Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:36 PM GMT

PDB ID	:	1BLX
Title	:	P19INK4D/CDK6 COMPLEX
Authors	:	Brotherton, D.H.; Dhanaraj, V.; Wick, S.; Brizuela, L.; Domaille, P.J.; Volyanik, E.; Xu, X.; Parisini, E.; Smith, B.O.; Archer, S.J.; Serrano, M.; Brenner, S.L.; Blundell, T.L.; Laue, E.D.
Deposited on	:	1998-07-21
Resolution	:	1.90 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:

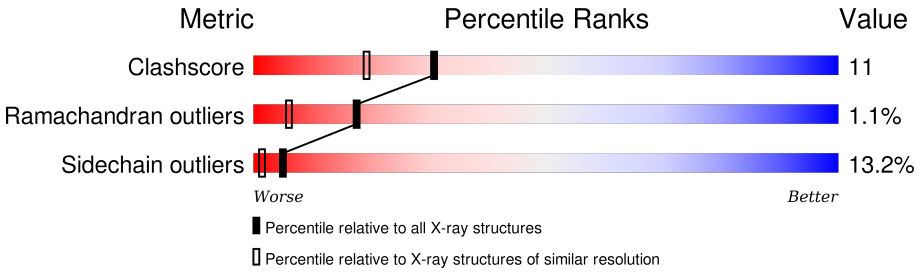
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	326	67% 20% 5% • 6%
2	B	166	63% 23% 8% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3858 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 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2369	1514	411	434	10			

- Molecule 2 is a protein called P19INK4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1194	738	225	225	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	ALA	ARG	VARIANT	UNP Q60773

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		
4	B	108	Total	O	0	0
			108	108		

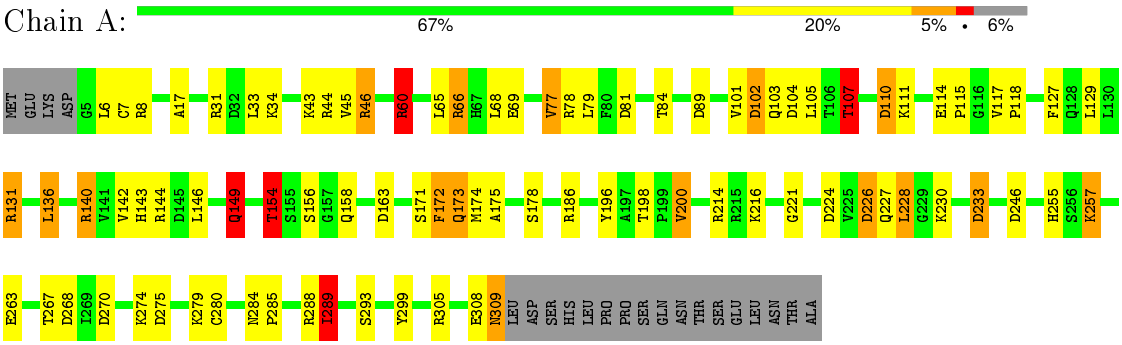
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

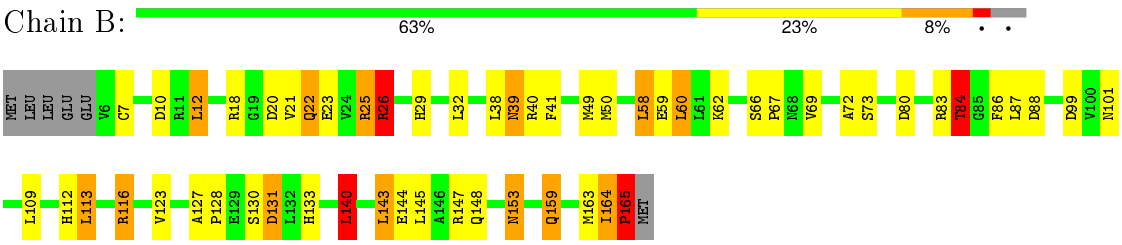
- Molecule 1: CYCLIN-DEPENDENT KINASE 6

Chain A:



- Molecule 2: P19INK4D

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.21Å 76.41Å 93.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.54 – 1.90	Depositor
% Data completeness (in resolution range)	98.5 (18.54-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3858	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.80	0/2420	1.61	44/3285 (1.3%)
2	B	0.88	1/1214 (0.1%)	1.89	29/1645 (1.8%)
All	All	0.83	1/3634 (0.0%)	1.71	73/4930 (1.5%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	165	PRO	N-CD	7.62	1.58	1.47

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	40	ARG	CD-NE-CZ	30.03	165.64	123.60
1	A	31	ARG	NE-CZ-NH2	-14.76	112.92	120.30
2	B	83	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	A	77	VAL	CG1-CB-CG2	11.23	128.87	110.90
2	B	40	ARG	NE-CZ-NH1	11.15	125.87	120.30
2	B	116	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	275	ASP	CB-CG-OD2	10.05	127.34	118.30
2	B	84	THR	N-CA-CB	-9.84	91.61	110.30
1	A	131	ARG	NE-CZ-NH1	9.47	125.04	120.30
2	B	88	ASP	CB-CG-OD1	9.34	126.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	ASP	CB-CG-OD2	9.29	126.66	118.30
1	A	154	THR	OG1-CB-CG2	9.05	130.81	110.00
2	B	20	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	A	246	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	A	60	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	299	TYR	CB-CG-CD2	-8.04	116.17	121.00
2	B	83	ARG	NH1-CZ-NH2	8.04	128.24	119.40
1	A	110	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	A	154	THR	N-CA-CB	-7.96	95.19	110.30
1	A	78	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	31	ARG	CD-NE-CZ	7.87	134.62	123.60
2	B	84	THR	OG1-CB-CG2	7.82	127.98	110.00
2	B	60	LEU	CA-CB-CG	7.76	133.16	115.30
1	A	81	ASP	CB-CG-OD2	-7.66	111.41	118.30
2	B	25	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	131	ARG	CD-NE-CZ	7.58	134.21	123.60
2	B	83	ARG	CD-NE-CZ	7.35	133.89	123.60
1	A	289	ILE	CB-CA-C	-7.14	97.31	111.60
2	B	147	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	77	VAL	N-CA-CB	-7.05	95.99	111.50
1	A	299	TYR	CB-CG-CD1	6.91	125.15	121.00
1	A	214	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	60	ARG	NH1-CZ-NH2	6.64	126.70	119.40
1	A	81	ASP	CB-CG-OD1	6.62	124.26	118.30
2	B	26	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	200	VAL	CA-CB-CG1	6.58	120.76	110.90
1	A	60	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	69	GLU	OE1-CD-OE2	-6.46	115.54	123.30
1	A	289	ILE	CA-CB-CG2	6.42	123.73	110.90
2	B	23	GLU	OE1-CD-OE2	6.24	130.78	123.30
2	B	133	HIS	CA-CB-CG	-6.17	103.11	113.60
1	A	246	ASP	CB-CG-OD1	6.04	123.73	118.30
2	B	165	PRO	CA-N-CD	-6.03	103.06	111.50
2	B	140	LEU	CA-CB-CG	6.00	129.09	115.30
2	B	12	LEU	CB-CG-CD2	5.99	121.18	111.00
1	A	140	ARG	CD-NE-CZ	5.77	131.67	123.60
1	A	186	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	149	GLN	CG-CD-NE2	5.66	130.29	116.70
1	A	226	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	163	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	288	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	136	LEU	CB-CG-CD1	5.49	120.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	ASP	CB-CG-OD2	5.48	123.23	118.30
2	B	18	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	B	116	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	31	ARG	NH1-CZ-NH2	5.34	125.27	119.40
1	A	200	VAL	N-CA-CB	-5.32	99.79	111.50
1	A	101	VAL	CA-CB-CG2	5.30	118.85	110.90
2	B	88	ASP	OD1-CG-OD2	-5.28	113.26	123.30
1	A	228	LEU	CA-CB-CG	5.27	127.43	115.30
2	B	147	ARG	NH1-CZ-NH2	5.23	125.16	119.40
1	A	200	VAL	CG1-CB-CG2	5.22	119.26	110.90
2	B	40	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
2	B	83	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	233	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	99	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	101	VAL	CA-CB-CG1	5.18	118.67	110.90
2	B	84	THR	O-C-N	-5.17	114.41	123.20
1	A	110	ASP	OD1-CG-OD2	5.15	133.09	123.30
1	A	17	ALA	N-CA-CB	5.13	117.29	110.10
2	B	113	LEU	CB-CG-CD1	5.10	119.67	111.00
2	B	131	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	A	107	THR	CA-CB-OG1	5.04	119.59	109.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	164	ILE	Mainchain

5.2 Too-close contacts (i)

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	2369	0	2341	45	0
2	B	1194	0	1191	33	0
3	A	1	0	0	0	0
4	A	186	0	0	6	1
4	B	108	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3858	0	3532	77	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 11.

All (77) 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:104:ASP:OD1	1:A:107:THR:HG23	1.77	0.84
2:B:49:MET:SD	4:B:244:HOH:O	2.37	0.83
1:A:154:THR:HG22	1:A:158:GLN:H	1.46	0.79
2:B:22:GLN:O	2:B:26:ARG:HG2	1.86	0.75
1:A:308:GLU:O	1:A:309:ASN:HB2	1.87	0.73
1:A:66:ARG:HG3	4:A:470:HOH:O	1.89	0.73
1:A:154:THR:HG23	1:A:156:SER:H	1.54	0.72
2:B:165:PRO:HD3	4:B:211:HOH:O	1.92	0.69
1:A:267:THR:O	1:A:268:ASP:HB2	1.92	0.68
2:B:84:THR:HG23	2:B:86:PHE:HD2	1.59	0.68
1:A:221:GLY:H	1:A:227:GLN:NE2	1.96	0.64
1:A:221:GLY:H	1:A:227:GLN:HE22	1.45	0.64
1:A:154:THR:HG21	4:A:429:HOH:O	1.98	0.63
1:A:279:LYS:HB3	1:A:289:ILE:HG12	1.81	0.62
1:A:255:HIS:HD2	1:A:257:LYS:HB3	1.64	0.62
2:B:165:PRO:HA	4:B:188:HOH:O	2.01	0.59
2:B:84:THR:HG23	2:B:86:PHE:CD2	2.37	0.59
2:B:29:HIS:HE1	2:B:59:GLU:OE1	1.86	0.58
1:A:226:ASP:O	1:A:230:LYS:HG2	2.04	0.58
2:B:80:ASP:O	2:B:84:THR:HB	2.05	0.57
2:B:143:LEU:HD11	2:B:159:GLN:NE2	2.20	0.57
2:B:39:ASN:HD22	2:B:39:ASN:C	2.09	0.56
1:A:127:PHE:CE2	1:A:131:ARG:HD2	2.41	0.55
1:A:44:ARG:NH1	1:A:44:ARG:HB3	2.23	0.54
1:A:143:HIS:O	1:A:144:ARG:HB2	2.07	0.54
2:B:101:ASN:HD21	2:B:131:ASP:H	1.56	0.53
1:A:66:ARG:HD2	1:A:79:LEU:CD2	2.38	0.53
1:A:263:GLU:HB2	4:A:441:HOH:O	2.08	0.53
2:B:153:ASN:H	2:B:153:ASN:HD22	1.56	0.53
2:B:58:LEU:HD22	2:B:62:LYS:HD2	1.91	0.52
1:A:60:ARG:HD2	1:A:60:ARG:N	2.24	0.52
1:A:289:ILE:HG22	1:A:293:SER:HB2	1.90	0.52
1:A:233:ASP:O	1:A:257:LYS:HE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ILE:O	2:B:165:PRO:C	2.48	0.50
1:A:172:PHE:O	1:A:173:GLN:C	2.49	0.50
1:A:280:CYS:SG	1:A:289:ILE:HD11	2.51	0.49
1:A:107:THR:HG21	2:B:50:MET:SD	2.53	0.49
2:B:116:ARG:NH2	4:B:222:HOH:O	2.46	0.49
1:A:172:PHE:O	1:A:175:ALA:N	2.43	0.48
1:A:263:GLU:HG3	1:A:274:LYS:NZ	2.27	0.48
1:A:174:MET:O	1:A:175:ALA:HB3	2.13	0.48
1:A:44:ARG:HB3	1:A:44:ARG:HH11	1.80	0.47
2:B:101:ASN:ND2	2:B:131:ASP:H	2.13	0.47
2:B:143:LEU:HD11	2:B:159:GLN:HE21	1.80	0.47
1:A:103:GLN:NE2	1:A:111:LYS:HE2	2.30	0.47
2:B:39:ASN:ND2	2:B:41:PHE:H	2.12	0.46
2:B:153:ASN:HD22	2:B:153:ASN:N	2.13	0.46
2:B:101:ASN:HD21	2:B:130:SER:HA	1.81	0.46
1:A:43:LYS:HB2	1:A:43:LYS:HE3	1.67	0.46
2:B:164:ILE:N	2:B:165:PRO:HD2	2.31	0.46
2:B:25:ARG:HD3	2:B:59:GLU:OE2	2.16	0.45
1:A:111:LYS:HB3	4:A:501:HOH:O	2.16	0.45
2:B:140:LEU:HD12	2:B:144:GLU:HB3	1.98	0.45
2:B:127:ALA:HB3	2:B:128:PRO:HD3	1.99	0.45
1:A:154:THR:CG2	1:A:158:GLN:H	2.25	0.45
1:A:149:GLN:H	1:A:149:GLN:NE2	2.14	0.45
2:B:109:LEU:H	2:B:112:HIS:HD2	1.64	0.45
1:A:66:ARG:HD2	1:A:79:LEU:HD23	1.99	0.45
1:A:255:HIS:HB3	4:A:468:HOH:O	2.17	0.44
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.82	0.44
1:A:224:ASP:HB2	4:A:485:HOH:O	2.17	0.44
2:B:21:VAL:O	2:B:25:ARG:HG3	2.18	0.43
1:A:7:CYS:SG	1:A:8:ARG:N	2.91	0.43
1:A:279:LYS:HB3	1:A:289:ILE:CG1	2.48	0.43
2:B:148:GLN:HG2	4:B:270:HOH:O	2.17	0.42
1:A:284:ASN:HA	1:A:285:PRO:HD2	1.94	0.42
1:A:142:VAL:HG11	1:A:196:TYR:HE2	1.83	0.42
2:B:163:MET:O	2:B:163:MET:HG3	2.20	0.42
1:A:142:VAL:HG22	1:A:198:THR:HG22	2.02	0.42
1:A:103:GLN:HE22	1:A:111:LYS:HE2	1.85	0.41
1:A:66:ARG:HD2	1:A:79:LEU:HD21	2.01	0.41
2:B:112:HIS:HE1	2:B:140:LEU:O	2.03	0.41
1:A:114:GLU:HA	1:A:115:PRO:HA	1.82	0.41
2:B:109:LEU:H	2:B:112:HIS:CD2	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:SER:HA	2:B:67:PRO:HD2	1.95	0.40
2:B:10:ASP:OD1	2:B:39:ASN:HB2	2.22	0.40
1:A:117:VAL:HA	1:A:118:PRO:HD2	1.97	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)
4:A:510:HOH:O	4:B:188:HOH:O[3_556]	1.80	0.40

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	303/326 (93%)	281 (93%)	18 (6%)	4 (1%)	15 4
2	B	158/166 (95%)	151 (96%)	6 (4%)	1 (1%)	30 17
All	All	461/492 (94%)	432 (94%)	24 (5%)	5 (1%)	17 6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	172	PHE
1	A	6	LEU
1	A	178	SER
2	B	72	ALA

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	253/289 (88%)	224 (88%)	29 (12%)	7 2
2	B	127/134 (95%)	106 (84%)	21 (16%)	3 1
All	All	380/423 (90%)	330 (87%)	50 (13%)	5 1

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	34	LYS
1	A	45	VAL
1	A	46	ARG
1	A	60	ARG
1	A	65	LEU
1	A	66	ARG
1	A	68	LEU
1	A	77	VAL
1	A	84	THR
1	A	89	ASP
1	A	102	ASP
1	A	105	LEU
1	A	107	THR
1	A	110	ASP
1	A	129	LEU
1	A	136	LEU
1	A	140	ARG
1	A	146	LEU
1	A	149	GLN
1	A	154	THR
1	A	171	SER
1	A	200	VAL
1	A	216	LYS
1	A	228	LEU
1	A	257	LYS
1	A	289	ILE
1	A	305	ARG
1	A	309	ASN
2	B	7	CYS
2	B	12	LEU

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Mol	Chain	Res	Type
2	B	22	GLN
2	B	26	ARG
2	B	32	LEU
2	B	38	LEU
2	B	39	ASN
2	B	58	LEU
2	B	60	LEU
2	B	69	VAL
2	B	73	SER
2	B	84	THR
2	B	87	LEU
2	B	113	LEU
2	B	123	VAL
2	B	140	LEU
2	B	143	LEU
2	B	145	LEU
2	B	153	ASN
2	B	159	GLN
2	B	165	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	139	HIS
1	A	158	GLN
1	A	227	GLN
1	A	301	GLN
2	B	29	HIS
2	B	39	ASN
2	B	96	HIS
2	B	101	ASN
2	B	112	HIS
2	B	153	ASN
2	B	159	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.