



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:25 AM UTC

PDB ID : 4MQ1 / pdb_00004mq1
Title : The crystal structure of DYRK1a with a bound pyrido[2,3-d]pyrimidine inhibitor
Authors : Lukacs, C.M.; Janson, C.A.; Garvie, C.; Liang, L.
Deposited on : 2013-09-15
Resolution : 2.35 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

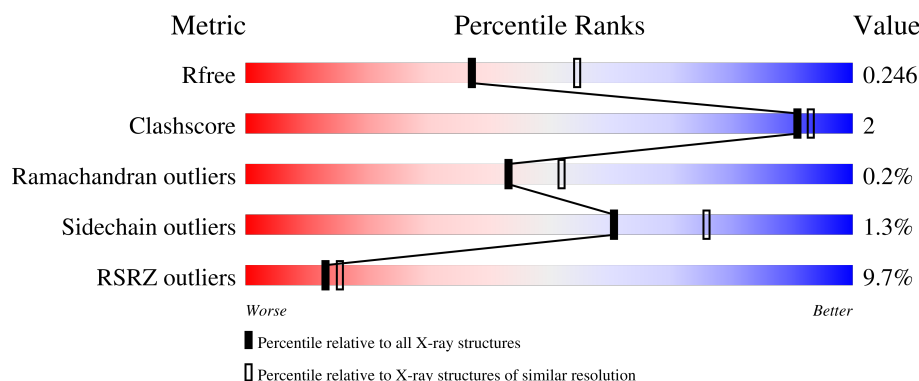
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	361	4% 93% • •
1	B	361	5% 87% 7% • 6%
1	C	361	18% 86% 6% 9%
1	D	361	10% 86% 6% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11696 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.

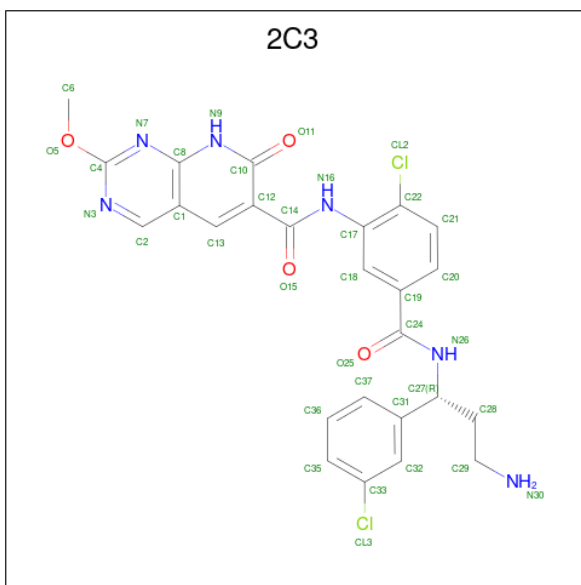
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	P	S	0	1	0
			2829	1818	482	510	2	17			
1	B	341	Total	C	N	O	P	S	0	0	0
			2771	1784	471	498	1	17			
1	C	329	Total	C	N	O	P	S	0	0	0
			2635	1704	438	476	1	16			
1	D	337	Total	C	N	O	P	S	0	1	0
			2710	1746	463	483	1	17			

There are 8 discrepancies between the modelled and reference sequences:

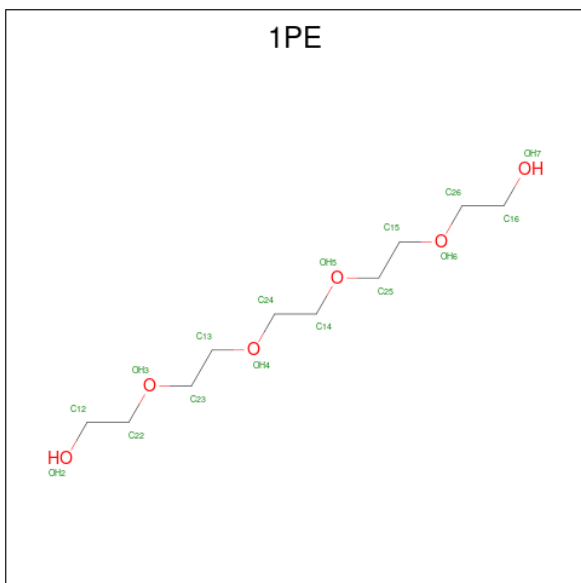
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627
D	126	MET	-	expression tag	UNP Q13627

- Molecule 2 is N-(5-([(1R)-3-amino-1-(3-chlorophenyl)propyl]carbamoyl)-2-chlorophenyl)-2-methoxy-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidine-6-carboxamide (CCD ID: 2C3) (formula: C₂₅H₂₂Cl₂N₆O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 37	C 25	Cl 2	N 6	O 4	0	0
2	B	1	Total 37	C 25	Cl 2	N 6	O 4	0	0
2	C	1	Total 37	C 25	Cl 2	N 6	O 4	0	0
2	D	1	Total 37	C 25	Cl 2	N 6	O 4	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		
5	B	162	Total	O	0	0
			162	162		
5	C	50	Total	O	0	0
			50	50		
5	D	55	Total	O	0	0
			55	55		

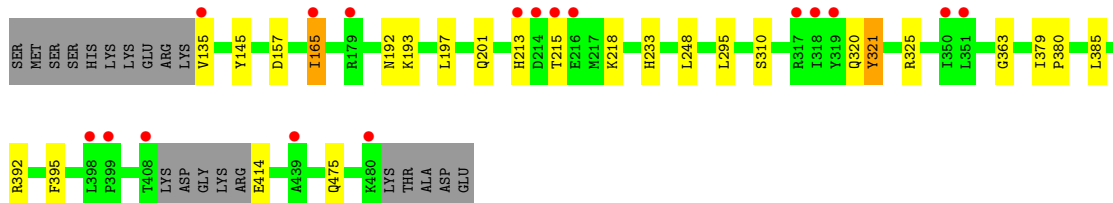
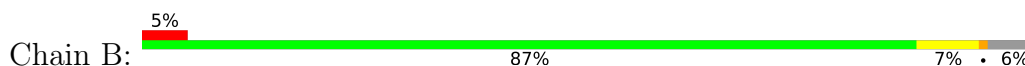
3 Residue-property plots

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

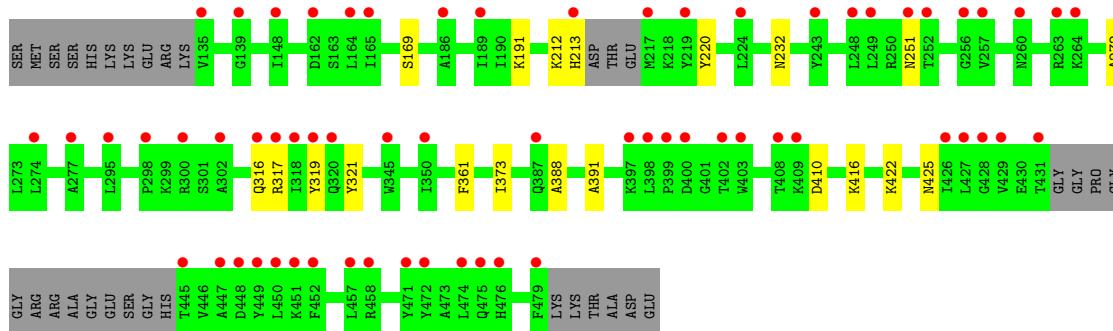
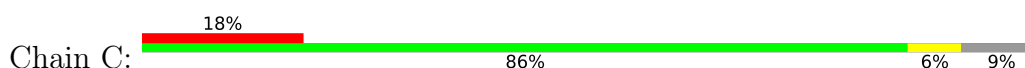
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



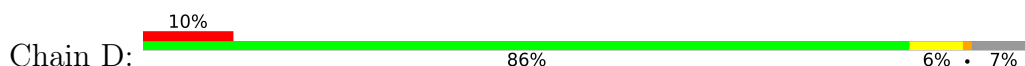
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

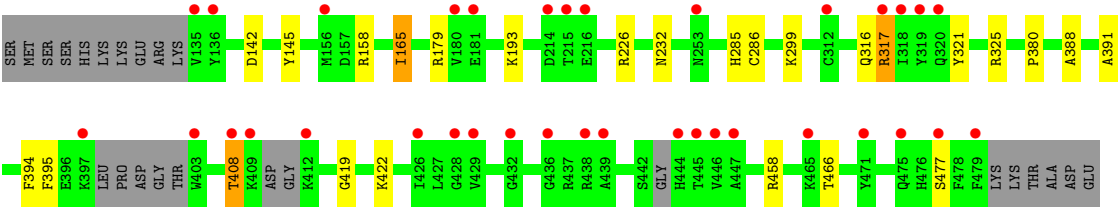


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	263.84Å 64.94Å 140.46Å 90.00° 115.16° 90.00°	Depositor
Resolution (Å)	39.83 – 2.35 39.83 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.83-2.35) 99.7 (39.83-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.246 0.205 , 0.246	Depositor DCC
R_{free} test set	4498 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11696	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: PTR, 2C3, SO4, 1PE

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	0.93	0/2862	0.93	2/3862 (0.1%)
1	B	0.83	0/2819	0.91	2/3806 (0.1%)
1	C	0.71	0/2679	0.87	2/3628 (0.1%)
1	D	0.75	0/2757	0.88	3/3725 (0.1%)
All	All	0.81	0/11117	0.90	9/15021 (0.1%)

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	C	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	LYS	CA-C-N	-6.56	113.62	120.38
1	C	416	LYS	C-N-CA	-6.56	113.62	120.38
1	A	289	LYS	CA-C-N	-5.69	112.73	119.05
1	A	289	LYS	C-N-CA	-5.69	112.73	119.05
1	D	165	ILE	CB-CA-C	-5.36	102.51	111.29
1	B	165	ILE	CB-CA-C	-5.32	102.56	111.29
1	B	379	ILE	N-CA-C	-5.16	104.22	109.02
1	D	325	ARG	N-CA-C	5.12	117.25	111.11
1	D	380	PRO	O-C-N	5.01	123.50	121.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	319	TYR	Peptide

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	2829	0	2803	5	0
1	B	2771	0	2748	11	0
1	C	2635	0	2561	6	0
1	D	2710	0	2653	15	0
2	A	37	0	22	1	0
2	B	37	0	22	1	0
2	C	37	0	22	1	0
2	D	37	0	22	1	0
3	A	32	0	44	0	0
3	B	29	0	39	0	0
3	C	16	0	22	0	0
3	D	16	0	22	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	203	0	0	0	0
5	B	162	0	0	0	0
5	C	50	0	0	0	0
5	D	55	0	0	2	0
All	All	11696	0	10980	38	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 2.

All (38) 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:192:ASN:HB2	1:A:233:HIS:CE1	2.31	0.66
1:B:325:ARG:HD2	1:B:363:GLY:O	1.99	0.62
1:A:316:GLN:O	1:A:317:ARG:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:THR:HG23	5:D:655:HOH:O	2.07	0.55
2:A:501:2C3:H12	2:A:501:2C3:O15	2.07	0.54
1:C:316:GLN:O	1:C:317:ARG:C	2.53	0.52
1:B:320:GLN:O	1:B:321:PTR:C	2.58	0.51
1:A:316:GLN:O	1:A:317:ARG:C	2.56	0.49
1:D:316:GLN:O	1:D:317:ARG:O	2.29	0.49
1:D:226[B]:ARG:NH2	5:D:601:HOH:O	2.42	0.49
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.94	0.49
1:C:169:SER:O	1:C:191:LYS:HE3	2.12	0.49
1:D:165:ILE:O	1:D:165:ILE:HG22	2.12	0.48
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.96	0.47
1:B:165:ILE:HG21	2:B:501:2C3:C13	2.46	0.46
1:A:381:PRO:HG2	1:A:384:ILE:HD12	1.98	0.46
1:D:285:HIS:O	1:D:286:CYS:HB2	2.17	0.45
1:D:158:ARG:O	1:D:179:ARG:HG3	2.17	0.45
1:B:414:GLU:OE1	1:D:299:LYS:NZ	2.44	0.45
1:D:145:TYR:CE1	1:D:193:LYS:HD3	2.53	0.44
1:B:145:TYR:CE1	1:B:193:LYS:HD2	2.53	0.43
1:B:213:HIS:O	1:B:218:LYS:HD3	2.19	0.43
1:B:248:LEU:HD21	1:B:295:LEU:HD11	2.01	0.43
2:C:501:2C3:C37	2:C:501:2C3:C29	2.97	0.42
1:B:197:LEU:O	1:B:201:GLN:HG3	2.19	0.42
1:B:392:ARG:HA	1:B:395:PHE:O	2.19	0.42
1:D:394:PHE:HB2	1:D:395:PHE:CD2	2.54	0.42
1:A:463:ASP:OD1	1:A:463:ASP:C	2.63	0.42
1:C:422:LYS:HB2	1:C:425:ASN:HD22	1.85	0.42
1:D:316:GLN:O	1:D:317:ARG:C	2.63	0.41
1:B:192:ASN:HB2	1:B:233:HIS:CE1	2.55	0.41
1:B:380:PRO:HG2	1:B:385:LEU:HD21	2.03	0.41
1:D:165:ILE:HG21	2:D:501:2C3:C13	2.51	0.41
1:D:142:ASP:OD1	1:D:142:ASP:C	2.64	0.41
1:D:419:GLY:O	1:D:422:LYS:HE3	2.21	0.41
1:D:458:ARG:NH1	1:D:466:THR:O	2.43	0.41
1:C:361:PHE:CE1	1:C:373:ILE:HA	2.56	0.40
1:C:220:TYR:HB3	1:C:272:ALA:HB2	2.04	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	343/361 (95%)	320 (93%)	22 (6%)	1 (0%)	36	43
1	B	336/361 (93%)	326 (97%)	10 (3%)	0	100	100
1	C	322/361 (89%)	305 (95%)	17 (5%)	0	100	100
1	D	329/361 (91%)	308 (94%)	20 (6%)	1 (0%)	36	43
All	All	1330/1444 (92%)	1259 (95%)	69 (5%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	ARG
1	D	317	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/320 (94%)	299 (99%)	2 (1%)	76	86
1	B	297/320 (93%)	292 (98%)	5 (2%)	53	68
1	C	277/320 (87%)	272 (98%)	5 (2%)	51	66
1	D	284/320 (89%)	281 (99%)	3 (1%)	65	79
All	All	1159/1280 (90%)	1144 (99%)	15 (1%)	61	76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	215	THR
1	B	135	VAL
1	B	157	ASP
1	B	215	THR
1	B	310	SER
1	B	475	GLN
1	C	212	LYS
1	C	213	HIS
1	C	232	ASN
1	C	251	ASN
1	C	410	ASP
1	D	232	ASN
1	D	408	THR
1	D	477	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	198	ASN
1	A	213	HIS
1	A	383	HIS
1	A	425	ASN
1	B	172	GLN
1	B	182	GLN
1	B	232	ASN
1	B	404	ASN
1	B	424	HIS
1	B	425	ASN
1	B	475	GLN
1	C	198	ASN
1	C	232	ASN
1	C	253	ASN
1	C	297	ASN
1	C	316	GLN
1	C	383	HIS
1	C	425	ASN
1	C	469	GLN
1	D	198	ASN
1	D	316	GLN
1	D	371	ASN
1	D	404	ASN

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Mol	Chain	Res	Type
1	D	424	HIS
1	D	469	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PTR	A	321[A]	1	15,16,17	0.93	0	17,22,24	1.24	2 (11%)
1	PTR	C	321	1	15,16,17	0.86	0	17,22,24	1.24	2 (11%)
1	PTR	D	321	1	15,16,17	0.89	1 (6%)	17,22,24	1.56	3 (17%)
1	PTR	B	321	1	15,16,17	1.52	3 (20%)	17,22,24	1.46	4 (23%)
1	PTR	A	321[B]	1	15,16,17	1.34	2 (13%)	17,22,24	1.59	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	321[A]	1	-	2/10/11/13	0/1/1/1
1	PTR	C	321	1	-	3/10/11/13	0/1/1/1
1	PTR	D	321	1	-	3/10/11/13	0/1/1/1
1	PTR	B	321	1	-	2/10/11/13	0/1/1/1
1	PTR	A	321[B]	1	-	2/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321[B]	PTR	P-OH	3.27	1.65	1.59
1	B	321	PTR	P-OH	3.02	1.65	1.59
1	B	321	PTR	CE2-CD2	2.71	1.43	1.38
1	A	321[B]	PTR	CE1-CD1	2.20	1.42	1.38
1	B	321	PTR	CE2-CZ	2.16	1.42	1.38
1	D	321	PTR	OH-CZ	-2.08	1.36	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	PTR	O2P-P-OH	-3.08	96.22	105.32
1	A	321[B]	PTR	P-OH-CZ	3.00	134.57	123.88
1	A	321[A]	PTR	O3P-P-O2P	2.96	118.91	107.80
1	C	321	PTR	O3P-P-O2P	2.89	118.65	107.80
1	D	321	PTR	O3P-P-O2P	2.88	118.61	107.80
1	B	321	PTR	P-OH-CZ	2.87	134.10	123.88
1	A	321[B]	PTR	CE2-CZ-CE1	-2.62	116.34	120.16
1	D	321	PTR	CD2-CG-CD1	2.55	122.03	118.23
1	B	321	PTR	OH-P-O1P	-2.54	101.01	109.48
1	A	321[A]	PTR	CB-CG-CD2	-2.52	116.20	120.90
1	D	321	PTR	P-OH-CZ	-2.51	114.96	123.88
1	B	321	PTR	CE2-CZ-CE1	-2.30	116.80	120.16
1	A	321[B]	PTR	OH-CZ-CE1	2.17	125.72	119.22
1	B	321	PTR	OH-CZ-CE2	2.15	125.66	119.22
1	A	321[B]	PTR	CD2-CE2-CZ	2.11	122.14	119.73
1	A	321[B]	PTR	OH-P-O1P	-2.09	102.50	109.48
1	A	321[B]	PTR	O2P-P-OH	2.05	111.38	105.32

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	321[A]	PTR	N-CA-CB-CG
1	A	321[A]	PTR	C-CA-CB-CG
1	A	321[B]	PTR	C-CA-CB-CG
1	C	321	PTR	O-C-CA-CB
1	C	321	PTR	N-CA-CB-CG
1	C	321	PTR	C-CA-CB-CG
1	D	321	PTR	N-CA-CB-CG
1	D	321	PTR	C-CA-CB-CG
1	A	321[B]	PTR	N-CA-CB-CG
1	B	321	PTR	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	D	321	PTR	CZ-OH-P-O3P
1	B	321	PTR	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	D	504	-	4,4,4	0.55	0	6,6,6	0.52	0
4	SO4	D	503	-	4,4,4	0.45	0	6,6,6	0.38	0
3	1PE	D	502	-	15,15,15	0.54	0	14,14,14	0.70	0
4	SO4	C	504	-	4,4,4	0.60	0	6,6,6	0.23	0
3	1PE	B	502	-	15,15,15	0.67	0	14,14,14	0.32	0
2	2C3	D	501	-	40,40,40	2.16	12 (30%)	49,56,56	2.50	17 (34%)
4	SO4	A	504	-	4,4,4	0.71	0	6,6,6	0.40	0
2	2C3	A	501	-	40,40,40	2.21	11 (27%)	49,56,56	2.28	17 (34%)
3	1PE	C	502	-	15,15,15	0.76	0	14,14,14	0.49	0
2	2C3	C	501	-	40,40,40	2.22	11 (27%)	49,56,56	2.22	13 (26%)
3	1PE	A	502	-	15,15,15	0.68	0	14,14,14	0.60	0
4	SO4	B	504	-	4,4,4	0.38	0	6,6,6	0.60	0
3	1PE	A	503	-	15,15,15	0.56	0	14,14,14	0.64	0
3	1PE	B	503	-	12,12,15	0.79	0	11,11,14	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	505	-	4,4,4	0.51	0	6,6,6	0.88	0
4	SO4	C	503	-	4,4,4	0.44	0	6,6,6	0.25	0
4	SO4	B	505	-	4,4,4	0.57	0	6,6,6	0.47	0
2	2C3	B	501	-	40,40,40	2.08	12 (30%)	49,56,56	2.12	15 (30%)

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	1PE	D	502	-	-	2/13/13/13	-
3	1PE	B	502	-	-	4/13/13/13	-
2	2C3	D	501	-	-	6/25/25/25	0/4/4/4
2	2C3	A	501	-	-	4/25/25/25	0/4/4/4
3	1PE	C	502	-	-	3/13/13/13	-
2	2C3	C	501	-	-	5/25/25/25	0/4/4/4
3	1PE	A	502	-	-	4/13/13/13	-
3	1PE	A	503	-	-	5/13/13/13	-
3	1PE	B	503	-	-	4/10/10/13	-
2	2C3	B	501	-	-	8/25/25/25	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	2C3	C31-C27	-9.42	1.39	1.52
2	D	501	2C3	C31-C27	-9.19	1.39	1.52
2	B	501	2C3	C31-C27	-8.29	1.40	1.52
2	A	501	2C3	C31-C27	-7.89	1.41	1.52
2	A	501	2C3	C10-N9	6.00	1.44	1.35
2	A	501	2C3	C19-C24	-5.12	1.39	1.50
2	C	501	2C3	C10-N9	4.65	1.42	1.35
2	B	501	2C3	C19-C24	-4.37	1.40	1.50
2	C	501	2C3	C19-C24	-4.01	1.41	1.50
2	D	501	2C3	C2-N3	3.42	1.41	1.34
2	B	501	2C3	C12-C14	-3.40	1.39	1.49
2	D	501	2C3	C22-CL2	3.29	1.81	1.73
2	D	501	2C3	C10-N9	3.28	1.40	1.35
2	B	501	2C3	C33-CL3	-3.18	1.67	1.74
2	D	501	2C3	C19-C24	-3.17	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	2C3	C17-N16	-3.01	1.35	1.41
2	D	501	2C3	C28-C27	-3.00	1.49	1.53
2	B	501	2C3	C1-C13	-2.96	1.37	1.43
2	A	501	2C3	C2-N3	2.94	1.40	1.34
2	B	501	2C3	C1-C8	-2.83	1.38	1.41
2	C	501	2C3	C1-C8	-2.77	1.38	1.41
2	C	501	2C3	C2-N3	2.76	1.40	1.34
2	D	501	2C3	C12-C14	-2.72	1.41	1.49
2	A	501	2C3	C27-N26	2.61	1.49	1.46
2	C	501	2C3	C33-CL3	-2.59	1.68	1.74
2	A	501	2C3	C17-N16	-2.59	1.36	1.41
2	A	501	2C3	C12-C10	-2.58	1.40	1.45
2	A	501	2C3	C12-C14	-2.54	1.42	1.49
2	C	501	2C3	C28-C27	-2.51	1.50	1.53
2	B	501	2C3	C2-N3	2.40	1.39	1.34
2	B	501	2C3	C13-C12	2.40	1.40	1.35
2	D	501	2C3	C17-N16	-2.36	1.37	1.41
2	C	501	2C3	C13-C12	2.36	1.40	1.35
2	D	501	2C3	C1-C8	-2.33	1.39	1.41
2	D	501	2C3	C1-C13	-2.32	1.39	1.43
2	B	501	2C3	C17-N16	-2.30	1.37	1.41
2	D	501	2C3	C13-C12	2.30	1.40	1.35
2	A	501	2C3	C33-CL3	-2.29	1.69	1.74
2	A	501	2C3	C4-N7	2.29	1.37	1.33
2	D	501	2C3	C4-N3	2.24	1.35	1.32
2	B	501	2C3	C12-C10	-2.15	1.40	1.45
2	A	501	2C3	C1-C13	-2.13	1.39	1.43
2	B	501	2C3	C22-CL2	-2.11	1.68	1.73
2	C	501	2C3	C1-C13	-2.08	1.39	1.43
2	C	501	2C3	C12-C14	-2.04	1.43	1.49
2	B	501	2C3	C2-C1	-2.02	1.36	1.40

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C3	N3-C4-N7	-10.12	119.63	128.35
2	A	501	2C3	N3-C4-N7	-8.14	121.33	128.35
2	C	501	2C3	N3-C4-N7	-7.99	121.46	128.35
2	B	501	2C3	N3-C4-N7	-7.81	121.62	128.35
2	D	501	2C3	C28-C27-N26	-6.21	101.94	109.56
2	B	501	2C3	C2-N3-C4	5.16	120.98	115.00
2	A	501	2C3	C2-N3-C4	4.98	120.77	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	2C3	C14-C12-C10	4.95	126.60	122.64
2	A	501	2C3	N9-C8-N7	4.73	122.54	116.36
2	D	501	2C3	C2-N3-C4	4.59	120.31	115.00
2	A	501	2C3	C22-C17-N16	-4.26	112.68	119.25
2	A	501	2C3	C14-C12-C10	4.02	125.86	122.64
2	C	501	2C3	C28-C27-C31	4.02	117.42	111.41
2	A	501	2C3	C12-C10-N9	3.96	121.41	114.51
2	D	501	2C3	C14-C12-C10	3.87	125.74	122.64
2	B	501	2C3	C22-C17-N16	-3.86	113.30	119.25
2	D	501	2C3	C8-N9-C10	-3.73	120.83	124.27
2	C	501	2C3	C8-N9-C10	-3.68	120.87	124.27
2	B	501	2C3	C28-C27-C31	3.63	116.84	111.41
2	C	501	2C3	C1-C8-N7	-3.62	119.89	123.87
2	D	501	2C3	C1-C8-N7	-3.58	119.93	123.87
2	C	501	2C3	C22-C17-N16	-3.48	113.89	119.25
2	D	501	2C3	C31-C27-N26	-3.46	106.18	112.07
2	B	501	2C3	C8-N9-C10	-3.43	121.10	124.27
2	C	501	2C3	C2-N3-C4	3.40	118.93	115.00
2	A	501	2C3	C8-N9-C10	-3.26	121.26	124.27
2	C	501	2C3	C12-C10-N9	3.22	120.11	114.51
2	B	501	2C3	C1-C13-C12	-3.20	118.93	122.06
2	C	501	2C3	N9-C8-N7	3.19	120.53	116.36
2	D	501	2C3	C22-C17-N16	-3.07	114.53	119.25
2	B	501	2C3	C12-C10-N9	3.06	119.83	114.51
2	C	501	2C3	C27-N26-C24	-3.00	118.77	122.34
2	A	501	2C3	O5-C4-N7	2.96	125.97	116.29
2	D	501	2C3	C12-C10-N9	2.93	119.61	114.51
2	A	501	2C3	O11-C10-C12	-2.83	119.73	125.98
2	C	501	2C3	O11-C10-N9	-2.83	116.40	121.61
2	D	501	2C3	N9-C8-N7	2.81	120.04	116.36
2	D	501	2C3	C27-N26-C24	2.79	125.66	122.34
2	B	501	2C3	C17-C22-CL2	-2.55	116.76	119.52
2	B	501	2C3	C6-O5-C4	-2.53	113.57	117.56
2	A	501	2C3	C1-C8-N7	-2.49	121.13	123.87
2	A	501	2C3	C18-C17-N16	2.48	128.45	121.95
2	A	501	2C3	C2-C1-C13	-2.46	117.90	123.01
2	B	501	2C3	C31-C27-N26	-2.42	107.95	112.07
2	D	501	2C3	O11-C10-N9	-2.41	117.17	121.61
2	A	501	2C3	C12-C14-N16	2.38	118.97	115.61
2	A	501	2C3	C13-C12-C10	-2.37	116.22	119.32
2	D	501	2C3	C18-C17-N16	2.34	128.07	121.95
2	D	501	2C3	C19-C18-C17	2.31	123.72	119.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C3	C6-O5-C4	-2.27	113.98	117.56
2	B	501	2C3	O11-C10-N9	-2.24	117.47	121.61
2	C	501	2C3	C13-C12-C10	-2.24	116.38	119.32
2	D	501	2C3	O15-C14-C12	-2.23	117.16	121.04
2	D	501	2C3	C20-C19-C18	-2.22	116.68	119.25
2	A	501	2C3	C28-C27-C31	-2.19	108.13	111.41
2	C	501	2C3	C18-C17-N16	2.16	127.61	121.95
2	A	501	2C3	C28-C27-N26	2.15	112.19	109.56
2	B	501	2C3	O15-C14-C12	-2.14	117.31	121.04
2	A	501	2C3	C31-C27-N26	-2.14	108.43	112.07
2	B	501	2C3	C28-C27-N26	-2.10	106.98	109.56
2	B	501	2C3	O5-C4-N7	2.06	123.01	116.29
2	B	501	2C3	C18-C17-N16	2.02	127.24	121.95

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	2C3	N3-C4-O5-C6
2	A	501	2C3	N7-C4-O5-C6
2	A	501	2C3	C31-C27-C28-C29
2	B	501	2C3	C31-C27-C28-C29
2	C	501	2C3	N3-C4-O5-C6
2	C	501	2C3	N7-C4-O5-C6
2	C	501	2C3	N26-C27-C28-C29
2	C	501	2C3	C31-C27-C28-C29
2	D	501	2C3	N3-C4-O5-C6
2	D	501	2C3	N7-C4-O5-C6
2	D	501	2C3	C27-C28-C29-N30
3	B	502	1PE	OH7-C16-C26-OH6
2	B	501	2C3	N7-C4-O5-C6
2	A	501	2C3	N26-C27-C28-C29
3	A	503	1PE	OH4-C13-C23-OH3
3	B	503	1PE	OH5-C14-C24-OH4
2	D	501	2C3	C28-C27-C31-C32
3	D	502	1PE	OH6-C15-C25-OH5
3	C	502	1PE	OH4-C13-C23-OH3
2	B	501	2C3	N3-C4-O5-C6
3	A	503	1PE	OH6-C15-C25-OH5
3	A	503	1PE	OH2-C12-C22-OH3
3	B	503	1PE	OH6-C15-C25-OH5
3	A	502	1PE	OH2-C12-C22-OH3

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Mol	Chain	Res	Type	Atoms
3	A	503	1PE	C12-C22-OH3-C23
2	D	501	2C3	C28-C27-C31-C37
3	B	503	1PE	OH2-C12-C22-OH3
3	C	502	1PE	OH7-C16-C26-OH6
3	B	502	1PE	C24-C14-OH5-C25
3	A	502	1PE	C25-C15-OH6-C26
2	B	501	2C3	N26-C27-C28-C29
3	A	502	1PE	OH7-C16-C26-OH6
3	B	502	1PE	C25-C15-OH6-C26
3	A	503	1PE	C16-C26-OH6-C15
3	B	503	1PE	C14-C24-OH4-C13
3	C	502	1PE	OH6-C15-C25-OH5
2	D	501	2C3	N26-C27-C31-C32
3	B	502	1PE	OH5-C14-C24-OH4
2	B	501	2C3	N26-C27-C31-C32
2	B	501	2C3	N26-C27-C31-C37
3	A	502	1PE	C16-C26-OH6-C15
3	D	502	1PE	OH2-C12-C22-OH3
2	C	501	2C3	C27-C28-C29-N30
2	B	501	2C3	C28-C27-C31-C37
2	B	501	2C3	C28-C27-C31-C32

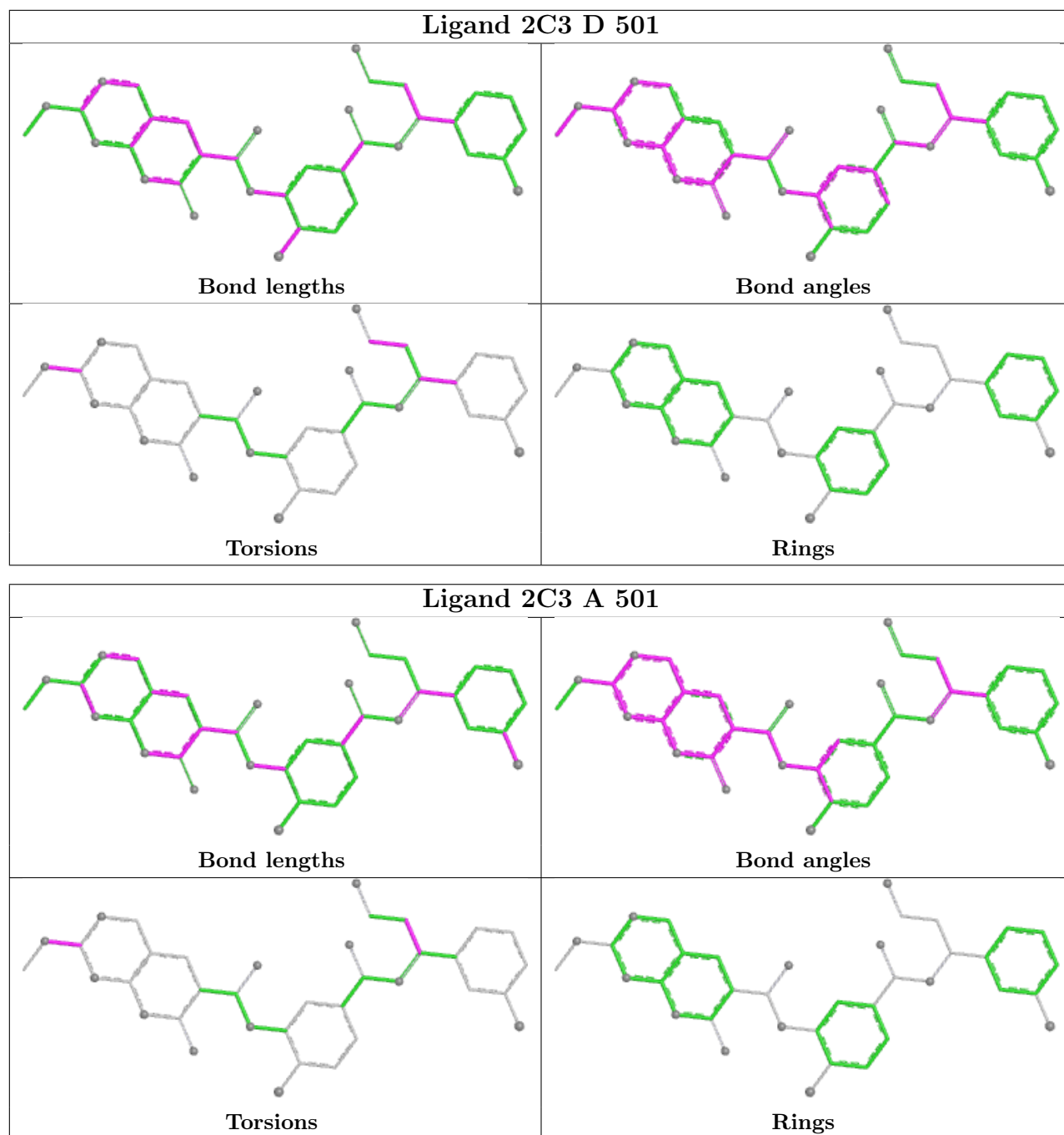
There are no ring outliers.

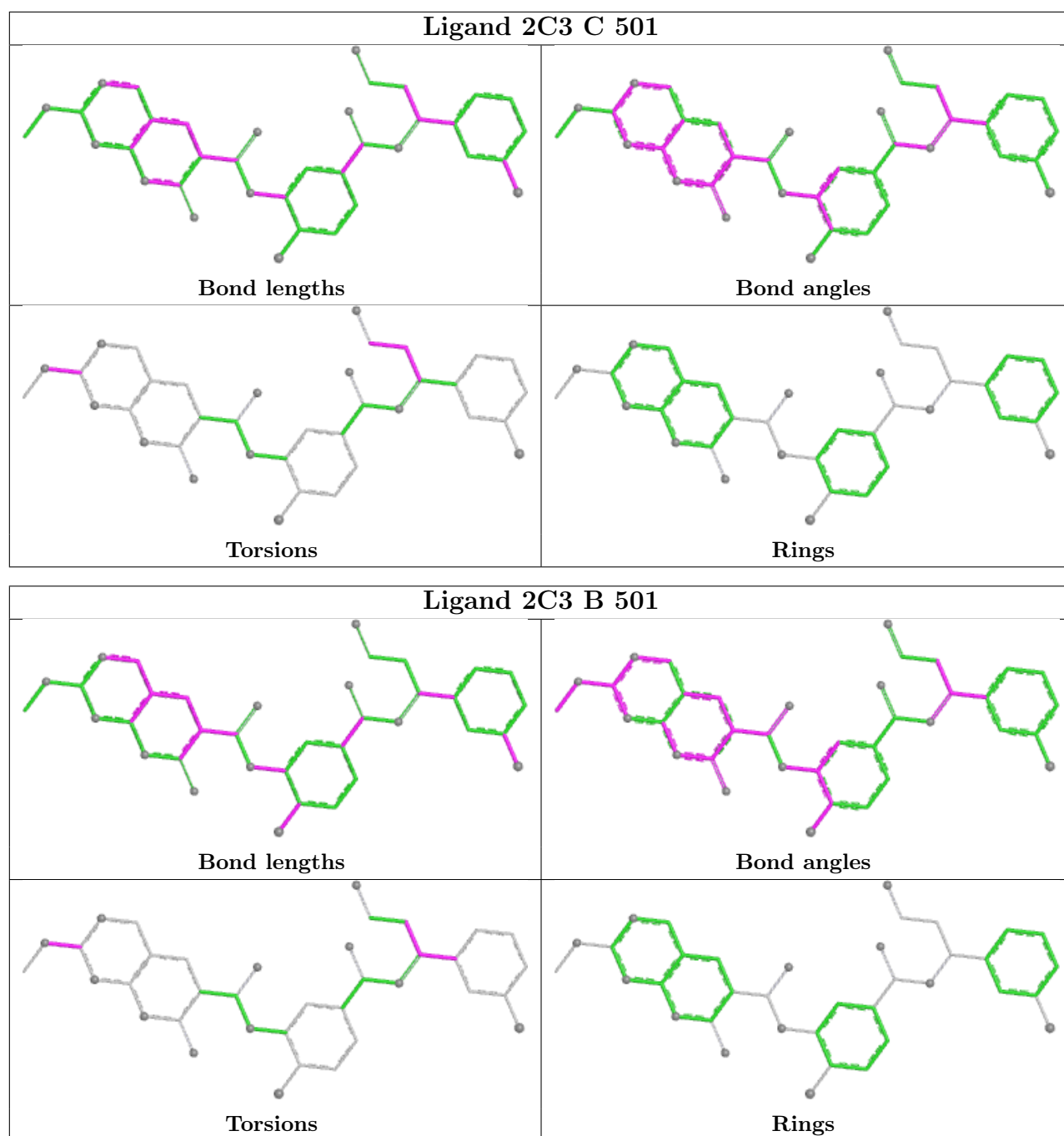
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	2C3	1	0
2	A	501	2C3	1	0
2	C	501	2C3	1	0
2	B	501	2C3	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.





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 [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	345/361 (95%)	0.13	15 (4%)	40	45	25, 38, 70, 94	0
1	B	340/361 (94%)	0.17	17 (5%)	34	40	27, 40, 67, 99	0
1	C	328/361 (90%)	1.13	64 (19%)	3	3	40, 62, 96, 115	0
1	D	336/361 (93%)	0.72	35 (10%)	11	13	23, 54, 87, 117	1 (0%)
All	All	1349/1444 (93%)	0.53	131 (9%)	13	15	23, 49, 86, 117	1 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	ILE	5.3
1	C	458	ARG	4.9
1	D	135	VAL	4.8
1	B	215	THR	4.6
1	C	445	THR	4.4
1	D	436	GLY	4.3
1	C	260	ASN	4.3
1	D	214	ASP	4.3
1	B	408	THR	4.3
1	B	216	GLU	4.2
1	C	472	TYR	4.2
1	C	295	LEU	4.0
1	C	317	ARG	4.0
1	A	319	TYR	4.0
1	B	135	VAL	4.0
1	C	451	LYS	3.9
1	D	318	ILE	3.8
1	C	318	ILE	3.8
1	D	479	PHE	3.7
1	C	447	ALA	3.7
1	C	398	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	428	GLY	3.7
1	C	252	THR	3.7
1	D	471	TYR	3.6
1	D	397	LYS	3.5
1	A	215	THR	3.5
1	C	217	MET	3.5
1	C	471	TYR	3.5
1	D	432	GLY	3.4
1	C	249	LEU	3.4
1	C	452	PHE	3.4
1	D	215	THR	3.4
1	D	429	VAL	3.4
1	C	428	GLY	3.4
1	D	319	TYR	3.4
1	D	409	LYS	3.3
1	C	248	LEU	3.3
1	C	300	ARG	3.3
1	C	409	LYS	3.3
1	C	475	GLN	3.2
1	D	180	VAL	3.2
1	C	320	GLN	3.2
1	C	403	TRP	3.1
1	D	408	THR	3.1
1	C	213	HIS	3.1
1	B	480	LYS	3.1
1	B	317	ARG	3.1
1	C	219	TYR	3.0
1	C	427	LEU	3.0
1	A	135	VAL	3.0
1	C	426	ILE	2.9
1	B	214	ASP	2.9
1	B	179	ARG	2.9
1	D	253	ASN	2.9
1	C	243	TYR	2.9
1	A	409	LYS	2.9
1	D	320	GLN	2.8
1	C	135	VAL	2.8
1	C	448	ASP	2.8
1	C	298	PRO	2.8
1	C	402	THR	2.8
1	C	319	TYR	2.7
1	C	277	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	256	GLY	2.7
1	B	213	HIS	2.6
1	A	316	GLN	2.6
1	C	251	ASN	2.6
1	C	397	LYS	2.6
1	D	445	THR	2.6
1	D	447	ALA	2.5
1	C	139	GLY	2.5
1	C	429	VAL	2.5
1	C	476	HIS	2.5
1	C	264	LYS	2.5
1	C	399	PRO	2.5
1	D	312	CYS	2.4
1	D	412	LYS	2.4
1	C	302	ALA	2.4
1	D	477	SER	2.4
1	B	398	LEU	2.4
1	D	317	ARG	2.4
1	B	399	PRO	2.4
1	B	439	ALA	2.3
1	C	186	ALA	2.3
1	D	181	GLU	2.3
1	C	257	VAL	2.3
1	D	475	GLN	2.3
1	C	450	LEU	2.3
1	A	136	TYR	2.3
1	D	403	TRP	2.3
1	C	408	THR	2.3
1	C	431	THR	2.3
1	A	317	ARG	2.3
1	B	318	ILE	2.3
1	C	165	ILE	2.3
1	D	426	ILE	2.3
1	B	165	ILE	2.3
1	D	136	TYR	2.2
1	C	457	LEU	2.2
1	D	446	VAL	2.2
1	C	263	ARG	2.2
1	C	345	TRP	2.2
1	C	148	ILE	2.2
1	C	350	ILE	2.2
1	B	351	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	162	ASP	2.2
1	C	400	ASP	2.2
1	B	319	TYR	2.2
1	A	156	MET	2.2
1	A	216	GLU	2.2
1	C	449	TYR	2.1
1	C	274	LEU	2.1
1	C	474	LEU	2.1
1	D	444	HIS	2.1
1	D	465	LYS	2.1
1	C	316	GLN	2.1
1	D	439	ALA	2.1
1	A	480	LYS	2.1
1	D	156	MET	2.1
1	A	157	ASP	2.1
1	A	213	HIS	2.1
1	A	320	GLN	2.1
1	C	224	LEU	2.1
1	C	479	PHE	2.1
1	D	216	GLU	2.0
1	C	164	LEU	2.0
1	C	189	ILE	2.0
1	A	180	VAL	2.0
1	C	387	GLN	2.0
1	B	350	ILE	2.0
1	D	438	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PTR	A	321[A]	16/17	0.84	0.21	28,33,47,53	16
1	PTR	A	321[B]	16/17	0.84	0.21	38,51,56,59	16
1	PTR	C	321	16/17	0.88	0.15	52,73,84,84	0
1	PTR	D	321	16/17	0.90	0.15	55,73,85,88	0
1	PTR	B	321	16/17	0.94	0.12	42,54,57,59	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

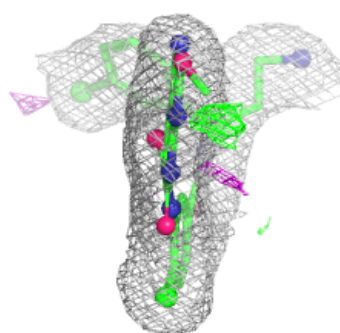
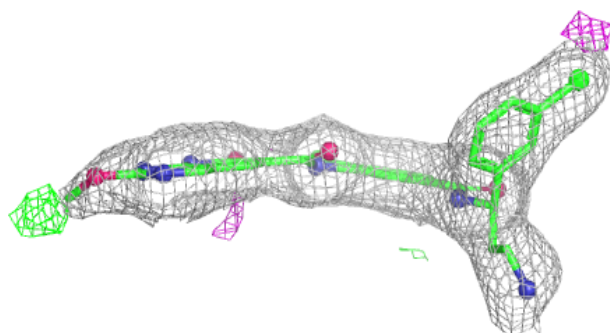
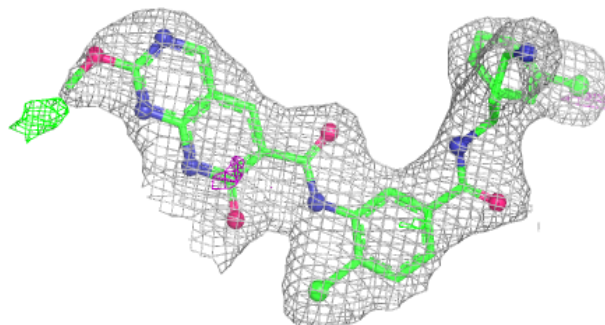
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	504	5/5	0.60	0.16	74,87,91,92	0
4	SO4	D	504	5/5	0.64	0.15	78,86,95,98	0
3	1PE	C	502	16/16	0.87	0.14	66,71,80,81	0
3	1PE	A	502	16/16	0.90	0.12	62,67,87,87	0
2	2C3	C	501	37/37	0.91	0.12	52,60,73,75	0
4	SO4	A	504	5/5	0.92	0.26	47,55,63,75	0
3	1PE	B	502	16/16	0.92	0.12	48,62,74,75	0
3	1PE	A	503	16/16	0.92	0.11	37,46,54,61	0
4	SO4	D	503	5/5	0.93	0.16	57,63,75,79	0
4	SO4	C	503	5/5	0.93	0.07	80,81,83,95	0
3	1PE	B	503	13/16	0.94	0.08	34,37,40,50	0
4	SO4	B	505	5/5	0.94	0.23	42,51,65,71	0
4	SO4	B	504	5/5	0.95	0.11	56,59,63,65	0
3	1PE	D	502	16/16	0.95	0.10	40,52,62,64	0
4	SO4	A	505	5/5	0.95	0.14	50,55,61,61	0
2	2C3	D	501	37/37	0.96	0.07	36,44,56,56	0
2	2C3	B	501	37/37	0.96	0.07	30,35,43,51	0
2	2C3	A	501	37/37	0.96	0.06	26,34,47,53	0

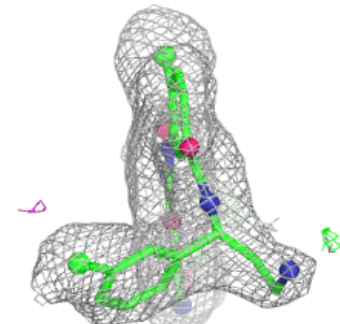
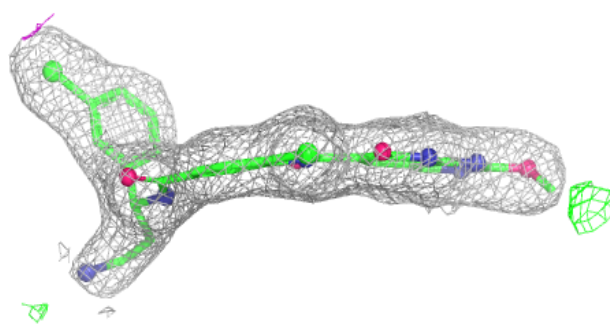
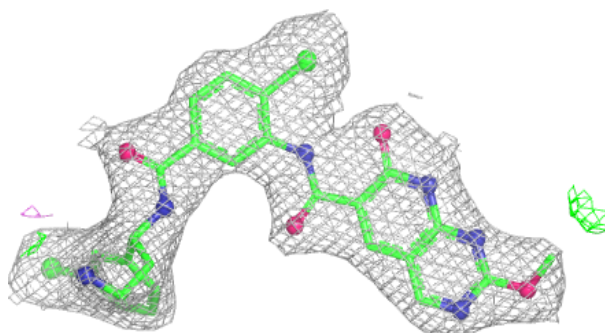
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2C3 C 501:

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

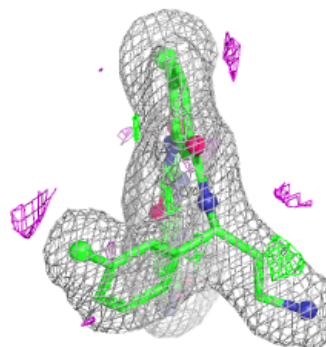
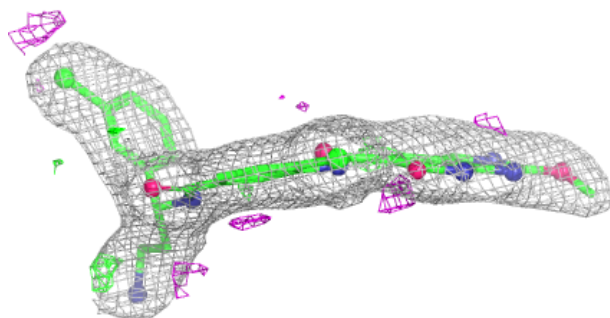
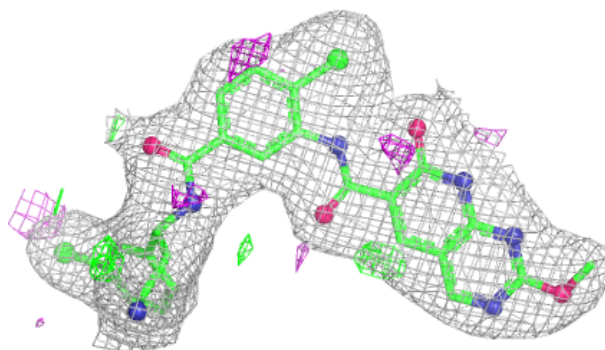
**Electron density around 2C3 D 501:**

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

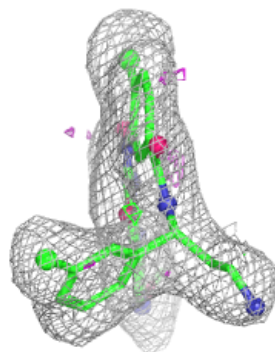
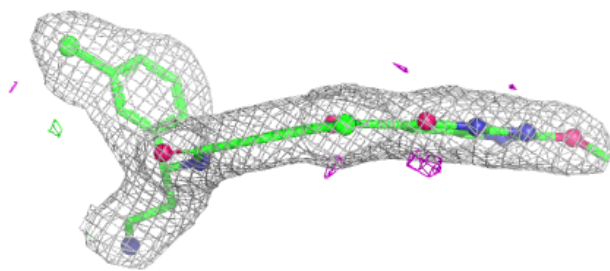
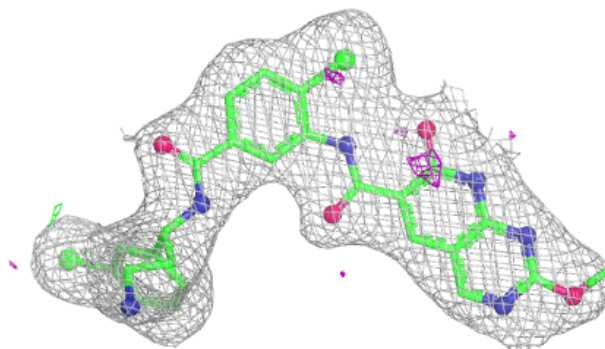


Electron density around 2C3 B 501:

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

**Electron density around 2C3 A 501:**

$2mF_o-DF_c$ (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.