



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:28 AM UTC

PDB ID : 2OJX / pdb_00002ojx
Title : Molecular and structural basis of polo-like kinase 1 substrate recognition: Implications in centrosomal localization
Authors : Garcia-Alvarez, B.; de Carcer, G.; Ibanez, S.; Bragado-Nilsson, E.; Montoya, G.
Deposited on : 2007-01-15
Resolution : 2.85 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
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

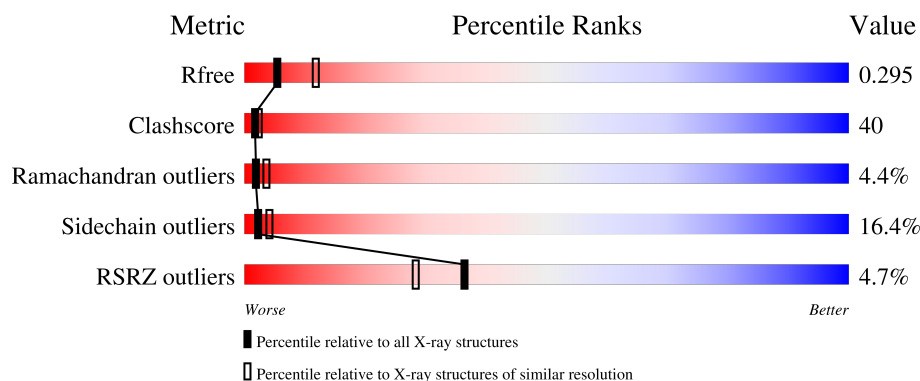
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	239	2% 29% 42% 13% 15%
2	E	9	56% 22% 22% 33% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1735 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 PLK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1675	1064	290	311	10			

- Molecule 2 is a protein called Synthetic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	S	0	0	0
			50	31	8	10	1			

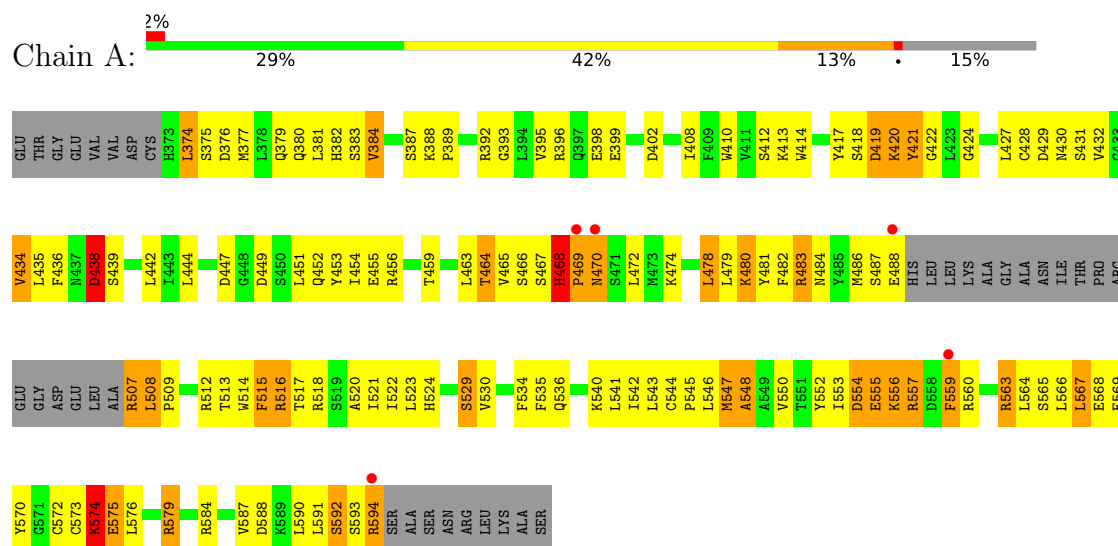
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	E	1	Total	O	0	0
			1	1		

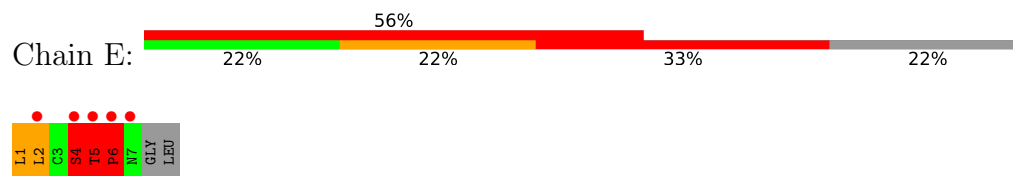
3 Residue-property plots [i](#)

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 PLK1



- Molecule 2: Synthetic peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.19Å 49.18Å 56.23Å 90.00° 109.48° 90.00°	Depositor
Resolution (Å)	18.94 – 2.85 18.94 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (18.94-2.85) 95.3 (18.94-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.230 , 0.270 0.238 , 0.295	Depositor DCC
R_{free} test set	230 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	1735	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.95% 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

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	0.65	0/1710	1.27	24/2309 (1.0%)
2	E	1.03	0/50	3.33	7/68 (10.3%)
All	All	0.67	0/1760	1.37	31/2377 (1.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	LYS	N-CA-C	-12.36	95.21	110.41
2	E	5	THR	CA-C-N	-11.99	107.41	119.76
2	E	5	THR	C-N-CA	-11.99	107.41	119.76
2	E	6	PRO	N-CA-C	9.18	125.45	111.14
1	A	566	LEU	N-CA-C	-8.66	101.84	111.28
2	E	4	SER	N-CA-C	8.61	129.15	110.80
2	E	2	LEU	N-CA-C	8.58	129.07	110.80
1	A	419	ASP	N-CA-C	-8.22	102.28	111.82
1	A	517	THR	N-CA-C	-8.22	93.30	110.80
1	A	402	ASP	CA-C-N	7.17	126.84	119.82
1	A	402	ASP	C-N-CA	7.17	126.84	119.82
1	A	393	GLY	N-CA-C	-6.95	103.88	112.77
1	A	474	LYS	N-CA-C	-6.95	103.32	111.03
1	A	554	ASP	N-CA-C	6.73	120.29	109.86
1	A	417	TYR	N-CA-C	-6.57	103.59	112.26
1	A	447	ASP	N-CA-C	-6.49	105.29	113.72
1	A	383	SER	N-CA-C	6.42	117.94	111.07
1	A	468	HIS	N-CA-C	6.20	123.50	109.81
1	A	431	SER	N-CA-C	-5.92	100.91	110.32
1	A	563	ARG	N-CA-C	-5.91	99.50	108.67
1	A	438	ASP	N-CA-C	-5.63	105.75	113.30
1	A	576	LEU	N-CA-C	-5.61	104.79	111.69
1	A	508	LEU	N-CA-C	5.48	120.61	109.60
2	E	6	PRO	CA-C-N	5.46	131.53	121.70
2	E	6	PRO	C-N-CA	5.46	131.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	508	LEU	CA-C-N	5.43	128.45	120.46
1	A	508	LEU	C-N-CA	5.43	128.45	120.46
1	A	520	ALA	N-CA-C	5.27	115.49	108.38
1	A	535	PHE	N-CA-C	5.24	116.69	110.97
1	A	486	MET	N-CA-C	5.21	117.87	111.82
1	A	548	ALA	N-CA-C	-5.21	104.22	111.30

There are no chirality outliers.

There are no planarity outliers.

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	1675	0	1662	125	0
2	E	50	0	54	22	0
3	A	9	0	0	6	0
3	E	1	0	0	0	0
All	All	1735	0	1716	139	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 40.

All (139) 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:512:ARG:HD3	3:A:2:HOH:O	1.34	1.28
1:A:516:ARG:HH22	2:E:2:LEU:HB2	1.16	1.09
1:A:541:LEU:HD11	1:A:579:ARG:HB3	1.44	0.97
2:E:1:LEU:HG	2:E:2:LEU:HG	1.43	0.96
2:E:4:SER:O	2:E:5:THR:HB	1.66	0.95
1:A:554:ASP:HB2	1:A:555:GLU:OE2	1.70	0.92
1:A:579:ARG:HG3	1:A:579:ARG:HH11	1.35	0.91
2:E:1:LEU:CG	2:E:2:LEU:HG	2.03	0.89
1:A:590:LEU:O	1:A:594:ARG:HB2	1.76	0.85
1:A:574:LYS:O	1:A:575:GLU:HB2	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASP:O	1:A:380:GLN:HG3	1.77	0.83
1:A:414:TRP:H	2:E:4:SER:HB3	1.43	0.82
1:A:464:THR:HG22	1:A:466:SER:H	1.49	0.78
1:A:449:ASP:OD2	1:A:464:THR:HG23	1.83	0.78
1:A:484:ASN:O	1:A:488:GLU:HB3	1.84	0.78
1:A:444:LEU:HB2	1:A:479:LEU:HD21	1.66	0.76
1:A:579:ARG:HG3	1:A:579:ARG:NH1	2.01	0.75
2:E:4:SER:C	2:E:6:PRO:HD3	2.11	0.75
1:A:513:THR:HG21	1:A:594:ARG:NH1	2.03	0.73
1:A:375:SER:O	1:A:379:GLN:HG3	1.88	0.72
1:A:584:ARG:HH11	1:A:584:ARG:HG3	1.55	0.72
1:A:594:ARG:CZ	1:A:594:ARG:HA	2.20	0.72
1:A:516:ARG:NH2	2:E:2:LEU:HB2	2.00	0.71
1:A:468:HIS:O	1:A:470:ASN:N	2.25	0.70
1:A:398:GLU:HG2	1:A:399:GLU:N	2.08	0.69
1:A:481:TYR:CE2	3:A:4:HOH:O	2.46	0.69
1:A:468:HIS:O	1:A:469:PRO:C	2.36	0.68
1:A:574:LYS:O	1:A:575:GLU:CB	2.42	0.68
2:E:1:LEU:HG	2:E:2:LEU:CG	2.24	0.67
1:A:513:THR:HG22	3:A:3:HOH:O	1.95	0.67
1:A:464:THR:HG22	1:A:466:SER:N	2.11	0.66
2:E:4:SER:O	2:E:6:PRO:HD3	1.95	0.65
2:E:1:LEU:HG	2:E:2:LEU:N	2.11	0.64
2:E:4:SER:O	2:E:5:THR:CB	2.45	0.64
1:A:556:LYS:O	1:A:557:ARG:HB2	1.98	0.64
1:A:464:THR:HG22	1:A:467:SER:H	1.64	0.63
1:A:555:GLU:CD	1:A:555:GLU:H	2.07	0.63
1:A:432:VAL:HG21	1:A:483:ARG:HG3	1.81	0.63
1:A:438:ASP:O	1:A:456:ARG:HG2	1.98	0.63
1:A:480:LYS:HG3	1:A:483:ARG:NH2	2.15	0.62
1:A:456:ARG:NH1	1:A:456:ARG:HB3	2.14	0.61
1:A:438:ASP:OD1	1:A:438:ASP:N	2.33	0.61
1:A:414:TRP:H	2:E:4:SER:CB	2.13	0.61
1:A:592:SER:OG	1:A:593:SER:N	2.33	0.61
1:A:514:TRP:O	1:A:515:PHE:HB3	1.99	0.61
1:A:438:ASP:O	1:A:439:SER:HB2	2.00	0.60
1:A:544:CYS:SG	1:A:546:LEU:HB2	2.42	0.60
1:A:384:VAL:O	1:A:389:PRO:HD3	2.03	0.59
1:A:377:MET:HB2	1:A:545:PRO:HB3	1.85	0.59
1:A:541:LEU:CD1	1:A:579:ARG:HB3	2.26	0.58
1:A:559:PHE:H	1:A:559:PHE:HD2	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:SER:OG	2:E:6:PRO:HD2	2.03	0.58
1:A:414:TRP:N	2:E:4:SER:HB3	2.17	0.58
1:A:573:CYS:C	1:A:574:LYS:O	2.39	0.57
1:A:464:THR:HB	1:A:467:SER:HB3	1.87	0.57
2:E:4:SER:C	2:E:6:PRO:CD	2.78	0.57
1:A:389:PRO:HA	1:A:392:ARG:NH2	2.20	0.56
1:A:507:ARG:NH1	1:A:508:LEU:HD13	2.20	0.56
1:A:552:TYR:CE1	1:A:579:ARG:HD3	2.41	0.56
1:A:567:LEU:HD21	1:A:572:CYS:HB3	1.86	0.55
1:A:436:PHE:HB2	1:A:438:ASP:OD1	2.07	0.55
1:A:524:HIS:HD2	3:A:3:HOH:O	1.89	0.55
1:A:374:LEU:HB2	1:A:591:LEU:HD21	1.87	0.55
1:A:456:ARG:HB3	1:A:456:ARG:CZ	2.37	0.54
1:A:418:SER:HA	1:A:422:GLY:N	2.22	0.54
1:A:507:ARG:O	1:A:509:PRO:HD3	2.08	0.53
1:A:594:ARG:HA	1:A:594:ARG:NH2	2.22	0.53
1:A:413:LYS:HG2	2:E:6:PRO:HG2	1.91	0.53
1:A:584:ARG:HG3	1:A:584:ARG:NH1	2.19	0.53
1:A:464:THR:CG2	1:A:466:SER:H	2.20	0.52
1:A:513:THR:CG2	3:A:3:HOH:O	2.56	0.52
1:A:529:SER:HA	1:A:543:LEU:O	2.10	0.51
1:A:429:ASP:O	1:A:430:ASN:HB2	2.10	0.51
1:A:540:LYS:HD2	1:A:553:ILE:HD12	1.93	0.51
2:E:5:THR:O	2:E:5:THR:CG2	2.59	0.51
1:A:522:ILE:N	1:A:522:ILE:HD12	2.26	0.51
1:A:412:SER:OG	1:A:428:CYS:HA	2.10	0.51
1:A:410:TRP:CB	1:A:542:ILE:HD13	2.41	0.50
1:A:434:VAL:HG12	1:A:479:LEU:HD13	1.94	0.50
1:A:521:ILE:C	1:A:522:ILE:HD12	2.36	0.50
1:A:374:LEU:HD23	1:A:587:VAL:HG13	1.94	0.49
1:A:442:LEU:HD11	1:A:451:LEU:HD13	1.94	0.49
1:A:484:ASN:O	1:A:488:GLU:CB	2.59	0.49
1:A:481:TYR:HE2	3:A:4:HOH:O	1.88	0.49
1:A:384:VAL:O	1:A:387:SER:OG	2.30	0.48
1:A:449:ASP:OD2	1:A:464:THR:CG2	2.57	0.48
1:A:392:ARG:HB3	1:A:395:VAL:HG22	1.94	0.48
1:A:444:LEU:CB	1:A:479:LEU:HD21	2.41	0.48
2:E:1:LEU:CD2	2:E:2:LEU:HG	2.43	0.47
1:A:554:ASP:OD1	1:A:556:LYS:HG3	2.14	0.47
1:A:396:ARG:O	1:A:570:TYR:HB3	2.14	0.47
1:A:483:ARG:HE	1:A:483:ARG:HB3	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LYS:HB3	1:A:421:TYR:CD1	2.51	0.46
1:A:384:VAL:HA	1:A:568:GLU:HG3	1.98	0.46
1:A:452:GLN:CD	1:A:454:ILE:HD11	2.41	0.46
1:A:381:LEU:O	1:A:382:HIS:C	2.58	0.46
1:A:547:MET:HE2	1:A:547:MET:HB3	1.70	0.46
1:A:414:TRP:CD1	2:E:4:SER:HB3	2.51	0.45
1:A:547:MET:O	1:A:548:ALA:C	2.57	0.45
1:A:424:GLY:HA3	1:A:482:PHE:CD2	2.51	0.45
1:A:454:ILE:HA	1:A:459:THR:O	2.17	0.45
1:A:421:TYR:CD1	1:A:421:TYR:N	2.84	0.44
1:A:544:CYS:SG	1:A:547:MET:HG2	2.57	0.44
1:A:587:VAL:O	1:A:588:ASP:C	2.59	0.44
1:A:467:SER:OG	1:A:469:PRO:HD3	2.18	0.44
1:A:380:GLN:O	1:A:384:VAL:HG13	2.18	0.44
1:A:480:LYS:CG	1:A:483:ARG:NH2	2.80	0.44
1:A:541:LEU:HD22	1:A:550:VAL:CG2	2.48	0.44
2:E:1:LEU:CD1	2:E:2:LEU:HG	2.48	0.44
1:A:374:LEU:HD11	1:A:524:HIS:NE2	2.33	0.43
1:A:421:TYR:CD2	1:A:478:LEU:HD11	2.53	0.43
1:A:514:TRP:HA	1:A:522:ILE:O	2.18	0.43
1:A:593:SER:O	1:A:594:ARG:O	2.36	0.43
1:A:392:ARG:HB3	1:A:395:VAL:CG2	2.48	0.43
1:A:453:TYR:CE2	1:A:455:GLU:HG3	2.54	0.43
1:A:565:SER:C	1:A:568:GLU:H	2.27	0.43
1:A:377:MET:HE1	1:A:530:VAL:HG23	2.01	0.43
1:A:408:ILE:N	1:A:408:ILE:HD12	2.32	0.43
1:A:456:ARG:NH1	1:A:456:ARG:CB	2.80	0.43
1:A:438:ASP:O	1:A:439:SER:CB	2.63	0.43
1:A:564:LEU:HD23	1:A:564:LEU:HA	1.86	0.42
2:E:5:THR:O	2:E:5:THR:HG22	2.20	0.42
1:A:434:VAL:HG12	1:A:479:LEU:CD1	2.49	0.42
1:A:579:ARG:NH1	1:A:579:ARG:CG	2.73	0.42
1:A:418:SER:HA	1:A:422:GLY:CA	2.49	0.42
1:A:512:ARG:O	1:A:513:THR:HB	2.20	0.41
1:A:413:LYS:HA	2:E:4:SER:CB	2.50	0.41
1:A:563:ARG:HH11	1:A:563:ARG:HG2	1.84	0.41
1:A:387:SER:O	1:A:388:LYS:C	2.62	0.41
1:A:463:LEU:CD1	1:A:472:LEU:HD12	2.51	0.41
1:A:463:LEU:HB3	1:A:469:PRO:HG3	2.02	0.41
1:A:514:TRP:HB2	1:A:523:LEU:HD23	2.03	0.41
1:A:590:LEU:O	1:A:594:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:CB	1:A:395:VAL:HG22	2.51	0.40
1:A:419:ASP:C	1:A:420:LYS:HD2	2.45	0.40
1:A:567:LEU:HA	1:A:567:LEU:HD23	1.83	0.40
1:A:392:ARG:HD3	1:A:392:ARG:HA	1.82	0.40
1:A:534:PHE:CE1	1:A:579:ARG:HG2	2.56	0.40
1:A:593:SER:O	1:A:594:ARG:C	2.64	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	200/239 (84%)	179 (90%)	14 (7%)	7 (4%)	3	6
2	E	5/9 (56%)	2 (40%)	1 (20%)	2 (40%)	0	0
All	All	205/248 (83%)	181 (88%)	15 (7%)	9 (4%)	2	3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	HIS
1	A	469	PRO
1	A	470	ASN
2	E	5	THR
1	A	515	PHE
1	A	575	GLU
2	E	4	SER
1	A	557	ARG
1	A	592	SER

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	188/215 (87%)	158 (84%)	30 (16%)	2	4
2	E	7/8 (88%)	5 (71%)	2 (29%)	0	0
All	All	195/223 (87%)	163 (84%)	32 (16%)	2	4

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

Mol	Chain	Res	Type
1	A	374	LEU
1	A	384	VAL
1	A	420	LYS
1	A	421	TYR
1	A	427	LEU
1	A	434	VAL
1	A	435	LEU
1	A	438	ASP
1	A	464	THR
1	A	465	VAL
1	A	468	HIS
1	A	478	LEU
1	A	480	LYS
1	A	483	ARG
1	A	487	SER
1	A	507	ARG
1	A	516	ARG
1	A	518	ARG
1	A	529	SER
1	A	536	GLN
1	A	547	MET
1	A	555	GLU
1	A	556	LYS
1	A	559	PHE
1	A	560	ARG
1	A	567	LEU
1	A	569	GLU

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Mol	Chain	Res	Type
1	A	574	LYS
1	A	579	ARG
1	A	594	ARG
2	E	1	LEU
2	E	6	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	GLN
1	A	468	HIS
1	A	484	ASN
1	A	538	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 [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	204/239 (85%)	-0.02	5 (2%) 58 49	12, 27, 46, 94	0
2	E	7/9 (77%)	2.57	5 (71%) 0 0	52, 64, 92, 98	0
All	All	211/248 (85%)	0.07	10 (4%) 36 28	12, 27, 51, 98	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	4	SER	4.2
2	E	5	THR	3.5
1	A	559	PHE	2.8
2	E	7	ASN	2.6
1	A	470	ASN	2.5
2	E	6	PRO	2.4
2	E	2	LEU	2.4
1	A	594	ARG	2.4
1	A	488	GLU	2.3
1	A	469	PRO	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.