



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:33 AM UTC

PDB ID : 8BYA / pdb_00008bya
EMDB ID : EMD-16325
Title : Cryo-EM structure of SKP1-SKP2-CKS1-CDK2-CyclinA-p27KIP1 Complex
Authors : Rowland, R.J.; Salamina, M.; Endicott, J.A.; Noble, M.E.
Deposited on : 2022-12-12
Resolution : 3.38 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

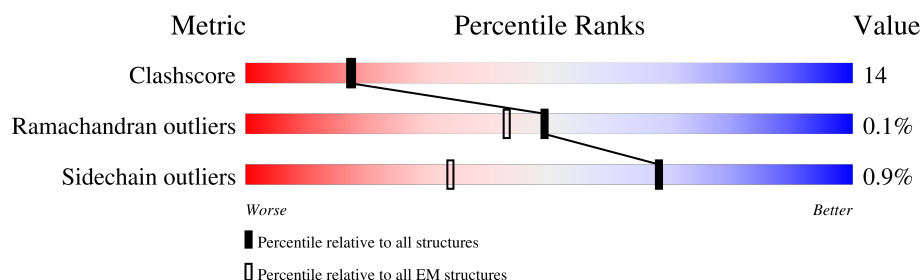
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	298	71% 22% 7%
2	B	432	46% 13% 41%
3	C	158	38% 6% 56%
4	D	163	67% 17% • 15%
5	E	424	56% 20% • 23%
6	F	79	62% 23% • 13%
7	G	10	60% 30% 10%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8389 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	277	Total	C	N	O	P	S	0	0
			2025	1322	340	358	1	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	TPO	TYR	conflict	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	257	Total	C	N	O	S		0	0
			1871	1216	309	338	8			

- Molecule 3 is a protein called Cyclin-dependent kinase inhibitor 1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	69	Total	C	N	O	S		0	0
			499	325	87	86	1			

- Molecule 4 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	138	Total	C	N	O	S		0	0
			855	535	152	164	4			

- Molecule 5 is a protein called S-phase kinase-associated protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	325	Total	C	N	O	S		0	0
			2481	1574	431	461	15			

- Molecule 6 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	69	Total	C	N	O	S	0	0
			589	382	102	102	3		

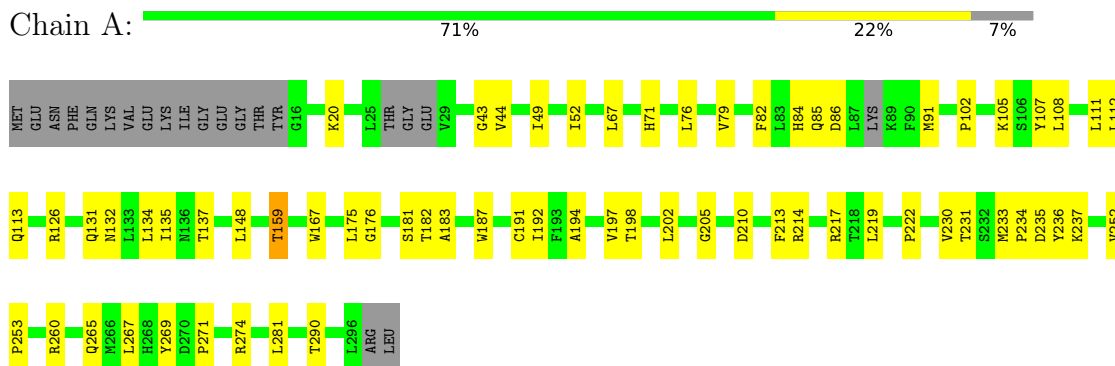
- Molecule 7 is a protein called p27 KIP1 C-terminus.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	10	Total	C	N	O	P	0	0
			69	38	11	19	1		

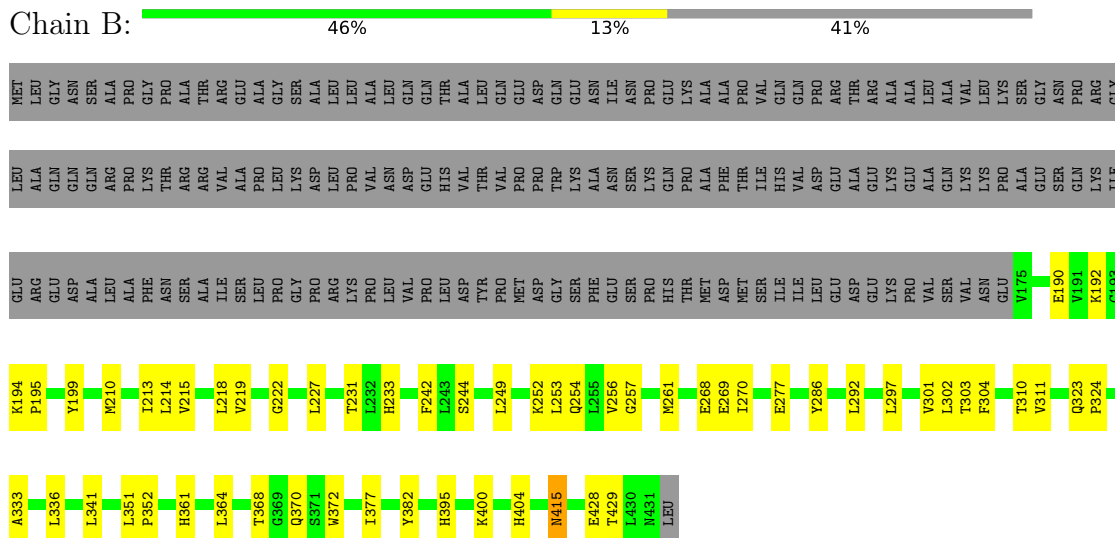
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

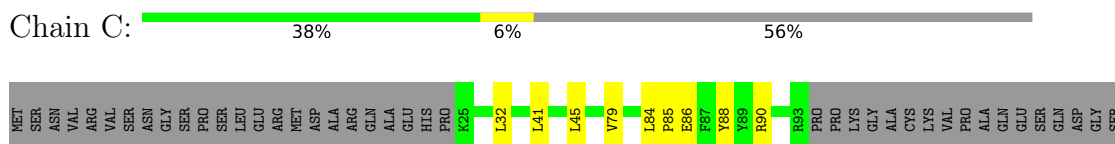
• Molecule 1: Cyclin-dependent kinase 2



• Molecule 2: Cyclin-A2



• Molecule 3: Cyclin-dependent kinase inhibitor 1B



GLY SER ARG PRO ALA PRO LEU ILE GLY ALA PRO ASP ASN SER GLU ASP THR HIS LEU VAL ASP PRO THR LYS ASP PRO SER ASP SER GLN THR GLY LEU ALA GLN CYS ALA GLY TLE ARG LYS ARG PRO ALA THR ASP

• Molecule 4: S-phase kinase-associated protein 1

Chain D:  67% 17% 15%

MET P1002 S1009 V1025 T1029 M1030 L1031 GLU ASP LEU GLY MET ASP ASP GLU P1041 P1044 V1045 P1048 M1051 I1054 L1055 V1058 H1064 HIS LYS ASP ASP PRO PRO PRO PRO GLU ASP ASP ASP ASN LYS E1079 K1080 R1081 T1082 D1083 D1084 I1085 D1089 G1114

V1118 N1126 M1126 I1127 K1128 P1132 E1133 I1135 R1136 F1139 E1147 E1148 M1157 E1162 LYS

• Molecule 5: S-phase kinase-associated protein 2

Chain E:  56% 20% 23%

MET HIS ARG LYS HIS LEU GLN GLU ILE PRO ASP LEU SER SER ASN VAL ASP THR SER PHE THR TRP GLY TRP ASP SER SER LYS THR SER GLU LEU LEU SER GLY MET GLY VAL SER ALA PRO TLE LEU LEU LYS GLU PRO ASP SER ASN TLE PRO GLN GLU LEU LEU SER ASN LEU GLY

HIS PRO GLU SER M1126 I1127 K1128 P1132 E1133 I1135 R1136 F1139 E1147 E1148 M1157 E1162 LYS

D2133 L2136 W2137 Q2138 T2139 L2140 D2141 N2146 L2147 H2148 P2149 L2155 R2161 C2165 P2167 Q2172 V2183 N2190 I2193 E2194 T2197 N2210 L2218 S2219 D2220 P2221 I2222 V2223 F2243 L2248 L2252 L2258 L2261 W2265 F2269 T2270 E2271 A2277 V2278

V2281 S2282 E2283 L2288 Y2293 R2294 L2297 L2302 V2306 R2307 R2308 L2312 L2315 D2316 L2317 S2318 V2321 F2332 L2337 L2340 R2344 C2345 L2348 T2352 E2355 E2358 L2362 L2365 T2395 I2401 N2406 Q2407 E2408 L2409 W2410 C2414

Q2419 LYS PRO SER CYS LEU

• Molecule 6: Cyclin-dependent kinases regulatory subunit 1

Chain F:  62% 23% 13%

MET SER HIS LYS Q3005 Y3008 Y3012 D3013 D3014 E3015 R3020 H3021 L3024 P3025 K3026 D3027 I3028 A3029 T3035 H3036 L3037 S3041 Q3049 Y3057 M3058 I3059 H3060 L3068 L3073 PRO LYS LYS PRO LYS

• Molecule 7: p27 KIP1 C-terminus

Chain G:  60% 30% 10%

K4181 E4185 Q4186 T4187 P4188 K4189 K4190

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	136325	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/2065	0.54	0/2826
2	B	0.28	0/1918	0.53	0/2632
3	C	0.33	0/517	0.48	0/711
4	D	0.32	0/864	0.56	0/1192
5	E	0.26	0/2530	0.47	0/3449
6	F	0.32	0/609	0.56	1/825 (0.1%)
7	G	0.28	0/57	0.60	0/73
All	All	0.29	0/8560	0.52	1/11708 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	3028	ILE	N-CA-C	-5.96	107.69	113.53

There are no chirality outliers.

There are no planarity outliers.

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	2025	0	1885	71	0
2	B	1871	0	1709	47	0
3	C	499	0	399	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	855	0	656	20	0
5	E	2481	0	2422	70	0
6	F	589	0	561	18	0
7	G	69	0	52	4	0
All	All	8389	0	7684	220	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 14.

All (220) 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)
5:E:2105:LEU:HD11	5:E:2130:LEU:CD1	1.43	1.44
5:E:2105:LEU:HD11	5:E:2130:LEU:HD13	1.15	1.15
2:B:218:LEU:HD22	2:B:261:MET:HE2	1.30	1.11
1:A:85:GLN:OE1	1:A:107:TYR:CE2	2.05	1.09
5:E:2105:LEU:HD11	5:E:2130:LEU:HD11	1.32	1.08
1:A:85:GLN:OE1	1:A:107:TYR:HE2	1.36	1.07
1:A:86:ASP:OD1	1:A:134:LEU:HD23	1.51	1.06
5:E:2105:LEU:CD1	5:E:2130:LEU:CD1	2.39	0.99
4:D:1045:VAL:HG13	4:D:1048:PRO:HD2	1.44	0.98
1:A:84:HIS:CE1	1:A:137:THR:HG23	1.99	0.97
1:A:85:GLN:NE2	1:A:107:TYR:OH	1.98	0.95
6:F:3008:TYR:HB3	6:F:3020:ARG:HH22	1.34	0.93
1:A:86:ASP:OD1	1:A:134:LEU:CD2	2.18	0.92
1:A:84:HIS:HE1	1:A:137:THR:HG23	1.33	0.90
2:B:302:LEU:O	2:B:303:THR:HG22	1.71	0.90
5:E:2105:LEU:CD1	5:E:2130:LEU:HD13	2.02	0.88
5:E:2105:LEU:CD1	5:E:2130:LEU:CD2	2.56	0.84
1:A:86:ASP:OD2	3:C:85:PRO:HB3	1.81	0.80
1:A:84:HIS:CE1	1:A:137:THR:CG2	2.64	0.79
6:F:3014:ASP:OD1	6:F:3015:GLU:N	2.16	0.79
4:D:1125:ASN:HA	4:D:1128:LYS:HG2	1.64	0.78
1:A:222:PRO:HB2	1:A:230:VAL:HG21	1.67	0.76
5:E:2105:LEU:CD1	5:E:2130:LEU:HD11	2.12	0.74
4:D:1045:VAL:HG13	4:D:1048:PRO:CD	2.17	0.72
1:A:235:ASP:OD1	6:F:3060:HIS:NE2	2.23	0.71
4:D:1128:LYS:HE3	5:E:2112:LEU:HD23	1.72	0.71
1:A:85:GLN:OE1	1:A:107:TYR:CZ	2.44	0.70
1:A:231:THR:HA	1:A:236:TYR:CD2	2.27	0.69
2:B:302:LEU:O	2:B:303:THR:CG2	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2252:LEU:HD12	5:E:2281:VAL:HA	1.74	0.68
1:A:132:ASN:HD22	3:C:90:ARG:HH12	1.38	0.68
5:E:2105:LEU:CD1	5:E:2130:LEU:HD22	2.22	0.68
5:E:2149:PRO:HG3	5:E:2172:GLN:HB3	1.78	0.66
1:A:85:GLN:CD	1:A:107:TYR:HH	2.04	0.65
1:A:183:ALA:HB1	1:A:274:ARG:HD2	1.78	0.65
5:E:2131:ALA:O	5:E:2136:LEU:HD12	1.95	0.65
1:A:85:GLN:CD	1:A:107:TYR:OH	2.38	0.65
1:A:210:ASP:O	1:A:214:ARG:HG3	1.96	0.65
5:E:2146:ASN:OD1	5:E:2147:LEU:N	2.28	0.65
3:C:79:VAL:HB	3:C:84:LEU:HD11	1.78	0.65
2:B:199:TYR:HB3	2:B:244:SER:HA	1.79	0.65
1:A:85:GLN:NE2	1:A:107:TYR:HH	1.92	0.65
1:A:102:PRO:HA	1:A:105:LYS:HD2	1.80	0.64
2:B:194:LYS:HZ3	2:B:352:PRO:HD3	1.63	0.64
4:D:1114:GLY:O	4:D:1118:VAL:HG23	1.97	0.64
1:A:43:GLY:HA2	2:B:292:LEU:HD11	1.80	0.63
5:E:2167:ARG:NH2	6:F:3035:THR:O	2.32	0.63
5:E:2105:LEU:HD12	5:E:2130:LEU:HD21	1.80	0.63
2:B:333:ALA:HA	2:B:336:LEU:HD12	1.81	0.62
6:F:3008:TYR:HB3	6:F:3020:ARG:NH2	2.12	0.62
2:B:210:MET:O	2:B:213:ILE:HG22	1.99	0.62
5:E:2105:LEU:HD21	5:E:2126:ARG:HH12	1.64	0.62
5:E:2105:LEU:HD13	5:E:2130:LEU:HD22	1.82	0.62
1:A:233:MET:CB	1:A:236:TYR:HB2	2.30	0.61
1:A:175:LEU:HA	1:A:235:ASP:HB3	1.83	0.61
1:A:252:VAL:HG13	1:A:253:PRO:HD3	1.81	0.61
1:A:260:ARG:O	1:A:265:GLN:NE2	2.33	0.61
1:A:84:HIS:NE2	1:A:137:THR:HG22	2.16	0.60
1:A:52:ILE:HD13	2:B:304:PHE:HD2	1.66	0.60
1:A:85:GLN:OE1	1:A:107:TYR:OH	2.20	0.60
2:B:213:ILE:HG23	3:C:32:LEU:HD11	1.83	0.60
2:B:218:LEU:CD2	2:B:261:MET:HE2	2.21	0.59
2:B:215:VAL:O	2:B:219:VAL:HG23	2.02	0.59
6:F:3012:TYR:OH	6:F:3021:HIS:NE2	2.32	0.59
5:E:2223:VAL:HG21	5:E:2243:PHE:HB3	1.83	0.59
5:E:2408:GLU:N	5:E:2408:GLU:OE1	2.35	0.59
5:E:2248:LEU:HD21	5:E:2277:ALA:HB2	1.85	0.59
5:E:2105:LEU:HD11	5:E:2130:LEU:CG	2.29	0.58
1:A:176:GLY:O	1:A:234:PRO:HG2	2.04	0.58
2:B:190:GLU:OE2	2:B:190:GLU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2105:LEU:CD1	5:E:2130:LEU:HD21	2.30	0.58
1:A:85:GLN:NE2	1:A:135:ILE:HG22	2.18	0.58
2:B:253:LEU:HA	2:B:256:VAL:HG12	1.85	0.58
5:E:2337:LEU:HD21	5:E:2340:LEU:HB2	1.85	0.58
1:A:82:PHE:HD1	3:C:88:TYR:HE1	1.51	0.57
4:D:1051:ASN:O	4:D:1055:LEU:HG	2.05	0.56
5:E:2316:ASP:OD1	5:E:2318:SER:OG	2.24	0.56
6:F:3008:TYR:HD2	6:F:3020:ARG:HH12	1.54	0.55
5:E:2123:VAL:C	5:E:2125:LYS:N	2.60	0.55
5:E:2265:TRP:NE1	6:F:3041:SER:OG	2.32	0.55
1:A:237:LYS:HD2	6:F:3058:MET:HE3	1.87	0.55
3:C:41:LEU:O	3:C:45:LEU:HG	2.07	0.55
5:E:2123:VAL:HG23	5:E:2127:TRP:CG	2.40	0.55
1:A:85:GLN:HB3	1:A:135:ILE:O	2.08	0.54
2:B:222:GLY:HA2	2:B:227:LEU:HD12	1.89	0.54
2:B:429:THR:HG22	2:B:429:THR:O	2.07	0.54
2:B:323:GLN:HG2	2:B:324:PRO:HD2	1.90	0.54
5:E:2123:VAL:C	5:E:2125:LYS:H	2.14	0.54
5:E:2105:LEU:CD2	5:E:2126:ARG:HH12	2.20	0.54
1:A:260:ARG:HB3	1:A:265:GLN:HE21	1.73	0.54
5:E:2117:LEU:HA	5:E:2120:VAL:HB	1.90	0.53
7:G:4185:GLU:N	7:G:4185:GLU:OE1	2.42	0.53
1:A:182:THR:HG22	1:A:183:ALA:H	1.72	0.53
1:A:194:ALA:HA	1:A:197:VAL:HG12	1.90	0.53
2:B:368:THR:HG23	2:B:370:GLN:H	1.74	0.52
4:D:1132:PRO:HA	4:D:1135:ILE:HB	1.92	0.52
5:E:2139:THR:HB	5:E:2414:CYS:HA	1.92	0.52
5:E:2105:LEU:HD11	5:E:2130:LEU:CD2	2.35	0.52
4:D:1157:ASN:N	4:D:1157:ASN:HD22	2.07	0.52
2:B:302:LEU:C	2:B:303:THR:HG22	2.35	0.52
5:E:2281:VAL:O	5:E:2308:ARG:NH2	2.43	0.52
2:B:277:GLU:N	2:B:277:GLU:OE2	2.43	0.51
2:B:297:LEU:O	2:B:301:VAL:HG22	2.10	0.51
7:G:4186:GLN:HG3	7:G:4186:GLN:O	2.10	0.51
2:B:253:LEU:HD21	3:C:32:LEU:HD22	1.91	0.51
1:A:235:ASP:OD1	6:F:3060:HIS:CD2	2.64	0.51
2:B:254:GLN:HG2	2:B:286:TYR:HE2	1.76	0.51
1:A:235:ASP:CG	6:F:3060:HIS:HE2	2.19	0.50
4:D:1054:ILE:O	4:D:1058:VAL:HG23	2.12	0.50
2:B:231:THR:HG22	2:B:268:GLU:HB3	1.94	0.50
5:E:2218:LEU:HD22	5:E:2222:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1132:PRO:O	4:D:1136:ARG:HG2	2.12	0.50
2:B:254:GLN:HG2	2:B:286:TYR:CE2	2.47	0.50
5:E:2161:ILE:HA	5:E:2183:VAL:HA	1.94	0.50
6:F:3005:GLN:HB3	6:F:3025:PRO:HB3	1.93	0.49
2:B:214:LEU:HD11	2:B:257:GLY:HA3	1.94	0.49
5:E:2193:ILE:HG22	5:E:2197:THR:HG23	1.94	0.49
5:E:2406:ASN:HB3	5:E:2408:GLU:OE1	2.12	0.49
5:E:2293:TYR:HB2	5:E:2297:LEU:HD12	1.95	0.49
4:D:1126:MET:HE1	4:D:1139:PHE:CZ	2.47	0.49
1:A:85:GLN:OE1	1:A:91:MET:HE2	2.13	0.49
5:E:2130:LEU:O	5:E:2130:LEU:HD23	2.13	0.48
5:E:2362:LEU:HD21	5:E:2365:LEU:HD13	1.94	0.48
5:E:2105:LEU:HA	5:E:2108:ILE:HG12	1.95	0.48
2:B:249:LEU:H	2:B:252:LYS:HD3	1.78	0.48
1:A:219:LEU:HD21	1:A:267:LEU:HB2	1.96	0.48
1:A:187:TRP:CZ2	1:A:192:ILE:HD11	2.48	0.48
1:A:20:LYS:HD2	1:A:82:PHE:CE1	2.49	0.48
4:D:1009:SER:HB3	4:D:1044:PRO:HD2	1.96	0.48
1:A:205:GLY:HA2	1:A:214:ARG:HD2	1.96	0.48
5:E:2294:ARG:HG2	5:E:2321:VAL:HG13	1.96	0.48
5:E:2124:CYS:SG	5:E:2124:CYS:O	2.72	0.47
1:A:20:LYS:HD2	1:A:82:PHE:CZ	2.49	0.47
1:A:252:VAL:CG1	1:A:253:PRO:HD3	2.45	0.47
2:B:194:LYS:NZ	2:B:352:PRO:HD3	2.29	0.47
2:B:395:HIS:NE2	2:B:428:GLU:HA	2.30	0.47
4:D:1085:ILE:HG12	4:D:1118:VAL:HG13	1.97	0.47
5:E:2395:THR:HB	5:E:2401:ILE:HD13	1.97	0.47
1:A:84:HIS:NE2	1:A:137:THR:CG2	2.77	0.47
2:B:242:PHE:CD2	2:B:301:VAL:HG21	2.50	0.47
5:E:2131:ALA:C	5:E:2133:ASP:H	2.23	0.47
6:F:3024:LEU:HD22	6:F:3028:ILE:HB	1.97	0.46
1:A:197:VAL:HG13	1:A:198:THR:HG23	1.97	0.46
5:E:2302:LEU:O	5:E:2306:VAL:HG22	2.15	0.46
5:E:2104:LEU:O	5:E:2108:ILE:HG23	2.14	0.46
2:B:218:LEU:HD22	2:B:261:MET:CE	2.21	0.46
2:B:310:THR:OG1	2:B:311:VAL:N	2.47	0.46
4:D:1025:VAL:O	4:D:1029:THR:HG23	2.14	0.46
1:A:67:LEU:HB2	1:A:79:VAL:HG23	1.98	0.46
1:A:175:LEU:HD23	1:A:235:ASP:OD2	2.15	0.46
1:A:290:THR:O	1:A:290:THR:OG1	2.33	0.46
5:E:2258:LEU:HD23	5:E:2261:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1127:ILE:O	4:D:1128:LYS:C	2.59	0.46
1:A:167:TRP:N	1:A:167:TRP:CD1	2.82	0.45
1:A:187:TRP:HA	1:A:191:CYS:HB2	1.99	0.45
4:D:1139:PHE:HE2	5:E:2095:VAL:HB	1.82	0.45
2:B:192:LYS:H	2:B:192:LYS:HG2	1.43	0.45
1:A:108:LEU:HG	1:A:112:LEU:HD12	1.98	0.45
1:A:126:ARG:HD2	1:A:148:LEU:HB3	1.97	0.45
6:F:3057:TYR:CE1	6:F:3068:LEU:HB3	2.52	0.45
1:A:213:PHE:O	1:A:217:ARG:HG3	2.17	0.45
5:E:2337:LEU:HD11	5:E:2340:LEU:HB2	1.99	0.45
5:E:2194:GLU:HB3	5:E:2197:THR:HG22	1.98	0.45
1:A:230:VAL:HG22	1:A:236:TYR:CE1	2.52	0.45
4:D:1081:ARG:HH12	4:D:1083:ASP:HB2	1.82	0.45
5:E:2190:ASN:ND2	6:F:3037:LEU:HD11	2.32	0.45
1:A:84:HIS:CG	1:A:85:GLN:H	2.35	0.44
1:A:181:SER:OG	1:A:182:THR:N	2.42	0.44
5:E:2332:PHE:HZ	5:E:2358:GLU:CB	2.31	0.44
2:B:194:LYS:HE3	2:B:351:LEU:HD23	1.99	0.44
5:E:2278:VAL:O	5:E:2308:ARG:NH1	2.51	0.44
2:B:194:LYS:HZ1	2:B:351:LEU:HA	1.82	0.44
1:A:159:TPO:HG22	2:B:270:ILE:HG21	1.99	0.43
2:B:194:LYS:HD3	2:B:195:PRO:HD2	2.00	0.43
2:B:233:HIS:CD2	2:B:341:LEU:HD11	2.53	0.43
1:A:269:TYR:O	1:A:271:PRO:HD3	2.18	0.43
5:E:2243:PHE:HE2	5:E:2269:PHE:CE1	2.37	0.43
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.83	0.43
5:E:2123:VAL:HG12	5:E:2125:LYS:CB	2.49	0.43
5:E:2114:LEU:O	5:E:2118:LEU:HG	2.19	0.43
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.87	0.42
3:C:88:TYR:N	3:C:88:TYR:CD2	2.86	0.42
6:F:3026:LYS:HA	6:F:3029:ALA:HB3	2.02	0.42
2:B:231:THR:HG21	2:B:269:GLU:HG2	2.02	0.42
5:E:2261:LEU:HB3	5:E:2288:LEU:HD12	2.01	0.42
6:F:3008:TYR:HD2	6:F:3020:ARG:NH1	2.18	0.42
1:A:71:HIS:HA	1:A:76:LEU:HD12	2.01	0.42
1:A:131:GLN:HE22	3:C:86:GLU:CB	2.33	0.42
5:E:2345:CYS:HB2	5:E:2348:ILE:HG13	2.01	0.42
2:B:400:LYS:O	2:B:404:HIS:N	2.48	0.42
2:B:415:ASN:OD1	2:B:415:ASN:N	2.52	0.42
5:E:2106:LEU:HD23	5:E:2106:LEU:HA	1.92	0.42
5:E:2132:SER:HA	5:E:2137:TRP:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:HIS:O	1:A:85:GLN:C	2.63	0.41
5:E:2243:PHE:HE2	5:E:2269:PHE:HE1	1.66	0.41
5:E:2352:THR:O	5:E:2355:GLU:HB3	2.20	0.41
6:F:3049:GLN:O	7:G:4188:PRO:HD3	2.20	0.41
1:A:44:VAL:HG21	1:A:49:ILE:HD11	2.01	0.41
1:A:84:HIS:CG	1:A:85:GLN:N	2.87	0.41
1:A:113:GLN:HG2	1:A:281:LEU:HD21	2.03	0.41
5:E:2141:ASP:HB2	5:E:2414:CYS:HB2	2.02	0.41
4:D:1147:GLU:O	4:D:1148:GLU:HG3	2.20	0.41
2:B:253:LEU:HD23	2:B:254:GLN:N	2.36	0.41
2:B:364:LEU:HD23	2:B:364:LEU:HA	1.91	0.41
2:B:253:LEU:HD23	2:B:254:GLN:H	1.84	0.41
2:B:361:HIS:HB2	2:B:372:TRP:CE3	2.55	0.41
1:A:182:THR:HG22	1:A:183:ALA:N	2.35	0.41
5:E:2165:CYS:N	5:E:2166:PRO:HD3	2.36	0.41
4:D:1089:ASP:HB3	4:D:1118:VAL:HG11	2.03	0.41
2:B:377:ILE:HD13	2:B:382:TYR:O	2.21	0.40
5:E:2220:ASP:HB2	5:E:2221:PRO:HD3	2.04	0.40
1:A:82:PHE:HD1	3:C:88:TYR:CE1	2.36	0.40
2:B:252:LYS:HE2	2:B:252:LYS:HB2	1.83	0.40
5:E:2140:LEU:HD21	5:E:2155:LEU:HD13	2.02	0.40
4:D:1133:GLU:HA	4:D:1136:ARG:CZ	2.52	0.40
5:E:2270:THR:HG22	5:E:2271:GLU:H	1.86	0.40
7:G:4187:TPO:HA	7:G:4188:PRO:HD3	1.75	0.40
1:A:107:TYR:CZ	1:A:135:ILE:HG21	2.57	0.40
5:E:2210:ASN:HB3	5:E:2410:TRP:CZ3	2.57	0.40
5:E:2312:LEU:HD22	5:E:2315:LEU:HD22	2.02	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 PDB entries followed by that with respect to all EM entries.

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	270/298 (91%)	250 (93%)	20 (7%)	0	100	100
2	B	255/432 (59%)	251 (98%)	4 (2%)	0	100	100
3	C	67/158 (42%)	64 (96%)	3 (4%)	0	100	100
4	D	132/163 (81%)	125 (95%)	7 (5%)	0	100	100
5	E	323/424 (76%)	305 (94%)	17 (5%)	1 (0%)	36	64
6	F	67/79 (85%)	62 (92%)	5 (8%)	0	100	100
7	G	7/10 (70%)	6 (86%)	1 (14%)	0	100	100
All	All	1121/1564 (72%)	1063 (95%)	57 (5%)	1 (0%)	49	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	2132	SER

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 PDB entries followed by that with respect to all EM entries.

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	186/262 (71%)	186 (100%)	0	100	100
2	B	172/378 (46%)	171 (99%)	1 (1%)	78	80
3	C	39/135 (29%)	39 (100%)	0	100	100
4	D	56/150 (37%)	55 (98%)	1 (2%)	51	67
5	E	276/392 (70%)	272 (99%)	4 (1%)	59	70
6	F	63/76 (83%)	62 (98%)	1 (2%)	55	68
7	G	5/7 (71%)	5 (100%)	0	100	100
All	All	797/1400 (57%)	790 (99%)	7 (1%)	68	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	415	ASN

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Mol	Chain	Res	Type
4	D	1128	LYS
5	E	2120	VAL
5	E	2283	GLU
5	E	2332	PHE
5	E	2344	ARG
6	F	3041	SER

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

Mol	Chain	Res	Type
1	A	85	GLN
1	A	132	ASN
2	B	228	GLN
2	B	321	HIS
4	D	1157	ASN
5	E	2172	GLN
5	E	2296	ASN
6	F	3052	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
7	TPO	G	4187	7	8,10,11	0.65	0	10,14,16	1.24	2 (20%)
1	TPO	A	159	1	8,10,11	0.88	0	10,14,16	0.98	1 (10%)

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
7	TPO	G	4187	7	-	1/9/11/13	-
1	TPO	A	159	1	-	4/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	TPO	O-C-CA	-2.47	118.41	124.77
7	G	4187	TPO	O-C-CA	-2.41	118.58	124.77
7	G	4187	TPO	P-OG1-CB	-2.21	117.32	123.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	159	TPO	N-CA-CB-OG1
1	A	159	TPO	C-CA-CB-CG2
1	A	159	TPO	O-C-CA-CB
1	A	159	TPO	N-CA-CB-CG2
7	G	4187	TPO	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	4187	TPO	1	0
1	A	159	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-16325. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.