



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:40 PM GMT

PDB ID : 1Q4O
Title : The structure of the polo box domain of human Plk1
Authors : Cheng, K.Y.; Lowe, E.D.; Sinclair, J.; Nigg, E.A.; Johnson, L.N.
Deposited on : 2003-08-04
Resolution : 2.20 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

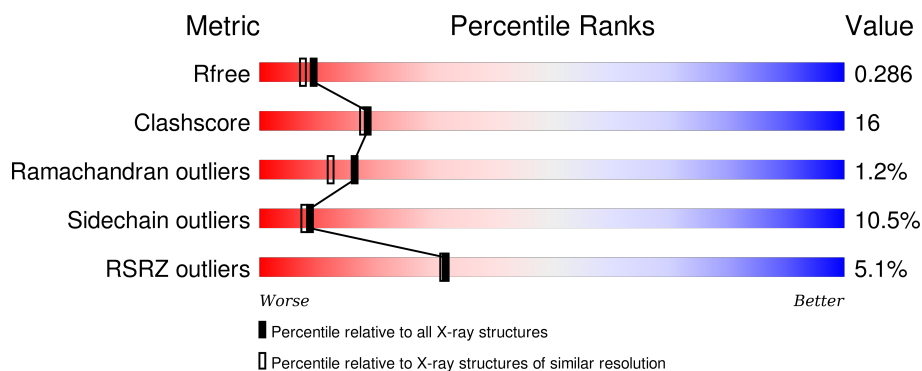
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	237	 3% 59% 22% 5% 13%
1	B	237	 6% 56% 27% 5% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3622 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	A	207	Total	C	N	O	S	0	0	0
			1694	1079	290	314	11			
1	B	208	Total	C	N	O	S	0	0	0
			1701	1083	291	316	11			

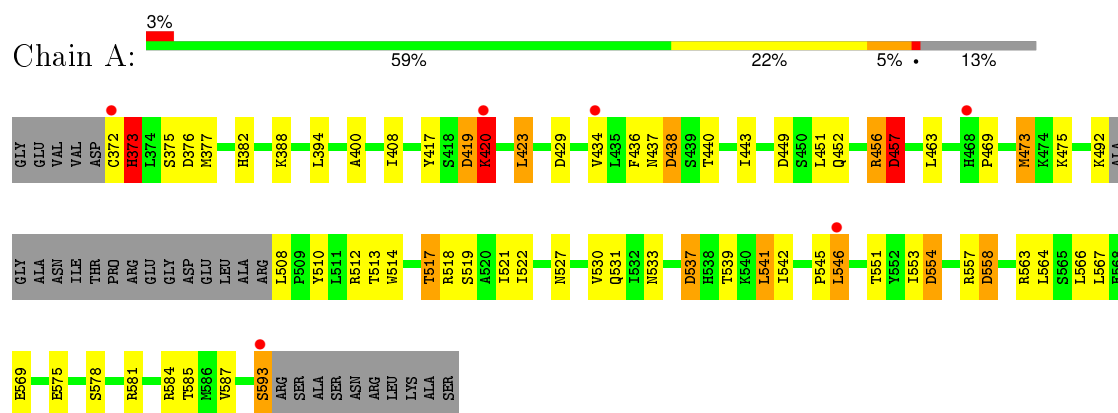
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	113	Total	O	0	0
			113	113		

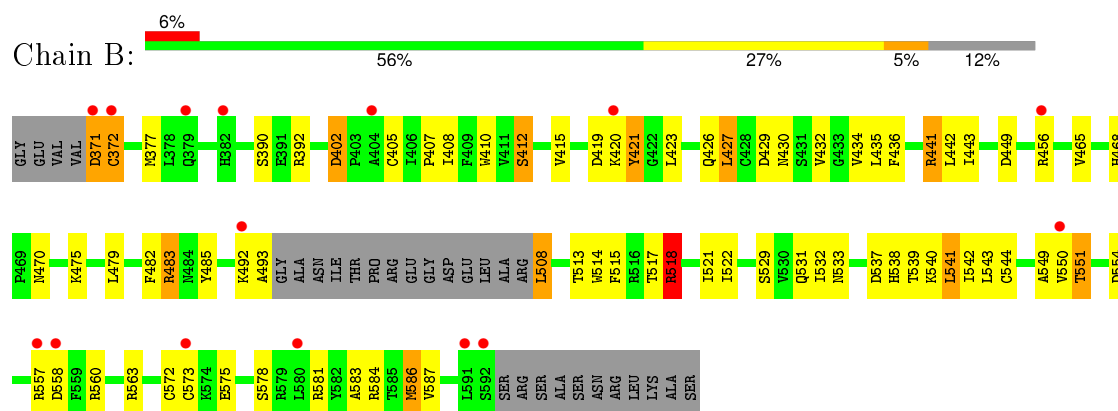
3 Residue-property plots

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

- Molecule 1: Serine/threonine-protein kinase PLK



- Molecule 1: Serine/threonine-protein kinase PLK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	32.74Å 42.02Å 80.73Å 103.16° 93.88° 91.32°	Depositor
Resolution (Å)	20.00 – 2.20 19.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-2.20) 87.9 (19.69-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.198 , 0.288 0.204 , 0.286	Depositor DCC
R_{free} test set	1041 reflections (5.45%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.4	EDS
Estimated twinning fraction	0.026 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20134 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3622	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.82	0/1730	1.07	11/2337 (0.5%)
1	B	0.81	1/1737 (0.1%)	1.00	4/2347 (0.2%)
All	All	0.81	1/3467 (0.0%)	1.04	15/4684 (0.3%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	421	TYR	CA-C	-5.48	1.38	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	ARG	N-CA-CB	-14.71	84.12	110.60
1	A	554	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	449	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	429	ASP	CB-CG-OD2	7.94	125.45	118.30
1	A	517	THR	N-CA-C	-7.87	89.76	111.00
1	A	517	THR	CB-CA-C	-7.35	91.75	111.60
1	A	581	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	419	ASP	CA-CB-CG	-6.55	98.98	113.40
1	A	581	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	402	ASP	CB-CG-OD2	6.33	123.99	118.30
1	A	438	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	457	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	421	TYR	N-CA-C	5.38	125.53	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	449	ASP	CB-CG-OD2	5.08	122.87	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	LYS	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	1694	0	1683	45	0
1	B	1701	0	1687	61	0
2	A	114	0	0	8	0
2	B	113	0	0	14	0
All	All	3622	0	3370	105	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 16.

All (105) 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:382:HIS:CE1	1:A:584:ARG:HD2	1.90	1.06
1:A:508:LEU:N	2:A:80:HOH:O	2.01	0.94
1:A:420:LYS:HA	1:A:437:ASN:HD22	1.37	0.87
1:B:531:GLN:HE21	1:B:533:ASN:HD21	1.18	0.87
1:B:586:MET:SD	2:B:189:HOH:O	2.34	0.84
1:B:479:LEU:HG	2:B:25:HOH:O	1.80	0.80
1:B:544:CYS:HB3	2:B:19:HOH:O	1.84	0.77
1:B:434:VAL:HG11	1:B:436:PHE:CZ	2.21	0.74
1:B:522:ILE:HG12	1:B:586:MET:HG2	1.67	0.73
1:A:531:GLN:HE21	1:A:533:ASN:HD21	1.38	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ARG:HD2	2:B:63:HOH:O	1.92	0.69
1:B:522:ILE:HG12	1:B:586:MET:CG	2.24	0.68
1:B:371:ASP:N	1:B:371:ASP:OD1	2.24	0.68
1:B:586:MET:CG	2:B:189:HOH:O	2.48	0.62
1:B:371:ASP:O	1:B:372:CYS:HB2	1.98	0.62
1:B:522:ILE:CG1	1:B:586:MET:HG2	2.31	0.61
1:A:372:CYS:SG	1:A:546:LEU:HD23	2.41	0.60
1:A:420:LYS:HA	1:A:437:ASN:ND2	2.12	0.59
1:B:508:LEU:N	2:B:119:HOH:O	2.35	0.59
1:A:443:ILE:HD12	2:A:1:HOH:O	2.02	0.59
1:B:415:VAL:HG11	1:B:485:TYR:CD2	2.37	0.59
1:A:457:ASP:OD1	1:A:457:ASP:C	2.43	0.57
1:A:440:THR:HG21	1:A:475:LYS:NZ	2.18	0.57
1:A:377:MET:SD	1:A:530:VAL:HG13	2.45	0.57
1:B:531:GLN:HA	1:B:541:LEU:O	2.04	0.57
1:A:373:HIS:CD2	2:A:87:HOH:O	2.57	0.56
1:B:493:ALA:HB3	2:B:94:HOH:O	2.05	0.56
1:B:508:LEU:N	2:B:180:HOH:O	2.39	0.55
1:A:537:ASP:HB3	1:A:539:THR:H	1.73	0.54
1:B:537:ASP:CB	1:B:539:THR:HG23	2.38	0.54
1:B:407:PRO:CD	1:B:551:THR:HG21	2.37	0.54
1:B:573:CYS:SG	1:B:575:GLU:HB2	2.48	0.54
1:B:513:THR:HA	2:B:78:HOH:O	2.09	0.53
1:A:443:ILE:HB	1:A:452:GLN:HB3	1.90	0.52
1:B:410:TRP:HB3	1:B:542:ILE:HD13	1.91	0.52
1:B:517:THR:C	1:B:518:ARG:HG3	2.30	0.52
1:B:465:VAL:O	1:B:468:HIS:HD2	1.92	0.52
1:A:382:HIS:ND1	1:A:584:ARG:HD2	2.21	0.52
1:B:537:ASP:HB2	1:B:539:THR:HG23	1.92	0.52
1:A:569:GLU:CD	1:B:475:LYS:HZ2	2.14	0.52
1:B:538:HIS:CE1	2:B:105:HOH:O	2.62	0.51
1:A:377:MET:CE	1:A:530:VAL:HG13	2.41	0.51
1:A:372:CYS:SG	1:A:527:ASN:O	2.69	0.50
1:A:469:PRO:HD2	1:A:473:MET:HE1	1.92	0.50
1:B:515:PHE:HZ	1:B:586:MET:HG3	1.75	0.50
1:A:423:LEU:HD13	1:A:514:TRP:CD2	2.46	0.50
1:B:586:MET:HB2	2:B:189:HOH:O	2.11	0.49
1:A:438:ASP:OD2	1:A:475:LYS:NZ	2.42	0.49
1:B:377:MET:CE	1:B:587:VAL:CG2	2.91	0.49
1:B:377:MET:CE	1:B:587:VAL:HG21	2.43	0.49
1:B:434:VAL:CG1	1:B:436:PHE:CZ	2.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:LEU:HD13	1:B:441:ARG:HD3	1.94	0.49
1:A:372:CYS:HA	1:A:546:LEU:HD23	1.94	0.48
1:B:531:GLN:NE2	1:B:533:ASN:HD21	1.98	0.48
1:B:415:VAL:HG21	1:B:482:PHE:HD2	1.79	0.48
1:B:465:VAL:O	1:B:468:HIS:CD2	2.67	0.47
1:B:426:GLN:HG2	1:B:427:LEU:O	2.13	0.47
1:A:584:ARG:NH2	1:A:585:THR:HG22	2.29	0.47
1:A:438:ASP:HB2	1:A:456:ARG:NH1	2.30	0.47
1:B:522:ILE:HD12	1:B:522:ILE:N	2.30	0.47
1:B:443:ILE:HG12	2:B:70:HOH:O	2.14	0.47
1:A:440:THR:HG21	1:A:475:LYS:HZ3	1.80	0.47
1:A:463:LEU:HD21	2:A:36:HOH:O	2.15	0.46
1:A:438:ASP:OD1	1:A:440:THR:HG22	2.16	0.46
1:B:420:LYS:HD2	1:B:421:TYR:CE2	2.51	0.46
1:A:517:THR:OG1	1:A:517:THR:O	2.31	0.45
1:B:415:VAL:HG11	1:B:485:TYR:HD2	1.82	0.45
1:A:584:ARG:HA	1:A:587:VAL:HG12	1.99	0.44
1:B:377:MET:HE3	1:B:587:VAL:HG21	1.99	0.44
1:B:412:SER:OG	1:B:492:LYS:HD3	2.17	0.44
1:A:584:ARG:HD3	2:A:55:HOH:O	2.17	0.44
1:A:436:PHE:HB2	1:A:440:THR:HG22	1.99	0.44
1:A:408:ILE:HD11	2:A:207:HOH:O	2.17	0.44
1:A:564:LEU:O	1:A:567:LEU:HB2	2.18	0.44
1:B:521:ILE:C	1:B:522:ILE:HD12	2.38	0.43
1:B:470:ASN:O	2:B:144:HOH:O	2.21	0.43
1:A:553:ILE:HA	1:A:558:ASP:O	2.19	0.43
1:A:521:ILE:C	1:A:522:ILE:HD12	2.39	0.43
1:B:493:ALA:HB1	1:B:540:LYS:NZ	2.33	0.43
1:B:432:VAL:HG21	1:B:483:ARG:HG3	2.01	0.43
1:B:531:GLN:HE21	1:B:533:ASN:ND2	2.00	0.43
1:A:492:LYS:HZ3	1:A:557:ARG:NH1	2.17	0.42
1:B:532:ILE:CD1	1:B:583:ALA:HA	2.49	0.42
1:B:515:PHE:CZ	1:B:586:MET:HG3	2.53	0.42
1:A:443:ILE:HD11	1:A:510:TYR:HB2	2.02	0.42
1:B:423:LEU:HD13	1:B:514:TRP:CD2	2.54	0.42
1:B:402:ASP:OD2	1:B:563:ARG:HD3	2.20	0.41
1:B:543:LEU:HD23	1:B:550:VAL:HG23	2.02	0.41
1:A:575:GLU:CD	2:A:121:HOH:O	2.58	0.41
1:B:537:ASP:HB3	1:B:539:THR:HG23	2.00	0.41
1:B:429:ASP:O	1:B:430:ASN:HB2	2.19	0.41
1:B:558:ASP:OD2	1:B:560:ARG:CZ	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:SER:HA	2:A:153:HOH:O	2.20	0.41
1:B:578:SER:O	1:B:581:ARG:HB2	2.21	0.41
1:B:390:SER:HA	1:B:572:CYS:O	2.21	0.41
1:B:442:LEU:C	1:B:443:ILE:HD13	2.40	0.41
1:A:492:LYS:HZ3	1:A:557:ARG:CZ	2.33	0.41
1:B:560:ARG:NE	2:B:145:HOH:O	2.54	0.41
1:A:542:ILE:HB	1:A:551:THR:HB	2.03	0.41
1:A:531:GLN:HA	1:A:541:LEU:O	2.22	0.40
1:A:522:ILE:HD12	1:A:522:ILE:N	2.37	0.40
1:A:377:MET:CE	1:A:545:PRO:HD3	2.51	0.40
1:B:405:CYS:HB3	1:B:549:ALA:HB2	2.03	0.40
1:A:443:ILE:O	1:A:451:LEU:HA	2.21	0.40
1:A:400:ALA:HA	1:A:566:LEU:HB3	2.03	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	203/237 (86%)	188 (93%)	12 (6%)	3 (2%)	13	9
1	B	204/237 (86%)	187 (92%)	15 (7%)	2 (1%)	19	16
All	All	407/474 (86%)	375 (92%)	27 (7%)	5 (1%)	16	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	CYS
1	B	518	ARG
1	A	420	LYS
1	A	419	ASP
1	A	373	HIS

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	191/213 (90%)	168 (88%)	23 (12%)	6	5
1	B	191/213 (90%)	174 (91%)	17 (9%)	12	11
All	All	382/426 (90%)	342 (90%)	40 (10%)	8	8

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	HIS
1	A	375	SER
1	A	388	LYS
1	A	394	LEU
1	A	417	TYR
1	A	419	ASP
1	A	420	LYS
1	A	423	LEU
1	A	434	VAL
1	A	456	ARG
1	A	457	ASP
1	A	473	MET
1	A	512	ARG
1	A	513	THR
1	A	519	SER
1	A	537	ASP
1	A	541	LEU
1	A	546	LEU
1	A	554	ASP
1	A	558	ASP
1	A	563	ARG
1	A	578	SER
1	A	593	SER
1	B	371	ASP
1	B	392	ARG
1	B	408	ILE
1	B	412	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	427	LEU
1	B	441	ARG
1	B	456	ARG
1	B	483	ARG
1	B	508	LEU
1	B	518	ARG
1	B	529	SER
1	B	541	LEU
1	B	551	THR
1	B	554	ASP
1	B	557	ARG
1	B	584	ARG
1	B	586	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	ASN
1	A	452	GLN
1	A	470	ASN
1	A	489	HIS
1	A	533	ASN
1	B	426	GLN
1	B	468	HIS
1	B	524	HIS
1	B	533	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

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	207/237 (87%)	0.17	6 (2%) 55 54	19, 30, 45, 53	0
1	B	208/237 (87%)	0.41	15 (7%) 18 18	22, 35, 52, 67	0
All	All	415/474 (87%)	0.29	21 (5%) 32 31	19, 32, 49, 67	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	CYS	6.1
1	A	593	SER	5.2
1	B	371	ASP	4.4
1	B	573	CYS	4.1
1	B	456	ARG	3.5
1	A	420	LYS	3.4
1	A	546	LEU	3.4
1	A	468	HIS	3.2
1	B	372	CYS	2.9
1	B	580	LEU	2.5
1	B	404	ALA	2.5
1	B	592	SER	2.4
1	B	557	ARG	2.4
1	B	591	LEU	2.4
1	B	550	VAL	2.2
1	B	379	GLN	2.1
1	A	434	VAL	2.1
1	B	382	HIS	2.1
1	B	420	LYS	2.1
1	B	558	ASP	2.1
1	B	492	LYS	2.0

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 carbohydrates 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.