



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:13 PM UTC

PDB ID : 4LUT / pdb_00004lut
Title : alanine racemase [Clostridium difficile 630] complex with cycloserine
Authors : Asojo, O.A.
Deposited on : 2013-07-25
Resolution : 2.26 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

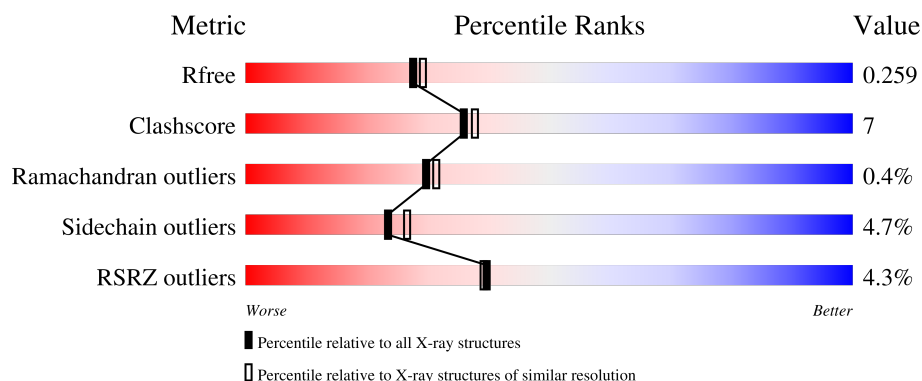
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	385	5% 77% 17% • • •
2	B	385	3% 81% 12% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6061 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.

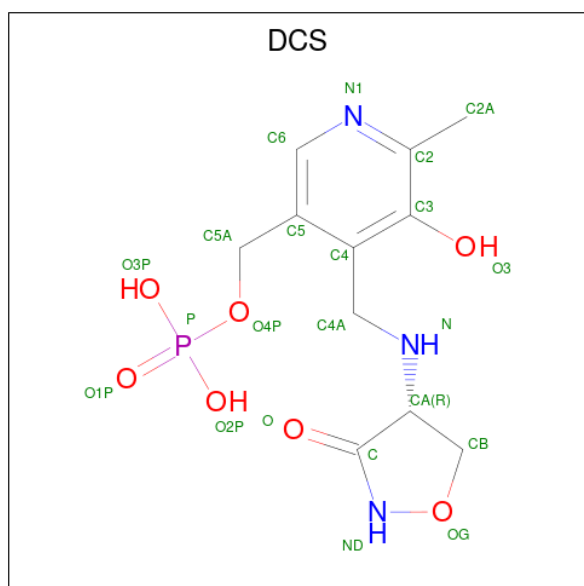
- Molecule 1 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2963	1886	493	569	15			

- Molecule 2 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	0	0
			2883	1830	483	554	16			

- Molecule 3 is D-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (CCD ID: DCS) (formula: $C_{11}H_{16}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
3	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

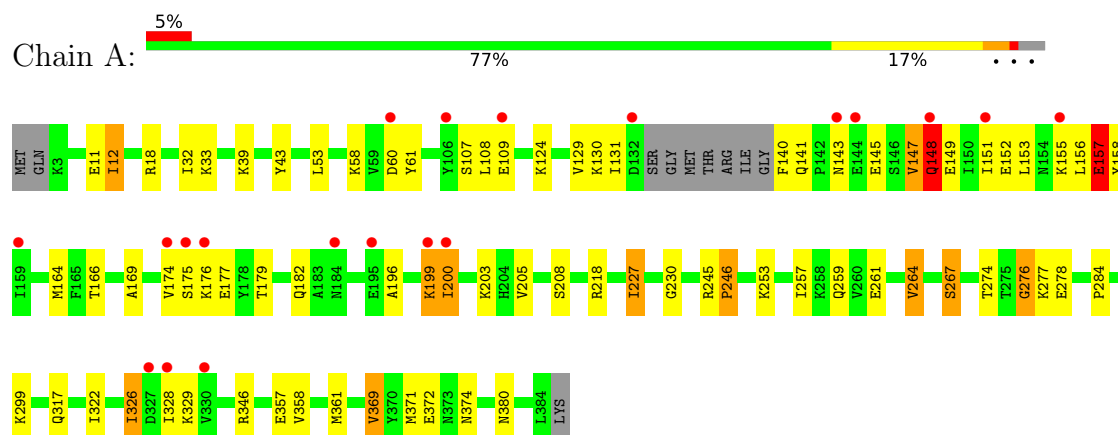
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total 82	O 82	0	0
4	B	89	Total 89	O 89	0	0

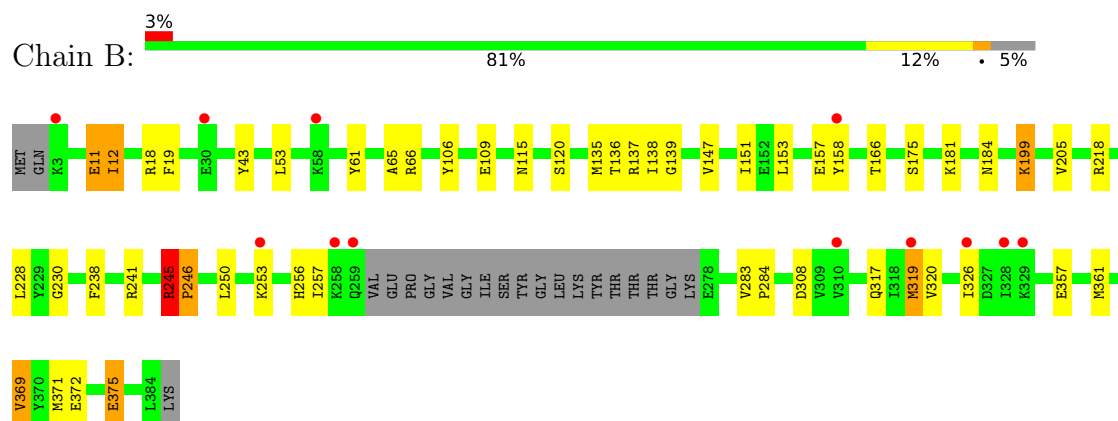
3 Residue-property plots [i](#)

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

• Molecule 1: Alanine racemase



• Molecule 2: Alanine racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.84Å 138.97Å 144.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.62 – 2.26 45.62 – 2.26	Depositor EDS
% Data completeness (in resolution range)	64.0 (45.62-2.26) 64.0 (45.62-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.210 , 0.248 0.224 , 0.259	Depositor DCC
R_{free} test set	1785 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6061	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.77	5/3005 (0.2%)	0.94	9/4054 (0.2%)
2	B	0.80	8/2909 (0.3%)	0.84	3/3921 (0.1%)
All	All	0.79	13/5914 (0.2%)	0.89	12/7975 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	ILE	C-O	-6.11	1.16	1.24
2	B	283	VAL	C-O	-5.95	1.18	1.23
1	A	246	PRO	C-O	-5.79	1.17	1.23
1	A	245	ARG	C-N	5.72	1.41	1.33
2	B	256	HIS	CG-ND1	-5.69	1.31	1.38
2	B	11	GLU	C-O	-5.65	1.17	1.24
2	B	250	LEU	C-O	-5.63	1.17	1.24
2	B	245	ARG	C-N	5.23	1.40	1.33
2	B	375	GLU	C-O	-5.22	1.17	1.24
2	B	246	PRO	C-O	-5.15	1.17	1.23
2	B	246	PRO	N-CD	5.04	1.54	1.47
1	A	148	GLN	C-O	-5.01	1.18	1.24
1	A	246	PRO	N-CD	5.00	1.54	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LYS	N-CA-C	13.75	125.99	111.14
1	A	157	GLU	N-CA-C	11.44	135.16	110.80
1	A	158	TYR	N-CA-CB	-11.32	94.72	111.25
1	A	158	TYR	N-CA-C	-7.04	100.97	111.81
1	A	245	ARG	CA-C-N	-6.29	113.28	119.76
1	A	245	ARG	C-N-CA	-6.29	113.28	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ILE	N-CA-C	6.25	122.33	109.34
2	B	139	GLY	N-CA-C	6.03	117.68	111.95
2	B	245	ARG	CA-C-N	-5.94	113.64	119.76
2	B	245	ARG	C-N-CA	-5.94	113.64	119.76
1	A	276	GLY	N-CA-C	-5.84	102.92	110.69
1	A	147	VAL	CB-CA-C	-5.05	105.32	112.14

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	2963	0	3022	65	0
2	B	2883	0	2936	24	0
3	A	22	0	13	2	0
3	B	22	0	14	0	0
4	A	82	0	0	4	0
4	B	89	0	0	1	0
All	All	6061	0	5985	87	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 7.

All (87) 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:326:ILE:HD12	1:A:328:ILE:CG2	2.09	0.82
1:A:33:LYS:HA	1:A:60:ASP:OD2	1.80	0.81
1:A:33:LYS:CA	1:A:60:ASP:OD2	2.34	0.75
1:A:326:ILE:HD12	1:A:328:ILE:HG23	1.67	0.75
1:A:33:LYS:CB	1:A:60:ASP:OD2	2.40	0.69
2:B:147:VAL:O	2:B:151:ILE:HD12	1.93	0.68
1:A:148:GLN:O	1:A:151:ILE:HG13	1.96	0.66
2:B:115:ASN:OD1	2:B:157:GLU:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:HG21	1:A:203:LYS:HE3	1.78	0.65
1:A:200:ILE:CG2	1:A:203:LYS:HG2	2.27	0.65
1:A:274:THR:CG2	1:A:276:GLY:O	2.46	0.64
1:A:267:SER:HA	2:B:135:MET:HE3	1.80	0.64
1:A:169:ALA:H	1:A:182:GLN:HE22	1.47	0.63
1:A:176:LYS:HA	4:A:519:HOH:O	1.97	0.63
2:B:369:VAL:HG23	2:B:371:MET:HE2	1.83	0.60
1:A:131:ILE:HD11	1:A:164:MET:SD	2.41	0.60
1:A:176:LYS:O	1:A:179:THR:N	2.35	0.60
1:A:176:LYS:O	1:A:177:GLU:C	2.44	0.60
1:A:369:VAL:HG23	1:A:371:MET:HE2	1.85	0.59
1:A:200:ILE:CG2	1:A:203:LYS:HE3	2.33	0.57
1:A:39:LYS:CE	3:A:401:DCS:H4A1	2.34	0.57
1:A:274:THR:HG22	1:A:276:GLY:O	2.03	0.57
1:A:200:ILE:HG22	1:A:203:LYS:HG2	1.88	0.56
2:B:18:ARG:NH2	2:B:372:GLU:OE2	2.38	0.56
1:A:257:ILE:HD11	1:A:328:ILE:HD11	1.88	0.56
1:A:322:ILE:HG13	1:A:328:ILE:CD1	2.35	0.56
1:A:33:LYS:HG2	1:A:60:ASP:CG	2.32	0.55
1:A:200:ILE:HG22	1:A:200:ILE:O	2.07	0.54
1:A:155:LYS:O	1:A:156:LEU:C	2.51	0.54
1:A:107:SER:OG	1:A:109:GLU:HG2	2.08	0.53
1:A:257:ILE:CD1	1:A:328:ILE:CD1	2.86	0.53
1:A:358:VAL:HA	1:A:361:MET:HE2	1.91	0.53
1:A:200:ILE:HG21	1:A:203:LYS:HG2	1.91	0.53
2:B:19:PHE:CD1	2:B:245:ARG:HG3	2.44	0.52
1:A:129:VAL:HG13	1:A:140:PHE:CD2	2.44	0.52
2:B:106:TYR:CD1	2:B:138:ILE:HG23	2.45	0.51
1:A:33:LYS:HB3	1:A:60:ASP:OD2	2.08	0.51
1:A:166:THR:HG22	1:A:205:VAL:HG12	1.93	0.51
1:A:259:GLN:HG2	1:A:277:LYS:HE2	1.93	0.50
1:A:200:ILE:CB	1:A:203:LYS:HE3	2.41	0.50
1:A:317:GLN:HG3	2:B:137:ARG:HD2	1.92	0.50
1:A:253:LYS:O	1:A:284:PRO:HD2	2.12	0.49
2:B:166:THR:HG22	2:B:205:VAL:HG12	1.93	0.49
1:A:299:LYS:HD2	1:A:346:ARG:NH2	2.27	0.49
1:A:357:GLU:O	1:A:361:MET:HG3	2.12	0.49
2:B:317:GLN:NE2	2:B:319:MET:HE1	2.28	0.48
1:A:108:LEU:HD21	1:A:152:GLU:HG2	1.96	0.48
2:B:11:GLU:C	2:B:12:ILE:HD12	2.39	0.48
1:A:230:GLY:HA3	1:A:246:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:HD12	1:A:328:ILE:HD12	1.96	0.47
1:A:274:THR:HG23	1:A:278:GLU:CD	2.39	0.47
1:A:261:GLU:O	1:A:264:VAL:HG13	2.14	0.47
2:B:253:LYS:O	2:B:284:PRO:HD2	2.15	0.47
2:B:357:GLU:O	2:B:361:MET:HG3	2.14	0.47
1:A:147:VAL:O	1:A:151:ILE:HG23	2.15	0.47
2:B:184:ASN:HD22	2:B:184:ASN:HA	1.60	0.47
1:A:200:ILE:HB	1:A:203:LYS:HE3	1.96	0.46
2:B:106:TYR:CZ	2:B:138:ILE:HD12	2.50	0.46
1:A:143:ASN:O	1:A:147:VAL:HG23	2.17	0.45
2:B:308:ASP:O	2:B:320:VAL:HG13	2.17	0.45
1:A:11:GLU:C	1:A:12:ILE:HD13	2.42	0.44
2:B:53:LEU:C	2:B:53:LEU:HD23	2.42	0.44
2:B:369:VAL:CG2	2:B:371:MET:HE2	2.47	0.43
1:A:124:LYS:NZ	1:A:157:GLU:O	2.51	0.43
1:A:374:ASN:HB2	4:A:534:HOH:O	2.18	0.43
2:B:199:LYS:HB2	2:B:199:LYS:HE3	1.86	0.43
1:A:326:ILE:HD12	1:A:328:ILE:HG21	1.98	0.43
1:A:157:GLU:HG2	4:A:573:HOH:O	2.17	0.43
1:A:18:ARG:NH2	1:A:372:GLU:OE1	2.48	0.43
1:A:369:VAL:CG2	1:A:371:MET:HE2	2.49	0.42
1:A:257:ILE:HD11	1:A:328:ILE:CD1	2.49	0.42
2:B:65:ALA:C	2:B:66:ARG:HG2	2.45	0.42
2:B:230:GLY:HA3	2:B:246:PRO:HA	2.01	0.42
1:A:208:SER:HB3	1:A:227:ILE:HG23	2.01	0.42
1:A:53:LEU:C	1:A:53:LEU:HD23	2.44	0.42
2:B:238:PHE:HB3	2:B:241:ARG:HG3	2.01	0.42
1:A:39:LYS:NZ	3:A:401:DCS:H4A1	2.35	0.41
1:A:259:GLN:HG2	1:A:277:LYS:CE	2.51	0.41
1:A:32:ILE:HD13	1:A:218:ARG:HB3	2.02	0.41
1:A:174:VAL:HG13	1:A:175:SER:N	2.35	0.41
1:A:322:ILE:HG13	1:A:328:ILE:HD13	2.03	0.41
1:A:380:ASN:ND2	4:A:529:HOH:O	2.54	0.41
1:A:257:ILE:HD12	1:A:328:ILE:CD1	2.49	0.41
1:A:145:GLU:O	1:A:149:GLU:HG3	2.22	0.40
1:A:200:ILE:HD12	1:A:203:LYS:HE3	2.03	0.40
2:B:157:GLU:O	2:B:158:TYR:HB2	2.21	0.40
2:B:218:ARG:NH2	4:B:527:HOH:O	2.54	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	371/385 (96%)	354 (95%)	14 (4%)	3 (1%)	16	14
2	B	359/385 (93%)	347 (97%)	12 (3%)	0	100	100
All	All	730/770 (95%)	701 (96%)	26 (4%)	3 (0%)	30	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	GLU
1	A	196	ALA
1	A	58	LYS

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	326/334 (98%)	313 (96%)	13 (4%)	28	34
2	B	316/333 (95%)	299 (95%)	17 (5%)	20	21
All	All	642/667 (96%)	612 (95%)	30 (5%)	23	26

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	43	TYR
1	A	61	TYR

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Mol	Chain	Res	Type
1	A	130	LYS
1	A	141	GLN
1	A	148	GLN
1	A	153	LEU
1	A	199	LYS
1	A	264	VAL
1	A	267	SER
1	A	326	ILE
1	A	329	LYS
1	A	369	VAL
2	B	12	ILE
2	B	43	TYR
2	B	61	TYR
2	B	109	GLU
2	B	120	SER
2	B	136	THR
2	B	153	LEU
2	B	175	SER
2	B	181	LYS
2	B	199	LYS
2	B	228	LEU
2	B	245	ARG
2	B	257	ILE
2	B	319	MET
2	B	326	ILE
2	B	369	VAL
2	B	375	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	75	GLN
1	A	141	GLN
1	A	154	ASN
1	A	182	GLN
1	A	374	ASN
1	A	380	ASN
2	B	115	ASN
2	B	184	ASN
2	B	256	HIS
2	B	317	GLN

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Mol	Chain	Res	Type
2	B	374	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	KCX	B	130	2	10,11,12	0.60	0	6,12,14	0.32	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
2	KCX	B	130	2	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	130	KCX	N-CA-CB-CG
2	B	130	KCX	C-CA-CB-CG
2	B	130	KCX	CG-CD-CE-NZ
2	B	130	KCX	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DCS	A	401	-	22,23,23	2.86	3 (13%)	27,33,33	1.97	8 (29%)
3	DCS	B	401	-	22,23,23	2.89	4 (18%)	27,33,33	2.23	9 (33%)

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	DCS	A	401	-	-	2/11/21/21	0/2/2/2
3	DCS	B	401	-	-	2/11/21/21	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	DCS	C3-C2	8.47	1.49	1.41
3	B	401	DCS	C3-C2	8.03	1.49	1.41
3	B	401	DCS	C3-C4	7.00	1.50	1.40
3	A	401	DCS	C5-C4	7.00	1.50	1.40
3	A	401	DCS	C3-C4	6.98	1.50	1.40
3	B	401	DCS	C5-C4	5.88	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	DCS	CA-C	-5.45	1.48	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	DCS	O-C-CA	-6.61	121.44	126.19
3	B	401	DCS	C4A-C4-C3	4.30	125.70	119.98
3	A	401	DCS	C3-C4-C5	-4.12	115.00	118.73
3	A	401	DCS	C4A-N-CA	4.07	121.47	113.84
3	A	401	DCS	C4A-C4-C3	3.73	124.94	119.98
3	A	401	DCS	C6-C5-C4	3.66	120.83	118.06
3	B	401	DCS	CA-C-ND	3.43	109.74	107.63
3	B	401	DCS	C4A-N-CA	3.16	119.77	113.84
3	A	401	DCS	CA-C-ND	3.07	109.52	107.63
3	A	401	DCS	O-C-CA	-2.64	124.29	126.19
3	B	401	DCS	C6-N1-C2	2.55	123.82	119.20
3	B	401	DCS	O-C-ND	2.51	128.81	125.73
3	A	401	DCS	CB-OG-ND	2.37	110.04	105.92
3	A	401	DCS	C6-N1-C2	2.35	123.47	119.20
3	B	401	DCS	CB-OG-ND	2.34	109.99	105.92
3	B	401	DCS	C3-C4-C5	-2.30	116.64	118.73
3	B	401	DCS	O3P-P-O2P	2.11	115.71	107.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	DCS	C5-C4-C4A-N
3	A	401	DCS	C5-C4-C4A-N
3	A	401	DCS	C3-C4-C4A-N
3	B	401	DCS	C3-C4-C4A-N

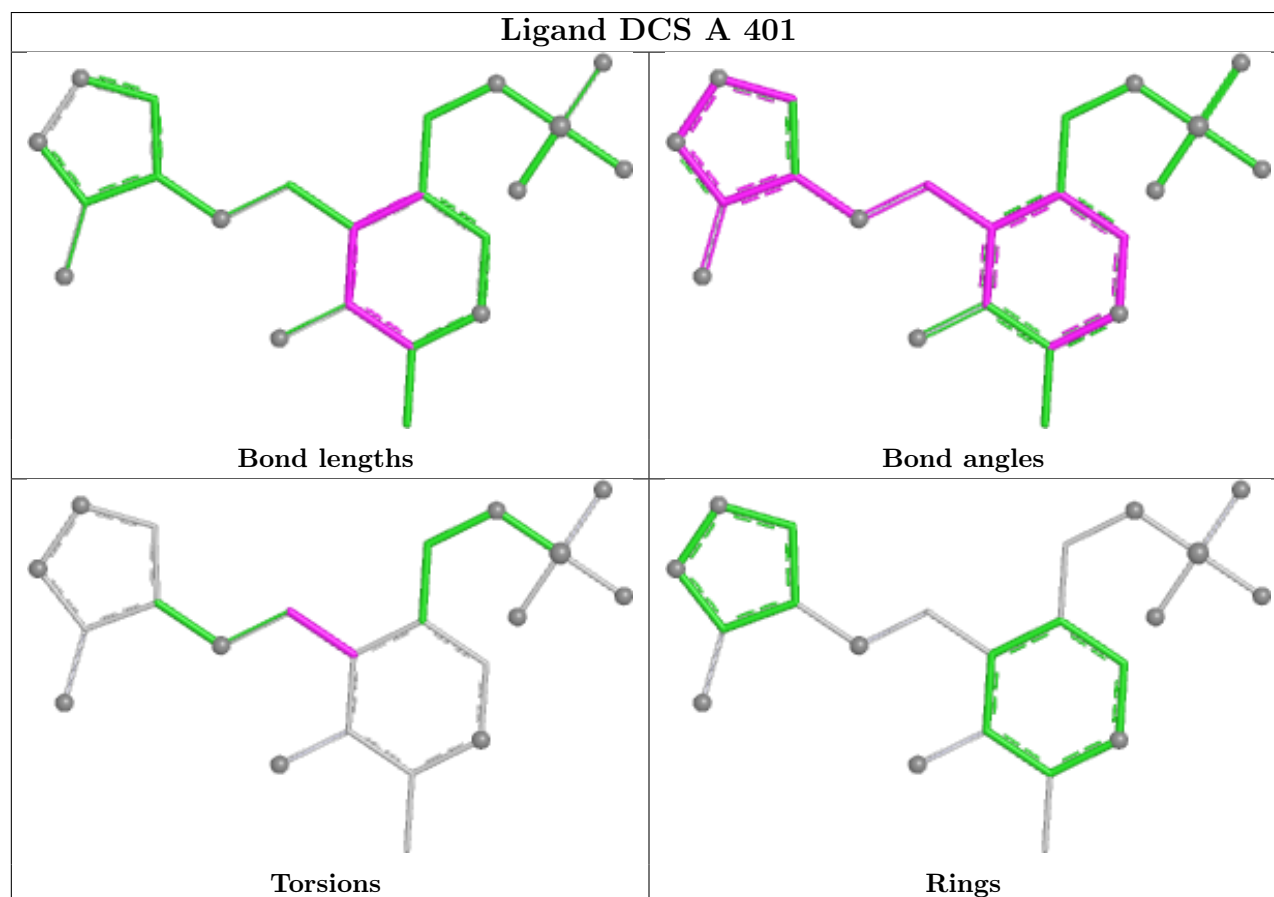
There are no ring outliers.

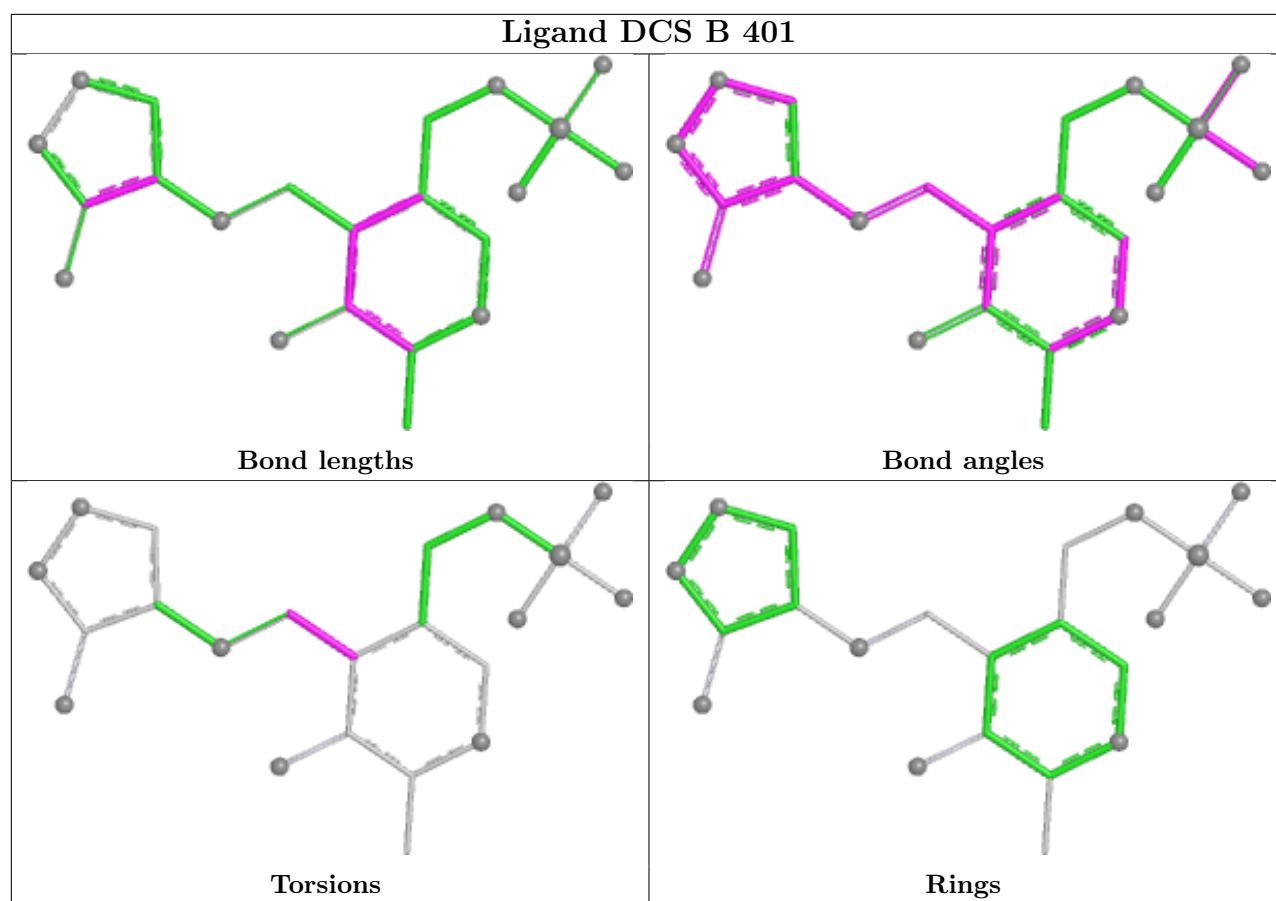
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	DCS	2	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	375/385 (97%)	0.29	20 (5%) 32 30	16, 30, 56, 72	0
2	B	363/385 (94%)	0.20	12 (3%) 49 49	16, 32, 52, 74	0
All	All	738/770 (95%)	0.24	32 (4%) 40 39	16, 31, 55, 74	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	ILE	4.3
1	A	199	LYS	3.8
1	A	106	TYR	3.7
1	A	174	VAL	3.4
2	B	259	GLN	3.3
1	A	60	ASP	3.2
1	A	132	ASP	3.1
1	A	148	GLN	3.1
2	B	58	LYS	3.0
1	A	109	GLU	2.9
1	A	328	ILE	2.8
2	B	258	LYS	2.8
2	B	319	MET	2.6
1	A	184	ASN	2.6
1	A	327	ASP	2.6
2	B	328	ILE	2.6
2	B	3	LYS	2.6
1	A	195	GLU	2.5
1	A	155	LYS	2.4
2	B	326	ILE	2.4
2	B	329	LYS	2.4
1	A	176	LYS	2.3
1	A	151	ILE	2.3
1	A	330	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	158	TYR	2.1
1	A	143	ASN	2.1
1	A	144	GLU	2.1
2	B	310	VAL	2.1
1	A	175	SER	2.1
1	A	159	ILE	2.1
2	B	253	LYS	2.0
2	B	30	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KCX	B	130	12/13	0.90	0.12	29,33,40,60	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

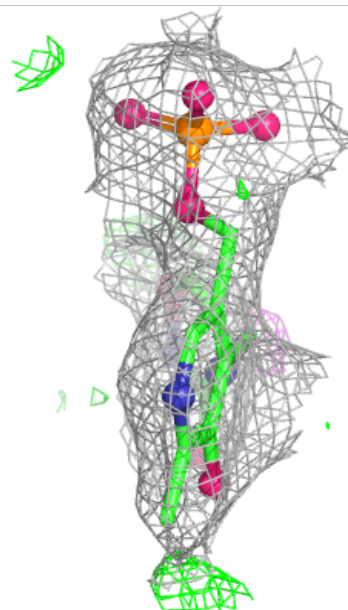
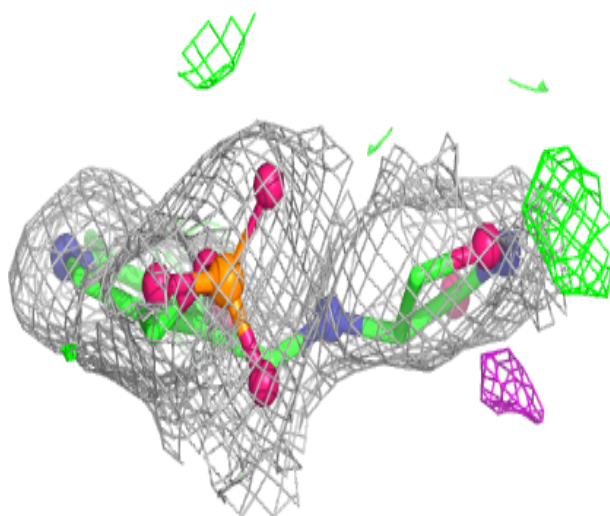
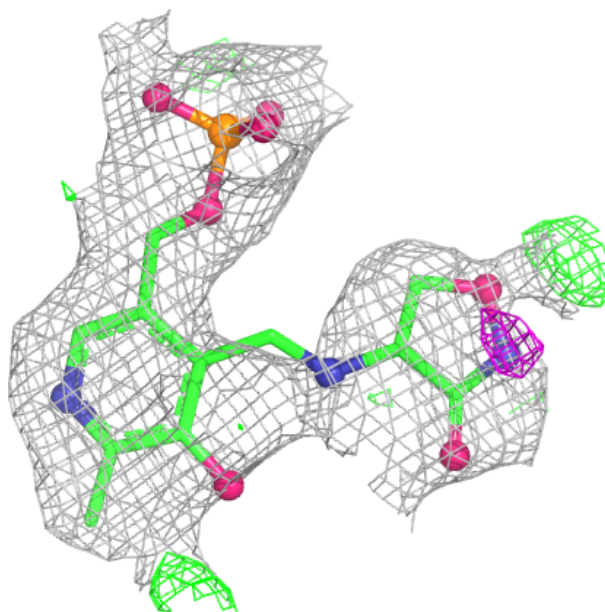
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DCS	A	401	22/22	0.96	0.11	19,38,60,65	0
3	DCS	B	401	22/22	0.97	0.07	17,24,43,57	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.

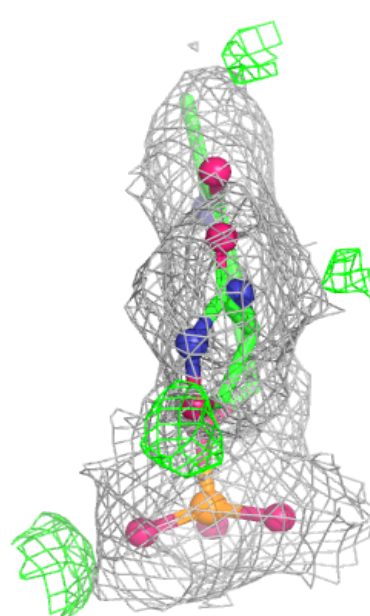
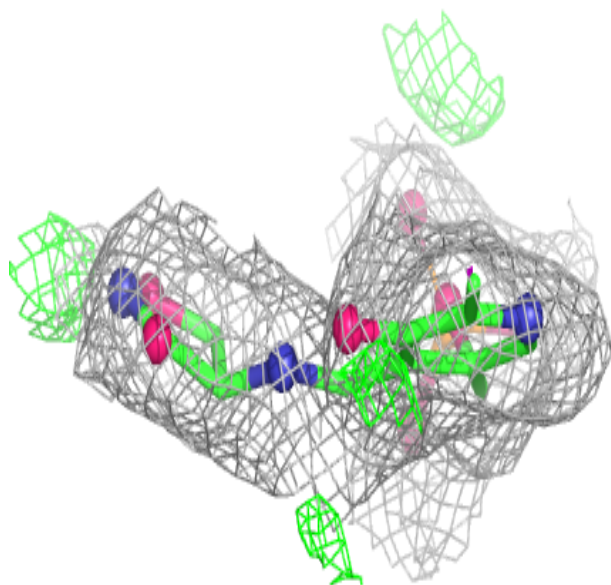
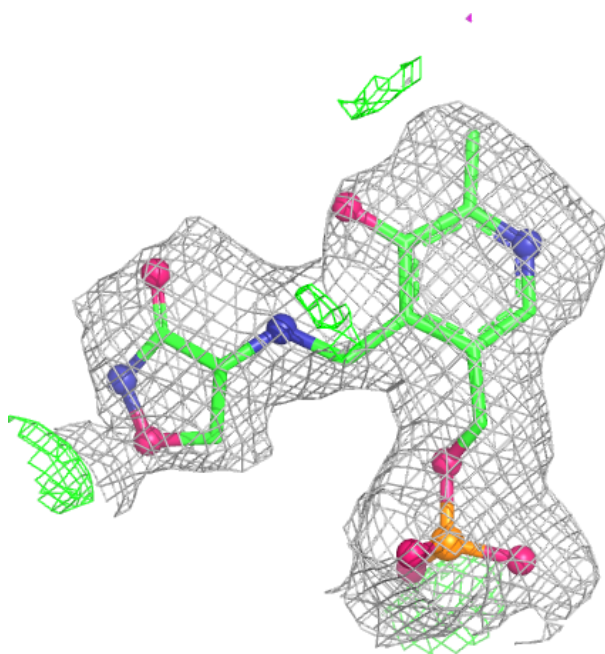
Electron density around DCS A 401:

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



Electron density around DCS 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 ⓘ

There are no such residues in this entry.