



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 06:11 AM EDT

PDB ID : 4MQ1
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

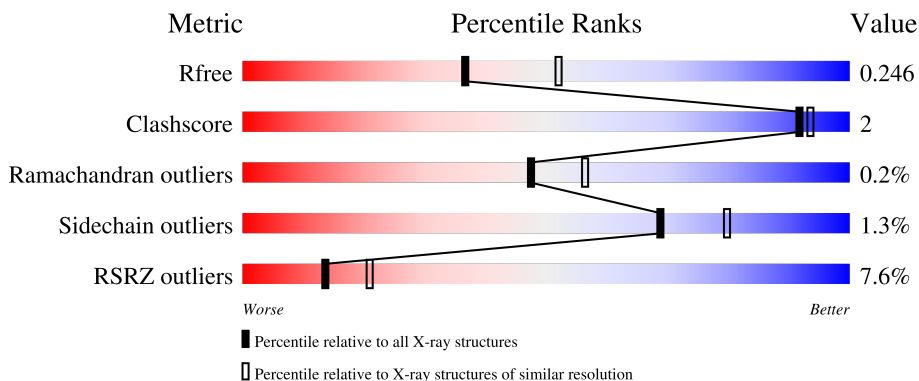
1 Overall quality at a glance

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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	 7% 92% 5% 2%
1	B	361	 6% 87% 7% 6%
1	C	361	 11% 86% 5% 9%
1	D	361	 5% 87% 6% 7%

2 Entry composition i

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.

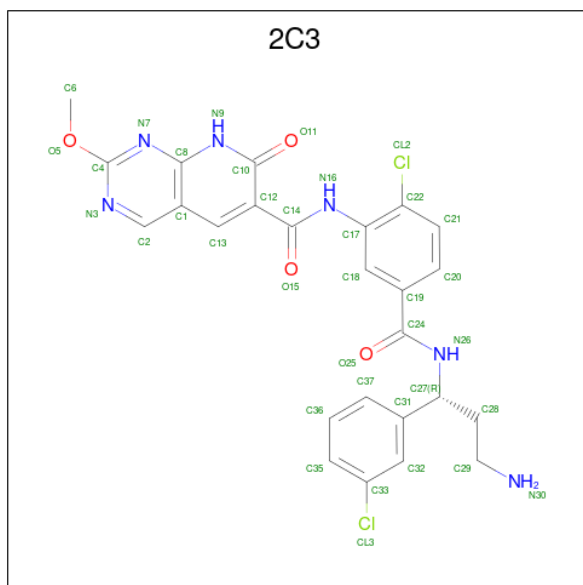
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

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

There are 8 discrepancies between the modelled and reference sequences:

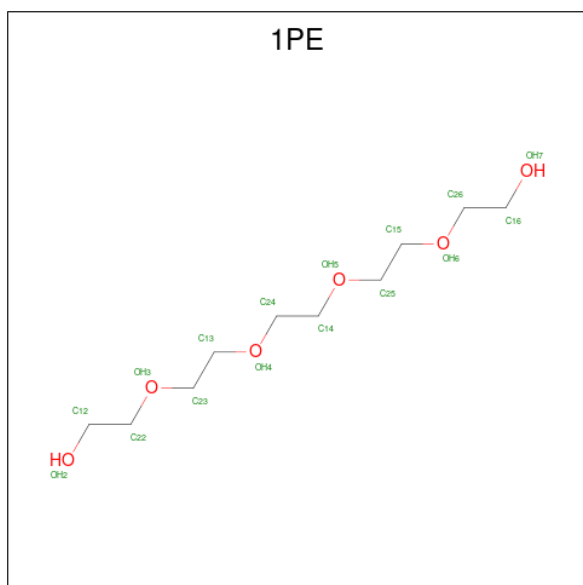
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	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 (three-letter code: 2C3) (formula: C₂₅H₂₂Cl₂N₆O₄).



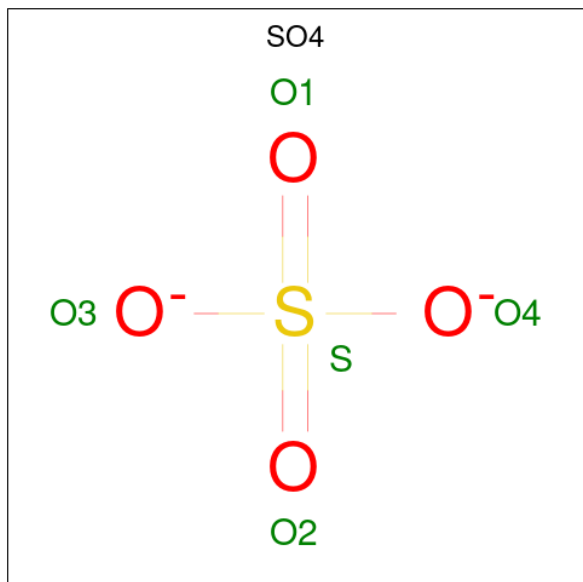
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
2	A	1	Total	C	Cl	N	O	0	0
			37	25	2	6	4		
2	B	1	Total	C	Cl	N	O	0	0
			37	25	2	6	4		
2	C	1	Total	C	Cl	N	O	0	0
			37	25	2	6	4		
2	D	1	Total	C	Cl	N	O	0	0
			37	25	2	6	4		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 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 (three-letter code: 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		

Continued on next page...

Continued from previous page...

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		

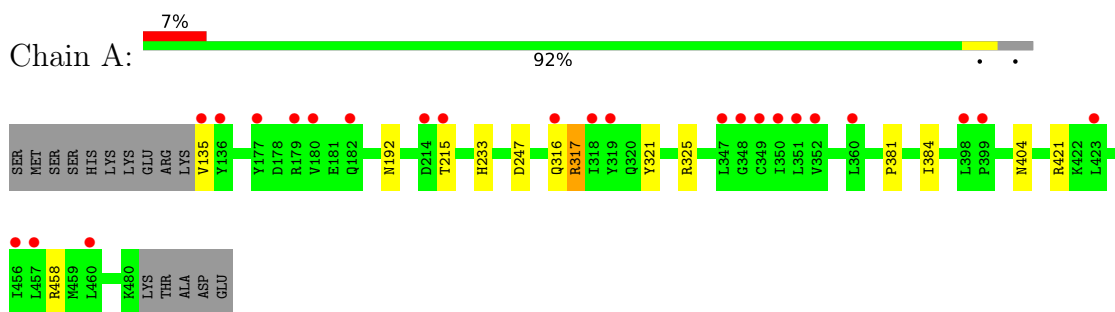
- Molecule 5 is water.

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		

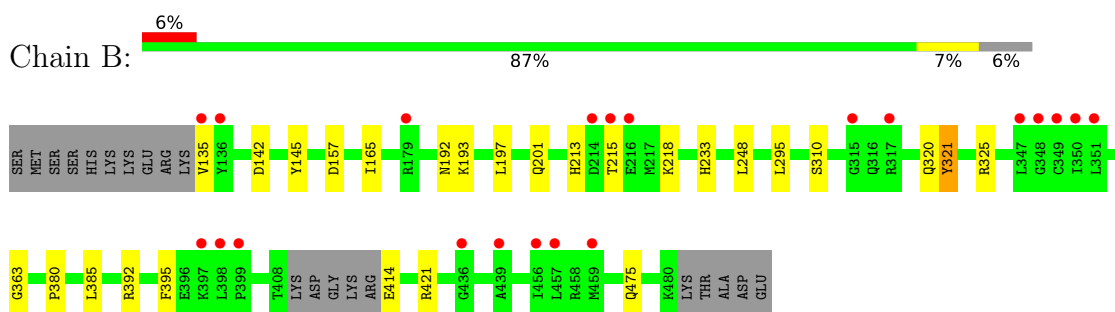
3 Residue-property plots [i](#)

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.

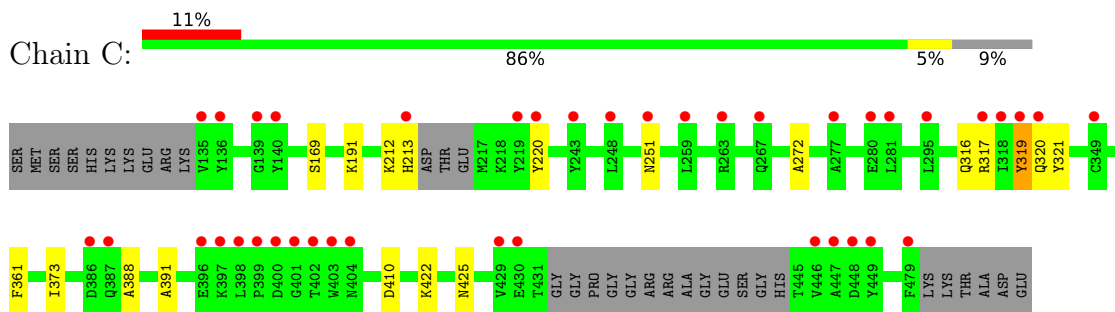
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



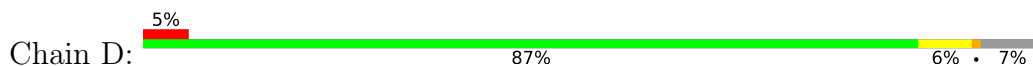
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

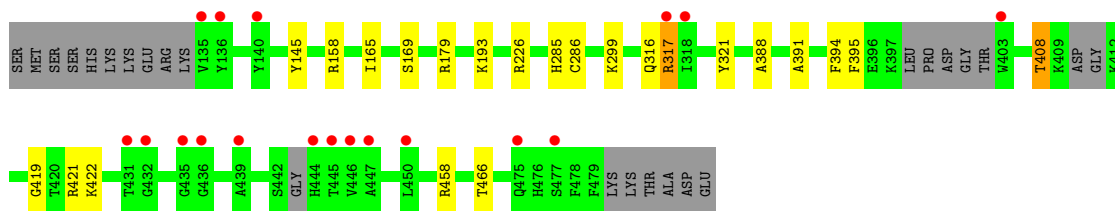


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- 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 39.44 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.83-2.35) 99.7 (39.44-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.34Å)	Xtrriage
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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, SO4, 1PE, 2C3

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	0.68	0/2862	0.79	6/3862 (0.2%)
1	B	0.61	0/2819	0.74	2/3806 (0.1%)
1	C	0.51	0/2679	0.67	1/3628 (0.0%)
1	D	0.54	0/2757	0.70	1/3725 (0.0%)
All	All	0.59	0/11117	0.73	10/15021 (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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	458	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	247	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	325	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	142	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	325	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	421	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	421	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	320	GLN	N-CA-C	-5.06	97.33	111.00
1	B	421	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2829	0	2803	4	0
1	B	2771	0	2748	11	0
1	C	2635	0	2561	6	0
1	D	2710	0	2653	13	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	35	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 (35) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:320:GLN:O	1:B:321:PTR:C	2.58	0.51
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:C:316:GLN:O	1:C:317:ARG:C	2.53	0.47
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:A:316:GLN:O	1:A:317:ARG:C	2.56	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:C:422:LYS:HB2	1:C:425:ASN:HD22	1.85	0.42
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: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%)	41	47
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%)	41	47
All	All	1330/1444 (92%)	1259 (95%)	69 (5%)	2 (0%)	47	56

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%)	298 (99%)	3 (1%)	76	85
1	B	297/320 (93%)	292 (98%)	5 (2%)	60	72
1	C	277/320 (87%)	272 (98%)	5 (2%)	59	70
1	D	284/320 (89%)	282 (99%)	2 (1%)	84	91
All	All	1159/1280 (90%)	1144 (99%)	15 (1%)	69	80

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

Mol	Chain	Res	Type
1	A	135	VAL
1	A	215	THR
1	A	404	ASN
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	251	ASN
1	C	319	TYR
1	C	410	ASP
1	D	169	SER
1	D	408	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	383	HIS
1	B	404	ASN
1	B	425	ASN
1	C	198	ASN
1	C	253	ASN
1	C	404	ASN
1	C	425	ASN
1	C	469	GLN
1	D	198	ASN
1	D	404	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	D	321	1	15,16,17	0.90	1 (6%)	19,22,24	2.00	5 (26%)
1	PTR	A	321[B]	1	15,16,17	1.47	1 (6%)	19,22,24	1.56	3 (15%)
1	PTR	C	321	1	15,16,17	0.96	1 (6%)	19,22,24	2.30	4 (21%)
1	PTR	A	321[A]	1	15,16,17	0.92	0	19,22,24	1.85	4 (21%)
1	PTR	B	321	1	15,16,17	1.59	3 (20%)	19,22,24	1.42	4 (21%)

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	D	321	1	-	3/10/11/13	0/1/1/1
1	PTR	A	321[B]	1	-	2/10/11/13	0/1/1/1
1	PTR	C	321	1	-	3/10/11/13	0/1/1/1
1	PTR	A	321[A]	1	-	2/10/11/13	0/1/1/1
1	PTR	B	321	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	4.22	1.65	1.59
1	B	321	PTR	P-OH	3.92	1.65	1.59
1	C	321	PTR	P-OH	2.64	1.63	1.59
1	B	321	PTR	CE2-CD2	2.44	1.43	1.38
1	B	321	PTR	CE2-CZ	2.08	1.42	1.38
1	D	321	PTR	OH-CZ	-2.05	1.36	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	PTR	CB-CA-C	7.59	125.69	111.47
1	A	321[A]	PTR	CG-CB-CA	-5.56	102.85	114.10
1	D	321	PTR	CG-CB-CA	-5.07	103.83	114.10
1	C	321	PTR	CG-CB-CA	4.28	122.76	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321[B]	PTR	P-OH-CZ	3.37	134.57	123.75
1	D	321	PTR	CB-CA-C	3.24	117.53	111.47
1	B	321	PTR	P-OH-CZ	3.23	134.10	123.75
1	A	321[A]	PTR	CB-CA-C	-3.18	105.51	111.47
1	A	321[A]	PTR	O3P-P-O2P	2.95	118.91	107.64
1	C	321	PTR	O2P-P-OH	-2.88	96.22	105.24
1	C	321	PTR	O3P-P-O2P	2.88	118.65	107.64
1	D	321	PTR	O3P-P-O2P	2.87	118.61	107.64
1	D	321	PTR	P-OH-CZ	-2.74	114.96	123.75
1	A	321[B]	PTR	CE2-CZ-CE1	-2.49	116.34	120.18
1	D	321	PTR	CD2-CG-CD1	2.46	122.03	118.17
1	A	321[A]	PTR	CB-CG-CD2	-2.37	116.20	120.91
1	B	321	PTR	OH-P-O1P	-2.20	101.01	109.31
1	B	321	PTR	CE2-CZ-CE1	-2.19	116.80	120.18
1	A	321[B]	PTR	OH-CZ-CE1	2.18	125.72	119.23
1	B	321	PTR	OH-CZ-CE2	2.16	125.66	119.23

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
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 monosaccharides 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
2	2C3	A	501	-	39,40,40	2.17	11 (28%)	52,56,56	2.38	17 (32%)
4	SO4	C	504	-	4,4,4	0.52	0	6,6,6	0.24	0
4	SO4	D	504	-	4,4,4	0.46	0	6,6,6	0.58	0
3	1PE	A	502	-	15,15,15	0.68	0	14,14,14	0.61	0
4	SO4	A	504	-	4,4,4	0.64	0	6,6,6	0.47	0
3	1PE	C	502	-	15,15,15	0.76	0	14,14,14	0.50	0
3	1PE	B	503	-	12,12,15	0.79	0	11,11,14	0.91	0
4	SO4	D	503	-	4,4,4	0.36	0	6,6,6	0.37	0
2	2C3	B	501	-	39,40,40	1.99	10 (25%)	52,56,56	2.21	17 (32%)
2	2C3	C	501	-	39,40,40	2.13	9 (23%)	52,56,56	2.18	14 (26%)
3	1PE	D	502	-	15,15,15	0.54	0	14,14,14	0.71	0
4	SO4	B	504	-	4,4,4	0.28	0	6,6,6	0.63	0
4	SO4	A	505	-	4,4,4	0.42	0	6,6,6	0.88	0
4	SO4	C	503	-	4,4,4	0.33	0	6,6,6	0.21	0
4	SO4	B	505	-	4,4,4	0.48	0	6,6,6	0.49	0
2	2C3	D	501	-	39,40,40	2.06	11 (28%)	52,56,56	2.55	19 (36%)
3	1PE	B	502	-	15,15,15	0.66	0	14,14,14	0.33	0
3	1PE	A	503	-	15,15,15	0.56	0	14,14,14	0.65	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	2C3	A	501	-	-	4/25/25/25	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	502	-	-	4/13/13/13	-
3	1PE	C	502	-	-	3/13/13/13	-
3	1PE	B	503	-	-	4/10/10/13	-
2	2C3	B	501	-	-	7/25/25/25	0/4/4/4
2	2C3	C	501	-	-	5/25/25/25	0/4/4/4
3	1PE	D	502	-	-	2/13/13/13	-
2	2C3	D	501	-	-	6/25/25/25	0/4/4/4
3	1PE	B	502	-	-	4/13/13/13	-
3	1PE	A	503	-	-	5/13/13/13	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	2C3	C31-C27	-8.64	1.39	1.52
2	D	501	2C3	C31-C27	-8.44	1.39	1.52
2	B	501	2C3	C31-C27	-7.60	1.40	1.52
2	A	501	2C3	C31-C27	-7.24	1.41	1.52
2	A	501	2C3	C10-N9	6.11	1.44	1.35
2	A	501	2C3	C19-C24	-5.38	1.39	1.50
2	C	501	2C3	C10-N9	4.74	1.42	1.35
2	B	501	2C3	C19-C24	-4.59	1.40	1.50
2	C	501	2C3	C19-C24	-4.21	1.41	1.50
2	B	501	2C3	C33-CL3	-3.45	1.67	1.74
2	D	501	2C3	C10-N9	3.35	1.40	1.35
2	D	501	2C3	C19-C24	-3.33	1.43	1.50
2	D	501	2C3	C2-N3	3.30	1.41	1.34
2	D	501	2C3	C22-CL2	3.27	1.81	1.73
2	B	501	2C3	C12-C14	-3.12	1.39	1.49
2	C	501	2C3	C17-N16	-3.12	1.35	1.41
2	B	501	2C3	C1-C13	-2.89	1.37	1.43
2	A	501	2C3	C2-N3	2.84	1.40	1.34
2	C	501	2C3	C33-CL3	-2.82	1.68	1.74
2	D	501	2C3	C28-C27	-2.82	1.49	1.53
2	A	501	2C3	C17-N16	-2.68	1.36	1.41
2	C	501	2C3	C2-N3	2.66	1.40	1.34
2	A	501	2C3	C12-C10	-2.65	1.40	1.45
2	A	501	2C3	C33-CL3	-2.50	1.69	1.74
2	D	501	2C3	C12-C14	-2.49	1.41	1.49
2	D	501	2C3	C17-N16	-2.44	1.37	1.41
2	A	501	2C3	C27-N26	2.40	1.49	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	2C3	C17-N16	-2.38	1.37	1.41
2	C	501	2C3	C28-C27	-2.35	1.50	1.53
2	A	501	2C3	C12-C14	-2.33	1.42	1.49
2	B	501	2C3	C2-N3	2.32	1.39	1.34
2	B	501	2C3	C13-C12	2.31	1.40	1.36
2	D	501	2C3	C1-C13	-2.27	1.39	1.43
2	C	501	2C3	C13-C12	2.27	1.40	1.36
2	B	501	2C3	C12-C10	-2.22	1.40	1.45
2	D	501	2C3	C13-C12	2.22	1.40	1.36
2	A	501	2C3	C4-N7	2.20	1.37	1.33
2	B	501	2C3	C22-CL2	-2.12	1.68	1.73
2	A	501	2C3	C1-C13	-2.09	1.39	1.43
2	D	501	2C3	C4-N3	2.07	1.35	1.32
2	C	501	2C3	C1-C13	-2.04	1.39	1.43

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C3	N3-C4-N7	-11.07	119.63	128.43
2	A	501	2C3	N3-C4-N7	-8.93	121.33	128.43
2	C	501	2C3	N3-C4-N7	-8.76	121.46	128.43
2	B	501	2C3	N3-C4-N7	-8.56	121.62	128.43
2	D	501	2C3	C28-C27-N26	-5.67	101.94	110.19
2	B	501	2C3	C2-N3-C4	4.95	120.98	114.97
2	A	501	2C3	C2-N3-C4	4.78	120.77	114.97
2	A	501	2C3	N9-C8-N7	4.55	122.54	116.53
2	D	501	2C3	C2-N3-C4	4.40	120.31	114.97
2	C	501	2C3	C2-C1-C8	4.39	119.14	114.61
2	A	501	2C3	C2-C1-C8	4.34	119.09	114.61
2	A	501	2C3	C22-C17-N16	-4.14	112.68	119.24
2	D	501	2C3	C2-C1-C8	4.12	118.87	114.61
2	A	501	2C3	C12-C10-N9	4.05	121.41	114.41
2	B	501	2C3	C2-C1-C8	3.91	118.65	114.61
2	B	501	2C3	C1-C2-N3	-3.87	118.32	123.70
2	D	501	2C3	C4-N7-C8	3.86	122.64	113.80
2	A	501	2C3	C1-C2-N3	-3.85	118.35	123.70
2	B	501	2C3	C22-C17-N16	-3.76	113.30	119.24
2	A	501	2C3	C8-C1-C13	3.74	123.00	118.52
2	D	501	2C3	C8-N9-C10	-3.74	120.83	124.14
2	C	501	2C3	C8-N9-C10	-3.69	120.87	124.14
2	D	501	2C3	C1-C2-N3	-3.66	118.61	123.70
2	B	501	2C3	C8-N9-C10	-3.43	121.10	124.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	2C3	C22-C17-N16	-3.38	113.89	119.24
2	C	501	2C3	C12-C10-N9	3.30	120.11	114.41
2	C	501	2C3	C4-N7-C8	3.29	121.33	113.80
2	B	501	2C3	C1-C13-C12	-3.28	118.93	122.10
2	C	501	2C3	C2-N3-C4	3.26	118.93	114.97
2	A	501	2C3	C8-N9-C10	-3.25	121.26	124.14
2	C	501	2C3	C1-C2-N3	-3.21	119.24	123.70
2	B	501	2C3	C12-C10-N9	3.14	119.83	114.41
2	D	501	2C3	C31-C27-N26	-3.11	106.18	112.00
2	C	501	2C3	N9-C8-N7	3.03	120.53	116.53
2	D	501	2C3	C12-C10-N9	3.01	119.61	114.41
2	A	501	2C3	O5-C4-N7	2.98	125.97	116.25
2	D	501	2C3	C22-C17-N16	-2.98	114.53	119.24
2	C	501	2C3	O11-C10-N9	-2.90	116.40	121.67
2	C	501	2C3	C14-C12-C10	2.88	126.60	120.32
2	B	501	2C3	C8-C1-C13	2.81	121.88	118.52
2	C	501	2C3	C27-N26-C24	-2.77	118.77	122.34
2	A	501	2C3	C13-C12-C10	-2.73	116.22	119.14
2	A	501	2C3	O11-C10-C12	-2.67	119.73	125.99
2	D	501	2C3	N9-C8-N7	2.66	120.04	116.53
2	D	501	2C3	C27-N26-C24	2.58	125.66	122.34
2	C	501	2C3	C13-C12-C10	-2.57	116.38	119.14
2	A	501	2C3	C14-C12-C10	2.54	125.86	120.32
2	B	501	2C3	C6-O5-C4	-2.51	113.57	117.58
2	D	501	2C3	C14-C12-C10	2.49	125.74	120.32
2	D	501	2C3	O11-C10-N9	-2.48	117.17	121.67
2	A	501	2C3	C18-C17-N16	2.48	128.45	121.90
2	A	501	2C3	C2-C1-C13	-2.45	117.90	122.46
2	B	501	2C3	C17-C22-CL2	-2.44	116.76	119.54
2	A	501	2C3	C4-N7-C8	2.40	119.30	113.80
2	A	501	2C3	C12-C14-N16	2.36	118.97	115.48
2	D	501	2C3	C18-C17-N16	2.33	128.07	121.90
2	B	501	2C3	O11-C10-N9	-2.31	117.47	121.67
2	D	501	2C3	C6-O5-C4	-2.25	113.98	117.58
2	B	501	2C3	C28-C27-N26	-2.21	106.98	110.19
2	D	501	2C3	C19-C18-C17	2.19	123.72	119.70
2	B	501	2C3	C31-C27-N26	-2.16	107.95	112.00
2	D	501	2C3	C20-C19-C18	-2.16	116.68	119.24
2	C	501	2C3	C18-C17-N16	2.16	127.61	121.90
2	D	501	2C3	O15-C14-C12	-2.11	117.16	121.05
2	B	501	2C3	O5-C4-N7	2.08	123.01	116.25
2	B	501	2C3	O15-C14-C12	-2.02	117.31	121.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	2C3	C18-C17-N16	2.02	127.24	121.90

There are no chirality outliers.

All (44) 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
3	B	502	1PE	OH7-C16-C26-OH6
2	A	501	2C3	N26-C27-C28-C29
2	B	501	2C3	N7-C4-O5-C6
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
2	B	501	2C3	N3-C4-O5-C6
3	C	502	1PE	OH4-C13-C23-OH3
3	A	503	1PE	OH2-C12-C22-OH3
3	A	503	1PE	OH6-C15-C25-OH5
3	A	502	1PE	OH2-C12-C22-OH3
3	B	503	1PE	OH6-C15-C25-OH5
2	D	501	2C3	C28-C27-C31-C37
3	A	503	1PE	C12-C22-OH3-C23
3	B	503	1PE	OH2-C12-C22-OH3
3	C	502	1PE	OH7-C16-C26-OH6
2	C	501	2C3	C27-C28-C29-N30
2	D	501	2C3	C27-C28-C29-N30
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

Continued on next page...

Continued from previous page...

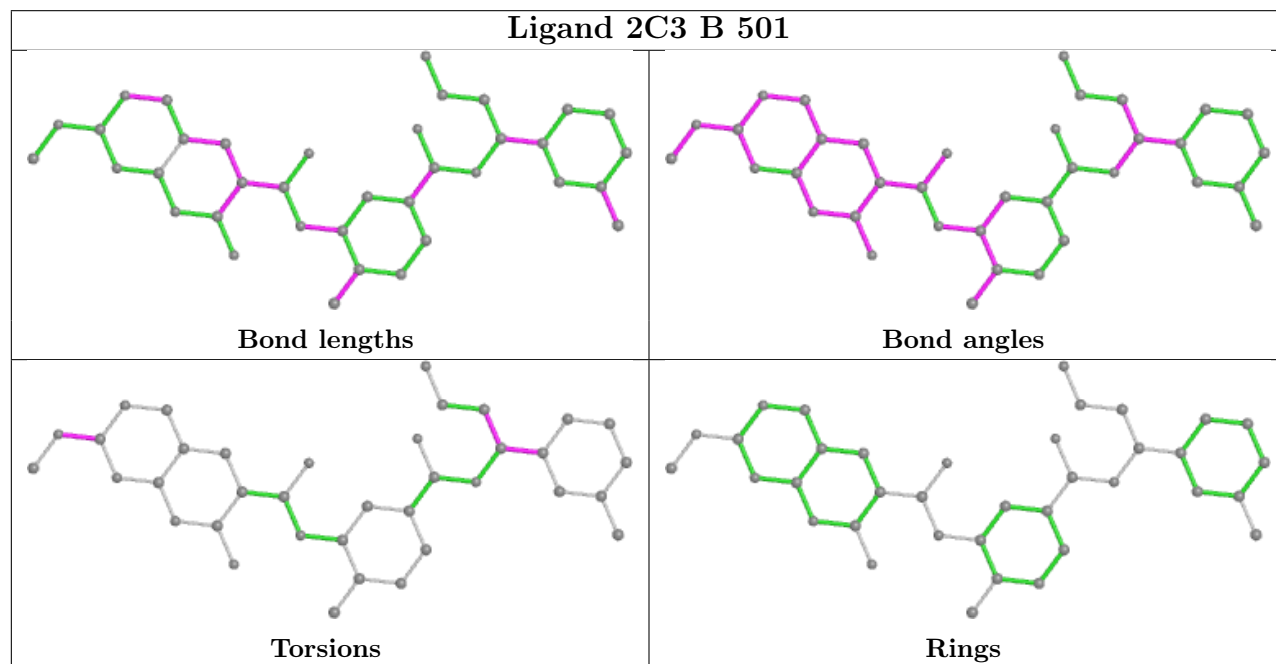
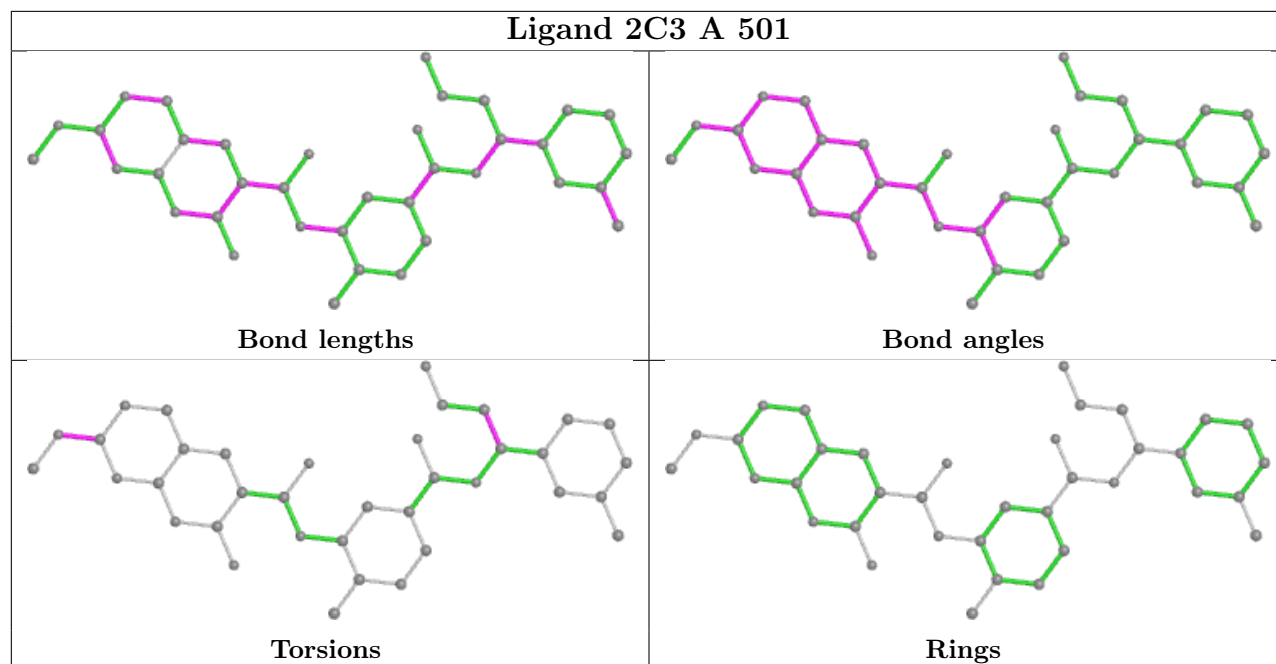
Mol	Chain	Res	Type	Atoms
3	C	502	1PE	OH6-C15-C25-OH5
2	B	501	2C3	N26-C27-C31-C32
2	D	501	2C3	N26-C27-C31-C32
3	B	502	1PE	OH5-C14-C24-OH4
3	A	502	1PE	C16-C26-OH6-C15
3	D	502	1PE	OH2-C12-C22-OH3
2	B	501	2C3	N26-C27-C31-C37
2	B	501	2C3	C28-C27-C31-C37

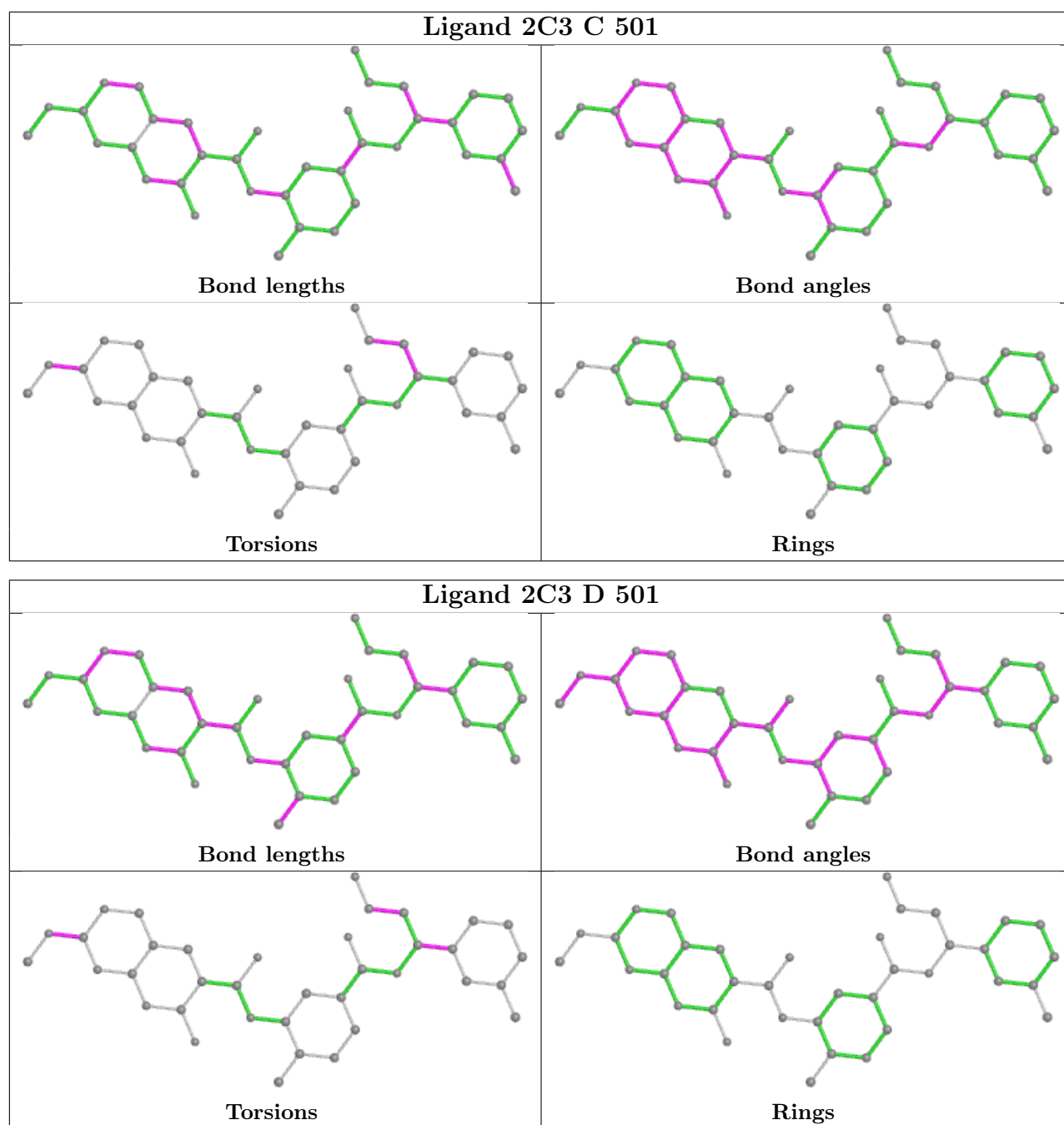
There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

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	345/361 (95%)	0.23	24 (6%) 16 24	25, 38, 70, 94	0
1	B	340/361 (94%)	0.21	21 (6%) 20 29	27, 40, 67, 99	0
1	C	328/361 (90%)	0.59	40 (12%) 4 7	40, 62, 96, 115	0
1	D	336/361 (93%)	0.20	18 (5%) 25 37	34, 54, 87, 117	0
All	All	1349/1444 (93%)	0.31	103 (7%) 13 21	25, 49, 86, 117	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	398	LEU	6.6
1	A	135	VAL	5.7
1	C	403	TRP	5.7
1	D	318	ILE	5.6
1	C	402	THR	5.5
1	C	399	PRO	5.0
1	C	401	GLY	4.8
1	B	215	THR	4.7
1	C	213	HIS	4.7
1	B	214	ASP	4.4
1	C	318	ILE	4.4
1	B	317	ARG	4.4
1	A	318	ILE	4.2
1	C	448	ASP	4.2
1	B	135	VAL	4.2
1	C	136	TYR	4.1
1	A	215	THR	4.1
1	C	397	LYS	4.0
1	D	136	TYR	3.9
1	D	445	THR	3.8
1	C	259	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	251	ASN	3.7
1	B	350	ILE	3.6
1	C	219	TYR	3.5
1	D	439	ALA	3.5
1	C	400	ASP	3.5
1	D	403	TRP	3.4
1	B	457	LEU	3.4
1	A	456	ILE	3.4
1	C	243	TYR	3.4
1	D	135	VAL	3.4
1	B	351	LEU	3.3
1	B	439	ALA	3.3
1	C	447	ALA	3.2
1	C	319	TYR	3.2
1	A	136	TYR	3.2
1	A	214	ASP	3.2
1	D	447	ALA	3.1
1	C	295	LEU	3.1
1	D	435	GLY	3.1
1	A	460	LEU	3.1
1	C	280	GLU	2.9
1	C	277	ALA	2.9
1	A	180	VAL	2.9
1	A	347	LEU	2.8
1	D	431	THR	2.8
1	B	179	ARG	2.8
1	A	457	LEU	2.7
1	D	432	GLY	2.7
1	C	317	ARG	2.7
1	C	135	VAL	2.7
1	A	350	ILE	2.7
1	C	349	CYS	2.7
1	D	444	HIS	2.7
1	D	450	LEU	2.7
1	B	347	LEU	2.7
1	C	404	ASN	2.6
1	D	436	GLY	2.6
1	C	430	GLU	2.6
1	C	479	PHE	2.6
1	C	263	ARG	2.6
1	B	456	ILE	2.6
1	C	396	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	139	GLY	2.5
1	D	446	VAL	2.5
1	D	475	GLN	2.5
1	B	216	GLU	2.5
1	B	399	PRO	2.4
1	A	182	GLN	2.4
1	A	349	CYS	2.4
1	B	136	TYR	2.4
1	A	398	LEU	2.4
1	B	398	LEU	2.4
1	C	248	LEU	2.4
1	D	477	SER	2.4
1	A	348	GLY	2.3
1	C	220	TYR	2.3
1	C	320	GLN	2.3
1	A	360	LEU	2.3
1	B	315	GLY	2.3
1	A	423	LEU	2.3
1	C	387	GLN	2.3
1	C	386	ASP	2.3
1	A	399	PRO	2.3
1	A	351	LEU	2.3
1	C	429	VAL	2.3
1	A	352	VAL	2.2
1	C	140	TYR	2.2
1	D	140	TYR	2.2
1	C	446	VAL	2.2
1	B	349	CYS	2.2
1	C	267	GLN	2.2
1	B	459	MET	2.2
1	A	316	GLN	2.2
1	A	319	TYR	2.1
1	B	397	LYS	2.1
1	C	281	LEU	2.1
1	C	449	TYR	2.1
1	B	348	GLY	2.1
1	B	436	GLY	2.1
1	D	317	ARG	2.1
1	A	177	TYR	2.0
1	A	179	ARG	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
1	PTR	A	321[A]	16/17	0.89	0.19	28,33,47,53	16
1	PTR	A	321[B]	16/17	0.89	0.19	38,51,56,59	16
1	PTR	C	321	16/17	0.92	0.17	52,73,84,84	0
1	PTR	D	321	16/17	0.93	0.16	55,73,85,88	0
1	PTR	B	321	16/17	0.95	0.15	42,54,57,59	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

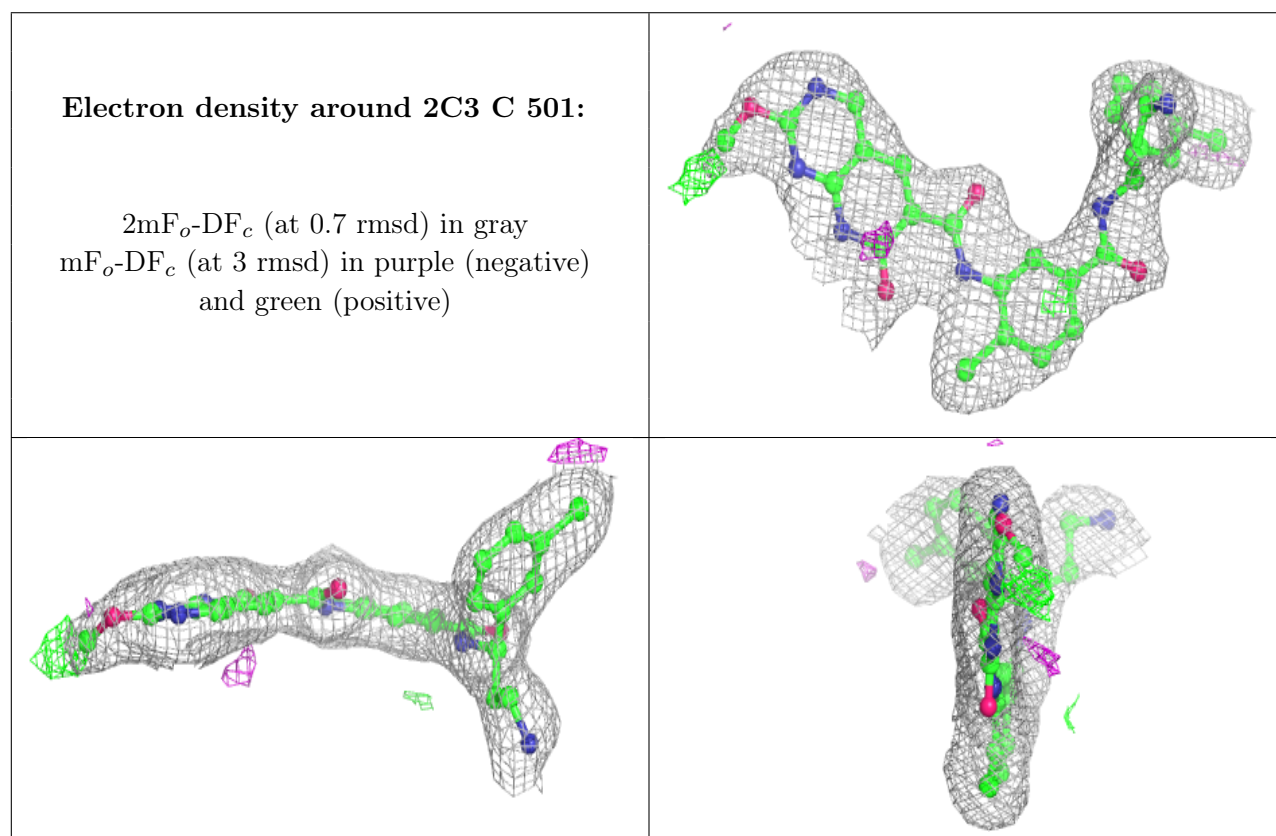
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	D	504	5/5	0.85	0.25	78,86,95,98	0
4	SO4	C	504	5/5	0.88	0.27	74,87,91,92	0
3	1PE	A	502	16/16	0.88	0.24	62,67,87,87	0
3	1PE	C	502	16/16	0.89	0.17	66,71,80,81	0
3	1PE	B	502	16/16	0.90	0.14	48,62,74,75	0
3	1PE	A	503	16/16	0.92	0.23	37,46,54,61	0
4	SO4	A	504	5/5	0.92	0.20	47,55,63,75	0
2	2C3	C	501	37/37	0.93	0.12	52,60,73,75	0
3	1PE	B	503	13/16	0.94	0.17	34,37,40,50	0
2	2C3	A	501	37/37	0.95	0.11	26,34,47,53	0
2	2C3	B	501	37/37	0.95	0.14	30,35,43,51	0
3	1PE	D	502	16/16	0.95	0.14	40,52,62,64	0
2	2C3	D	501	37/37	0.96	0.11	36,44,56,56	0
4	SO4	B	505	5/5	0.96	0.12	42,51,65,71	0
4	SO4	A	505	5/5	0.97	0.10	50,55,61,61	0
4	SO4	D	503	5/5	0.97	0.09	57,63,75,79	0
4	SO4	C	503	5/5	0.97	0.12	80,81,83,95	0

Continued on next page...

Continued from previous page...

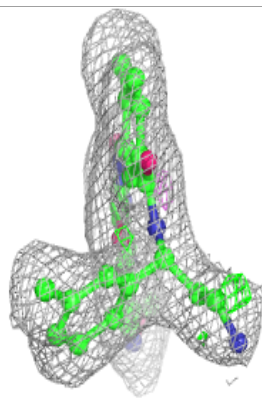
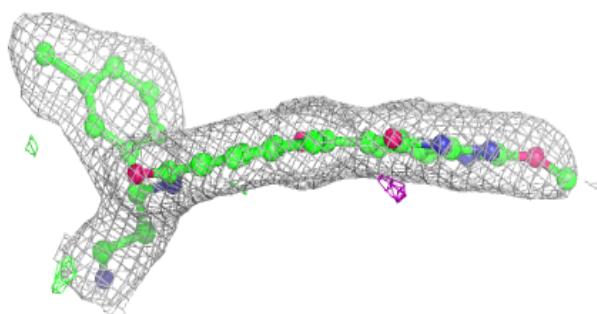
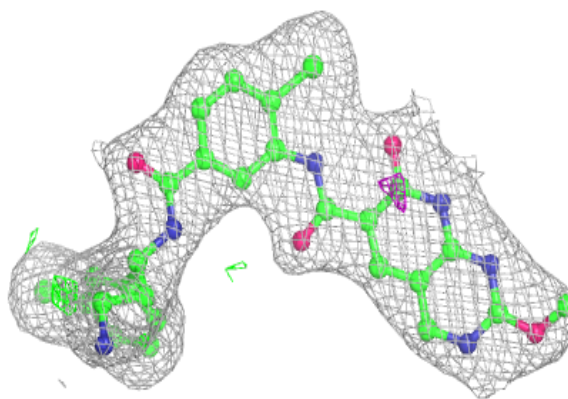
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	504	5/5	0.98	0.11	56,59,63,65	0

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.

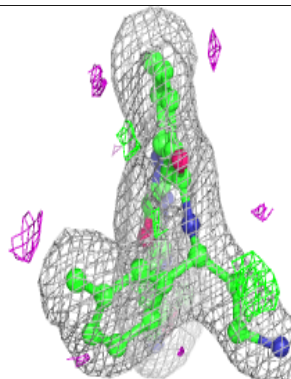
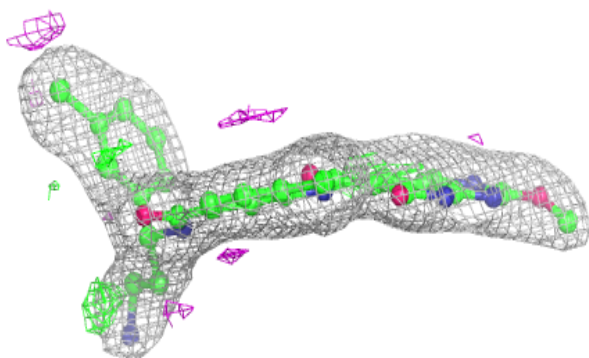
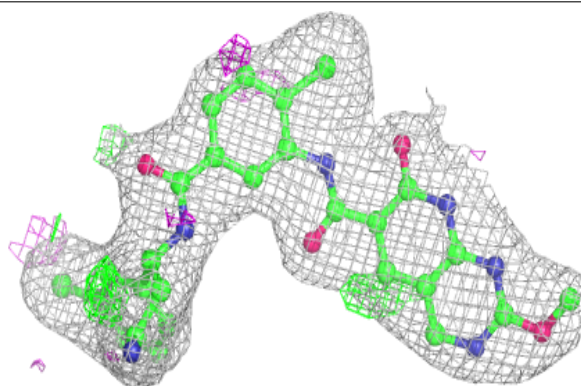


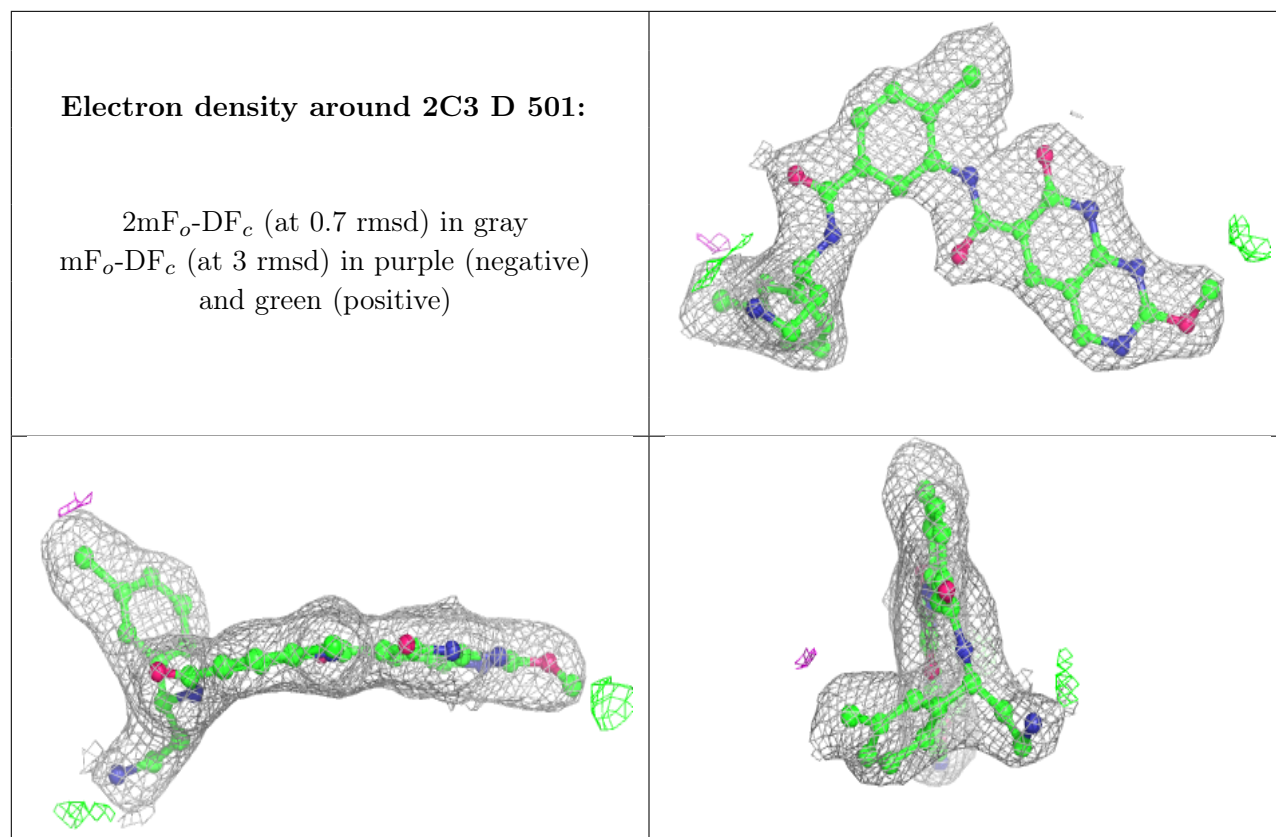
Electron density around 2C3 A 501:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.