



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:38 PM GMT

PDB ID : 2EUF  
Title : X-ray structure of human CDK6-Vcyclin in complex with the inhibitor PD0332991  
Authors : Schulze-Gahmen, U.; Lu, H.  
Deposited on : 2005-10-28  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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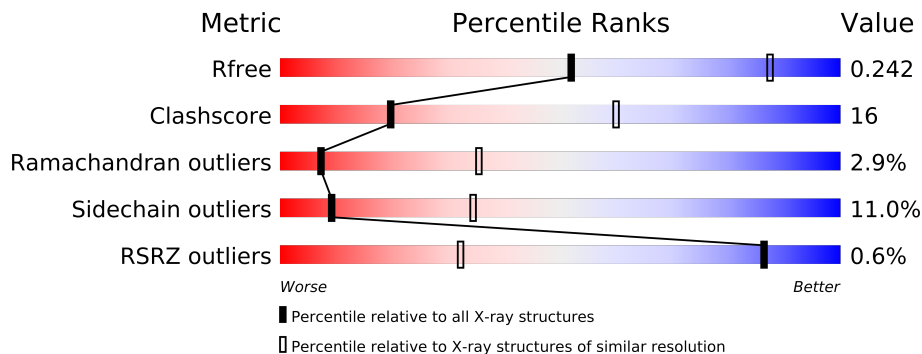
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	254	
2	B	308	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	LQQ	B	401	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4084 atoms, of which 0 are hydrogen and 0 are deuterium.

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 viral Cyclin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1908	1230	307	360	11			

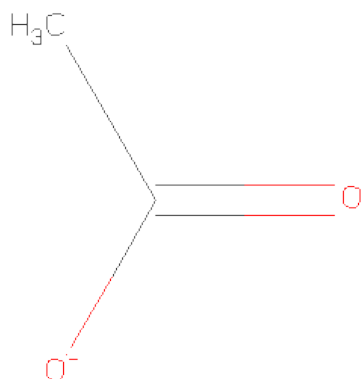
- Molecule 2 is a protein called Cell division protein kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	282	Total	C	N	O	S	0	0	0
			2133	1375	355	396	7			

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

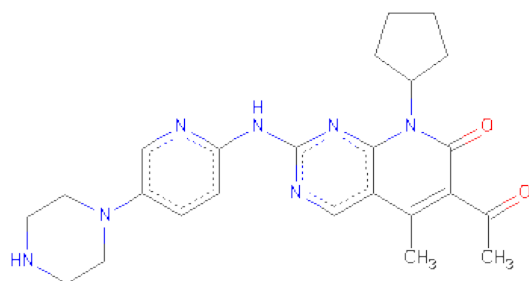
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



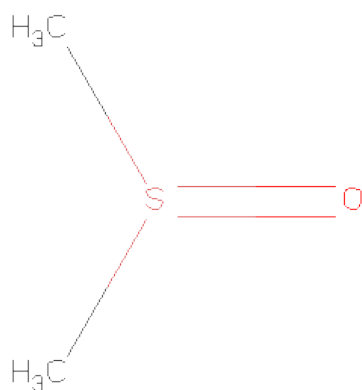
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 6-ACETYL-8-CYCLOPENTYL-5-METHYL-2-[(5-PIPERAZIN-1-YL)PYRIDIN-2-YL)AMINO]PYRIDO[2,3-D]PYRIMIDIN-7(8H)-ONE (three-letter code: LQQ) (formula:  $C_{24}H_{29}N_7O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			33	24	7	2		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is water.

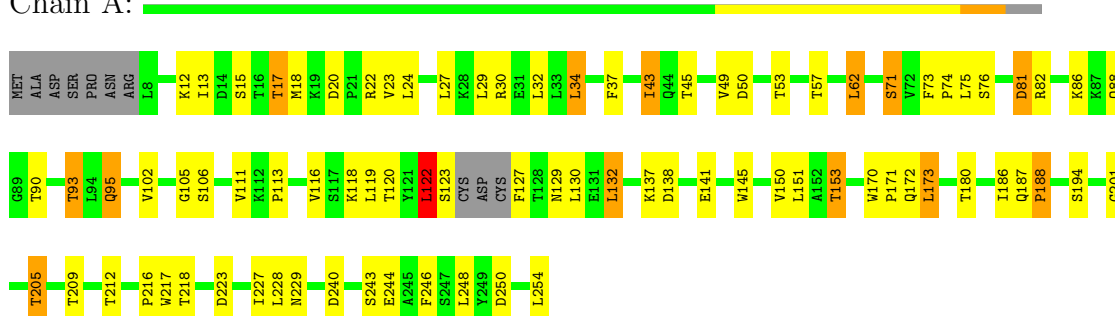
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		

### 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.

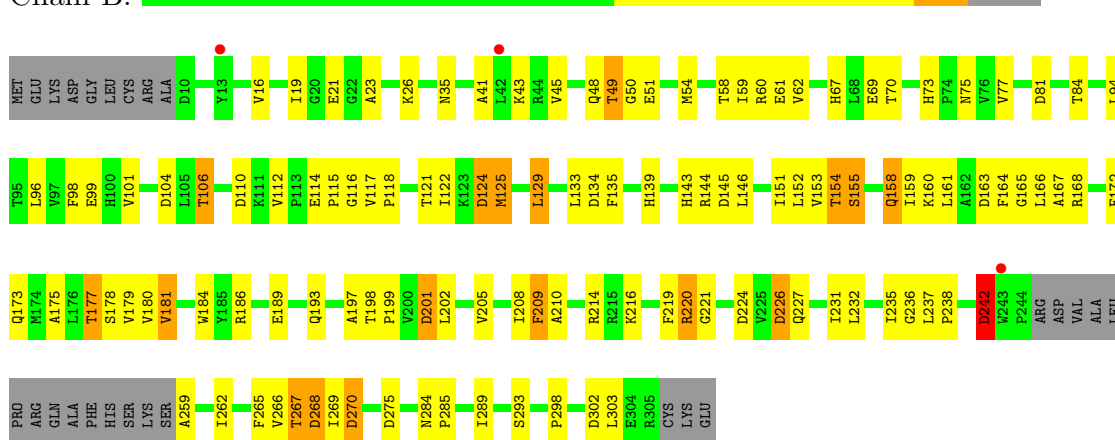
#### • Molecule 1: viral Cyclin

Chain A:



#### • Molecule 2: Cell division protein kinase 6

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.15Å 71.15Å 446.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 47.47 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 93.7 (47.47-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.229 , 0.306 0.241 , 0.242	Depositor DCC
$R_{free}$ test set	687 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.5	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 74.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 13632 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4084	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.56	0/1939	0.85	6/2639 (0.2%)
2	B	0.53	0/2180	0.81	11/2970 (0.4%)
All	All	0.54	0/4119	0.83	17/5609 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	81	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	50	ASP	CB-CG-OD2	6.55	124.19	118.30
2	B	134	ASP	CB-CG-OD2	6.41	124.06	118.30
2	B	124	ASP	CB-CG-OD2	6.13	123.82	118.30
2	B	201	ASP	CB-CG-OD2	5.98	123.68	118.30
2	B	81	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	34	LEU	CA-CB-CG	5.76	128.56	115.30
2	B	268	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	138	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	275	ASP	CB-CG-OD2	5.53	123.28	118.30
2	B	302	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	250	ASP	CB-CG-OD2	5.51	123.25	118.30
1	A	122	LEU	CA-CB-CG	5.31	127.51	115.30
2	B	226	ASP	CB-CG-OD2	5.14	122.93	118.30
2	B	242	ASP	CB-CG-OD2	5.02	122.82	118.30
2	B	270	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1908	0	1970	59	0
2	B	2133	0	2038	83	0
3	A	1	0	0	0	0
4	B	4	0	3	11	0
5	B	33	0	29	4	0
6	B	4	0	6	1	0
7	B	1	0	0	3	0
All	All	4084	0	4046	131	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (131) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:77:VAL:HG21	5:B:401:LQQ:H052	1.39	1.01
2:B:23:ALA:CB	7:B:403:HOH:O	2.19	0.89
1:A:30:ARG:HH11	2:B:139:HIS:HD2	1.18	0.89
1:A:43:ILE:HD12	1:A:43:ILE:H	1.36	0.88
1:A:30:ARG:HD3	2:B:139:HIS:CD2	2.16	0.81
2:B:23:ALA:HB2	7:B:403:HOH:O	1.81	0.80
2:B:143:HIS:HA	4:B:309:ACT:H3	1.60	0.80
2:B:189:GLU:HG2	2:B:285:PRO:HG3	1.63	0.79
1:A:30:ARG:NH1	2:B:139:HIS:HD2	1.81	0.78
1:A:53:THR:O	1:A:57:THR:HG23	1.85	0.76
2:B:145:ASP:HB3	4:B:309:ACT:OXT	1.87	0.75
1:A:30:ARG:HH11	2:B:139:HIS:CD2	2.04	0.74
2:B:144:ARG:N	4:B:309:ACT:CH3	2.52	0.73
2:B:69:GLU:HA	6:B:402:DMS:S	2.28	0.72
1:A:45:THR:H	1:A:88:GLN:NE2	1.88	0.70
2:B:61:GLU:HB2	2:B:165:GLY:HA2	1.74	0.69
2:B:184:TRP:CD1	2:B:220:ARG:HA	2.27	0.69
1:A:244:GLU:O	1:A:248:LEU:HD12	1.92	0.69
2:B:144:ARG:N	4:B:309:ACT:H1	2.09	0.68
2:B:73:HIS:HE1	2:B:75:ASN:HD22	1.40	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:LEU:HD22	1:A:150:VAL:HG13	1.77	0.67
1:A:43:ILE:H	1:A:43:ILE:CD1	2.01	0.67
2:B:189:GLU:CG	2:B:285:PRO:HG3	2.25	0.67
2:B:133:LEU:HD11	2:B:146:LEU:HD11	1.80	0.64
2:B:54:MET:CE	2:B:94:LEU:HD11	2.27	0.64
2:B:117:VAL:HG23	2:B:122:ILE:HG13	1.80	0.63
1:A:119:LEU:O	1:A:122:LEU:O	2.17	0.62
2:B:77:VAL:HG21	5:B:401:LQQ:C05	2.22	0.62
1:A:122:LEU:O	1:A:123:SER:CB	2.48	0.62
1:A:205:THR:HG23	1:A:243:SER:HB2	1.83	0.61
1:A:111:VAL:CG2	2:B:177:THR:HG23	2.31	0.60
2:B:54:MET:HB2	2:B:59:ILE:HD11	1.84	0.60
2:B:125:MET:HE1	2:B:153:VAL:HG22	1.82	0.60
2:B:144:ARG:H	4:B:309:ACT:CH3	2.15	0.59
5:B:401:LQQ:H20	5:B:401:LQQ:N02	2.16	0.59
2:B:189:GLU:HG2	2:B:285:PRO:CG	2.31	0.59
2:B:165:GLY:HA3	7:B:403:HOH:O	2.02	0.59
2:B:146:LEU:HD21	2:B:161:LEU:HD22	1.84	0.58
1:A:111:VAL:HG23	2:B:177:THR:HG23	1.85	0.58
2:B:180:VAL:HG12	2:B:181:VAL:HG23	1.86	0.57
2:B:154:THR:HG22	2:B:158:GLN:H	1.69	0.57
1:A:30:ARG:HD3	2:B:139:HIS:HD2	1.66	0.57
1:A:170:TRP:N	1:A:171:PRO:HD2	2.20	0.57
1:A:30:ARG:NH1	2:B:139:HIS:CD2	2.67	0.56
2:B:143:HIS:CA	4:B:309:ACT:H3	2.32	0.56
1:A:223:ASP:O	1:A:227:ILE:HG12	2.07	0.55
1:A:90:THR:H	1:A:93:THR:HG22	1.71	0.55
2:B:201:ASP:O	2:B:205:VAL:HG23	2.06	0.55
1:A:111:VAL:HG12	2:B:175:ALA:HB3	1.88	0.55
1:A:116:VAL:HG22	1:A:129:ASN:HB2	1.90	0.54
1:A:57:THR:HG22	1:A:186:ILE:HG21	1.90	0.54
1:A:76:SER:OG	1:A:102:VAL:HA	2.08	0.53
2:B:60:ARG:HD3	2:B:167:ALA:O	2.09	0.53
2:B:98:PHE:CE1	5:B:401:LQQ:H012	2.43	0.53
2:B:114:GLU:HA	2:B:116:GLY:H	1.74	0.52
2:B:21:GLU:HA	2:B:26:LYS:HA	1.90	0.52
2:B:172:PHE:CD2	2:B:173:GLN:HG3	2.44	0.52
2:B:210:ALA:O	2:B:214:ARG:HG3	2.10	0.52
1:A:45:THR:N	1:A:88:GLN:NE2	2.57	0.51
2:B:75:ASN:HA	2:B:159:ILE:O	2.10	0.51
1:A:17:THR:HG22	1:A:18:MET:HG3	1.93	0.51
2:B:202:LEU:HD13	2:B:289:ILE:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:VAL:HG23	1:A:132:LEU:HD12	1.93	0.50
1:A:30:ARG:HE	2:B:67:HIS:CE1	2.29	0.50
1:A:145:TRP:HB3	2:B:62:VAL:HG11	1.94	0.50
2:B:266:VAL:O	2:B:269:ILE:HG22	2.11	0.50
1:A:137:LYS:O	1:A:141:GLU:HG2	2.11	0.50
2:B:118:PRO:HG2	2:B:121:THR:OG1	2.11	0.50
2:B:214:ARG:HD2	2:B:265:PHE:O	2.13	0.49
2:B:129:LEU:HD11	2:B:151:ILE:HD13	1.94	0.49
1:A:49:VAL:HG11	1:A:188:PRO:HB3	1.93	0.49
1:A:45:THR:N	1:A:88:GLN:HE22	2.11	0.49
2:B:112:VAL:HG21	2:B:117:VAL:HG12	1.95	0.49
2:B:101:VAL:HG11	2:B:152:LEU:HB3	1.94	0.48
1:A:57:THR:HG22	1:A:186:ILE:HD13	1.96	0.47
2:B:48:GLN:C	2:B:50:GLY:H	2.16	0.47
1:A:180:THR:HG22	1:A:246:PHE:CE1	2.50	0.47
1:A:30:ARG:HE	2:B:67:HIS:HE1	1.61	0.47
1:A:12:LYS:CD	1:A:13:ILE:H	2.28	0.47
2:B:242:ASP:OD1	2:B:284:ASN:HB2	2.14	0.46
2:B:221:GLY:HA3	2:B:227:GLN:OE1	2.16	0.46
1:A:71:SER:HB2	1:A:153:THR:HG21	1.97	0.46
2:B:219:PHE:CE1	2:B:231:ILE:HA	2.51	0.46
1:A:172:GLN:HG3	1:A:173:LEU:H	1.81	0.46
1:A:45:THR:H	1:A:88:GLN:HE21	1.62	0.45
2:B:237:LEU:HD12	2:B:238:PRO:HD2	1.97	0.45
2:B:181:VAL:HB	2:B:186:ARG:HG3	1.99	0.45
1:A:62:LEU:HA	1:A:62:LEU:HD12	1.63	0.45
2:B:117:VAL:HG23	2:B:122:ILE:CG1	2.47	0.45
1:A:75:LEU:HB2	1:A:151:LEU:HD11	1.99	0.45
2:B:104:ASP:OD2	2:B:106:THR:HB	2.17	0.44
2:B:45:VAL:HB	2:B:94:LEU:HB2	1.99	0.44
2:B:41:ALA:HB3	2:B:98:PHE:HB2	2.00	0.44
2:B:144:ARG:O	2:B:181:VAL:HG22	2.17	0.44
1:A:106:SER:HB2	1:A:113:PRO:HA	1.99	0.44
1:A:20:ASP:HB3	1:A:23:VAL:HG23	2.00	0.44
1:A:20:ASP:OD1	1:A:22:ARG:HG2	2.18	0.44
1:A:43:ILE:HD12	1:A:43:ILE:N	2.16	0.43
1:A:75:LEU:HD12	1:A:105:GLY:HA2	1.98	0.43
2:B:236:GLY:HA3	2:B:259:ALA:HB2	2.00	0.43
1:A:240:ASP:O	1:A:244:GLU:HG2	2.18	0.43
1:A:81:ASP:O	1:A:82:ARG:C	2.57	0.43
2:B:143:HIS:C	4:B:309:ACT:H1	2.37	0.43
1:A:116:VAL:CG2	1:A:129:ASN:HB2	2.47	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.72	0.43
2:B:143:HIS:C	4:B:309:ACT:CH3	2.88	0.42
1:A:116:VAL:O	1:A:120:THR:HG23	2.19	0.42
2:B:99:GLU:OE2	2:B:160:LYS:HE3	2.19	0.42
2:B:164:PHE:C	4:B:309:ACT:O	2.58	0.42
2:B:214:ARG:O	2:B:216:LYS:N	2.43	0.42
2:B:43:LYS:HB3	2:B:96:LEU:HB3	1.99	0.42
2:B:193:GLN:HA	2:B:193:GLN:HE21	1.84	0.42
2:B:154:THR:HG23	2:B:155:SER:N	2.34	0.42
2:B:73:HIS:CD2	2:B:135:PHE:CG	3.08	0.42
2:B:54:MET:HB3	2:B:54:MET:HE3	1.94	0.41
2:B:167:ALA:N	4:B:309:ACT:O	2.53	0.41
1:A:49:VAL:CG1	1:A:188:PRO:HB3	2.50	0.41
2:B:284:ASN:OD1	2:B:285:PRO:HD2	2.21	0.41
1:A:201:GLY:O	1:A:205:THR:OG1	2.39	0.41
1:A:118:LYS:O	1:A:122:LEU:HD22	2.19	0.41
2:B:216:LYS:HD3	2:B:220:ARG:HH12	1.85	0.41
1:A:120:THR:HG22	1:A:127:PHE:HE2	1.85	0.41
1:A:187:GLN:HA	1:A:188:PRO:HD2	1.69	0.41
1:A:228:LEU:O	1:A:229:ASN:CB	2.68	0.41
2:B:267:THR:O	2:B:268:ASP:HB2	2.21	0.41
2:B:208:ILE:O	2:B:209:PHE:C	2.59	0.41
1:A:73:PHE:HB3	1:A:74:PRO:HD3	2.03	0.40
2:B:198:THR:N	2:B:199:PRO:CD	2.84	0.40
1:A:95:GLN:HA	1:A:95:GLN:HE21	1.86	0.40
2:B:145:ASP:N	4:B:309:ACT:H1	2.37	0.40
2:B:232:LEU:HA	2:B:232:LEU:HD23	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	240/254 (94%)	211 (88%)	26 (11%)	3 (1%)	18 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	278/308 (90%)	241 (87%)	25 (9%)	12 (4%)	4	23
All	All	518/562 (92%)	452 (87%)	51 (10%)	15 (3%)	7	35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	84	THR
2	B	181	VAL
2	B	303	LEU
1	A	218	THR
2	B	35	ASN
2	B	51	GLU
2	B	163	ASP
2	B	298	PRO
1	A	37	PHE
2	B	19	ILE
2	B	49	THR
2	B	197	ALA
2	B	16	VAL
1	A	188	PRO
2	B	115	PRO

### 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	218/234 (93%)	195 (89%)	23 (11%)	10	36
2	B	218/272 (80%)	193 (88%)	25 (12%)	8	32
All	All	436/506 (86%)	388 (89%)	48 (11%)	9	34

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	17	THR
1	A	24	LEU

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Mol	Chain	Res	Type
1	A	29	LEU
1	A	32	LEU
1	A	34	LEU
1	A	43	ILE
1	A	62	LEU
1	A	71	SER
1	A	86	LYS
1	A	93	THR
1	A	95	GLN
1	A	122	LEU
1	A	130	LEU
1	A	132	LEU
1	A	153	THR
1	A	173	LEU
1	A	194	SER
1	A	205	THR
1	A	209	THR
1	A	212	THR
1	A	216	PRO
1	A	217	TRP
2	B	49	THR
2	B	58	THR
2	B	70	THR
2	B	106	THR
2	B	124	ASP
2	B	125	MET
2	B	129	LEU
2	B	154	THR
2	B	155	SER
2	B	158	GLN
2	B	166	LEU
2	B	168	ARG
2	B	177	THR
2	B	178	SER
2	B	179	VAL
2	B	209	PHE
2	B	220	ARG
2	B	224	ASP
2	B	226	ASP
2	B	235	ILE
2	B	242	ASP
2	B	262	ILE

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Mol	Chain	Res	Type
2	B	267	THR
2	B	270	ASP
2	B	293	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	88	GLN
1	A	95	GLN
2	B	67	HIS
2	B	75	ASN
2	B	139	HIS
2	B	158	GLN
2	B	193	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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
4	ACT	B	309	-	1,3,3	0.88	0	0,3,3	0.00	-
5	LQQ	B	401	-	37,37,37	1.31	3 (8%)	50,53,53	2.46	14 (28%)
6	DMS	B	402	-	3,3,3	2.83	1 (33%)	3,3,3	0.95	0

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
4	ACT	B	309	-	-	0/0/0/0	0/0/0/0
5	LQQ	B	401	-	-	0/12/31/31	0/3/5/5
6	DMS	B	402	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	402	DMS	O-S	4.73	1.82	1.50
5	B	401	LQQ	C07-C06	4.05	1.46	1.42
5	B	401	LQQ	C06-C09	3.62	1.46	1.41
5	B	401	LQQ	C15-N03	2.99	1.43	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	LQQ	C06-C07-N01	-7.12	119.46	124.68
5	B	401	LQQ	N01-C08-N02	-6.57	120.59	126.62
5	B	401	LQQ	C14-C10-N03	-6.30	108.96	114.00
5	B	401	LQQ	C08-N02-C09	6.25	123.00	115.15
5	B	401	LQQ	C06-C09-N02	-5.42	116.65	123.55
5	B	401	LQQ	C23-N07-C22	3.17	121.19	110.14
5	B	401	LQQ	C21-N06-C18	-3.13	109.54	118.05
5	B	401	LQQ	C04-C03-C02	3.00	121.72	119.41
5	B	401	LQQ	C07-N01-C08	3.00	121.67	116.03
5	B	401	LQQ	C17-N05-C16	2.99	121.11	117.99
5	B	401	LQQ	C24-N06-C18	-2.83	110.35	118.05
5	B	401	LQQ	N02-C09-N03	2.74	123.18	115.97
5	B	401	LQQ	N04-C08-N02	2.55	124.52	116.99
5	B	401	LQQ	C14-C10-C11	2.19	106.87	104.28

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	244/254 (96%)	-0.10	0 100 100	41, 52, 66, 83	0
2	B	282/308 (91%)	0.02	3 (1%) 77 21	44, 52, 61, 76	0
All	All	526/562 (93%)	-0.03	3 (0%) 86 32	41, 52, 64, 83	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	42	LEU	2.8
2	B	243	TRP	2.1
2	B	13	TYR	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	LQQ	B	401	33/33	0.56	2.14	52,53,54,54	0
6	DMS	B	402	4/4	0.29	0.92	71,72,72,72	0
4	ACT	B	309	4/4	0.26	0.80	83,83,83,84	0
3	CA	A	255	1/1	0.18	-0.84	70,70,70,70	0

## 6.5 Other polymers

There are no such residues in this entry.