



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:40 pm GMT

PDB ID : 5IF1
Title : Crystal structure apo CDK2/cyclin A
Authors : Ayaz, P.; Andres, D.; Kwiatkowski, D.A.; Kolbe, C.; Lienau, P.; Siemeister, G.; Luecking, U.; Stegmann, C.M.
Deposited on : 2016-02-25
Resolution : 2.61 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

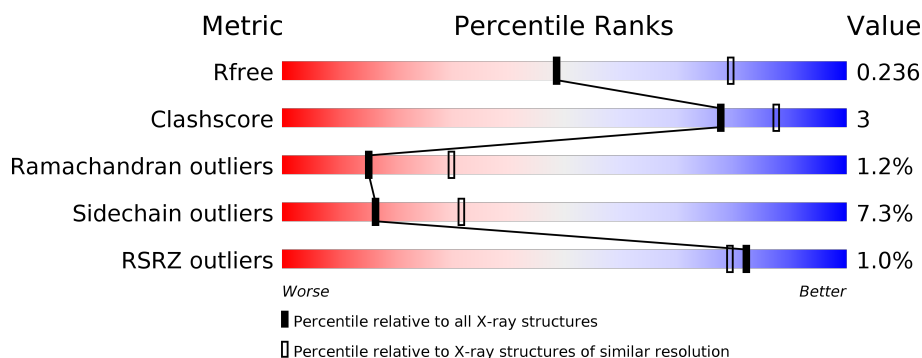
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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	298	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>
1	C	298	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
2	B	265	<div> <div></div> <div> <div>83%</div> <div>12%</div> <div>..</div> </div> </div>
2	D	265	<div> <div></div> <div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9059 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	1	0
			2400	1561	411	420	8			
1	C	296	Total	C	N	O	S	0	0	0
			2372	1544	403	417	8			

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	1	0
			2083	1349	338	385	11			
2	D	257	Total	C	N	O	S	0	1	0
			2083	1349	339	384	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	168	HIS	-	expression tag	UNP P20248
B	169	HIS	-	expression tag	UNP P20248
B	170	HIS	-	expression tag	UNP P20248
B	171	HIS	-	expression tag	UNP P20248
B	172	HIS	-	expression tag	UNP P20248
B	173	HIS	-	expression tag	UNP P20248
D	168	HIS	-	expression tag	UNP P20248
D	169	HIS	-	expression tag	UNP P20248
D	170	HIS	-	expression tag	UNP P20248
D	171	HIS	-	expression tag	UNP P20248
D	172	HIS	-	expression tag	UNP P20248
D	173	HIS	-	expression tag	UNP P20248

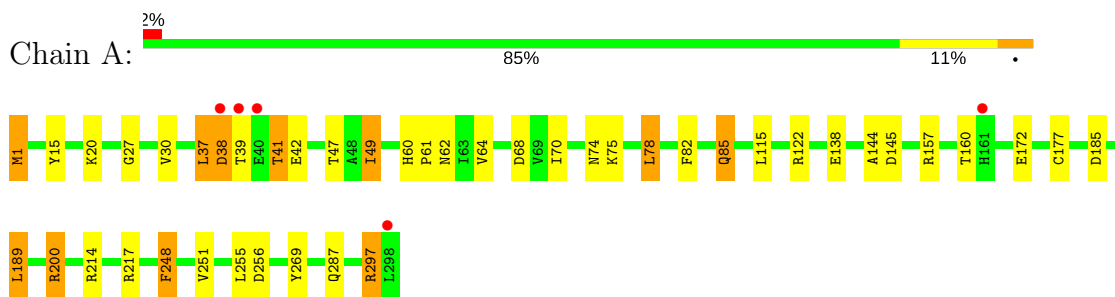
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	20	Total 20	O 20	0	0
3	C	17	Total 17	O 17	0	0
3	D	29	Total 29	O 29	0	0

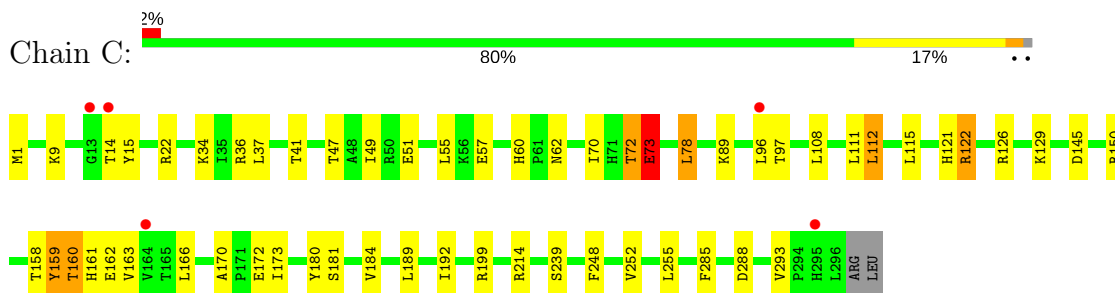
3 Residue-property plots [i](#)

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.

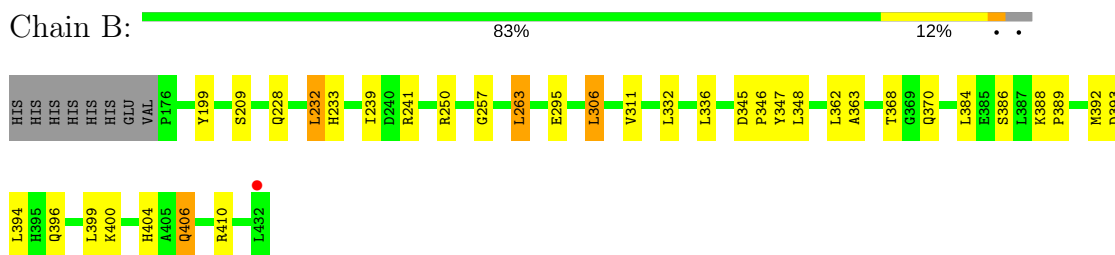
• Molecule 1: Cyclin-dependent kinase 2



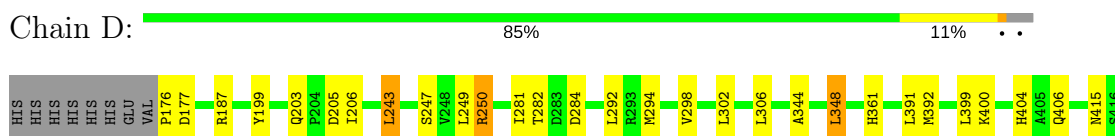
• Molecule 1: Cyclin-dependent kinase 2



• Molecule 2: Cyclin-A2



• Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	186.57Å 186.57Å 213.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.07 – 2.61 48.07 – 2.61	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.07-2.61) 100.0 (48.07-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.187 , 0.236 0.194 , 0.236	Depositor DCC
R_{free} test set	3312 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9059	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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	0.84	2/2465 (0.1%)	1.02	6/3344 (0.2%)
1	C	0.74	0/2434	0.98	5/3305 (0.2%)
2	B	0.71	0/2136	0.89	3/2898 (0.1%)
2	D	0.75	0/2136	0.90	2/2898 (0.1%)
All	All	0.76	2/9171 (0.0%)	0.95	16/12445 (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	C	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	TYR	CG-CD2	5.20	1.46	1.39
1	A	256	ASP	CB-CG	5.05	1.62	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	36	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	214	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	B	241	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	217	ARG	NE-CZ-NH2	-6.01	117.29	120.30
2	B	232	LEU	CA-CB-CG	5.94	128.97	115.30
1	C	159	TYR	CA-CB-CG	5.84	124.49	113.40
2	D	187	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	297	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	200	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	68	ASP	CB-CG-OD1	5.34	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	393	ASP	CB-CG-OD1	5.24	123.01	118.30
1	C	126	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	37	LEU	CA-CB-CG	5.12	127.09	115.30
2	D	250	ARG	CG-CD-NE	5.12	122.56	111.80
1	C	214	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	36	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	37	LEU	Peptide
1	C	72	THR	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	2400	0	2454	19	0
1	C	2372	0	2417	18	0
2	B	2083	0	2105	13	0
2	D	2083	0	2107	15	0
3	A	55	0	0	2	1
3	B	20	0	0	2	0
3	C	17	0	0	0	0
3	D	29	0	0	2	0
All	All	9059	0	9083	62	1

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 3.

All (62) 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)
2:D:391:LEU:HD23	2:D:432:LEU:HD11	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:O	1:C:122:ARG:HG2	1.93	0.67
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.80	0.62
2:B:239:ILE:HD11	2:B:257:GLY:HA2	1.82	0.61
2:B:404:HIS:HD2	2:B:406:GLN:H	1.46	0.61
1:A:60:HIS:HD2	1:A:62:ASN:H	1.49	0.60
1:A:60:HIS:CD2	1:A:62:ASN:H	2.19	0.60
2:D:203:GLN:NE2	2:D:247:SER:HA	2.17	0.59
2:D:205:ASP:OD2	2:D:250:ARG:HG2	2.05	0.56
2:B:368:THR:HG22	2:B:368:THR:O	2.04	0.56
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.86	0.56
1:A:248:PHE:HA	1:A:251:VAL:HG12	1.87	0.56
1:C:160:THR:HA	1:C:161:HIS:CG	2.40	0.56
2:D:404:HIS:HD2	2:D:406:GLN:H	1.53	0.56
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.87	0.56
1:C:163:VAL:HG22	1:C:180:TYR:OH	2.07	0.54
1:A:37:LEU:HA	1:A:38:ASP:C	2.29	0.53
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.91	0.53
1:C:161:HIS:CB	1:C:162:GLU:HA	2.39	0.52
2:D:404:HIS:CD2	2:D:406:GLN:H	2.29	0.51
1:C:161:HIS:HB3	1:C:162:GLU:HA	1.93	0.50
1:C:150:ARG:HD2	3:D:510:HOH:O	2.12	0.50
1:A:41:THR:OG1	1:A:42:GLU:N	2.45	0.49
2:B:228:GLN:HG3	3:B:508:HOH:O	2.12	0.49
2:D:294:MET:O	2:D:298:VAL:HG23	2.12	0.49
2:D:203:GLN:HG2	2:D:206:ILE:CG1	2.43	0.49
2:D:205:ASP:OD1	2:D:250:ARG:NH1	2.46	0.49
1:C:1:MET:HE3	1:C:70:ILE:HG21	1.95	0.49
2:B:263:LEU:HD13	2:B:295:GLU:HG3	1.94	0.48
2:B:368:THR:HG21	2:B:370:GLN:OE1	2.13	0.48
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.49	0.48
1:C:57:GLU:OE1	1:C:122:ARG:NH1	2.41	0.48
1:A:115:LEU:HD21	1:A:185:ASP:HB3	1.95	0.47
1:C:51:GLU:O	1:C:55:LEU:HB2	2.15	0.47
1:A:78:LEU:HD23	1:A:78:LEU:N	2.30	0.46
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.97	0.46
2:D:199:TYR:CE1	2:D:243:LEU:HB3	2.50	0.46
2:D:203:GLN:HE22	2:D:247:SER:HA	1.81	0.46
1:A:157:ARG:NH2	3:A:303:HOH:O	2.49	0.45
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.51	0.45
1:A:49:ILE:HG23	2:B:306:LEU:HD23	1.99	0.45
1:C:72:THR:HB	1:C:73:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:HIS:HD2	3:B:509:HOH:O	1.99	0.45
1:A:115:LEU:HD22	1:A:189:LEU:HD22	1.98	0.44
1:C:60:HIS:HD2	1:C:62:ASN:H	1.65	0.44
1:A:172:GLU:HB3	1:A:177:CYS:SG	2.58	0.43
1:C:158:THR:HA	1:C:180:TYR:CE1	2.54	0.43
1:A:20:LYS:HG3	1:A:82:PHE:CE1	2.54	0.43
1:A:64:VAL:HG21	1:A:144:ALA:HB2	2.01	0.42
1:C:163:VAL:HG21	1:C:173:ILE:HG21	2.02	0.42
2:D:400:LYS:NZ	3:D:503:HOH:O	2.52	0.42
1:C:78:LEU:N	1:C:78:LEU:HD23	2.35	0.42
2:B:347:TYR:OH	2:B:394:LEU:HA	2.20	0.42
1:A:27:GLY:HA3	2:D:249:LEU:HD22	2.02	0.41
1:C:108:LEU:O	1:C:112:LEU:HB2	2.20	0.41
1:A:85:GLN:HE21	1:A:85:GLN:HB2	1.60	0.41
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.03	0.41
1:A:160:THR:HG22	3:A:318:HOH:O	2.20	0.41
1:A:1:MET:HE1	1:A:70:ILE:HB	2.01	0.41
2:B:345:ASP:HA	2:B:346:PRO:HA	1.91	0.41
1:A:248:PHE:HA	1:A:251:VAL:CG1	2.51	0.40
1:C:170:ALA:HB1	1:C:172:GLU:OE2	2.22	0.40

All (1) 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)
3:A:343:HOH:O	3:A:343:HOH:O[11_455]	0.83	1.37

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	297/298 (100%)	277 (93%)	14 (5%)	6 (2%)	9 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	294/298 (99%)	270 (92%)	18 (6%)	6 (2%)	9	16
2	B	256/265 (97%)	251 (98%)	4 (2%)	1 (0%)	38	61
2	D	256/265 (97%)	252 (98%)	4 (2%)	0	100	100
All	All	1103/1126 (98%)	1050 (95%)	40 (4%)	13 (1%)	15	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
2	B	250	ARG
1	C	14	THR
1	C	73	GLU
1	A	39	THR
1	A	41	THR
1	A	38	ASP
1	A	145	ASP
1	C	239	SER
1	C	160	THR
1	A	287	GLN
1	C	41	THR
1	C	285	PHE

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	262/263 (100%)	247 (94%)	15 (6%)	24	45
1	C	259/263 (98%)	232 (90%)	27 (10%)	8	14
2	B	232/239 (97%)	217 (94%)	15 (6%)	20	38
2	D	232/239 (97%)	217 (94%)	15 (6%)	20	38
All	All	985/1004 (98%)	913 (93%)	72 (7%)	16	32

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	VAL
1	A	47	THR
1	A	49	ILE
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	85	GLN
1	A	122	ARG
1	A	138	GLU
1	A	189	LEU
1	A	200	ARG
1	A	248	PHE
1	A	255	LEU
1	A	297	ARG
2	B	199	TYR
2	B	209	SER
2	B	232	LEU
2	B	263	LEU
2	B	306	LEU
2	B	311	VAL
2	B	348	LEU
2	B	384	LEU
2	B	386	SER
2	B	392	MET
2	B	396	GLN
2	B	399	LEU
2	B	400	LYS
2	B	406	GLN
2	B	410	ARG
1	C	9	LYS
1	C	15	TYR
1	C	22	ARG
1	C	34	LYS
1	C	47	THR
1	C	73	GLU
1	C	78	LEU
1	C	89	LYS
1	C	96	LEU
1	C	97	THR
1	C	111	LEU
1	C	112	LEU
1	C	115	LEU

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Mol	Chain	Res	Type
1	C	121	HIS
1	C	122	ARG
1	C	145	ASP
1	C	159	TYR
1	C	166	LEU
1	C	181	SER
1	C	184	VAL
1	C	189	LEU
1	C	199	ARG
1	C	248	PHE
1	C	252	VAL
1	C	255	LEU
1	C	288	ASP
1	C	293	VAL
2	D	176	PRO
2	D	177	ASP
2	D	243	LEU
2	D	281	ILE
2	D	282	THR
2	D	284	ASP
2	D	292	LEU
2	D	302	LEU
2	D	348	LEU
2	D	392	MET
2	D	399	LEU
2	D	415	ASN
2	D	417	LYS
2	D	424	LEU
2	D	431	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
2	B	179	HIS
2	B	203	GLN
2	B	208	ASN
2	B	317	GLN
2	B	323	GLN
2	B	404	HIS
1	C	71	HIS
1	C	85	GLN

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Mol	Chain	Res	Type
2	D	203	GLN
2	D	208	ASN
2	D	404	HIS
2	D	419	HIS
2	D	425	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 [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	298/298 (100%)	-0.48	5 (1%) 70 65	36, 50, 92, 143	0
1	C	296/298 (99%)	-0.25	5 (1%) 70 65	41, 67, 107, 151	0
2	B	257/265 (96%)	-0.42	1 (0%) 92 91	36, 58, 86, 110	0
2	D	257/265 (96%)	-0.53	0 100 100	35, 49, 83, 102	0
All	All	1108/1126 (98%)	-0.42	11 (0%) 82 79	35, 56, 94, 151	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	4.2
1	C	14	THR	3.6
1	A	39	THR	3.4
1	C	13	GLY	2.9
1	C	295	HIS	2.6
2	B	432	LEU	2.5
1	A	38	ASP	2.2
1	A	161	HIS	2.1
1	C	164	VAL	2.1
1	A	298	LEU	2.0
1	C	96	LEU	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.