



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:03 AM UTC

PDB ID : 3A8X / pdb_00003a8x
Title : Crystal Structure of PKC α kinase domain
Authors : Takimura, T.; Kamata, K.
Deposited on : 2009-10-11
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

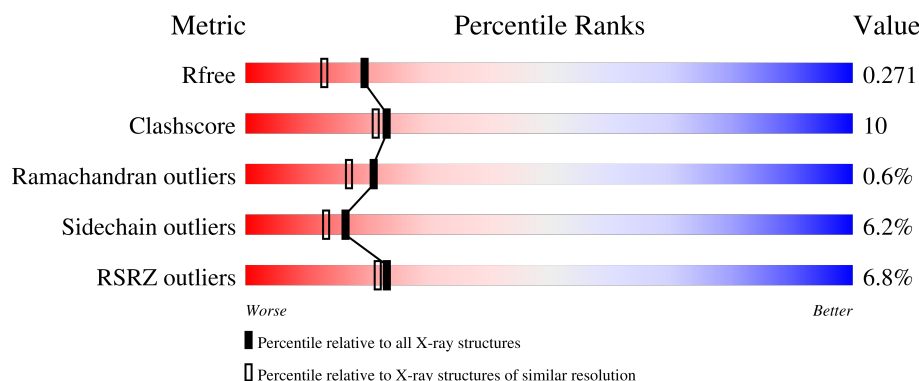
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	345	4% 79% 15% • •
1	B	345	9% 72% 20% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5651 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.

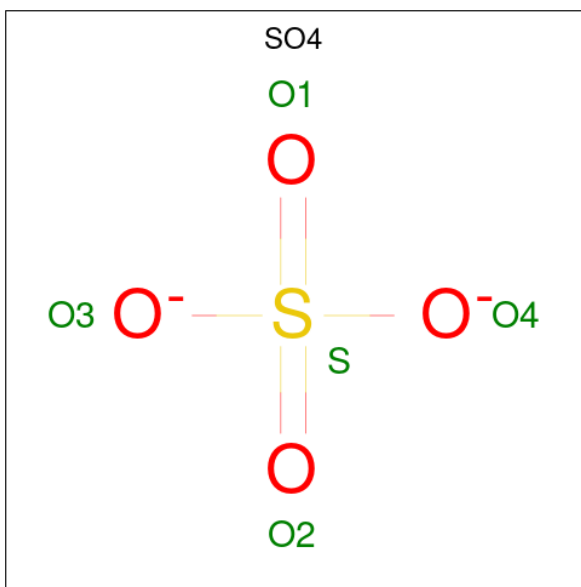
- Molecule 1 is a protein called Protein kinase C iota type.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	P	S	0	0	0
			2740	1749	458	517	2	14			
1	B	331	Total	C	N	O	P	S	0	0	0
			2702	1730	452	504	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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

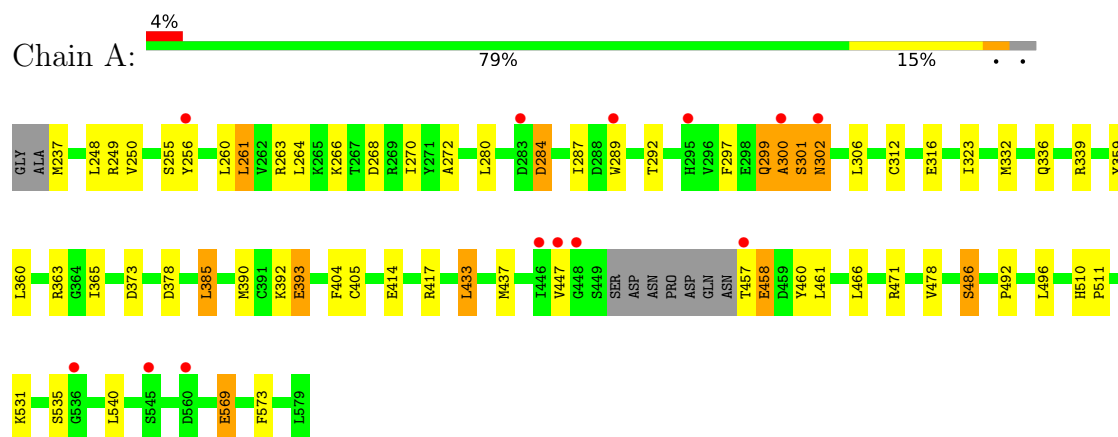
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	69	Total	O	0	0
			69	69		

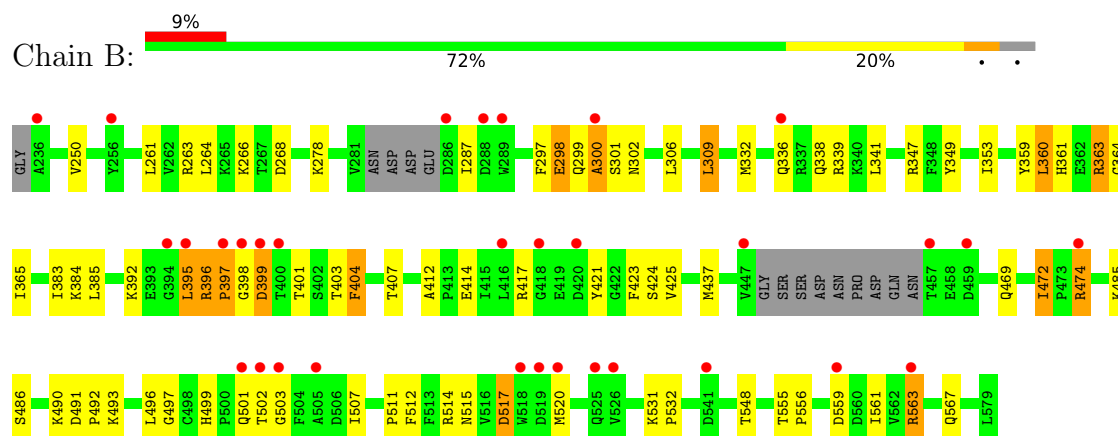
3 Residue-property plots [i](#)

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

• Molecule 1: 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	84.90Å 89.15Å 204.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.40 – 2.00 30.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.40-2.00) 91.8 (30.40-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.52 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.223 , 0.271 0.222 , 0.271	Depositor DCC
R_{free} test set	2448 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5651	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: TPO, 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	0.43	0/2782	0.70	0/3752
1	B	0.37	0/2743	0.67	2/3698 (0.1%)
All	All	0.40	0/5525	0.69	2/7450 (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	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	407	THR	CA-C-N	5.23	126.38	119.84
1	B	407	THR	C-N-CA	5.23	126.38	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	PHE	Peptide
1	B	300	ALA	Peptide
1	B	404	PHE	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	2740	0	2660	53	0
1	B	2702	0	2636	59	0
2	A	15	0	0	2	0
2	B	5	0	0	0	0
3	A	120	0	0	3	0
3	B	69	0	0	2	0
All	All	5651	0	5296	111	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 10.

All (111) 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:341:LEU:CD1	1:B:437:MET:HE2	1.87	1.05
1:A:292:THR:HG23	1:A:393:GLU:HG2	1.50	0.94
1:B:341:LEU:HD12	1:B:437:MET:HE2	1.50	0.92
1:A:299:GLN:C	1:A:301:SER:H	1.75	0.90
1:A:302:ASN:H	1:A:302:ASN:HD22	1.22	0.88
1:B:341:LEU:HD11	1:B:437:MET:HE2	1.62	0.80
1:B:474:ARG:HE	1:B:474:ARG:H	1.32	0.77
1:A:299:GLN:O	1:A:301:SER:N	2.18	0.77
1:A:256:TYR:CE2	1:A:289:TRP:HH2	2.05	0.74
1:A:359:TYR:CE1	1:A:363:ARG:NH2	2.57	0.73
1:A:302:ASN:H	1:A:302:ASN:ND2	1.85	0.72
1:A:302:ASN:HD22	1:A:302:ASN:N	1.86	0.70
1:B:364:GLY:HA3	1:B:395:LEU:H	1.56	0.70
1:A:237:MET:HE3	1:B:298:GLU:HB2	1.74	0.70
1:A:299:GLN:C	1:A:301:SER:N	2.41	0.69
1:A:266:LYS:HG3	3:A:736:HOH:O	1.93	0.68
1:B:365:ILE:HA	1:B:392:LYS:O	1.95	0.67
1:B:472:ILE:HD11	1:B:485:LYS:HG2	1.77	0.67
1:A:447:VAL:O	1:A:447:VAL:HG23	1.95	0.66
1:A:414:GLU:HG2	1:A:492:PRO:HG3	1.77	0.65
1:B:364:GLY:CA	1:B:395:LEU:H	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:SER:HB2	1:A:496:LEU:HB2	1.79	0.64
1:A:457:THR:HB	1:A:460:TYR:CB	2.28	0.63
1:B:472:ILE:CD1	1:B:485:LYS:HG2	2.28	0.63
1:B:298:GLU:HG3	1:B:299:GLN:N	2.15	0.62
1:A:332:MET:O	1:A:336:GLN:HG3	2.00	0.61
1:A:256:TYR:CE2	1:A:289:TRP:CH2	2.87	0.61
1:B:364:GLY:O	1:B:395:LEU:HB2	2.00	0.60
1:A:414:GLU:CG	1:A:492:PRO:HG3	2.33	0.59
1:B:297:PHE:O	1:B:301:SER:OG	2.09	0.59
1:B:349:TYR:CD2	1:B:437:MET:HE1	2.38	0.59
1:B:417:ARG:NH2	1:B:490:LYS:O	2.36	0.58
1:A:471:ARG:HD3	2:A:604:SO4:O3	2.03	0.58
1:A:457:THR:HB	1:A:460:TYR:HB2	1.86	0.57
1:B:306:LEU:HD23	1:B:385:LEU:HB2	1.87	0.57
1:A:433:LEU:HD23	1:A:437:MET:HE2	1.86	0.57
1:B:474:ARG:H	1:B:474:ARG:NE	2.02	0.56
1:B:401:THR:OG1	1:B:403:TPO:O3P	2.18	0.56
1:A:457:THR:HB	1:A:460:TYR:HB3	1.88	0.55
1:A:249:ARG:HG3	1:A:540:LEU:HD11	1.88	0.55
1:B:497:GLY:HA3	1:B:507:ILE:HD11	1.90	0.54
1:B:491:ASP:OD2	1:B:493:LYS:HG2	2.07	0.54
1:B:349:TYR:O	1:B:353:ILE:HG13	2.06	0.54
1:B:396:ARG:O	1:B:398:GLY:N	2.42	0.53
1:B:332:MET:HG3	1:B:336:GLN:HE21	1.74	0.53
1:A:260:LEU:N	1:A:260:LEU:HD22	2.23	0.53
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.75	0.51
1:A:287:ILE:HG21	1:A:569:GLU:HG3	1.92	0.51
1:B:278:LYS:NZ	1:B:567:GLN:HE22	2.08	0.51
1:A:256:TYR:CD2	1:A:289:TRP:HH2	2.28	0.51
1:B:301:SER:CB	3:B:813:HOH:O	2.58	0.50
1:B:278:LYS:HZ2	1:B:567:GLN:HE22	1.59	0.50
1:B:399:ASP:OD1	1:B:399:ASP:N	2.44	0.50
1:A:250:VAL:HG22	1:A:260:LEU:CD1	2.42	0.50
1:A:540:LEU:HD12	2:A:602:SO4:S	2.52	0.49
1:A:261:LEU:HD21	1:A:270:ILE:CG2	2.42	0.49
1:A:478:VAL:HG23	3:A:837:HOH:O	2.12	0.49
1:A:359:TYR:HE1	1:A:363:ARG:NH2	2.11	0.49
1:B:396:ARG:O	1:B:397:PRO:C	2.55	0.49
1:B:338:GLN:O	1:B:339:ARG:HB2	2.13	0.48
1:B:561:ILE:HD12	1:B:561:ILE:N	2.28	0.48
1:B:297:PHE:HB3	1:B:309:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:HIS:HE1	1:B:501:GLN:HB2	1.79	0.48
1:B:486:SER:HB3	1:B:496:LEU:HB2	1.96	0.47
1:B:361:HIS:C	1:B:363:ARG:H	2.22	0.47
1:A:458:GLU:HG2	1:A:458:GLU:O	2.13	0.47
1:A:447:VAL:O	1:A:447:VAL:CG2	2.62	0.47
1:A:300:ALA:O	1:A:301:SER:C	2.58	0.47
1:A:390:MET:HG3	1:A:405:CYS:SG	2.55	0.47
1:B:559:ASP:O	1:B:563:ARG:HB2	2.15	0.47
1:B:347:ARG:NH2	1:B:512:PHE:O	2.46	0.47
1:B:263:ARG:HH21	1:B:263:ARG:HG3	1.81	0.46
1:A:417:ARG:HG3	1:A:466:LEU:HD21	1.98	0.46
1:B:412:ALA:HB3	1:B:425:VAL:HG12	1.96	0.46
1:B:511:PRO:O	1:B:514:ARG:HB2	2.15	0.46
1:B:403:TPO:O	1:B:421:TYR:OH	2.30	0.46
1:A:312:CYS:HB3	1:A:573:PHE:CE2	2.51	0.45
1:A:339:ARG:HA	1:A:339:ARG:HD2	1.83	0.45
1:A:359:TYR:CE1	1:A:363:ARG:CZ	3.00	0.45
1:A:363:ARG:HH11	1:A:363:ARG:HG2	1.81	0.45
1:B:414:GLU:HG3	1:B:492:PRO:HG3	1.98	0.45
1:B:359:TYR:OH	1:B:363:ARG:NH1	2.50	0.45
1:B:414:GLU:CG	1:B:492:PRO:HG3	2.48	0.44
1:B:563:ARG:HH11	1:B:563:ARG:HB3	1.82	0.44
1:B:531:LYS:HD3	1:B:532:PRO:O	2.18	0.44
1:B:423:PHE:O	1:B:424:SER:C	2.61	0.44
1:A:250:VAL:HA	1:A:260:LEU:HD13	2.00	0.43
1:B:300:ALA:O	1:B:302:ASN:N	2.51	0.43
1:B:517:ASP:OD1	1:B:520:MET:HB2	2.18	0.43
1:B:359:TYR:CZ	1:B:363:ARG:NH1	2.87	0.43
1:B:414:GLU:H	1:B:414:GLU:CD	2.25	0.43
1:A:248:LEU:C	1:A:249:ARG:HG2	2.43	0.43
1:A:378:ASP:OD1	1:A:378:ASP:C	2.62	0.43
1:A:263:ARG:HD2	1:A:268:ASP:OD1	2.19	0.42
1:B:306:LEU:HD21	1:B:360:LEU:HD21	2.01	0.42
1:B:499:HIS:CE1	1:B:501:GLN:HB2	2.53	0.42
1:B:250:VAL:O	1:B:548:THR:HA	2.20	0.42
1:B:347:ARG:NE	3:B:875:HOH:O	2.26	0.42
1:B:555:TPO:HA	1:B:556:PRO:HD3	1.93	0.42
1:A:447:VAL:HG11	1:A:461:LEU:HA	2.01	0.42
1:A:248:LEU:O	1:A:249:ARG:HD3	2.20	0.41
1:A:280:LEU:HD12	3:A:770:HOH:O	2.21	0.41
1:A:510:HIS:CG	1:A:511:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ALA:HB3	1:A:323:ILE:HG13	2.03	0.41
1:B:502:THR:O	1:B:503:GLY:C	2.64	0.41
1:A:306:LEU:HD23	1:A:385:LEU:HB2	2.03	0.41
1:B:561:ILE:N	1:B:561:ILE:CD1	2.83	0.41
1:A:297:PHE:CZ	1:A:323:ILE:HG21	2.56	0.40
1:A:365:ILE:HA	1:A:392:LYS:O	2.20	0.40
1:B:306:LEU:HD21	1:B:360:LEU:CD2	2.51	0.40
1:B:403:TPO:HG23	1:B:404:PHE:O	2.21	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	330/345 (96%)	321 (97%)	6 (2%)	3 (1%)	14	9
1	B	323/345 (94%)	315 (98%)	7 (2%)	1 (0%)	36	35
All	All	653/690 (95%)	636 (97%)	13 (2%)	4 (1%)	21	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ASP
1	A	300	ALA
1	A	301	SER
1	B	397	PRO

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	299/306 (98%)	282 (94%)	17 (6%)	18	15
1	B	294/306 (96%)	274 (93%)	20 (7%)	14	11
All	All	593/612 (97%)	556 (94%)	37 (6%)	16	13

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	SER
1	A	261	LEU
1	A	264	LEU
1	A	284	ASP
1	A	299	GLN
1	A	302	ASN
1	A	316	GLU
1	A	360	LEU
1	A	373	ASP
1	A	385	LEU
1	A	393	GLU
1	A	433	LEU
1	A	458	GLU
1	A	486	SER
1	A	531	LYS
1	A	535	SER
1	A	569	GLU
1	B	261	LEU
1	B	264	LEU
1	B	266	LYS
1	B	268	ASP
1	B	287	ILE
1	B	298	GLU
1	B	309	LEU
1	B	360	LEU
1	B	363	ARG
1	B	383	ILE
1	B	384	LYS
1	B	395	LEU
1	B	396	ARG
1	B	399	ASP
1	B	469	GLN
1	B	472	ILE

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Mol	Chain	Res	Type
1	B	474	ARG
1	B	515	ASN
1	B	517	ASP
1	B	563	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	299	GLN
1	A	302	ASN
1	A	336	GLN
1	A	358	ASN
1	A	469	GLN
1	A	542	ASN
1	B	291	GLN
1	B	302	ASN
1	B	336	GLN
1	B	533	ASN
1	B	546	GLN
1	B	567	GLN

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	TPO	B	403	1	8,10,11	0.72	0	10,14,16	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	A	403	1	8,10,11	0.74	0	10,14,16	1.12	0
1	TPO	B	555	1	8,10,11	0.76	0	10,14,16	1.20	0
1	TPO	A	555	1	8,10,11	0.83	0	10,14,16	1.00	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
1	TPO	B	403	1	-	0/9/11/13	-
1	TPO	A	403	1	-	0/9/11/13	-
1	TPO	B	555	1	-	0/9/11/13	-
1	TPO	A	555	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	403	TPO	3	0
1	B	555	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	SO4	A	604	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	603	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	601	-	4,4,4	0.23	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	SO4	1	0
2	A	602	SO4	1	0

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	334/345 (96%)	0.25	13 (3%) 43 42	19, 32, 51, 65	0
1	B	329/345 (95%)	0.71	32 (9%) 13 12	24, 40, 63, 82	0
All	All	663/690 (96%)	0.48	45 (6%) 23 22	19, 35, 59, 82	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	ALA	5.7
1	B	256	TYR	3.6
1	B	418	GLY	3.5
1	B	541	ASP	3.5
1	A	457	THR	3.3
1	A	302	ASN	3.2
1	B	300	ALA	3.0
1	A	256	TYR	3.0
1	B	474	ARG	2.9
1	A	448	GLY	2.9
1	B	563	ARG	2.8
1	B	397	PRO	2.8
1	B	399	ASP	2.8
1	B	505	ALA	2.8
1	B	336	GLN	2.7
1	B	400	THR	2.6
1	B	420	ASP	2.6
1	A	536	GLY	2.6
1	A	295	HIS	2.6
1	A	289	TRP	2.6
1	B	526	VAL	2.6
1	B	286	ASP	2.5
1	B	502	THR	2.5
1	A	545	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	395	LEU	2.4
1	B	394	GLY	2.4
1	B	398	GLY	2.4
1	B	519	ASP	2.4
1	B	518	TRP	2.3
1	A	300	ALA	2.3
1	B	501	GLN	2.3
1	B	447	VAL	2.2
1	A	446	ILE	2.2
1	A	560	ASP	2.2
1	B	520	MET	2.2
1	B	457	THR	2.2
1	A	283	ASP	2.1
1	B	525	GLN	2.1
1	B	289	TRP	2.1
1	B	459	ASP	2.1
1	B	559	ASP	2.1
1	B	288	ASP	2.0
1	B	503	GLY	2.0
1	A	447	VAL	2.0
1	B	416	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. 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	TPO	B	403	11/12	0.85	0.13	52,55,56,59	0
1	TPO	A	403	11/12	0.94	0.10	36,41,44,44	0
1	TPO	B	555	11/12	0.95	0.07	32,36,39,40	0
1	TPO	A	555	11/12	0.96	0.07	32,34,36,38	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	603	5/5	0.74	0.11	73,74,75,75	0
2	SO4	A	602	5/5	0.82	0.13	76,78,79,83	0
2	SO4	A	604	5/5	0.84	0.10	56,56,58,58	0
2	SO4	A	601	5/5	0.95	0.08	44,44,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.