



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2W96 / pdb_00002w96
Title : Crystal Structure of CDK4 in complex with a D-type cyclin
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Deposited on : 2009-01-21
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

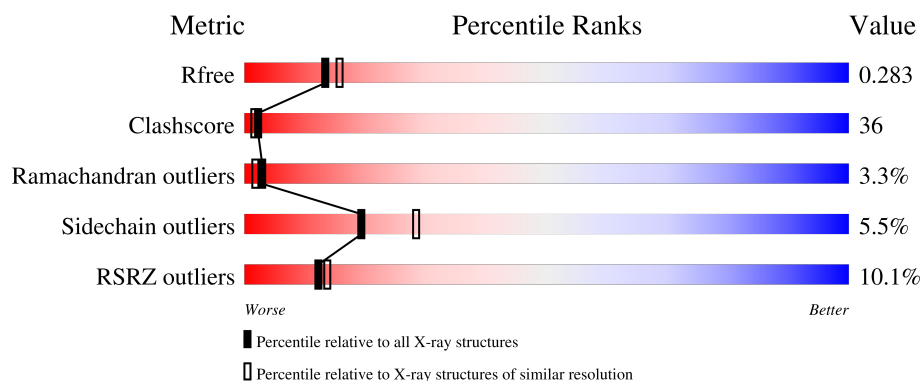
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 4 unique types of molecules in this entry. The entry contains 4306 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	249	Total	C	N	O	S	0	1	0
			1983	1260	336	365	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	267	Total	C	N	O	S	0	1	0
			2127	1365	366	385	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	ASP	THR	engineered mutation	UNP P11802

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	68	Total	O	0	0
			68	68		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.91Å 64.69Å 168.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.22 – 2.30 84.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (84.22-2.30) 99.2 (84.22-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.29Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.203 , 0.259 0.218 , 0.283	Depositor DCC
R_{free} test set	1356 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4306	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

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

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	0.44	0/2018	0.85	4/2723 (0.1%)
2	B	0.33	0/2181	0.85	13/2963 (0.4%)
All	All	0.39	0/4199	0.85	17/5686 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	SER	CA-C-N	8.43	128.55	119.28
1	A	219	SER	C-N-CA	8.43	128.55	119.28
1	A	12	THR	N-CA-C	-8.34	103.55	114.31
2	B	172	ASP	CA-C-N	-7.98	112.23	120.85
2	B	172	ASP	C-N-CA	-7.98	112.23	120.85
2	B	112	LEU	C-N-CD	-6.67	105.92	120.60
2	B	7	GLU	CA-C-N	6.65	128.16	119.84
2	B	7	GLU	C-N-CA	6.65	128.16	119.84
2	B	107	ALA	CA-C-N	6.27	126.83	120.38
2	B	107	ALA	C-N-CA	6.27	126.83	120.38
2	B	279	ASN	CA-C-N	6.21	125.95	119.05
2	B	279	ASN	C-N-CA	6.21	125.95	119.05
2	B	211	LYS	CA-C-N	5.71	126.98	119.84
2	B	211	LYS	C-N-CA	5.71	126.98	119.84
2	B	108	PRO	CA-C-N	5.35	125.89	120.38
2	B	108	PRO	C-N-CA	5.35	125.89	120.38
1	A	7	CYS	N-CA-C	5.32	117.87	108.24

There are no chirality outliers.

There are no planarity outliers.

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	1983	0	2036	81	0
2	B	2127	0	2133	231	0
3	A	6	0	8	3	0
4	A	122	0	0	7	0
4	B	68	0	0	8	0
All	All	4306	0	4177	300	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 36.

All (300) 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:32:VAL:HG11	2:B:92:VAL:HG13	1.38	1.06
2:B:173:PRO:HA	2:B:174:VAL:HB	1.38	1.03
2:B:190:THR:HA	2:B:191:TYR:HB2	1.46	0.98
1:A:142:LEU:HD13	2:B:82:ARG:HD3	1.48	0.95
2:B:279:ASN:HD22	2:B:282:LYS:HG2	1.29	0.95
2:B:178:LEU:HD13	2:B:181:ARG:HB2	1.51	0.92
2:B:193:THR:HG22	2:B:194:PRO:HD3	1.53	0.91
2:B:179:TRP:CH2	2:B:216:GLY:HA2	2.06	0.90
2:B:64:GLU:HG3	2:B:73:ARG:HD2	1.55	0.88
2:B:179:TRP:CZ3	2:B:216:GLY:HA2	2.07	0.88
2:B:186:LEU:HD13	2:B:223:LEU:HD12	1.54	0.87
1:A:58:LYS:O	1:A:62:THR:HG22	1.77	0.83
2:B:232:LEU:HD12	2:B:233:PRO:HD2	1.59	0.83
1:A:142:LEU:HD13	2:B:82:ARG:CD	2.08	0.83
2:B:121:MET:SD	2:B:207:MET:HE1	2.19	0.82
1:A:60:VAL:HG21	1:A:99:LEU:HG	1.60	0.81
2:B:196:ASP:O	2:B:200:VAL:HG23	1.80	0.80
2:B:32:VAL:HG11	2:B:92:VAL:CG1	2.11	0.80
2:B:213:LEU:HD23	2:B:213:LEU:H	1.45	0.80
2:B:59:LEU:HD21	4:B:2009:HOH:O	1.81	0.80
2:B:102:THR:HG22	2:B:106:LYS:HE3	1.64	0.80
2:B:188:GLN:HB3	2:B:189:SER:OG	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ILE:O	2:B:230:ILE:HG22	1.84	0.78
2:B:170:ALA:C	2:B:171:LEU:HD12	2.09	0.78
2:B:136[A]:ILE:HD11	2:B:159:PHE:HB2	1.66	0.77
2:B:264:MET:HE3	2:B:269:ALA:CA	2.15	0.77
2:B:122:ARG:O	2:B:126:ARG:HG3	1.86	0.76
2:B:118:LYS:HE2	2:B:294:TYR:CE1	2.18	0.76
2:B:187:LEU:HG	2:B:188:GLN:HA	1.68	0.76
1:A:116:THR:HG22	4:A:2038:HOH:O	1.84	0.76
2:B:264:MET:HE3	2:B:269:ALA:HA	1.68	0.75
2:B:198:TRP:HB2	2:B:283:ARG:NH2	2.01	0.75
1:A:237:ILE:CG2	1:A:239:CYS:HB3	2.17	0.75
2:B:187:LEU:CG	2:B:188:GLN:HA	2.17	0.75
2:B:140:ASP:OD1	2:B:142:LYS:HE3	1.86	0.74
2:B:187:LEU:CD2	2:B:188:GLN:HA	2.18	0.74
1:A:237:ILE:HG21	1:A:239:CYS:HB3	1.69	0.73
2:B:172:ASP:H	2:B:173:PRO:CD	2.03	0.72
2:B:190:THR:HA	2:B:191:TYR:CB	2.18	0.72
2:B:51:ILE:O	2:B:54:VAL:HG22	1.90	0.71
2:B:187:LEU:HD23	2:B:188:GLN:HA	1.73	0.71
1:A:79:PRO:HG2	1:A:158:HIS:CE1	2.26	0.70
2:B:24:ARG:O	2:B:26:PRO:HD3	1.90	0.70
2:B:215:CYS:H	2:B:225:LYS:HD3	1.56	0.70
2:B:261:VAL:HG23	4:B:2064:HOH:O	1.91	0.69
2:B:199:SER:O	2:B:203:ILE:HG12	1.93	0.69
1:A:237:ILE:HG22	1:A:239:CYS:N	2.07	0.69
2:B:170:ALA:O	2:B:171:LEU:HD12	1.92	0.69
2:B:227:PHE:CE2	2:B:233:PRO:HD3	2.28	0.69
2:B:101:ARG:NE	2:B:144:GLU:HG3	2.08	0.68
2:B:187:LEU:HA	2:B:188:GLN:C	2.18	0.68
2:B:279:ASN:ND2	2:B:282:LYS:HG2	2.07	0.68
2:B:55:ARG:O	2:B:59:LEU:HD13	1.94	0.68
2:B:101:ARG:CZ	2:B:144:GLU:HG3	2.24	0.68
2:B:184:GLU:HB3	2:B:190:THR:O	1.93	0.68
1:A:10:VAL:HG12	1:A:11:GLU:N	2.08	0.68
1:A:185:PHE:HE1	1:A:255:LEU:HD22	1.59	0.67
2:B:229:LEU:O	2:B:229:LEU:HD23	1.93	0.67
2:B:171:LEU:N	2:B:172:ASP:HA	2.10	0.67
2:B:101:ARG:HD3	2:B:144:GLU:OE2	1.95	0.67
2:B:193:THR:CG2	2:B:194:PRO:HD3	2.24	0.67
2:B:49:LEU:HD23	2:B:87:ILE:HD13	1.77	0.66
2:B:235:GLU:HA	2:B:237:ASP:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:SER:O	2:B:82:ARG:HG3	1.96	0.66
2:B:65:ALA:HB2	4:B:2021:HOH:O	1.96	0.66
2:B:178:LEU:CD1	2:B:181:ARG:HB2	2.26	0.66
2:B:187:LEU:HD12	2:B:191:TYR:CE2	2.32	0.65
2:B:36:SER:OG	2:B:88:LYS:HE2	1.95	0.65
2:B:144:GLU:N	2:B:144:GLU:OE1	2.28	0.65
1:A:28:LEU:HD21	1:A:236:VAL:HG12	1.79	0.65
2:B:192:ALA:O	2:B:195:VAL:HG22	1.96	0.65
1:A:204:ALA:O	1:A:208:VAL:HG23	1.97	0.64
1:A:248:GLN:NE2	1:A:252:GLU:OE2	2.30	0.64
2:B:140:ASP:O	2:B:145:ASN:ND2	2.30	0.64
2:B:186:LEU:CD1	2:B:223:LEU:HD12	2.27	0.64
2:B:149:THR:CG2	2:B:153:THR:H	2.09	0.64
2:B:232:LEU:CD1	2:B:233:PRO:HD2	2.27	0.64
1:A:71:GLN:NE2	1:A:127:TYR:OH	2.25	0.64
1:A:162:GLU:OE1	1:A:179:ARG:NH1	2.30	0.64
1:A:145:VAL:HG12	1:A:150:TRP:CD1	2.33	0.64
2:B:40:PRO:HA	2:B:85:ARG:O	1.98	0.63
2:B:190:THR:CA	2:B:191:TYR:HB2	2.27	0.63
2:B:149:THR:HG21	2:B:153:THR:HB	1.78	0.63
2:B:5:ARG:O	2:B:26:PRO:HG2	1.97	0.63
2:B:186:LEU:HD11	2:B:219:GLU:HB3	1.81	0.63
2:B:115:GLU:OE1	2:B:118:LYS:HD2	1.98	0.63
2:B:184:GLU:OE2	2:B:280:PRO:HB3	1.99	0.63
2:B:80:THR:OG1	2:B:88:LYS:HD2	1.98	0.62
2:B:149:THR:CG2	2:B:153:THR:HB	2.29	0.62
1:A:164:PHE:HB3	1:A:168:MET:HE3	1.81	0.62
2:B:187:LEU:HD23	2:B:188:GLN:CA	2.30	0.62
2:B:213:LEU:HD23	2:B:213:LEU:N	2.13	0.62
2:B:142:LYS:N	2:B:145:ASN:HD22	1.98	0.61
2:B:102:THR:O	2:B:106:LYS:HG2	2.01	0.61
1:A:9:GLU:OE2	2:B:288:ARG:NH1	2.34	0.60
1:A:101:LEU:HG	1:A:140:MET:HG3	1.83	0.60
2:B:39:VAL:HG22	2:B:87:ILE:O	2.01	0.60
2:B:96:VAL:HB	2:B:147:LEU:HD13	1.83	0.60
2:B:176:VAL:HB	2:B:178:LEU:HD23	1.83	0.60
2:B:32:VAL:HG13	2:B:93:PHE:O	2.01	0.59
1:A:162:GLU:OE2	1:A:179:ARG:HD3	2.02	0.59
2:B:35:LYS:NZ	2:B:158:ASP:OD1	2.29	0.59
1:A:10:VAL:HG21	2:B:287:PHE:CE2	2.38	0.59
1:A:185:PHE:CE1	1:A:255:LEU:HD22	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLN:HA	1:A:264:GLN:HG2	1.85	0.59
2:B:209:ARG:NH2	2:B:213:LEU:HD13	2.18	0.59
2:B:70:ASN:HD21	2:B:123:GLN:HE21	1.51	0.59
2:B:213:LEU:H	2:B:213:LEU:CD2	2.15	0.59
2:B:123:GLN:HE22	2:B:153:THR:HA	1.68	0.58
1:A:118:PRO:HG2	2:B:51:ILE:CD1	2.33	0.58
2:B:167:TYR:O	2:B:171:LEU:HD13	2.02	0.58
2:B:49:LEU:CD2	2:B:87:ILE:HD13	2.34	0.58
2:B:215:CYS:O	2:B:222:GLN:NE2	2.36	0.58
2:B:173:PRO:HA	2:B:174:VAL:CB	2.20	0.58
1:A:34:ALA:HB1	4:A:2078:HOH:O	2.03	0.57
2:B:71:VAL:HG13	2:B:159:PHE:CE2	2.39	0.57
2:B:223:LEU:HD23	2:B:223:LEU:O	2.04	0.57
2:B:217:ASN:HB3	2:B:221:ASP:CB	2.35	0.57
1:A:10:VAL:HG21	2:B:287:PHE:CD2	2.39	0.57
2:B:186:LEU:CD1	2:B:219:GLU:HB3	2.34	0.57
1:A:234:SER:OG	1:A:241:PRO:HA	2.04	0.57
2:B:214:PHE:HA	2:B:225:LYS:HD3	1.85	0.56
1:A:142:LEU:HD21	2:B:49:LEU:HD21	1.88	0.56
2:B:190:THR:HB	2:B:191:TYR:C	2.31	0.56
2:B:124:PHE:CD1	2:B:156:LEU:HD21	2.40	0.56
2:B:206:GLU:OE2	2:B:212:PRO:HD3	2.04	0.56
1:A:95:LYS:NZ	4:A:2051:HOH:O	2.37	0.56
2:B:179:TRP:N	2:B:179:TRP:CE3	2.74	0.56
1:A:33:LYS:HB3	4:B:2024:HOH:O	2.06	0.56
1:A:11:GLU:O	1:A:11:GLU:HG2	2.05	0.56
1:A:87:ARG:HH21	3:A:1266:GOL:H2	1.71	0.56
2:B:32:VAL:CG1	2:B:92:VAL:HG13	2.26	0.56
2:B:142:LYS:HB3	2:B:144:GLU:OE1	2.06	0.55
2:B:264:MET:CE	2:B:269:ALA:HA	2.36	0.55
1:A:182:ALA:O	1:A:186:VAL:HG23	2.07	0.55
2:B:49:LEU:HD23	2:B:87:ILE:CD1	2.37	0.55
2:B:183:PRO:HG2	4:B:2059:HOH:O	2.06	0.55
2:B:209:ARG:O	2:B:210:ARG:HG3	2.07	0.54
1:A:240:ASP:HB3	1:A:243:CYS:SG	2.47	0.54
2:B:264:MET:HE3	2:B:269:ALA:N	2.22	0.54
1:A:27:VAL:HG13	1:A:28:LEU:H	1.73	0.54
2:B:172:ASP:N	2:B:173:PRO:CD	2.71	0.54
2:B:294:TYR:O	2:B:295:LEU:HB2	2.07	0.54
2:B:35:LYS:HZ2	2:B:158:ASP:CG	2.15	0.54
2:B:142:LYS:O	2:B:146:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:HH12	1:A:231:ARG:NH1	2.06	0.53
2:B:14:VAL:HG12	2:B:14:VAL:O	2.08	0.53
1:A:63:TRP:CZ3	1:A:107:MET:HE2	2.44	0.53
2:B:41:ASN:HB2	2:B:87:ILE:HG13	1.89	0.53
2:B:204:PHE:HA	2:B:207:MET:CE	2.39	0.53
1:A:142:LEU:HD13	2:B:82:ARG:HH11	1.75	0.52
1:A:170:GLU:O	1:A:175:LYS:HE3	2.09	0.52
2:B:217:ASN:HB3	2:B:221:ASP:HB2	1.92	0.52
2:B:227:PHE:O	2:B:231:GLY:N	2.39	0.51
2:B:205:ALA:HB2	2:B:272:LEU:HD21	1.92	0.51
1:A:157:PRO:HG2	1:A:186:VAL:HG13	1.93	0.51
1:A:79:PRO:HG2	1:A:158:HIS:HE1	1.72	0.51
2:B:205:ALA:HB1	2:B:209:ARG:HE	1.75	0.51
2:B:64:GLU:HB2	4:B:2023:HOH:O	2.10	0.51
2:B:4:SER:HB3	2:B:6:TYR:CZ	2.46	0.51
2:B:215:CYS:O	2:B:216:GLY:O	2.28	0.51
1:A:108:PHE:CE2	1:A:112:LYS:HE3	2.46	0.50
2:B:172:ASP:OD1	2:B:172:ASP:O	2.29	0.50
1:A:225:SER:O	1:A:229:LEU:HD13	2.12	0.50
2:B:178:LEU:HD12	2:B:222:GLN:HG2	1.92	0.50
2:B:190:THR:CA	2:B:191:TYR:CB	2.89	0.50
2:B:17:TYR:CD2	2:B:165:TYR:CG	2.99	0.50
2:B:172:ASP:H	2:B:173:PRO:HD2	1.76	0.50
2:B:227:PHE:CD2	2:B:233:PRO:HD3	2.46	0.49
1:A:79:PRO:CG	1:A:158:HIS:HE1	2.25	0.49
2:B:235:GLU:HB3	2:B:236:ASP:HA	1.94	0.49
2:B:111:GLY:HA3	2:B:112:LEU:HB3	1.93	0.49
2:B:274:GLU:OE1	2:B:284:ILE:HD12	2.13	0.49
1:A:237:ILE:O	1:A:238:LYS:HB2	2.12	0.49
2:B:71:VAL:HG21	2:B:131:LEU:HD13	1.93	0.49
2:B:261:VAL:N	2:B:262:PRO:HD3	2.27	0.49
2:B:17:TYR:HD2	2:B:165:TYR:CD2	2.31	0.49
2:B:114:ALA:O	2:B:118:LYS:HG3	2.12	0.49
2:B:261:VAL:HG12	2:B:261:VAL:O	2.13	0.49
2:B:277:THR:O	2:B:279:ASN:N	2.45	0.49
2:B:8:PRO:O	2:B:9:VAL:HG23	2.12	0.49
2:B:20:VAL:HB	2:B:35:LYS:HG2	1.94	0.49
2:B:96:VAL:HB	2:B:147:LEU:CD1	2.43	0.49
2:B:34:LEU:CD2	2:B:92:VAL:HG22	2.43	0.48
1:A:31:MET:HE3	1:A:155:MET:HE1	1.95	0.48
2:B:209:ARG:HH21	2:B:213:LEU:HD13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:HH21	3:A:1266:GOL:C2	2.26	0.48
2:B:180:TYR:OH	2:B:206:GLU:OE1	2.28	0.48
2:B:149:THR:HG22	2:B:153:THR:O	2.14	0.48
1:A:112:LYS:O	2:B:55:ARG:NH1	2.43	0.48
2:B:206:GLU:HA	2:B:209:ARG:HB2	1.95	0.48
2:B:142:LYS:H	2:B:145:ASN:HD22	1.61	0.48
2:B:223:LEU:HD22	2:B:227:PHE:CE1	2.49	0.48
2:B:71:VAL:CG1	2:B:159:PHE:CZ	2.97	0.47
2:B:138:HIS:CD2	2:B:141:LEU:HD13	2.49	0.47
2:B:88:LYS:NZ	2:B:90:THR:HG22	2.30	0.47
2:B:235:GLU:CB	2:B:236:ASP:HA	2.43	0.47
2:B:9:VAL:O	2:B:10:ALA:HB2	2.15	0.47
2:B:204:PHE:HA	2:B:207:MET:HE3	1.96	0.47
2:B:149:THR:HG22	2:B:153:THR:N	2.29	0.47
2:B:285:SER:HB2	2:B:288:ARG:HG3	1.96	0.47
2:B:97:ASP:OD1	2:B:97:ASP:O	2.32	0.46
2:B:143:PRO:HD3	2:B:203:ILE:HD11	1.96	0.46
1:A:145:VAL:HG12	1:A:150:TRP:CG	2.51	0.46
2:B:69:PRO:O	2:B:155:LYS:HD3	2.15	0.46
2:B:88:LYS:NZ	2:B:90:THR:CG2	2.79	0.46
1:A:93:PRO:HG3	4:A:2018:HOH:O	2.14	0.46
2:B:193:THR:N	2:B:194:PRO:CD	2.79	0.45
1:A:63:TRP:CZ3	1:A:107:MET:CE	3.00	0.45
2:B:149:THR:CG2	2:B:153:THR:N	2.79	0.45
2:B:188:GLN:HB3	2:B:189:SER:HG	1.80	0.45
1:A:237:ILE:HG22	1:A:239:CYS:HB3	1.98	0.45
1:A:168:MET:C	1:A:170:GLU:H	2.24	0.45
1:A:173:GLU:O	1:A:177:ILE:HG13	2.15	0.45
1:A:9:GLU:O	1:A:9:GLU:HG3	2.17	0.45
2:B:214:PHE:CD1	2:B:214:PHE:N	2.84	0.45
2:B:223:LEU:CD2	2:B:227:PHE:CE1	2.99	0.45
2:B:227:PHE:CE2	2:B:233:PRO:CD	2.99	0.45
1:A:28:LEU:CD2	1:A:236:VAL:CG1	2.95	0.45
1:A:237:ILE:HG22	1:A:239:CYS:H	1.80	0.45
2:B:101:ARG:O	2:B:104:LEU:N	2.50	0.45
1:A:142:LEU:HD13	2:B:82:ARG:HD2	1.94	0.45
2:B:66:PHE:CD2	2:B:130:PHE:HE1	2.34	0.45
2:B:293:SER:O	2:B:295:LEU:HD12	2.16	0.45
2:B:235:GLU:HA	2:B:237:ASP:N	2.29	0.45
1:A:168:MET:HE1	1:A:208:VAL:HG11	1.99	0.45
1:A:6:LEU:N	1:A:6:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123[B]:LYS:NZ	4:A:2065:HOH:O	2.49	0.44
2:B:8:PRO:C	2:B:9:VAL:HG23	2.43	0.44
2:B:82:ARG:NH1	4:B:2030:HOH:O	2.30	0.44
1:A:28:LEU:HD21	1:A:236:VAL:CG1	2.44	0.44
2:B:51:ILE:O	2:B:55:ARG:HG3	2.17	0.44
2:B:62:ARG:O	2:B:62:ARG:HG2	2.18	0.44
1:A:167:LYS:HG2	4:A:2086:HOH:O	2.16	0.44
1:A:255:LEU:O	1:A:258:SER:HB2	2.18	0.44
2:B:111:GLY:CA	2:B:112:LEU:CB	2.95	0.44
2:B:96:VAL:CG1	2:B:147:LEU:HB3	2.48	0.44
2:B:209:ARG:HH22	2:B:229:LEU:HD11	1.83	0.43
2:B:127:GLY:O	2:B:130:PHE:HB3	2.18	0.43
2:B:187:LEU:HD23	2:B:188:GLN:N	2.33	0.43
1:A:112:LYS:NZ	2:B:49:LEU:O	2.52	0.43
1:A:149:LYS:HB2	3:A:1266:GOL:H32	1.99	0.43
2:B:111:GLY:HA3	2:B:112:LEU:CB	2.48	0.43
2:B:66:PHE:HB2	2:B:130:PHE:HZ	1.83	0.43
2:B:99:ASP:HA	2:B:147:LEU:HA	2.00	0.43
2:B:266:GLU:O	2:B:270:GLN:HG2	2.18	0.43
1:A:198:ASN:HA	1:A:199:PRO:HD3	1.79	0.43
2:B:174:VAL:HG12	2:B:174:VAL:O	2.17	0.43
2:B:212:PRO:HB2	2:B:215:CYS:SG	2.59	0.43
2:B:109:PRO:HA	2:B:110:PRO:HA	1.64	0.43
2:B:179:TRP:HB3	2:B:214:PHE:O	2.19	0.43
2:B:214:PHE:HA	2:B:225:LYS:CD	2.49	0.42
2:B:34:LEU:HD22	2:B:92:VAL:HG22	2.01	0.42
2:B:211:LYS:HA	2:B:212:PRO:HD2	1.84	0.42
2:B:267:SER:HA	2:B:270:GLN:HG2	2.01	0.42
1:A:78:PHE:HB3	1:A:79:PRO:HD3	2.01	0.42
1:A:153:ALA:HB3	4:B:2019:HOH:O	2.19	0.42
2:B:182:ALA:HB3	2:B:185:VAL:HG23	2.01	0.42
2:B:88:LYS:HZ3	2:B:90:THR:CG2	2.32	0.42
2:B:215:CYS:HB3	2:B:216:GLY:H	1.51	0.42
1:A:35:GLU:OE2	1:A:200:PRO:HD2	2.19	0.42
1:A:10:VAL:HG12	1:A:12:THR:H	1.84	0.42
2:B:40:PRO:O	2:B:50:PRO:HG3	2.19	0.42
2:B:71:VAL:HG21	2:B:131:LEU:CD1	2.50	0.42
2:B:233:PRO:HA	2:B:234:PRO:HD2	1.91	0.42
2:B:81:SER:OG	2:B:82:ARG:N	2.53	0.42
1:A:260:ARG:O	1:A:264:GLN:N	2.52	0.42
2:B:107:ALA:HA	2:B:108:PRO:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:THR:HA	2:B:191:TYR:CD2	2.54	0.42
2:B:39:VAL:O	2:B:86:GLU:HA	2.18	0.42
2:B:110:PRO:HD2	2:B:112:LEU:HD23	2.02	0.42
2:B:229:LEU:HD23	2:B:229:LEU:C	2.44	0.42
1:A:31:MET:HE3	1:A:159:ASP:HB3	2.02	0.41
2:B:217:ASN:CB	2:B:221:ASP:CB	2.97	0.41
2:B:11:GLU:HG3	2:B:19:THR:CG2	2.50	0.41
1:A:123[A]:LYS:HE3	1:A:123[A]:LYS:HB2	1.95	0.41
2:B:82:ARG:HG2	2:B:87:ILE:HG12	2.02	0.41
2:B:233:PRO:HG2	2:B:238:TRP:CZ3	2.55	0.41
2:B:261:VAL:N	2:B:262:PRO:CD	2.83	0.41
2:B:88:LYS:HZ3	2:B:90:THR:HG22	1.86	0.41
2:B:235:GLU:CD	2:B:235:GLU:N	2.78	0.41
2:B:111:GLY:CA	2:B:112:LEU:HB3	2.50	0.41
1:A:142:LEU:CD1	2:B:82:ARG:HD3	2.33	0.41
2:B:71:VAL:HG13	2:B:159:PHE:CZ	2.55	0.41
2:B:169:MET:O	2:B:173:PRO:O	2.38	0.41
1:A:62:THR:HG23	4:A:2026:HOH:O	2.21	0.41
1:A:76:GLU:C	1:A:79:PRO:HD2	2.46	0.41
1:A:124:LEU:O	1:A:128:THR:HG23	2.21	0.41
2:B:208:PHE:CE1	2:B:264:MET:HB3	2.55	0.41
2:B:219:GLU:O	2:B:223:LEU:HB2	2.21	0.41
2:B:124:PHE:CZ	2:B:141:LEU:HD21	2.56	0.41
2:B:5:ARG:NE	2:B:5:ARG:HA	2.35	0.40
2:B:51:ILE:CG2	2:B:55:ARG:CZ	2.99	0.40
2:B:215:CYS:N	2:B:225:LYS:HD3	2.31	0.40
2:B:232:LEU:HD12	2:B:233:PRO:CD	2.41	0.40
1:A:27:VAL:HG13	1:A:28:LEU:N	2.35	0.40
1:A:44:TYR:C	1:A:44:TYR:CD2	2.99	0.40
2:B:193:THR:CG2	2:B:194:PRO:CD	2.98	0.40
2:B:112:LEU:HD12	2:B:112:LEU:O	2.22	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	246/271 (91%)	239 (97%)	4 (2%)	3 (1%)	10	12
2	B	264/306 (86%)	222 (84%)	28 (11%)	14 (5%)	1	1
All	All	510/577 (88%)	461 (90%)	32 (6%)	17 (3%)	3	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	CYS
1	A	11	GLU
2	B	9	VAL
2	B	209	ARG
2	B	216	GLY
2	B	278	PHE
2	B	110	PRO
2	B	111	GLY
2	B	172	ASP
2	B	176	VAL
2	B	187	LEU
2	B	210	ARG
1	A	10	VAL
2	B	174	VAL
2	B	212	PRO
2	B	108	PRO
2	B	214	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	225/243 (93%)	214 (95%)	11 (5%)	22	34
2	B	232/265 (88%)	217 (94%)	15 (6%)	15	22
All	All	457/508 (90%)	431 (94%)	26 (6%)	19	27

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	12	THR
1	A	27	VAL
1	A	44	TYR
1	A	50	LYS
1	A	62	THR
1	A	65	LEU
1	A	89	LEU
1	A	116	THR
1	A	237	ILE
1	A	264	GLN
2	B	5	ARG
2	B	20	VAL
2	B	59	LEU
2	B	90	THR
2	B	112	LEU
2	B	120	LEU
2	B	131	LEU
2	B	136[A]	ILE
2	B	136[B]	ILE
2	B	139	ARG
2	B	154	VAL
2	B	178	LEU
2	B	179	TRP
2	B	186	LEU
2	B	213	LEU

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

Mol	Chain	Res	Type
1	A	71	GLN
1	A	139	GLN
1	A	158	HIS
1	A	183	GLN
1	A	213	GLN
1	A	261	GLN
2	B	27	HIS
2	B	30	HIS
2	B	98	GLN
2	B	123	GLN
2	B	145	ASN

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Mol	Chain	Res	Type
2	B	279	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
3	GOL	A	1266	-	5,5,5	0.31	0	5,5,5	0.30	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
3	GOL	A	1266	-	-	0/4/4/4	-

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1266	GOL	3	0

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	249/271 (91%)	0.29	10 (4%)	42 44	25, 44, 97, 163	1 (0%)
2	B	267/306 (87%)	1.14	42 (15%)	5 6	35, 77, 125, 140	1 (0%)
All	All	516/577 (89%)	0.73	52 (10%)	12 14	25, 58, 121, 163	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	174	VAL	4.4
2	B	261	VAL	4.2
2	B	238	TRP	4.0
2	B	175	VAL	4.0
2	B	209	ARG	3.9
2	B	295	LEU	3.8
1	A	10	VAL	3.7
1	A	6	LEU	3.6
2	B	9	VAL	3.6
1	A	259	LEU	3.4
1	A	13	ILE	3.4
2	B	220	ALA	3.4
2	B	172	ASP	3.3
2	B	226	ILE	3.2
2	B	10	ALA	3.2
2	B	262	PRO	3.2
2	B	230	ILE	3.2
1	A	262	ALA	3.1
2	B	112	LEU	3.0
2	B	173	PRO	3.0
2	B	223	LEU	2.8
2	B	188	GLN	2.7
1	A	12	THR	2.7
2	B	103	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	257	SER	2.6
2	B	12	ILE	2.6
2	B	234	PRO	2.6
2	B	191	TYR	2.6
1	A	263	GLN	2.5
1	A	256	GLU	2.5
2	B	236	ASP	2.5
2	B	268	GLY	2.5
2	B	278	PHE	2.5
2	B	14	VAL	2.5
2	B	176	VAL	2.5
2	B	82	ARG	2.4
2	B	66	PHE	2.4
2	B	227	PHE	2.4
2	B	267	SER	2.3
2	B	179	TRP	2.3
2	B	192	ALA	2.2
2	B	185	VAL	2.2
2	B	269	ALA	2.2
2	B	183	PRO	2.2
1	A	28	LEU	2.1
2	B	232	LEU	2.1
2	B	273	LEU	2.1
2	B	205	ALA	2.1
2	B	26	PRO	2.1
2	B	178	LEU	2.0
2	B	8	PRO	2.0
2	B	24	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum,

median, 95th 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1266	6/6	0.88	0.13	59,62,63,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.