



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 11:12 PM EDT

PDB ID : 3A8W
Title : Crystal Structure of PKC α kinase domain
Authors : Takimura, T.; Kamata, K.
Deposited on : unknown
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

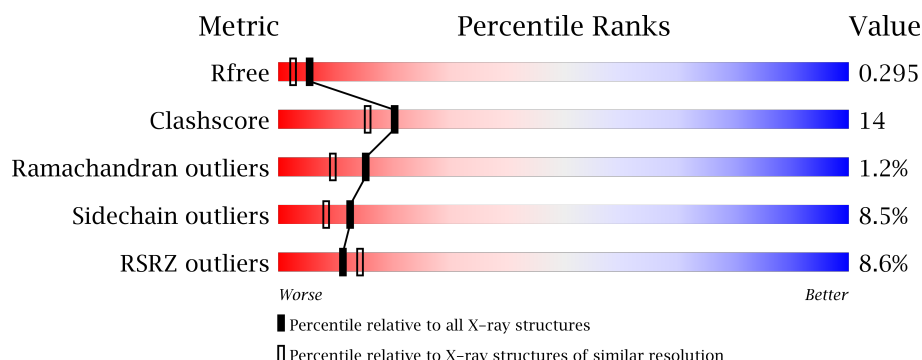
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	345	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	B	345	<div> <div>13%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>6%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5598 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 Protein kinase C iota type.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	P	S	0	0	0
			2681	1716	450	499	2	14			
1	B	329	Total	C	N	O	P	S	0	0	0
			2688	1716	448	508	2	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLY	-	EXPRESSION TAG	UNP P41743
A	236	ALA	-	EXPRESSION TAG	UNP P41743
A	237	MET	-	EXPRESSION TAG	UNP P41743
A	238	ASP	-	EXPRESSION TAG	UNP P41743
A	239	PRO	-	EXPRESSION TAG	UNP P41743
B	235	GLY	-	EXPRESSION TAG	UNP P41743
B	236	ALA	-	EXPRESSION TAG	UNP P41743
B	237	MET	-	EXPRESSION TAG	UNP P41743
B	238	ASP	-	EXPRESSION TAG	UNP P41743
B	239	PRO	-	EXPRESSION TAG	UNP P41743

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

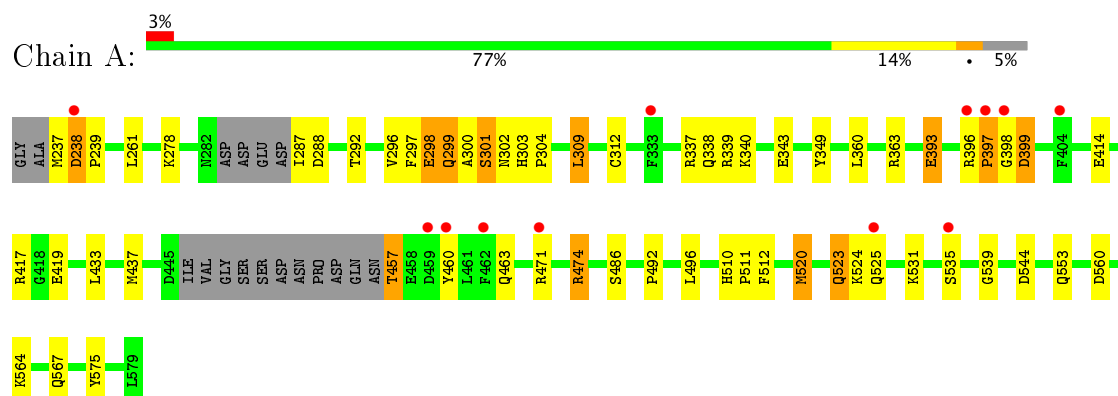
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total 87	O 87	0	0
4	B	75	Total 75	O 75	0	0

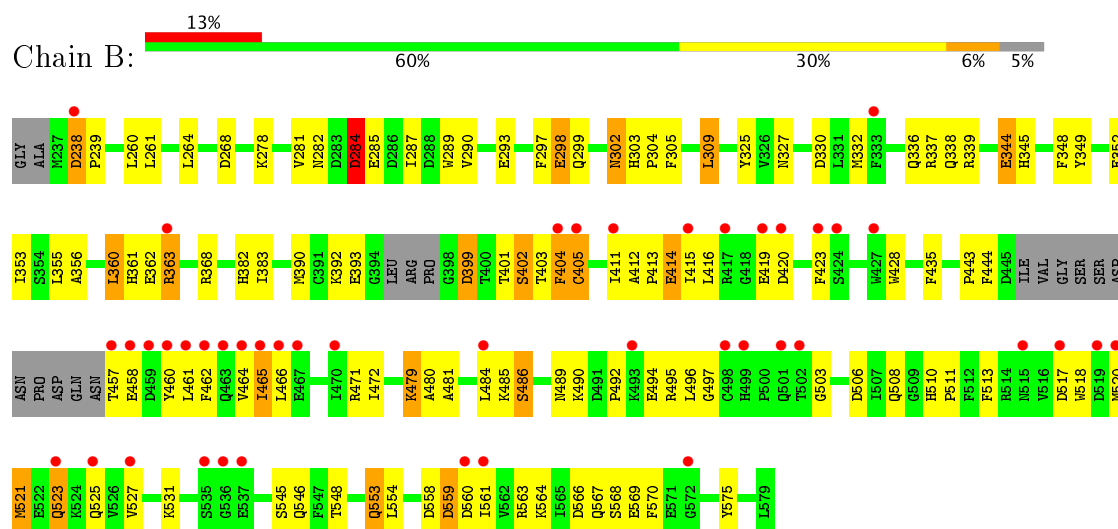
3 Residue-property plots [i](#)

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

• Molecule 1: Protein kinase C iota type



• Molecule 1: Protein kinase C iota type



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.04Å 89.14Å 206.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.92 – 2.10 40.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.92-2.10) 99.9 (40.92-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.14 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.247 , 0.301 0.245 , 0.295	Depositor DCC
R_{free} test set	2332 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5598	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: TPO, SO4, ATP

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	0.46	1/2722 (0.0%)	0.56	0/3670
1	B	0.49	0/2728	0.61	0/3678
All	All	0.47	1/5450 (0.0%)	0.59	0/7348

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	CYS	CB-SG	-5.54	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	399	ASP	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	2681	0	2613	52	0
1	B	2688	0	2599	103	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
3	B	5	0	0	0	0
4	A	87	0	0	1	0
4	B	75	0	0	2	0
All	All	5598	0	5236	149	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 14.

All (149) 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:287:ILE:HD12	1:A:288:ASP:H	1.07	1.18
1:A:396:ARG:HB3	1:A:397:PRO:HD3	1.18	1.12
1:A:237:MET:CE	1:B:298:GLU:HB2	1.88	1.03
1:A:237:MET:HE1	1:B:298:GLU:HB2	1.38	1.02
1:A:397:PRO:HD2	1:A:399:ASP:HB2	1.39	1.01
1:B:523:GLN:HB2	1:B:525:GLN:OE1	1.62	0.97
1:B:559:ASP:O	1:B:563:ARG:HB2	1.65	0.96
1:B:414:GLU:HG2	1:B:492:PRO:CG	1.97	0.95
1:B:414:GLU:HG2	1:B:492:PRO:HG3	1.49	0.92
1:A:287:ILE:CD1	1:A:288:ASP:H	1.86	0.87
1:A:287:ILE:HD12	1:A:288:ASP:N	1.89	0.86
1:B:472:ILE:HG21	1:B:481:ALA:HB2	1.58	0.85
1:A:396:ARG:HB3	1:A:397:PRO:CD	2.05	0.85
1:B:401:THR:O	1:B:420:ASP:HB2	1.78	0.83
1:B:414:GLU:CG	1:B:492:PRO:HG3	2.09	0.82
1:B:299:GLN:HG2	1:B:363:ARG:HG2	1.63	0.80
1:A:398:GLY:O	1:A:399:ASP:O	1.99	0.80
1:B:405:CYS:HB3	4:B:874:HOH:O	1.82	0.79
1:B:297:PHE:HB3	1:B:309:LEU:HG	1.65	0.78
1:A:396:ARG:CB	1:A:397:PRO:HD3	2.07	0.77
1:B:349:TYR:O	1:B:353:ILE:HG13	1.84	0.77
1:B:489:ASN:ND2	1:B:494:GLU:HB3	2.04	0.73
1:B:278:LYS:HZ3	1:B:567:GLN:HE22	1.38	0.72
1:B:303:HIS:CG	1:B:304:PRO:HD2	2.25	0.71
1:B:414:GLU:HG2	1:B:492:PRO:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LEU:HD11	1:B:521:MET:HG2	1.74	0.70
1:A:292:THR:HG23	1:A:393:GLU:HG2	1.73	0.69
1:B:497:GLY:HA2	1:B:503:GLY:O	1.94	0.68
1:A:520:MET:HG3	1:A:525:GLN:HB2	1.77	0.67
1:A:300:ALA:O	1:A:301:SER:O	2.12	0.66
1:A:457:THR:O	1:A:460:TYR:N	2.28	0.66
1:B:416:LEU:HB2	1:B:466:LEU:HD21	1.78	0.66
1:B:508:GLN:HG2	1:B:518:TRP:CE2	2.31	0.66
1:B:472:ILE:HG21	1:B:481:ALA:CB	2.26	0.66
1:A:298:GLU:HG3	1:A:299:GLN:N	2.11	0.65
1:A:417:ARG:HD2	1:A:419:GLU:OE2	1.97	0.64
1:A:278:LYS:HZ2	1:A:567:GLN:HE22	1.44	0.64
1:A:560:ASP:O	1:A:564:LYS:HD2	1.97	0.64
1:B:361:HIS:CE1	1:B:423:PHE:HB3	2.34	0.62
1:A:301:SER:O	1:A:302:ASN:HB3	1.97	0.62
1:A:474:ARG:H	1:A:474:ARG:HE	1.48	0.62
1:B:403:TPO:O	1:B:404:PHE:HB3	2.01	0.61
1:B:352:GLU:OE2	1:B:382:HIS:ND1	2.23	0.61
1:A:238:ASP:OD2	1:A:239:PRO:HD2	2.00	0.61
1:B:238:ASP:HB2	1:B:239:PRO:CD	2.31	0.61
1:B:298:GLU:HG3	1:B:299:GLN:N	2.16	0.60
1:A:237:MET:HE3	1:B:298:GLU:HB2	1.80	0.60
1:B:457:THR:HG22	1:B:460:TYR:H	1.66	0.60
1:A:414:GLU:HG3	1:A:492:PRO:HG3	1.82	0.60
1:B:518:TRP:O	1:B:521:MET:HB3	2.02	0.60
1:B:305:PHE:HB2	1:B:356:ALA:HB2	1.83	0.60
1:A:237:MET:HE1	1:B:298:GLU:CB	2.23	0.59
1:B:460:TYR:O	1:B:464:VAL:HG23	2.04	0.58
1:B:355:LEU:CD1	1:B:521:MET:HG2	2.34	0.58
1:B:278:LYS:NZ	1:B:567:GLN:HE22	2.00	0.57
1:A:278:LYS:NZ	1:A:567:GLN:HE22	2.03	0.57
1:A:553:GLN:OE1	4:A:866:HOH:O	2.17	0.57
1:B:413:PRO:HA	1:B:416:LEU:HD12	1.87	0.57
1:B:305:PHE:CZ	1:B:352:GLU:HG2	2.40	0.56
1:B:348:PHE:CE1	1:B:521:MET:HE1	2.41	0.56
1:A:474:ARG:H	1:A:474:ARG:NE	2.02	0.56
1:B:489:ASN:HD21	1:B:494:GLU:HB3	1.68	0.56
1:B:332:MET:HE2	1:B:336:GLN:HG3	1.88	0.56
1:A:303:HIS:CG	1:A:304:PRO:HD2	2.40	0.56
1:B:303:HIS:CD2	1:B:304:PRO:HD2	2.42	0.55
1:B:413:PRO:O	1:B:416:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:HIS:ND1	1:B:304:PRO:HD2	2.22	0.54
1:A:535:SER:O	1:A:539:GLY:HA2	2.08	0.53
1:B:344:GLU:CD	1:B:344:GLU:H	2.11	0.53
1:B:278:LYS:HE2	1:B:570:PHE:CD1	2.43	0.53
1:B:503:GLY:O	1:B:506:ASP:HB2	2.08	0.53
1:B:303:HIS:CE1	1:B:304:PRO:HD2	2.43	0.53
1:B:510:HIS:CG	1:B:511:PRO:HD2	2.43	0.53
1:B:435:PHE:CE2	1:B:443:PRO:HA	2.45	0.52
1:B:368:ARG:CZ	1:B:392:LYS:HB2	2.40	0.51
1:B:403:TPO:O1P	1:B:403:TPO:N	2.43	0.51
1:B:490:LYS:O	1:B:492:PRO:HD3	2.10	0.51
1:A:349:TYR:CD2	1:A:437:MET:HE1	2.46	0.51
1:B:309:LEU:HD13	1:B:575:TYR:CD2	2.46	0.51
1:B:287:ILE:HG21	1:B:569:GLU:HB3	1.93	0.51
1:A:349:TYR:HD2	1:A:437:MET:HE1	1.76	0.50
1:B:281:VAL:HG22	1:B:281:VAL:O	2.12	0.50
1:B:545:SER:HA	1:B:548:THR:OG1	2.12	0.50
1:A:292:THR:O	1:A:296:VAL:HG23	2.12	0.50
1:B:462:PHE:HA	1:B:465:ILE:HG13	1.93	0.50
1:A:486:SER:OG	1:A:496:LEU:HB2	2.12	0.49
1:B:414:GLU:CG	1:B:492:PRO:CG	2.75	0.49
1:A:301:SER:O	1:A:302:ASN:CB	2.60	0.49
1:B:289:TRP:CH2	1:B:293:GLU:HG3	2.48	0.49
1:B:461:LEU:O	1:B:465:ILE:HG13	2.12	0.49
1:A:338:GLN:O	1:A:339:ARG:HB2	2.13	0.48
1:B:428:TRP:HE3	1:B:495:ARG:HH21	1.52	0.48
1:B:508:GLN:HG2	1:B:518:TRP:CD2	2.48	0.48
1:B:492:PRO:HA	1:B:495:ARG:HH11	1.78	0.48
1:B:560:ASP:O	1:B:564:LYS:HB2	2.14	0.48
1:B:444:PHE:CZ	1:B:465:ILE:HG23	2.49	0.48
1:A:523:GLN:O	1:A:524:LYS:HB2	2.13	0.47
1:A:460:TYR:O	1:A:463:GLN:N	2.48	0.47
1:B:428:TRP:CE3	1:B:495:ARG:NH2	2.67	0.47
1:B:558:ASP:OD2	1:B:561:ILE:HG13	2.15	0.47
1:B:510:HIS:O	1:B:513:PHE:N	2.35	0.47
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.79	0.47
1:A:309:LEU:HD13	1:A:575:TYR:CD2	2.50	0.47
1:B:461:LEU:O	1:B:465:ILE:CG1	2.63	0.46
1:A:297:PHE:HB3	1:A:309:LEU:HB2	1.97	0.45
1:A:297:PHE:O	1:A:301:SER:OG	2.28	0.45
1:A:343:GLU:CG	1:A:512:PHE:HE1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:GLN:HA	1:A:523:GLN:HE21	1.82	0.45
1:B:330:ASP:C	1:B:330:ASP:OD2	2.55	0.45
1:B:553:GLN:HG2	1:B:554:LEU:N	2.31	0.45
1:B:338:GLN:NE2	4:B:777:HOH:O	2.43	0.45
1:A:523:GLN:CA	1:A:523:GLN:HE21	2.29	0.45
1:B:492:PRO:HA	1:B:495:ARG:NH1	2.32	0.44
1:B:559:ASP:OD1	1:B:559:ASP:N	2.51	0.44
1:B:412:ALA:O	1:B:416:LEU:HG	2.18	0.44
1:B:497:GLY:O	1:B:503:GLY:HA3	2.17	0.44
1:B:284:ASP:HB2	1:B:285:GLU:H	1.58	0.44
1:B:353:ILE:HG12	1:B:383:ILE:HD13	2.00	0.44
1:B:486:SER:HB3	1:B:496:LEU:HB2	1.99	0.43
1:B:238:ASP:HB2	1:B:239:PRO:HD2	2.00	0.43
1:B:393:GLU:O	1:B:393:GLU:HG2	2.17	0.43
1:A:567:GLN:HE21	1:A:567:GLN:HA	1.82	0.43
1:B:282:ASN:ND2	1:B:282:ASN:C	2.72	0.43
1:A:460:TYR:O	1:A:463:GLN:HB2	2.19	0.43
1:B:281:VAL:CG2	1:B:290:VAL:HG23	2.49	0.43
1:B:479:LYS:HE3	1:B:479:LYS:HB2	1.44	0.43
1:B:558:ASP:OD1	1:B:558:ASP:C	2.57	0.43
1:B:360:LEU:HA	1:B:360:LEU:HD12	1.91	0.42
1:B:462:PHE:N	1:B:462:PHE:CD1	2.88	0.42
1:B:484:LEU:HD23	1:B:484:LEU:HA	1.81	0.42
1:B:402:SER:O	1:B:403:TPO:C	2.67	0.42
1:B:412:ALA:H	1:B:415:ILE:HD12	1.83	0.42
1:A:396:ARG:CB	1:A:397:PRO:CD	2.83	0.42
1:B:413:PRO:HD2	1:B:414:GLU:OE2	2.19	0.42
1:A:510:HIS:HA	1:A:511:PRO:HD3	1.95	0.42
1:B:489:ASN:C	1:B:489:ASN:OD1	2.59	0.42
1:A:237:MET:HE2	1:B:575:TYR:CE1	2.55	0.42
1:B:480:ALA:O	1:B:484:LEU:HB2	2.20	0.41
1:B:527:VAL:O	1:B:527:VAL:HG13	2.19	0.41
1:A:237:MET:CE	1:B:298:GLU:CB	2.79	0.41
1:B:325:TYR:CZ	1:B:327:ASN:HB3	2.55	0.41
1:B:401:THR:O	1:B:420:ASP:CB	2.60	0.41
1:B:281:VAL:HG21	1:B:290:VAL:CG2	2.50	0.41
1:B:566:ASP:OD2	1:B:568:SER:OG	2.38	0.41
1:A:338:GLN:C	1:A:340:LYS:H	2.24	0.41
1:B:553:GLN:HE21	1:B:553:GLN:HB3	1.68	0.41
1:B:517:ASP:CG	1:B:520:MET:HG3	2.41	0.40
1:B:435:PHE:CD1	1:B:443:PRO:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:CG1	1:A:288:ASP:H	2.32	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	320/345 (93%)	293 (92%)	24 (8%)	3 (1%)	20	14
1	B	321/345 (93%)	293 (91%)	23 (7%)	5 (2%)	11	5
All	All	641/690 (93%)	586 (91%)	47 (7%)	8 (1%)	15	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	SER
1	A	397	PRO
1	A	399	ASP
1	B	284	ASP
1	B	302	ASN
1	B	399	ASP
1	B	390	MET
1	B	404	PHE

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	292/306 (95%)	275 (94%)	17 (6%)	23	20
1	B	293/306 (96%)	260 (89%)	33 (11%)	7	3
All	All	585/612 (96%)	535 (92%)	50 (8%)	12	8

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ASP
1	A	261	LEU
1	A	298	GLU
1	A	299	GLN
1	A	309	LEU
1	A	337	ARG
1	A	360	LEU
1	A	363	ARG
1	A	393	GLU
1	A	433	LEU
1	A	457	THR
1	A	471	ARG
1	A	474	ARG
1	A	520	MET
1	A	523	GLN
1	A	531	LYS
1	A	544	ASP
1	B	238	ASP
1	B	260	LEU
1	B	261	LEU
1	B	264	LEU
1	B	268	ASP
1	B	284	ASP
1	B	298	GLU
1	B	302	ASN
1	B	309	LEU
1	B	337	ARG
1	B	339	ARG
1	B	344	GLU
1	B	345	HIS
1	B	360	LEU
1	B	362	GLU
1	B	363	ARG
1	B	402	SER
1	B	405	CYS

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Mol	Chain	Res	Type
1	B	411	ILE
1	B	414	GLU
1	B	419	GLU
1	B	458	GLU
1	B	465	ILE
1	B	471	ARG
1	B	479	LYS
1	B	485	LYS
1	B	486	SER
1	B	521	MET
1	B	523	GLN
1	B	531	LYS
1	B	546	GLN
1	B	553	GLN
1	B	559	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	508	GLN
1	A	523	GLN
1	A	567	GLN
1	B	546	GLN
1	B	553	GLN
1	B	567	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	TPO	A	403	1	9,10,11	0.58	0	10,14,16	1.28	0
1	TPO	A	555	1	9,10,11	0.78	0	10,14,16	1.04	0
1	TPO	B	403	1	9,10,11	0.86	0	10,14,16	1.77	2 (20%)
1	TPO	B	555	1	9,10,11	1.05	0	10,14,16	1.41	1 (10%)

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	TPO	A	403	1	-	0/8/11/13	0/0/0/0
1	TPO	A	555	1	-	0/8/11/13	0/0/0/0
1	TPO	B	403	1	-	0/8/11/13	0/0/0/0
1	TPO	B	555	1	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	TPO	O-C-CA	-2.12	120.19	125.15
1	B	555	TPO	C-CA-N	2.79	115.48	109.86
1	B	403	TPO	C-CA-N	4.31	118.55	109.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	403	TPO	3	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 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	ATP	A	601	-	27,33,33	0.94	1 (3%)	25,52,52	1.74	3 (12%)
2	ATP	B	601	-	27,33,33	1.03	2 (7%)	25,52,52	1.92	4 (16%)
3	SO4	B	611	-	4,4,4	0.13	0	6,6,6	0.27	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	ATP	A	601	-	-	0/18/38/38	0/3/3/3
2	ATP	B	601	-	-	0/18/38/38	0/3/3/3
3	SO4	B	611	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ATP	PG-O3B	2.55	1.64	1.60
2	B	601	ATP	C5-C4	2.89	1.47	1.40
2	A	601	ATP	C5-C4	2.96	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ATP	N3-C2-N1	-7.62	122.22	128.86
2	A	601	ATP	N3-C2-N1	-6.92	122.83	128.86
2	A	601	ATP	C4-C5-N7	-3.22	106.30	109.41
2	A	601	ATP	C2-N1-C6	2.12	122.48	118.77
2	B	601	ATP	C2-N1-C6	2.15	122.52	118.77
2	B	601	ATP	O3G-PG-O2G	2.24	116.64	107.61
2	B	601	ATP	N6-C6-N1	2.27	123.26	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	326/345 (94%)	0.29	12 (3%) 42 49	14, 30, 49, 62	0
1	B	327/345 (94%)	0.86	44 (13%) 3 5	8, 33, 55, 70	0
All	All	653/690 (94%)	0.58	56 (8%) 11 14	8, 31, 53, 70	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	PHE	7.2
1	B	420	ASP	6.8
1	B	536	GLY	5.9
1	B	460	TYR	5.6
1	B	461	LEU	4.5
1	B	470	ILE	4.5
1	B	462	PHE	4.2
1	A	397	PRO	3.7
1	B	238	ASP	3.7
1	B	467	GLU	3.7
1	B	466	LEU	3.6
1	B	502	THR	3.6
1	B	423	PHE	3.5
1	A	460	TYR	3.5
1	B	405	CYS	3.5
1	B	459	ASP	3.4
1	B	417	ARG	3.4
1	A	238	ASP	3.3
1	B	424	SER	3.3
1	B	517	ASP	3.3
1	B	458	GLU	3.3
1	B	515	ASN	3.3
1	A	333	PHE	3.2
1	B	457	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	493	LYS	3.1
1	A	535	SER	3.0
1	B	537	GLU	3.0
1	B	463	GLN	2.9
1	B	499	HIS	2.9
1	B	519	ASP	2.9
1	B	415	ILE	2.8
1	B	333	PHE	2.8
1	A	404	PHE	2.7
1	A	396	ARG	2.7
1	A	471	ARG	2.7
1	B	572	GLY	2.6
1	B	465	ILE	2.6
1	B	525	GLN	2.6
1	B	535	SER	2.5
1	B	501	GLN	2.5
1	A	398	GLY	2.5
1	B	498	CYS	2.4
1	B	520	MET	2.4
1	B	363	ARG	2.3
1	B	523	GLN	2.3
1	A	525	GLN	2.3
1	B	560	ASP	2.2
1	B	484	LEU	2.2
1	A	459	ASP	2.2
1	B	419	GLU	2.1
1	B	527	VAL	2.1
1	B	411	ILE	2.1
1	B	464	VAL	2.1
1	B	427	TRP	2.1
1	A	462	PHE	2.0
1	B	561	ILE	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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	TPO	B	403	11/12	0.70	0.20	-	53,54,58,60	0
1	TPO	A	403	11/12	0.97	0.09	-	31,33,35,35	0
1	TPO	B	555	11/12	0.96	0.11	-	19,32,36,36	0
1	TPO	A	555	11/12	0.98	0.10	-	18,25,32,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ATP	B	601	31/31	0.98	0.11	-1.51	8,15,28,33	0
2	ATP	A	601	31/31	0.97	0.10	-1.55	14,20,24,27	0
3	SO4	B	611	5/5	0.98	0.12	-2.07	31,33,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.