



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 03:31 PM EDT

PDB ID : 3B1E
Title : Crystal structure of betaC-S lyase from Streptococcus anginosus in complex with L-serine: alpha-Aminoacrylate form
Authors : Kezuka, Y.; Yoshida, Y.; Nonaka, T.
Deposited on : 2011-06-29
Resolution : 1.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

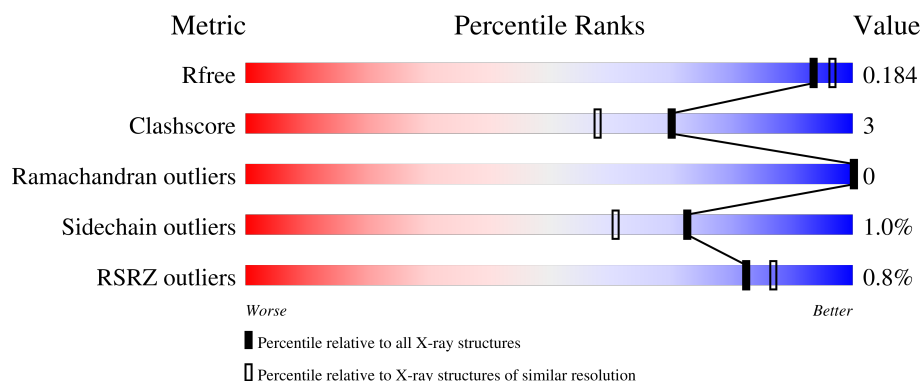
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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

Mol	Chain	Length	Quality of chain
1	A	392	<div> <div>%</div> <div>94% 5% .</div> </div>
1	B	392	<div> <div>%</div> <div>94% . .</div> </div>
1	C	392	<div> <div>%</div> <div>91% 7% .</div> </div>
1	D	392	<div> <div>%</div> <div>90% 8% .</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OJO	C	401	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14723 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.

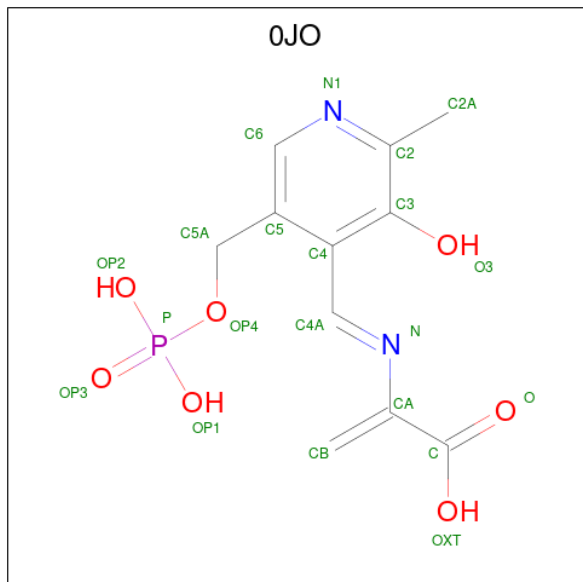
- Molecule 1 is a protein called BetaC-S lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	15	0
			3216	2066	530	609	11			
1	B	387	Total	C	N	O	S	0	14	0
			3196	2053	527	604	12			
1	C	385	Total	C	N	O	S	0	11	0
			3168	2035	524	599	10			
1	D	385	Total	C	N	O	S	0	13	0
			3185	2047	528	599	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A6BMJ3
A	-2	PRO	-	expression tag	UNP A6BMJ3
A	-1	LEU	-	expression tag	UNP A6BMJ3
A	0	GLY	-	expression tag	UNP A6BMJ3
A	1	SER	-	expression tag	UNP A6BMJ3
B	-3	GLY	-	expression tag	UNP A6BMJ3
B	-2	PRO	-	expression tag	UNP A6BMJ3
B	-1	LEU	-	expression tag	UNP A6BMJ3
B	0	GLY	-	expression tag	UNP A6BMJ3
B	1	SER	-	expression tag	UNP A6BMJ3
C	-3	GLY	-	expression tag	UNP A6BMJ3
C	-2	PRO	-	expression tag	UNP A6BMJ3
C	-1	LEU	-	expression tag	UNP A6BMJ3
C	0	GLY	-	expression tag	UNP A6BMJ3
C	1	SER	-	expression tag	UNP A6BMJ3
D	-3	GLY	-	expression tag	UNP A6BMJ3
D	-2	PRO	-	expression tag	UNP A6BMJ3
D	-1	LEU	-	expression tag	UNP A6BMJ3
D	0	GLY	-	expression tag	UNP A6BMJ3
D	1	SER	-	expression tag	UNP A6BMJ3

- Molecule 2 is 2-{[(E)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyldiene]amino}prop-2-enoic acid (three-letter code: OJO) (formula: $C_{11}H_{13}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	11	0
			15	8	2	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

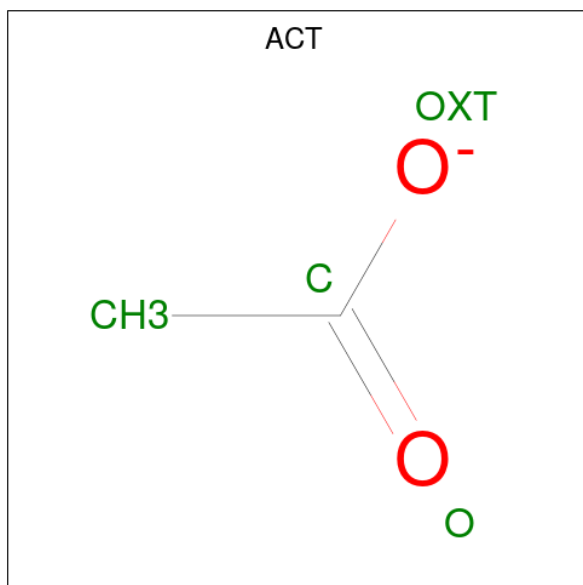
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	463	Total	O	0	4
			463	463		
6	B	466	Total	O	0	6
			466	466		
6	C	385	Total	O	0	11
			385	385		
6	D	387	Total	O	0	7
			387	387		

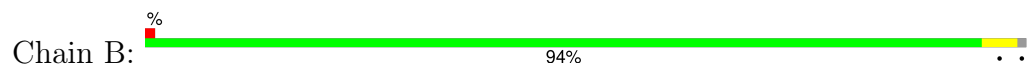
3 Residue-property plots [i](#)

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

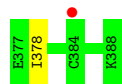
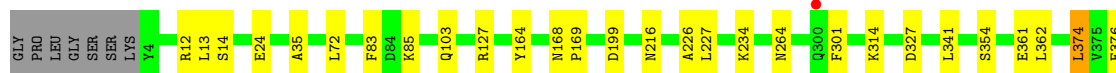
- Molecule 1: BetaC-S lyase



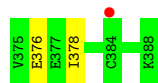
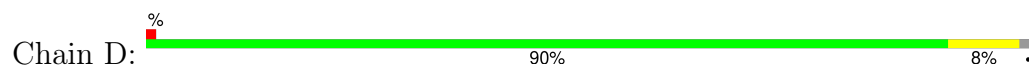
- Molecule 1: BetaC-S lyase



- Molecule 1: BetaC-S lyase



- Molecule 1: BetaC-S lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.20Å 111.21Å 217.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 1.78 49.27 – 1.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-1.78) 99.6 (49.27-1.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.55 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.142 , 0.177 0.152 , 0.184	Depositor DCC
R_{free} test set	7800 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14723	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0JO, NA, EPE, ACT

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	0.58	0/3329	0.65	0/4525
1	B	0.56	0/3317	0.64	0/4509
1	C	0.56	0/3274	0.62	0/4453
1	D	0.54	0/3297	0.62	0/4483
All	All	0.56	0/13217	0.63	0/17970

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3216	0	3150	17	0
1	B	3196	0	3138	17	0
1	C	3168	0	3104	30	0
1	D	3185	0	3131	24	0
2	A	21	0	9	6	0
2	B	21	0	9	6	0
2	C	21	0	9	8	0
2	D	21	0	9	6	0
3	A	45	0	51	0	0
3	B	30	0	34	0	0
3	C	45	0	52	0	0
3	D	45	0	52	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	4	0	3	0	0
6	A	463	0	0	5	0
6	B	466	0	0	1	0
6	C	385	0	0	0	0
6	D	387	0	0	2	0
All	All	14723	0	12751	86	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 (86) 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:D:13[B]:LEU:O	1:D:14[B]:SER:OG	1.61	1.14
1:C:13[A]:LEU:O	1:C:14[A]:SER:OG	1.68	1.09
1:B:234:LYS:HE3	2:B:401:OJO:H4	1.63	0.81
1:C:234:LYS:CE	2:C:401:OJO:H4	2.13	0.78
1:B:234:LYS:CE	2:B:401:OJO:H4	2.13	0.78
1:A:234:LYS:CE	2:A:401:OJO:H4	2.16	0.75
1:A:234:LYS:HE3	2:A:401:OJO:H4	1.69	0.73
1:D:234:LYS:CE	2:D:401:OJO:H4	2.18	0.73
1:A:234:LYS:NZ	2:A:401:OJO:H3	2.05	0.72
1:B:341:LEU:HD13	1:B:345:GLN:NE2	2.05	0.71
1:D:234:LYS:HE3	2:D:401:OJO:H4	1.74	0.70
1:C:234:LYS:NZ	2:C:401:OJO:H3	2.07	0.69
1:D:72:LEU:HD12	1:D:83:PHE:CE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13[B]:LEU:O	1:D:14[B]:SER:CB	2.41	0.68
1:D:103:GLN:NE2	1:D:264:ASN:HD21	1.89	0.68
1:A:85:LYS:NZ	6:A:1028:HOH:O	2.29	0.66
1:D:234:LYS:NZ	2:D:401:OJO:H3	2.09	0.66
1:C:103:GLN:NE2	1:C:264:ASN:HD21	1.93	0.65
1:C:234:LYS:HE3	2:C:401:OJO:H4	1.79	0.64
1:D:103:GLN:HE22	1:D:264:ASN:HD21	1.43	0.64
1:C:103:GLN:HE22	1:C:264:ASN:HD21	1.46	0.63
1:C:13[A]:LEU:O	1:C:14[A]:SER:CB	2.47	0.62
1:C:341:LEU:HD23	1:C:341:LEU:C	2.21	0.60
1:B:234:LYS:HE3	2:B:401:OJO:C4A	2.31	0.60
1:B:234:LYS:NZ	2:B:401:OJO:H3	2.16	0.60
1:B:381:ARG:O	1:B:384[B]:CYS:SG	2.59	0.60
1:B:183[B]:GLU:HG2	1:B:187:HIS:CE1	2.37	0.59
1:A:234:LYS:HZ1	2:A:401:OJO:H3	1.68	0.59
1:B:341:LEU:CD1	1:B:345:GLN:NE2	2.66	0.59
1:D:211:GLU:HG3	6:D:1170:HOH:O	2.04	0.58
1:C:234:LYS:HZ1	2:C:401:OJO:H3	1.66	0.58
1:A:261:GLN:NE2	6:A:850:HOH:O	2.37	0.58
1:C:35:ALA:HB3	2:C:401:OJO:CB	2.34	0.58
1:A:2:SER:N	6:A:968:HOH:O	2.37	0.57
1:C:234:LYS:HE2	2:C:401:OJO:H4	1.84	0.57
1:A:234:LYS:HE3	2:A:401:OJO:C4A	2.32	0.57
1:B:35:ALA:HB3	2:B:401:OJO:CB	2.36	0.56
1:C:168[B]:ASN:HD22	1:C:169:PRO:HA	1.69	0.56
1:D:234:LYS:HZ1	2:D:401:OJO:H3	1.71	0.56
1:C:374:LEU:HD22	1:C:378:ILE:HD11	1.88	0.56
1:A:35:ALA:HB3	2:A:401:OJO:CB	2.36	0.55
1:D:282:ARG:HG3	1:D:283:TYR:CD2	2.41	0.55
1:D:13[B]:LEU:C	1:D:14[B]:SER:HG	1.88	0.55
1:D:234:LYS:HE3	2:D:401:OJO:C4A	2.38	0.54
1:C:361[B]:GLU:OE1	1:C:361[B]:GLU:HA	2.09	0.53
1:C:72:LEU:HD11	1:C:85:LYS:CG	2.39	0.53
1:C:234:LYS:HE3	2:C:401:OJO:C4A	2.38	0.53
1:B:361:GLU:HG2	6:B:1052:HOH:O	2.09	0.52
1:B:301:PHE:CZ	1:B:376:GLU:HG2	2.44	0.52
1:D:374:LEU:HD22	1:D:378:ILE:HD11	1.92	0.52
1:D:5:ASN:HD21	1:D:8:THR:HB	1.76	0.51
1:C:361[B]:GLU:OE1	1:C:361[B]:GLU:CA	2.59	0.50
1:C:72:LEU:HD11	1:C:85:LYS:HG2	1.94	0.49
1:D:35:ALA:HB3	2:D:401:OJO:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:GLN:NE2	6:D:1074:HOH:O	2.45	0.49
1:B:234:LYS:HZ1	2:B:401:OJO:H3	1.75	0.48
1:D:374:LEU:HD22	1:D:378:ILE:CD1	2.42	0.48
1:C:361[A]:GLU:HG2	1:C:362[A]:LEU:HD23	1.95	0.48
1:B:72:LEU:HD12	1:B:88:ILE:HD11	1.96	0.47
1:D:279:THR:HA	1:D:282:ARG:HE	1.80	0.47
1:A:304:GLU:HG3	6:A:1149:HOH:O	2.15	0.46
1:C:354:SER:HB3	1:C:361[B]:GLU:OE1	2.14	0.46
1:C:216:ASN:HD21	1:C:226:ALA:HB3	1.81	0.46
1:A:72:LEU:C	1:A:72:LEU:HD23	2.35	0.46
1:D:301:PHE:CZ	1:D:376[A]:GLU:HG2	2.51	0.46
1:D:132:LYS:NZ	1:D:159:ASN:HD22	2.14	0.45
1:C:314:LYS:HB2	1:C:327:ASP:HB3	1.98	0.45
1:A:42[B]:MET:CE	1:A:236:PHE:CD1	3.00	0.45
1:B:333:LEU:O	1:C:127[A]:ARG:HG2	2.17	0.45
1:C:199:ASP:OD2	2:C:401:OJO:N1	2.51	0.44
1:A:13[A]:LEU:HD22	1:A:24:GLU:HG3	2.00	0.43
1:B:96:PRO:HB3	1:B:266:HIS:CE1	2.54	0.43
1:C:13[A]:LEU:HD22	1:C:24:GLU:HG3	2.01	0.43
1:C:301:PHE:CZ	1:C:376:GLU:HG2	2.54	0.42
1:C:12:ARG:HH12	1:D:55:GLN:HE21	1.67	0.42
1:B:341:LEU:HD12	1:B:345:GLN:HB2	2.01	0.42
1:C:72:LEU:HD23	1:C:83:PHE:CE1	2.55	0.41
1:A:96:PRO:HB3	1:A:266:HIS:CE1	2.55	0.41
1:D:361:GLU:HG2	1:D:362[A]:LEU:HD23	2.03	0.41
1:A:301:PHE:CZ	1:A:376:GLU:HG2	2.56	0.41
1:C:13[A]:LEU:HD22	1:C:24:GLU:CG	2.51	0.41
1:D:233:THR:HB	1:D:239:ALA:HA	2.02	0.41
1:A:13[A]:LEU:O	1:A:14[A]:SER:OG	2.31	0.40
1:A:300:GLN:NE2	6:A:1105:HOH:O	2.46	0.40
1:C:374:LEU:HD22	1:C:378:ILE:CD1	2.51	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	400/392 (102%)	389 (97%)	11 (3%)	0	100	100
1	B	399/392 (102%)	389 (98%)	10 (2%)	0	100	100
1	C	394/392 (100%)	383 (97%)	11 (3%)	0	100	100
1	D	396/392 (101%)	384 (97%)	12 (3%)	0	100	100
All	All	1589/1568 (101%)	1545 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	357/345 (104%)	355 (99%)	2 (1%)	84	78
1	B	356/345 (103%)	353 (99%)	3 (1%)	79	70
1	C	351/345 (102%)	348 (99%)	3 (1%)	75	65
1	D	353/345 (102%)	347 (98%)	6 (2%)	56	38
All	All	1417/1380 (103%)	1403 (99%)	14 (1%)	73	61

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	TYR
1	A	227	LEU
1	B	72	LEU
1	B	164	TYR
1	B	227	LEU
1	C	164	TYR
1	C	227	LEU
1	C	374	LEU
1	D	7	GLN
1	D	12	ARG

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Mol	Chain	Res	Type
1	D	92	GLU
1	D	164	TYR
1	D	227	LEU
1	D	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	261	GLN
1	A	351	ASN
1	B	261	GLN
1	B	298	ASN
1	B	308	GLN
1	B	345	GLN
1	C	16	HIS
1	C	55	GLN
1	C	80	GLN
1	C	103	GLN
1	C	151	GLN
1	C	187	HIS
1	C	190	GLN
1	C	216	ASN
1	C	261	GLN
1	D	47	GLN
1	D	55	GLN
1	D	103	GLN
1	D	130	ASN
1	D	159	ASN
1	D	261	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
3	EPE	A	502	-	15,15,15	0.87	1 (6%)	19,20,20	1.08	2 (10%)
3	EPE	D	502	-	15,15,15	0.76	1 (6%)	19,20,20	1.04	0
2	OJO	A	401	-	20,21,21	2.04	6 (30%)	23,30,30	1.56	5 (21%)
3	EPE	D	501	-	15,15,15	0.69	1 (6%)	19,20,20	0.89	0
2	OJO	D	401	-	20,21,21	1.98	6 (30%)	23,30,30	1.47	4 (17%)
3	EPE	A	503	-	15,15,15	0.81	1 (6%)	19,20,20	1.03	1 (5%)
3	EPE	C	502	-	15,15,15	0.77	1 (6%)	19,20,20	1.05	1 (5%)
3	EPE	A	501	-	15,15,15	0.50	0	19,20,20	1.17	2 (10%)
3	EPE	B	501	-	15,15,15	0.65	1 (6%)	19,20,20	1.02	1 (5%)
3	EPE	B	502	-	15,15,15	0.65	1 (6%)	19,20,20	1.09	3 (15%)
3	EPE	C	501	-	15,15,15	0.61	0	19,20,20	0.93	0
3	EPE	C	503	-	15,15,15	0.77	1 (6%)	19,20,20	1.10	3 (15%)
2	OJO	C	401	-	20,21,21	1.79	6 (30%)	23,30,30	1.51	3 (13%)
5	ACT	C	701	-	3,3,3	0.78	0	3,3,3	1.35	0
3	EPE	D	503	-	15,15,15	1.68	1 (6%)	19,20,20	1.71	2 (10%)
2	OJO	B	401	-	20,21,21	1.96	6 (30%)	23,30,30	1.33	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	502	-	-	0/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	D	502	-	-	1/9/19/19	0/1/1/1
2	OJO	A	401	-	-	4/11/15/15	0/1/1/1
3	EPE	D	501	-	-	0/9/19/19	0/1/1/1
2	OJO	D	401	-	-	5/11/15/15	0/1/1/1
3	EPE	A	503	-	-	1/9/19/19	0/1/1/1
3	EPE	C	502	-	-	2/9/19/19	0/1/1/1
3	EPE	A	501	-	-	0/9/19/19	0/1/1/1
3	EPE	B	501	-	-	0/9/19/19	0/1/1/1
3	EPE	B	502	-	-	1/9/19/19	0/1/1/1
3	EPE	C	501	-	-	0/9/19/19	0/1/1/1
3	EPE	C	503	-	-	1/9/19/19	0/1/1/1
2	OJO	C	401	-	-	5/11/15/15	0/1/1/1
3	EPE	D	503	-	-	1/9/19/19	0/1/1/1
2	OJO	B	401	-	-	5/11/15/15	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	503	EPE	C10-S	6.07	1.86	1.77
2	A	401	OJO	C4A-N	5.02	1.35	1.28
2	D	401	OJO	C4A-N	4.87	1.34	1.28
2	C	401	OJO	C4A-N	4.68	1.34	1.28
2	B	401	OJO	C4A-N	4.06	1.33	1.28
2	B	401	OJO	C2A-C2	3.99	1.56	1.50
2	A	401	OJO	P-OP1	-3.40	1.42	1.54
2	A	401	OJO	P-OP2	-3.07	1.43	1.54
3	A	502	EPE	C10-S	2.98	1.81	1.77
2	A	401	OJO	C4-C4A	2.88	1.52	1.46
2	D	401	OJO	P-OP1	-2.83	1.44	1.54
2	D	401	OJO	P-OP2	-2.82	1.44	1.54
2	B	401	OJO	OXT-C	-2.76	1.23	1.30
3	A	503	EPE	C10-S	2.73	1.81	1.77
3	C	502	EPE	C10-S	2.68	1.81	1.77
2	D	401	OJO	C4-C4A	2.65	1.52	1.46
2	D	401	OJO	OXT-C	-2.56	1.23	1.30
3	D	502	EPE	C10-S	2.53	1.81	1.77
2	B	401	OJO	C4-C4A	2.51	1.52	1.46
3	C	503	EPE	C10-S	2.41	1.81	1.77
2	C	401	OJO	C3-C2	-2.40	1.38	1.41
2	C	401	OJO	C4-C4A	2.38	1.51	1.46
2	B	401	OJO	CA-N	2.38	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	OJO	P-OP2	-2.38	1.46	1.54
3	D	501	EPE	C10-S	2.37	1.80	1.77
3	B	501	EPE	C10-S	2.27	1.80	1.77
2	D	401	OJO	C2A-C2	2.22	1.53	1.50
2	B	401	OJO	C4-C5	-2.21	1.38	1.42
2	C	401	OJO	OXT-C	-2.17	1.24	1.30
2	A	401	OJO	C6-C5	2.17	1.42	1.37
2	A	401	OJO	CA-N	2.11	1.46	1.36
3	B	502	EPE	C10-S	2.11	1.80	1.77
2	C	401	OJO	CA-N	2.04	1.45	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	EPE	O1S-S-C10	5.91	115.66	106.73
2	A	401	OJO	C4-C4A-N	-3.93	113.96	123.01
2	C	401	OJO	C4-C4A-N	-3.81	114.23	123.01
2	D	401	OJO	C4-C4A-N	-3.80	114.25	123.01
2	B	401	OJO	C4-C4A-N	-3.49	114.95	123.01
2	C	401	OJO	C5-C4-C4A	-3.15	116.61	121.47
2	C	401	OJO	C3-C4-C4A	3.07	125.95	120.40
3	B	502	EPE	O2S-S-C10	2.98	111.23	106.73
2	A	401	OJO	C5-C6-N1	-2.72	119.41	123.83
3	A	503	EPE	C5-N4-C3	-2.54	103.36	108.84
3	D	503	EPE	C5-N4-C3	-2.54	103.36	108.84
2	D	401	OJO	C5-C4-C4A	-2.49	117.62	121.47
2	A	401	OJO	C5-C4-C4A	-2.48	117.64	121.47
3	A	501	EPE	O1S-S-C10	2.44	110.41	106.73
2	B	401	OJO	OP2-P-OP1	2.35	116.61	107.80
2	D	401	OJO	C3-C4-C4A	2.30	124.56	120.40
3	A	502	EPE	C2-C3-N4	2.30	115.29	110.65
3	A	501	EPE	O2S-S-O1S	-2.26	106.48	113.82
3	C	502	EPE	C8-C7-N4	2.24	121.31	113.44
3	B	501	EPE	C5-N4-C3	-2.16	104.19	108.84
3	B	502	EPE	C5-N4-C3	-2.15	104.21	108.84
3	A	502	EPE	C7-N4-C5	-2.15	105.51	111.24
3	C	503	EPE	C5-N4-C3	-2.15	104.21	108.84
3	C	503	EPE	C7-N4-C5	-2.14	105.54	111.24
2	A	401	OJO	C3-C4-C4A	2.12	124.23	120.40
2	A	401	OJO	C6-N1-C2	2.10	123.00	119.20
3	B	502	EPE	C7-N4-C5	-2.10	105.65	111.24
3	C	503	EPE	C2-C3-N4	2.07	114.82	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	OJO	OP2-P-OP1	2.04	115.44	107.80
2	B	401	OJO	C3-C4-C4A	2.01	124.03	120.40

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	OJO	C5A-OP4-P-OP3
2	A	401	OJO	C5A-OP4-P-OP1
2	A	401	OJO	C5A-OP4-P-OP2
2	B	401	OJO	C4-C4A-N-CA
2	B	401	OJO	C5A-OP4-P-OP3
2	B	401	OJO	C5A-OP4-P-OP1
2	B	401	OJO	C5A-OP4-P-OP2
2	C	401	OJO	C5A-OP4-P-OP3
2	C	401	OJO	C5A-OP4-P-OP1
2	C	401	OJO	C5A-OP4-P-OP2
2	D	401	OJO	C5A-OP4-P-OP3
2	D	401	OJO	C5A-OP4-P-OP1
2	D	401	OJO	C5A-OP4-P-OP2
3	C	502	EPE	C8-C7-N4-C5
2	D	401	OJO	C4-C4A-N-CA
3	D	502	EPE	N4-C7-C8-O8
2	C	401	OJO	C4-C4A-N-CA
2	A	401	OJO	C3-C4-C4A-N
2	B	401	OJO	C3-C4-C4A-N
2	D	401	OJO	C3-C4-C4A-N
3	B	502	EPE	C8-C7-N4-C3
2	C	401	OJO	C3-C4-C4A-N
3	A	503	EPE	C8-C7-N4-C5
3	D	503	EPE	C8-C7-N4-C5
3	C	503	EPE	N4-C7-C8-O8
3	C	502	EPE	C8-C7-N4-C3

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	OJO	6	0
2	D	401	OJO	6	0
2	C	401	OJO	8	0

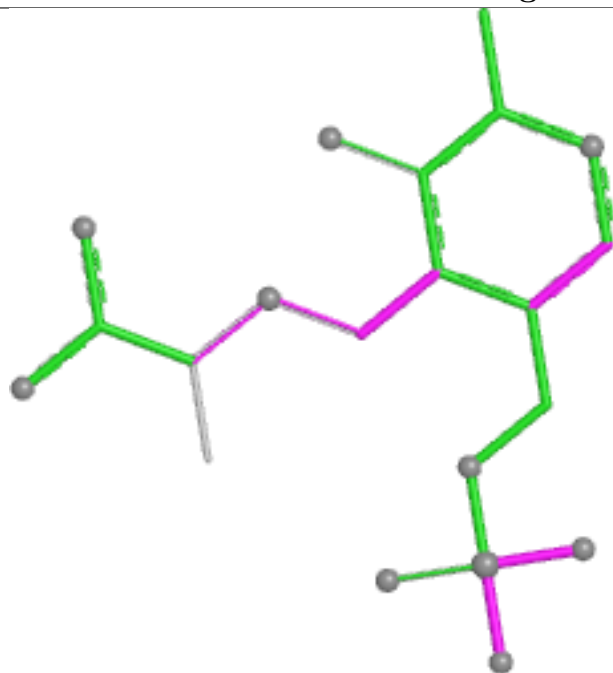
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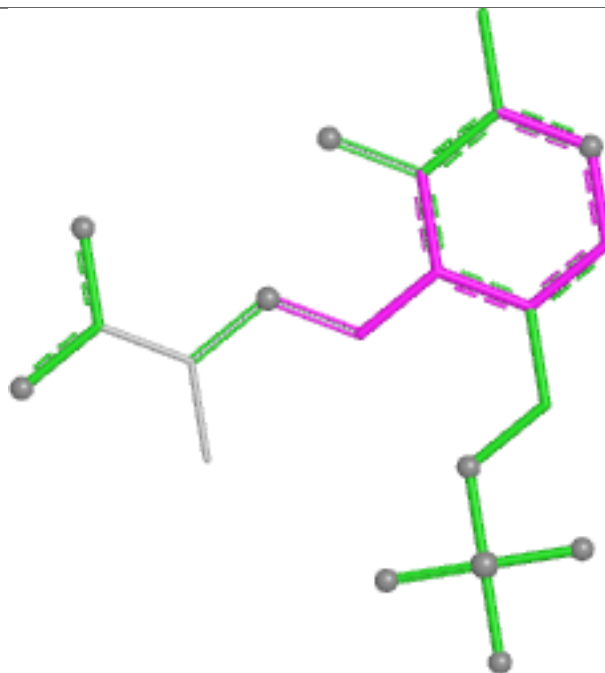
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	OJO	6	0

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.

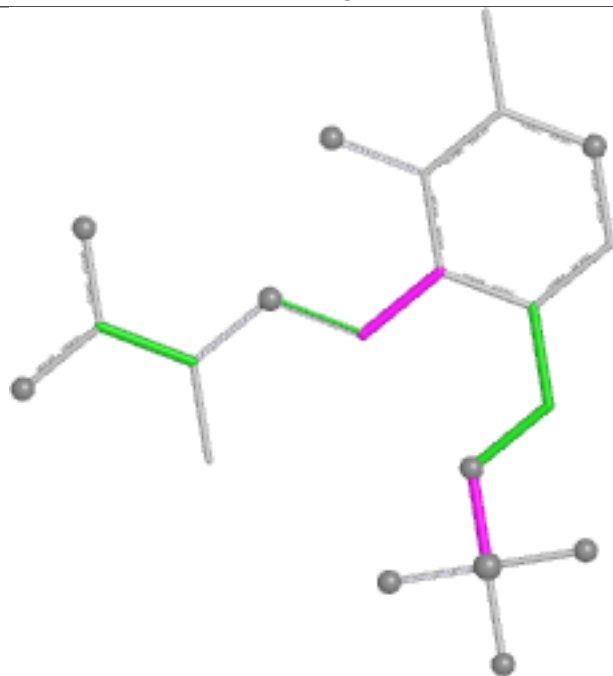
Ligand 0JO A 401



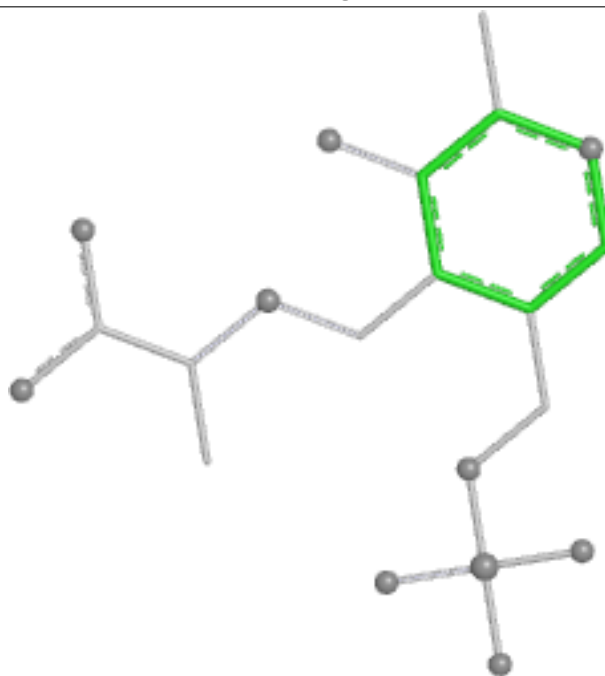
Bond lengths



Bond angles

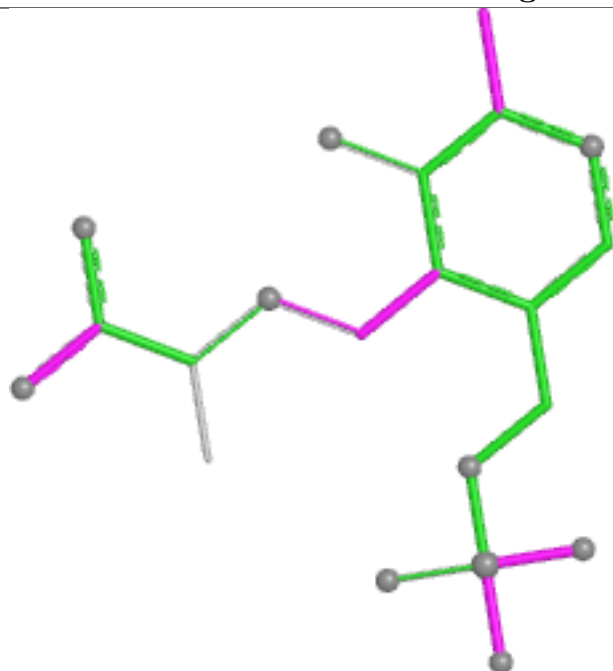


Torsions

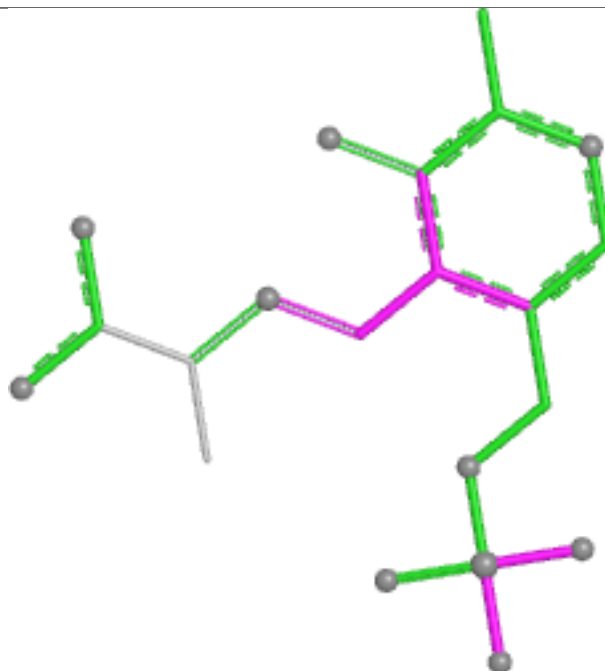


Rings

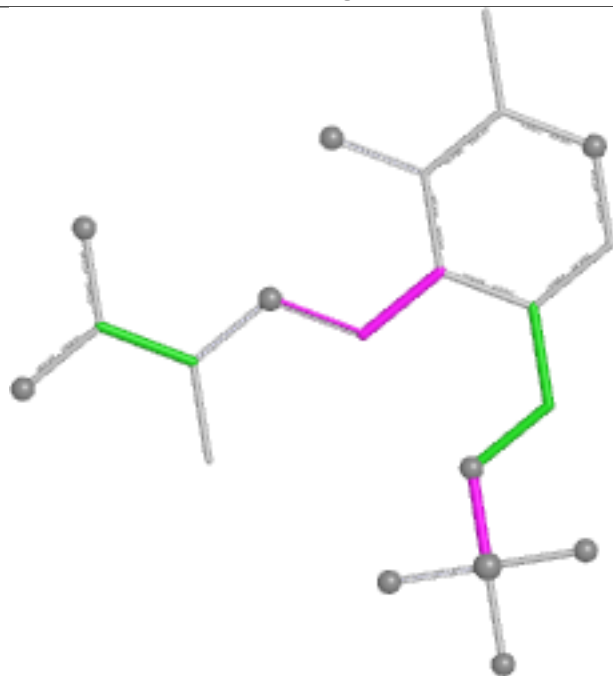
Ligand 0JO D 401



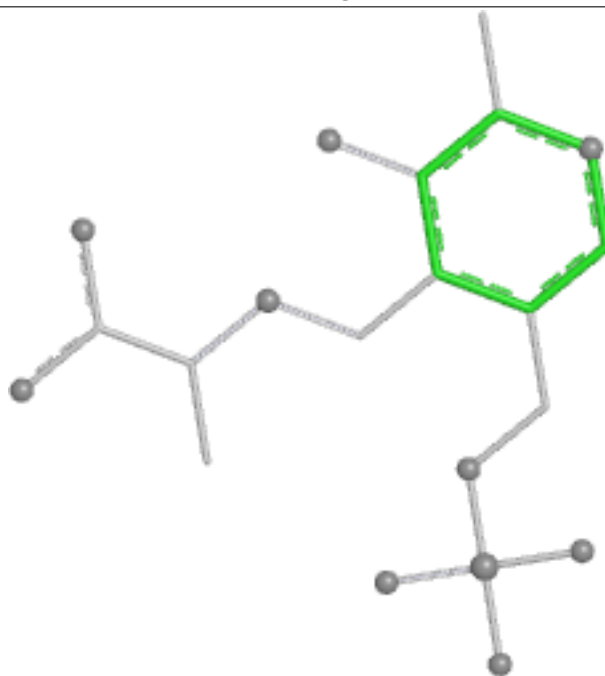
Bond lengths



Bond angles

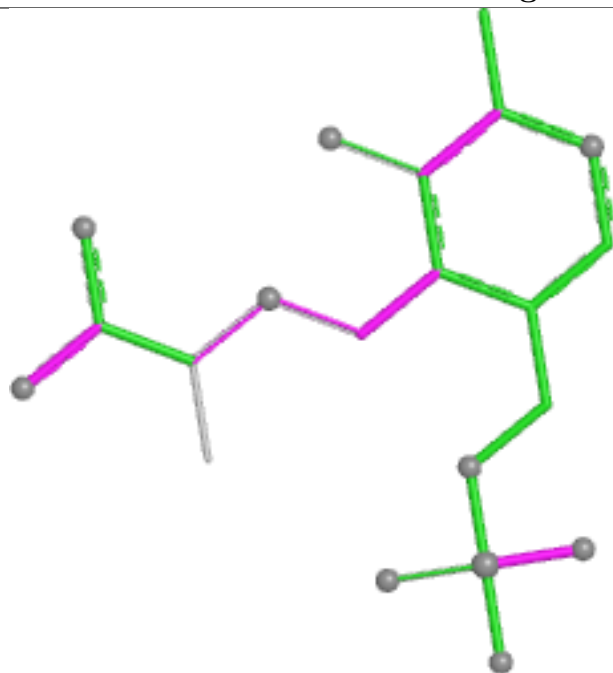


Torsions

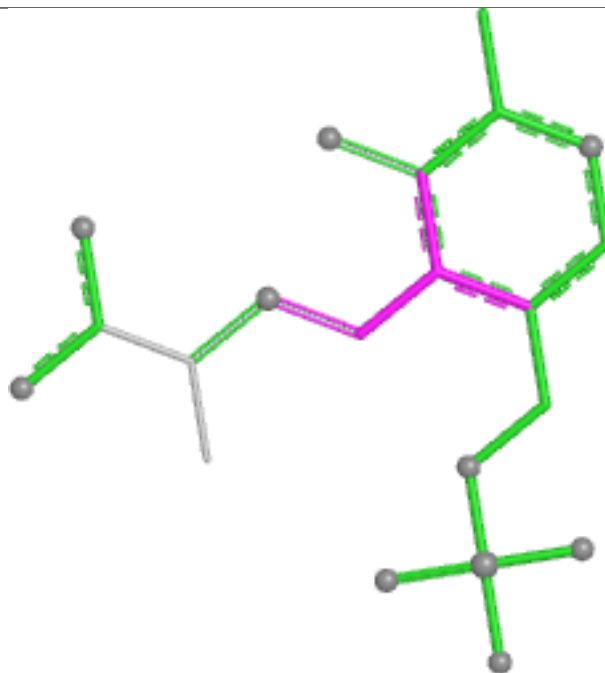


Rings

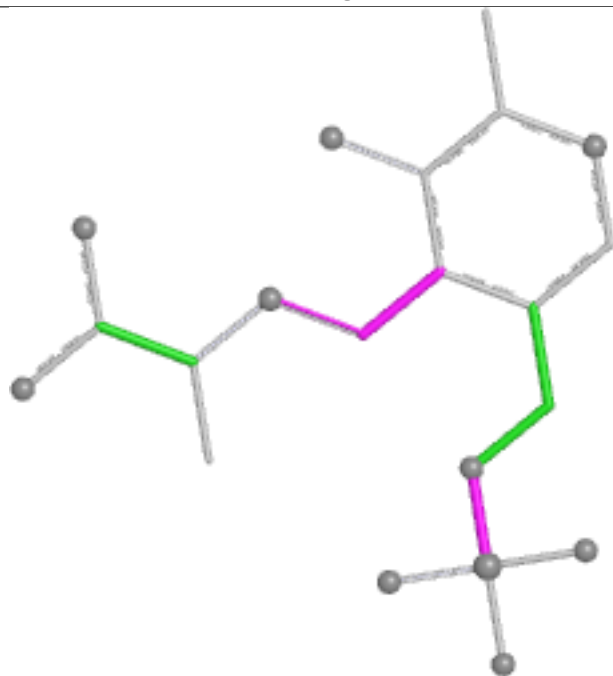
Ligand 0JO C 401



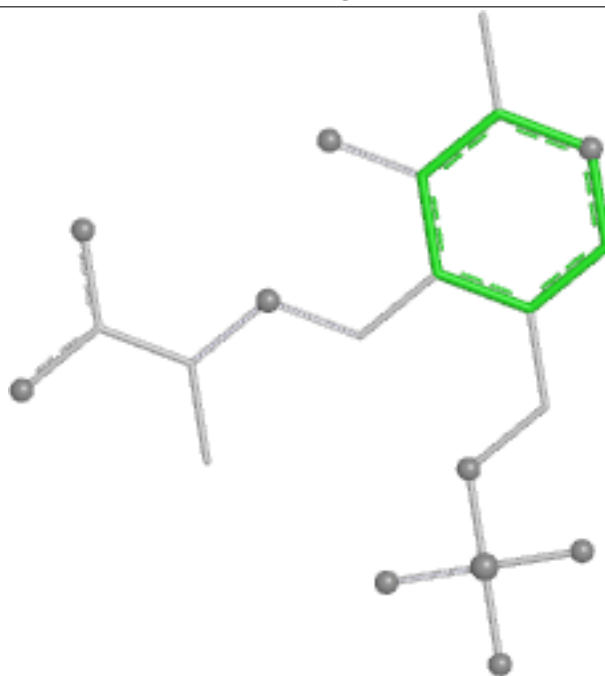
Bond lengths



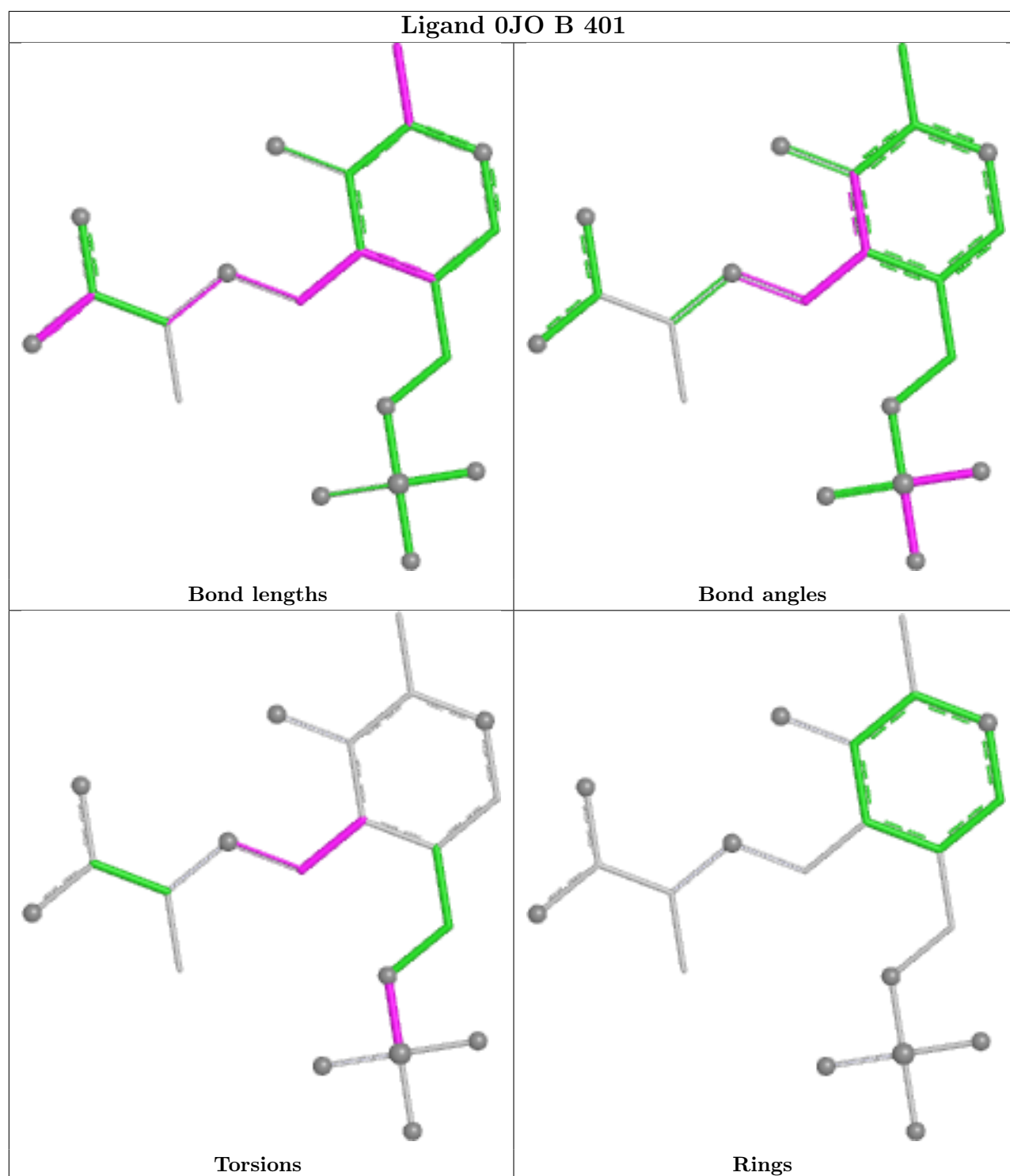
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/392 (98%)	-0.52	3 (0%) 82 87	3, 8, 17, 29	15 (3%)
1	B	387/392 (98%)	-0.48	3 (0%) 82 87	4, 9, 17, 30	14 (3%)
1	C	385/392 (98%)	-0.33	2 (0%) 87 91	5, 11, 20, 28	11 (2%)
1	D	385/392 (98%)	-0.37	4 (1%) 79 84	4, 10, 20, 28	13 (3%)
All	All	1544/1568 (98%)	-0.43	12 (0%) 82 87	3, 10, 19, 30	53 (3%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13[A]	LEU	3.8
1	D	282	ARG	3.1
1	B	2	SER	2.9
1	A	308	GLN	2.6
1	B	25	THR	2.6
1	A	2	SER	2.4
1	D	384	CYS	2.2
1	C	384	CYS	2.2
1	D	11	ASN	2.1
1	B	3	LYS	2.1
1	A	384	CYS	2.1
1	C	300	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

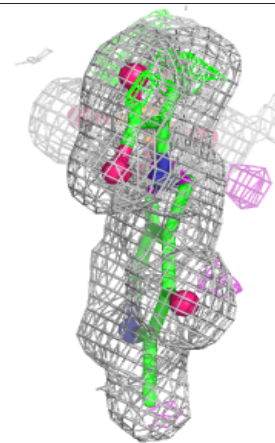
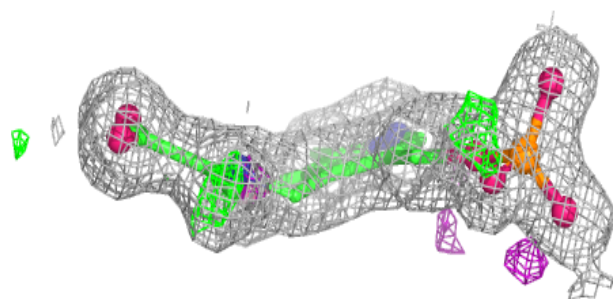
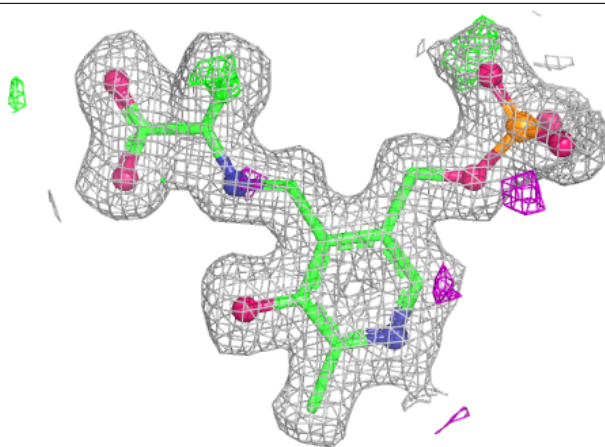
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	C	701	4/4	0.82	0.16	30,31,31,31	0
3	EPE	A	503	15/15	0.86	0.15	31,40,47,48	0
3	EPE	D	503	15/15	0.90	0.15	38,41,46,47	11
3	EPE	B	502	15/15	0.90	0.13	26,33,40,42	0
3	EPE	A	502	15/15	0.93	0.12	20,25,32,32	0
3	EPE	C	503	15/15	0.93	0.12	21,27,35,36	0
3	EPE	D	502	15/15	0.95	0.11	16,25,35,37	0
3	EPE	C	502	15/15	0.95	0.10	16,23,34,37	0
3	EPE	D	501	15/15	0.95	0.07	12,13,26,26	0
4	NA	C	601	1/1	0.96	0.07	20,20,20,20	0
3	EPE	C	501	15/15	0.96	0.06	8,10,21,22	0
2	OJO	C	401	21/21	0.97	0.05	5,8,10,12	0
3	EPE	A	501	15/15	0.97	0.06	9,10,22,24	0
3	EPE	B	501	15/15	0.97	0.06	9,11,21,23	0
2	OJO	A	401	21/21	0.98	0.04	3,7,9,10	0
4	NA	B	601	1/1	0.98	0.07	18,18,18,18	0
2	OJO	D	401	21/21	0.98	0.04	5,7,10,11	0
2	OJO	B	401	21/21	0.98	0.05	5,6,9,11	0
4	NA	D	601	1/1	0.99	0.08	16,16,16,16	0
4	NA	A	601	1/1	0.99	0.05	15,15,15,15	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.

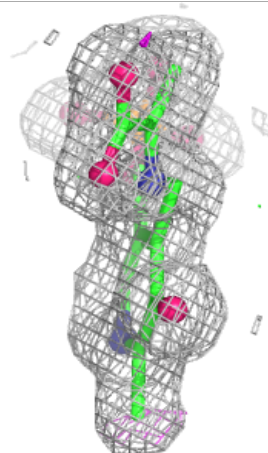
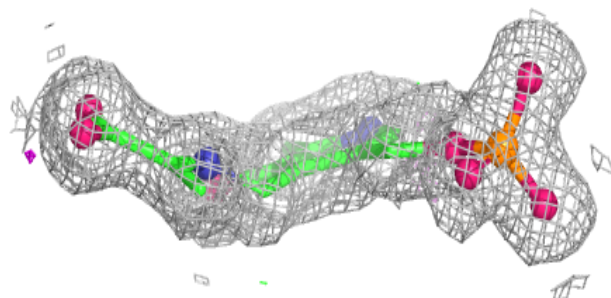
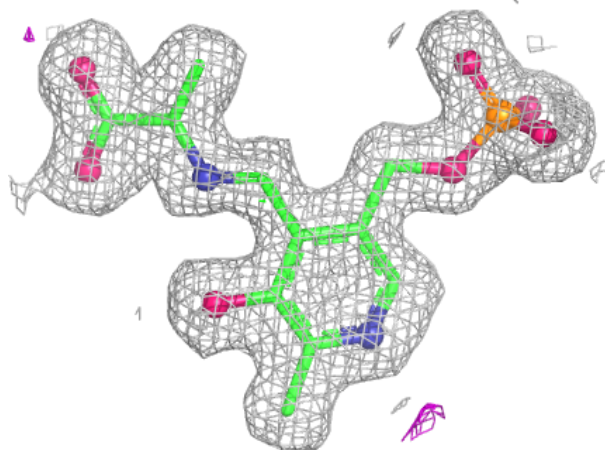
Electron density around 0JO C 401:

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



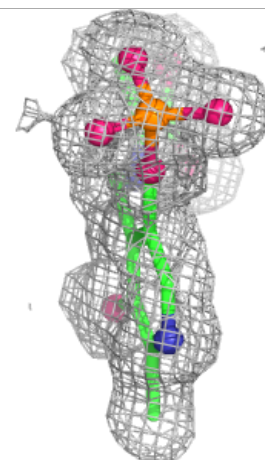
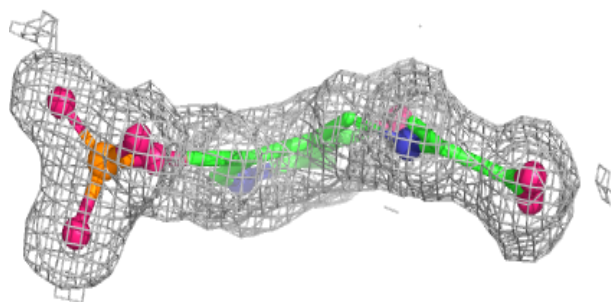
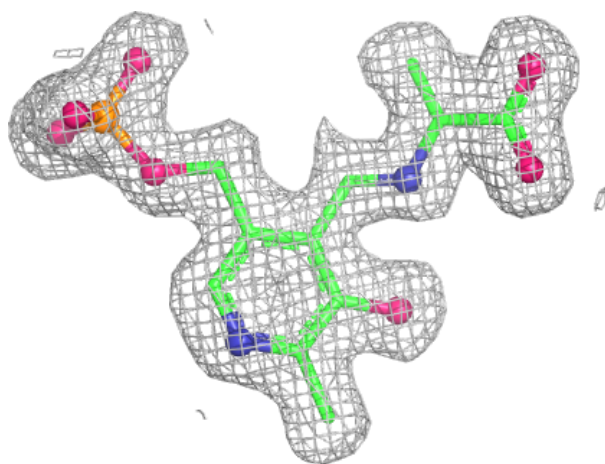
Electron density around 0JO A 401:

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



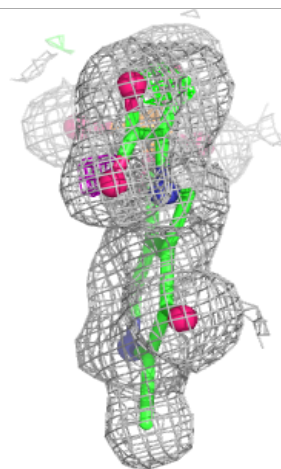
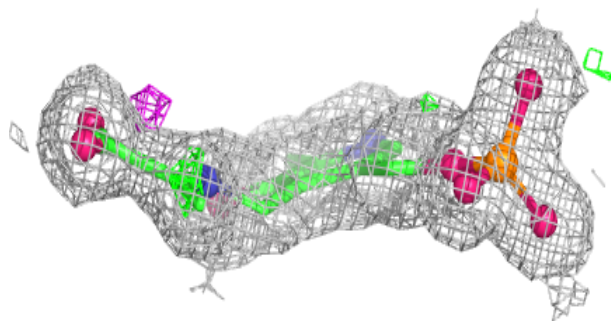
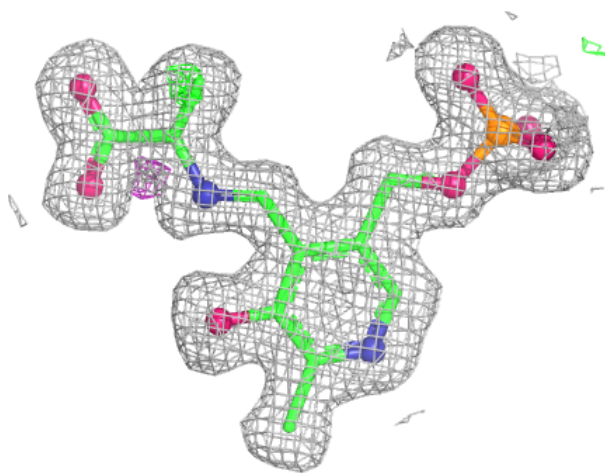
Electron density around 0JO D 401:

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



Electron density around 0JO B 401:

$2mF_o-DF_c$ (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.