



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:50 pm GMT

PDB ID : 2W9F
Title : CRYSTAL STRUCTURE OF CDK4 IN COMPLEX WITH A D-TYPE CYCLIN
Authors : Day, P.J.; Cleasby, A.; Tickle, I.J.; Reilly, M.O.; Coyle, J.E.; Holding, F.P.; Mcmenamin, R.L.; Yon, J.; Chopra, R.; Lengauer, C.; Jhoti, H.
Deposited on : 2009-01-23
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

<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

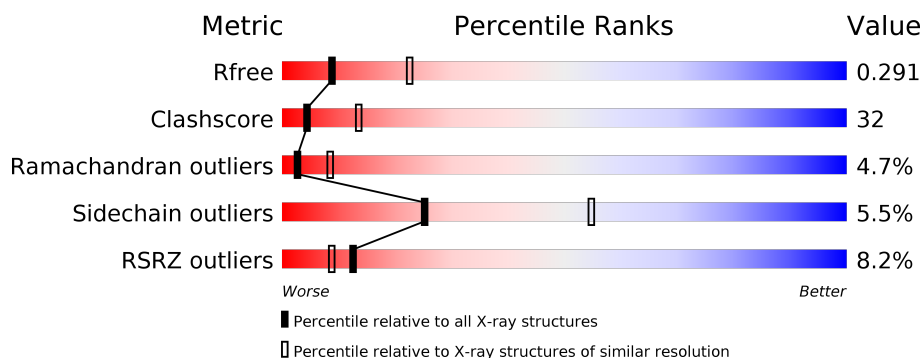
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	271	
2	B	306	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4036 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 G1/S-SPECIFIC CYCLIN-D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1889	1204	320	345	20			

- Molecule 2 is a protein called CELL DIVISION PROTEIN KINASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			2077	1329	363	374	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	43	GLU	GLY	ENGINEERED MUTATION	UNP P11802
B	44	GLU	GLY	ENGINEERED MUTATION	UNP P11802
B	172	PHE	THR	ENGINEERED MUTATION	UNP P11802

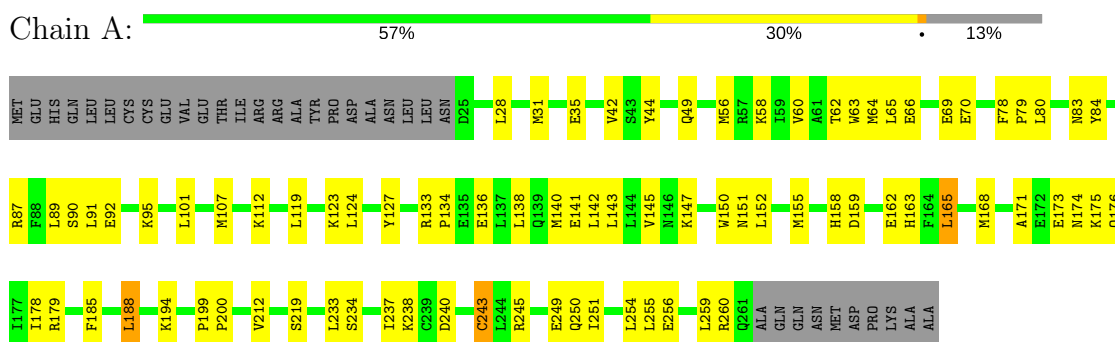
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	19	Total	O	0	0
			19	19		

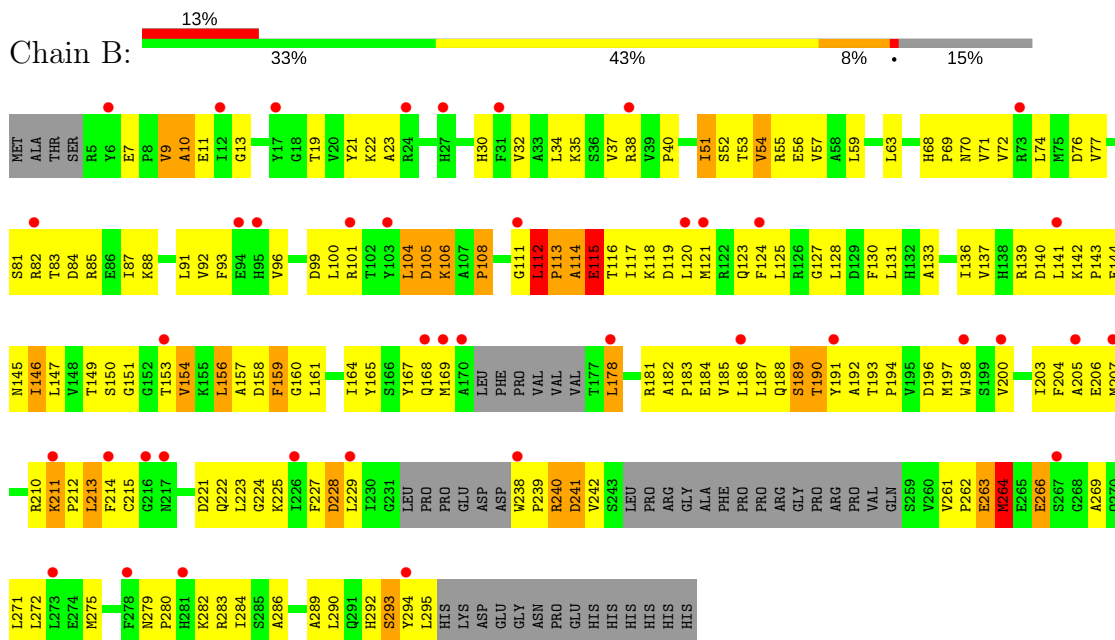
3 Residue-property plots [i](#)

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: G1/S-SPECIFIC CYCLIN-D1



• Molecule 2: CELL DIVISION PROTEIN KINASE 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.00Å 64.28Å 187.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.66 – 2.85 60.81 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.0 (93.66-2.85) 98.1 (60.81-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.86Å)	Xtriage
Refinement program	BUSTER/TNT	Depositor
R, R_{free}	0.225 , 0.300 0.227 , 0.291	Depositor DCC
R_{free} test set	801 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 86.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4036	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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	0.29	0/1922	0.42	0/2595
2	B	0.24	0/2124	0.50	1/2878 (0.0%)
All	All	0.26	0/4046	0.46	1/5473 (0.0%)

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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	112	LEU	C-N-CD	-6.74	105.78	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	156	LEU	Peptide
2	B	211	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	1889	0	1946	74	0
2	B	2077	0	2079	182	0
3	A	51	0	0	1	0
3	B	19	0	0	0	0
All	All	4036	0	4025	253	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 32.

All (253) 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:B:212:PRO:HB2	2:B:215:CYS:HB3	1.26	1.14
2:B:145:ASN:HB3	2:B:157:ALA:HB3	1.35	1.04
2:B:100:LEU:HG	2:B:104:LEU:HD11	1.46	0.95
2:B:40:PRO:HD3	2:B:167:TYR:CD2	2.02	0.94
2:B:32:VAL:HG11	2:B:92:VAL:HG13	1.46	0.94
2:B:185:VAL:HG12	2:B:186:LEU:HG	1.50	0.92
2:B:211:LYS:HB3	2:B:212:PRO:HD3	1.52	0.89
2:B:118:LYS:HE3	2:B:294:TYR:CE2	2.08	0.89
2:B:197:MET:HE2	2:B:284:ILE:HG23	1.58	0.85
2:B:190:THR:HG22	2:B:192:ALA:H	1.45	0.82
2:B:213:LEU:H	2:B:213:LEU:HD23	1.45	0.82
2:B:205:ALA:HB3	2:B:213:LEU:HD21	1.62	0.82
2:B:32:VAL:CG1	2:B:92:VAL:HG13	2.13	0.79
1:A:35:GLU:OE2	1:A:199:PRO:HB2	1.84	0.79
2:B:161:LEU:HA	2:B:164:ILE:HD13	1.65	0.79
1:A:58:LYS:O	1:A:62:THR:HG23	1.84	0.77
1:A:259:LEU:HD12	1:A:260:ARG:N	2.00	0.76
2:B:196:ASP:O	2:B:200:VAL:HG23	1.85	0.76
1:A:31:MET:HG2	1:A:155:MET:CE	2.16	0.76
1:A:188:LEU:HD22	1:A:254:LEU:HG	1.67	0.76
2:B:211:LYS:HB3	2:B:212:PRO:CD	2.17	0.74
2:B:197:MET:CE	2:B:284:ILE:HG23	2.17	0.74
2:B:212:PRO:HB2	2:B:215:CYS:CB	2.11	0.74
2:B:221:ASP:O	2:B:225:LYS:HG3	1.88	0.74
2:B:181:ARG:HD3	2:B:186:LEU:HD11	1.70	0.74
2:B:127:GLY:O	2:B:131:LEU:HD13	1.89	0.73
2:B:204:PHE:HD1	2:B:207:MET:HE2	1.53	0.73
2:B:117:ILE:HG23	2:B:207:MET:CE	2.19	0.73
2:B:263:GLU:O	2:B:264:MET:HB2	1.89	0.73
1:A:35:GLU:HG3	1:A:200:PRO:HD2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:GLN:OE1	2:B:154:VAL:HG13	1.90	0.71
1:A:162:GLU:OE2	1:A:179:ARG:HD3	1.92	0.70
2:B:145:ASN:O	2:B:147:LEU:N	2.25	0.69
2:B:211:LYS:CB	2:B:212:PRO:HD3	2.22	0.69
2:B:123:GLN:HB3	2:B:154:VAL:HG22	1.75	0.68
2:B:142:LYS:H	2:B:145:ASN:HD22	1.42	0.68
2:B:271:LEU:HD13	2:B:292:HIS:CG	2.30	0.67
1:A:155:MET:HE3	1:A:159:ASP:CB	2.24	0.67
1:A:78:PHE:HB3	1:A:79:PRO:HD3	1.78	0.66
2:B:111:GLY:O	2:B:112:LEU:HD23	1.96	0.66
1:A:238:LYS:NZ	3:A:2050:HOH:O	2.29	0.66
2:B:178:LEU:HD13	2:B:181:ARG:HD2	1.77	0.66
2:B:178:LEU:HD22	2:B:181:ARG:HH11	1.60	0.65
1:A:171:ALA:HB1	1:A:173:GLU:OE1	1.97	0.65
1:A:240:ASP:HB3	1:A:243:CYS:SG	2.37	0.64
2:B:279:ASN:HB3	2:B:282:LYS:HG2	1.79	0.64
2:B:279:ASN:HB3	2:B:282:LYS:CG	2.28	0.64
2:B:185:VAL:HG12	2:B:186:LEU:CG	2.23	0.64
2:B:145:ASN:HB3	2:B:157:ALA:CB	2.19	0.63
1:A:79:PRO:HG2	1:A:158:HIS:CE1	2.34	0.63
2:B:99:ASP:HA	2:B:147:LEU:HA	1.80	0.63
2:B:143:PRO:HD3	2:B:203:ILE:HD11	1.80	0.63
1:A:112:LYS:O	2:B:55:ARG:HD3	2.00	0.61
2:B:19:THR:HG21	2:B:21:TYR:CZ	2.35	0.61
2:B:72:VAL:HG13	2:B:156:LEU:O	2.00	0.60
2:B:63:LEU:HD11	2:B:136:ILE:HD12	1.82	0.60
2:B:101:ARG:HA	2:B:104:LEU:HD12	1.84	0.60
2:B:114:ALA:O	2:B:118:LYS:N	2.30	0.60
2:B:117:ILE:HG23	2:B:207:MET:HE1	1.84	0.60
2:B:145:ASN:CB	2:B:157:ALA:HB3	2.21	0.60
2:B:190:THR:CG2	2:B:192:ALA:HB2	2.32	0.60
2:B:193:THR:HG22	2:B:194:PRO:HD3	1.83	0.60
1:A:145:VAL:HG13	1:A:152:LEU:HD11	1.82	0.59
1:A:31:MET:HG2	1:A:155:MET:HE2	1.83	0.59
2:B:91:LEU:HB3	2:B:93:PHE:CE1	2.37	0.59
2:B:206:GLU:O	2:B:210:ARG:HA	2.02	0.59
2:B:165:TYR:HB3	2:B:169:MET:HG3	1.84	0.59
2:B:241:ASP:O	2:B:242:VAL:HG23	2.01	0.59
1:A:80:LEU:O	1:A:83:ASN:HB3	2.03	0.58
2:B:178:LEU:HD22	2:B:181:ARG:NH1	2.19	0.58
2:B:190:THR:HG22	2:B:192:ALA:N	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLU:H	1:A:173:GLU:CD	2.06	0.58
2:B:112:LEU:HB3	2:B:113:PRO:CA	2.34	0.57
2:B:51:ILE:O	2:B:55:ARG:HG3	2.04	0.57
2:B:124:PHE:CE2	2:B:200:VAL:HG22	2.39	0.57
2:B:205:ALA:HB3	2:B:213:LEU:CD2	2.33	0.57
2:B:206:GLU:HG3	2:B:211:LYS:HA	1.86	0.57
2:B:121:MET:CG	2:B:207:MET:HE1	2.34	0.57
1:A:64:MET:HG2	1:A:107:MET:CE	2.35	0.57
2:B:137:VAL:HG22	2:B:193:THR:HA	1.87	0.57
1:A:92:GLU:HG2	1:A:147:LYS:HZ2	1.70	0.57
2:B:284:ILE:HD11	2:B:289:ALA:HA	1.87	0.56
2:B:188:GLN:O	2:B:189:SER:HB2	2.05	0.56
1:A:92:GLU:OE2	1:A:147:LYS:NZ	2.29	0.56
2:B:76:ASP:OD1	2:B:77:VAL:N	2.38	0.56
2:B:178:LEU:HD12	2:B:222:GLN:HG2	1.87	0.56
2:B:52:SER:O	2:B:56:GLU:HG2	2.06	0.56
1:A:174:ASN:O	1:A:178:ILE:HG13	2.05	0.56
2:B:124:PHE:CZ	2:B:200:VAL:HG22	2.41	0.56
2:B:271:LEU:HD13	2:B:292:HIS:ND1	2.21	0.56
1:A:141:GLU:O	1:A:145:VAL:HG23	2.06	0.56
1:A:155:MET:HE3	1:A:159:ASP:HB2	1.87	0.56
1:A:35:GLU:CG	1:A:200:PRO:HD2	2.35	0.56
2:B:139:ARG:HD2	2:B:191:TYR:HD1	1.71	0.56
2:B:192:ALA:HB1	2:B:194:PRO:HD2	1.88	0.55
2:B:181:ARG:HD3	2:B:186:LEU:CD1	2.36	0.55
2:B:124:PHE:CZ	2:B:141:LEU:HD21	2.42	0.55
1:A:90:SER:O	1:A:91:LEU:HD23	2.06	0.55
2:B:192:ALA:CB	2:B:194:PRO:HD2	2.37	0.55
2:B:124:PHE:HE2	2:B:200:VAL:HG13	1.70	0.55
2:B:185:VAL:CG1	2:B:186:LEU:HG	2.31	0.54
2:B:100:LEU:HG	2:B:104:LEU:CD1	2.30	0.54
2:B:279:ASN:HD22	2:B:282:LYS:HG2	1.72	0.54
1:A:178:ILE:HD13	1:A:212:VAL:HG22	1.89	0.54
2:B:112:LEU:CB	2:B:113:PRO:CA	2.38	0.54
1:A:185:PHE:CE2	1:A:255:LEU:HD22	2.43	0.53
1:A:245:ARG:O	1:A:249:GLU:HG3	2.09	0.53
1:A:62:THR:O	1:A:66:GLU:HG3	2.09	0.53
2:B:181:ARG:HH11	2:B:186:LEU:HD11	1.73	0.53
2:B:112:LEU:CB	2:B:113:PRO:CA	2.87	0.53
2:B:182:ALA:HB2	2:B:198:TRP:HB3	1.90	0.53
2:B:223:LEU:C	2:B:223:LEU:HD23	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:ARG:HD2	2:B:191:TYR:CD1	2.45	0.52
1:A:254:LEU:HD12	1:A:254:LEU:O	2.10	0.52
2:B:200:VAL:O	2:B:204:PHE:HB2	2.09	0.52
2:B:70:ASN:O	2:B:71:VAL:HG23	2.10	0.52
1:A:65:LEU:HD13	1:A:78:PHE:CD2	2.45	0.52
2:B:240:ARG:CG	2:B:241:ASP:N	2.72	0.52
1:A:168:MET:HE2	1:A:233:LEU:HD21	1.91	0.52
2:B:224:GLY:O	2:B:228:ASP:OD1	2.28	0.52
2:B:204:PHE:CD1	2:B:207:MET:HE2	2.40	0.51
2:B:74:LEU:HD12	2:B:92:VAL:O	2.10	0.51
2:B:140:ASP:OD1	2:B:142:LYS:HE3	2.11	0.51
2:B:229:LEU:HD23	2:B:229:LEU:C	2.31	0.51
2:B:32:VAL:HG11	2:B:92:VAL:CG1	2.32	0.51
2:B:223:LEU:HD21	2:B:227:PHE:HE1	1.75	0.51
2:B:142:LYS:O	2:B:145:ASN:HB2	2.10	0.51
2:B:266:GLU:O	2:B:269:ALA:N	2.40	0.51
2:B:114:ALA:O	2:B:118:LYS:HG3	2.10	0.51
2:B:9:VAL:O	2:B:10:ALA:HB2	2.10	0.51
2:B:113:PRO:HG2	2:B:114:ALA:H	1.76	0.51
2:B:11:GLU:HG2	2:B:13:GLY:N	2.26	0.51
2:B:124:PHE:CE2	2:B:200:VAL:HG13	2.46	0.51
2:B:193:THR:N	2:B:194:PRO:CD	2.74	0.50
2:B:128:LEU:HD12	2:B:286:ALA:HB2	1.94	0.50
2:B:137:VAL:CG2	2:B:193:THR:HA	2.41	0.50
2:B:34:LEU:CD2	2:B:92:VAL:HG22	2.41	0.50
2:B:181:ARG:CD	2:B:186:LEU:HD11	2.39	0.50
2:B:9:VAL:HG22	2:B:9:VAL:O	2.12	0.50
1:A:101:LEU:HG	1:A:140:MET:HG3	1.93	0.50
1:A:28:LEU:HD22	1:A:163:HIS:NE2	2.27	0.50
2:B:272:LEU:HD12	2:B:272:LEU:O	2.12	0.50
1:A:31:MET:HG2	1:A:155:MET:HE1	1.94	0.49
1:A:119:LEU:HD13	1:A:124:LEU:HD21	1.93	0.49
2:B:186:LEU:HD12	2:B:186:LEU:N	2.27	0.49
2:B:204:PHE:HD1	2:B:207:MET:CE	2.21	0.49
2:B:149:THR:CG2	2:B:153:THR:H	2.26	0.49
2:B:118:LYS:HE3	2:B:294:TYR:CD2	2.48	0.49
2:B:11:GLU:HG2	2:B:13:GLY:H	1.77	0.49
1:A:70:GLU:HG2	1:A:127:TYR:OH	2.12	0.49
2:B:121:MET:HG2	2:B:207:MET:HE1	1.94	0.49
2:B:182:ALA:HB1	2:B:183:PRO:HD2	1.94	0.48
2:B:108:PRO:O	2:B:111:GLY:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PHE:HZ	2:B:141:LEU:HD21	1.78	0.48
2:B:115:GLU:N	2:B:115:GLU:OE1	2.47	0.48
1:A:35:GLU:OE2	1:A:200:PRO:HD2	2.13	0.48
2:B:116:THR:O	2:B:120:LEU:HD13	2.13	0.48
2:B:71:VAL:HG13	2:B:159:PHE:CE2	2.49	0.47
1:A:155:MET:CE	1:A:159:ASP:HB3	2.44	0.47
2:B:213:LEU:H	2:B:213:LEU:CD2	2.23	0.47
1:A:237:ILE:O	1:A:238:LYS:HB2	2.15	0.47
1:A:42:VAL:O	1:A:42:VAL:HG22	2.14	0.47
2:B:282:LYS:O	2:B:282:LYS:HG3	2.13	0.47
1:A:65:LEU:O	1:A:69:GLU:HG3	2.14	0.47
2:B:19:THR:CG2	2:B:21:TYR:CZ	2.98	0.47
1:A:155:MET:HE3	1:A:159:ASP:HB3	1.97	0.47
1:A:84:TYR:OH	1:A:152:LEU:O	2.31	0.46
2:B:37:VAL:HA	2:B:168:GLN:OE1	2.16	0.46
2:B:210:ARG:O	2:B:211:LYS:CB	2.63	0.46
2:B:275:MET:O	2:B:283:ARG:HD2	2.15	0.46
2:B:38:ARG:HE	2:B:88:LYS:HE2	1.79	0.46
2:B:167:TYR:HD1	2:B:168:GLN:N	2.13	0.46
2:B:181:ARG:NH1	2:B:186:LEU:HD11	2.30	0.46
2:B:213:LEU:HD12	2:B:214:PHE:CE1	2.50	0.46
1:A:49:GLN:NE2	1:A:92:GLU:O	2.44	0.46
2:B:35:LYS:NZ	2:B:158:ASP:OD2	2.39	0.46
1:A:31:MET:HE2	1:A:155:MET:HE2	1.97	0.46
2:B:83:THR:C	2:B:85:ARG:H	2.19	0.46
1:A:185:PHE:CD2	1:A:251:ILE:HG22	2.51	0.46
1:A:79:PRO:HG2	1:A:158:HIS:HE1	1.78	0.46
2:B:114:ALA:C	2:B:116:THR:H	2.18	0.46
2:B:161:LEU:HA	2:B:164:ILE:CD1	2.42	0.46
2:B:184:GLU:HB3	2:B:190:THR:HB	1.98	0.45
2:B:130:PHE:O	2:B:133:ALA:HB3	2.16	0.45
2:B:159:PHE:C	2:B:161:LEU:H	2.20	0.45
1:A:134:PRO:O	1:A:138:LEU:HG	2.16	0.45
1:A:188:LEU:HD12	1:A:255:LEU:HD13	1.98	0.45
1:A:56:MET:O	1:A:60:VAL:HG23	2.16	0.45
1:A:142:LEU:CD1	2:B:82:ARG:HD3	2.46	0.45
2:B:19:THR:HG21	2:B:21:TYR:CE1	2.52	0.45
2:B:142:LYS:HB3	2:B:143:PRO:HD2	1.98	0.45
2:B:112:LEU:HB3	2:B:113:PRO:HA	1.95	0.45
2:B:96:VAL:HB	2:B:147:LEU:HB3	1.98	0.45
2:B:157:ALA:O	2:B:158:ASP:OD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:MET:CE	1:A:233:LEU:HD21	2.46	0.45
1:A:185:PHE:CD2	1:A:251:ILE:CG2	3.00	0.45
2:B:210:ARG:O	2:B:211:LYS:HB2	2.15	0.45
2:B:7:GLU:O	2:B:23:ALA:HB1	2.18	0.44
1:A:165:LEU:O	1:A:175:LYS:HE2	2.16	0.44
1:A:176:GLN:O	1:A:176:GLN:NE2	2.50	0.44
1:A:188:LEU:HD11	1:A:255:LEU:HA	1.99	0.44
2:B:54:VAL:CG2	2:B:55:ARG:N	2.79	0.44
1:A:101:LEU:O	1:A:101:LEU:HD12	2.16	0.44
1:A:194:LYS:HB3	1:A:194:LYS:HE3	1.75	0.44
2:B:292:HIS:O	2:B:294:TYR:N	2.51	0.44
2:B:293:SER:C	2:B:295:LEU:H	2.20	0.44
2:B:159:PHE:O	2:B:161:LEU:N	2.49	0.44
2:B:53:THR:O	2:B:57:VAL:HG23	2.18	0.44
1:A:185:PHE:HD2	1:A:251:ILE:CG2	2.31	0.44
2:B:228:ASP:OD1	2:B:228:ASP:N	2.51	0.44
2:B:204:PHE:HD2	2:B:272:LEU:HD13	1.82	0.44
2:B:68:HIS:ND1	2:B:69:PRO:HD2	2.32	0.44
2:B:167:TYR:CD1	2:B:168:GLN:N	2.86	0.43
1:A:194:LYS:HD2	1:A:250:GLN:HB3	1.99	0.43
2:B:161:LEU:HD23	2:B:164:ILE:HD13	1.99	0.43
2:B:271:LEU:HD22	2:B:292:HIS:ND1	2.33	0.43
2:B:63:LEU:HD11	2:B:136:ILE:CD1	2.47	0.43
2:B:51:ILE:CG2	2:B:55:ARG:CZ	2.97	0.43
2:B:204:PHE:CD1	2:B:207:MET:CE	2.99	0.43
1:A:92:GLU:HG2	1:A:147:LYS:NZ	2.34	0.43
2:B:146:ILE:O	2:B:146:ILE:HG22	2.18	0.43
1:A:147:LYS:HD3	1:A:147:LYS:HA	1.87	0.43
1:A:145:VAL:HG12	1:A:150:TRP:CD1	2.54	0.42
1:A:234:SER:O	1:A:238:LYS:N	2.49	0.42
2:B:9:VAL:N	2:B:22:LYS:O	2.50	0.42
1:A:95:LYS:HB3	1:A:95:LYS:HE2	1.88	0.42
2:B:38:ARG:NE	2:B:88:LYS:HE2	2.35	0.42
2:B:279:ASN:HB3	2:B:282:LYS:HG3	2.02	0.42
2:B:178:LEU:CD2	2:B:181:ARG:HH11	2.31	0.42
2:B:261:VAL:N	2:B:262:PRO:HD3	2.34	0.42
2:B:182:ALA:HB2	2:B:198:TRP:CB	2.50	0.42
2:B:11:GLU:HA	2:B:21:TYR:HA	2.01	0.42
2:B:204:PHE:O	2:B:207:MET:HE2	2.20	0.42
2:B:118:LYS:NZ	2:B:294:TYR:O	2.33	0.41
1:A:256:GLU:O	1:A:259:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:SER:O	2:B:87:ILE:HG23	2.20	0.41
2:B:184:GLU:OE2	2:B:280:PRO:HB3	2.20	0.41
2:B:125:LEU:HA	2:B:125:LEU:HD23	1.92	0.41
2:B:145:ASN:O	2:B:147:LEU:HG	2.20	0.41
2:B:275:MET:HA	2:B:284:ILE:HG22	2.02	0.41
1:A:63:TRP:CZ3	1:A:107:MET:HE1	2.56	0.41
2:B:96:VAL:CG1	2:B:147:LEU:HB3	2.50	0.41
2:B:190:THR:CG2	2:B:192:ALA:CB	2.98	0.41
2:B:83:THR:O	2:B:85:ARG:N	2.53	0.41
2:B:105:ASP:O	2:B:106:LYS:C	2.59	0.41
2:B:112:LEU:HB2	2:B:113:PRO:HA	2.02	0.41
1:A:123:LYS:HE3	1:A:123:LYS:HB2	1.86	0.40
2:B:113:PRO:O	2:B:114:ALA:HB2	2.20	0.40
1:A:142:LEU:HD13	2:B:82:ARG:HD3	2.03	0.40
1:A:133:ARG:O	1:A:136:GLU:N	2.54	0.40
1:A:87:ARG:HH22	1:A:151:ASN:HB3	1.86	0.40
1:A:31:MET:CG	1:A:155:MET:HE2	2.50	0.40
2:B:292:HIS:O	2:B:295:LEU:N	2.53	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	235/271 (87%)	220 (94%)	15 (6%)	0	100	100
2	B	253/306 (83%)	195 (77%)	35 (14%)	23 (9%)	1	1
All	All	488/577 (85%)	415 (85%)	50 (10%)	23 (5%)	3	8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	VAL
2	B	112	LEU
2	B	146	ILE
2	B	189	SER
2	B	190	THR
2	B	239	PRO
2	B	264	MET
2	B	106	LYS
2	B	108	PRO
2	B	114	ALA
2	B	240	ARG
2	B	10	ALA
2	B	51	ILE
2	B	151	GLY
2	B	241	ASP
2	B	293	SER
2	B	105	ASP
2	B	113	PRO
2	B	160	GLY
2	B	84	ASP
2	B	115	GLU
2	B	150	SER
2	B	30	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	214/243 (88%)	207 (97%)	7 (3%)	43	74
2	B	225/265 (85%)	208 (92%)	17 (8%)	15	38
All	All	439/508 (86%)	415 (94%)	24 (6%)	25	55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	TYR

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Mol	Chain	Res	Type
1	A	89	LEU
1	A	143	LEU
1	A	165	LEU
1	A	188	LEU
1	A	219	SER
1	A	243	CYS
2	B	54	VAL
2	B	59	LEU
2	B	104	LEU
2	B	115	GLU
2	B	119	ASP
2	B	144	GLU
2	B	154	VAL
2	B	159	PHE
2	B	178	LEU
2	B	187	LEU
2	B	213	LEU
2	B	228	ASP
2	B	238	TRP
2	B	263	GLU
2	B	264	MET
2	B	266	GLU
2	B	290	LEU

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	139	GLN
1	A	158	HIS
1	A	183	GLN
1	A	261	GLN
2	B	138	HIS
2	B	145	ASN
2	B	222	GLN
2	B	279	ASN

5.3.3 RNA ⓘ

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	237/271 (87%)	0.19	0 100 100	33, 55, 89, 117	0
2	B	261/306 (85%)	0.91	41 (15%) 2 2	56, 109, 143, 161	0
All	All	498/577 (86%)	0.57	41 (8%) 12 9	33, 80, 135, 161	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	217	ASN	6.4
2	B	229	LEU	5.9
2	B	31	PHE	4.7
2	B	214	PHE	4.6
2	B	6	TYR	4.1
2	B	153	THR	3.6
2	B	191	TYR	3.4
2	B	267	SER	3.4
2	B	124	PHE	3.3
2	B	24	ARG	3.1
2	B	211	LYS	3.1
2	B	103	TYR	3.1
2	B	207	MET	3.1
2	B	111	GLY	3.0
2	B	169	MET	2.9
2	B	170	ALA	2.9
2	B	38	ARG	2.8
2	B	198	TRP	2.8
2	B	95	HIS	2.6
2	B	120	LEU	2.6
2	B	121	MET	2.6
2	B	82	ARG	2.6
2	B	12	ILE	2.4
2	B	226	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	273	LEU	2.4
2	B	186	LEU	2.4
2	B	281	HIS	2.3
2	B	101	ARG	2.3
2	B	168	GLN	2.3
2	B	200	VAL	2.3
2	B	94	GLU	2.3
2	B	238	TRP	2.2
2	B	73	ARG	2.2
2	B	216	GLY	2.2
2	B	205	ALA	2.1
2	B	141	LEU	2.1
2	B	27	HIS	2.1
2	B	278	PHE	2.1
2	B	178	LEU	2.0
2	B	294	TYR	2.0
2	B	17	TYR	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.