



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 02:56 AM EDT

PDB ID : 4MQ2 / pdb_00004mq2
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 : 2.80 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

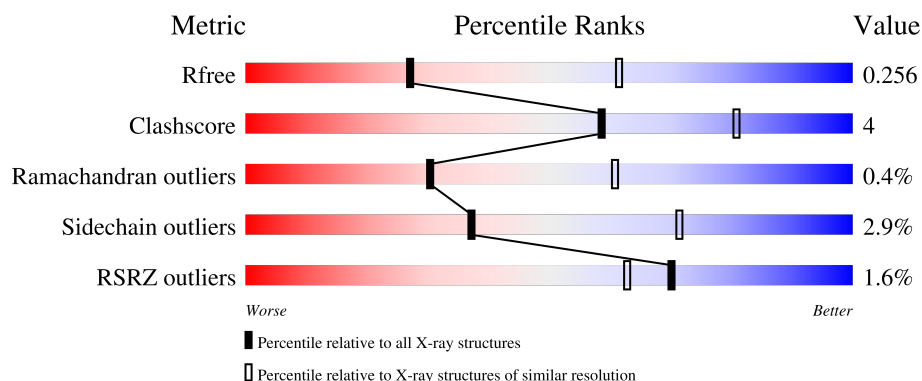
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	
1	B	361	
1	C	361	
1	D	361	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11273 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.

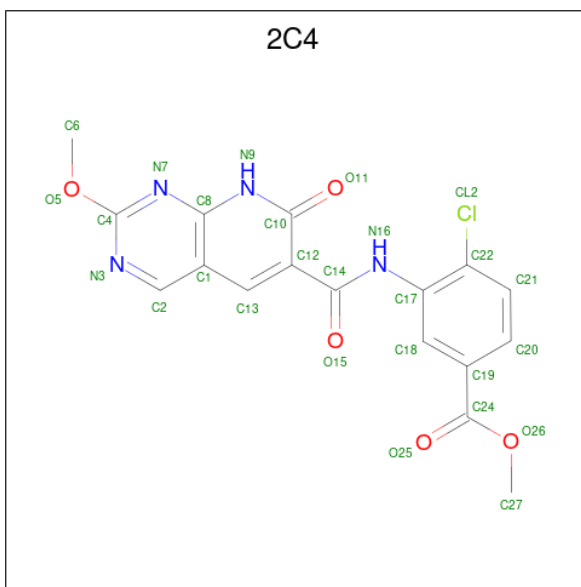
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	P	S	0	0	0
			2800	1800	480	502	1	17			
1	B	339	Total	C	N	O	P	S	0	0	0
			2752	1773	468	493	1	17			
1	C	340	Total	C	N	O	P	S	0	0	0
			2712	1750	457	488	1	16			
1	D	330	Total	C	N	O	P	S	0	1	0
			2662	1722	445	477	1	17			

There are 8 discrepancies between the modelled and reference sequences:

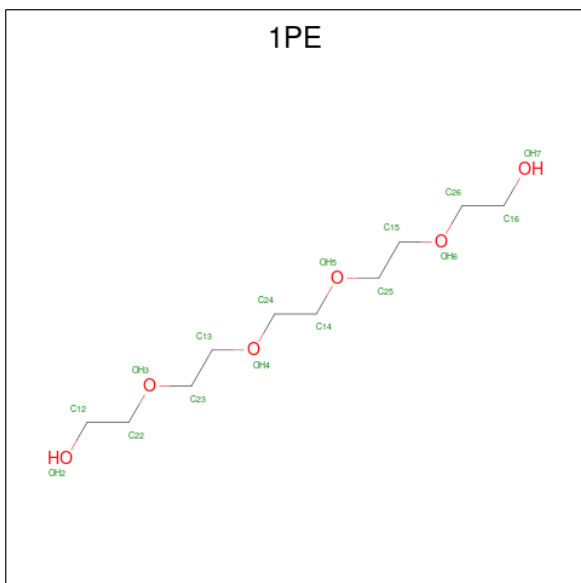
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	125	SER	-	expression tag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

- Molecule 2 is methyl 4-chloro-3-[(2-methoxy-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-6-yl) carbonyl]amino}benzoate (CCD ID: 2C4) (formula: C₁₇H₁₃ClN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	17	1	4	5		
2	B	1	Total	C	Cl	N	O	0	0
			27	17	1	4	5		
2	C	1	Total	C	Cl	N	O	0	0
			27	17	1	4	5		
2	D	1	Total	C	Cl	N	O	0	0
			27	17	1	4	5		

- 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	B	1	Total	O	S	0	0
			5	4	1		

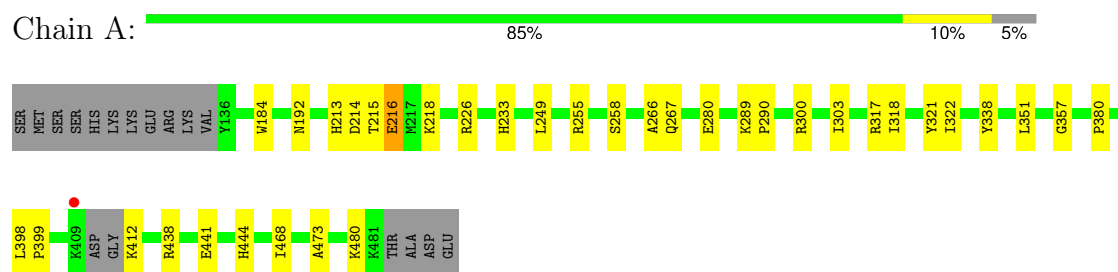
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total 53	O 53	0	0
5	B	33	Total 33	O 33	0	0
5	C	16	Total 16	O 16	0	0
5	D	19	Total 19	O 19	0	0

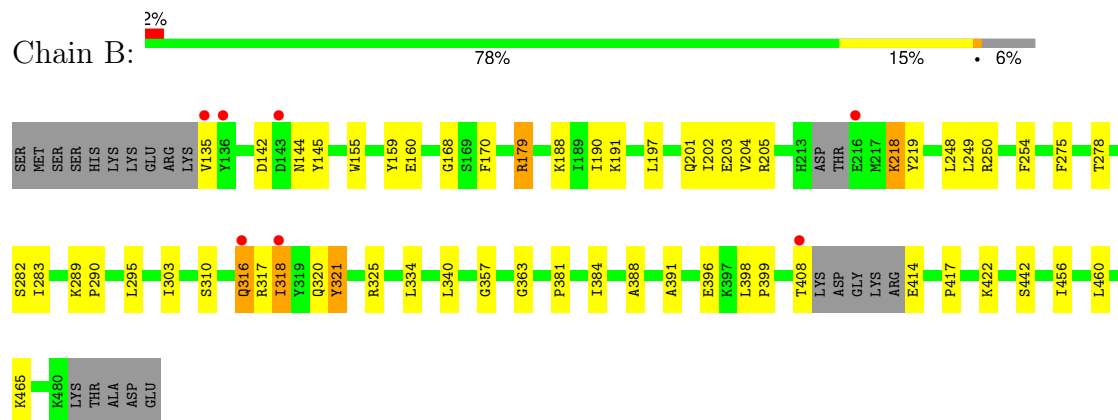
3 Residue-property plots

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.

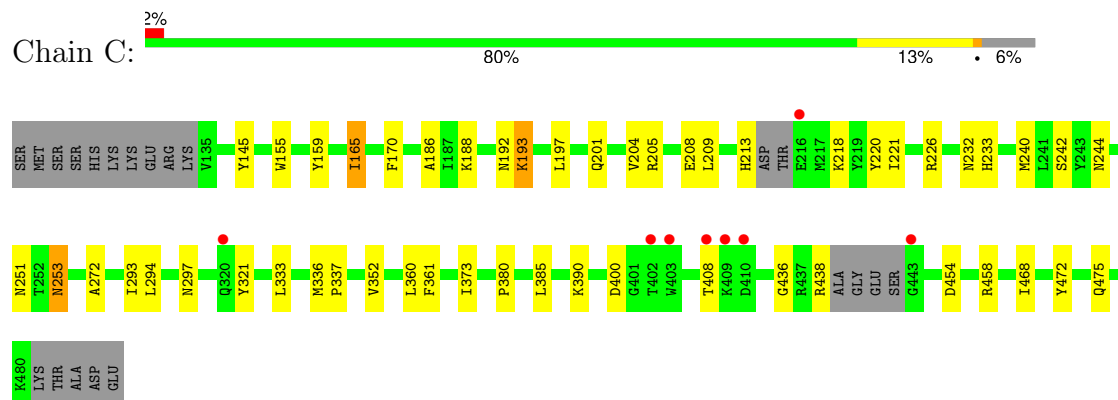
• Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



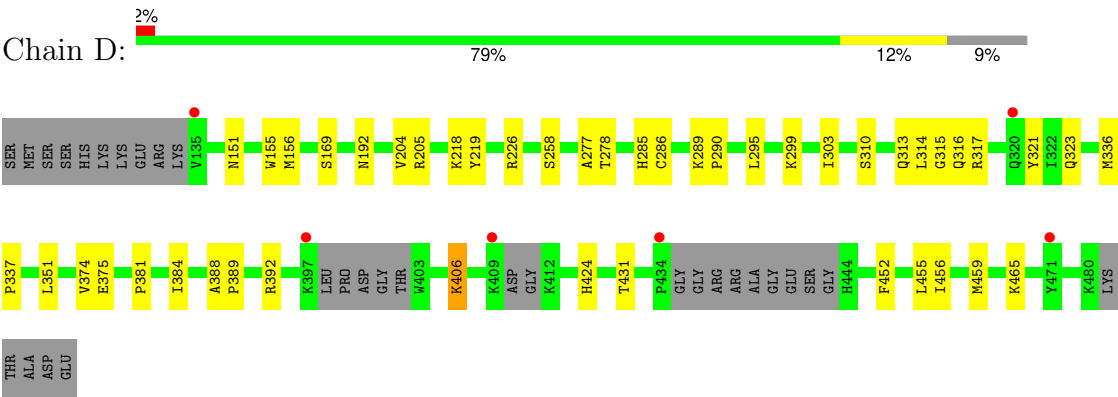
• Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



• 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	264.10Å 65.16Å 138.43Å 90.00° 115.01° 90.00°	Depositor
Resolution (Å)	36.78 – 2.80 36.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.78-2.80) 99.9 (36.78-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.258 0.194 , 0.256	Depositor DCC
R_{free} test set	2652 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11273	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: SO4, 1PE, 2C4, PTR

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	0.98	0/2848	1.04	2/3842 (0.1%)
1	B	0.86	0/2799	1.00	6/3778 (0.2%)
1	C	0.81	0/2759	0.96	2/3733 (0.1%)
1	D	0.80	0/2710	0.94	0/3666
All	All	0.86	0/11116	0.99	10/15019 (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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	GLU	N-CA-C	-6.11	100.19	109.85
1	B	218	LYS	N-CA-C	-5.86	102.62	110.24
1	C	165	ILE	N-CA-C	5.63	117.52	112.17
1	B	417	PRO	O-C-N	5.57	123.77	121.15
1	A	380	PRO	O-C-N	5.53	123.75	121.15
1	C	251	ASN	N-CA-C	5.44	118.71	111.75
1	B	316	GLN	N-CA-C	5.36	116.97	108.67
1	B	283	ILE	CB-CA-C	-5.32	104.31	110.91
1	B	417	PRO	CA-C-N	5.17	126.30	119.84
1	B	417	PRO	C-N-CA	5.17	126.30	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	LYS	Peptide
1	B	316	GLN	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	2800	0	2778	18	0
1	B	2752	0	2726	27	0
1	C	2712	0	2636	24	0
1	D	2662	0	2597	26	0
2	A	27	0	13	2	0
2	B	27	0	13	0	0
2	C	27	0	13	0	0
2	D	27	0	13	0	0
3	A	32	0	44	1	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	15	0	0	0	0
5	A	53	0	0	0	0
5	B	33	0	0	0	0
5	C	16	0	0	1	0
5	D	19	0	0	2	0
All	All	11273	0	10916	95	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 4.

All (95) 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:B:317:ARG:CB	1:B:318:ILE:HG13	1.67	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:CB	1:B:318:ILE:CG1	2.41	0.98
1:D:151:ASN:HB3	5:D:609:HOH:O	1.82	0.80
1:A:213:HIS:O	1:A:218:LYS:HD3	1.86	0.75
1:A:258:SER:HA	1:A:438:ARG:HH21	1.57	0.70
1:D:455:LEU:HG	1:D:459:MET:HE2	1.74	0.68
1:B:414:GLU:OE2	1:D:299:LYS:NZ	2.26	0.67
1:B:325:ARG:HD2	1:B:363:GLY:O	1.98	0.64
1:B:250:ARG:HG2	1:B:254:PHE:CZ	2.34	0.62
1:D:226[A]:ARG:NH2	1:D:226[A]:ARG:HG3	2.15	0.61
1:A:322:ILE:HD11	1:A:338:TYR:CZ	2.37	0.59
2:A:501:2C4:O15	2:A:501:2C4:H10	2.04	0.58
1:D:226[A]:ARG:HG3	1:D:226[A]:ARG:HH21	1.69	0.57
1:B:317:ARG:CB	1:B:318:ILE:HG12	2.35	0.56
1:C:361:PHE:CE1	1:C:373:ILE:HA	2.41	0.56
1:A:322:ILE:CD1	1:A:338:TYR:CZ	2.89	0.56
1:A:192:ASN:HB2	1:A:233:HIS:CE1	2.42	0.55
1:D:226[A]:ARG:HH21	1:D:226[A]:ARG:CG	2.18	0.55
1:A:322:ILE:HD11	1:A:338:TYR:CE2	2.43	0.54
1:D:392:ARG:O	1:D:406:LYS:HE3	2.08	0.53
1:A:398:LEU:O	1:A:399:PRO:C	2.50	0.53
1:D:424:HIS:HB2	5:D:607:HOH:O	2.08	0.53
1:C:186:ALA:HB2	1:C:240:MET:HE3	1.91	0.52
1:A:438:ARG:HG3	1:A:444:HIS:CD2	2.45	0.52
1:B:320:GLN:O	1:B:321:PTR:C	2.59	0.51
1:A:266:ALA:HB2	1:A:351:LEU:HD22	1.93	0.51
1:D:286:CYS:O	1:D:323:GLN:HA	2.11	0.50
1:D:351:LEU:HD12	1:D:459:MET:HE1	1.94	0.50
1:A:213:HIS:O	1:A:218:LYS:CD	2.59	0.49
1:A:317:ARG:HD2	1:A:338:TYR:CZ	2.47	0.49
1:A:216:GLU:HG3	1:C:297:ASN:HD21	1.77	0.49
1:B:197:LEU:O	1:B:201:GLN:HG3	2.13	0.49
1:D:452:PHE:CE1	1:D:456:ILE:HD11	2.48	0.49
1:A:184:TRP:NE1	3:A:502:1PE:H252	2.28	0.48
1:B:188:LYS:NZ	1:B:203:GLU:OE1	2.47	0.48
1:D:374:VAL:O	1:D:375:GLU:C	2.55	0.48
1:D:388:ALA:O	1:D:389:PRO:C	2.56	0.48
1:B:381:PRO:HG2	1:B:384:ILE:HD12	1.95	0.48
1:C:472:TYR:HA	1:C:475:GLN:HG3	1.96	0.48
1:B:249:LEU:HD22	1:B:357:GLY:HA2	1.97	0.47
1:C:213:HIS:C	1:C:218:LYS:HD3	2.40	0.47
1:C:155:TRP:HB2	1:C:159:TYR:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:TRP:O	1:D:156:MET:C	2.58	0.46
1:D:285:HIS:O	1:D:286:CYS:HB2	2.15	0.46
1:C:436:GLY:O	1:C:438:ARG:N	2.49	0.46
1:B:144:ASN:O	1:B:145:TYR:HB2	2.16	0.45
1:C:352:VAL:HG11	1:C:360:LEU:HD13	1.98	0.45
1:D:277:ALA:O	1:D:278:THR:C	2.59	0.45
1:C:454:ASP:O	1:C:458:ARG:HG2	2.15	0.45
1:C:145:TYR:CE2	1:C:193:LYS:HD3	2.52	0.45
1:B:289:LYS:HB2	1:B:290:PRO:HD2	1.99	0.45
1:C:165:ILE:CD1	1:C:240:MET:HE1	2.47	0.45
1:B:398:LEU:HB3	1:B:399:PRO:HD2	1.99	0.45
1:B:142:ASP:OD1	1:B:142:ASP:C	2.60	0.45
2:A:501:2C4:O11	2:A:501:2C4:N16	2.46	0.44
1:D:289:LYS:O	1:D:290:PRO:C	2.58	0.44
1:B:190:ILE:HG22	1:B:191:LYS:N	2.32	0.44
1:B:334:LEU:HB3	1:B:388:ALA:HB1	1.99	0.44
1:A:258:SER:CA	1:A:438:ARG:HH21	2.30	0.43
1:C:380:PRO:HG2	1:C:385:LEU:HD21	1.99	0.43
1:B:218:LYS:O	1:B:219:TYR:CB	2.67	0.43
1:A:214:ASP:O	1:A:214:ASP:CG	2.61	0.43
1:C:170:PHE:CD1	1:C:188:LYS:HE3	2.53	0.43
1:C:204:VAL:O	1:C:205:ARG:C	2.61	0.43
1:C:220:TYR:HB3	1:C:272:ALA:HB2	2.01	0.43
1:B:456:ILE:O	1:B:460:LEU:HG	2.19	0.43
1:C:244:ASN:HA	1:C:294:LEU:HA	2.00	0.42
1:B:295:LEU:HD23	1:B:303:ILE:HG22	2.00	0.42
1:D:204:VAL:O	1:D:205:ARG:C	2.60	0.42
1:B:155:TRP:HB2	1:B:159:TYR:HB2	2.01	0.42
1:C:192:ASN:HB2	1:C:233:HIS:CE1	2.55	0.42
1:C:208:GLU:O	1:C:209:LEU:C	2.60	0.42
1:B:275:PHE:O	1:B:278:THR:HG23	2.20	0.42
1:B:340:LEU:HD12	1:B:340:LEU:N	2.34	0.42
1:D:295:LEU:HD23	1:D:303:ILE:HG22	2.01	0.42
1:D:218:LYS:HE2	1:D:219:TYR:CE1	2.55	0.41
1:A:249:LEU:HD22	1:A:357:GLY:HA2	2.03	0.41
1:C:293:ILE:C	1:C:294:LEU:HD12	2.46	0.41
1:D:351:LEU:CD1	1:D:459:MET:HE1	2.51	0.41
1:B:204:VAL:O	1:B:205:ARG:C	2.61	0.41
1:C:226:ARG:HD3	5:C:601:HOH:O	2.19	0.41
1:C:333:LEU:O	1:C:390:LYS:HE2	2.20	0.41
1:A:289:LYS:O	1:A:290:PRO:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:MET:HB3	1:C:337:PRO:HD2	2.03	0.41
1:C:458:ARG:HB3	1:C:468:ILE:HB	2.03	0.41
1:B:388:ALA:HB3	1:B:391:ALA:HB2	2.01	0.41
1:D:192:ASN:O	1:D:192:ASN:CG	2.63	0.41
1:D:315:GLY:O	1:D:317:ARG:N	2.51	0.41
1:C:197:LEU:O	1:C:201:GLN:HG3	2.21	0.40
1:D:192:ASN:O	1:D:192:ASN:OD1	2.39	0.40
1:D:381:PRO:HB2	1:D:384:ILE:HD12	2.04	0.40
1:B:160:GLU:OE1	1:B:179:ARG:HD3	2.22	0.40
1:B:168:GLY:HA3	1:B:170:PHE:CE1	2.56	0.40
1:D:336:MET:HB3	1:D:337:PRO:HD2	2.04	0.40
1:A:468:ILE:HD11	1:A:473:ALA:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/361 (94%)	311 (92%)	28 (8%)	0	100	100
1	B	332/361 (92%)	305 (92%)	27 (8%)	0	100	100
1	C	333/361 (92%)	304 (91%)	27 (8%)	2 (1%)	22	51
1	D	322/361 (89%)	289 (90%)	30 (9%)	3 (1%)	14	42
All	All	1326/1444 (92%)	1209 (91%)	112 (8%)	5 (0%)	30	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	ASN
1	C	400	ASP
1	D	258	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	316	GLN
1	D	406	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/320 (93%)	289 (97%)	10 (3%)	33	67
1	B	294/320 (92%)	282 (96%)	12 (4%)	26	59
1	C	283/320 (88%)	277 (98%)	6 (2%)	48	80
1	D	281/320 (88%)	275 (98%)	6 (2%)	48	80
All	All	1157/1280 (90%)	1123 (97%)	34 (3%)	37	71

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	THR
1	A	216	GLU
1	A	226	ARG
1	A	255	ARG
1	A	267	GLN
1	A	280	GLU
1	A	300	ARG
1	A	303	ILE
1	A	318	ILE
1	A	412	LYS
1	B	135	VAL
1	B	179	ARG
1	B	202	ILE
1	B	248	LEU
1	B	282	SER
1	B	310	SER
1	B	318	ILE
1	B	396	GLU
1	B	408	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	422	LYS
1	B	442	SER
1	B	465	LYS
1	C	193	LYS
1	C	221	ILE
1	C	232	ASN
1	C	242	SER
1	C	253	ASN
1	C	408	THR
1	D	169	SER
1	D	310	SER
1	D	313	GLN
1	D	314	LEU
1	D	431	THR
1	D	465	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	267	GLN
1	A	383	HIS
1	B	182	GLN
1	B	267	GLN
1	B	297	ASN
1	B	387	GLN
1	B	424	HIS
1	B	425	ASN
1	C	201	GLN
1	C	313	GLN
1	C	371	ASN
1	C	469	GLN
1	D	137	ASN
1	D	198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	0.91	0	17,22,24	1.13	1 (5%)
1	PTR	C	321	1	15,16,17	0.89	1 (6%)	17,22,24	0.99	1 (5%)
1	PTR	B	321	1	15,16,17	1.58	3 (20%)	17,22,24	1.68	4 (23%)
1	PTR	A	321	1	15,16,17	1.02	0	17,22,24	1.26	1 (5%)

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	-	0/10/11/13	0/1/1/1
1	PTR	C	321	1	-	0/10/11/13	0/1/1/1
1	PTR	B	321	1	-	1/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	PTR	P-OH	4.18	1.67	1.59
1	B	321	PTR	CE2-CD2	2.26	1.42	1.38
1	C	321	PTR	P-OH	2.11	1.63	1.59
1	B	321	PTR	CE1-CD1	2.06	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PTR	CE2-CZ-CE1	-3.63	114.86	120.16
1	B	321	PTR	CD2-CE2-CZ	2.95	123.11	119.73
1	B	321	PTR	P-OH-CZ	2.60	133.14	123.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	PTR	OH-P-O1P	-2.57	100.89	109.48
1	C	321	PTR	O3P-P-O2P	2.36	116.63	107.80
1	B	321	PTR	CD1-CE1-CZ	2.19	122.23	119.73
1	A	321	PTR	O2P-P-OH	-2.09	99.12	105.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	321	PTR	O-C-CA-CB
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](#)

15 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	2C4	B	501	-	29,29,29	1.91	8 (27%)	35,41,41	2.19	11 (31%)
3	1PE	A	503	-	15,15,15	0.91	0	14,14,14	0.57	0
3	1PE	B	503	-	12,12,15	0.82	0	11,11,14	0.58	0
3	1PE	A	502	-	15,15,15	0.84	0	14,14,14	0.51	0
4	SO4	A	505	-	4,4,4	0.52	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2C4	C	501	-	29,29,29	1.95	6 (20%)	35,41,41	2.47	14 (40%)
4	SO4	B	504	-	4,4,4	0.55	0	6,6,6	0.43	0
2	2C4	D	501	-	29,29,29	1.78	9 (31%)	35,41,41	2.86	20 (57%)
3	1PE	B	502	-	15,15,15	0.92	0	14,14,14	0.59	0
3	1PE	D	502	-	15,15,15	0.71	0	14,14,14	0.78	0
4	SO4	A	504	-	4,4,4	0.69	0	6,6,6	0.99	0
4	SO4	B	506	-	4,4,4	0.54	0	6,6,6	0.32	0
3	1PE	C	502	-	15,15,15	0.94	0	14,14,14	0.50	0
4	SO4	B	505	-	4,4,4	0.44	0	6,6,6	0.46	0
2	2C4	A	501	-	29,29,29	1.96	9 (31%)	35,41,41	2.40	13 (37%)

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	2C4	B	501	-	-	4/16/16/16	0/3/3/3
3	1PE	A	503	-	-	3/13/13/13	-
3	1PE	B	503	-	-	2/10/10/13	-
3	1PE	A	502	-	-	5/13/13/13	-
2	2C4	C	501	-	-	8/16/16/16	0/3/3/3
2	2C4	D	501	-	-	4/16/16/16	0/3/3/3
3	1PE	B	502	-	-	6/13/13/13	-
3	1PE	D	502	-	-	1/13/13/13	-
3	1PE	C	502	-	-	1/13/13/13	-
2	2C4	A	501	-	-	2/16/16/16	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	2C4	C10-N9	5.98	1.44	1.35
2	D	501	2C4	C10-N9	5.15	1.43	1.35
2	C	501	2C4	C19-C24	-4.45	1.40	1.50
2	A	501	2C4	C19-C24	-4.34	1.40	1.50
2	B	501	2C4	C19-C24	-4.29	1.40	1.50
2	A	501	2C4	C17-N16	-4.11	1.33	1.41
2	A	501	2C4	C10-N9	3.93	1.41	1.35
2	B	501	2C4	C10-N9	3.75	1.41	1.35
2	B	501	2C4	C2-N3	3.63	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	2C4	C2-N3	3.51	1.41	1.34
2	B	501	2C4	C12-C14	-3.46	1.39	1.49
2	B	501	2C4	C17-N16	-3.11	1.35	1.41
2	C	501	2C4	C12-C14	-3.10	1.40	1.49
2	D	501	2C4	C19-C24	-3.01	1.43	1.50
2	A	501	2C4	C12-C14	-2.91	1.41	1.49
2	C	501	2C4	C2-N3	2.84	1.40	1.34
2	B	501	2C4	C12-C10	-2.70	1.39	1.45
2	C	501	2C4	C13-C12	2.66	1.41	1.35
2	D	501	2C4	C13-C12	2.65	1.41	1.35
2	D	501	2C4	C2-N3	2.64	1.39	1.34
2	A	501	2C4	C12-C10	-2.54	1.40	1.45
2	C	501	2C4	C17-N16	-2.49	1.36	1.41
2	D	501	2C4	C17-N16	-2.44	1.37	1.41
2	D	501	2C4	C12-C14	-2.39	1.42	1.49
2	D	501	2C4	C22-CL2	2.22	1.78	1.73
2	B	501	2C4	C4-N3	2.21	1.35	1.32
2	A	501	2C4	C4-N7	2.17	1.37	1.33
2	B	501	2C4	C1-C13	-2.17	1.39	1.43
2	A	501	2C4	C1-C13	-2.16	1.39	1.43
2	D	501	2C4	C1-C8	-2.16	1.39	1.41
2	D	501	2C4	C18-C17	2.10	1.42	1.39
2	A	501	2C4	C8-N9	2.05	1.40	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C4	N3-C4-N7	-8.50	121.03	128.35
2	C	501	2C4	N3-C4-N7	-8.00	121.46	128.35
2	B	501	2C4	N3-C4-N7	-7.34	122.03	128.35
2	A	501	2C4	N3-C4-N7	-7.31	122.06	128.35
2	D	501	2C4	C8-N9-C10	-6.07	118.66	124.27
2	C	501	2C4	C27-O26-C24	-4.88	106.43	115.81
2	A	501	2C4	C6-O5-C4	-4.82	109.95	117.56
2	A	501	2C4	C22-C17-N16	-4.77	111.90	119.25
2	A	501	2C4	N9-C8-N7	4.55	122.32	116.36
2	C	501	2C4	C8-N9-C10	-4.47	120.14	124.27
2	D	501	2C4	C12-C10-N9	4.19	121.80	114.51
2	A	501	2C4	C2-N3-C4	4.12	119.77	115.00
2	D	501	2C4	C22-C17-N16	-3.95	113.16	119.25
2	D	501	2C4	C27-O26-C24	-3.83	108.44	115.81
2	C	501	2C4	C2-N3-C4	3.81	119.41	115.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C4	C1-C8-N7	-3.79	119.70	123.87
2	B	501	2C4	C8-N9-C10	-3.73	120.82	124.27
2	B	501	2C4	C2-N3-C4	3.66	119.24	115.00
2	B	501	2C4	C12-C10-N9	3.54	120.68	114.51
2	D	501	2C4	C2-N3-C4	3.54	119.09	115.00
2	B	501	2C4	C22-C17-N16	-3.50	113.86	119.25
2	B	501	2C4	N9-C8-N7	3.46	120.89	116.36
2	D	501	2C4	O26-C24-C19	3.35	117.33	112.31
2	C	501	2C4	C22-C17-N16	-3.26	114.23	119.25
2	C	501	2C4	C1-C8-N7	-3.23	120.31	123.87
2	D	501	2C4	C6-O5-C4	-3.23	112.46	117.56
2	C	501	2C4	O26-C24-C19	3.19	117.09	112.31
2	C	501	2C4	C17-C22-CL2	3.14	122.93	119.52
2	A	501	2C4	C1-C8-N7	-3.05	120.51	123.87
2	D	501	2C4	C20-C19-C18	-3.04	115.73	119.25
2	C	501	2C4	C12-C10-N9	3.01	119.76	114.51
2	A	501	2C4	C12-C10-N9	2.93	119.61	114.51
2	D	501	2C4	C14-C12-C10	2.67	124.78	122.64
2	A	501	2C4	C8-N9-C10	-2.62	121.85	124.27
2	D	501	2C4	C18-C17-N16	2.57	128.69	121.95
2	C	501	2C4	N9-C8-N7	2.55	119.70	116.36
2	D	501	2C4	O15-C14-C12	-2.53	116.64	121.04
2	D	501	2C4	N9-C8-N7	2.42	119.53	116.36
2	B	501	2C4	C6-O5-C4	-2.36	113.84	117.56
2	D	501	2C4	O11-C10-C12	-2.35	120.80	125.98
2	C	501	2C4	C18-C17-N16	2.32	128.02	121.95
2	D	501	2C4	O11-C10-N9	-2.30	117.37	121.61
2	A	501	2C4	O5-C4-N7	2.29	123.77	116.29
2	D	501	2C4	C18-C19-C24	2.26	124.48	120.09
2	A	501	2C4	C18-C17-C22	2.25	120.51	118.21
2	A	501	2C4	O11-C10-C12	-2.25	121.02	125.98
2	A	501	2C4	C17-N16-C14	-2.22	120.66	126.84
2	C	501	2C4	O11-C10-C12	-2.17	121.20	125.98
2	C	501	2C4	C20-C19-C24	-2.14	115.68	120.40
2	C	501	2C4	C18-C19-C24	2.14	124.24	120.09
2	D	501	2C4	C12-C14-N16	2.13	118.62	115.61
2	B	501	2C4	C18-C17-N16	2.13	127.52	121.95
2	A	501	2C4	C18-C17-N16	2.11	127.47	121.95
2	D	501	2C4	C21-C20-C19	2.09	123.03	120.80
2	B	501	2C4	C1-C8-N7	-2.08	121.58	123.87
2	D	501	2C4	C19-C18-C17	2.06	123.26	119.43
2	B	501	2C4	O11-C10-N9	-2.05	117.83	121.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	2C4	O11-C10-C12	-2.04	121.49	125.98

There are no chirality outliers.

All (36) torsion outliers are listed below:

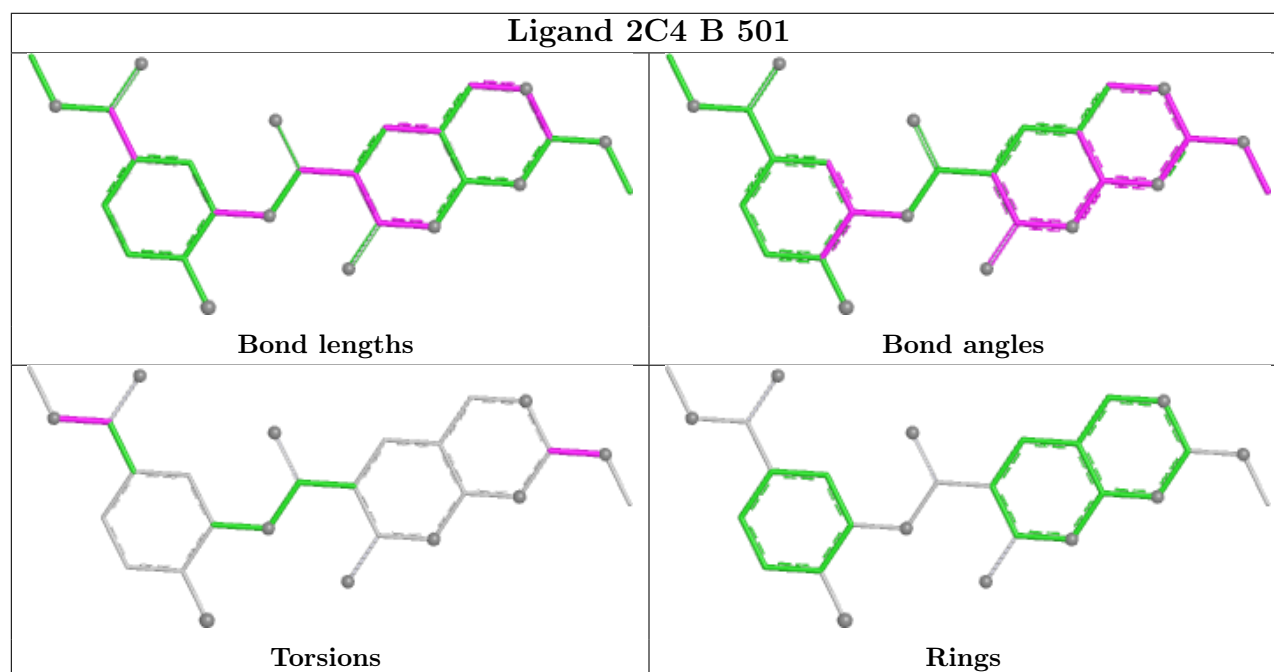
Mol	Chain	Res	Type	Atoms
2	A	501	2C4	N3-C4-O5-C6
2	A	501	2C4	N7-C4-O5-C6
2	B	501	2C4	N3-C4-O5-C6
2	B	501	2C4	N7-C4-O5-C6
2	C	501	2C4	N3-C4-O5-C6
2	D	501	2C4	N3-C4-O5-C6
2	D	501	2C4	N7-C4-O5-C6
2	C	501	2C4	C19-C24-O26-C27
2	D	501	2C4	C19-C24-O26-C27
2	D	501	2C4	O25-C24-O26-C27
2	C	501	2C4	O25-C24-O26-C27
2	B	501	2C4	C19-C24-O26-C27
2	C	501	2C4	N7-C4-O5-C6
3	B	502	1PE	OH4-C13-C23-OH3
3	A	502	1PE	OH4-C13-C23-OH3
3	A	503	1PE	OH2-C12-C22-OH3
2	B	501	2C4	O25-C24-O26-C27
3	C	502	1PE	OH6-C15-C25-OH5
3	A	502	1PE	OH7-C16-C26-OH6
3	B	503	1PE	OH6-C15-C25-OH5
3	B	502	1PE	OH7-C16-C26-OH6
3	B	502	1PE	OH5-C14-C24-OH4
3	A	503	1PE	OH4-C13-C23-OH3
3	D	502	1PE	OH4-C13-C23-OH3
2	C	501	2C4	C20-C19-C24-O26
3	B	502	1PE	C12-C22-OH3-C23
3	A	503	1PE	C25-C15-OH6-C26
3	A	502	1PE	C16-C26-OH6-C15
2	C	501	2C4	C18-C19-C24-O26
3	B	503	1PE	OH5-C14-C24-OH4
3	A	502	1PE	OH2-C12-C22-OH3
3	A	502	1PE	C15-C25-OH5-C14
3	B	502	1PE	C14-C24-OH4-C13
2	C	501	2C4	C20-C19-C24-O25
3	B	502	1PE	C16-C26-OH6-C15
2	C	501	2C4	C18-C19-C24-O25

There are no ring outliers.

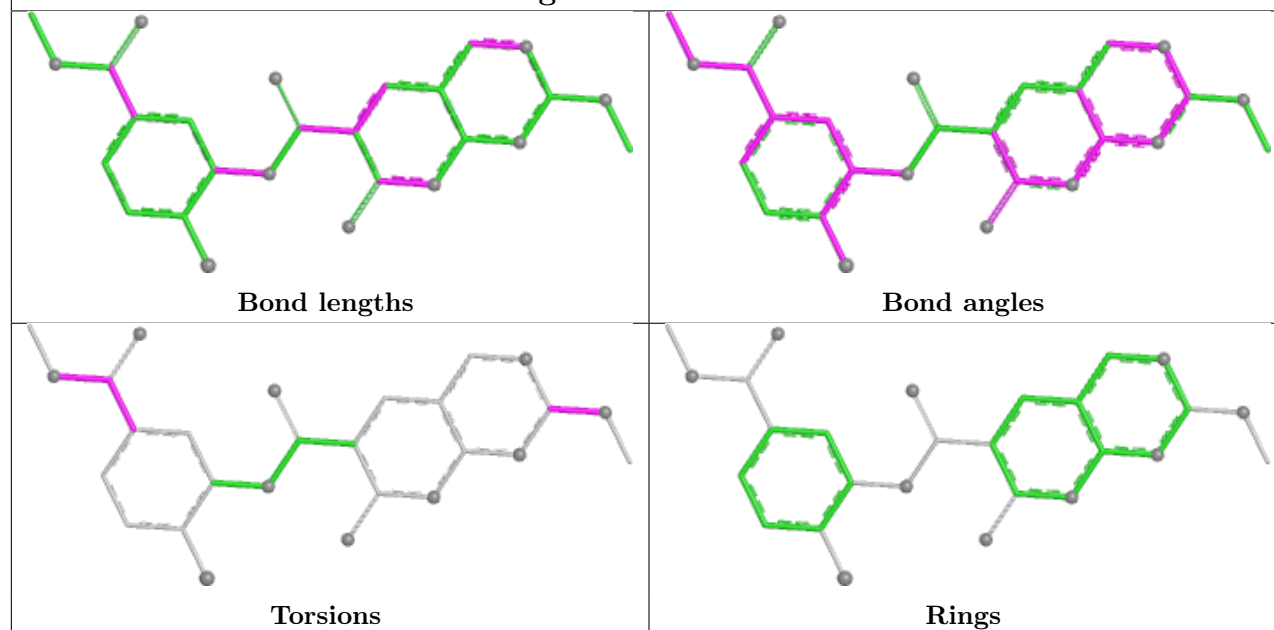
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	1PE	1	0
2	A	501	2C4	2	0

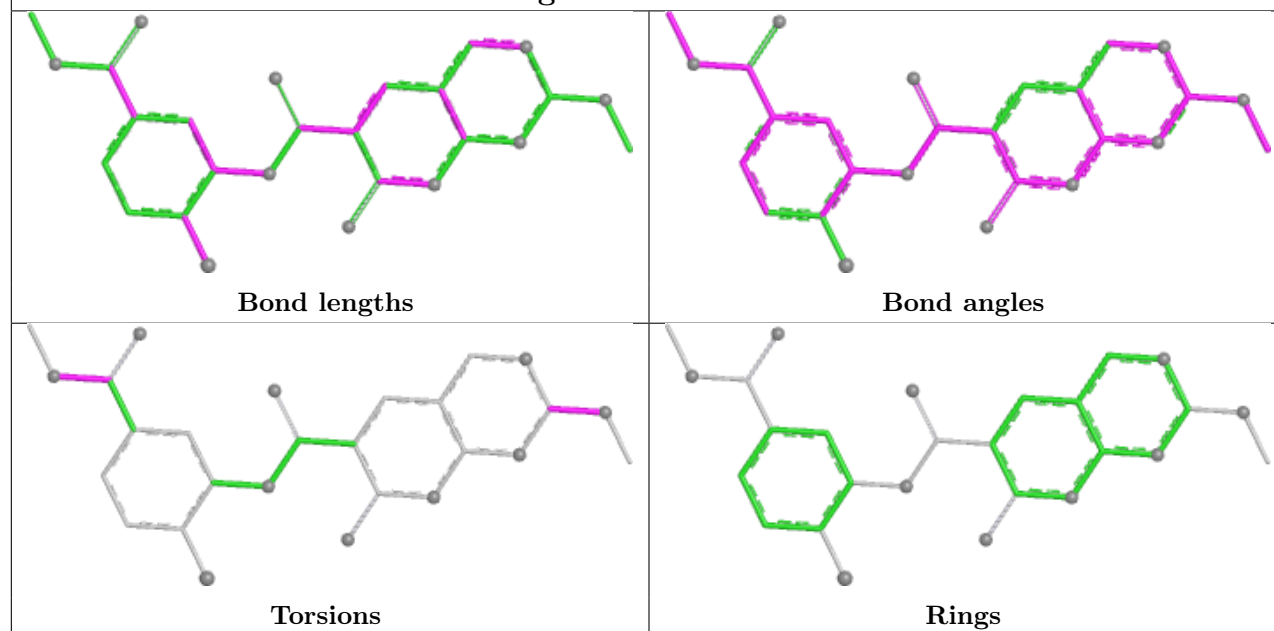
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

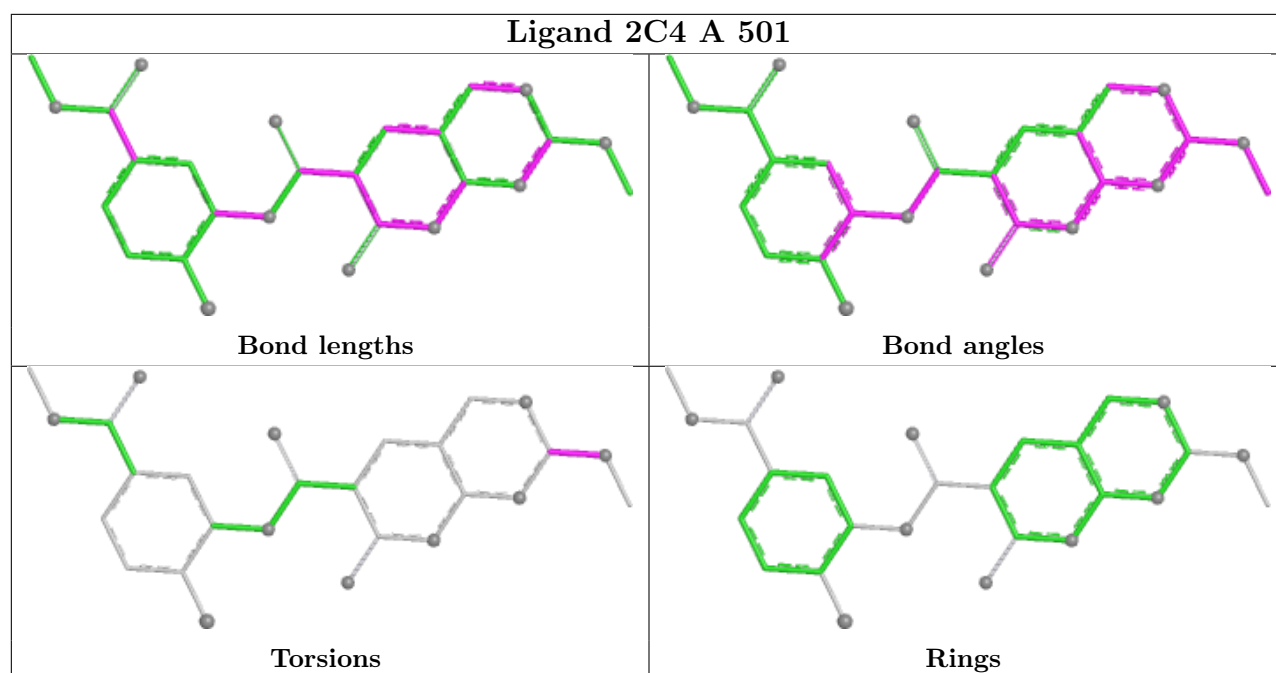


Ligand 2C4 C 501



Ligand 2C4 D 501





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	343/361 (95%)	-0.53	1 (0%) 90 87	25, 40, 70, 88	0
1	B	338/361 (93%)	-0.40	7 (2%) 63 55	28, 46, 76, 118	0
1	C	339/361 (93%)	-0.04	8 (2%) 59 51	39, 62, 94, 115	0
1	D	329/361 (91%)	-0.14	6 (1%) 67 60	21, 59, 90, 114	1 (0%)
All	All	1349/1444 (93%)	-0.28	22 (1%) 70 63	21, 52, 86, 118	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	408	THR	3.7
1	C	410	ASP	3.4
1	A	409	LYS	3.2
1	B	135	VAL	3.0
1	B	136	TYR	2.8
1	D	409	LYS	2.7
1	D	471	TYR	2.7
1	D	434	PRO	2.6
1	C	443	GLY	2.5
1	B	318	ILE	2.5
1	C	409	LYS	2.5
1	D	135	VAL	2.4
1	B	316	GLN	2.3
1	D	320	GLN	2.2
1	C	402	THR	2.2
1	B	216	GLU	2.2
1	C	320	GLN	2.2
1	D	397	LYS	2.1
1	C	403	TRP	2.1
1	B	408	THR	2.1
1	C	216	GLU	2.1
1	B	143	ASP	2.1

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	B	321	16/17	0.91	0.15	64,72,80,82	0
1	PTR	C	321	16/17	0.91	0.11	59,69,82,84	0
1	PTR	D	321	16/17	0.92	0.12	61,77,85,88	0
1	PTR	A	321	16/17	0.95	0.09	34,38,51,54	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

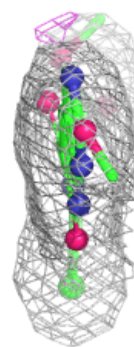
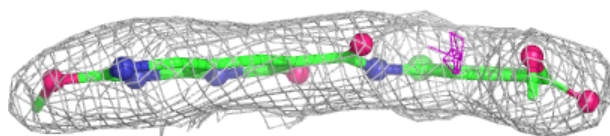
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	505	5/5	0.81	0.13	97,107,108,126	0
3	1PE	B	502	16/16	0.86	0.15	63,70,78,79	0
4	SO4	B	505	5/5	0.87	0.20	82,88,100,103	0
3	1PE	C	502	16/16	0.90	0.12	64,68,79,83	0
4	SO4	B	504	5/5	0.92	0.28	55,57,74,75	0
4	SO4	A	504	5/5	0.93	0.26	53,62,70,71	0
3	1PE	A	502	16/16	0.93	0.10	64,68,74,76	0
3	1PE	A	503	16/16	0.94	0.11	37,46,54,58	0
4	SO4	B	506	5/5	0.94	0.13	62,62,70,73	0
3	1PE	D	502	16/16	0.95	0.08	39,45,52,54	0
2	2C4	C	501	27/27	0.96	0.08	51,59,66,70	0
3	1PE	B	503	13/16	0.96	0.09	32,38,45,47	0
2	2C4	D	501	27/27	0.96	0.07	41,46,53,54	0
2	2C4	B	501	27/27	0.97	0.07	32,37,46,50	0
2	2C4	A	501	27/27	0.98	0.05	34,37,46,48	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.

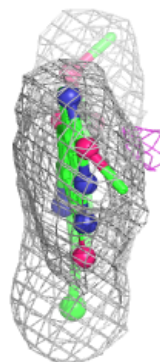
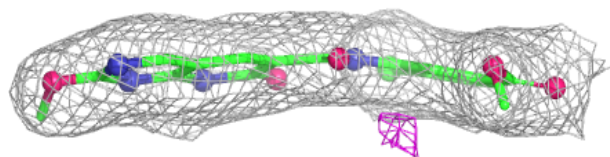
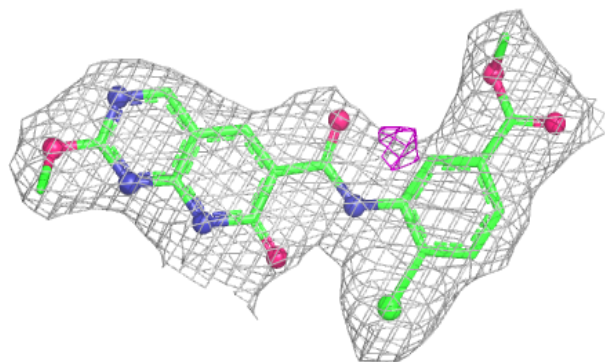
Electron density around 2C4 C 501:

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



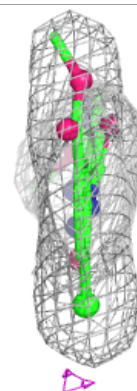
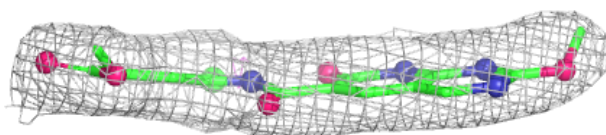
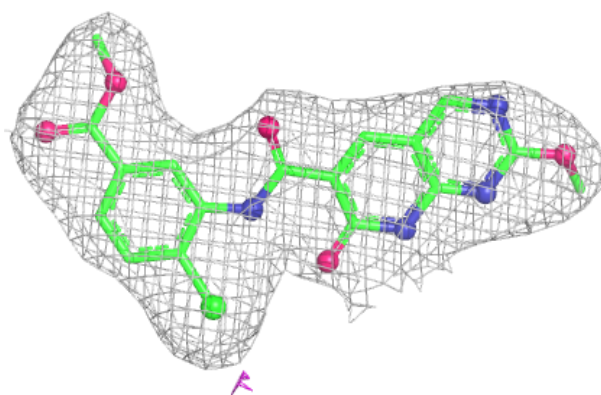
Electron density around 2C4 D 501:

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

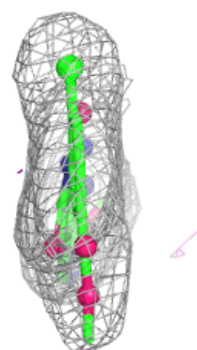
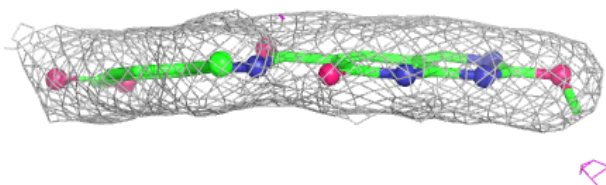
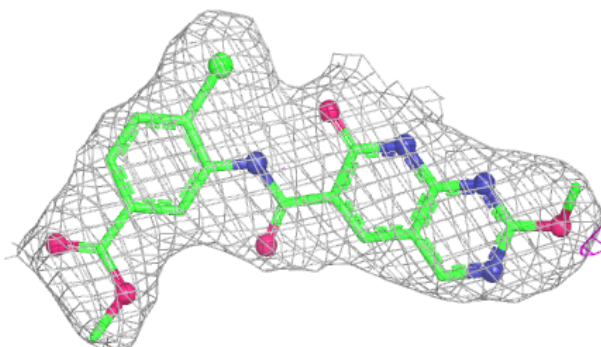


Electron density around 2C4 B 501:

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

**Electron density around 2C4 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.