Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 01:14 AM EDT

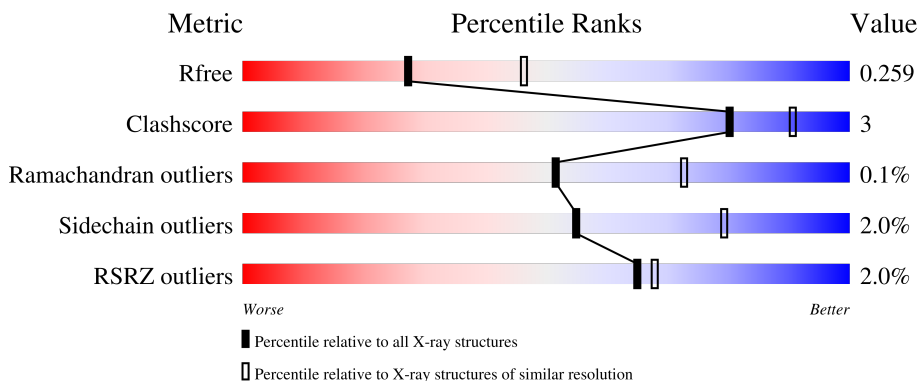|		
PDB ID	:	7M2N
Title	:	Crystal structure of Human Lactate Dehydrogenase A with Inhibitor Compound 15
Authors	:	Gumpena, R.; Ding, J.; Powell, D.A.; Lowther, W.T.
Deposited on	:	2021-03-17
Resolution	:	2.50 Å(reported)

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 2.50 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	Percentile Ranks	Value
Rfree		0.259
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		2.0%
RSRZ outliers		2.0%

Worse ——— *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	% 91% 6% ·
1	B	338	% 92% 6% ·
1	C	338	2% 90% 7% ··
1	D	338	3% 91% 7% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	D	412	-	-	X	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 11585 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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2515	1608	430	464	13			
1	B	331	Total	C	N	O	S	0	1	0
			2559	1635	440	471	13			
1	C	331	Total	C	N	O	S	0	2	0
			2558	1635	435	475	13			
1	D	331	Total	C	N	O	S	0	0	0
			2555	1631	437	474	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	HIS	-	expression tag	UNP P00338
A	333	HIS	-	expression tag	UNP P00338
A	334	HIS	-	expression tag	UNP P00338
A	335	HIS	-	expression tag	UNP P00338
A	336	HIS	-	expression tag	UNP P00338
A	337	HIS	-	expression tag	UNP P00338
B	332	HIS	-	expression tag	UNP P00338
B	333	HIS	-	expression tag	UNP P00338
B	334	HIS	-	expression tag	UNP P00338
B	335	HIS	-	expression tag	UNP P00338
B	336	HIS	-	expression tag	UNP P00338
B	337	HIS	-	expression tag	UNP P00338
C	332	HIS	-	expression tag	UNP P00338
C	333	HIS	-	expression tag	UNP P00338
C	334	HIS	-	expression tag	UNP P00338
C	335	HIS	-	expression tag	UNP P00338
C	336	HIS	-	expression tag	UNP P00338
C	337	HIS	-	expression tag	UNP P00338
D	332	HIS	-	expression tag	UNP P00338
D	333	HIS	-	expression tag	UNP P00338
D	334	HIS	-	expression tag	UNP P00338

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Chain	Residue	Modelled	Actual	Comment	Reference
D	335	HIS	-	expression tag	UNP P00338
D	336	HIS	-	expression tag	UNP P00338
D	337	HIS	-	expression tag	UNP P00338

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

NAI
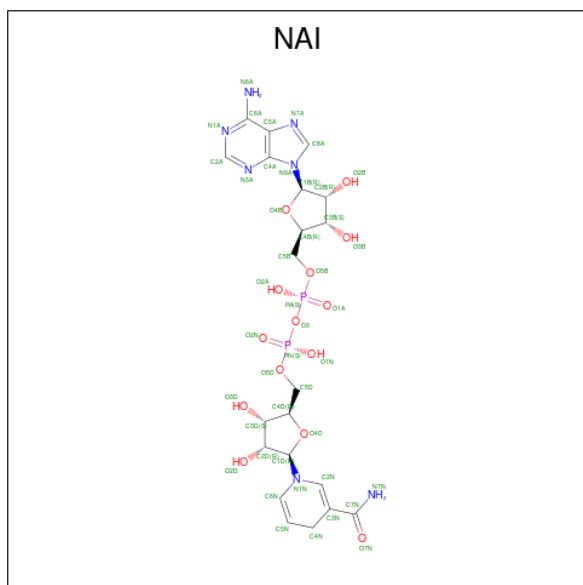
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

C1

O2
OH

C2

HO

O1
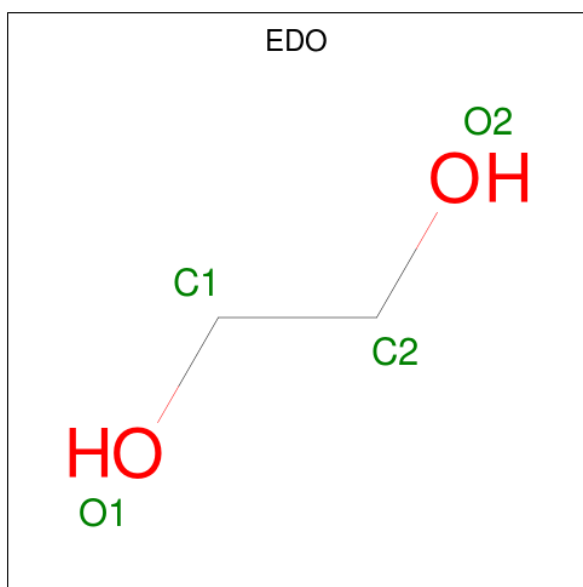
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0
4	A	1	Total C O 4 2 2			0	0

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

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
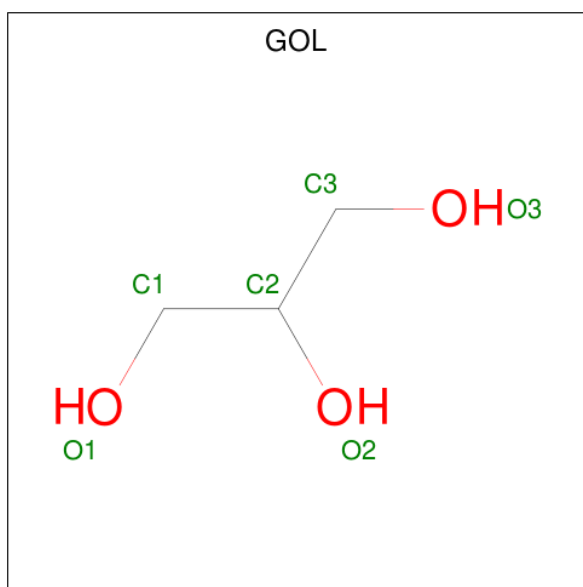
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG
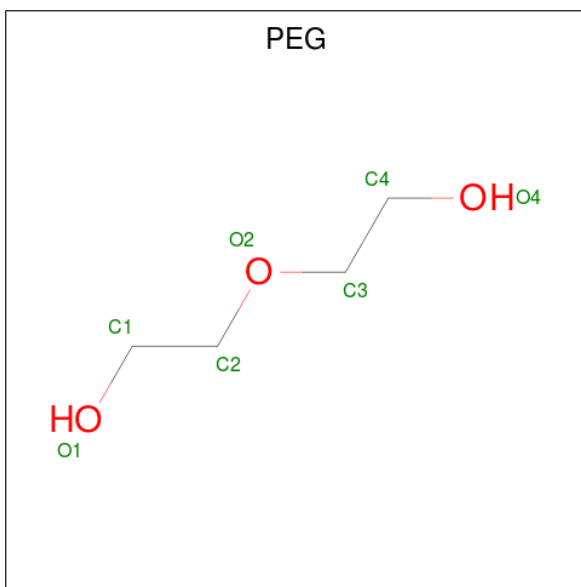
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 7	C 4	O 3	0	0
6	A	1	Total 7	C 4	O 3	0	0
6	A	1	Total 7	C 4	O 3	0	0
6	B	1	Total 7	C 4	O 3	0	0
6	B	1	Total 7	C 4	O 3	0	0
6	B	1	Total 7	C 4	O 3	0	0

- Molecule 7 is 5-[(5'-{1-(4-carboxy-1,3-thiazol-2-yl)-5-(cyclopropylmethyl)-4-[(3-fluoro-4-sulf amoylphenyl)methyl]-1H-pyrazol-3-yl}-2'-fluoro[1,1'-biphenyl]-4-yl)oxy]-1H-1,2,3-triazole-4-carboxylic acid (three-letter code: YOJ) (formula: $C_{33}H_{25}F_2N_7O_7S_2$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	S	0	1
			102	66	4	14	14	4		
7	B	1	Total	C	F	N	O	S	0	0
			51	33	2	7	7	2		
7	C	1	Total	C	F	N	O	S	0	0
			51	33	2	7	7	2		
7	D	1	Total	C	F	N	O	S	0	0
			51	33	2	7	7	2		

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	153	Total	O	0	2
			155	155		
8	B	143	Total	O	0	0
			143	143		
8	C	119	Total	O	0	0
			119	119		
8	D	122	Total	O	0	0
			122	122		

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.
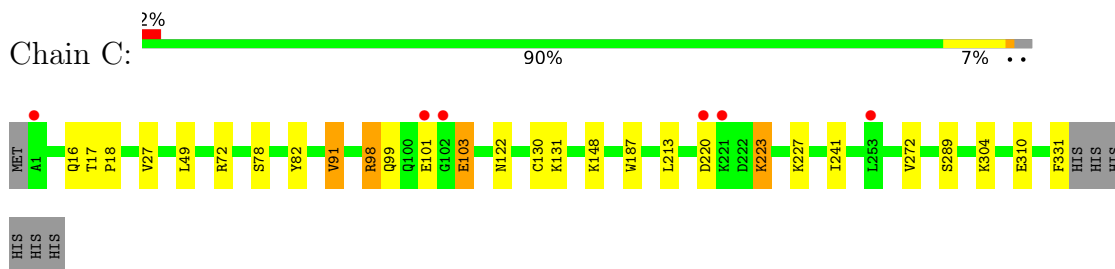
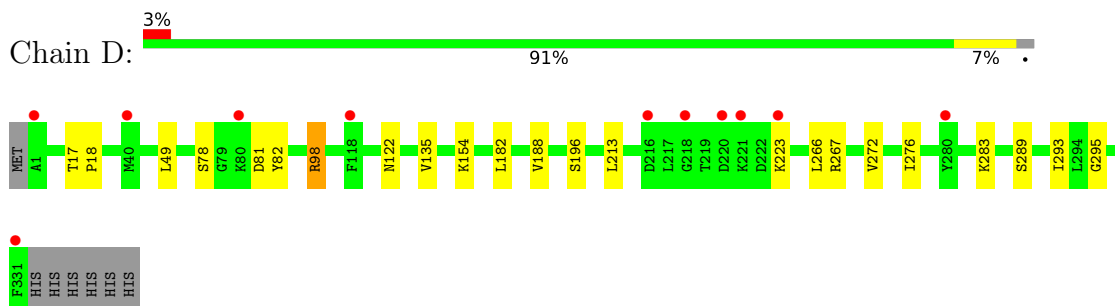- Molecule 1: L-lactate dehydrogenase A chain
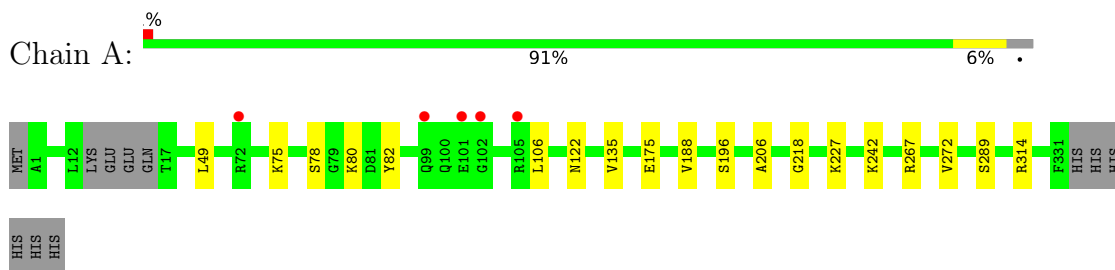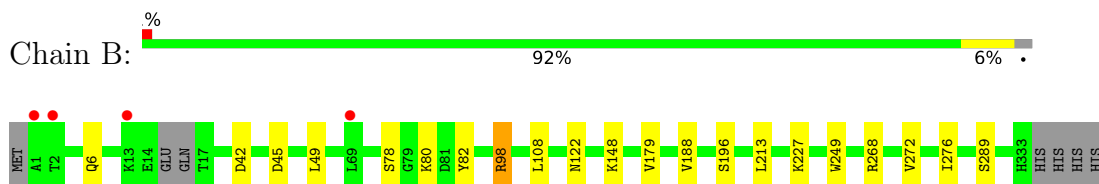
Chain A:

- Molecule 1: L-lactate dehydrogenase A chain

Chain B:

- Molecule 1: L-lactate dehydrogenase A chain

Chain C:

- Molecule 1: L-lactate dehydrogenase A chain

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	83.93Å 131.05Å 215.52Å 90.00° 99.30° 90.00°	Depositor
Resolution (Å)	48.89 – 2.50 48.85 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.89-2.50) 97.6 (48.85-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.258 0.213 , 0.259	Depositor DCC
R_{free} test set	3910 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.2	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11585	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YOJ, EDO, PEG, GOL, NAI, SO4

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	0.70	0/2558	0.79	0/3464
1	B	0.70	0/2607	0.78	0/3529
1	C	0.68	0/2608	0.80	0/3531
1	D	0.68	0/2599	0.78	0/3519
All	All	0.69	0/10372	0.78	0/14043

There are no bond length outliers.

There are no bond angle outliers.

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	2515	0	2590	15	0
1	B	2559	0	2631	13	0
1	C	2558	0	2633	17	0
1	D	2555	0	2630	15	0
2	A	44	0	27	2	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	1	0
3	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	76	0	114	2	0
4	B	80	0	120	5	0
4	C	68	0	102	0	0
4	D	76	0	114	8	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	18	0	24	2	0
5	D	6	0	8	0	0
6	A	21	0	30	0	0
6	B	21	0	30	0	0
7	A	102	0	0	2	0
7	B	51	0	0	1	0
7	C	51	0	0	0	0
7	D	51	0	0	0	0
8	A	155	0	0	2	0
8	B	143	0	0	2	0
8	C	119	0	0	3	0
8	D	122	0	0	2	0
All	All	11585	0	11150	60	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 3.

All (60) 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:314:ARG:HD2	8:A:617[B]:HOH:O	1.98	0.61
1:C:27:VAL:CG1	1:C:27:VAL:O	2.48	0.60
1:C:27:VAL:O	1:C:27:VAL:HG12	2.02	0.59
1:D:266:LEU:O	4:D:412:EDO:H22	2.05	0.57
4:B:416:EDO:H11	8:B:595:HOH:O	2.05	0.55
1:C:131:LYS:NZ	8:C:502:HOH:O	2.41	0.53
1:D:81:ASP:HB2	8:D:589:HOH:O	2.07	0.53
1:B:82:TYR:CG	1:B:122:ASN:HB3	2.45	0.51
1:C:99:GLN:HA	1:C:103:GLU:OE2	2.09	0.51
1:D:267:ARG:HD3	4:D:412:EDO:C1	2.41	0.51
1:D:295:GLY:HA3	4:D:413:EDO:H22	1.92	0.51
1:D:82:TYR:CG	1:D:122:ASN:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:CG	1:A:122:ASN:HB3	2.46	0.51
1:D:17:THR:HG22	1:D:18:PRO:O	2.11	0.51
1:D:267:ARG:HD3	4:D:412:EDO:H12	1.93	0.50
1:C:82:TYR:CG	1:C:122:ASN:HB3	2.46	0.50
1:C:148:LYS:HE2	1:C:331:PHE:HE2	1.76	0.50
1:B:108:LEU:HD23	7:B:422:YOJ:F31	2.03	0.49
1:A:175:GLU:OE2	4:A:425:EDO:H22	2.13	0.48
1:C:272:VAL:O	1:C:289:SER:HA	2.13	0.48
1:A:242:LYS:NZ	8:A:505:HOH:O	2.44	0.48
1:A:272:VAL:O	1:A:289:SER:HA	2.14	0.48
1:D:135:VAL:O	2:D:411:NAI:H2N	2.13	0.48
1:A:218:GLY:O	1:A:227:LYS:HE2	2.14	0.47
1:D:267:ARG:HB2	4:D:412:EDO:H21	1.96	0.47
5:C:420:GOL:O3	5:C:420:GOL:O1	2.31	0.46
1:B:272:VAL:O	1:B:289:SER:HA	2.16	0.46
1:D:272:VAL:O	1:D:289:SER:HA	2.15	0.46
1:B:249:TRP:CH2	4:B:417:EDO:H11	2.50	0.46
1:A:49:LEU:O	1:A:78:SER:HA	2.16	0.46
1:B:6:GLN:O	1:C:304:LYS:HE3	2.15	0.46
1:C:241:ILE:HD13	5:C:423:GOL:H2	1.96	0.45
1:C:17:THR:HG22	1:C:18:PRO:O	2.15	0.45
1:A:218:GLY:O	1:A:227:LYS:CE	2.64	0.45
1:C:49:LEU:O	1:C:78:SER:HA	2.16	0.45
1:A:206:ALA:HA	1:C:187:TRP:CE2	2.51	0.45
1:A:267:ARG:HD3	4:D:402:EDO:H21	1.99	0.44
1:D:49:LEU:O	1:D:78:SER:HA	2.17	0.44
1:C:91:VAL:HG13	1:C:130:CYS:SG	2.58	0.44
1:B:98:ARG:H	4:B:425:EDO:C1	2.32	0.43
1:D:98:ARG:H	4:D:407:EDO:C1	2.31	0.43
1:C:98:ARG:NH2	8:C:509:HOH:O	2.51	0.43
1:D:188:VAL:CG1	1:D:196:SER:HB2	2.48	0.43
1:A:206:ALA:HA	1:C:187:TRP:CZ2	2.54	0.42
1:A:135:VAL:O	2:A:401:NAI:H2N	2.20	0.42
1:B:49:LEU:O	1:B:78:SER:HA	2.18	0.42
2:A:401:NAI:H42N	7:A:420[B]:YOJ:C20	2.50	0.42
1:B:42:ASP:OD1	4:B:405:EDO:C1	2.68	0.42
1:A:188:VAL:CG1	1:A:196:SER:HB2	2.50	0.42
1:B:45:ASP:HB3	8:B:547:HOH:O	2.18	0.42
1:C:148:LYS:HE2	1:C:331:PHE:CE2	2.54	0.42
8:C:552:HOH:O	1:D:182:LEU:HD11	2.19	0.42
1:B:188:VAL:CG1	1:B:196:SER:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:HA	4:A:404:EDO:H11	2.02	0.41
1:C:223:LYS:H	1:C:223:LYS:CD	2.33	0.41
1:A:106:LEU:HB2	7:A:420[B]:YOJ:O44	2.20	0.41
4:D:410:EDO:H12	8:D:544:HOH:O	2.21	0.41
1:B:179:VAL:HG22	1:D:293:ILE:HD13	2.02	0.40
1:B:148:LYS:HD2	1:B:148:LYS:HA	1.90	0.40
1:B:268:ARG:NH2	4:B:428:EDO:H21	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/338 (96%)	316 (98%)	7 (2%)	0	100	100
1	B	328/338 (97%)	321 (98%)	7 (2%)	0	100	100
1	C	331/338 (98%)	321 (97%)	9 (3%)	1 (0%)	41	61
1	D	329/338 (97%)	319 (97%)	10 (3%)	0	100	100
All	All	1311/1352 (97%)	1277 (97%)	33 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	16	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/294 (95%)	278 (100%)	1 (0%)	91	97
1	B	284/294 (97%)	279 (98%)	5 (2%)	59	81
1	C	284/294 (97%)	274 (96%)	10 (4%)	36	62
1	D	284/294 (97%)	278 (98%)	6 (2%)	53	78
All	All	1131/1176 (96%)	1109 (98%)	22 (2%)	55	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	B	80	LYS
1	B	98	ARG
1	B	213	LEU
1	B	227	LYS
1	B	276	ILE
1	C	72	ARG
1	C	91	VAL
1	C	98	ARG
1	C	101	GLU
1	C	103	GLU
1	C	213	LEU
1	C	220	ASP
1	C	223	LYS
1	C	227	LYS
1	C	310	GLU
1	D	98	ARG
1	D	154	LYS
1	D	213	LEU
1	D	223	LYS
1	D	276	ILE
1	D	283	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	107	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

106 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	$\#|Z| > 2$
4	EDO	B	406	-	3,3,3	0.26	0	2,2,2	0.30	0
3	SO4	B	403	-	4,4,4	0.34	0	6,6,6	0.16	0
7	YOJ	A	420[A]	-	50,57,57	1.75	10 (20%)	66,85,85	2.08	12 (18%)
3	SO4	A	402	-	4,4,4	0.45	0	6,6,6	0.15	0
4	EDO	D	422	-	3,3,3	0.10	0	2,2,2	0.08	0
4	EDO	D	408	-	3,3,3	0.07	0	2,2,2	0.30	0
7	YOJ	C	421	-	50,57,57	1.87	9 (18%)	66,85,85	2.50	21 (31%)
3	SO4	B	419	-	4,4,4	0.41	0	6,6,6	0.24	0
4	EDO	D	413	-	3,3,3	0.28	0	2,2,2	0.39	0
4	EDO	B	407	-	3,3,3	0.14	0	2,2,2	0.26	0
4	EDO	C	408	-	3,3,3	0.13	0	2,2,2	0.18	0
4	EDO	B	428	-	3,3,3	0.20	0	2,2,2	0.42	0
4	EDO	C	418	-	3,3,3	0.15	0	2,2,2	0.34	0
2	NAI	C	404	-	42,48,48	0.54	0	47,73,73	0.87	2 (4%)
4	EDO	B	424	-	3,3,3	0.30	0	2,2,2	0.31	0
4	EDO	D	404	-	3,3,3	0.07	0	2,2,2	0.11	0
4	EDO	A	424	-	3,3,3	0.11	0	2,2,2	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	427	-	4,4,4	0.35	0	6,6,6	0.27	0
4	EDO	B	405	-	3,3,3	0.10	0	2,2,2	0.15	0
5	GOL	C	419	-	5,5,5	0.19	0	5,5,5	0.40	0
3	SO4	D	401	-	4,4,4	0.40	0	6,6,6	0.22	0
4	EDO	B	416	-	3,3,3	0.42	0	2,2,2	0.55	0
4	EDO	A	411	-	3,3,3	0.22	0	2,2,2	0.20	0
4	EDO	A	426	-	3,3,3	0.11	0	2,2,2	0.16	0
2	NAI	A	401	-	42,48,48	0.68	0	47,73,73	1.00	4 (8%)
4	EDO	B	414	-	3,3,3	0.10	0	2,2,2	0.23	0
4	EDO	C	410	-	3,3,3	0.06	0	2,2,2	0.08	0
5	GOL	D	409	-	5,5,5	0.19	0	5,5,5	0.45	0
4	EDO	A	416	-	3,3,3	0.07	0	2,2,2	0.15	0
4	EDO	B	413	-	3,3,3	0.15	0	2,2,2	0.21	0
4	EDO	D	405	-	3,3,3	0.34	0	2,2,2	0.53	0
4	EDO	C	406	-	3,3,3	0.22	0	2,2,2	0.25	0
4	EDO	A	414	-	3,3,3	0.18	0	2,2,2	0.43	0
4	EDO	A	403	-	3,3,3	0.08	0	2,2,2	0.07	0
3	SO4	A	423	-	4,4,4	0.31	0	6,6,6	0.14	0
4	EDO	A	412	-	3,3,3	0.24	0	2,2,2	0.29	0
4	EDO	A	408	-	3,3,3	0.10	0	2,2,2	0.17	0
7	YOJ	A	420[B]	-	50,57,57	1.79	9 (18%)	66,85,85	2.42	18 (27%)
6	PEG	B	412	-	6,6,6	0.26	0	5,5,5	0.17	0
6	PEG	B	429	-	6,6,6	0.25	0	5,5,5	0.22	0
4	EDO	D	406	-	3,3,3	0.07	0	2,2,2	0.13	0
2	NAI	D	411	-	42,48,48	0.58	0	47,73,73	0.95	3 (6%)
4	EDO	C	407	-	3,3,3	0.16	0	2,2,2	0.23	0
3	SO4	C	402	-	4,4,4	0.40	0	6,6,6	0.29	0
7	YOJ	D	421	-	50,57,57	1.78	9 (18%)	66,85,85	2.57	31 (46%)
6	PEG	A	417	-	6,6,6	0.40	0	5,5,5	0.31	0
4	EDO	A	405	-	3,3,3	0.13	0	2,2,2	0.34	0
6	PEG	B	423	-	6,6,6	0.29	0	5,5,5	0.18	0
4	EDO	C	405	-	3,3,3	0.11	0	2,2,2	0.16	0
4	EDO	D	416	-	3,3,3	0.06	0	2,2,2	0.16	0
4	EDO	D	415	-	3,3,3	0.30	0	2,2,2	0.41	0
4	EDO	D	402	-	3,3,3	0.53	0	2,2,2	0.62	0
4	EDO	B	415	-	3,3,3	0.11	0	2,2,2	0.18	0
5	GOL	C	423	-	5,5,5	0.09	0	5,5,5	0.38	0
3	SO4	B	408	-	4,4,4	0.33	0	6,6,6	0.18	0
3	SO4	D	423	-	4,4,4	0.36	0	6,6,6	0.07	0
4	EDO	D	407	-	3,3,3	0.12	0	2,2,2	0.43	0
5	GOL	C	420	-	5,5,5	0.14	0	5,5,5	0.42	0
4	EDO	D	412	-	3,3,3	0.37	0	2,2,2	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	EDO	A	415	-	3,3,3	0.13	0	2,2,2	0.35	0
4	EDO	C	414	-	3,3,3	0.14	0	2,2,2	0.23	0
4	EDO	B	411	-	3,3,3	0.12	0	2,2,2	0.28	0
4	EDO	A	407	-	3,3,3	0.30	0	2,2,2	0.57	0
4	EDO	B	409	-	3,3,3	0.39	0	2,2,2	0.55	0
4	EDO	A	421	-	3,3,3	0.13	0	2,2,2	0.34	0
4	EDO	D	417	-	3,3,3	0.12	0	2,2,2	0.07	0
3	SO4	B	402	-	4,4,4	0.35	0	6,6,6	0.19	0
4	EDO	C	403	-	3,3,3	0.25	0	2,2,2	0.13	0
4	EDO	C	413	-	3,3,3	0.19	0	2,2,2	0.30	0
4	EDO	C	401	-	3,3,3	0.28	0	2,2,2	0.49	0
4	EDO	D	410	-	3,3,3	0.14	0	2,2,2	0.29	0
4	EDO	D	419	-	3,3,3	0.07	0	2,2,2	0.02	0
7	YOJ	B	422	-	50,57,57	1.68	8 (16%)	66,85,85	2.70	23 (34%)
4	EDO	C	412	-	3,3,3	0.13	0	2,2,2	0.26	0
4	EDO	B	401	-	3,3,3	0.07	0	2,2,2	0.14	0
4	EDO	D	403	-	3,3,3	0.25	0	2,2,2	0.35	0
4	EDO	A	422	-	3,3,3	0.41	0	2,2,2	0.48	0
4	EDO	D	420	-	3,3,3	0.10	0	2,2,2	0.11	0
6	PEG	A	410	-	6,6,6	0.17	0	5,5,5	0.11	0
4	EDO	B	417	-	3,3,3	0.24	0	2,2,2	0.29	0
4	EDO	C	411	-	3,3,3	0.11	0	2,2,2	0.24	0
4	EDO	C	415	-	3,3,3	0.12	0	2,2,2	0.25	0
4	EDO	A	413	-	3,3,3	0.09	0	2,2,2	0.05	0
4	EDO	B	421	-	3,3,3	0.07	0	2,2,2	0.13	0
4	EDO	D	414	-	3,3,3	0.21	0	2,2,2	0.12	0
4	EDO	D	424	-	3,3,3	0.18	0	2,2,2	0.44	0
5	GOL	A	409	-	5,5,5	0.14	0	5,5,5	0.40	0
4	EDO	C	416	-	3,3,3	0.14	0	2,2,2	0.21	0
4	EDO	A	406	-	3,3,3	0.11	0	2,2,2	0.15	0
4	EDO	A	419	-	3,3,3	0.10	0	2,2,2	0.39	0
4	EDO	A	418	-	3,3,3	0.18	0	2,2,2	0.45	0
4	EDO	B	427	-	3,3,3	0.29	0	2,2,2	0.51	0
2	NAI	B	404	-	42,48,48	0.60	0	47,73,73	0.95	3 (6%)
4	EDO	C	417	-	3,3,3	0.10	0	2,2,2	0.19	0
4	EDO	C	422	-	3,3,3	0.13	0	2,2,2	0.27	0
4	EDO	B	420	-	3,3,3	0.10	0	2,2,2	0.10	0
4	EDO	A	404	-	3,3,3	0.09	0	2,2,2	0.32	0
4	EDO	C	409	-	3,3,3	0.38	0	2,2,2	0.56	0
5	GOL	B	426	-	5,5,5	0.18	0	5,5,5	0.53	0
4	EDO	B	418	-	3,3,3	0.14	0	2,2,2	0.33	0
6	PEG	A	428	-	6,6,6	0.20	0	5,5,5	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	B	425	-	3,3,3	0.23	0	2,2,2	0.24	0
4	EDO	B	430	-	3,3,3	0.08	0	2,2,2	0.19	0
4	EDO	A	425	-	3,3,3	0.39	0	2,2,2	0.66	0
4	EDO	D	418	-	3,3,3	0.13	0	2,2,2	0.27	0
4	EDO	B	410	-	3,3,3	0.18	0	2,2,2	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	406	-	-	1/1/1/1	-
7	YOJ	A	420[A]	-	-	6/29/40/40	0/7/7/7
4	EDO	D	422	-	-	0/1/1/1	-
4	EDO	D	408	-	-	0/1/1/1	-
7	YOJ	C	421	-	-	7/29/40/40	0/7/7/7
4	EDO	D	413	-	-	0/1/1/1	-
4	EDO	B	407	-	-	1/1/1/1	-
4	EDO	C	408	-	-	1/1/1/1	-
4	EDO	B	428	-	-	1/1/1/1	-
4	EDO	C	418	-	-	1/1/1/1	-
2	NAI	C	404	-	-	5/25/72/72	0/5/5/5
4	EDO	B	424	-	-	1/1/1/1	-
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	A	424	-	-	1/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-
5	GOL	C	419	-	-	4/4/4/4	-
4	EDO	B	416	-	-	1/1/1/1	-
4	EDO	A	411	-	-	0/1/1/1	-
4	EDO	A	426	-	-	0/1/1/1	-
2	NAI	A	401	-	-	5/25/72/72	0/5/5/5
4	EDO	B	414	-	-	1/1/1/1	-
4	EDO	C	410	-	-	1/1/1/1	-
5	GOL	D	409	-	-	4/4/4/4	-
4	EDO	A	416	-	-	1/1/1/1	-
4	EDO	B	413	-	-	1/1/1/1	-
4	EDO	D	405	-	-	1/1/1/1	-
4	EDO	C	406	-	-	1/1/1/1	-
4	EDO	A	414	-	-	0/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	412	-	-	0/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
7	YOJ	A	420[B]	-	-	5/29/40/40	0/7/7/7
6	PEG	B	412	-	-	1/4/4/4	-
6	PEG	B	429	-	-	2/4/4/4	-
4	EDO	D	406	-	-	1/1/1/1	-
2	NAI	D	411	-	-	5/25/72/72	0/5/5/5
4	EDO	C	407	-	-	0/1/1/1	-
7	YOJ	D	421	-	-	8/29/40/40	0/7/7/7
6	PEG	A	417	-	-	1/4/4/4	-
4	EDO	A	405	-	-	1/1/1/1	-
6	PEG	B	423	-	-	0/4/4/4	-
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	D	416	-	-	1/1/1/1	-
4	EDO	D	415	-	-	0/1/1/1	-
4	EDO	D	402	-	-	0/1/1/1	-
4	EDO	B	415	-	-	1/1/1/1	-
5	GOL	C	423	-	-	2/4/4/4	-
4	EDO	D	407	-	-	0/1/1/1	-
5	GOL	C	420	-	-	3/4/4/4	-
4	EDO	D	412	-	-	1/1/1/1	-
4	EDO	A	415	-	-	1/1/1/1	-
4	EDO	C	414	-	-	1/1/1/1	-
4	EDO	B	411	-	-	1/1/1/1	-
4	EDO	A	407	-	-	1/1/1/1	-
4	EDO	B	409	-	-	1/1/1/1	-
4	EDO	A	421	-	-	1/1/1/1	-
4	EDO	D	417	-	-	0/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-
4	EDO	C	413	-	-	1/1/1/1	-
4	EDO	C	401	-	-	0/1/1/1	-
4	EDO	D	410	-	-	0/1/1/1	-
4	EDO	D	419	-	-	1/1/1/1	-
7	YOJ	B	422	-	-	12/29/40/40	0/7/7/7
4	EDO	C	412	-	-	1/1/1/1	-
4	EDO	B	401	-	-	0/1/1/1	-
4	EDO	D	403	-	-	1/1/1/1	-
4	EDO	A	422	-	-	1/1/1/1	-
4	EDO	D	420	-	-	1/1/1/1	-
6	PEG	A	410	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	417	-	-	1/1/1/1	-
4	EDO	C	411	-	-	0/1/1/1	-
4	EDO	C	415	-	-	1/1/1/1	-
4	EDO	A	413	-	-	1/1/1/1	-
4	EDO	B	421	-	-	1/1/1/1	-
4	EDO	D	414	-	-	1/1/1/1	-
4	EDO	D	424	-	-	1/1/1/1	-
5	GOL	A	409	-	-	1/4/4/4	-
4	EDO	C	416	-	-	1/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	A	419	-	-	1/1/1/1	-
4	EDO	A	418	-	-	0/1/1/1	-
4	EDO	B	427	-	-	1/1/1/1	-
2	NAI	B	404	-	-	3/25/72/72	0/5/5/5
4	EDO	C	417	-	-	0/1/1/1	-
4	EDO	C	422	-	-	1/1/1/1	-
4	EDO	B	420	-	-	1/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	C	409	-	-	0/1/1/1	-
5	GOL	B	426	-	-	4/4/4/4	-
4	EDO	B	418	-	-	0/1/1/1	-
6	PEG	A	428	-	-	2/4/4/4	-
4	EDO	B	425	-	-	1/1/1/1	-
4	EDO	B	430	-	-	1/1/1/1	-
4	EDO	A	425	-	-	1/1/1/1	-
4	EDO	D	418	-	-	1/1/1/1	-
4	EDO	B	410	-	-	0/1/1/1	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	421	YOJ	C27-C26	-6.19	1.42	1.49
7	D	421	YOJ	S02-N01	6.18	1.72	1.60
7	B	422	YOJ	C27-C26	-6.11	1.42	1.49
7	A	420[B]	YOJ	C27-C26	-5.69	1.42	1.49
7	C	421	YOJ	S02-N01	5.06	1.70	1.60
7	A	420[A]	YOJ	C27-C26	-5.06	1.43	1.49
7	A	420[B]	YOJ	S02-N01	5.02	1.70	1.60
7	A	420[A]	YOJ	S02-N01	4.60	1.69	1.60
7	D	421	YOJ	C27-C26	-4.29	1.44	1.49
7	A	420[B]	YOJ	C12-C11	4.09	1.57	1.49
7	A	420[A]	YOJ	C12-C11	4.08	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	422	YOJ	C32-C33	-3.95	1.42	1.49
7	C	421	YOJ	C26-N25	-3.77	1.32	1.35
7	A	420[B]	YOJ	C32-C33	-3.61	1.42	1.49
7	C	421	YOJ	C32-C33	-3.54	1.43	1.49
7	C	421	YOJ	C12-C11	3.49	1.56	1.49
7	D	421	YOJ	C12-C11	3.40	1.56	1.49
7	D	421	YOJ	C32-C33	-3.38	1.43	1.49
7	A	420[A]	YOJ	C05-S02	3.35	1.81	1.77
7	A	420[B]	YOJ	C26-N25	-3.30	1.32	1.35
7	C	421	YOJ	C19-C20	3.10	1.55	1.50
7	D	421	YOJ	C26-N25	-3.09	1.32	1.35
7	B	422	YOJ	C12-C11	3.04	1.55	1.49
7	B	422	YOJ	O04-S02	2.99	1.49	1.43
7	A	420[B]	YOJ	C50-C05	-2.96	1.37	1.39
7	B	422	YOJ	S02-N01	2.92	1.66	1.60
7	A	420[A]	YOJ	C32-C33	-2.76	1.44	1.49
7	C	421	YOJ	C23-S24	2.52	1.74	1.70
7	B	422	YOJ	C50-C05	2.51	1.40	1.39
7	C	421	YOJ	O04-S02	2.43	1.48	1.43
7	A	420[A]	YOJ	O04-S02	2.40	1.48	1.43
7	D	421	YOJ	C23-S24	2.38	1.74	1.70
7	D	421	YOJ	C32-C30	2.32	1.42	1.39
7	A	420[A]	YOJ	C42-C43	2.23	1.55	1.51
7	B	422	YOJ	C05-S02	2.17	1.80	1.77
7	A	420[A]	YOJ	C23-S24	2.16	1.74	1.70
7	A	420[B]	YOJ	N25-N16	-2.13	1.35	1.39
7	A	420[A]	YOJ	C26-N25	-2.13	1.33	1.35
7	A	420[B]	YOJ	O04-S02	2.12	1.47	1.43
7	C	421	YOJ	C05-S02	2.12	1.80	1.77
7	D	421	YOJ	O03-S02	2.11	1.47	1.43
7	B	422	YOJ	C42-N41	-2.10	1.31	1.36
7	A	420[A]	YOJ	C09-C10	2.10	1.57	1.52
7	D	421	YOJ	C42-N41	-2.08	1.31	1.36
7	A	420[B]	YOJ	C23-S24	2.00	1.73	1.70

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	422	YOJ	O04-S02-O03	-11.96	99.10	118.76
7	C	421	YOJ	O04-S02-O03	-10.61	101.32	118.76
7	A	420[A]	YOJ	O04-S02-O03	-8.76	104.37	118.76
7	D	421	YOJ	O04-S02-O03	-7.41	106.58	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	420[B]	YOJ	O04-S02-O03	-7.33	106.71	118.76
7	B	422	YOJ	C19-C23-S24	-6.73	103.52	111.79
7	B	422	YOJ	O04-S02-N01	6.59	117.13	107.36
7	A	420[B]	YOJ	C09-C10-C11	-6.57	120.62	126.41
7	D	421	YOJ	C06-C05-C50	6.56	122.78	118.43
7	A	420[B]	YOJ	C49-C50-C05	-6.51	119.33	123.10
7	A	420[B]	YOJ	C06-C05-C50	6.35	122.64	118.43
7	C	421	YOJ	O03-S02-N01	6.18	116.52	107.36
7	B	422	YOJ	C49-C50-C05	-5.49	119.92	123.10
7	A	420[A]	YOJ	C19-C23-S24	-5.21	105.40	111.79
7	C	421	YOJ	O04-S02-C05	5.12	114.79	107.29
7	D	421	YOJ	C38-C42-C43	-5.00	122.12	131.57
7	A	420[A]	YOJ	O03-S02-C05	4.99	114.60	107.29
7	B	422	YOJ	C06-C05-C50	4.89	121.67	118.43
7	B	422	YOJ	O03-S02-N01	4.81	114.49	107.36
7	A	420[B]	YOJ	C19-C23-S24	-4.75	105.95	111.79
7	D	421	YOJ	F31-C30-C32	4.62	125.84	118.89
7	D	421	YOJ	C19-C23-S24	-4.61	106.13	111.79
7	C	421	YOJ	C06-C05-C50	4.60	121.48	118.43
7	A	420[B]	YOJ	C12-C11-C10	-4.45	122.75	130.34
7	A	420[B]	YOJ	C05-S02-N01	4.38	116.35	108.28
7	C	421	YOJ	C49-C50-C05	-4.36	120.57	123.10
7	D	421	YOJ	C12-C11-C10	-4.22	123.15	130.34
7	C	421	YOJ	C36-O37-C38	-4.16	109.92	118.16
7	C	421	YOJ	C38-C42-C43	-4.15	123.72	131.57
7	C	421	YOJ	C19-C23-S24	-4.14	106.71	111.79
7	D	421	YOJ	C49-C50-C05	-4.06	120.75	123.10
7	B	422	YOJ	C43-C42-N41	4.03	127.93	120.39
7	A	420[A]	YOJ	O04-S02-C05	4.02	113.19	107.29
7	D	421	YOJ	C43-C42-N41	3.94	127.76	120.39
7	A	420[B]	YOJ	C09-C10-C26	3.88	133.25	127.36
7	D	421	YOJ	C09-C10-C11	-3.86	123.00	126.41
7	D	421	YOJ	C11-N16-N25	-3.86	107.64	111.13
7	A	420[B]	YOJ	O03-S02-C05	-3.86	101.63	107.29
7	B	422	YOJ	C12-C11-C10	-3.83	123.81	130.34
7	A	420[A]	YOJ	C12-C11-C10	-3.81	123.83	130.34
7	B	422	YOJ	C09-C10-C11	-3.76	123.09	126.41
7	A	420[A]	YOJ	C06-C05-S02	3.68	122.57	117.52
7	C	421	YOJ	C09-C10-C11	-3.61	123.23	126.41
7	A	420[B]	YOJ	C43-C42-N41	3.54	127.03	120.39
7	D	421	YOJ	O03-S02-C05	3.54	112.47	107.29
7	D	421	YOJ	O37-C36-C35	3.48	131.61	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	420[B]	YOJ	C38-C42-C43	-3.47	125.02	131.57
7	C	421	YOJ	C43-C42-N41	3.42	126.80	120.39
7	D	421	YOJ	C29-C30-C32	-3.40	119.14	123.30
7	A	420[A]	YOJ	N41-N40-N39	-3.38	107.04	111.24
7	C	421	YOJ	N41-N40-N39	-3.38	107.04	111.24
7	C	421	YOJ	O21-C20-C19	3.35	122.31	114.69
7	D	421	YOJ	C34-C33-C32	3.30	126.26	120.91
7	D	421	YOJ	C47-C33-C32	-3.26	115.62	120.91
7	A	420[A]	YOJ	C11-N16-N25	-3.20	108.24	111.13
7	A	420[A]	YOJ	C09-C10-C11	-3.20	123.59	126.41
7	A	420[B]	YOJ	C07-C08-C49	3.20	123.02	118.54
7	D	421	YOJ	C38-C42-N41	3.17	110.11	107.94
7	B	422	YOJ	C38-C42-C43	-3.16	125.60	131.57
7	C	421	YOJ	C11-N16-N25	-3.05	108.38	111.13
7	A	420[B]	YOJ	O03-S02-N01	3.04	111.86	107.36
7	D	421	YOJ	N41-N40-N39	-3.02	107.48	111.24
7	B	422	YOJ	C11-N16-N25	-3.00	108.42	111.13
7	C	421	YOJ	C12-C11-C10	-3.00	125.22	130.34
7	D	421	YOJ	C36-O37-C38	2.98	124.06	118.16
7	A	420[A]	YOJ	C06-C05-C50	2.92	120.37	118.43
7	D	421	YOJ	C47-C46-C36	2.91	123.30	119.73
2	B	404	NAI	O4B-C1B-C2B	-2.91	102.67	106.93
7	A	420[B]	YOJ	O04-S02-C05	2.83	111.44	107.29
7	B	422	YOJ	N41-N40-N39	-2.81	107.74	111.24
7	D	421	YOJ	F51-C50-C05	2.73	121.61	118.89
7	B	422	YOJ	C09-C10-C26	2.68	131.43	127.36
2	A	401	NAI	O4D-C1D-C2D	-2.68	100.80	106.64
7	D	421	YOJ	C08-C49-C50	-2.65	117.65	119.37
7	C	421	YOJ	C11-C12-C13	-2.65	108.10	114.15
7	A	420[A]	YOJ	C49-C50-C05	-2.61	121.59	123.10
7	D	421	YOJ	O37-C36-C46	-2.60	110.22	119.38
2	B	404	NAI	C5A-C6A-N6A	2.56	124.25	120.35
2	D	411	NAI	C5A-C6A-N6A	2.55	124.22	120.35
7	A	420[B]	YOJ	C29-C30-C32	-2.51	120.24	123.30
7	B	422	YOJ	C34-C33-C32	2.49	124.94	120.91
7	A	420[B]	YOJ	N41-N40-N39	-2.43	108.22	111.24
7	B	422	YOJ	O22-C20-C19	-2.40	116.38	121.24
7	D	421	YOJ	C48-C32-C30	2.39	119.49	116.15
2	A	401	NAI	O4D-C1D-N1N	2.39	112.72	108.06
2	A	401	NAI	C5A-C6A-N6A	2.31	123.87	120.35
7	D	421	YOJ	O04-S02-C05	2.31	110.68	107.29
7	A	420[A]	YOJ	O44-C43-O45	-2.31	118.23	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	422	YOJ	C10-C11-N16	2.29	108.92	106.86
7	A	420[B]	YOJ	C48-C32-C30	2.28	119.33	116.15
7	D	421	YOJ	C48-C27-C26	2.26	124.49	120.15
7	C	421	YOJ	F51-C50-C05	-2.26	116.63	118.89
7	C	421	YOJ	C38-C42-N41	2.25	109.48	107.94
7	B	422	YOJ	C29-C30-C32	-2.23	120.58	123.30
2	D	411	NAI	O4B-C1B-C2B	-2.21	103.69	106.93
7	C	421	YOJ	C09-C10-C26	2.21	130.71	127.36
7	D	421	YOJ	O21-C20-C19	2.20	119.69	114.69
7	B	422	YOJ	F51-C50-C05	2.20	121.09	118.89
7	B	422	YOJ	O21-C20-C19	2.20	119.68	114.69
2	C	404	NAI	C1D-N1N-C2N	-2.19	117.46	121.11
7	B	422	YOJ	C23-C19-C20	-2.19	121.97	128.42
7	D	421	YOJ	C10-C11-N16	2.18	108.82	106.86
7	D	421	YOJ	O45-C43-C42	-2.17	116.27	120.73
7	D	421	YOJ	C11-C12-C13	-2.17	109.19	114.15
7	D	421	YOJ	C07-C06-C05	-2.17	116.71	120.03
7	B	422	YOJ	O44-C43-C42	2.17	121.48	114.46
7	B	422	YOJ	C38-C42-N41	-2.17	106.46	107.94
2	A	401	NAI	C3N-C7N-N7N	2.15	121.49	117.67
7	D	421	YOJ	C09-C10-C26	2.14	130.61	127.36
2	B	404	NAI	O2A-PA-O1A	2.13	122.78	112.24
7	A	420[B]	YOJ	C11-N16-N25	-2.13	109.21	111.13
7	C	421	YOJ	F51-C50-C49	2.11	122.80	118.61
2	D	411	NAI	O4D-C1D-C2D	-2.09	102.08	106.64
7	C	421	YOJ	O21-C20-O22	-2.09	118.71	123.35
7	C	421	YOJ	C06-C05-S02	2.08	120.38	117.52
7	B	422	YOJ	C28-C27-C26	-2.08	117.31	120.61
2	C	404	NAI	O4B-C1B-C2B	-2.07	103.90	106.93

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	413	EDO	O1-C1-C2-O2
4	C	415	EDO	O1-C1-C2-O2
5	B	426	GOL	C1-C2-C3-O3
5	C	419	GOL	O1-C1-C2-O2
5	C	419	GOL	O1-C1-C2-C3
5	C	419	GOL	C1-C2-C3-O3
5	C	419	GOL	O2-C2-C3-O3
5	D	409	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	D	409	GOL	O1-C1-C2-C3
7	A	420[A]	YOJ	C10-C26-C27-C48
7	A	420[A]	YOJ	C38-C42-C43-O44
7	A	420[A]	YOJ	C38-C42-C43-O45
7	A	420[A]	YOJ	N41-C42-C43-O44
7	A	420[B]	YOJ	C38-C42-C43-O44
7	A	420[B]	YOJ	C38-C42-C43-O45
7	A	420[B]	YOJ	N41-C42-C43-O44
7	B	422	YOJ	C38-C42-C43-O44
7	B	422	YOJ	C38-C42-C43-O45
7	B	422	YOJ	N41-C42-C43-O44
7	C	421	YOJ	C11-C12-C13-C15
7	C	421	YOJ	C38-C42-C43-O44
7	C	421	YOJ	C38-C42-C43-O45
7	C	421	YOJ	N41-C42-C43-O44
7	D	421	YOJ	C10-C26-C27-C28
7	D	421	YOJ	C10-C26-C27-C48
7	D	421	YOJ	C38-C42-C43-O44
7	D	421	YOJ	C38-C42-C43-O45
7	D	421	YOJ	N41-C42-C43-O44
7	B	422	YOJ	C48-C32-C33-C34
7	B	422	YOJ	C48-C32-C33-C47
7	A	420[A]	YOJ	C10-C26-C27-C28
7	A	420[B]	YOJ	C10-C26-C27-C28
7	A	420[B]	YOJ	C10-C26-C27-C48
7	C	421	YOJ	C10-C26-C27-C28
7	C	421	YOJ	C10-C26-C27-C48
4	C	418	EDO	O1-C1-C2-O2
4	D	419	EDO	O1-C1-C2-O2
7	B	422	YOJ	C10-C26-C27-C48
6	A	410	PEG	O1-C1-C2-O2
6	B	412	PEG	O2-C3-C4-O4
5	B	426	GOL	O1-C1-C2-C3
5	C	420	GOL	O1-C1-C2-C3
5	D	409	GOL	C1-C2-C3-O3
7	B	422	YOJ	C10-C26-C27-C28
6	A	428	PEG	O2-C3-C4-O4
4	A	403	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2
4	A	416	EDO	O1-C1-C2-O2
4	A	424	EDO	O1-C1-C2-O2
4	A	425	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	406	EDO	O1-C1-C2-O2
4	B	411	EDO	O1-C1-C2-O2
4	B	415	EDO	O1-C1-C2-O2
4	B	416	EDO	O1-C1-C2-O2
4	B	420	EDO	O1-C1-C2-O2
4	B	421	EDO	O1-C1-C2-O2
4	B	424	EDO	O1-C1-C2-O2
4	B	428	EDO	O1-C1-C2-O2
4	C	410	EDO	O1-C1-C2-O2
4	C	412	EDO	O1-C1-C2-O2
4	C	422	EDO	O1-C1-C2-O2
4	D	405	EDO	O1-C1-C2-O2
4	D	406	EDO	O1-C1-C2-O2
4	D	414	EDO	O1-C1-C2-O2
4	D	416	EDO	O1-C1-C2-O2
4	D	418	EDO	O1-C1-C2-O2
6	A	410	PEG	O2-C3-C4-O4
6	B	429	PEG	O1-C1-C2-O2
4	C	414	EDO	O1-C1-C2-O2
4	D	412	EDO	O1-C1-C2-O2
4	D	424	EDO	O1-C1-C2-O2
7	D	421	YOJ	C35-C36-O37-C38
5	C	420	GOL	C1-C2-C3-O3
7	B	422	YOJ	C30-C32-C33-C34
7	B	422	YOJ	C30-C32-C33-C47
6	A	417	PEG	O1-C1-C2-O2
7	D	421	YOJ	C46-C36-O37-C38
4	A	404	EDO	O1-C1-C2-O2
4	A	421	EDO	O1-C1-C2-O2
4	A	422	EDO	O1-C1-C2-O2
4	B	407	EDO	O1-C1-C2-O2
4	B	413	EDO	O1-C1-C2-O2
4	B	425	EDO	O1-C1-C2-O2
4	D	420	EDO	O1-C1-C2-O2
7	D	421	YOJ	N41-C42-C43-O45
5	A	409	GOL	O1-C1-C2-O2
6	A	428	PEG	O1-C1-C2-O2
4	B	414	EDO	O1-C1-C2-O2
4	C	406	EDO	O1-C1-C2-O2
4	D	403	EDO	O1-C1-C2-O2
6	B	429	PEG	O2-C3-C4-O4
4	A	419	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	408	EDO	O1-C1-C2-O2
4	C	416	EDO	O1-C1-C2-O2
2	A	401	NAI	O4D-C1D-N1N-C2N
2	C	404	NAI	O4D-C1D-N1N-C2N
7	B	422	YOJ	C35-C36-O37-C38
5	D	409	GOL	O2-C2-C3-O3
2	B	404	NAI	O4B-C4B-C5B-O5B
2	D	411	NAI	O4D-C1D-N1N-C2N
2	C	404	NAI	C2D-C1D-N1N-C2N
2	D	411	NAI	C2D-C1D-N1N-C2N
2	B	404	NAI	O4D-C1D-N1N-C2N
2	B	404	NAI	C2D-C1D-N1N-C2N
2	D	411	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	C2D-C1D-N1N-C2N
2	C	404	NAI	C2D-C1D-N1N-C6N
5	C	423	GOL	O1-C1-C2-C3
7	A	420[A]	YOJ	N41-C42-C43-O45
7	B	422	YOJ	N41-C42-C43-O45
5	C	420	GOL	O1-C1-C2-O2
5	C	423	GOL	O1-C1-C2-O2
7	B	422	YOJ	C46-C36-O37-C38
2	D	411	NAI	O4B-C4B-C5B-O5B
4	A	406	EDO	O1-C1-C2-O2
4	A	413	EDO	O1-C1-C2-O2
4	A	415	EDO	O1-C1-C2-O2
4	B	409	EDO	O1-C1-C2-O2
4	B	417	EDO	O1-C1-C2-O2
4	B	427	EDO	O1-C1-C2-O2
4	B	430	EDO	O1-C1-C2-O2
2	C	404	NAI	O4D-C1D-N1N-C6N
5	B	426	GOL	O1-C1-C2-O2
5	B	426	GOL	O2-C2-C3-O3
2	A	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	C2N-C3N-C7N-N7N
2	D	411	NAI	C2N-C3N-C7N-N7N
2	C	404	NAI	O4B-C4B-C5B-O5B
4	A	407	EDO	O1-C1-C2-O2
7	C	421	YOJ	C11-C12-C13-C14
2	A	401	NAI	C2D-C1D-N1N-C6N

There are no ring outliers.

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	413	EDO	1	0
4	B	428	EDO	1	0
4	B	405	EDO	1	0
4	B	416	EDO	1	0
2	A	401	NAI	2	0
7	A	420[B]	YOJ	2	0
2	D	411	NAI	1	0
4	D	402	EDO	1	0
5	C	423	GOL	1	0
4	D	407	EDO	1	0
5	C	420	GOL	1	0
4	D	412	EDO	4	0
4	D	410	EDO	1	0
7	B	422	YOJ	1	0
4	B	417	EDO	1	0
4	A	404	EDO	1	0
4	B	425	EDO	1	0
4	A	425	EDO	1	0

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

Ligand YOJ A 420 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand YOJ C 421

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI C 404

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand YOJ A 420 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI D 411

Bond lengths

Bond angles

Torsions

Rings

Ligand YOJ D 421

Bond lengths

Bond angles

Torsions

Rings

Ligand YOJ B 422

Bond lengths

Bond angles

Torsions

Rings

Ligand NAI B 404

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	327/338 (96%)	-0.19	5 (1%)	73	75	20, 31, 59, 92	0
1	B	331/338 (97%)	-0.22	4 (1%)	79	80	21, 34, 58, 98	0
1	C	331/338 (97%)	0.01	6 (1%)	68	71	24, 38, 73, 112	0
1	D	331/338 (97%)	-0.05	11 (3%)	46	50	22, 37, 70, 98	0
All	All	1320/1352 (97%)	-0.11	26 (1%)	65	68	20, 35, 65, 112	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	102	GLY	4.3
1	C	101	GLU	4.2
1	B	1	ALA	3.9
1	B	13	LYS	3.6
1	D	220	ASP	3.5
1	A	99	GLN	3.4
1	A	102	GLY	3.3
1	D	221	LYS	3.2
1	D	218	GLY	3.2
1	A	105	ARG	3.0
1	D	1	ALA	2.8
1	D	331	PHE	2.6
1	D	216	ASP	2.6
1	D	40	MET	2.6
1	D	223	LYS	2.5
1	A	72	ARG	2.4
1	D	118	PHE	2.4
1	C	1	ALA	2.4
1	C	253	LEU	2.3
1	C	220	ASP	2.2
1	A	101	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2	THR	2.2
1	D	80	LYS	2.2
1	D	280	TYR	2.1
1	C	221	LYS	2.1
1	B	69	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	413	4/4	0.54	0.30	81,86,87,87	0
4	EDO	C	415	4/4	0.62	0.21	66,67,69,69	0
4	EDO	C	411	4/4	0.64	0.39	72,74,75,76	0
4	EDO	C	422	4/4	0.64	0.30	76,76,78,81	0
6	PEG	A	417	7/7	0.64	0.36	68,72,75,75	0
4	EDO	A	416	4/4	0.66	0.29	66,66,67,71	0
5	GOL	C	423	6/6	0.70	0.26	75,81,83,88	0
5	GOL	D	409	6/6	0.71	0.36	61,65,71,75	0
4	EDO	D	402	4/4	0.71	0.34	52,55,57,58	0
4	EDO	D	415	4/4	0.72	0.37	57,67,69,71	0
6	PEG	B	423	7/7	0.72	0.26	66,71,77,78	0
4	EDO	B	424	4/4	0.73	0.22	57,59,62,63	0
4	EDO	B	406	4/4	0.73	0.28	60,61,61,64	0
4	EDO	D	408	4/4	0.74	0.21	70,72,73,78	0
4	EDO	D	407	4/4	0.75	0.25	69,73,75,75	0
6	PEG	B	429	7/7	0.75	0.25	71,75,77,78	0
4	EDO	D	405	4/4	0.77	0.28	53,59,60,66	0
4	EDO	C	412	4/4	0.77	0.36	67,70,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	426	4/4	0.77	0.30	74,78,81,87	0
4	EDO	D	412	4/4	0.77	0.27	44,56,58,59	0
4	EDO	D	403	4/4	0.77	0.23	64,67,70,72	0
4	EDO	A	424	4/4	0.78	0.16	65,73,77,80	0
4	EDO	B	401	4/4	0.78	0.23	71,76,77,79	0
4	EDO	C	401	4/4	0.79	0.21	65,65,69,69	0
4	EDO	A	418	4/4	0.80	0.29	56,63,66,66	0
4	EDO	B	421	4/4	0.80	0.18	71,74,74,75	0
4	EDO	B	416	4/4	0.81	0.14	48,49,53,54	0
4	EDO	B	425	4/4	0.81	0.22	60,61,67,72	0
4	EDO	D	416	4/4	0.81	0.19	54,59,61,71	0
4	EDO	C	417	4/4	0.81	0.27	70,71,77,80	0
4	EDO	B	430	4/4	0.82	0.16	70,72,73,75	0
4	EDO	A	412	4/4	0.82	0.30	70,74,75,79	0
4	EDO	C	414	4/4	0.83	0.24	57,57,61,63	0
4	EDO	B	409	4/4	0.83	0.42	51,61,61,65	0
4	EDO	C	416	4/4	0.83	0.44	67,72,73,73	0
6	PEG	A	410	7/7	0.83	0.18	68,75,80,81	0
4	EDO	B	413	4/4	0.83	0.22	63,65,67,71	0
4	EDO	A	421	4/4	0.83	0.69	57,64,67,69	0
4	EDO	B	427	4/4	0.83	0.21	56,58,60,62	0
4	EDO	A	425	4/4	0.84	0.25	54,60,66,67	0
4	EDO	D	420	4/4	0.84	0.22	64,67,72,73	0
5	GOL	B	426	6/6	0.84	0.25	44,52,53,53	0
4	EDO	A	422	4/4	0.85	0.20	49,56,57,57	0
5	GOL	C	419	6/6	0.85	0.46	61,67,68,70	0
6	PEG	B	412	7/7	0.85	0.15	55,63,66,69	0
4	EDO	C	410	4/4	0.85	0.17	61,67,69,73	0
4	EDO	D	422	4/4	0.85	0.17	72,76,82,82	0
4	EDO	D	417	4/4	0.86	0.21	64,73,73,76	0
5	GOL	C	420	6/6	0.86	0.25	60,65,69,71	0
4	EDO	B	418	4/4	0.86	0.16	56,56,57,59	0
4	EDO	B	411	4/4	0.87	0.19	61,68,71,72	0
4	EDO	B	415	4/4	0.87	0.22	50,55,58,58	0
4	EDO	C	409	4/4	0.87	0.23	65,68,69,72	0
4	EDO	B	428	4/4	0.87	0.46	60,60,60,60	0
4	EDO	D	406	4/4	0.88	0.29	60,60,61,65	0
4	EDO	D	418	4/4	0.88	0.12	57,66,66,68	0
4	EDO	C	406	4/4	0.88	0.42	53,61,66,70	0
4	EDO	C	413	4/4	0.88	0.32	50,53,55,56	0
6	PEG	A	428	7/7	0.88	0.86	69,74,80,84	0
4	EDO	A	419	4/4	0.88	0.22	62,69,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
4	EDO	A	403	4/4	0.88	0.12	47,54,57,59	0
4	EDO	A	414	4/4	0.88	0.41	65,67,69,70	0
5	GOL	A	409	6/6	0.89	0.23	57,68,70,70	0
4	EDO	A	408	4/4	0.89	0.24	59,59,60,63	0
4	EDO	C	418	4/4	0.89	0.17	50,52,53,58	0
4	EDO	B	405	4/4	0.90	0.62	51,54,55,62	0
4	EDO	D	424	4/4	0.90	0.51	57,61,62,64	0
4	EDO	C	408	4/4	0.90	0.31	45,52,54,70	0
4	EDO	A	407	4/4	0.90	0.44	45,47,52,53	0
4	EDO	A	405	4/4	0.90	0.22	61,68,70,71	0
4	EDO	D	419	4/4	0.90	0.29	59,65,67,68	0
4	EDO	D	414	4/4	0.90	0.27	49,51,54,57	0
4	EDO	D	410	4/4	0.91	0.66	54,58,62,62	0
4	EDO	B	414	4/4	0.91	0.17	65,66,68,70	0
4	EDO	D	413	4/4	0.91	0.28	42,44,49,51	0
4	EDO	A	411	4/4	0.91	0.38	43,43,48,50	0
4	EDO	A	415	4/4	0.92	0.14	51,54,56,57	0
4	EDO	B	420	4/4	0.92	0.29	60,62,63,65	0
3	SO4	A	423	5/5	0.92	0.40	75,77,86,86	0
4	EDO	B	417	4/4	0.92	0.35	47,57,63,84	0
4	EDO	A	406	4/4	0.93	0.28	56,60,64,65	0
4	EDO	B	410	4/4	0.93	0.19	56,57,61,68	0
4	EDO	C	407	4/4	0.93	0.60	52,53,54,56	0
4	EDO	C	403	4/4	0.94	0.11	43,50,53,55	0
4	EDO	D	404	4/4	0.94	0.37	65,69,70,72	0
4	EDO	B	407	4/4	0.94	0.17	61,70,73,75	0
3	SO4	D	423	5/5	0.95	0.13	71,72,75,75	5
3	SO4	B	402	5/5	0.95	0.09	54,57,62,71	0
4	EDO	C	405	4/4	0.95	0.14	56,59,60,64	0
3	SO4	B	403	5/5	0.95	0.14	64,65,70,78	0
7	YOJ	A	420[A]	51/51	0.95	0.19	31,36,68,70	51
7	YOJ	A	420[B]	51/51	0.95	0.19	23,30,67,69	51
2	NAI	D	411	44/44	0.96	0.12	26,34,44,46	0
3	SO4	B	419	5/5	0.96	0.10	40,53,60,73	0
4	EDO	A	404	4/4	0.96	0.17	37,46,46,50	0
7	YOJ	B	422	51/51	0.96	0.13	29,41,62,75	0
7	YOJ	C	421	51/51	0.96	0.15	33,45,100,106	0
7	YOJ	D	421	51/51	0.96	0.15	33,43,93,106	0
2	NAI	C	404	44/44	0.97	0.10	30,37,44,47	0
2	NAI	A	401	44/44	0.97	0.11	24,32,35,36	0
2	NAI	B	404	44/44	0.97	0.10	26,30,43,43	0
3	SO4	C	402	5/5	0.98	0.10	45,45,55,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	402	5/5	0.99	0.14	33,36,38,40	0
3	SO4	A	427	5/5	0.99	0.17	31,34,36,38	0
3	SO4	D	401	5/5	0.99	0.09	32,33,36,42	0
3	SO4	B	408	5/5	1.00	0.09	35,37,40,42	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 YOJ A 420 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
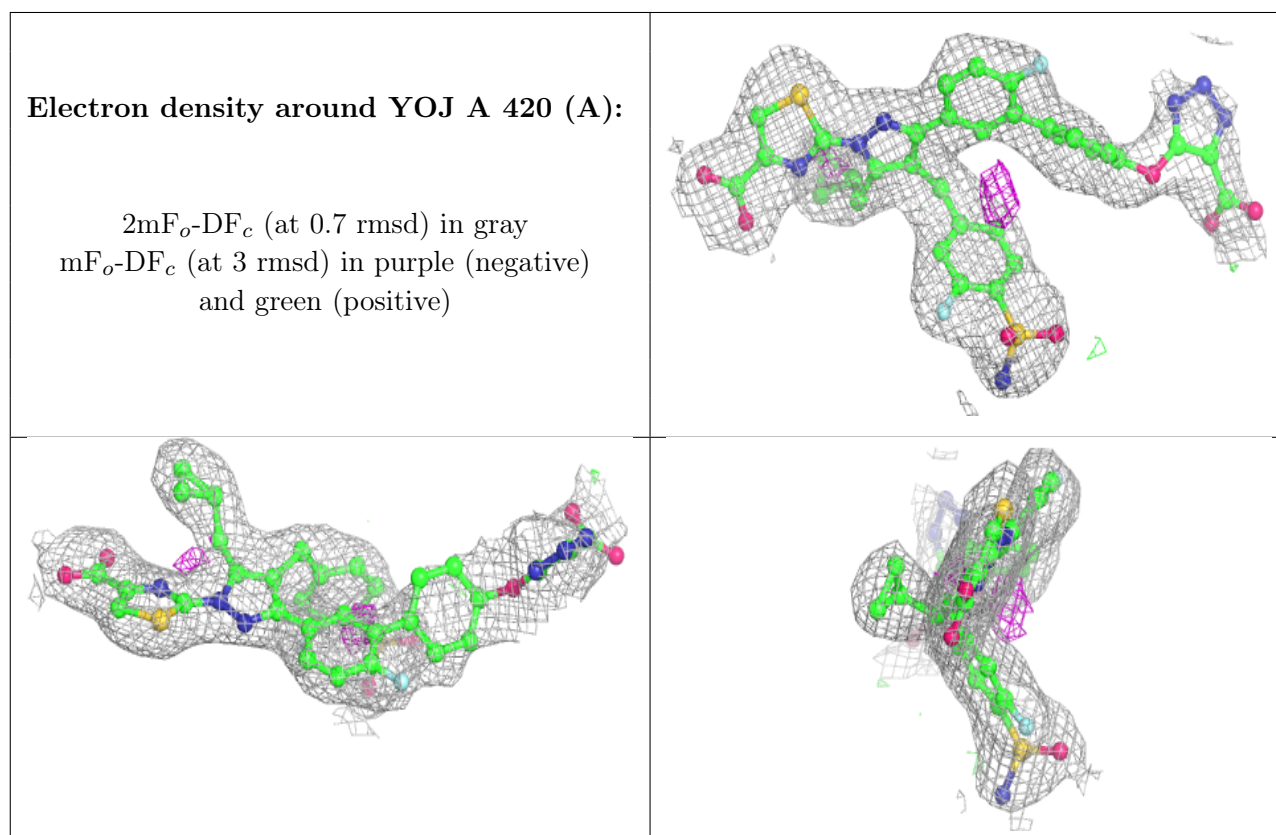
Electron density around YOJ A 420 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
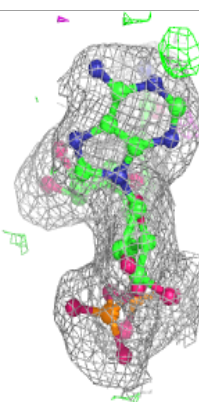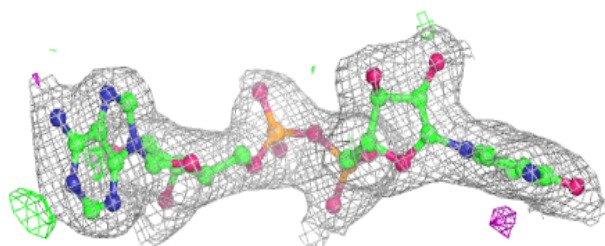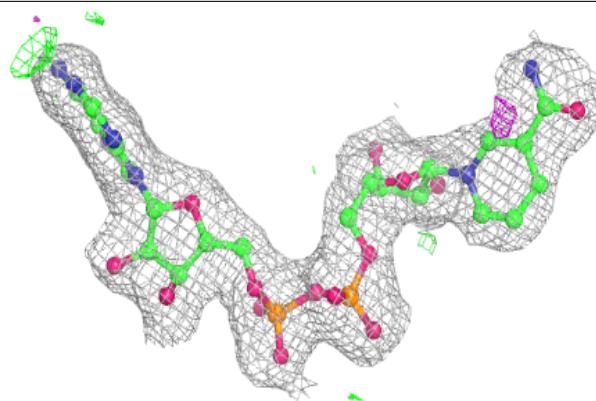mF_o-DF_c (at 3 rmsd) in purple (negative)
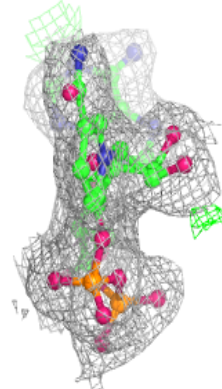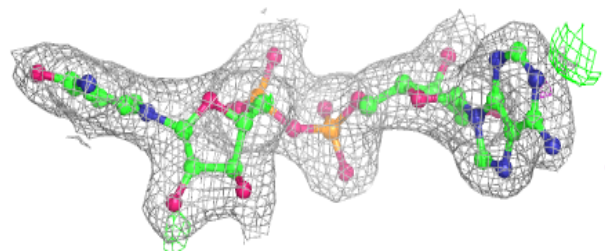and green (positive)
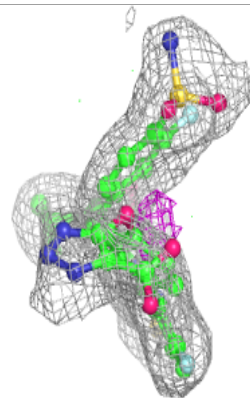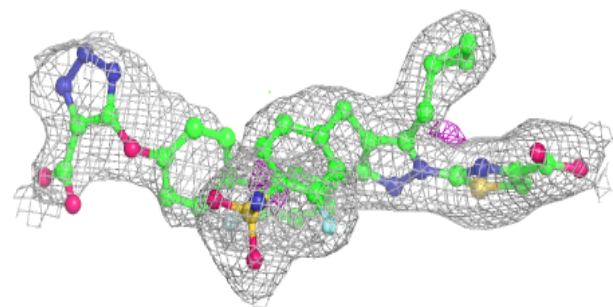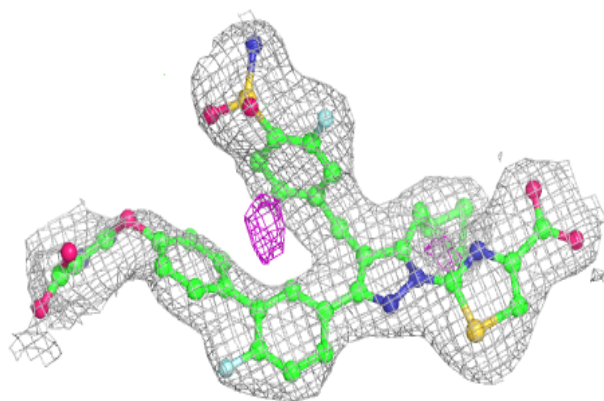
Electron density around NAI D 411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
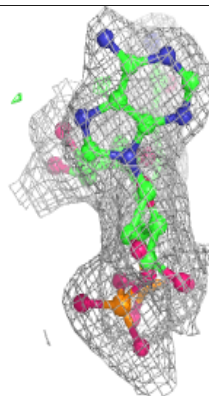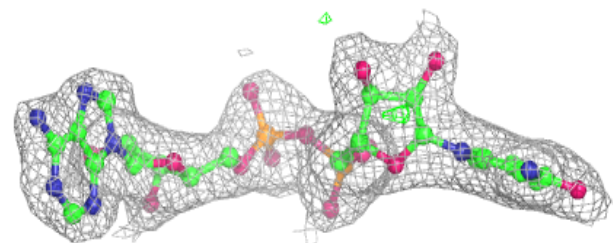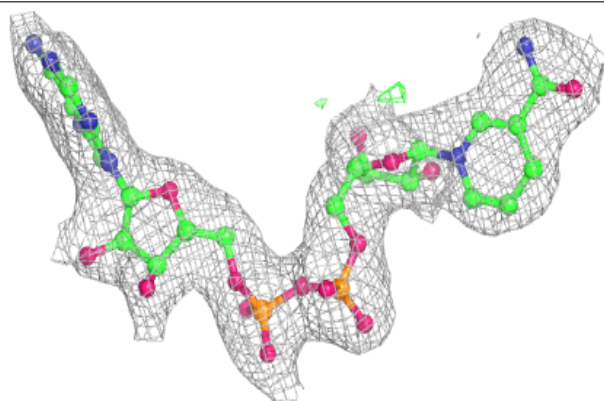
Electron density around YOJ B 422:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
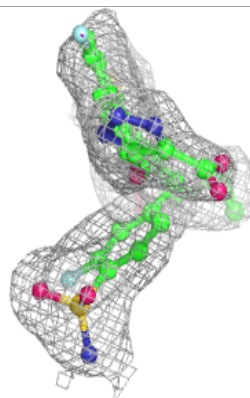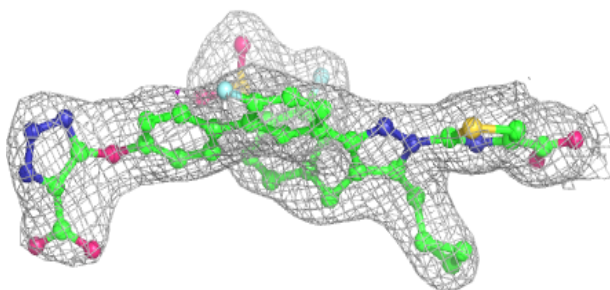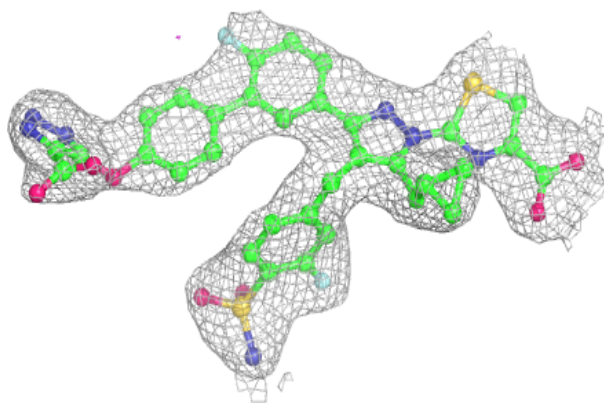
Electron density around YOJ C 421:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
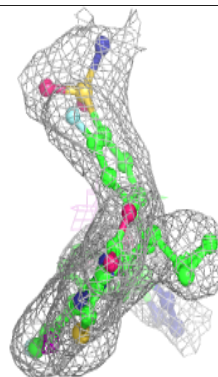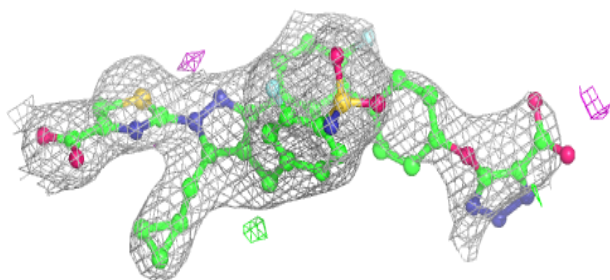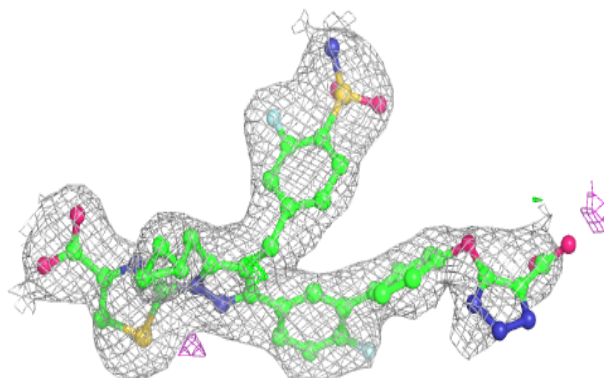
Electron density around YOJ D 421:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
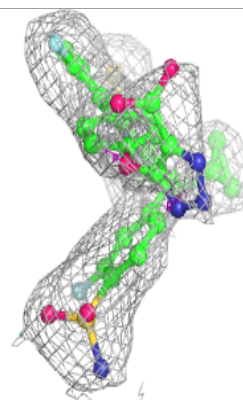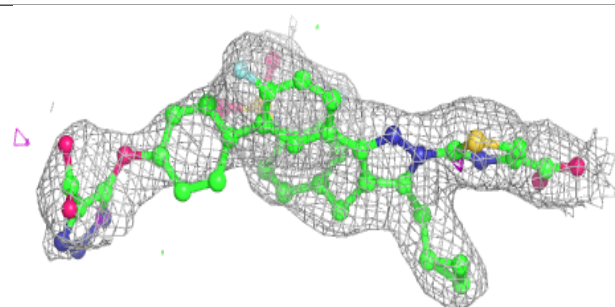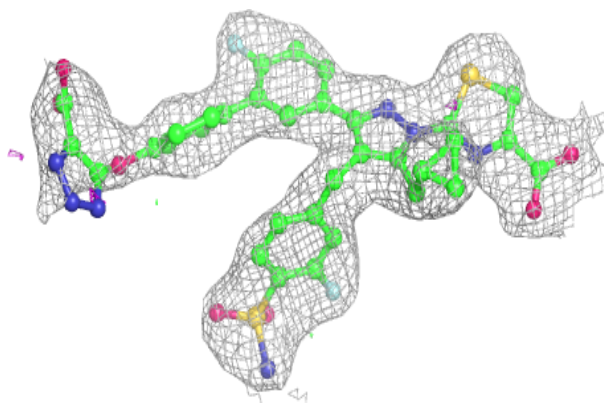
Electron density around NAI C 404:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
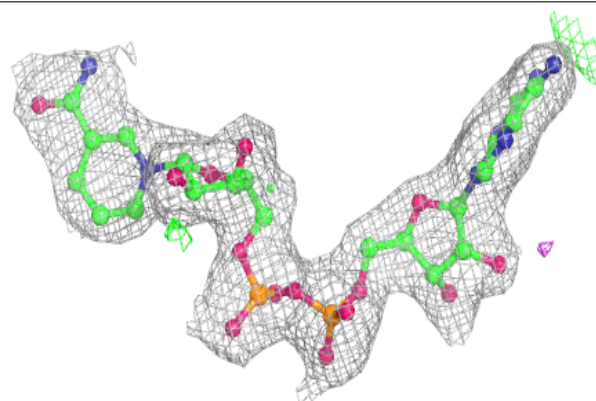$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
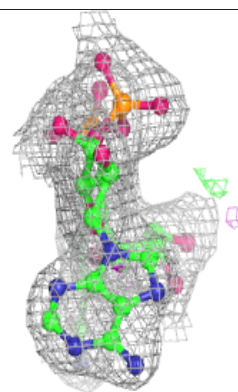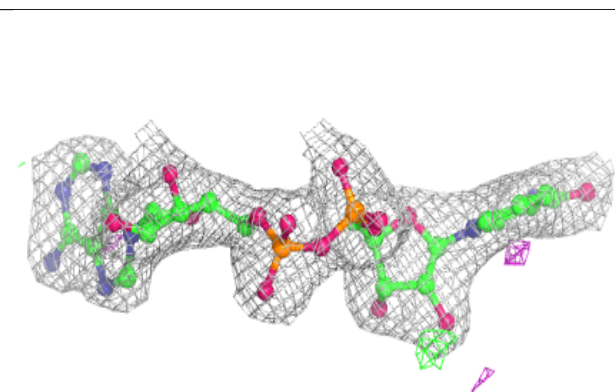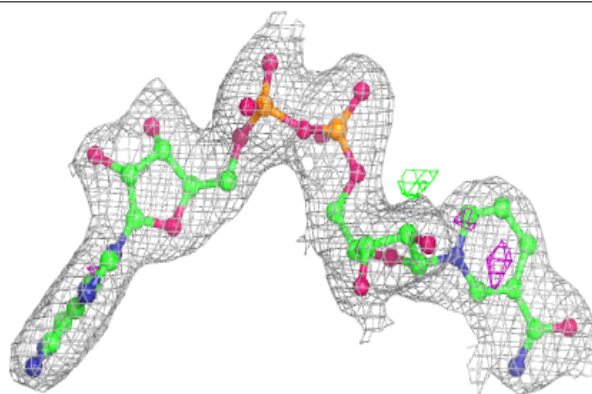
Electron density around NAI A 401:

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

Electron density around NAI B 404:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.