



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:11 AM UTC

PDB ID : 1Q4K / pdb_00001q4k
Title : The polo-box domain of Plk1 in complex with a phospho-peptide
Authors : Cheng, K.; Lowe, E.D.; Sinclair, J.; Nigg, E.A.; Johnson, L.N.
Deposited on : 2003-08-04
Resolution : 2.30 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:

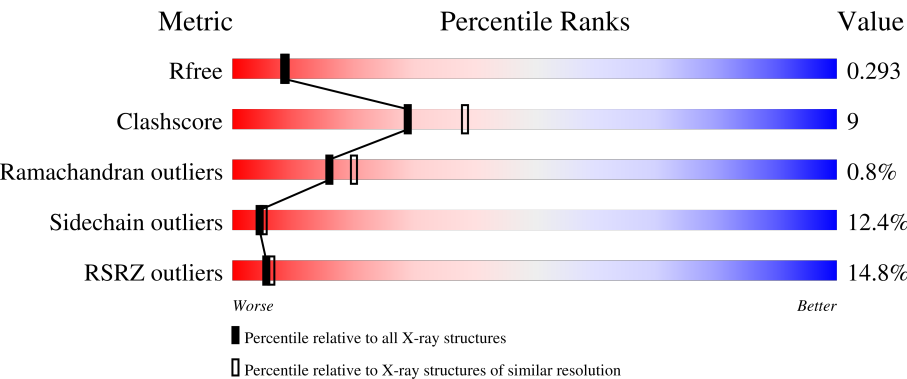
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	259	9% 64% 17% • 14%
1	B	259	8% 64% 20% • 14%
1	C	259	20% 60% 20% • 17%
2	D	6	33% 50% 50%
2	E	6	67% 33%

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Mol	Chain	Length	Quality of chain
2	F	6	33% 33% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5707 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 Serine/threonine-protein kinase PLK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	224	Total	C	N	O	S	0	0	0
			1822	1153	317	341	11			
1	A	222	Total	C	N	O	S	0	0	0
			1803	1143	312	337	11			
1	C	214	Total	C	N	O	S	0	0	0
			1744	1108	300	325	11			

- Molecule 2 is a protein called Phospho-peptide sequence Met.Gln.Ser.pThr.Pro.Leu.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	P	S	0	0	0
			49	28	7	12	1	1			
2	E	6	Total	C	N	O	P	S	0	0	0
			49	28	7	12	1	1			
2	F	6	Total	C	N	O	P	S	0	0	0
			49	28	7	12	1	1			

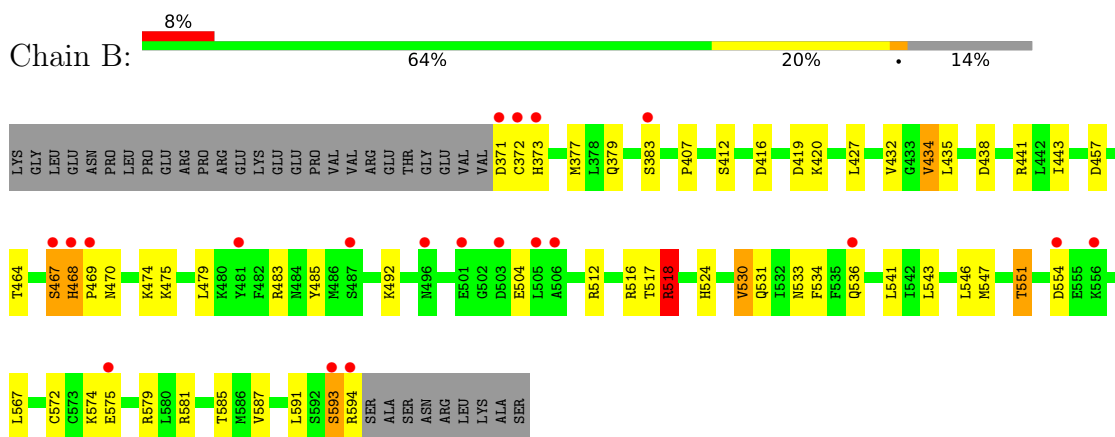
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	78	Total	O	0	0
			78	78		
3	A	55	Total	O	0	0
			55	55		
3	C	43	Total	O	0	0
			43	43		
3	D	2	Total	O	0	0
			2	2		
3	E	8	Total	O	0	0
			8	8		
3	F	5	Total	O	0	0
			5	5		

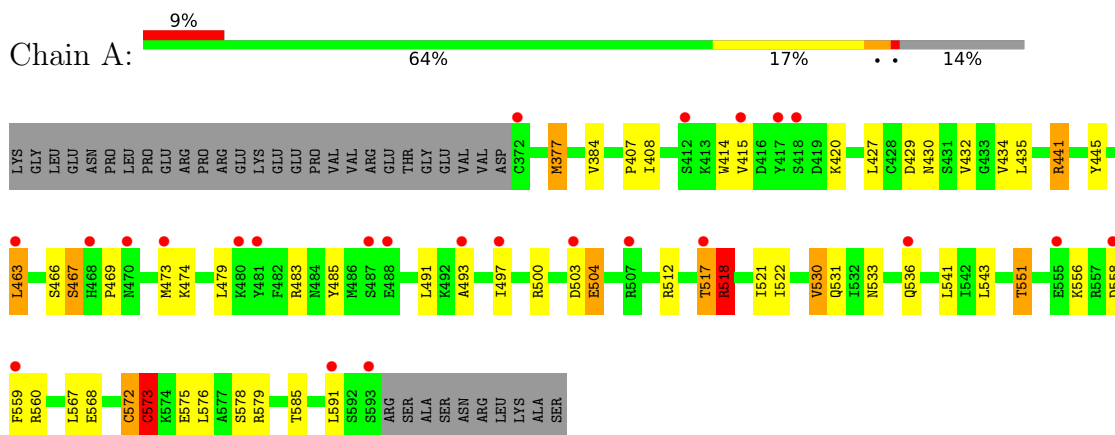
3 Residue-property plots [i](#)

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.

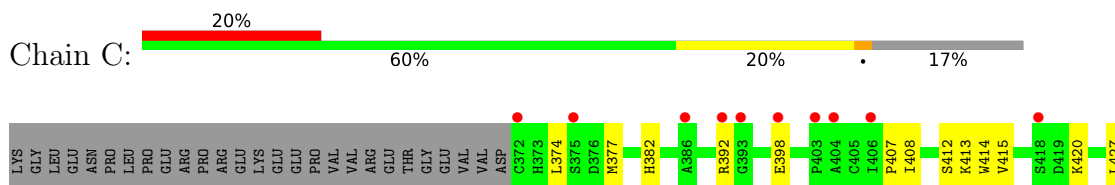
- Molecule 1: Serine/threonine-protein kinase PLK

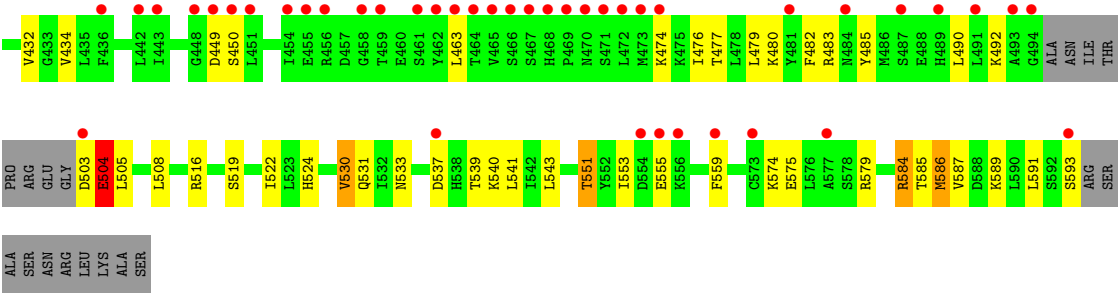


- Molecule 1: Serine/threonine-protein kinase PLK

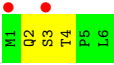


- Molecule 1: Serine/threonine-protein kinase PLK





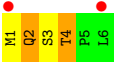
● Molecule 2: Phospho-peptide sequence Met.Gln.Ser.pThr.Pro.Leu



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.07Å 56.89Å 85.05Å 91.45° 103.21° 118.50°	Depositor
Resolution (Å)	29.36 – 2.30 29.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.36-2.30) 96.2 (29.36-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.245 , 0.312 0.237 , 0.293	Depositor DCC
R_{free} test set	1943 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5707	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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

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	0.73	1/1841 (0.1%)	0.97	5/2489 (0.2%)
1	B	0.77	0/1860	0.94	2/2514 (0.1%)
1	C	0.60	0/1780	0.85	0/2404
2	D	0.62	0/37	0.76	0/46
2	E	0.80	0/37	1.19	0/46
2	F	0.66	0/37	0.77	0/46
All	All	0.70	1/5592 (0.0%)	0.92	7/7545 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	MET	SD-CE	-6.19	1.64	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	THR	N-CA-C	9.16	124.95	111.02
1	A	518	ARG	N-CA-C	7.79	123.93	112.94
1	B	518	ARG	N-CA-C	-5.60	107.45	114.56
1	B	420	LYS	N-CA-C	5.44	122.20	114.16
1	A	573	CYS	CB-CA-C	-5.32	99.84	110.42
1	A	517	THR	CA-C-N	5.21	130.40	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	THR	C-N-CA	5.21	130.40	122.37

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	517	THR	Peptide
1	A	572	CYS	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	1803	0	1789	36	1
1	B	1822	0	1806	29	1
1	C	1744	0	1730	32	1
2	D	49	0	48	2	0
2	E	49	0	48	1	0
2	F	49	0	48	3	0
3	A	55	0	0	1	0
3	B	78	0	0	5	1
3	C	43	0	0	3	0
3	D	2	0	0	0	0
3	E	8	0	0	0	0
3	F	5	0	0	0	0
All	All	5707	0	5469	96	2

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 9.

All (96) 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:463:LEU:HD21	1:A:469:PRO:HD2	1.54	0.89
1:B:517:THR:C	3:B:36:HOH:O	2.16	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:MET:HE3	1:C:586:MET:HA	1.65	0.77
1:A:493:ALA:O	3:A:21:HOH:O	2.04	0.75
1:B:432:VAL:HG12	1:B:479:LEU:HD11	1.69	0.74
1:B:547:MET:HA	1:B:547:MET:HE2	1.70	0.72
1:A:384:VAL:HA	1:A:568:GLU:HG2	1.72	0.71
1:C:537:ASP:HB3	1:C:539:THR:HG23	1.71	0.70
1:B:531:GLN:HE21	1:B:533:ASN:HD21	1.41	0.69
1:B:416:ASP:OD2	1:B:516:ARG:NH1	2.27	0.67
1:A:463:LEU:HD21	1:A:469:PRO:CD	2.25	0.66
1:A:518:ARG:NE	1:A:518:ARG:H	1.93	0.66
1:C:374:LEU:HD21	1:C:524:HIS:ND1	2.11	0.66
1:A:377:MET:CE	1:A:543:LEU:HD13	2.29	0.63
1:A:432:VAL:HG12	1:A:479:LEU:HD11	1.82	0.61
1:B:377:MET:CE	1:B:543:LEU:HD13	2.29	0.61
1:C:476:ILE:O	1:C:480:LYS:HG3	2.00	0.60
1:C:377:MET:CE	1:C:543:LEU:HD13	2.31	0.60
1:A:531:GLN:HE21	1:A:533:ASN:HD21	1.49	0.60
1:B:407:PRO:HD3	1:B:551:THR:HG21	1.86	0.58
1:A:522:ILE:N	1:A:522:ILE:HD12	2.19	0.57
1:A:567:LEU:HD22	1:A:572:CYS:HB3	1.90	0.54
1:A:435:LEU:HD13	1:A:441:ARG:HD3	1.89	0.54
1:B:434:VAL:HG12	1:B:479:LEU:HD13	1.90	0.54
1:B:534:PHE:CE1	1:B:579:ARG:HD2	2.43	0.54
1:C:531:GLN:HE21	1:C:533:ASN:HD21	1.55	0.54
1:A:377:MET:HE1	1:A:530:VAL:HG22	1.91	0.53
1:A:573:CYS:HB3	1:A:576:LEU:H	1.74	0.53
1:A:485:TYR:OH	2:D:2:GLN:NE2	2.43	0.52
1:B:377:MET:HE3	1:B:543:LEU:HD13	1.92	0.52
1:B:468:HIS:N	1:B:468:HIS:ND1	2.57	0.52
1:A:518:ARG:H	1:A:518:ARG:CD	2.19	0.52
1:B:469:PRO:HD2	3:B:23:HOH:O	2.09	0.52
1:A:463:LEU:CD2	1:A:469:PRO:HD2	2.35	0.51
1:C:485:TYR:OH	2:F:2:GLN:NE2	2.44	0.51
1:C:585:THR:HG21	3:C:73:HOH:O	2.10	0.51
1:B:377:MET:SD	1:B:530:VAL:HG13	2.51	0.50
1:C:522:ILE:HG12	1:C:586:MET:HG2	1.93	0.50
1:B:575:GLU:O	1:B:579:ARG:HG2	2.12	0.49
1:A:377:MET:HE3	1:A:543:LEU:HD13	1.95	0.49
1:C:586:MET:HA	1:C:586:MET:CE	2.39	0.49
1:A:497:ILE:HG13	1:A:559:PHE:CD1	2.48	0.49
1:C:374:LEU:HD21	1:C:524:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:MET:HE2	1:C:587:VAL:HG21	1.94	0.48
1:B:373:HIS:CD2	1:B:546:LEU:HD21	2.49	0.48
1:B:377:MET:HE2	1:B:587:VAL:HG21	1.95	0.48
1:A:466:SER:O	1:A:467:SER:CB	2.62	0.47
1:A:377:MET:HE3	1:A:543:LEU:CB	2.44	0.47
1:A:429:ASP:O	1:A:430:ASN:HB2	2.14	0.47
1:A:432:VAL:HG21	1:A:483:ARG:HG3	1.95	0.47
1:B:432:VAL:HG12	1:B:479:LEU:CD1	2.42	0.47
1:C:414:TRP:CD1	2:F:3:SER:HB3	2.49	0.47
1:C:415:VAL:HG21	1:C:482:PHE:HD2	1.80	0.47
1:B:485:TYR:OH	2:E:2:GLN:NE2	2.46	0.47
1:C:503:ASP:C	1:C:504:GLU:HG3	2.40	0.46
1:C:575:GLU:O	1:C:579:ARG:HG2	2.16	0.46
1:C:522:ILE:HG12	1:C:586:MET:CG	2.46	0.46
1:C:407:PRO:CD	1:C:551:THR:HG21	2.46	0.45
1:C:477:THR:HA	1:C:480:LYS:HE3	1.99	0.45
1:C:463:LEU:N	1:C:463:LEU:HD12	2.31	0.45
1:B:524:HIS:CD2	1:B:524:HIS:C	2.95	0.45
1:B:593:SER:HB2	3:B:55:HOH:O	2.15	0.45
1:C:413:LYS:HD3	1:C:490:LEU:HB2	1.98	0.45
1:A:432:VAL:HG21	1:A:483:ARG:CG	2.47	0.45
1:B:373:HIS:NE2	1:B:546:LEU:HD21	2.32	0.44
1:B:438:ASP:OD2	1:B:475:LYS:NZ	2.49	0.44
1:C:540:LYS:NZ	2:F:4:TPO:O1P	2.49	0.44
1:A:384:VAL:HA	1:A:568:GLU:CG	2.46	0.44
1:C:553:ILE:HD11	1:C:559:PHE:CE1	2.53	0.44
1:B:468:HIS:HA	3:B:23:HOH:O	2.18	0.43
1:C:524:HIS:CD2	1:C:524:HIS:C	2.97	0.43
1:B:518:ARG:NH1	1:A:568:GLU:O	2.48	0.42
1:B:567:LEU:HD22	1:B:572:CYS:HB3	2.01	0.42
1:A:521:ILE:C	1:A:522:ILE:HD12	2.44	0.42
1:A:377:MET:SD	1:A:530:VAL:HG13	2.59	0.42
1:C:382:HIS:ND1	1:C:584:ARG:NH2	2.68	0.42
1:C:503:ASP:O	1:C:505:LEU:N	2.44	0.42
1:C:377:MET:HE3	1:C:543:LEU:HD13	1.99	0.42
1:B:464:THR:O	1:B:467:SER:O	2.38	0.41
1:A:407:PRO:CD	1:A:551:THR:HG21	2.50	0.41
1:A:415:VAL:HG23	1:A:415:VAL:O	2.19	0.41
1:A:377:MET:HE3	1:A:543:LEU:HB3	2.01	0.41
1:C:377:MET:SD	1:C:530:VAL:HG13	2.60	0.41
1:C:432:VAL:HG12	1:C:479:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ARG:HB2	1:B:524:HIS:CD2	2.55	0.41
1:A:575:GLU:OE1	1:A:579:ARG:NH2	2.54	0.41
1:A:408:ILE:HD13	1:A:500:ARG:CG	2.51	0.41
1:A:435:LEU:HD13	1:A:441:ARG:HH11	1.86	0.41
1:A:522:ILE:N	1:A:522:ILE:CD1	2.83	0.41
1:C:551:THR:HG22	3:C:46:HOH:O	2.20	0.41
1:B:457:ASP:OD1	1:B:457:ASP:C	2.64	0.40
1:A:414:TRP:CD1	2:D:3:SER:HB3	2.56	0.40
1:C:408:ILE:HD12	1:C:503:ASP:CG	2.47	0.40
1:C:504:GLU:OE1	3:C:3:HOH:O	2.22	0.40
1:A:407:PRO:HD3	1:A:551:THR:HG21	2.02	0.40
1:B:581:ARG:NH1	3:B:58:HOH:O	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:LYS:NZ	3:B:13:HOH:O[1_554]	1.91	0.29
1:B:419:ASP:OD2	1:A:445:TYR:OH[1_455]	2.19	0.01

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	220/259 (85%)	206 (94%)	11 (5%)	3 (1%)	9	9
1	B	222/259 (86%)	206 (93%)	15 (7%)	1 (0%)	24	31
1	C	210/259 (81%)	198 (94%)	11 (5%)	1 (0%)	24	31
2	D	3/6 (50%)	3 (100%)	0	0	100	100
2	E	3/6 (50%)	3 (100%)	0	0	100	100
2	F	3/6 (50%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	661/795 (83%)	619 (94%)	37 (6%)	5 (1%)	16	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	SER
1	A	504	GLU
1	A	573	CYS
1	C	504	GLU
1	B	504	GLU

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	201/234 (86%)	178 (89%)	23 (11%)	5	6
1	B	203/234 (87%)	176 (87%)	27 (13%)	4	4
1	C	195/234 (83%)	171 (88%)	24 (12%)	4	5
2	D	5/5 (100%)	5 (100%)	0	100	100
2	E	5/5 (100%)	5 (100%)	0	100	100
2	F	5/5 (100%)	3 (60%)	2 (40%)	0	0
All	All	614/717 (86%)	538 (88%)	76 (12%)	4	5

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	371	ASP
1	B	372	CYS
1	B	379	GLN
1	B	383	SER
1	B	412	SER
1	B	427	LEU
1	B	434	VAL

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Mol	Chain	Res	Type
1	B	435	LEU
1	B	441	ARG
1	B	443	ILE
1	B	467	SER
1	B	468	HIS
1	B	470	ASN
1	B	474	LYS
1	B	483	ARG
1	B	492	LYS
1	B	518	ARG
1	B	530	VAL
1	B	536	GLN
1	B	541	LEU
1	B	551	THR
1	B	554	ASP
1	B	574	LYS
1	B	585	THR
1	B	591	LEU
1	B	593	SER
1	B	594	ARG
1	A	420	LYS
1	A	427	LEU
1	A	434	VAL
1	A	441	ARG
1	A	463	LEU
1	A	473	MET
1	A	474	LYS
1	A	491	LEU
1	A	503	ASP
1	A	504	GLU
1	A	512	ARG
1	A	518	ARG
1	A	530	VAL
1	A	536	GLN
1	A	541	LEU
1	A	551	THR
1	A	556	LYS
1	A	558	ASP
1	A	560	ARG
1	A	573	CYS
1	A	578	SER
1	A	585	THR

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Mol	Chain	Res	Type
1	A	591	LEU
1	C	392	ARG
1	C	398	GLU
1	C	412	SER
1	C	420	LYS
1	C	427	LEU
1	C	434	VAL
1	C	449	ASP
1	C	450	SER
1	C	474	LYS
1	C	483	ARG
1	C	492	LYS
1	C	504	GLU
1	C	508	LEU
1	C	516	ARG
1	C	519	SER
1	C	530	VAL
1	C	541	LEU
1	C	551	THR
1	C	555	GLU
1	C	574	LYS
1	C	584	ARG
1	C	586	MET
1	C	591	LEU
1	C	593	SER
2	F	1	MET
2	F	2	GLN

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

Mol	Chain	Res	Type
1	B	489	HIS
1	B	524	HIS
1	B	533	ASN
1	A	426	GLN
1	A	533	ASN
1	C	426	GLN
1	C	468	HIS
1	C	484	ASN
1	C	524	HIS
1	C	533	ASN
2	D	2	GLN

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Mol	Chain	Res	Type
2	E	2	GLN
2	F	2	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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
2	TPO	F	4	2	8,10,11	3.72	4 (50%)	10,14,16	3.06	3 (30%)
2	TPO	D	4	2	8,10,11	3.57	4 (50%)	10,14,16	2.99	5 (50%)
2	TPO	E	4	2	8,10,11	3.33	4 (50%)	10,14,16	2.85	4 (40%)

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	TPO	F	4	2	-	1/9/11/13	-
2	TPO	D	4	2	-	0/9/11/13	-
2	TPO	E	4	2	-	0/9/11/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	TPO	P-O1P	6.45	1.70	1.50
2	D	4	TPO	P-O1P	6.03	1.69	1.50
2	F	4	TPO	O-C	5.93	1.42	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	TPO	O-C	5.89	1.42	1.20
2	D	4	TPO	O-C	5.81	1.42	1.20
2	E	4	TPO	P-O1P	5.31	1.67	1.50
2	F	4	TPO	P-O3P	4.04	1.69	1.54
2	F	4	TPO	P-O2P	3.86	1.69	1.54
2	D	4	TPO	P-O2P	3.83	1.69	1.54
2	D	4	TPO	P-O3P	3.70	1.68	1.54
2	E	4	TPO	P-O3P	3.65	1.68	1.54
2	E	4	TPO	P-O2P	3.47	1.67	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	TPO	O2P-P-OG1	-7.16	77.96	105.85
2	D	4	TPO	O2P-P-OG1	-6.13	81.96	105.85
2	E	4	TPO	O3P-P-O2P	4.88	126.10	107.80
2	E	4	TPO	O2P-P-OG1	-4.57	88.06	105.85
2	F	4	TPO	O3P-P-O2P	4.49	124.63	107.80
2	D	4	TPO	O-C-CA	-4.24	113.87	124.77
2	E	4	TPO	O3P-P-OG1	-3.89	90.68	105.85
2	E	4	TPO	O-C-CA	-3.83	114.93	124.77
2	F	4	TPO	O-C-CA	-3.37	116.11	124.77
2	D	4	TPO	O3P-P-O2P	2.91	118.72	107.80
2	D	4	TPO	O3P-P-O1P	2.84	121.89	110.83
2	D	4	TPO	O3P-P-OG1	-2.55	95.91	105.85

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	4	TPO	CB-OG1-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	222/259 (85%)	0.92	24 (10%) 11 12	30, 45, 59, 67	0
1	B	224/259 (86%)	0.77	20 (8%) 15 17	27, 41, 57, 65	0
1	C	214/259 (82%)	1.37	52 (24%) 2 2	35, 53, 91, 95	0
2	D	5/6 (83%)	1.71	2 (40%) 1 0	51, 53, 55, 57	0
2	E	5/6 (83%)	1.08	0 100 100	38, 40, 42, 44	0
2	F	5/6 (83%)	1.59	2 (40%) 1 0	48, 52, 56, 57	0
All	All	675/795 (84%)	1.02	100 (14%) 5 6	27, 46, 65, 95	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	TYR	5.9
1	A	372	CYS	5.6
1	C	372	CYS	5.5
1	B	372	CYS	4.9
1	B	468	HIS	4.8
1	C	465	VAL	4.8
1	A	517	THR	4.7
1	A	559	PHE	4.5
1	A	487	SER	4.4
1	C	503	ASP	4.4
1	C	481	TYR	4.3
1	C	464	THR	4.1
1	C	462	TYR	4.0
1	B	554	ASP	4.0
1	B	371	ASP	3.9
1	C	403	PRO	3.8
1	C	473	MET	3.7
1	C	449	ASP	3.7
1	C	406	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	554	ASP	3.4
1	C	559	PHE	3.4
1	C	593	SER	3.3
1	B	503	ASP	3.2
1	C	375	SER	3.1
1	A	481	TYR	3.1
1	C	489	HIS	3.1
1	B	487	SER	3.0
1	C	472	LEU	3.0
1	B	536	GLN	3.0
1	C	537	ASP	3.0
1	A	470	ASN	3.0
1	B	469	PRO	3.0
1	A	503	ASP	2.9
1	C	484	ASN	2.9
1	C	469	PRO	2.9
1	C	404	ALA	2.9
1	A	536	GLN	2.9
1	C	471	SER	2.8
1	B	575	GLU	2.8
1	C	461	SER	2.8
1	B	501	GLU	2.8
1	B	467	SER	2.7
1	C	467	SER	2.7
1	B	506	ALA	2.7
1	C	459	THR	2.7
1	C	487	SER	2.6
1	C	491	LEU	2.6
1	A	418	SER	2.6
1	B	373	HIS	2.6
2	F	6	LEU	2.6
1	A	493	ALA	2.6
1	C	451	LEU	2.5
1	A	558	ASP	2.5
1	C	466	SER	2.5
1	C	468	HIS	2.5
1	C	392	ARG	2.4
1	C	418	SER	2.4
1	C	443	ILE	2.4
1	C	556	LYS	2.4
1	C	456	ARG	2.4
1	A	415	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	386	ALA	2.3
2	D	1	MET	2.3
1	C	436	PHE	2.3
1	A	593	SER	2.3
1	A	507	ARG	2.3
1	C	454	ILE	2.3
1	C	463	LEU	2.3
1	C	470	ASN	2.3
1	B	593	SER	2.3
2	D	3	SER	2.3
1	C	398	GLU	2.3
1	A	497	ILE	2.3
1	A	463	LEU	2.2
1	B	594	ARG	2.2
1	A	488	GLU	2.2
1	A	555	GLU	2.2
1	B	505	LEU	2.2
2	F	1	MET	2.2
1	C	455	GLU	2.2
1	B	556	LYS	2.2
1	A	468	HIS	2.2
1	B	481	TYR	2.2
1	C	474	LYS	2.2
1	C	393	GLY	2.2
1	A	412	SER	2.2
1	A	480	LYS	2.1
1	C	493	ALA	2.1
1	A	473	MET	2.1
1	A	591	LEU	2.1
1	C	573	CYS	2.1
1	B	383	SER	2.1
1	C	442	LEU	2.1
1	C	494	GLY	2.1
1	C	450	SER	2.1
1	B	496	ASN	2.1
1	C	448	GLY	2.1
1	C	458	GLY	2.1
1	C	577	ALA	2.0
1	C	555	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TPO	F	4	11/12	0.93	0.11	44,47,49,49	0
2	TPO	D	4	11/12	0.94	0.12	47,49,50,51	0
2	TPO	E	4	11/12	0.97	0.11	32,35,36,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.