



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:03 PM GMT

PDB ID : 4MQ2
Title : The crystal structure of DYRK1a with a bound pyrido[2,3-d]pyrimidin
einhibitor
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

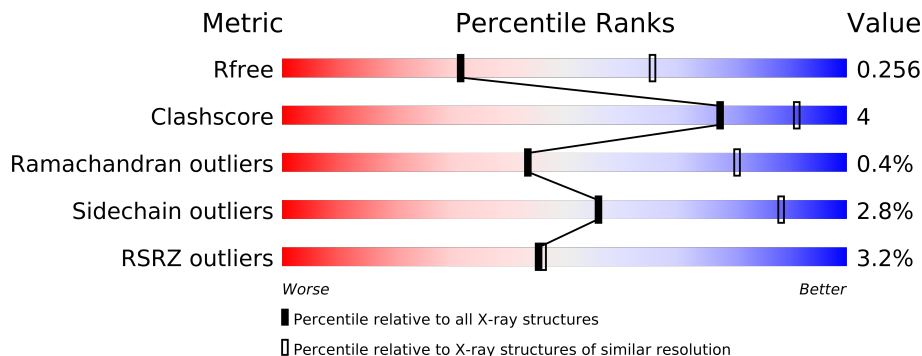
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	361	
1	B	361	
1	C	361	
1	D	361	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	1PE	A	502	-	X
3	1PE	A	503	-	X
4	SO4	B	504	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11273 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

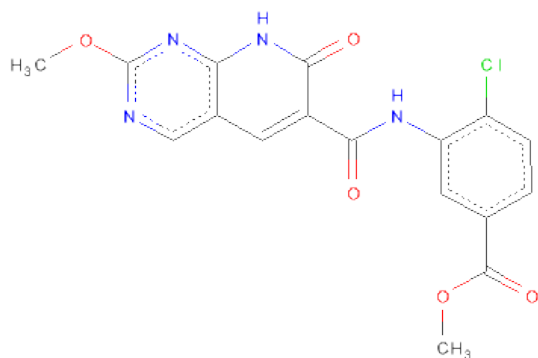
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

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:

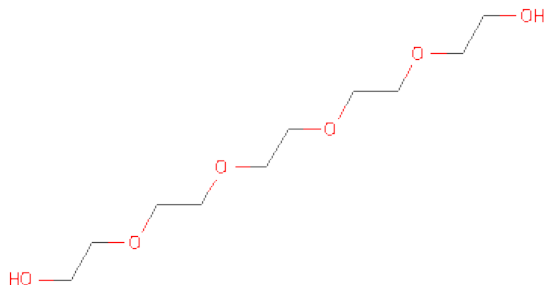
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	EXPRESSION TAG	UNP Q13627
A	126	MET	-	EXPRESSION TAG	UNP Q13627
B	125	SER	-	EXPRESSION TAG	UNP Q13627
B	126	MET	-	EXPRESSION TAG	UNP Q13627
C	125	SER	-	EXPRESSION TAG	UNP Q13627
C	126	MET	-	EXPRESSION TAG	UNP Q13627
D	125	SER	-	EXPRESSION TAG	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 (three-letter code: 2C4) (formula: C₁₇H₁₃ClN₄O₅).



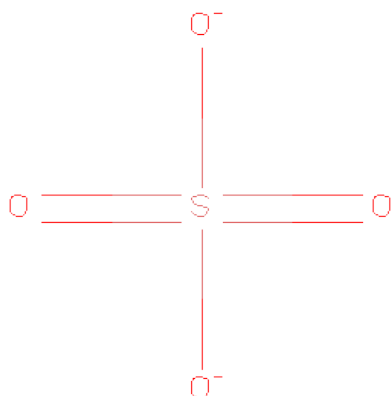
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	17	1	4	5		
2	B	1	Total	C	Cl	N	O	0	0
			27	17	1	4	5		
2	C	1	Total	C	Cl	N	O	0	0
			27	17	1	4	5		
2	D	1	Total	C	Cl	N	O	0	0
			27	17	1	4	5		

- Molecule 3 is PENTAETHYLENE GLYCOL (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	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

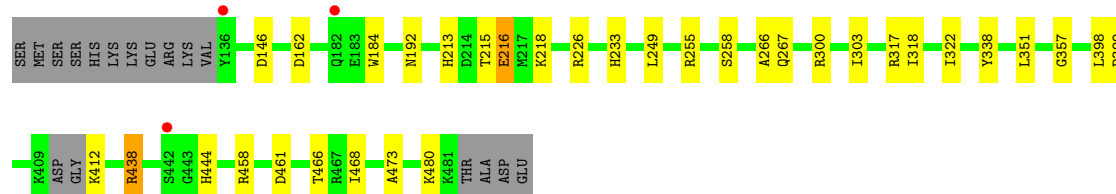
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total 53	O 53	0	0
5	B	33	Total 33	O 33	0	0
5	C	16	Total 16	O 16	0	0
5	D	19	Total 19	O 19	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

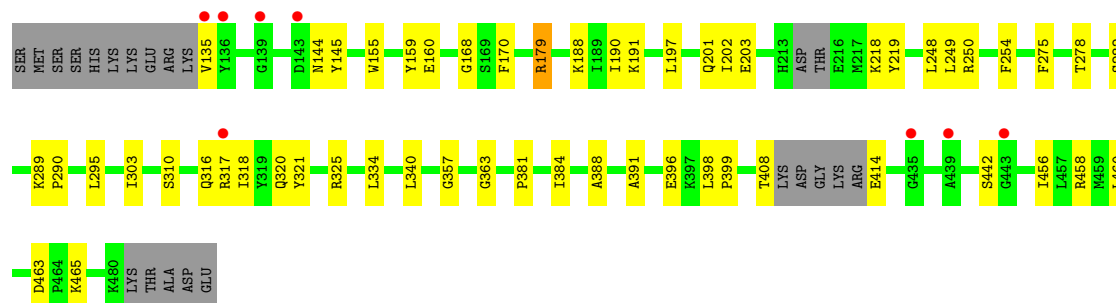
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulatedkinase 1A

Chain A: 



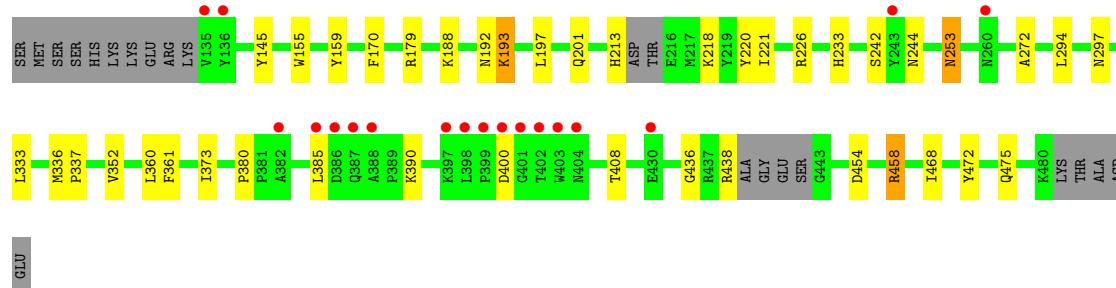
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulatedkinase 1A

Chain B: 



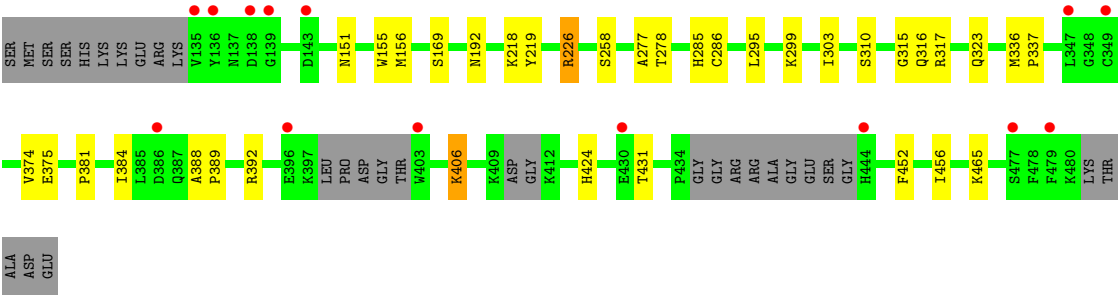
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulatedkinase 1A

Chain C: 



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulatedkinase 1A

Chain D: 



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 36.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.78-2.80) 100.0 (36.30-2.80)	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 0.193 , 0.256	Depositor DCC
R_{free} test set	2652 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53114 reflections	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.

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: 2C4, 1PE, PTR, SO4

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	0.71	0/2848	0.84	1/3842 (0.0%)
1	B	0.63	0/2799	0.79	2/3778 (0.1%)
1	C	0.59	0/2759	0.76	1/3733 (0.0%)
1	D	0.58	0/2710	0.74	2/3666 (0.1%)
All	All	0.63	0/11116	0.78	6/15019 (0.0%)

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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	458	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	458	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	B	463	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	226[A]	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	226[B]	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2800	0	2778	17	0
1	B	2752	0	2725	25	0
1	C	2712	0	2636	19	0
1	D	2662	0	2597	20	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	10915	81	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:317:ARG:CB	1:B:318:ILE:HG13	1.67	1.23
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:258:SER:HA	1:A:438:ARG:HH21	1.57	0.70
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:CG	1:D:226[A]:ARG:HH21	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:D:424:HIS:HB2	5:D:607:HOH:O	2.08	0.53
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: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:D:452:PHE:CE1	1:D:456:ILE:HD11	2.48	0.49
1:B:197:LEU:O	1:B:201:GLN:HG3	2.13	0.49
1:A:398:LEU:O	1:A:399:PRO:C	2.50	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: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:155:TRP:HB2	1:C:159:TYR:HB2	1.96	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: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:B:398:LEU:HB3	1:B:399:PRO:HD2	1.99	0.45
2:A:501:2C4:O11	2:A:501:2C4:N16	2.46	0.44
1:B:190:ILE:HG22	1:B:191:LYS:N	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:334:LEU:HB3	1:B:388:ALA:HB1	1.99	0.44
1:D:374:VAL:O	1:D:375:GLU:C	2.55	0.43
1:D:388:ALA:O	1:D:389:PRO:C	2.56	0.43
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:C:220:TYR:HB3	1:C:272:ALA:HB2	2.01	0.43
1:C:170:PHE:CD1	1:C:188:LYS:HE3	2.53	0.43
1:B:456:ILE:O	1:B:460:LEU:HG	2.19	0.43
1:A:461:ASP:OD2	1:A:466:THR:OG1	2.30	0.42
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: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:213:HIS:C	1:C:218:LYS:HD3	2.40	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:D:155:TRP:O	1:D:156:MET:C	2.58	0.41
1:A:249:LEU:HD22	1:A:357:GLY:HA2	2.03	0.41
1:C:333:LEU:O	1:C:390:LYS:HE2	2.20	0.41
1:C:226:ARG:HD3	5:C:601:HOH:O	2.19	0.41
1:C:458:ARG:HB3	1:C:468:ILE:HB	2.03	0.41
1:C:336:MET:HB3	1:C:337:PRO:HD2	2.03	0.41
1:B:388:ALA:HB3	1:B:391:ALA:HB2	2.01	0.41
1:D:277:ALA:O	1:D:278:THR:C	2.59	0.41
1:D:315:GLY:O	1:D:317:ARG:N	2.51	0.41
1:D:381:PRO:HB2	1:D:384:ILE:HD12	2.04	0.40
1:C:197:LEU:O	1:C:201:GLN:HG3	2.21	0.40
1:D:192:ASN:OD1	1:D:192:ASN:O	2.39	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%)	33	72
1	D	322/361 (89%)	289 (90%)	30 (9%)	3 (1%)	25	63
All	All	1326/1444 (92%)	1209 (91%)	112 (8%)	5 (0%)	43	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	ASN
1	C	400	ASP
1	D	258	SER
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%)	287 (96%)	12 (4%)	42	79
1	B	294/320 (92%)	284 (97%)	10 (3%)	49	84
1	C	283/320 (88%)	277 (98%)	6 (2%)	66	93
1	D	281/320 (88%)	277 (99%)	4 (1%)	78	96
All	All	1157/1280 (90%)	1125 (97%)	32 (3%)	56	88

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ASP
1	A	162	ASP
1	A	215	THR
1	A	216	GLU
1	A	226	ARG
1	A	255	ARG
1	A	267	GLN
1	A	300	ARG
1	A	303	ILE
1	A	318	ILE
1	A	412	LYS
1	A	438	ARG
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	396	GLU
1	B	408	THR
1	B	442	SER
1	B	465	LYS
1	C	179	ARG
1	C	193	LYS
1	C	221	ILE
1	C	242	SER
1	C	253	ASN
1	C	408	THR
1	D	169	SER
1	D	310	SER
1	D	431	THR
1	D	465	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	B	267	GLN
1	B	425	ASN
1	C	469	GLN
1	D	137	ASN
1	D	404	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	A	321	1	16,16,17	3.90	2 (12%)	20,22,24	1.46	3 (15%)
1	PTR	B	321	1	16,16,17	4.44	3 (18%)	20,22,24	1.50	3 (15%)
1	PTR	C	321	1	16,16,17	4.15	2 (12%)	20,22,24	1.02	1 (5%)
1	PTR	D	321	1	16,16,17	4.90	1 (6%)	20,22,24	1.06	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	A	321	1	-	0/9/11/13	0/1/1/1
1	PTR	B	321	1	-	0/9/11/13	0/1/1/1
1	PTR	C	321	1	-	0/9/11/13	0/1/1/1
1	PTR	D	321	1	-	0/9/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	321	PTR	O-C	19.30	1.24	1.11
1	B	321	PTR	O-C	16.41	1.22	1.11
1	C	321	PTR	O-C	16.16	1.22	1.11
1	A	321	PTR	O-C	15.01	1.21	1.11
1	B	321	PTR	P-OH	4.83	1.67	1.60
1	B	321	PTR	CA-C	2.77	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	PTR	CA-C	2.47	1.52	1.48
1	C	321	PTR	P-OH	2.33	1.63	1.60

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PTR	P-OH-CZ	3.40	133.14	123.55
1	B	321	PTR	CE2-CZ-CE1	-3.12	114.86	120.21
1	A	321	PTR	C-CA-N	-3.07	110.76	113.83
1	B	321	PTR	CD2-CE2-CZ	2.50	123.11	119.76
1	A	321	PTR	P-OH-CZ	2.44	130.44	123.55
1	D	321	PTR	O3P-P-O1P	2.34	118.10	110.44
1	C	321	PTR	O3P-P-O2P	2.32	116.63	107.61
1	A	321	PTR	O2P-P-O1P	2.31	117.98	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	501	-	29,29,29	2.37	7 (24%)	38,41,41	2.58	14 (36%)
3	1PE	A	502	-	15,15,15	0.84	0	14,14,14	0.46	0
3	1PE	A	503	-	15,15,15	0.90	0	14,14,14	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	504	-	4,4,4	0.79	0	6,6,6	1.16	1 (16%)
4	SO4	A	505	-	4,4,4	0.56	0	6,6,6	0.46	0
2	2C4	B	501	-	29,29,29	2.39	8 (27%)	38,41,41	2.46	10 (26%)
3	1PE	B	502	-	15,15,15	0.93	0	14,14,14	0.55	0
3	1PE	B	503	-	12,12,15	0.91	0	11,11,14	0.63	0
4	SO4	B	504	-	4,4,4	0.68	0	6,6,6	0.37	0
4	SO4	B	505	-	4,4,4	0.57	0	6,6,6	0.60	0
4	SO4	B	506	-	4,4,4	0.66	0	6,6,6	0.27	0
2	2C4	C	501	-	29,29,29	2.26	7 (24%)	38,41,41	2.67	14 (36%)
3	1PE	C	502	-	15,15,15	0.94	0	14,14,14	0.47	0
2	2C4	D	501	-	29,29,29	2.03	9 (31%)	38,41,41	3.01	15 (39%)
3	1PE	D	502	-	15,15,15	0.72	0	14,14,14	0.75	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	2C4	A	501	-	-	0/16/16/16	0/1/3/3
3	1PE	A	502	-	-	0/13/13/13	0/0/0/0
3	1PE	A	503	-	-	0/13/13/13	0/0/0/0
4	SO4	A	504	-	-	0/0/0/0	0/0/0/0
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	2C4	B	501	-	-	0/16/16/16	0/1/3/3
3	1PE	B	502	-	-	0/13/13/13	0/0/0/0
3	1PE	B	503	-	-	0/10/10/13	0/0/0/0
4	SO4	B	504	-	-	0/0/0/0	0/0/0/0
4	SO4	B	505	-	-	0/0/0/0	0/0/0/0
4	SO4	B	506	-	-	0/0/0/0	0/0/0/0
2	2C4	C	501	-	-	0/16/16/16	0/1/3/3
3	1PE	C	502	-	-	0/13/13/13	0/0/0/0
2	2C4	D	501	-	-	0/16/16/16	0/1/3/3
3	1PE	D	502	-	-	0/13/13/13	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	2C4	C12-C14	-7.24	1.39	1.50
2	B	501	2C4	C2-N3	7.15	1.41	1.31
2	A	501	2C4	C2-N3	6.96	1.41	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	2C4	C12-C14	-6.55	1.40	1.50
2	A	501	2C4	C12-C14	-6.17	1.41	1.50
2	C	501	2C4	C2-N3	5.97	1.40	1.31
2	D	501	2C4	C2-N3	5.68	1.39	1.31
2	D	501	2C4	C12-C14	-5.14	1.42	1.50
2	C	501	2C4	C10-N9	4.19	1.44	1.37
2	A	501	2C4	C17-N16	-4.10	1.33	1.41
2	C	501	2C4	C19-C24	-4.02	1.40	1.49
2	A	501	2C4	C19-C24	-3.93	1.40	1.49
2	B	501	2C4	C19-C24	-3.88	1.40	1.49
2	D	501	2C4	C10-N9	3.49	1.43	1.37
2	B	501	2C4	C17-N16	-3.10	1.35	1.41
2	A	501	2C4	C4-N7	3.10	1.37	1.33
2	C	501	2C4	C13-C12	2.83	1.41	1.37
2	D	501	2C4	C13-C12	2.81	1.41	1.37
2	D	501	2C4	C19-C24	-2.70	1.43	1.49
2	A	501	2C4	C8-N9	2.60	1.40	1.37
2	C	501	2C4	C17-N16	-2.50	1.36	1.41
2	D	501	2C4	C8-N7	-2.48	1.32	1.34
2	A	501	2C4	C10-N9	2.47	1.41	1.37
2	D	501	2C4	C17-N16	-2.45	1.37	1.41
2	C	501	2C4	C8-N9	2.41	1.40	1.37
2	B	501	2C4	C10-N9	2.32	1.41	1.37
2	B	501	2C4	C4-N3	2.29	1.35	1.33
2	B	501	2C4	C4-N7	2.22	1.36	1.33
2	B	501	2C4	C8-N9	2.18	1.40	1.37
2	D	501	2C4	C22-CL2	2.06	1.78	1.73
2	D	501	2C4	C18-C17	2.02	1.42	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C4	N3-C4-N7	-10.18	121.03	128.42
2	C	501	2C4	N3-C4-N7	-9.59	121.46	128.42
2	B	501	2C4	N3-C4-N7	-8.81	122.03	128.42
2	A	501	2C4	N3-C4-N7	-8.77	122.06	128.42
2	D	501	2C4	C12-C10-N9	7.60	121.80	115.40
2	A	501	2C4	C2-N3-C4	6.43	119.77	114.60
2	B	501	2C4	C12-C10-N9	6.26	120.68	115.40
2	D	501	2C4	C4-N7-C8	6.03	122.14	114.95
2	C	501	2C4	C2-N3-C4	5.98	119.41	114.60
2	B	501	2C4	C2-N3-C4	5.77	119.24	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C4	C2-N3-C4	5.59	119.09	114.60
2	C	501	2C4	C4-N7-C8	5.33	121.31	114.95
2	C	501	2C4	C12-C10-N9	5.17	119.76	115.40
2	A	501	2C4	C12-C10-N9	5.00	119.61	115.40
2	C	501	2C4	C27-O26-C24	-4.31	106.43	115.87
2	A	501	2C4	C22-C17-N16	-4.31	111.90	119.46
2	B	501	2C4	C4-N7-C8	3.82	119.51	114.95
2	A	501	2C4	C4-N7-C8	3.80	119.49	114.95
2	A	501	2C4	C6-O5-C4	-3.66	109.95	117.73
2	D	501	2C4	C22-C17-N16	-3.59	113.16	119.46
2	D	501	2C4	C27-O26-C24	-3.40	108.44	115.87
2	B	501	2C4	C22-C17-N16	-3.19	113.86	119.46
2	D	501	2C4	O15-C14-C12	-3.11	116.64	121.51
2	A	501	2C4	N9-C8-N7	3.04	122.32	116.35
2	C	501	2C4	C22-C17-N16	-2.98	114.23	119.46
2	A	501	2C4	C1-C2-N3	-2.83	118.64	123.83
2	D	501	2C4	C20-C19-C18	-2.79	115.73	119.24
2	D	501	2C4	O26-C24-C19	2.69	117.33	112.37
2	D	501	2C4	C12-C14-N16	2.65	118.62	114.51
2	C	501	2C4	C1-C2-N3	-2.65	118.98	123.83
2	C	501	2C4	C17-C22-CL2	2.61	122.93	119.45
2	C	501	2C4	O26-C24-C19	2.56	117.09	112.37
2	B	501	2C4	O15-C14-C12	-2.52	117.57	121.51
2	D	501	2C4	C1-C2-N3	-2.52	119.22	123.83
2	B	501	2C4	C1-C2-N3	-2.50	119.25	123.83
2	D	501	2C4	C1-C8-N7	-2.49	119.70	125.39
2	D	501	2C4	C6-O5-C4	-2.48	112.46	117.73
2	D	501	2C4	C18-C17-N16	2.47	128.69	122.17
4	A	504	SO4	O2-S-O1	2.45	117.64	109.53
2	B	501	2C4	N9-C8-N7	2.31	120.89	116.35
2	B	501	2C4	C13-C1-C8	2.27	121.46	118.44
2	A	501	2C4	O5-C4-N7	2.27	123.77	116.33
2	C	501	2C4	C1-C8-N7	-2.23	120.31	125.39
2	C	501	2C4	C18-C17-N16	2.21	128.02	122.17
2	A	501	2C4	C17-N16-C14	-2.18	120.66	126.83
2	A	501	2C4	C18-C17-C22	2.17	120.51	117.99
2	A	501	2C4	C13-C1-C8	2.16	121.32	118.44
2	D	501	2C4	C18-C19-C24	2.14	124.48	120.08
2	A	501	2C4	C1-C8-N7	-2.14	120.51	125.39
2	C	501	2C4	O15-C14-C12	-2.13	118.18	121.51
2	C	501	2C4	C20-C19-C24	-2.04	115.68	120.37
2	C	501	2C4	C18-C19-C24	2.03	124.24	120.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	2C4	C18-C17-N16	2.03	127.52	122.17
2	A	501	2C4	C18-C17-N16	2.00	127.47	122.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	344/361 (95%)	-0.26	3 (0%) 81 81	25, 40, 70, 88	0
1	B	339/361 (93%)	-0.11	8 (2%) 56 57	28, 46, 76, 118	0
1	C	340/361 (94%)	-0.04	18 (5%) 25 26	39, 62, 94, 115	0
1	D	330/361 (91%)	-0.04	14 (4%) 35 35	35, 60, 90, 114	0
All	All	1353/1444 (93%)	-0.11	43 (3%) 45 46	25, 52, 86, 118	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	VAL	5.4
1	C	402	THR	5.2
1	B	136	TYR	4.8
1	C	399	PRO	4.1
1	D	136	TYR	4.0
1	C	403	TRP	3.8
1	C	401	GLY	3.6
1	A	136	TYR	3.5
1	D	403	TRP	3.4
1	D	135	VAL	3.1
1	D	139	GLY	3.1
1	C	387	GLN	3.0
1	C	400	ASP	3.0
1	C	136	TYR	3.0
1	B	139	GLY	2.9
1	C	404	ASN	2.9
1	C	398	LEU	2.8
1	B	439	ALA	2.7
1	D	396	GLU	2.7
1	C	135	VAL	2.7
1	C	386	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	138	ASP	2.6
1	D	479	PHE	2.5
1	D	349	CYS	2.5
1	D	386	ASP	2.5
1	A	442	SER	2.5
1	C	260	ASN	2.4
1	C	382	ALA	2.4
1	C	397	LYS	2.3
1	B	143	ASP	2.3
1	D	347	LEU	2.3
1	D	430	GLU	2.3
1	A	182	GLN	2.3
1	C	243	TYR	2.3
1	C	430	GLU	2.2
1	B	443	GLY	2.2
1	B	317	ARG	2.2
1	D	444	HIS	2.1
1	B	435	GLY	2.1
1	C	388	ALA	2.1
1	D	477	SER	2.0
1	D	143	ASP	2.0
1	C	385	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	B	321	16/17	0.28	1.57	64,72,80,82	0
1	PTR	D	321	16/17	0.20	0.08	61,77,85,88	0
1	PTR	C	321	16/17	0.17	-0.63	59,69,82,84	0
1	PTR	A	321	16/17	0.16	-0.74	34,38,51,54	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	1PE	A	502	16/16	0.28	2.62	64,68,74,76	0
4	SO4	B	504	5/5	0.23	2.48	55,57,74,75	0
3	1PE	A	503	16/16	0.20	2.31	37,46,54,58	0
4	SO4	A	504	5/5	0.21	1.52	53,62,70,71	0
3	1PE	C	502	16/16	0.23	1.34	64,68,79,83	0
4	SO4	B	505	5/5	0.26	1.27	82,88,100,103	0
3	1PE	B	502	16/16	0.22	1.04	63,70,78,79	0
4	SO4	A	505	5/5	0.24	0.98	97,107,108,126	0
3	1PE	B	503	13/16	0.16	0.54	32,38,45,47	0
2	2C4	D	501	27/27	0.15	0.06	41,46,53,54	0
4	SO4	B	506	5/5	0.22	-0.22	62,62,70,73	0
2	2C4	C	501	27/27	0.13	-0.73	51,59,66,70	0
2	2C4	A	501	27/27	0.13	-0.75	34,37,46,48	0
2	2C4	B	501	27/27	0.15	-0.87	32,37,46,50	0
3	1PE	D	502	16/16	0.12	-1.12	39,45,52,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.