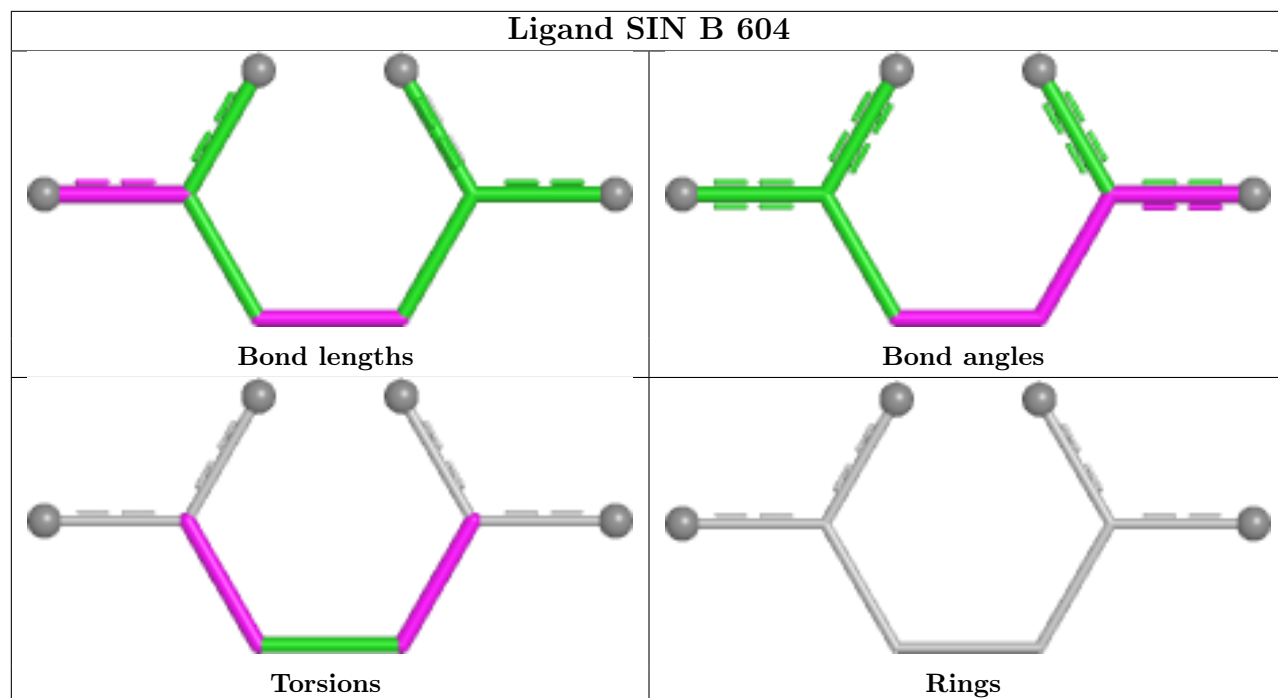
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	SIN	2	0
3	B	603	EDO	2	0
3	A	603	EDO	1	0
3	A	605	EDO	1	0
5	C	604	GOL	3	0
3	A	602	EDO	13	0

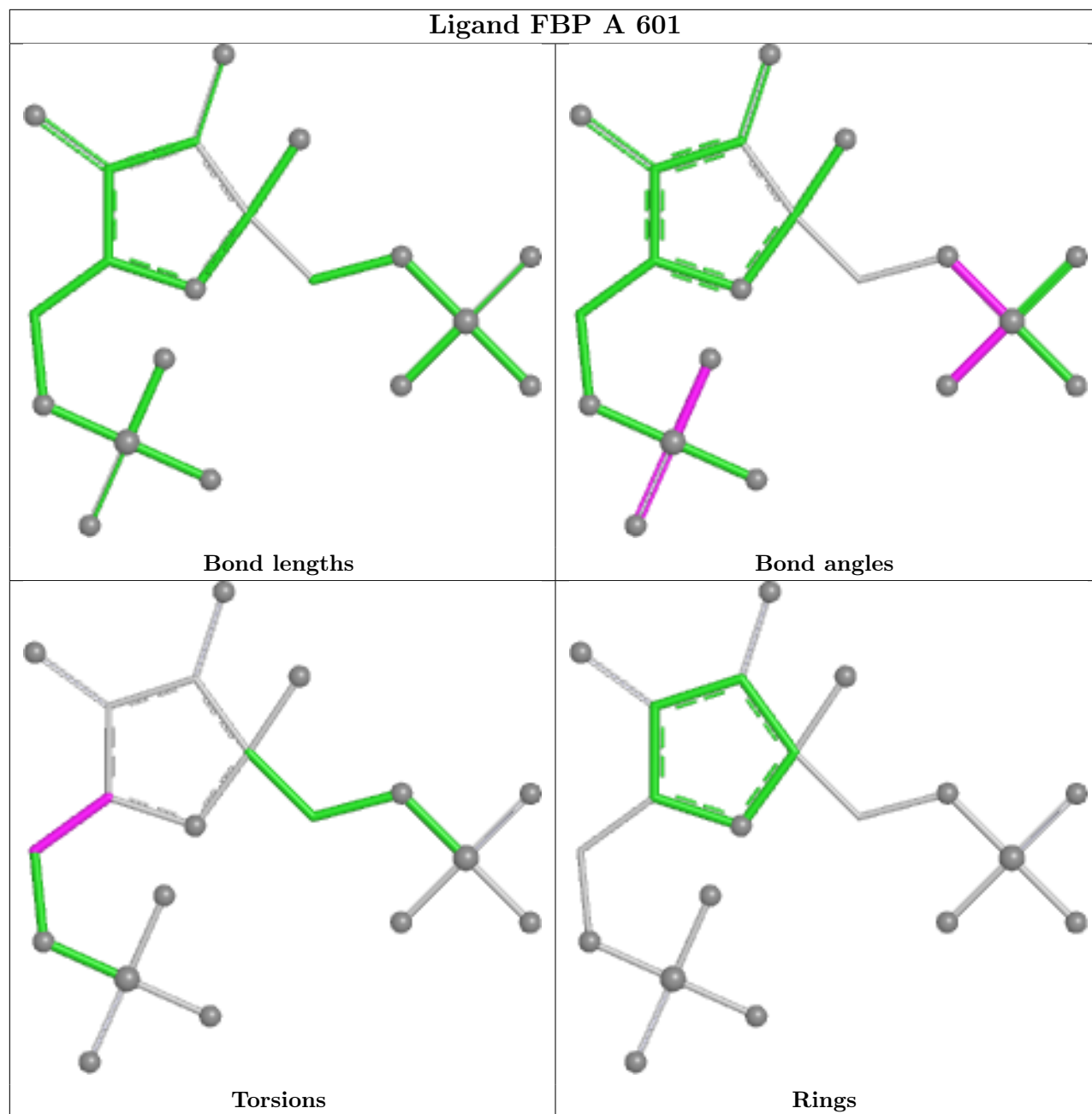
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

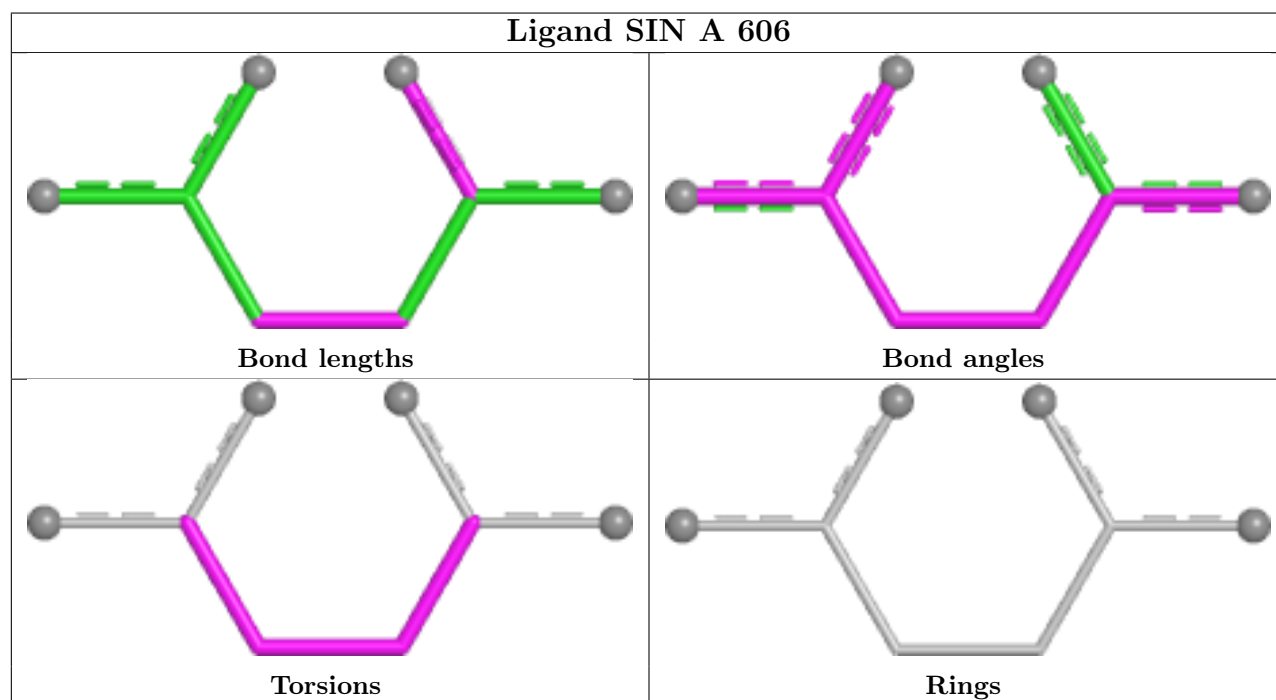
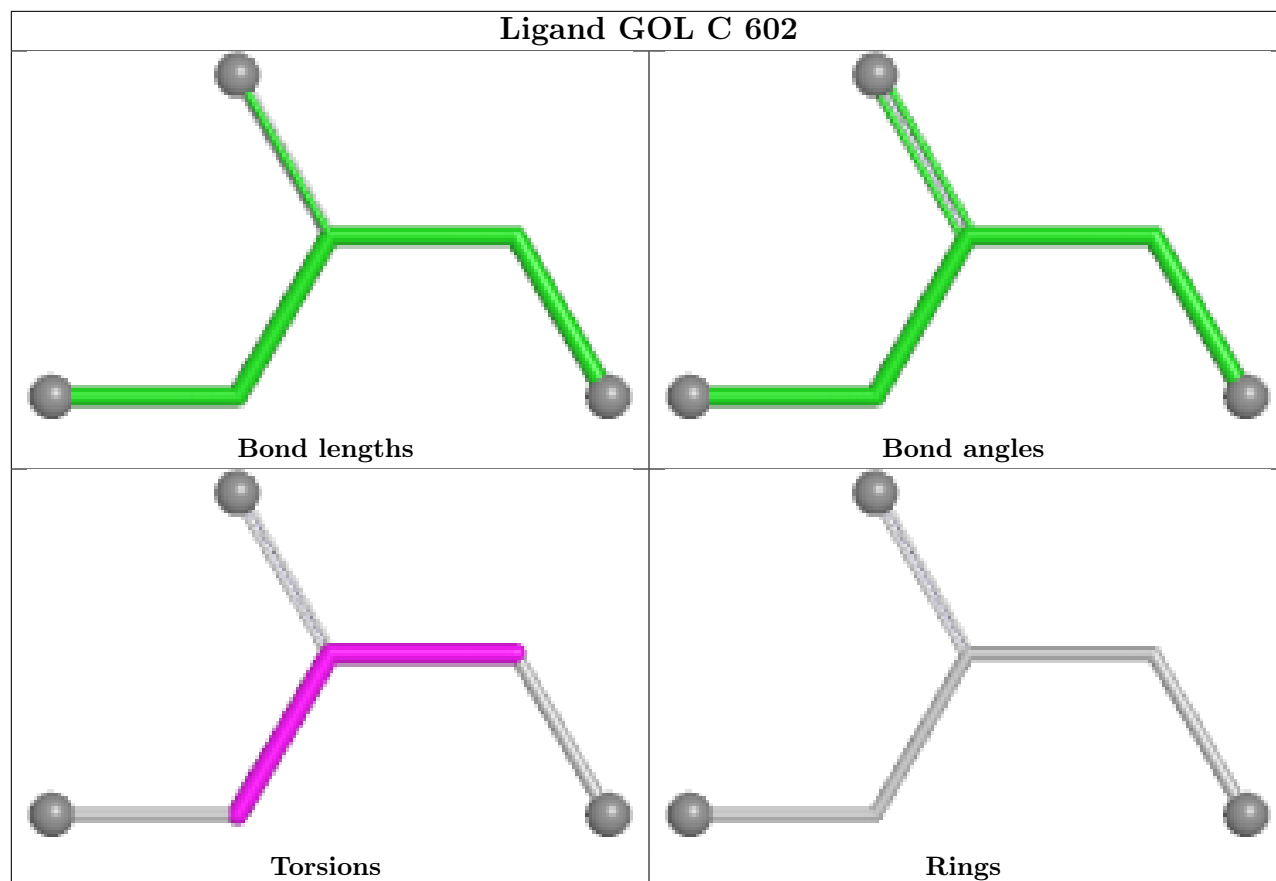


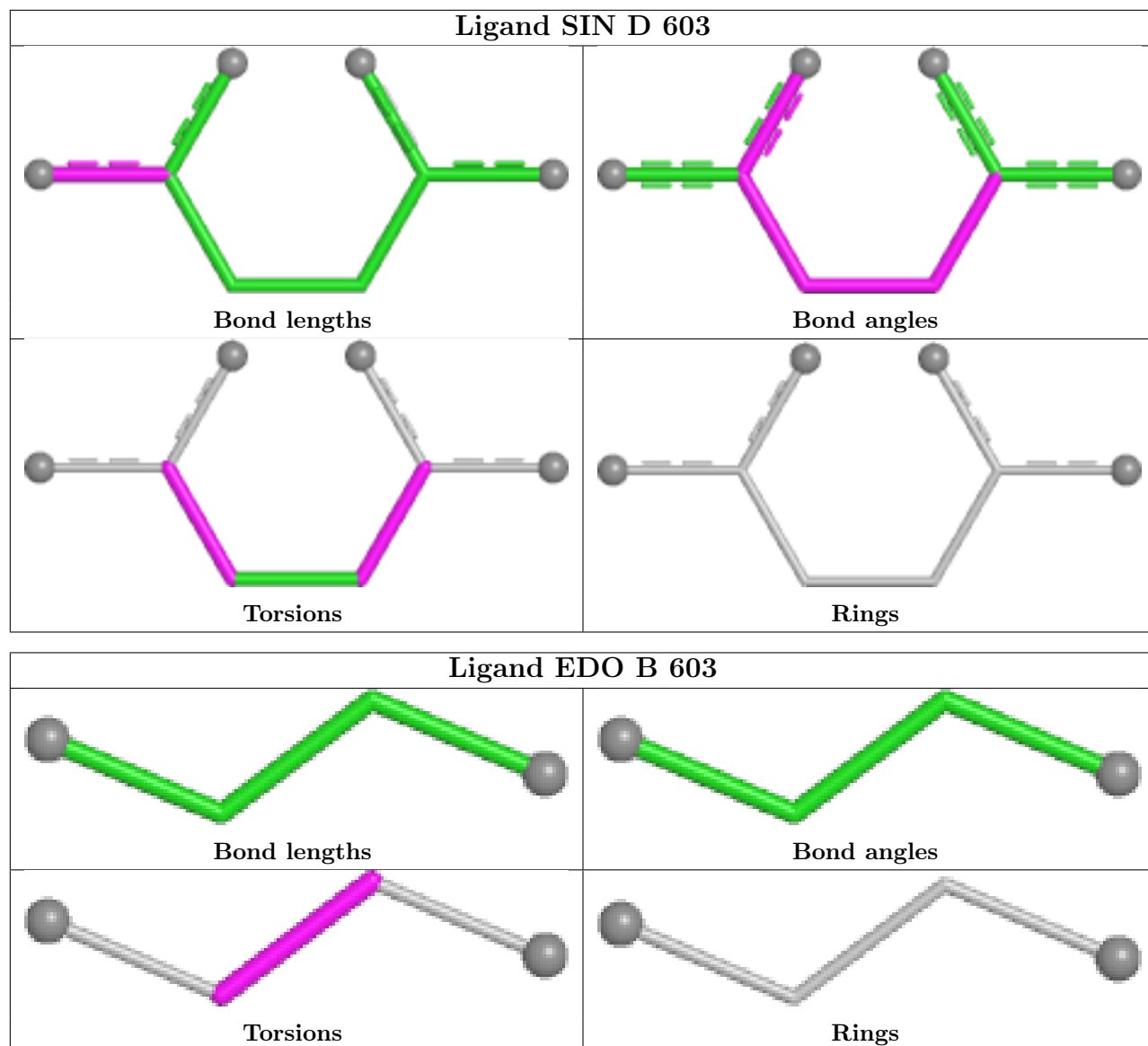
Ligand FBP B 601

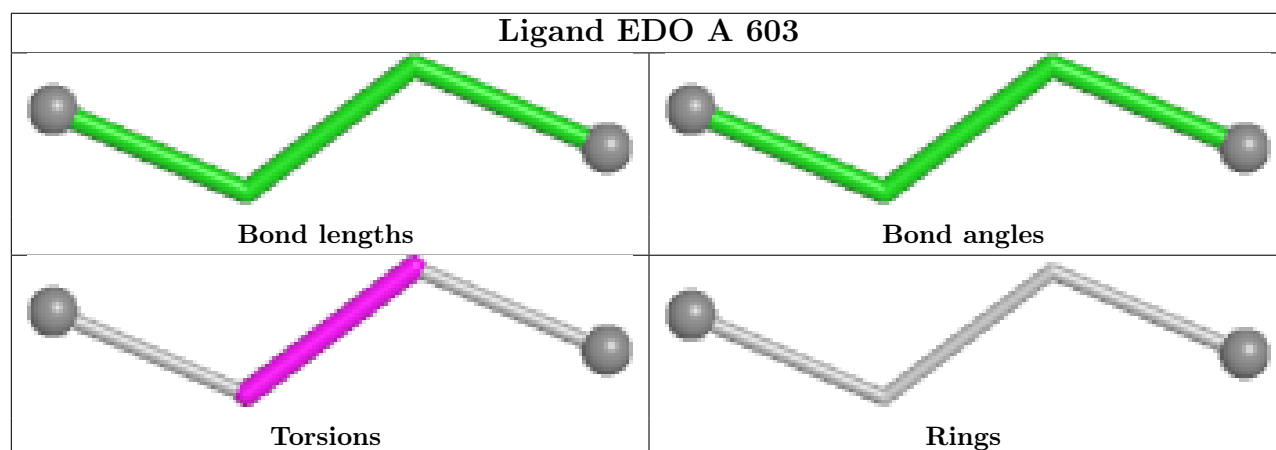
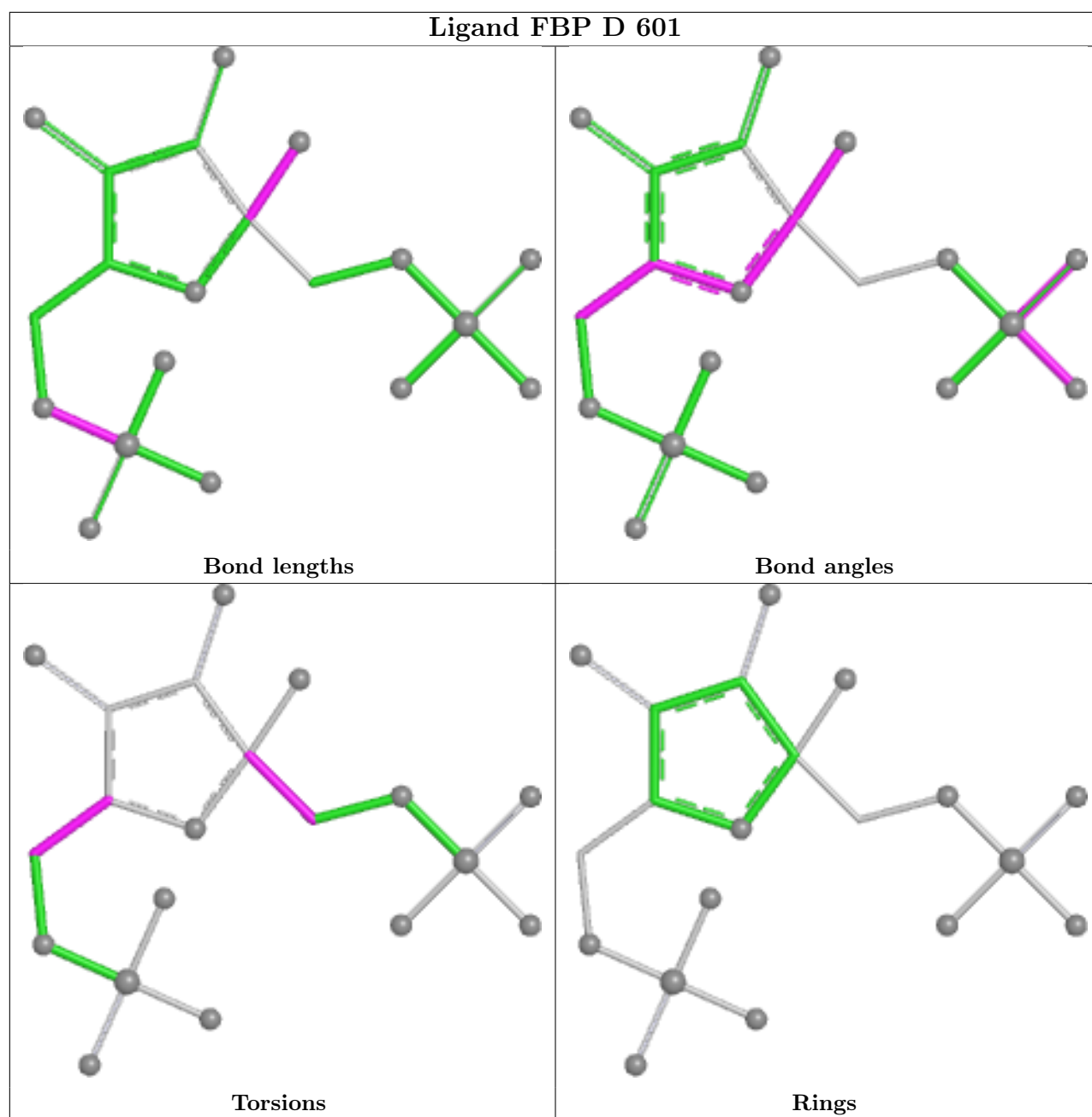


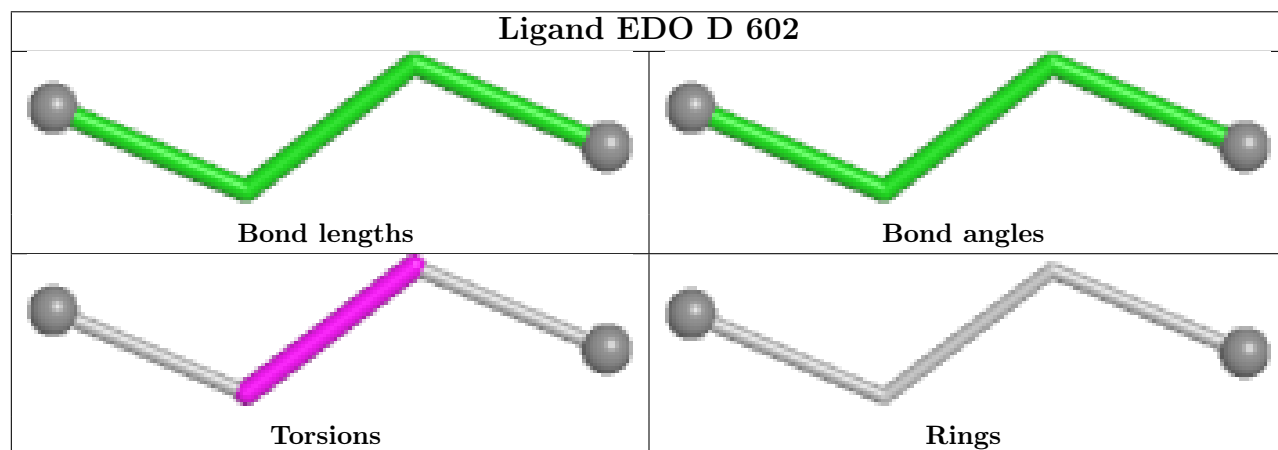
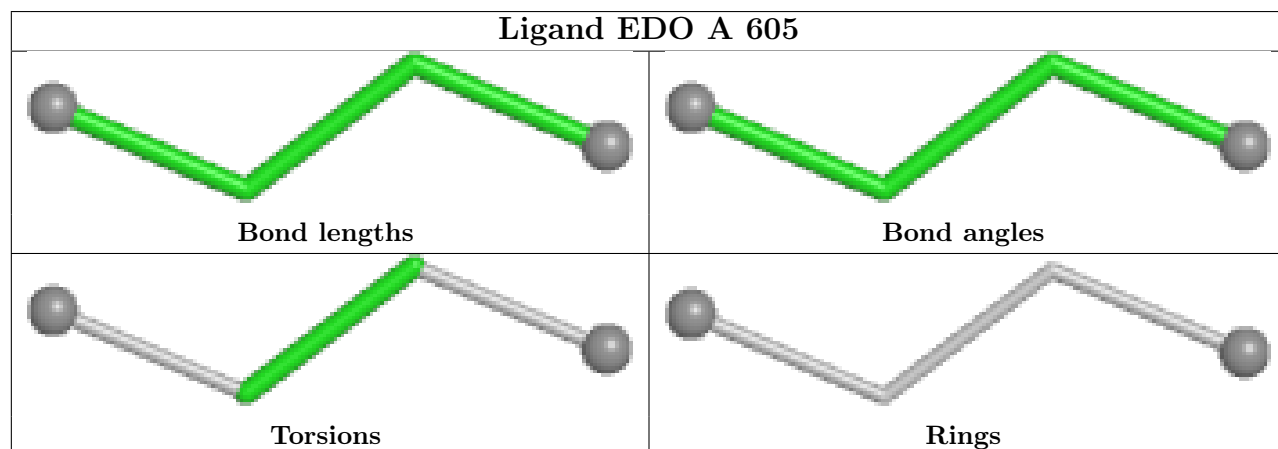
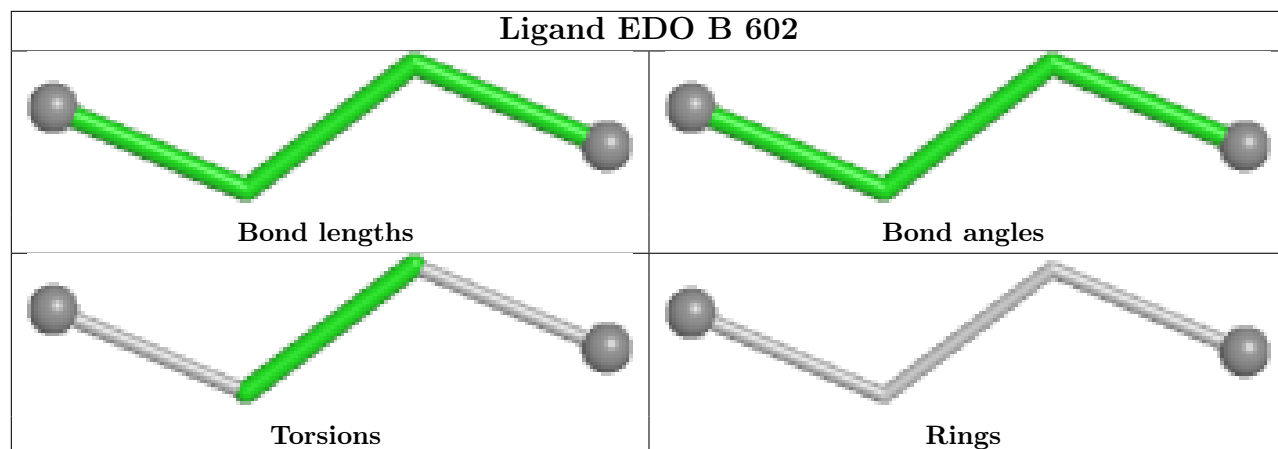


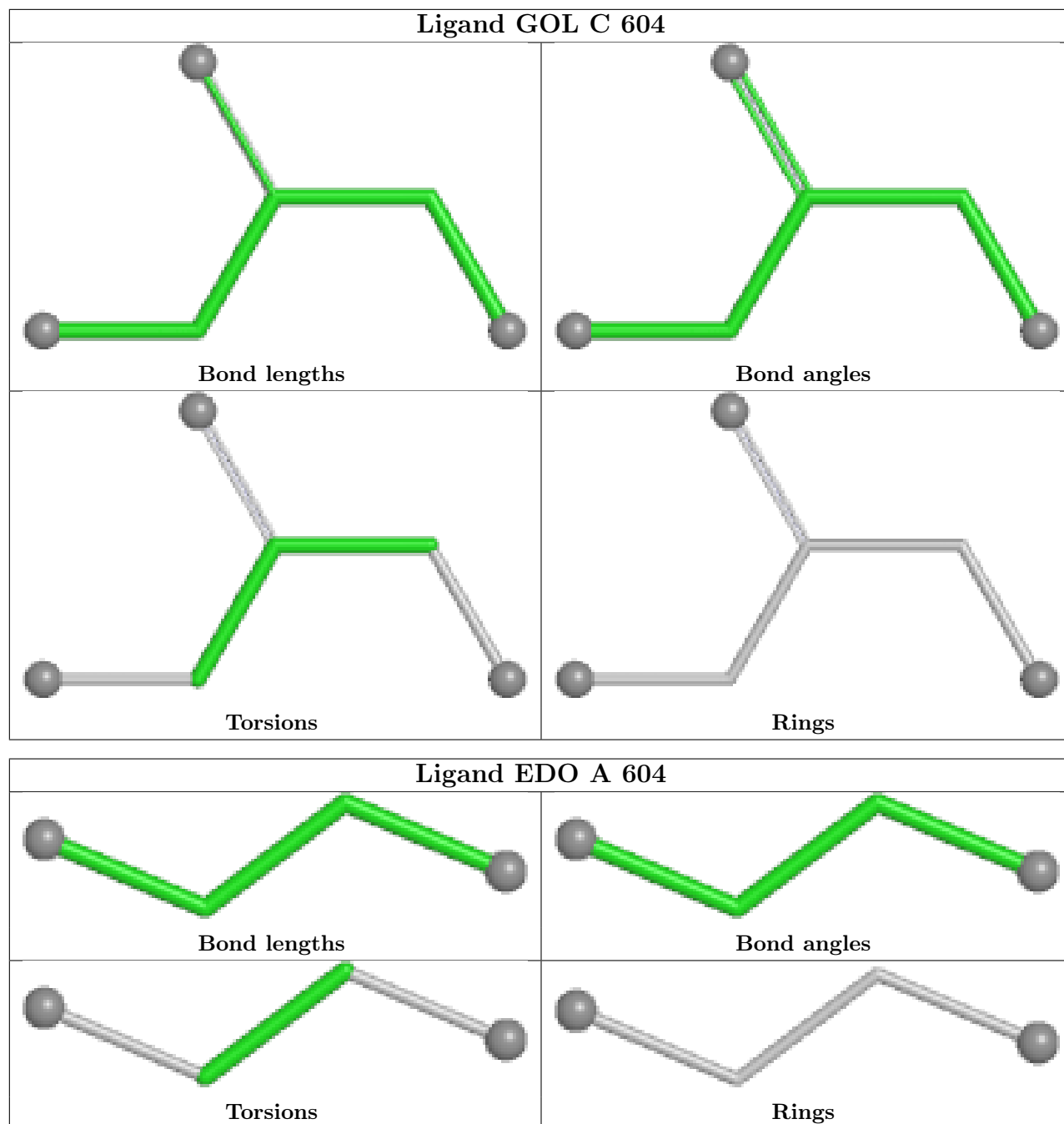




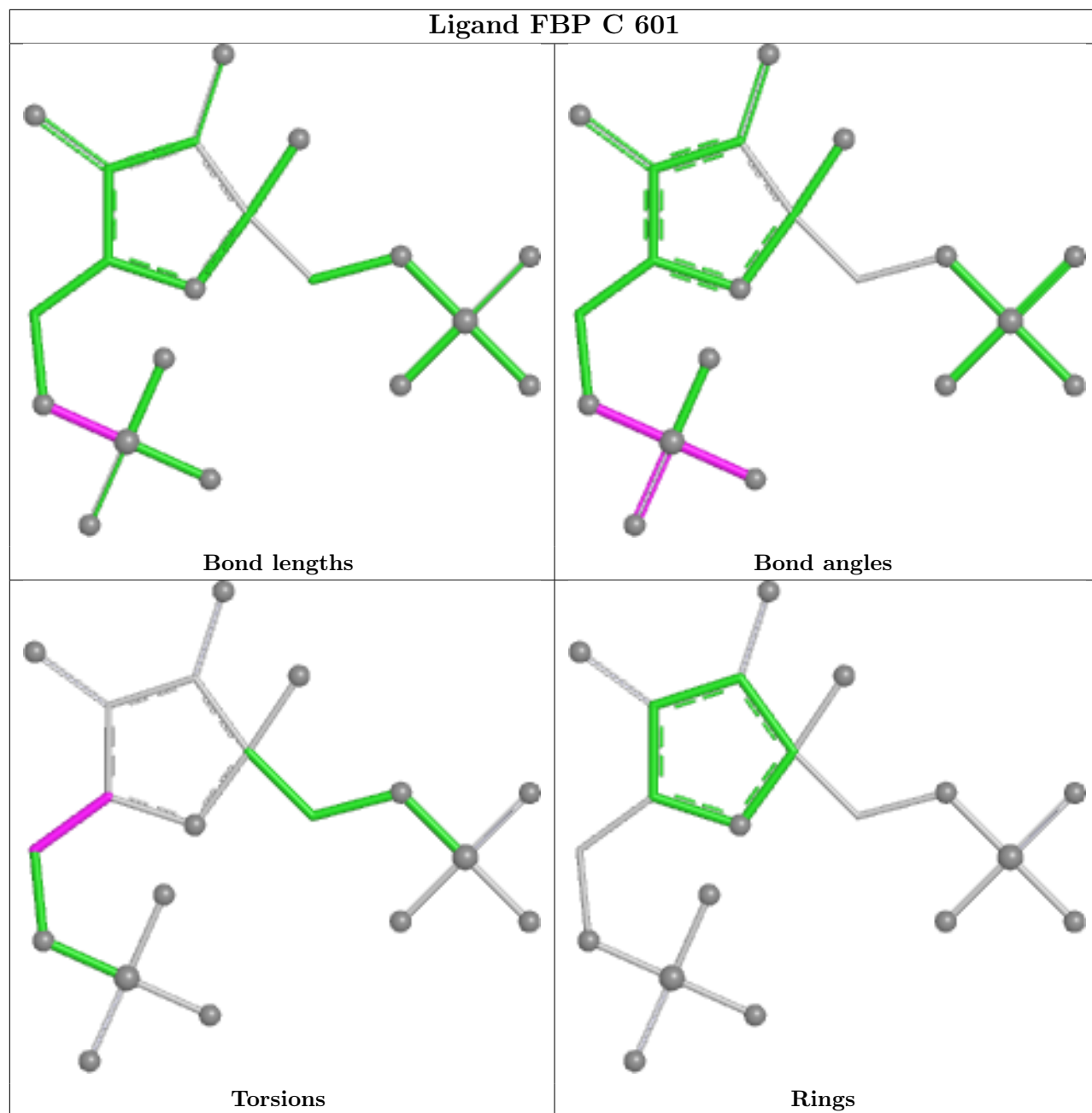




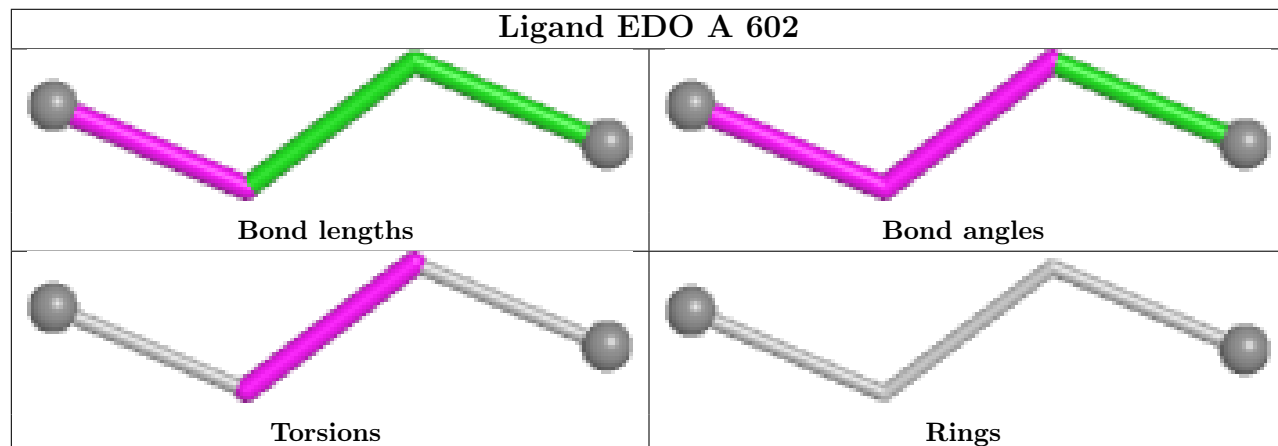




Ligand FBP C 601



Ligand EDO A 602



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	518/537 (96%)	-0.73	1 (0%) 91 91	15, 25, 50, 76	0
1	B	518/537 (96%)	-0.65	4 (0%) 82 83	15, 25, 60, 93	0
1	C	517/537 (96%)	-0.34	3 (0%) 85 86	23, 35, 72, 83	1 (0%)
1	D	517/537 (96%)	0.11	32 (6%) 26 25	23, 40, 90, 120	1 (0%)
All	All	2070/2148 (96%)	-0.40	40 (1%) 66 66	15, 31, 73, 120	2 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	ALA	6.0
1	D	170	VAL	4.2
1	D	203	LEU	3.8
1	D	194	VAL	3.6
1	D	204	GLY	3.3
1	D	132	VAL	3.3
1	D	156	ILE	3.1
1	D	192	PHE	3.1
1	D	166	LYS	3.1
1	D	143	THR	3.0
1	D	197	VAL	3.0
1	B	404	ILE	3.0
1	D	144	LEU	2.9
1	A	404	ILE	2.9
1	D	148	TYR	2.9
1	D	141	LYS	2.8
1	D	130	ALA	2.7
1	D	176	VAL	2.7
1	B	401	LEU	2.7
1	D	123	LEU	2.7
1	D	158	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	401	LEU	2.6
1	D	152	CYS	2.6
1	D	209	VAL	2.5
1	C	470	PHE	2.4
1	D	124	ILE	2.4
1	D	189	GLY	2.3
1	D	121	THR	2.2
1	D	185	VAL	2.2
1	D	128	GLY	2.2
1	D	147	ALA	2.2
1	D	180	LEU	2.2
1	C	404	ILE	2.2
1	B	403	PRO	2.2
1	D	403	PRO	2.1
1	D	119	ILE	2.1
1	D	506	GLY	2.1
1	D	140	LEU	2.1
1	B	190	ALA	2.1
1	C	126	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	ALY	D	115	12/13	0.88	0.12	46,53,71,71	0
1	ALY	C	115	12/13	0.91	0.11	36,40,51,52	0
1	ALY	A	115	12/13	0.95	0.09	24,27,45,48	0
1	ALY	B	115	12/13	0.97	0.07	21,24,37,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

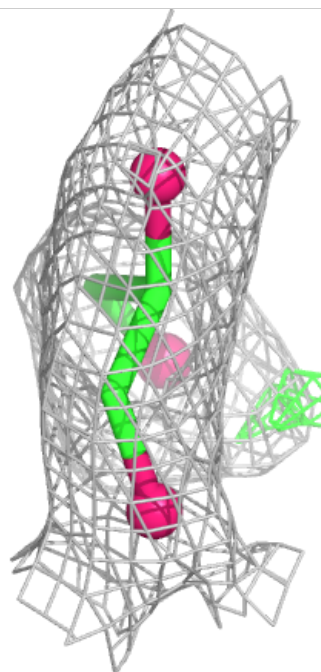
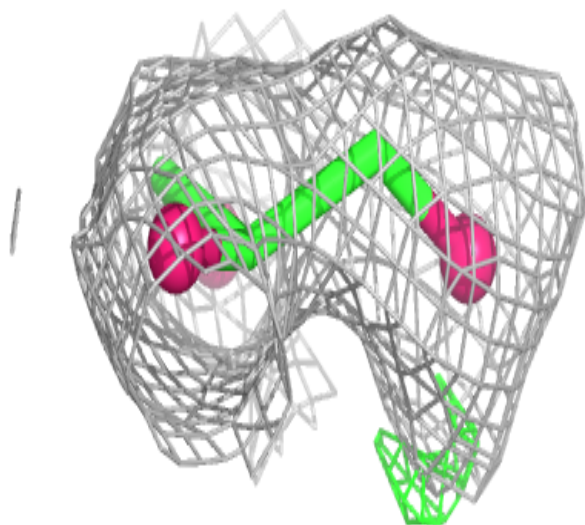
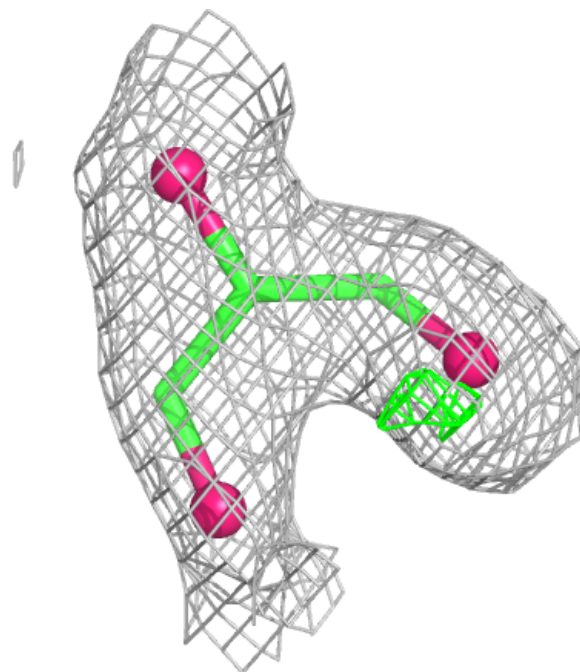
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	C	602	6/6	0.90	0.09	41,42,43,46	0
5	GOL	C	604	6/6	0.90	0.10	49,57,61,62	0
4	SIN	D	603	8/8	0.92	0.10	46,49,52,57	0
3	EDO	A	603	4/4	0.92	0.09	25,30,33,35	0
3	EDO	A	605	4/4	0.92	0.09	48,50,51,56	0
3	EDO	D	602	4/4	0.93	0.09	42,43,46,51	0
4	SIN	C	603	8/8	0.94	0.08	34,37,47,54	0
3	EDO	A	602	4/4	0.94	0.18	33,35,35,40	0
2	FBP	D	601	20/20	0.95	0.07	29,31,34,34	0
4	SIN	B	604	8/8	0.95	0.08	21,25,30,31	0
3	EDO	B	602	4/4	0.95	0.07	32,35,38,41	0
4	SIN	A	606	8/8	0.96	0.10	26,29,34,41	0
3	EDO	B	603	4/4	0.96	0.07	28,30,32,36	0
2	FBP	B	601	20/20	0.96	0.05	23,28,32,32	0
3	EDO	A	604	4/4	0.98	0.05	34,35,36,37	0
6	K	C	605	1/1	0.98	0.12	55,55,55,55	0
6	K	C	606	1/1	0.98	0.09	59,59,59,59	0
2	FBP	A	601	20/20	0.99	0.03	19,23,26,26	0
2	FBP	C	601	20/20	0.99	0.04	26,28,31,32	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.

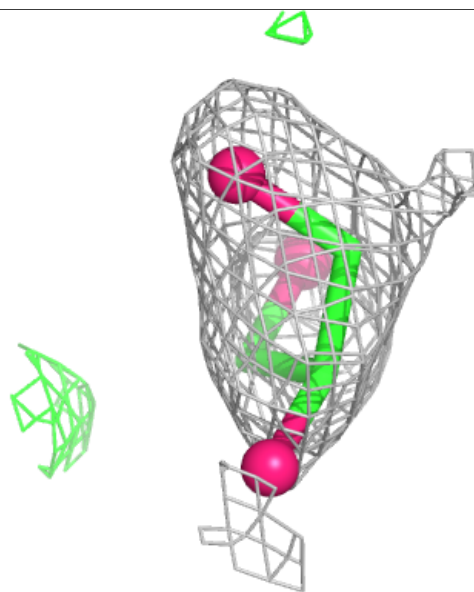
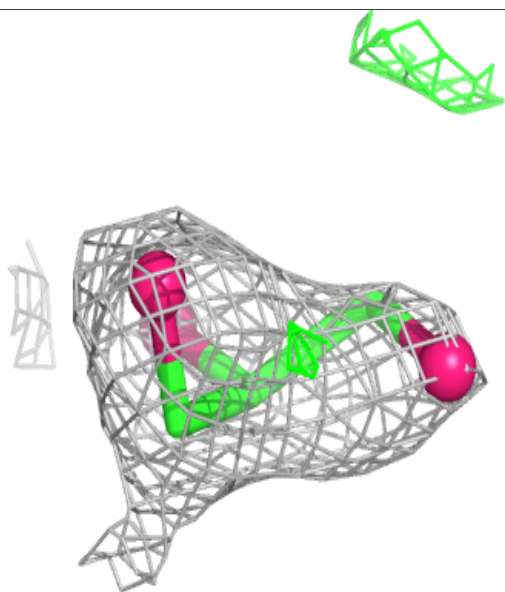
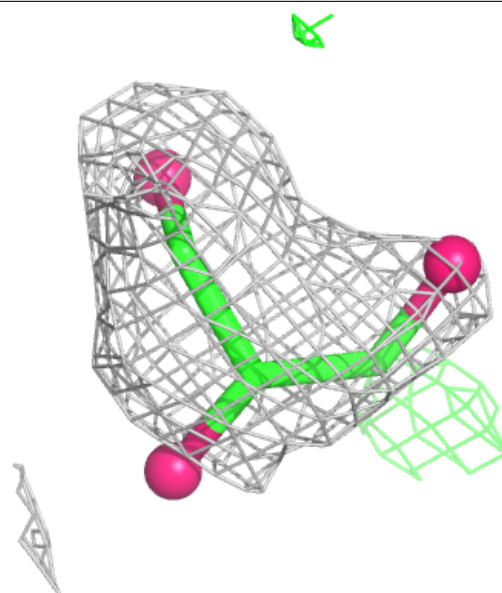
Electron density around GOL C 602:

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



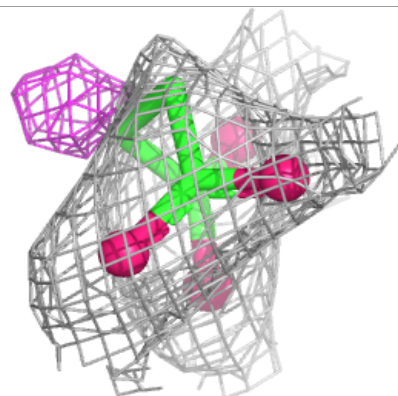
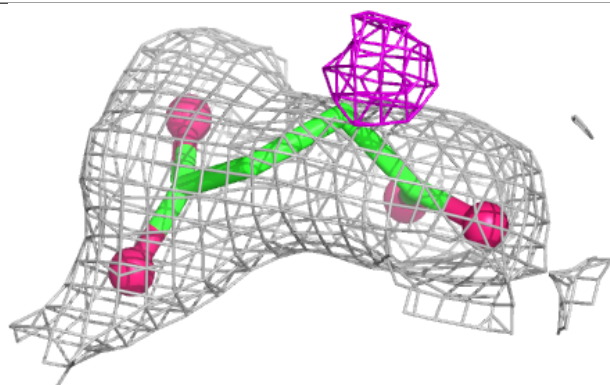
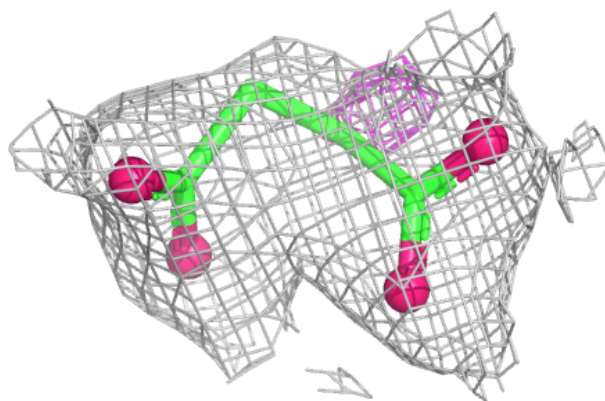
Electron density around GOL C 604:

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and green (positive)

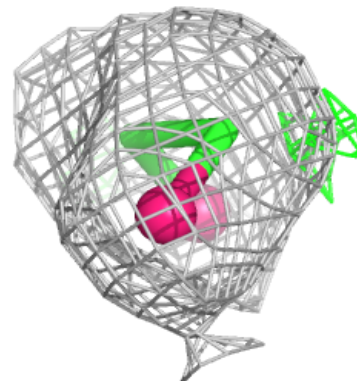
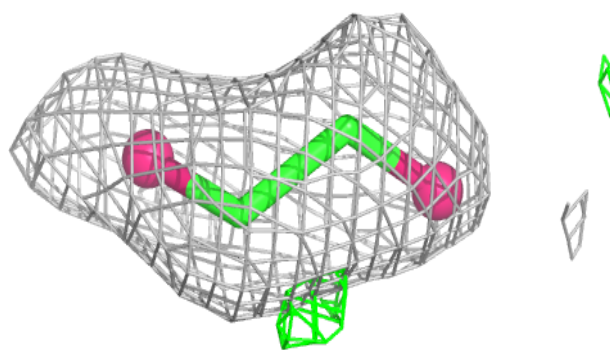
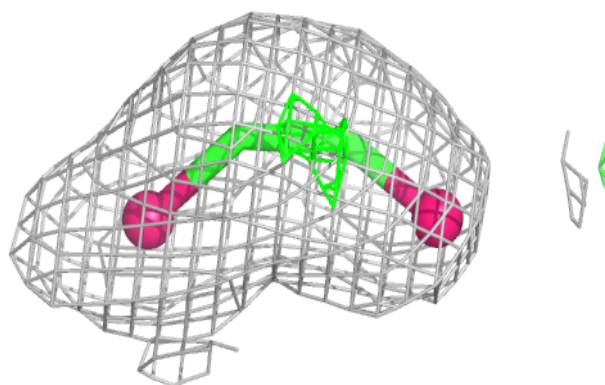


Electron density around SIN D 603:

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and green (positive)

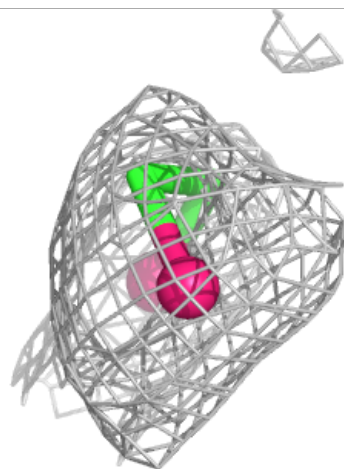
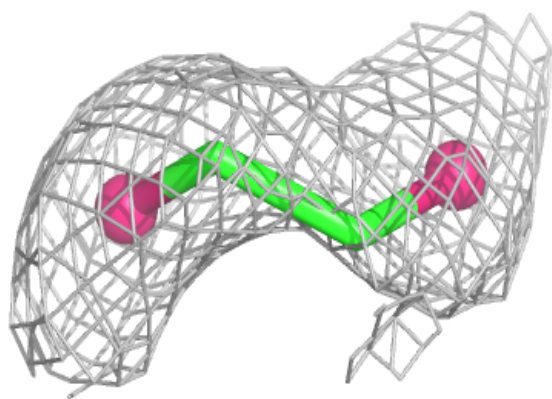
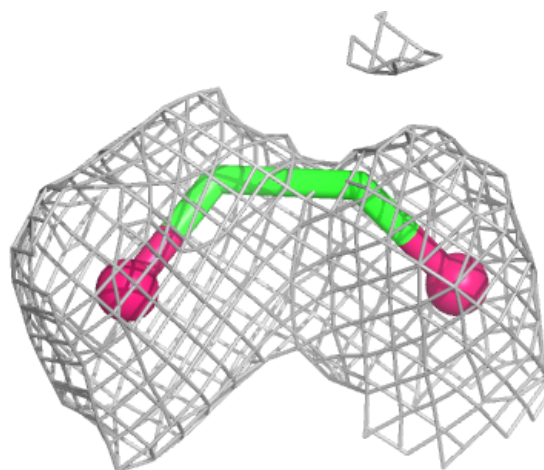
**Electron density around EDO A 603:**

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and green (positive)



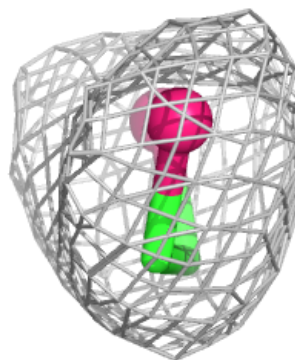
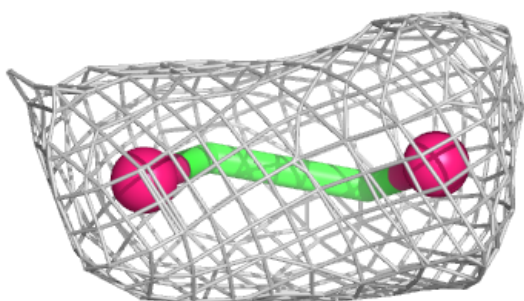
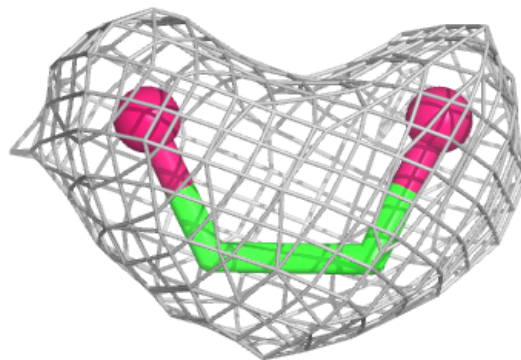
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and green (positive)

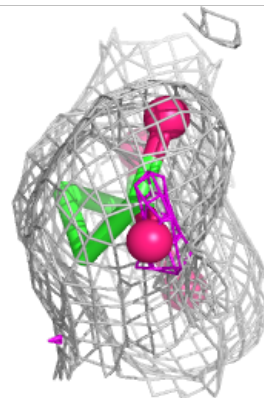
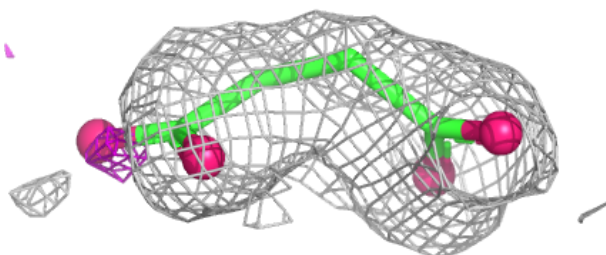
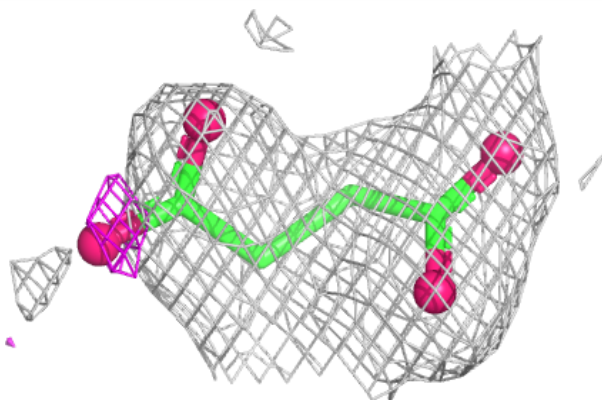


Electron density around EDO D 602:

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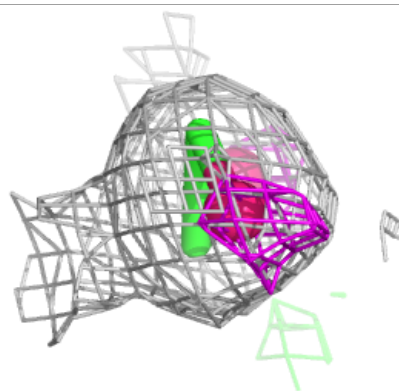
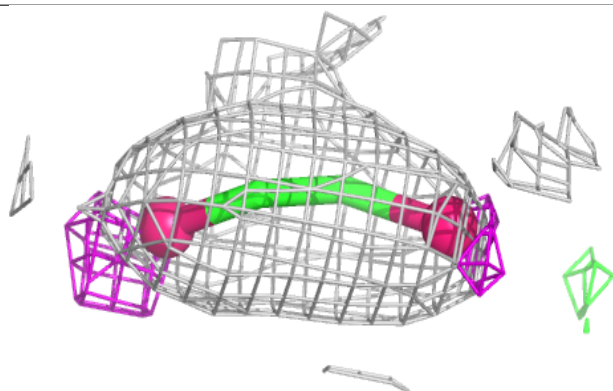
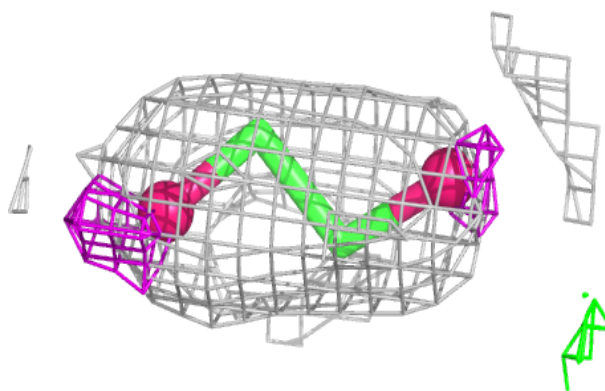
**Electron density around SIN C 603:**

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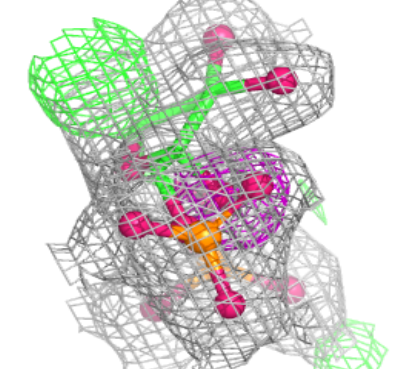
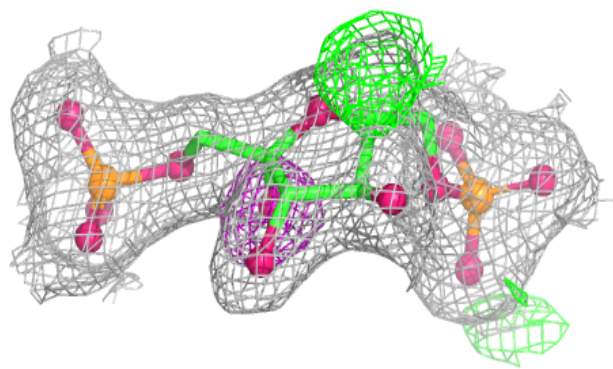
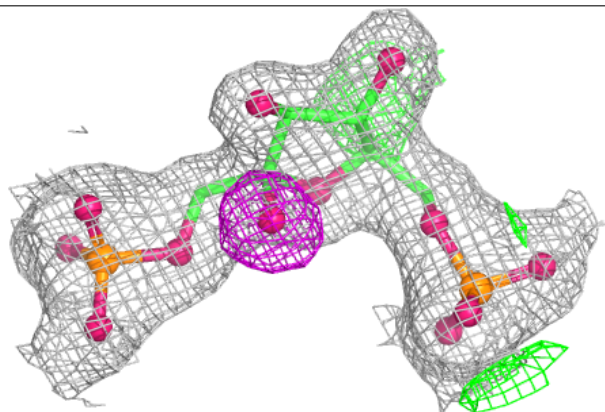


Electron density around EDO A 602:

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and green (positive)

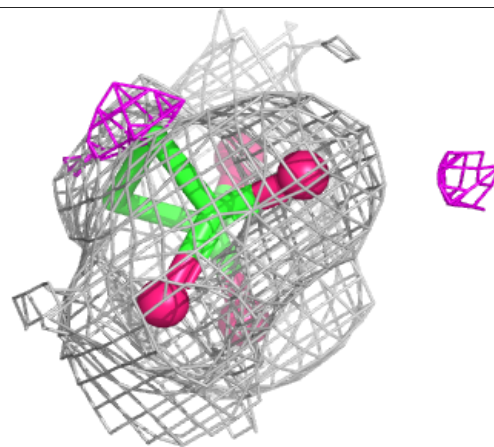
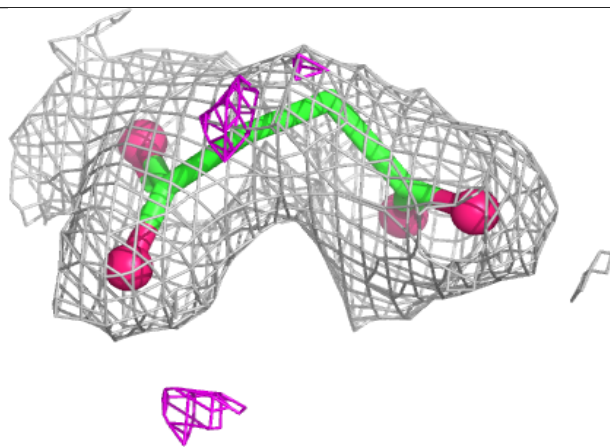
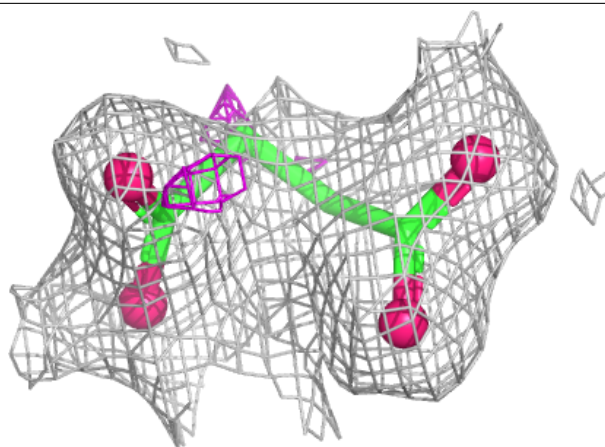
**Electron density around FBP D 601:**

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and green (positive)



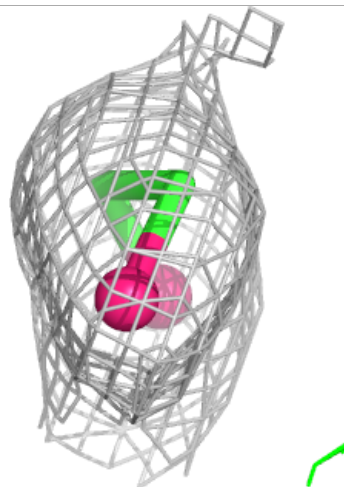
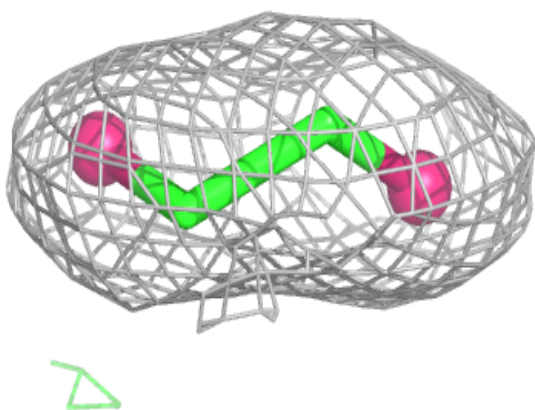
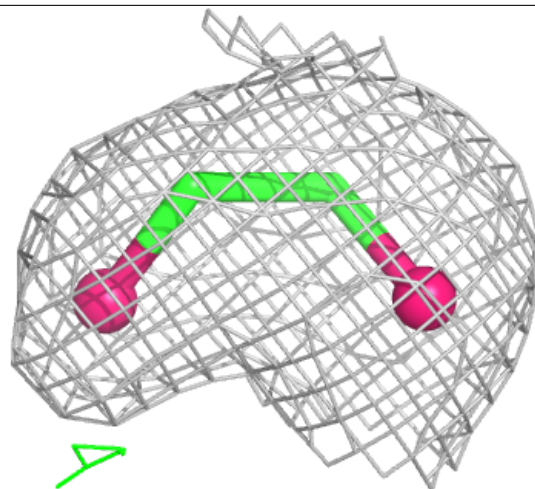
Electron density around SIN B 604:

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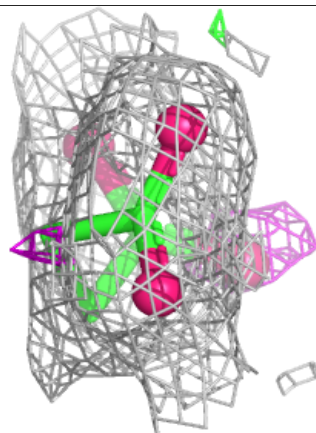
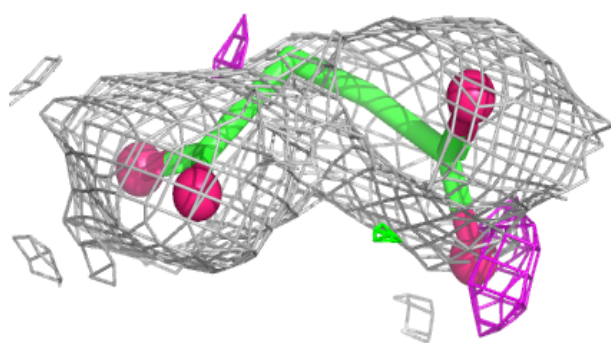
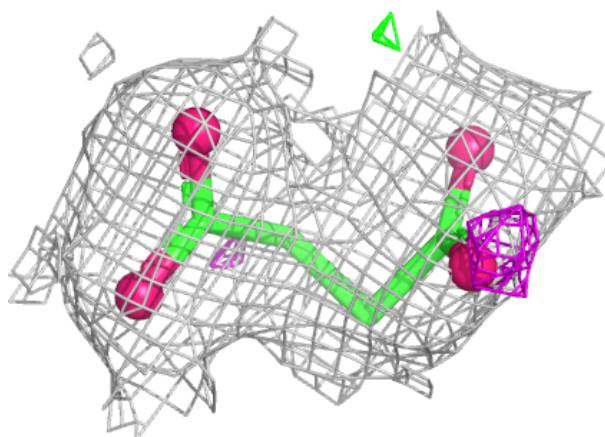
Electron density around EDO B 602:

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and green (positive)



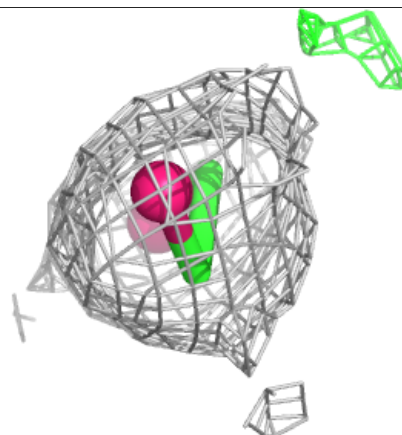
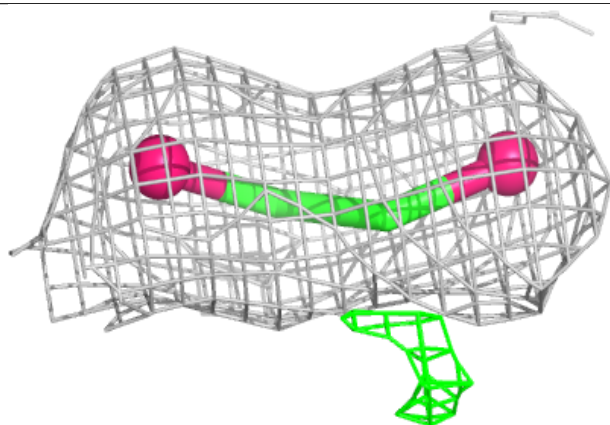
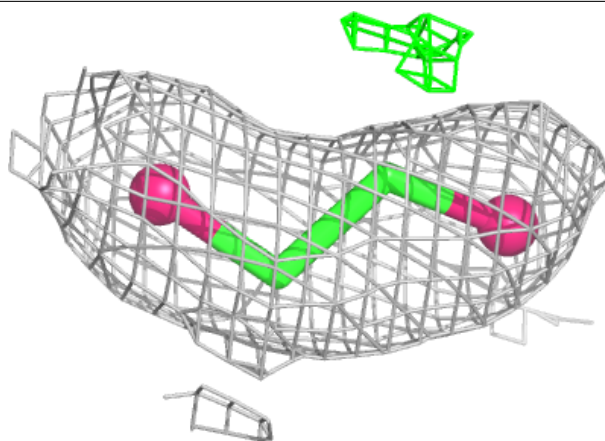
Electron density around SIN A 606:

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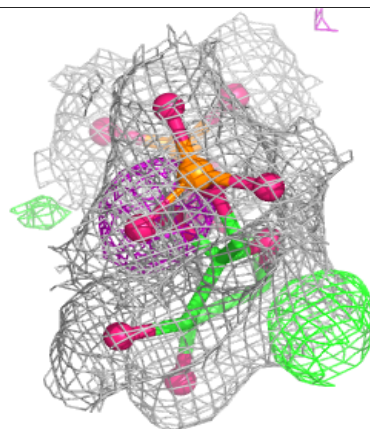
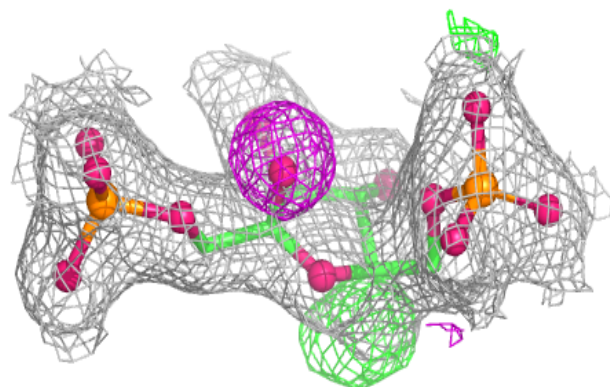
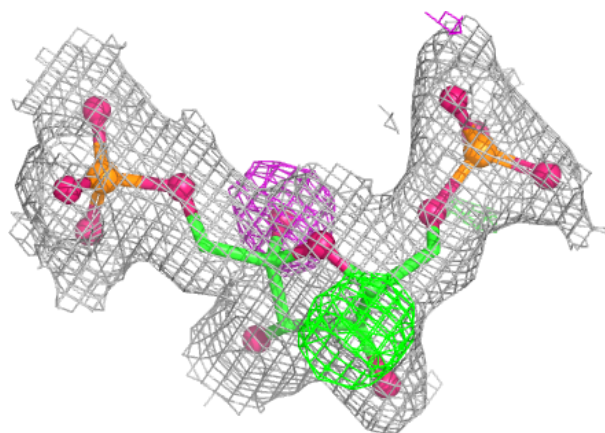
Electron density around EDO B 603:

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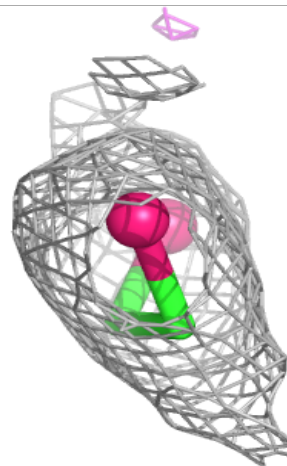
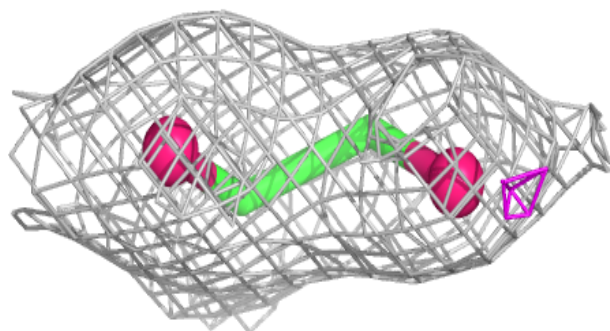
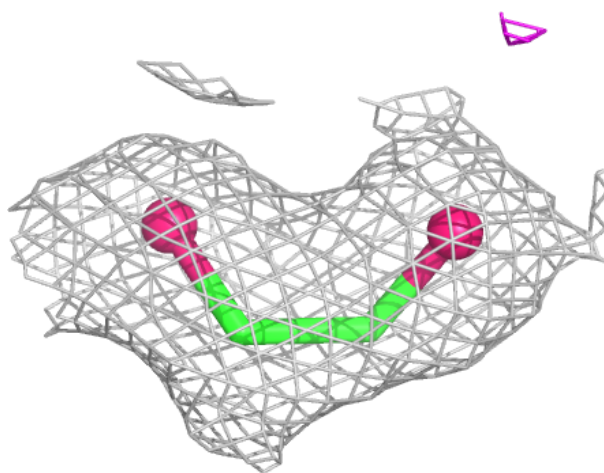
Electron density around FBP B 601:

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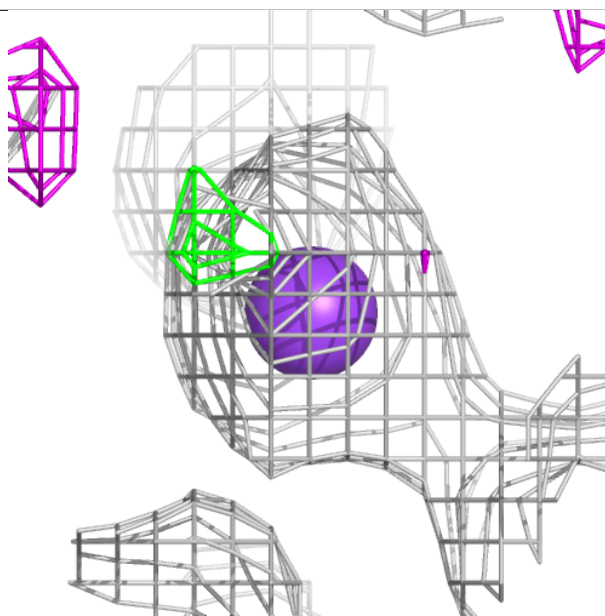
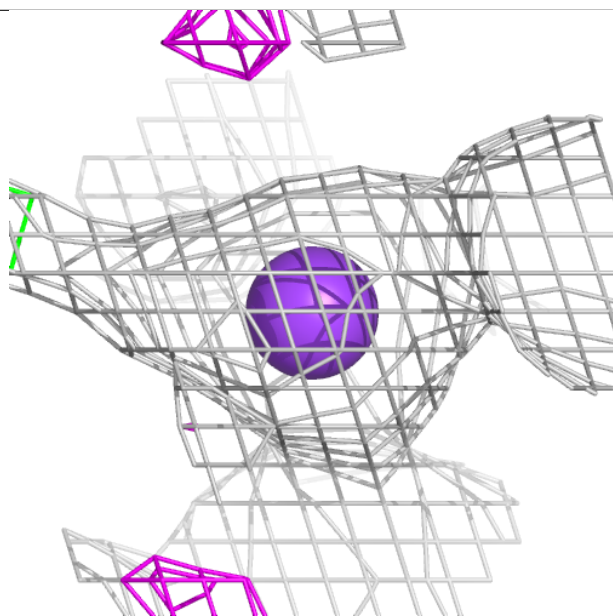
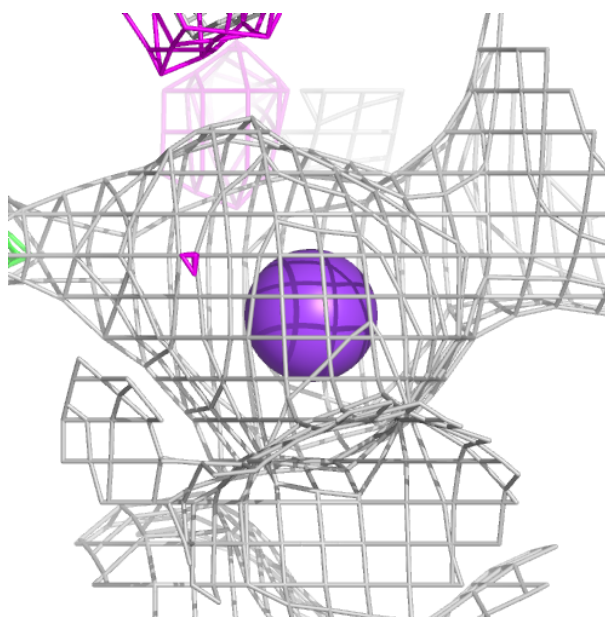
Electron density around EDO A 604:

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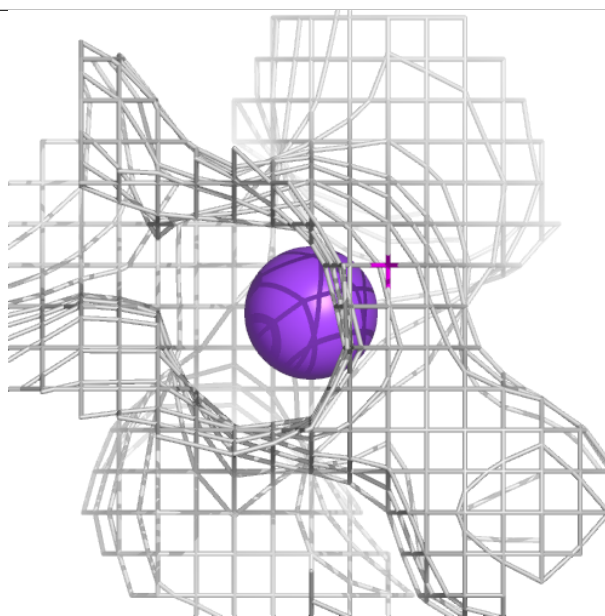
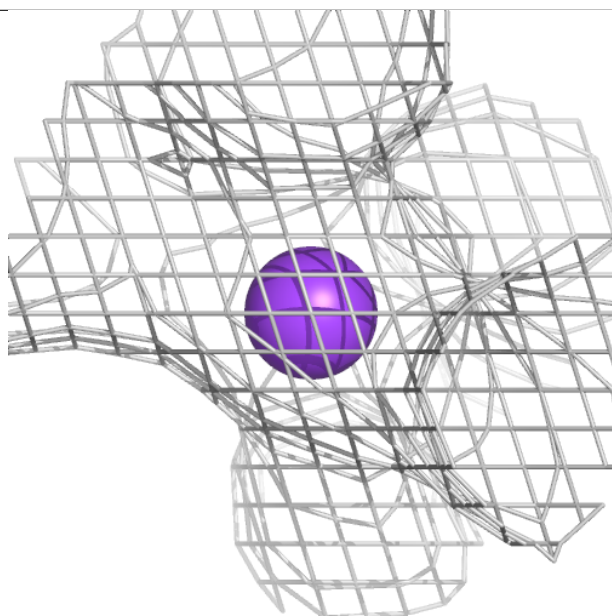
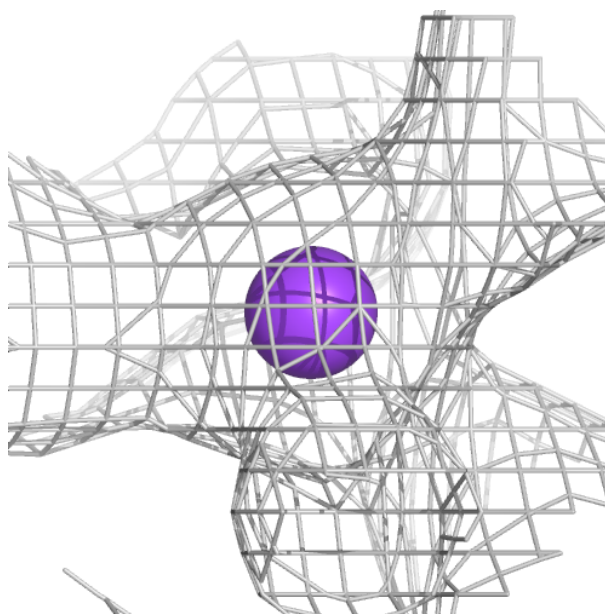
Electron density around K C 605:

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and green (positive)



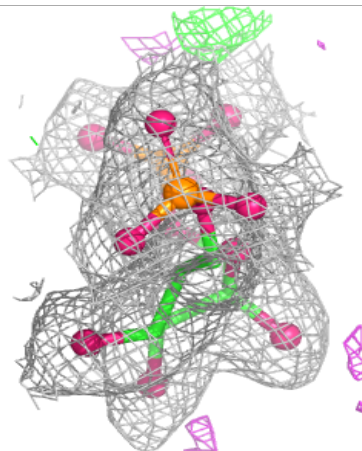
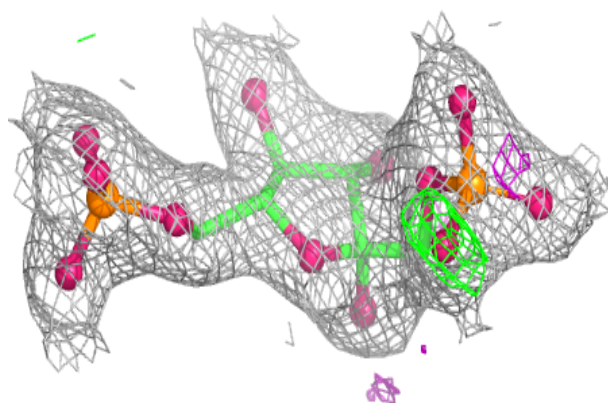
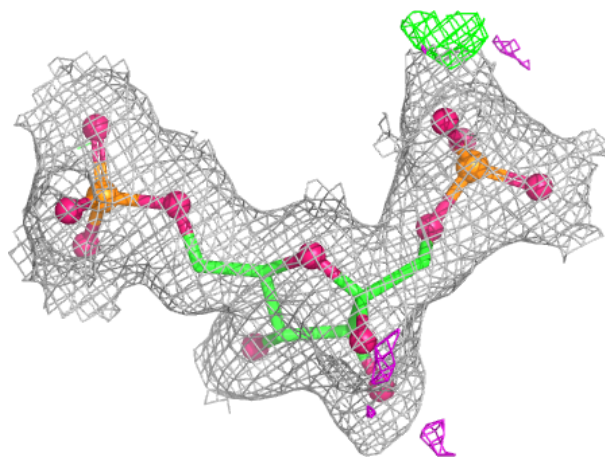
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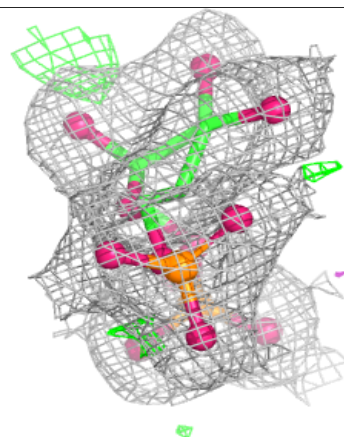
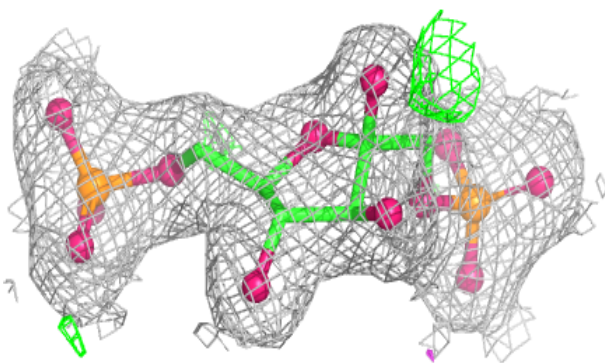
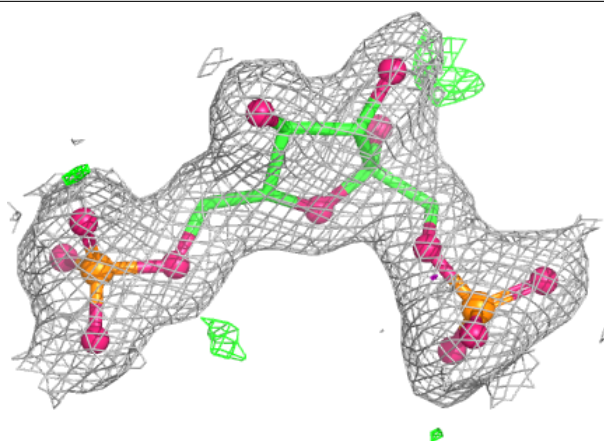
Electron density around FBP A 601:

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



Electron density around FBP C 601:

$2mF_o - DF_c$ (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.