



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 05:05 am BST

PDB ID : 6K3E
Title : LSD1/Co-Rest structure with an inhibitor
Authors : Wang, J.
Deposited on : 2019-05-17
Resolution : 2.87 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

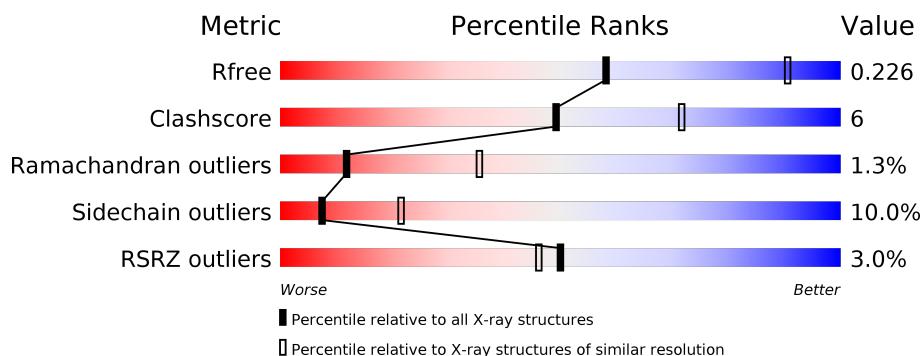
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 on 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	662	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	B	140	<div> <div>4%</div> <div>62%</div> <div>27%</div> <div>6%</div> <div>5%</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
10	PEG	A	924	-	-	-	X
10	PEG	A	925	-	-	-	X
10	PEG	A	926	-	-	-	X
12	CVO	A	929[B]	-	-	-	X
3	CW0	A	901[A]	-	-	-	X
4	DTT	A	902	-	-	-	X
5	ACT	B	501	-	-	-	X
6	MLA	A	906	-	-	-	X
7	GOL	A	910	-	-	-	X
9	EDO	A	912	-	-	-	X
9	EDO	A	913	-	-	-	X
9	EDO	A	914	-	-	-	X
9	EDO	A	916	-	-	-	X
9	EDO	A	917	-	-	-	X
9	EDO	A	918	-	-	-	X
9	EDO	A	919	-	-	-	X
9	EDO	A	920	-	-	-	X
9	EDO	A	922	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 6502 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5177	3297	901	959	20			

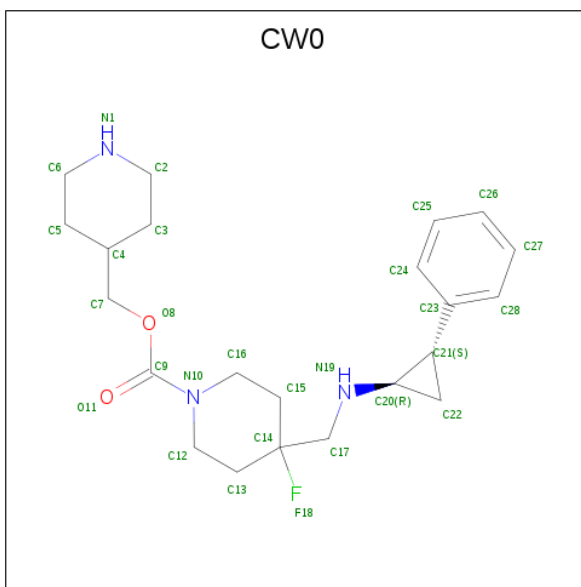
- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

There are 7 discrepancies between the modelled and reference sequences:

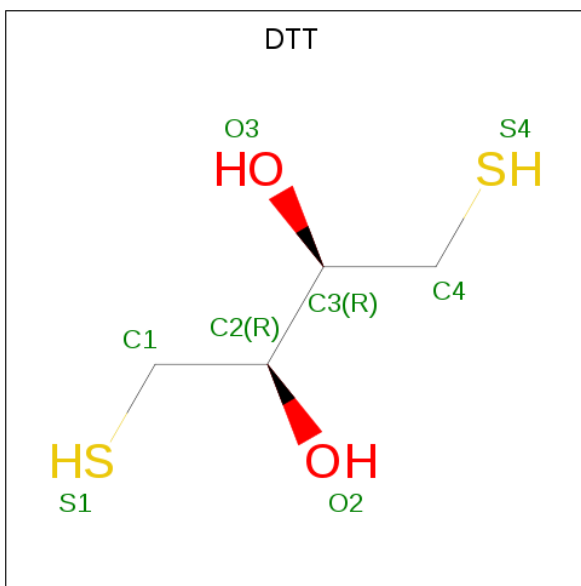
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	GLY	-	expression tag	UNP Q9UKL0
B	302	SER	-	expression tag	UNP Q9UKL0
B	303	SER	-	expression tag	UNP Q9UKL0
B	304	GLY	-	expression tag	UNP Q9UKL0
B	305	SER	-	expression tag	UNP Q9UKL0
B	306	ALA	-	expression tag	UNP Q9UKL0
B	307	SER	-	expression tag	UNP Q9UKL0

- Molecule 3 is piperidin-4-ylmethyl 4-fluoranyl-4-[[[(1 {R},2 {S})-2-phenylcyclopropyl]amino]methyl]piperidine-1-carboxylate (three-letter code: CW0) (formula: C₂₂H₃₂FN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	1
			28	22	1	3	2		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



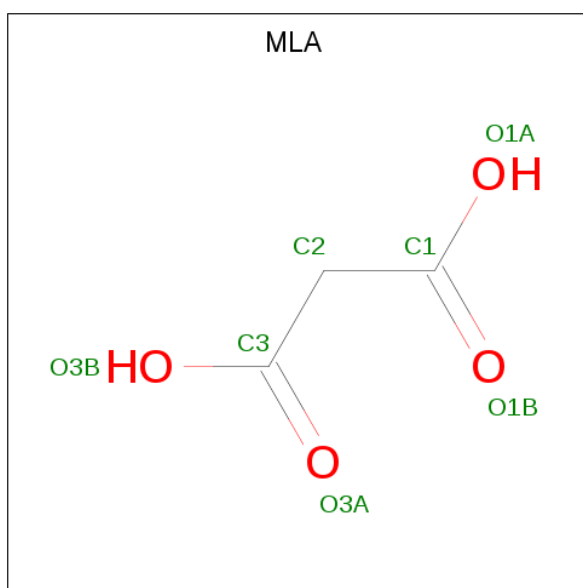
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



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

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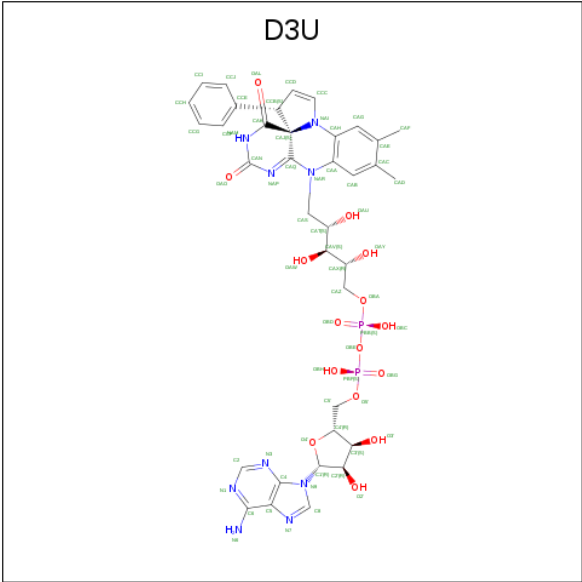
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



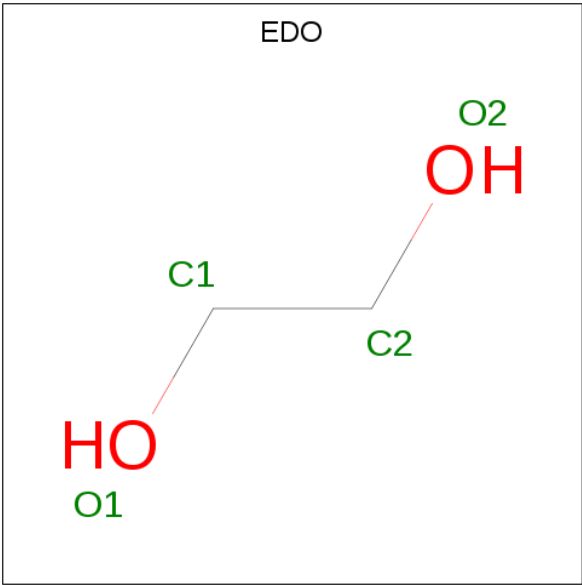
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 2-PCPA derivative (three-letter code: D3U) (formula: $C_{36}H_{41}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			62	36	9	15	2		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



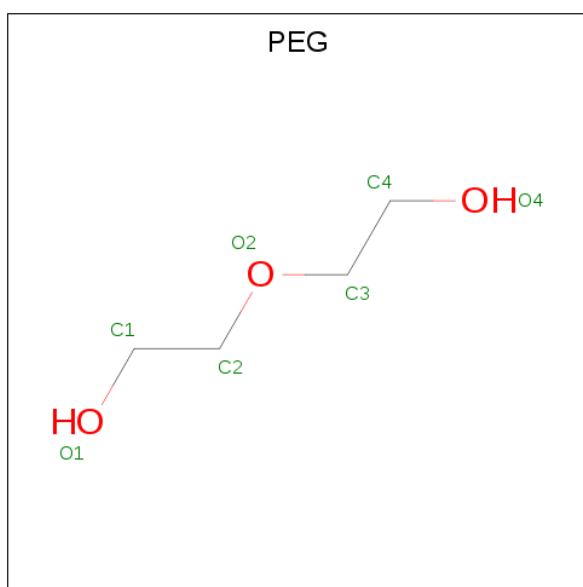
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	A	1	Total	C	O	0	0
			7	4	3		

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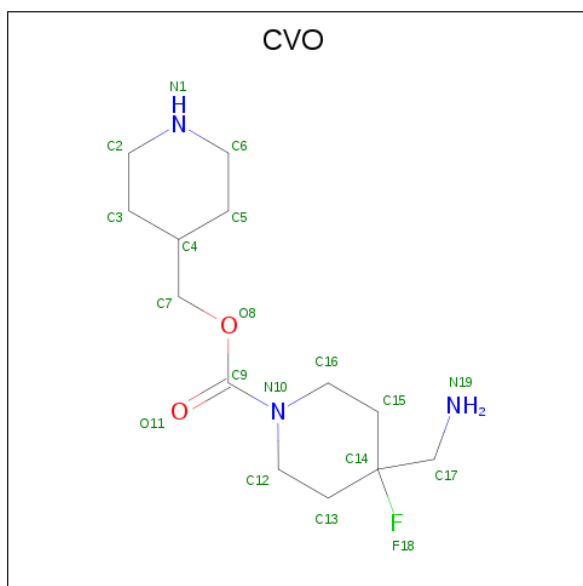
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Cl	0	0
			2	2		

- Molecule 12 is piperidin-4-ylmethyl 4-(aminomethyl)-4-fluoranyl-piperidine-1-carboxylate (three-letter code: CVO) (formula: C₁₃H₂₄FN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	F	N	O	0	1
			19	13	1	3	2		

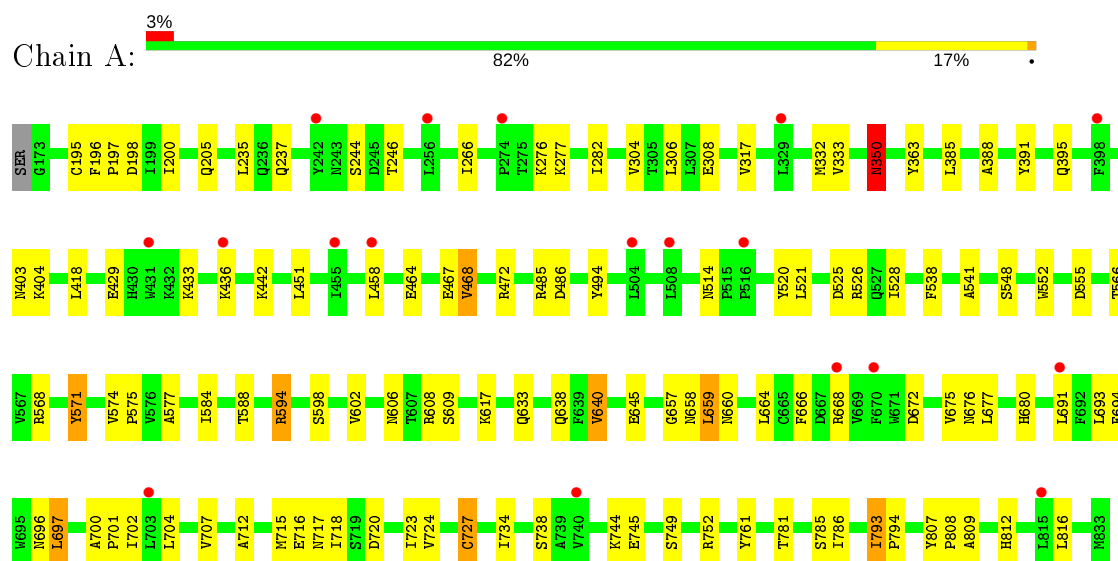
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	8	Total	O	0	0
			8	8		

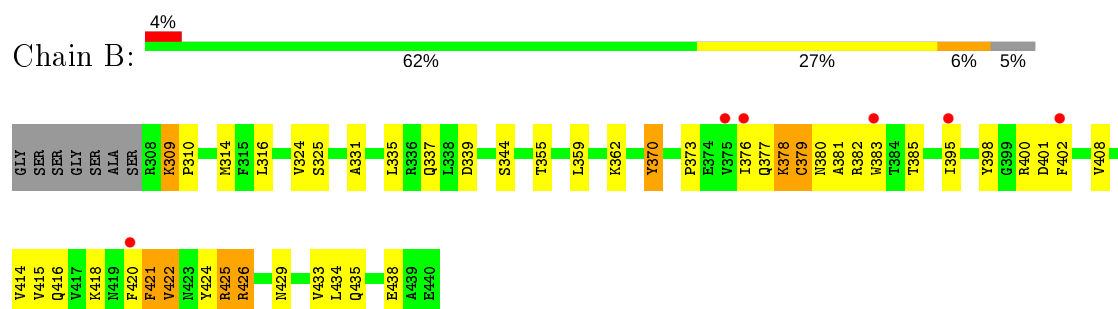
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Lysine-specific histone demethylase 1A



• Molecule 2: REST corepressor 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.51Å 179.44Å 234.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.46 – 2.87 76.34 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.7 (76.46-2.87) 98.7 (76.34-2.87)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.202 , 0.229 0.205 , 0.226	Depositor DCC
R_{free} test set	2828 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	93.3	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 83.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6502	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: GOL, MLA, CL, CW0, D3U, EDO, CVO, ACT, PEG, DTT

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	0.64	0/5289	0.78	0/7174
2	B	0.67	0/1091	0.79	0/1471
All	All	0.65	0/6380	0.78	0/8645

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	5177	0	5212	56	0
2	B	1076	0	1091	25	0
3	A	28	0	0	0	0
4	A	8	0	10	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	21	0	6	0	0
7	A	24	0	32	0	0
8	A	62	0	0	1	0
9	A	48	0	72	0	0
10	A	21	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	2	0	0	0	0
12	A	19	0	0	0	0
13	A	8	0	0	0	0
All	All	6502	0	6459	76	0

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

All (76) 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:566:THR:HG21	1:A:697:LEU:HD12	1.64	0.80
2:B:309:LYS:HE3	2:B:309:LYS:HA	1.70	0.73
2:B:309:LYS:HG3	2:B:310:PRO:HD2	1.84	0.60
2:B:309:LYS:HD3	2:B:310:PRO:HD2	1.84	0.59
1:A:807:TYR:N	1:A:808:PRO:HD3	2.16	0.59
1:A:308:GLU:OE2	8:A:911:D3U:O3'	2.20	0.59
1:A:548:SER:O	1:A:552:TRP:HB3	2.03	0.59
2:B:381:ALA:HA	2:B:416:GLN:NE2	2.18	0.59
1:A:385:LEU:O	1:A:388:ALA:HB3	2.04	0.57
2:B:309:LYS:CG	2:B:310:PRO:HD2	2.34	0.57
1:A:660:ASN:HA	1:A:749:SER:OG	2.04	0.57
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.45	0.56
1:A:195:CYS:SG	4:A:902:DTT:S4	3.03	0.56
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.87	0.56
2:B:424:TYR:O	2:B:426:ARG:N	2.40	0.55
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.36	0.55
1:A:672:ASP:O	1:A:675:VAL:HG12	2.05	0.55
1:A:793:ILE:HD13	1:A:793:ILE:N	2.21	0.55
2:B:309:LYS:HD3	2:B:310:PRO:CD	2.37	0.55
1:A:693:LEU:HD12	1:A:694:PHE:N	2.24	0.53
1:A:391:TYR:CE1	2:B:310:PRO:HD3	2.45	0.52
1:A:677:LEU:N	1:A:677:LEU:HD23	2.26	0.51
1:A:658:ASN:ND2	1:A:752:ARG:HB2	2.26	0.51
2:B:309:LYS:HA	2:B:309:LYS:CE	2.41	0.51
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.47	0.50
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.47	0.50
1:A:350:ASN:O	1:A:350:ASN:ND2	2.44	0.49
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.94	0.49
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.47	0.49
1:A:541:ALA:O	1:A:657:GLY:HA3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.94	0.49
2:B:422:VAL:O	2:B:425:ARG:HB2	2.13	0.49
1:A:566:THR:HG21	1:A:697:LEU:CD1	2.39	0.49
1:A:332:MET:CE	1:A:704:LEU:HD13	2.43	0.48
1:A:468:VAL:O	1:A:472:ARG:NH1	2.46	0.48
1:A:707:VAL:HG11	1:A:715:MET:HG3	1.96	0.48
1:A:720:ASP:O	1:A:724:VAL:HG23	2.14	0.48
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.28	0.48
1:A:666:PHE:O	1:A:701:PRO:HG2	2.14	0.47
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.49	0.47
1:A:418:LEU:HD12	2:B:324:VAL:HG21	1.96	0.47
2:B:381:ALA:HA	2:B:416:GLN:HE22	1.79	0.47
1:A:664:LEU:HD11	1:A:727:CYS:SG	2.54	0.47
2:B:309:LYS:CD	2:B:310:PRO:HD2	2.45	0.47
1:A:266:ILE:CD1	1:A:577:ALA:HB1	2.45	0.47
1:A:660:ASN:HD21	1:A:716:GLU:CG	2.29	0.46
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.98	0.46
1:A:266:ILE:HD12	1:A:577:ALA:HB1	1.98	0.45
1:A:594:ARG:HA	1:A:640:VAL:O	2.16	0.45
2:B:414:VAL:O	2:B:418:LYS:HG3	2.17	0.45
1:A:196:PHE:N	1:A:197:PRO:CD	2.79	0.45
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.99	0.45
1:A:332:MET:HG2	1:A:333:VAL:HG23	1.98	0.44
1:A:520:TYR:CE2	1:A:521:LEU:HD12	2.53	0.44
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.99	0.44
1:A:807:TYR:N	1:A:808:PRO:CD	2.82	0.43
1:A:723:ILE:O	1:A:727:CYS:HB2	2.18	0.43
2:B:324:VAL:HG12	2:B:324:VAL:O	2.19	0.43
1:A:793:ILE:N	1:A:793:ILE:CD1	2.82	0.43
1:A:306:LEU:HD13	1:A:584:ILE:HG12	2.00	0.43
2:B:400:ARG:O	2:B:402:PHE:N	2.52	0.43
1:A:317:VAL:HG13	1:A:571:TYR:HB3	2.01	0.43
1:A:606:ASN:HD22	1:A:609:SER:H	1.67	0.43
2:B:383:TRP:CZ2	2:B:420:PHE:HB2	2.54	0.42
1:A:606:ASN:HD21	1:A:608:ARG:HE	1.65	0.42
2:B:370:TYR:N	2:B:370:TYR:CD1	2.88	0.42
1:A:694:PHE:HA	1:A:704:LEU:O	2.20	0.41
2:B:359:LEU:N	2:B:359:LEU:HD23	2.36	0.41
1:A:574:VAL:HB	1:A:575:PRO:HD3	2.03	0.41
2:B:378:LYS:O	2:B:380:ASN:N	2.53	0.41
1:A:235:LEU:HD21	1:A:246:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLU:O	1:A:467:GLU:HB2	2.21	0.41
1:A:781:THR:OG1	1:A:794:PRO:HB3	2.21	0.40
1:A:525:ASP:O	1:A:528:ILE:N	2.54	0.40
1:A:812:HIS:O	1:A:816:LEU:HG	2.22	0.40
2:B:421:PHE:HE1	2:B:434:LEU:HD11	1.86	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	659/662 (100%)	585 (89%)	69 (10%)	5 (1%)	19	48
2	B	131/140 (94%)	109 (83%)	17 (13%)	5 (4%)	3	11
All	All	790/802 (98%)	694 (88%)	86 (11%)	10 (1%)	12	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	VAL
2	B	379	CYS
2	B	425	ARG
1	A	244	SER
2	B	373	PRO
2	B	401	ASP
1	A	659	LEU
1	A	350	ASN
1	A	403	ASN
2	B	331	ALA

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	561/562 (100%)	517 (92%)	44 (8%)	12	33
2	B	117/121 (97%)	93 (80%)	24 (20%)	1	3
All	All	678/683 (99%)	610 (90%)	68 (10%)	7	21

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	200	ILE
1	A	205	GLN
1	A	237	GLN
1	A	276	LYS
1	A	277	LYS
1	A	304	VAL
1	A	350	ASN
1	A	404	LYS
1	A	429	GLU
1	A	433	LYS
1	A	436	LYS
1	A	458	LEU
1	A	485	ARG
1	A	514	ASN
1	A	526	ARG
1	A	538	PHE
1	A	555	ASP
1	A	568	ARG
1	A	571	TYR
1	A	588	THR
1	A	594	ARG
1	A	598	SER
1	A	617	LYS
1	A	633	GLN
1	A	638	GLN
1	A	640	VAL

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Mol	Chain	Res	Type
1	A	645	GLU
1	A	659	LEU
1	A	668	ARG
1	A	676	ASN
1	A	680	HIS
1	A	696	ASN
1	A	697	LEU
1	A	702	ILE
1	A	717	ASN
1	A	718	ILE
1	A	727	CYS
1	A	738	SER
1	A	744	LYS
1	A	745	GLU
1	A	785	SER
1	A	786	ILE
1	A	793	ILE
2	B	309	LYS
2	B	314	MET
2	B	316	LEU
2	B	325	SER
2	B	335	LEU
2	B	337	GLN
2	B	339	ASP
2	B	344	SER
2	B	362	LYS
2	B	370	TYR
2	B	376	ILE
2	B	377	GLN
2	B	378	LYS
2	B	379	CYS
2	B	382	ARG
2	B	385	THR
2	B	408	VAL
2	B	415	VAL
2	B	421	PHE
2	B	422	VAL
2	B	426	ARG
2	B	429	ASN
2	B	435	GLN
2	B	438	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	350	ASN
1	A	358	GLN
1	A	395	GLN
1	A	422	HIS
1	A	633	GLN
1	A	660	ASN
1	A	717	ASN
2	B	337	GLN
2	B	348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\# Z > 2$
7	GOL	A	908	-	5,5,5	0.15	0	5,5,5	0.39	0
10	PEG	A	926	-	6,6,6	0.21	0	5,5,5	0.10	0
5	ACT	B	501	-	1,3,3	4.43	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	920	-	3,3,3	0.10	0	2,2,2	0.18	0
10	PEG	A	924	-	6,6,6	0.15	0	5,5,5	0.06	0
7	GOL	A	909	-	5,5,5	0.09	0	5,5,5	0.27	0
9	EDO	A	921	-	3,3,3	0.08	0	2,2,2	0.13	0
8	D3U	A	911	-	62,69,69	3.61	19 (30%)	70,107,107	1.89	14 (20%)
9	EDO	A	916	-	3,3,3	0.12	0	2,2,2	0.36	0
9	EDO	A	913	-	3,3,3	0.16	0	2,2,2	0.35	0
5	ACT	A	903	-	1,3,3	4.53	1 (100%)	0,3,3	0.00	-
6	MLA	A	905	-	0,6,6	0.00	-	0,7,7	0.00	-
12	CVO	A	929[B]	-	18,20,20	0.55	0	21,27,27	3.23	9 (42%)
7	GOL	A	910	-	5,5,5	0.13	0	5,5,5	0.36	0
3	CW0	A	901[A]	-	28,31,31	0.97	1 (3%)	35,43,43	2.98	10 (28%)
10	PEG	A	925	-	6,6,6	0.21	0	5,5,5	0.09	0
9	EDO	A	922	-	3,3,3	0.19	0	2,2,2	0.45	0
6	MLA	A	904	-	0,6,6	0.00	-	0,7,7	0.00	-
7	GOL	A	907	-	5,5,5	0.14	0	5,5,5	0.34	0
9	EDO	A	919	-	3,3,3	0.14	0	2,2,2	0.26	0
9	EDO	A	915	-	3,3,3	0.11	0	2,2,2	0.29	0
6	MLA	A	906	-	0,6,6	0.00	-	0,7,7	0.00	-
9	EDO	A	918	-	3,3,3	0.07	0	2,2,2	0.15	0
4	DTT	A	902	-	7,7,7	0.26	0	4,8,8	0.47	0
9	EDO	A	914	-	3,3,3	0.07	0	2,2,2	0.14	0
9	EDO	A	917	-	3,3,3	0.06	0	2,2,2	0.18	0
9	EDO	A	923	-	3,3,3	0.13	0	2,2,2	0.11	0
9	EDO	A	912	-	3,3,3	0.14	0	2,2,2	0.45	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
7	GOL	A	908	-	-	3/4/4/4	-
10	PEG	A	926	-	-	2/4/4/4	-
9	EDO	A	920	-	-	1/1/1/1	-
10	PEG	A	924	-	-	2/4/4/4	-
7	GOL	A	909	-	-	4/4/4/4	-
9	EDO	A	921	-	-	1/1/1/1	-
8	D3U	A	911	-	-	1/34/103/103	0/8/8/8
9	EDO	A	916	-	-	1/1/1/1	-
9	EDO	A	913	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MLA	A	905	-	-	0/0/4/4	-
12	CVO	A	929[B]	-	-	5/11/32/32	1/2/2/2
7	GOL	A	910	-	-	3/4/4/4	-
3	CW0	A	901[A]	-	-	6/16/44/44	1/4/4/4
10	PEG	A	925	-	-	2/4/4/4	-
9	EDO	A	922	-	-	0/1/1/1	-
6	MLA	A	904	-	-	0/0/4/4	-
7	GOL	A	907	-	-	0/4/4/4	-
9	EDO	A	919	-	-	1/1/1/1	-
9	EDO	A	915	-	-	0/1/1/1	-
6	MLA	A	906	-	-	0/0/4/4	-
9	EDO	A	918	-	-	0/1/1/1	-
4	DTT	A	902	-	-	4/8/8/8	-
9	EDO	A	914	-	-	1/1/1/1	-
9	EDO	A	917	-	-	0/1/1/1	-
9	EDO	A	923	-	-	0/1/1/1	-
9	EDO	A	912	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	911	D3U	CAJ-CAK	-17.90	1.35	1.54
8	A	911	D3U	CCB-CCD	-10.09	1.39	1.52
8	A	911	D3U	CCE-CCB	-9.27	1.44	1.52
8	A	911	D3U	C2-N3	5.75	1.41	1.32
8	A	911	D3U	CAF-CAE	-5.41	1.40	1.51
8	A	911	D3U	C2-N1	5.38	1.43	1.33
8	A	911	D3U	CAH-NAI	-5.35	1.29	1.40
8	A	911	D3U	CAD-CAC	-5.01	1.41	1.51
8	A	911	D3U	CAK-NAM	4.77	1.44	1.37
5	A	903	ACT	CH3-C	4.53	1.54	1.48
5	B	501	ACT	CH3-C	4.43	1.54	1.48
8	A	911	D3U	CAJ-CCB	4.40	1.64	1.58
8	A	911	D3U	CAS-CAT	4.36	1.58	1.52
3	A	901[A]	CW0	C22-C20	3.57	1.54	1.49
8	A	911	D3U	PBB-OBH	3.33	1.62	1.50
8	A	911	D3U	PBF-OBH	3.29	1.70	1.55
8	A	911	D3U	CCC-NAI	-3.18	1.34	1.39
8	A	911	D3U	CAJ-NAI	2.89	1.50	1.47
8	A	911	D3U	CAN-NAM	2.13	1.44	1.39
8	A	911	D3U	CAS-NAR	2.13	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	911	D3U	PBB-OBA	2.04	1.67	1.59
8	A	911	D3U	C6-C5	-2.02	1.35	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901[A]	CW0	O8-C9-N10	10.03	123.97	111.66
12	A	929[B]	CVO	O8-C9-N10	8.83	122.51	111.66
8	A	911	D3U	CAH-NAI-CCC	-7.90	111.32	123.82
12	A	929[B]	CVO	C15-C14-C13	7.28	116.03	110.75
3	A	901[A]	CW0	C15-C14-C13	6.80	115.69	110.75
3	A	901[A]	CW0	C13-C14-C17	5.95	121.47	109.39
8	A	911	D3U	N3-C2-N1	-5.43	120.18	128.68
3	A	901[A]	CW0	C15-C14-C17	5.27	120.10	109.39
8	A	911	D3U	O4'-C1'-C2'	-4.95	99.69	106.93
12	A	929[B]	CVO	C16-C15-C14	-4.92	108.50	112.38
3	A	901[A]	CW0	C22-C21-C23	-4.65	113.30	122.24
12	A	929[B]	CVO	C12-C13-C14	-4.18	109.08	112.38
3	A	901[A]	CW0	C16-C15-C14	-3.93	109.28	112.38
3	A	901[A]	CW0	O11-C9-N10	-3.91	117.78	124.32
3	A	901[A]	CW0	O8-C9-O11	-3.83	118.25	124.78
8	A	911	D3U	PBF-OBE-PBB	-3.64	120.33	132.83
12	A	929[B]	CVO	O8-C9-O11	-3.63	118.59	124.78
12	A	929[B]	CVO	O11-C9-N10	-3.24	118.90	124.32
8	A	911	D3U	CAB-CAA-CAH	-3.16	115.30	120.11
12	A	929[B]	CVO	C6-C5-C4	-2.97	107.54	112.14
3	A	901[A]	CW0	C16-N10-C12	2.95	118.30	112.62
8	A	911	D3U	CAA-CAH-NAI	-2.72	113.71	118.04
8	A	911	D3U	CAZ-CAX-CAV	-2.66	107.06	112.20
3	A	901[A]	CW0	O8-C7-C4	2.65	113.49	108.56
8	A	911	D3U	CAH-CAA-NAR	2.62	122.33	118.92
8	A	911	D3U	CAK-NAM-CAN	-2.62	121.48	125.42
12	A	929[B]	CVO	C16-N10-C12	2.61	117.65	112.62
8	A	911	D3U	C5-C6-N6	-2.59	116.42	120.35
8	A	911	D3U	CCE-CCB-CCD	-2.33	108.31	114.84
8	A	911	D3U	CAG-CAH-NAI	2.20	122.12	120.52
8	A	911	D3U	OBA-CAZ-CAX	2.14	115.08	109.36
12	A	929[B]	CVO	O8-C7-C4	2.13	112.53	108.56
8	A	911	D3U	N6-C6-N1	2.02	122.77	118.57

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	929[B]	CVO	C3-C4-C7-O8
12	A	929[B]	CVO	N10-C9-O8-C7
12	A	929[B]	CVO	C13-C14-C17-N19
3	A	901[A]	CW0	C13-C14-C17-N19
4	A	902	DTT	S1-C1-C2-O2
4	A	902	DTT	S1-C1-C2-C3
4	A	902	DTT	C2-C3-C4-S4
4	A	902	DTT	O3-C3-C4-S4
12	A	929[B]	CVO	O11-C9-O8-C7
3	A	901[A]	CW0	N10-C9-O8-C7
12	A	929[B]	CVO	C5-C4-C7-O8
10	A	925	PEG	O1-C1-C2-O2
7	A	908	GOL	O1-C1-C2-C3
7	A	908	GOL	C1-C2-C3-O3
7	A	909	GOL	O1-C1-C2-C3
7	A	909	GOL	C1-C2-C3-O3
7	A	910	GOL	C1-C2-C3-O3
10	A	924	PEG	O1-C1-C2-O2
10	A	924	PEG	O2-C3-C4-O4
7	A	908	GOL	O2-C2-C3-O3
7	A	909	GOL	O2-C2-C3-O3
3	A	901[A]	CW0	O11-C9-O8-C7
9	A	920	EDO	O1-C1-C2-O2
9	A	913	EDO	O1-C1-C2-O2
9	A	919	EDO	O1-C1-C2-O2
9	A	914	EDO	O1-C1-C2-O2
9	A	912	EDO	O1-C1-C2-O2
7	A	910	GOL	O2-C2-C3-O3
9	A	921	EDO	O1-C1-C2-O2
10	A	926	PEG	O2-C3-C4-O4
3	A	901[A]	CW0	C14-C17-N19-C20
10	A	926	PEG	C1-C2-O2-C3
7	A	909	GOL	O1-C1-C2-O2
7	A	910	GOL	O1-C1-C2-O2
8	A	911	D3U	O4'-C4'-C5'-O5'
3	A	901[A]	CW0	C22-C21-C23-C24
10	A	925	PEG	O2-C3-C4-O4
3	A	901[A]	CW0	C22-C21-C23-C28
9	A	916	EDO	O1-C1-C2-O2

All (2) ring outliers are listed below:

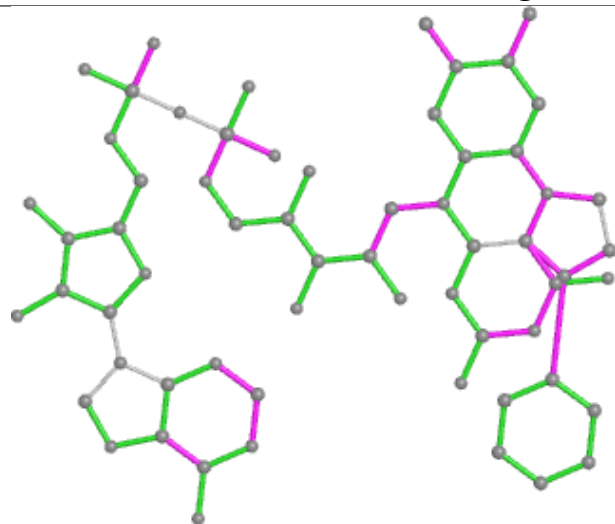
Mol	Chain	Res	Type	Atoms
3	A	901[A]	CW0	C12-C13-C14-C15-C16-N10
12	A	929[B]	CVO	C12-C13-C14-C15-C16-N10

2 monomers are involved in 2 short contacts:

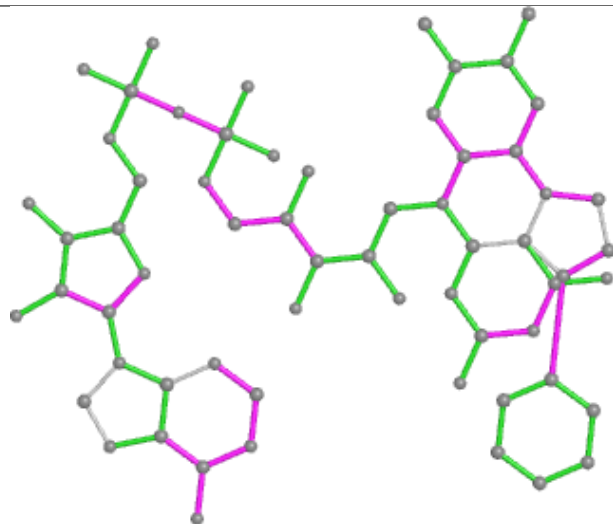
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	911	D3U	1	0
4	A	902	DTT	1	0

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 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.

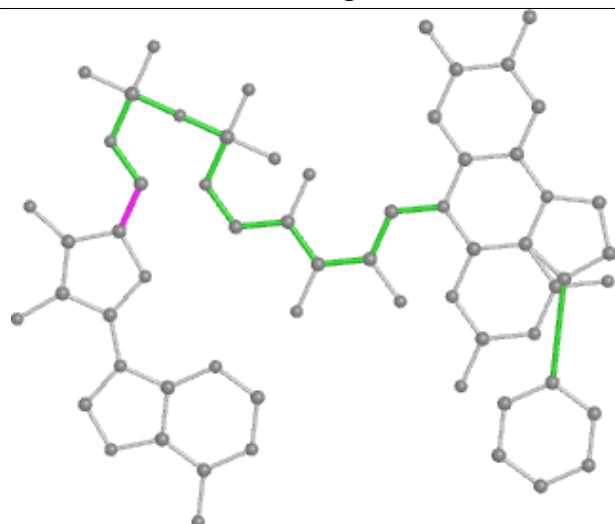
Ligand D3U A 911



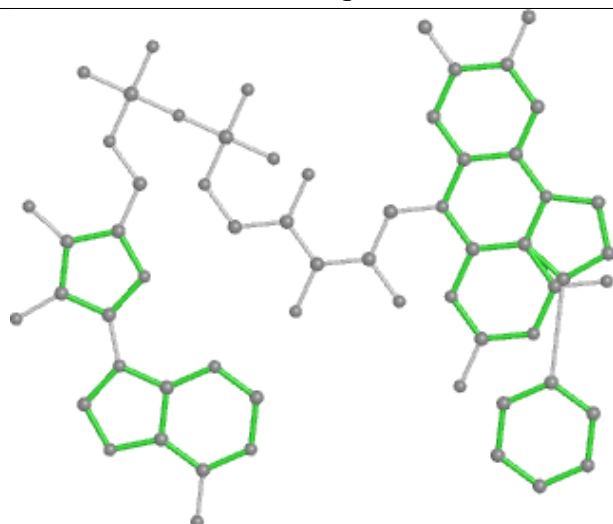
Bond lengths



Bond angles

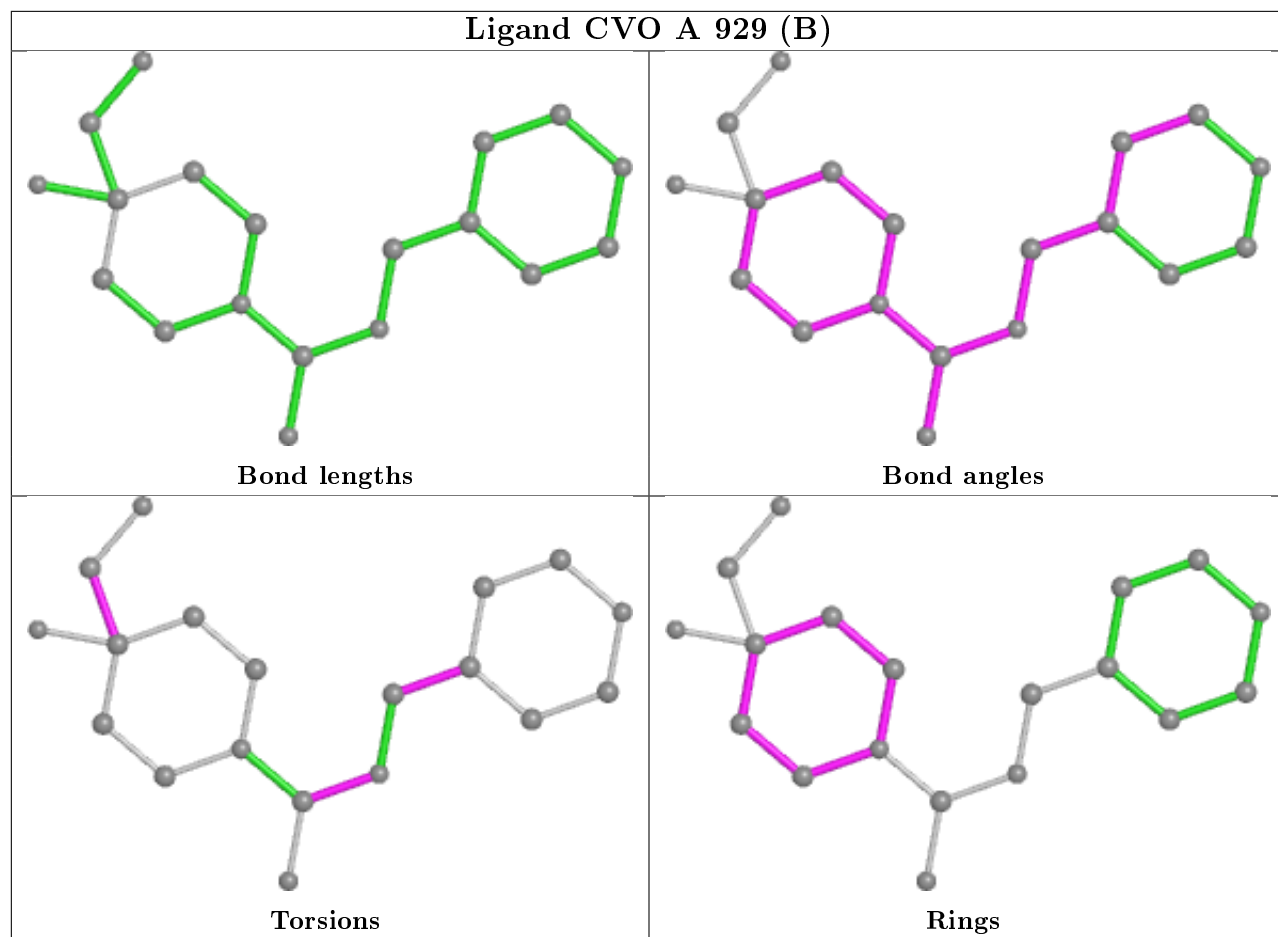


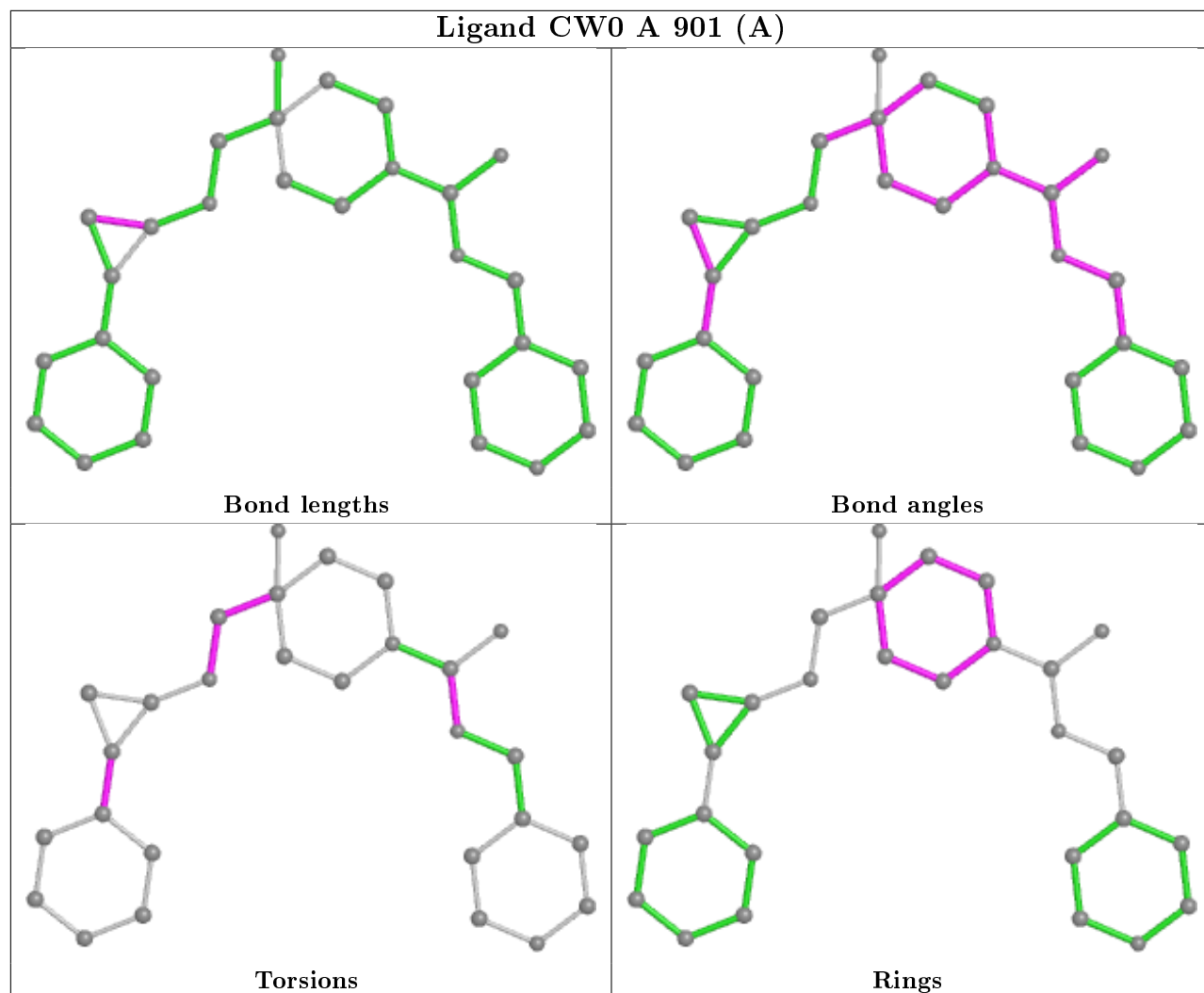
Torsions



Rings

Ligand CVO A 929 (B)





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	661/662 (99%)	0.45	18 (2%) 54 51	71, 107, 150, 191	0
2	B	133/140 (95%)	0.34	6 (4%) 33 29	101, 143, 172, 201	0
All	All	794/802 (99%)	0.43	24 (3%) 50 46	71, 115, 158, 201	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	376	ILE	3.1
1	A	508	LEU	3.0
2	B	402	PHE	2.9
1	A	691	LEU	2.7
1	A	242	TYR	2.5
2	B	375	VAL	2.4
1	A	504	LEU	2.4
2	B	395	ILE	2.4
1	A	431	TRP	2.3
1	A	329	LEU	2.3
1	A	274	PRO	2.3
1	A	703	LEU	2.3
1	A	668	ARG	2.2
1	A	455	ILE	2.2
2	B	420	PHE	2.2
1	A	436	LYS	2.2
1	A	516	PRO	2.1
1	A	815	LEU	2.1
1	A	398	PHE	2.1
2	B	383	TRP	2.1
1	A	740	VAL	2.0
1	A	458	LEU	2.0
1	A	256	LEU	2.0
1	A	670	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.

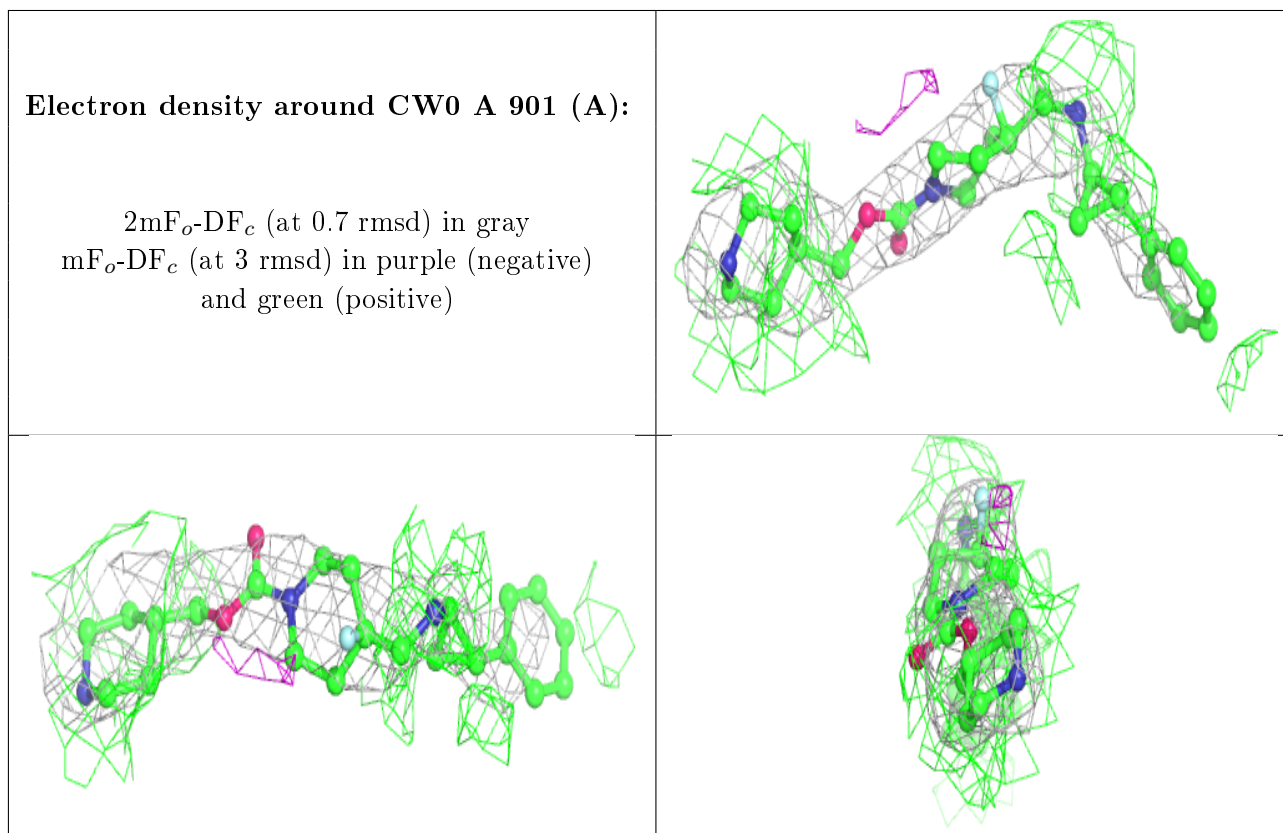
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	PEG	A	924	7/7	0.26	0.76	150,156,162,162	0
7	GOL	A	910	6/6	0.38	0.57	161,174,177,178	0
4	DTT	A	902	8/8	0.45	0.42	178,194,206,217	0
10	PEG	A	925	7/7	0.46	0.60	151,165,175,176	0
9	EDO	A	914	4/4	0.47	0.58	151,151,151,153	0
9	EDO	A	912	4/4	0.54	0.48	122,127,129,134	0
9	EDO	A	915	4/4	0.56	0.37	132,135,136,137	0
9	EDO	A	922	4/4	0.56	0.48	128,133,135,136	0
10	PEG	A	926	7/7	0.59	0.46	152,163,173,182	0
9	EDO	A	919	4/4	0.59	0.55	124,130,134,139	0
9	EDO	A	921	4/4	0.59	0.31	142,148,148,149	0
6	MLA	A	906	7/7	0.61	0.47	161,175,178,178	0
9	EDO	A	918	4/4	0.62	0.58	141,142,145,146	0
3	CW0	A	901[A]	28/28	0.64	0.54	159,172,178,179	19
9	EDO	A	916	4/4	0.67	0.58	119,134,139,141	0
12	CVO	A	929[B]	19/19	0.70	0.44	181,199,210,220	19
9	EDO	A	923	4/4	0.70	0.29	137,138,138,139	0
9	EDO	A	913	4/4	0.70	0.54	118,132,133,139	0
5	ACT	B	501	4/4	0.71	0.40	138,142,147,149	0
7	GOL	A	907	6/6	0.73	0.38	111,125,135,137	0
9	EDO	A	920	4/4	0.74	0.50	133,137,137,138	0
11	CL	A	927	1/1	0.75	0.21	144,144,144,144	0
9	EDO	A	917	4/4	0.76	0.47	153,153,157,159	0
7	GOL	A	908	6/6	0.82	0.35	126,146,155,158	0
7	GOL	A	909	6/6	0.82	0.38	153,160,165,169	6
6	MLA	A	905	7/7	0.82	0.26	105,120,127,132	0

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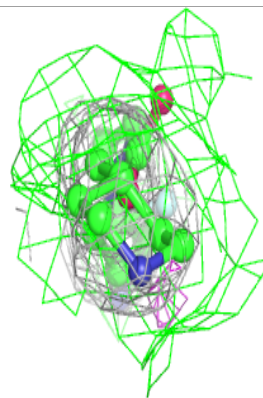
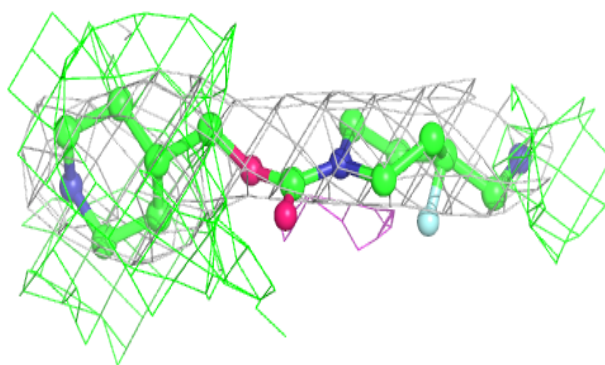
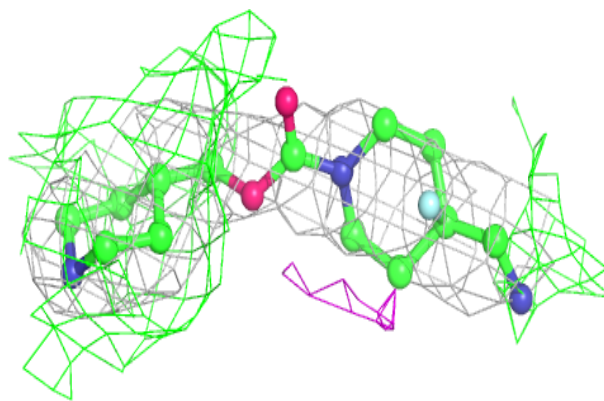
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MLA	A	904	7/7	0.84	0.39	120,127,129,135	0
11	CL	A	928	1/1	0.86	0.64	139,139,139,139	0
5	ACT	A	903	4/4	0.92	0.26	91,94,96,100	0
8	D3U	A	911	62/62	0.98	0.21	61,92,108,113	0

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.

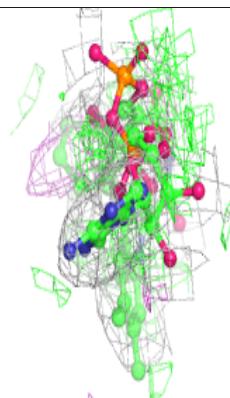
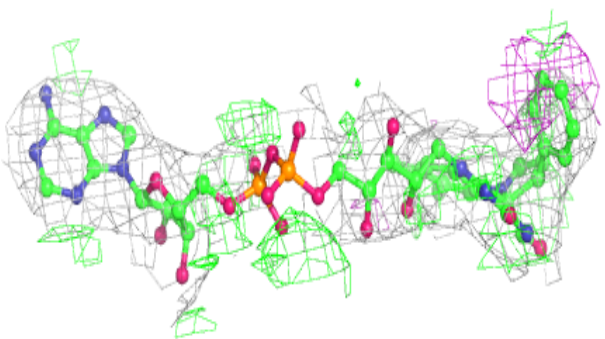
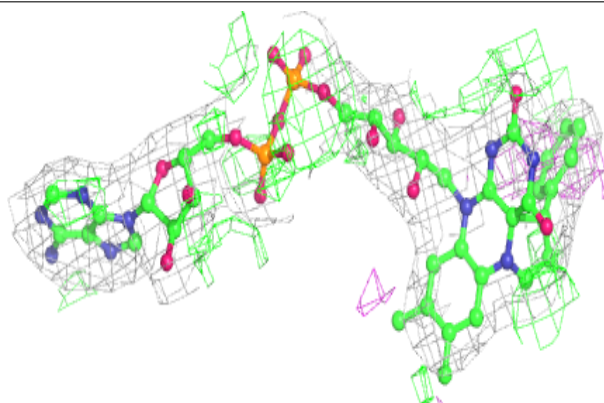


Electron density around CVO A 929 (B):

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

**Electron density around D3U A 911:**

$2mF_o-DF_c$ (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.