



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:47 PM UTC

PDB ID : 2ZXX / pdb_00002zxx
Title : Crystal structure of Cdt1/geminin complex
Authors : Cho, Y.; Lee, C.; Hong, B.S.; Choi, J.M.
Deposited on : 2009-01-08
Resolution : 2.80 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:

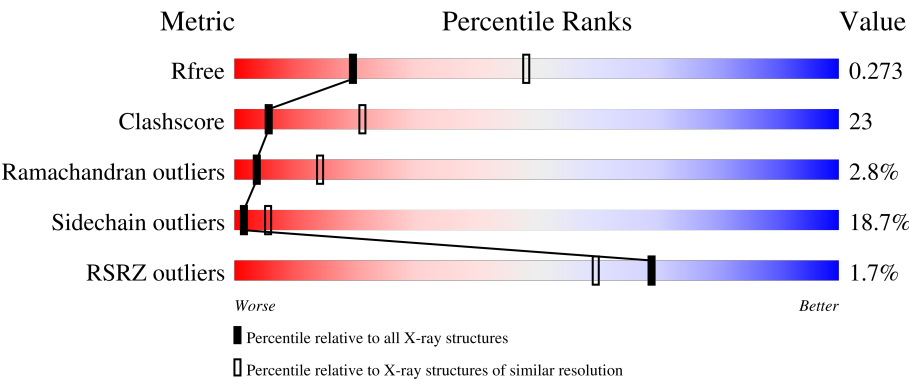
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	79	43%32%13%11% %
1	B	79	3%52%41%5% 3%
1	D	79	43%32%8%18%
1	E	79	4%61%34% 4%
2	C	197	2%44%39%11%6% 2%

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Mol	Chain	Length	Quality of chain
2	F	197	% 41% 43% 7% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5476 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 Geminin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	70	Total	C	N	O	Se	0	0	0
			590	365	107	117	1			
1	B	78	Total	C	N	O	Se	0	0	0
			653	406	115	131	1			
1	D	65	Total	C	N	O	Se	0	0	0
			551	342	100	108	1			
1	E	78	Total	C	N	O	Se	0	0	0
			653	406	115	131	1			

- Molecule 2 is a protein called DNA replication factor Cdt1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	185	Total	C	N	O	S	Se	0	0
			1512	962	271	271	2	6		
2	F	184	Total	C	N	O	S	Se	0	0
			1508	960	270	270	2	6		

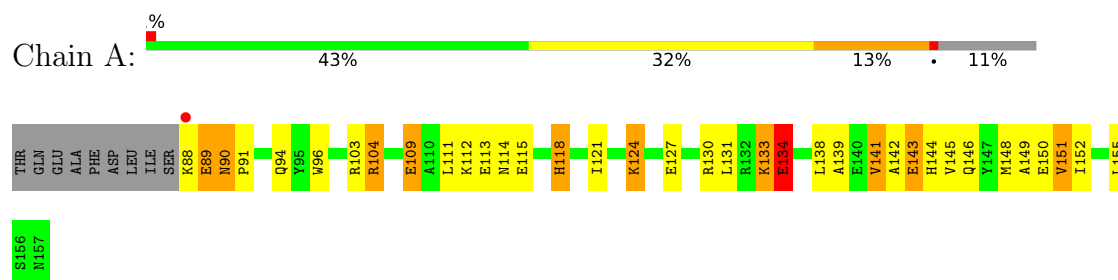
- Molecule 3 is water.

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

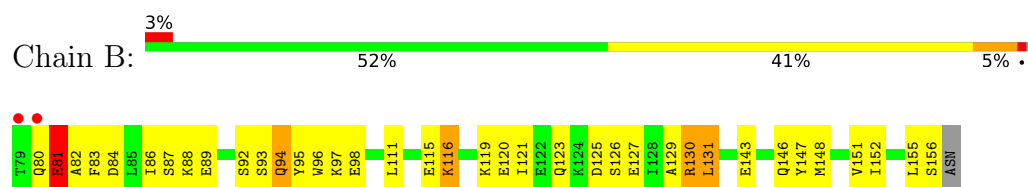
3 Residue-property plots

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 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.

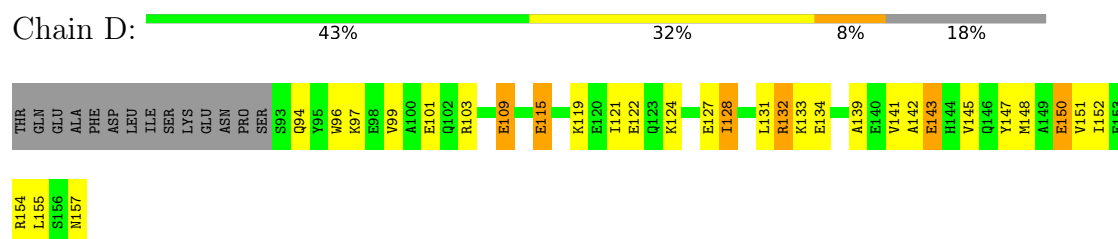
• Molecule 1: Geminin



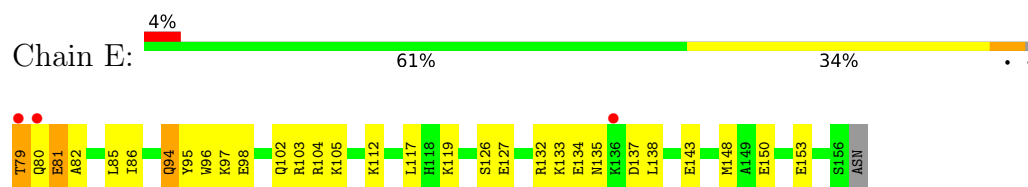
• Molecule 1: Geminin



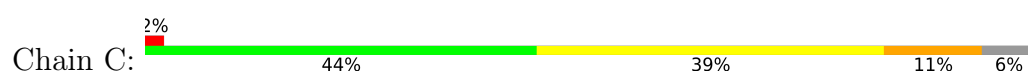
• Molecule 1: Geminin

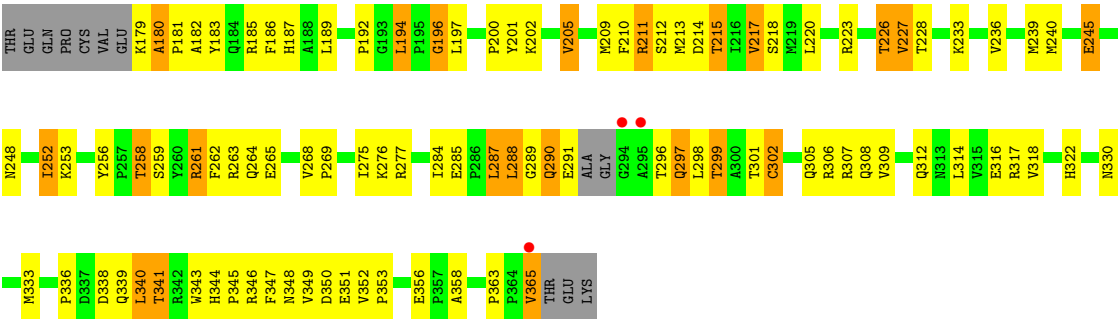


• Molecule 1: Geminin

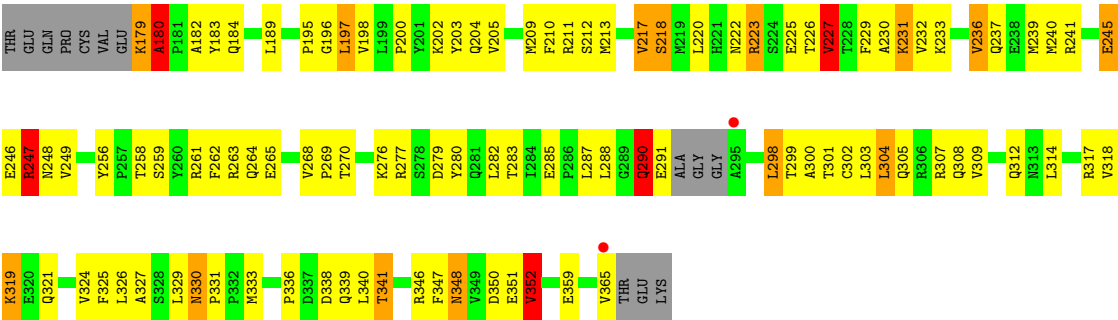


• Molecule 2: DNA replication factor Cdt1





● Molecule 2: DNA replication factor Cdt1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.77Å 94.33Å 115.57Å 90.00° 103.66° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.00-2.80) 95.2 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.277 0.231 , 0.273	Depositor DCC
R_{free} test set	1437 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5476	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% 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	0.74	0/596	0.92	0/794
1	B	0.85	0/660	0.98	0/881
1	D	0.81	0/556	0.99	2/740 (0.3%)
1	E	0.84	0/660	1.00	0/881
2	C	0.87	0/1541	1.07	2/2078 (0.1%)
2	F	0.86	0/1537	1.08	6/2073 (0.3%)
All	All	0.84	0/5550	1.03	10/7447 (0.1%)

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	C	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	119	LYS	N-CA-C	-6.17	104.47	111.07
1	D	115	GLU	N-CA-C	-5.36	105.36	111.14
2	C	285	GLU	CA-C-N	5.29	126.74	120.23
2	C	285	GLU	C-N-CA	5.29	126.74	120.23
2	F	352	VAL	N-CA-C	5.20	120.11	108.88
2	F	226	THR	CA-C-N	-5.15	116.56	122.95
2	F	226	THR	C-N-CA	-5.15	116.56	122.95
2	F	180	ALA	CA-C-N	5.10	125.09	119.89
2	F	180	ALA	C-N-CA	5.10	125.09	119.89
2	F	227	VAL	N-CA-C	5.07	114.59	106.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	330	ASN	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	590	0	586	30	0
1	B	653	0	646	30	0
1	D	551	0	549	28	0
1	E	653	0	646	28	0
2	C	1512	0	1526	93	0
2	F	1508	0	1523	88	0
3	C	6	0	0	2	0
3	F	3	0	0	0	0
All	All	5476	0	5476	256	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 23.

All (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:GLU:OE2	2:F:346:ARG:HD3	1.30	1.23
2:F:209:MSE:HG2	2:F:240:MSE:HE1	1.25	1.14
1:D:147:TYR:CE1	1:D:148:MSE:HE3	1.82	1.12
2:C:290:GLN:HG3	2:C:291:GLU:H	1.16	1.10
1:E:80:GLN:HE22	1:E:94:GLN:HB3	1.19	1.06
2:C:211:ARG:O	2:C:215:THR:HG22	1.60	1.00
2:F:209:MSE:CG	2:F:240:MSE:HE1	1.90	1.00
1:D:147:TYR:CE1	1:D:148:MSE:CE	2.47	0.98
1:D:147:TYR:CD1	1:D:148:MSE:HE3	1.98	0.97
2:F:222:ASN:HD21	2:F:298:LEU:H	1.07	0.95
2:C:277:ARG:HB2	2:C:365:VAL:HG21	1.50	0.94
1:D:131:LEU:HD21	1:E:132:ARG:HG3	1.53	0.89
1:B:147:TYR:HE1	1:B:148:MSE:HE2	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:196:GLY:O	2:F:197:LEU:HB2	1.75	0.87
2:C:277:ARG:HD2	2:C:365:VAL:HG21	1.55	0.87
2:C:317:ARG:HH11	2:C:317:ARG:HG3	1.39	0.87
2:C:302:CYS:O	2:C:306:ARG:HG3	1.75	0.86
2:C:194:LEU:H	2:C:194:LEU:HD12	1.40	0.85
2:C:277:ARG:HD2	2:C:365:VAL:CG2	2.08	0.84
2:F:209:MSE:HG2	2:F:240:MSE:CE	2.05	0.82
1:D:147:TYR:HE1	1:D:148:MSE:HE3	1.40	0.82
2:C:299:THR:HG23	2:C:302:CYS:HB2	1.63	0.80
2:F:218:SER:HB2	2:F:298:LEU:HD13	1.65	0.79
2:C:290:GLN:CG	2:C:291:GLU:H	1.93	0.79
2:C:245:GLU:H	2:C:248:ASN:ND2	1.82	0.78
2:C:268:VAL:HG13	2:C:269:PRO:HD2	1.64	0.78
2:F:222:ASN:HD21	2:F:298:LEU:N	1.84	0.76
2:F:261:ARG:HE	2:F:262:PHE:H	1.34	0.76
1:D:147:TYR:HE1	1:D:148:MSE:CE	1.93	0.75
1:B:147:TYR:CE1	1:B:148:MSE:HE2	2.21	0.75
1:A:104:ARG:HH21	2:C:192:PRO:HB3	1.51	0.75
1:B:82:ALA:HB2	2:C:333:MSE:HE3	1.69	0.74
2:C:290:GLN:HG3	2:C:291:GLU:N	1.99	0.74
2:C:245:GLU:H	2:C:248:ASN:HD22	1.34	0.74
2:F:301:THR:O	2:F:305:GLN:HG3	1.86	0.73
2:C:209:MSE:HG2	2:C:240:MSE:HE1	1.70	0.73
1:A:130:ARG:HH12	2:F:241:ARG:HD2	1.53	0.73
2:C:196:GLY:O	2:C:197:LEU:HB2	1.89	0.72
2:F:261:ARG:HE	2:F:262:PHE:N	1.86	0.72
1:B:143:GLU:CD	2:F:307:ARG:HH22	1.97	0.72
2:C:261:ARG:HG3	2:C:261:ARG:HH11	1.55	0.71
1:A:90:ASN:C	1:A:90:ASN:HD22	1.99	0.70
2:C:214:ASP:OD1	2:C:306:ARG:NH1	2.25	0.69
1:A:109:GLU:HA	1:A:109:GLU:OE1	1.92	0.68
1:B:86:ILE:HA	2:C:341:THR:HB	1.76	0.68
1:E:80:GLN:NE2	1:E:94:GLN:HB3	2.02	0.67
1:A:104:ARG:NH2	2:C:192:PRO:HB3	2.09	0.67
2:F:347:PHE:O	2:F:348:ASN:HB3	1.95	0.66
2:F:330:ASN:HB3	2:F:331:PRO:HD3	1.78	0.66
2:C:277:ARG:CD	2:C:365:VAL:HG21	2.25	0.64
2:F:222:ASN:ND2	2:F:298:LEU:H	1.88	0.64
2:C:352:VAL:HB	2:C:353:PRO:HD2	1.78	0.64
2:C:261:ARG:HH11	2:C:261:ARG:CG	2.10	0.64
2:C:197:LEU:HA	2:C:343:TRP:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:HG3	2:C:183:TYR:CE1	2.34	0.62
1:E:82:ALA:HB2	2:F:333:MSE:HE3	1.80	0.62
2:C:277:ARG:CB	2:C:365:VAL:HG21	2.27	0.62
1:D:124:LYS:O	1:D:128:ILE:HG13	1.99	0.61
2:F:330:ASN:CB	2:F:331:PRO:HD3	2.30	0.61
1:B:80:GLN:O	1:B:81:GLU:C	2.44	0.61
2:C:317:ARG:HG3	2:C:317:ARG:NH1	2.12	0.60
2:C:256:TYR:CG	2:C:259:SER:HB2	2.37	0.60
1:D:103:ARG:HE	1:E:104:ARG:HB2	1.66	0.60
2:C:291:GLU:HB2	2:C:296:THR:HG23	1.83	0.60
2:C:180:ALA:O	2:C:185:ARG:HD3	2.01	0.60
2:C:211:ARG:HG3	2:C:307:ARG:HH11	1.65	0.60
2:F:245:GLU:H	2:F:248:ASN:ND2	1.98	0.60
1:A:115:GLU:HG3	2:C:183:TYR:CD1	2.36	0.59
2:F:305:GLN:O	2:F:309:VAL:HG23	2.01	0.59
2:C:287:LEU:C	2:C:288:LEU:HD23	2.28	0.59
1:B:127:GLU:HG3	1:B:130:ARG:NH1	2.17	0.59
1:D:109:GLU:HA	1:D:109:GLU:OE1	2.02	0.58
2:F:200:PRO:HG3	2:F:352:VAL:HG21	1.83	0.58
1:A:124:LYS:HE3	1:B:125:ASP:OD1	2.02	0.58
2:F:261:ARG:HB2	2:F:287:LEU:HD11	1.85	0.58
1:B:87:SER:O	2:C:341:THR:HG21	2.02	0.58
1:B:98:GLU:HG2	2:C:345:PRO:HB2	1.85	0.57
2:C:200:PRO:HB3	2:C:350:ASP:HA	1.86	0.57
1:E:133:LYS:O	1:E:135:ASN:N	2.37	0.57
2:F:213:MSE:O	2:F:217:VAL:HG13	2.04	0.57
1:E:98:GLU:O	1:E:102:GLN:HG2	2.03	0.57
2:C:262:PHE:CE1	2:C:284:ILE:HG23	2.40	0.57
1:D:147:TYR:CD1	1:D:148:MSE:CE	2.81	0.57
2:F:200:PRO:HB3	2:F:350:ASP:HA	1.87	0.57
2:C:187:HIS:HB2	2:C:201:TYR:HB2	1.87	0.56
2:F:264:GLN:HE21	2:F:280:TYR:HB3	1.71	0.56
2:C:187:HIS:CB	2:C:201:TYR:HB2	2.35	0.56
2:F:210:PHE:C	2:F:212:SER:H	2.12	0.56
1:A:109:GLU:OE1	1:A:109:GLU:CA	2.54	0.56
1:B:143:GLU:CD	2:F:307:ARG:NH2	2.64	0.56
2:C:338:ASP:OD2	2:C:338:ASP:N	2.39	0.56
2:F:304:LEU:O	2:F:308:GLN:HG3	2.06	0.56
1:A:138:LEU:O	1:A:141:VAL:HG13	2.06	0.55
2:C:263:ARG:HD3	2:C:265:GLU:OE1	2.06	0.55
2:C:318:VAL:HG22	2:C:352:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLU:CG	1:B:130:ARG:NH1	2.70	0.54
1:A:104:ARG:HH21	2:C:192:PRO:CB	2.19	0.54
2:C:252:ILE:HD13	2:C:252:ILE:C	2.33	0.54
2:C:212:SER:O	2:C:215:THR:HG23	2.06	0.54
1:A:142:ALA:O	1:A:145:VAL:HB	2.08	0.54
1:E:95:TYR:OH	2:F:195:PRO:HG2	2.08	0.54
2:F:261:ARG:NE	2:F:262:PHE:H	2.04	0.53
1:A:148:MSE:O	1:A:152:ILE:HG13	2.09	0.53
2:C:264:GLN:HG2	2:C:363:PRO:HA	1.89	0.53
2:F:202:LYS:NZ	2:F:352:VAL:O	2.40	0.53
2:F:239:MSE:O	2:F:241:ARG:NH1	2.41	0.53
1:B:127:GLU:HG3	1:B:130:ARG:HH12	1.74	0.53
1:D:121:ILE:HD12	1:E:117:LEU:HD22	1.90	0.53
1:E:79:THR:HG21	2:F:346:ARG:HH22	1.73	0.53
1:D:96:TRP:CE2	1:E:97:LYS:HD2	2.43	0.53
2:C:259:SER:O	2:C:306:ARG:NH2	2.42	0.52
2:F:321:GLN:HA	2:F:321:GLN:NE2	2.25	0.52
1:B:96:TRP:O	1:B:97:LYS:C	2.52	0.52
2:C:194:LEU:H	2:C:194:LEU:CD1	2.13	0.52
2:F:179:LYS:O	2:F:180:ALA:HB3	2.10	0.52
2:F:263:ARG:NH2	2:F:285:GLU:OE1	2.43	0.52
2:F:330:ASN:CG	2:F:331:PRO:HD3	2.35	0.51
2:C:290:GLN:CG	2:C:291:GLU:N	2.63	0.51
1:E:81:GLU:OE2	1:E:81:GLU:HA	2.10	0.51
1:A:88:LYS:C	1:A:90:ASN:H	2.19	0.51
1:A:118:HIS:CE1	2:C:181:PRO:HB3	2.46	0.51
1:A:146:GLN:O	1:A:149:ALA:HB3	2.12	0.50
2:C:322:HIS:HD1	2:C:340:LEU:HD21	1.75	0.50
2:C:201:TYR:O	2:C:205:VAL:HG12	2.11	0.50
1:B:127:GLU:CG	1:B:130:ARG:HH12	2.25	0.50
2:C:349:VAL:C	2:C:351:GLU:H	2.19	0.50
2:C:196:GLY:O	2:C:197:LEU:CB	2.59	0.49
2:F:209:MSE:HG3	2:F:240:MSE:HE1	1.89	0.49
2:C:305:GLN:O	2:C:309:VAL:HG23	2.11	0.49
2:F:347:PHE:O	2:F:348:ASN:CB	2.59	0.49
1:A:127:GLU:OE2	1:A:127:GLU:HA	2.12	0.49
2:C:317:ARG:NH1	2:C:317:ARG:CG	2.74	0.49
2:C:213:MSE:HE3	2:C:284:ILE:HD13	1.94	0.49
2:C:351:GLU:HG3	3:C:1:HOH:O	2.11	0.49
2:F:233:LYS:NZ	2:F:237:GLN:OE1	2.44	0.49
1:A:133:LYS:O	1:A:134:GLU:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:245:GLU:O	2:F:248:ASN:HB2	2.13	0.49
1:D:154:ARG:HA	1:D:157:ASN:ND2	2.28	0.48
1:E:150:GLU:O	1:E:153:GLU:HB3	2.13	0.48
2:F:256:TYR:CG	2:F:259:SER:HB3	2.47	0.48
2:C:287:LEU:HB3	3:C:2:HOH:O	2.12	0.48
2:C:277:ARG:HD2	2:C:365:VAL:HG23	1.90	0.48
2:F:290:GLN:CD	2:F:291:GLU:H	2.22	0.48
2:C:197:LEU:HA	2:C:343:TRP:CZ2	2.49	0.48
2:C:217:VAL:HB	2:C:227:VAL:HG21	1.96	0.48
2:F:200:PRO:HG3	2:F:352:VAL:CG2	2.43	0.48
2:F:324:VAL:O	2:F:327:ALA:HB3	2.14	0.48
1:E:104:ARG:HH11	1:E:104:ARG:HG2	1.79	0.48
2:F:351:GLU:O	2:F:352:VAL:O	2.32	0.48
2:F:268:VAL:CG1	2:F:269:PRO:HD2	2.44	0.48
2:C:210:PHE:C	2:C:210:PHE:CD2	2.92	0.47
1:D:148:MSE:HE2	1:D:148:MSE:HA	1.96	0.47
1:D:150:GLU:O	1:D:154:ARG:HB2	2.14	0.47
1:A:91:PRO:HA	1:B:93:SER:HB3	1.96	0.47
1:E:137:ASP:O	1:E:138:LEU:C	2.57	0.47
2:F:218:SER:HA	2:F:298:LEU:HD12	1.96	0.47
2:C:352:VAL:HB	2:C:353:PRO:CD	2.44	0.47
1:D:131:LEU:HD21	1:E:132:ARG:CG	2.33	0.47
1:E:85:LEU:O	2:F:341:THR:HB	2.15	0.47
2:F:225:GLU:OE2	2:F:231:LYS:NZ	2.44	0.47
1:A:96:TRP:CE2	1:B:97:LYS:HG3	2.49	0.47
2:C:253:LYS:HB3	2:C:358:ALA:HB3	1.96	0.47
1:A:130:ARG:HH22	2:F:241:ARG:NE	2.13	0.47
2:C:268:VAL:CG1	2:C:269:PRO:HD2	2.42	0.46
1:E:98:GLU:CD	2:F:346:ARG:HH11	2.22	0.46
2:C:347:PHE:O	2:C:348:ASN:HB3	2.15	0.46
2:F:210:PHE:C	2:F:212:SER:N	2.73	0.46
2:C:322:HIS:ND1	2:C:340:LEU:HD21	2.31	0.46
1:D:115:GLU:HG3	2:F:183:TYR:CD1	2.50	0.46
2:F:330:ASN:CB	2:F:331:PRO:CD	2.93	0.46
2:C:220:LEU:HD23	2:C:223:ARG:HH21	1.81	0.46
2:C:245:GLU:N	2:C:248:ASN:HD22	2.07	0.46
1:D:115:GLU:HG3	2:F:183:TYR:CE1	2.50	0.46
1:D:132:ARG:NH1	1:E:127:GLU:OE2	2.49	0.46
2:C:220:LEU:CD2	2:C:223:ARG:HH21	2.29	0.46
1:A:148:MSE:HA	1:A:151:VAL:HG13	1.96	0.46
1:B:143:GLU:OE1	2:F:307:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLN:HE21	1:B:94:GLN:HB3	1.54	0.45
2:C:233:LYS:NZ	2:C:245:GLU:OE1	2.50	0.45
2:C:277:ARG:HH11	2:C:365:VAL:HG23	1.81	0.45
2:C:336:PRO:HG2	2:C:339:GLN:HB2	1.97	0.45
1:D:101:GLU:OE2	1:D:101:GLU:HA	2.16	0.45
2:C:226:THR:CG2	2:C:228:THR:HG23	2.46	0.45
1:A:90:ASN:C	1:A:90:ASN:ND2	2.69	0.45
1:B:120:GLU:HA	1:B:123:GLN:NE2	2.32	0.45
1:D:127:GLU:HA	1:D:127:GLU:OE2	2.17	0.45
1:D:147:TYR:HD1	1:D:148:MSE:HE3	1.72	0.45
1:B:81:GLU:C	1:B:83:PHE:N	2.74	0.45
2:F:330:ASN:HB3	2:F:331:PRO:CD	2.46	0.45
1:E:103:ARG:O	1:E:104:ARG:C	2.59	0.45
2:F:239:MSE:O	2:F:241:ARG:CZ	2.65	0.45
2:F:256:TYR:CD1	2:F:259:SER:HB3	2.52	0.45
2:C:261:ARG:CG	2:C:261:ARG:NH1	2.74	0.45
2:C:215:THR:HG21	2:C:239:MSE:HE1	1.98	0.45
1:A:114:ASN:ND2	2:C:182:ALA:HB3	2.32	0.44
2:F:263:ARG:HD2	2:F:265:GLU:OE1	2.17	0.44
1:D:139:ALA:O	1:D:142:ALA:HB3	2.17	0.44
2:F:245:GLU:H	2:F:248:ASN:HD22	1.64	0.44
2:C:256:TYR:CD1	2:C:258:THR:HG23	2.52	0.44
2:F:325:PHE:CZ	2:F:329:LEU:HD21	2.53	0.44
1:A:130:ARG:NH1	2:F:241:ARG:HD2	2.28	0.44
1:B:129:ALA:C	1:B:131:LEU:H	2.25	0.44
2:C:226:THR:HG22	2:C:228:THR:HG23	2.00	0.43
1:D:97:LYS:HG3	1:E:96:TRP:CE2	2.53	0.43
1:D:133:LYS:O	1:D:134:GLU:C	2.61	0.43
2:F:202:LYS:CE	2:F:352:VAL:O	2.66	0.43
2:F:277:ARG:C	2:F:279:ASP:H	2.27	0.43
1:B:119:LYS:C	1:B:123:GLN:HE21	2.25	0.43
1:E:104:ARG:HG2	1:E:104:ARG:NH1	2.33	0.43
1:B:92:SER:O	1:B:95:TYR:HB3	2.18	0.43
2:C:344:HIS:CE1	2:C:346:ARG:HB2	2.54	0.43
2:F:213:MSE:HE1	2:F:249:VAL:HG13	2.00	0.43
1:D:103:ARG:HH21	1:E:104:ARG:HB2	1.84	0.43
1:D:131:LEU:CD2	1:E:132:ARG:HG3	2.37	0.43
2:F:299:THR:O	2:F:300:ALA:C	2.60	0.43
2:F:227:VAL:O	2:F:227:VAL:HG22	2.18	0.43
1:B:155:LEU:O	1:B:156:SER:C	2.61	0.43
2:F:220:LEU:O	2:F:223:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:222:ASN:HD22	2:F:222:ASN:HA	1.60	0.43
2:F:351:GLU:CD	2:F:352:VAL:N	2.77	0.43
2:C:301:THR:OG1	1:E:150:GLU:OE1	2.31	0.42
2:F:203:TYR:CD1	2:F:203:TYR:N	2.86	0.42
1:A:141:VAL:O	1:A:145:VAL:HG23	2.19	0.42
2:F:232:VAL:O	2:F:236:VAL:HG12	2.19	0.42
2:F:245:GLU:OE1	2:F:245:GLU:HA	2.19	0.42
2:C:186:PHE:O	2:C:187:HIS:C	2.62	0.42
1:A:111:LEU:HD22	2:C:183:TYR:HA	2.01	0.42
2:C:212:SER:HA	2:C:215:THR:CG2	2.49	0.42
2:C:288:LEU:HB2	2:C:289:GLY:H	1.61	0.42
1:A:139:ALA:O	1:A:142:ALA:HB3	2.20	0.42
2:F:262:PHE:O	2:F:263:ARG:HG3	2.20	0.41
2:F:318:VAL:O	2:F:319:LYS:C	2.63	0.41
1:B:115:GLU:O	1:B:116:LYS:C	2.60	0.41
1:A:143:GLU:O	1:A:144:HIS:C	2.63	0.41
2:F:203:TYR:N	2:F:203:TYR:HD1	2.19	0.41
2:C:211:ARG:NH1	1:E:143:GLU:OE1	2.54	0.41
2:F:232:VAL:O	2:F:233:LYS:C	2.62	0.41
1:A:124:LYS:HE2	1:B:121:ILE:HG23	2.03	0.41
2:F:330:ASN:ND2	2:F:331:PRO:HD3	2.35	0.41
2:C:312:GLN:NE2	2:C:316:GLU:HG3	2.36	0.41
2:F:211:ARG:O	2:F:211:ARG:HG2	2.21	0.41
2:F:336:PRO:HG2	2:F:339:GLN:OE1	2.21	0.41
2:F:229:PHE:O	2:F:230:ALA:C	2.61	0.41
1:B:147:TYR:CD1	1:B:147:TYR:C	2.98	0.41
1:B:151:VAL:O	1:B:152:ILE:C	2.63	0.41
2:C:214:ASP:CG	2:C:306:ARG:HH11	2.28	0.41
2:C:180:ALA:HA	2:C:181:PRO:HD3	1.89	0.40
2:F:182:ALA:C	2:F:184:GLN:N	2.75	0.40
2:F:220:LEU:HD22	2:F:225:GLU:CD	2.46	0.40
1:B:129:ALA:C	1:B:131:LEU:N	2.78	0.40
2:C:344:HIS:HA	2:C:345:PRO:HD2	1.85	0.40
2:F:265:GLU:HB2	2:F:283:THR:HG21	2.04	0.40
1:D:142:ALA:O	1:D:143:GLU:C	2.65	0.40
2:F:246:GLU:O	2:F:247:ARG:C	2.63	0.40
2:F:336:PRO:HB2	2:F:339:GLN:HB2	2.04	0.40
1:E:81:GLU:O	1:E:82:ALA:C	2.65	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	68/79 (86%)	56 (82%)	10 (15%)	2 (3%)	3	13
1	B	76/79 (96%)	61 (80%)	13 (17%)	2 (3%)	4	15
1	D	63/79 (80%)	55 (87%)	8 (13%)	0	100	100
1	E	76/79 (96%)	63 (83%)	11 (14%)	2 (3%)	4	15
2	C	181/197 (92%)	160 (88%)	17 (9%)	4 (2%)	5	19
2	F	180/197 (91%)	148 (82%)	24 (13%)	8 (4%)	2	7
All	All	644/710 (91%)	543 (84%)	83 (13%)	18 (3%)	4	14

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	290	GLN
1	E	134	GLU
2	F	352	VAL
1	B	84	ASP
1	E	81	GLU
2	F	247	ARG
2	F	330	ASN
2	F	340	LEU
2	F	348	ASN
1	A	89	GLU
1	B	81	GLU
2	C	180	ALA
2	F	180	ALA
2	F	197	LEU
1	A	134	GLU
2	C	297	GLN
2	F	290	GLN
2	C	196	GLY

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	63/70 (90%)	44 (70%)	19 (30%)	0	1
1	B	70/70 (100%)	60 (86%)	10 (14%)	3	11
1	D	58/70 (83%)	45 (78%)	13 (22%)	1	3
1	E	70/70 (100%)	62 (89%)	8 (11%)	5	19
2	C	169/173 (98%)	139 (82%)	30 (18%)	2	6
2	F	169/173 (98%)	137 (81%)	32 (19%)	1	5
All	All	599/626 (96%)	487 (81%)	112 (19%)	1	5

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	90	ASN
1	A	94	GLN
1	A	103	ARG
1	A	104	ARG
1	A	109	GLU
1	A	112	LYS
1	A	113	GLU
1	A	118	HIS
1	A	121	ILE
1	A	124	LYS
1	A	131	LEU
1	A	133	LYS
1	A	134	GLU
1	A	141	VAL
1	A	143	GLU
1	A	150	GLU
1	A	151	VAL
1	A	155	LEU
1	B	81	GLU
1	B	88	LYS
1	B	89	GLU

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Mol	Chain	Res	Type
1	B	94	GLN
1	B	111	LEU
1	B	116	LYS
1	B	126	SER
1	B	130	ARG
1	B	131	LEU
1	B	146	GLN
2	C	179	LYS
2	C	189	LEU
2	C	194	LEU
2	C	202	LYS
2	C	205	VAL
2	C	211	ARG
2	C	215	THR
2	C	217	VAL
2	C	218	SER
2	C	226	THR
2	C	227	VAL
2	C	236	VAL
2	C	245	GLU
2	C	252	ILE
2	C	258	THR
2	C	261	ARG
2	C	275	ILE
2	C	276	LYS
2	C	287	LEU
2	C	288	LEU
2	C	297	GLN
2	C	298	LEU
2	C	299	THR
2	C	302	CYS
2	C	308	GLN
2	C	314	LEU
2	C	340	LEU
2	C	341	THR
2	C	356	GLU
2	C	365	VAL
1	D	94	GLN
1	D	99	VAL
1	D	109	GLU
1	D	122	GLU
1	D	128	ILE

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Mol	Chain	Res	Type
1	D	132	ARG
1	D	141	VAL
1	D	143	GLU
1	D	145	VAL
1	D	150	GLU
1	D	151	VAL
1	D	152	ILE
1	D	155	LEU
1	E	79	THR
1	E	86	ILE
1	E	94	GLN
1	E	105	LYS
1	E	112	LYS
1	E	119	LYS
1	E	126	SER
1	E	148	MSE
2	F	179	LYS
2	F	189	LEU
2	F	198	VAL
2	F	204	GLN
2	F	205	VAL
2	F	217	VAL
2	F	218	SER
2	F	223	ARG
2	F	227	VAL
2	F	231	LYS
2	F	236	VAL
2	F	245	GLU
2	F	247	ARG
2	F	258	THR
2	F	270	THR
2	F	276	LYS
2	F	282	LEU
2	F	288	LEU
2	F	290	GLN
2	F	298	LEU
2	F	302	CYS
2	F	303	LEU
2	F	304	LEU
2	F	312	GLN
2	F	314	LEU
2	F	317	ARG

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Mol	Chain	Res	Type
2	F	319	LYS
2	F	326	LEU
2	F	338	ASP
2	F	341	THR
2	F	359	GLU
2	F	365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	94	GLN
1	A	135	ASN
1	A	144	HIS
1	A	146	GLN
1	A	157	ASN
1	B	90	ASN
1	B	94	GLN
1	B	102	GLN
1	B	123	GLN
1	B	135	ASN
1	B	144	HIS
2	C	184	GLN
2	C	248	ASN
2	C	308	GLN
2	C	312	GLN
2	C	330	ASN
1	D	94	GLN
1	D	102	GLN
1	D	118	HIS
1	D	157	ASN
1	E	80	GLN
1	E	94	GLN
1	E	123	GLN
1	E	144	HIS
2	F	184	GLN
2	F	191	GLN
2	F	204	GLN
2	F	222	ASN
2	F	248	ASN
2	F	264	GLN
2	F	267	ASN

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Mol	Chain	Res	Type
2	F	297	GLN
2	F	308	GLN
2	F	312	GLN
2	F	313	ASN
2	F	321	GLN
2	F	348	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](#)

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	69/79 (87%)	-0.16	1 (1%) 73 64	44, 61, 83, 90	0
1	B	77/79 (97%)	-0.14	2 (2%) 57 47	41, 54, 74, 82	0
1	D	64/79 (81%)	-0.16	0 100 100	40, 63, 89, 93	0
1	E	77/79 (97%)	-0.09	3 (3%) 43 34	35, 59, 76, 85	0
2	C	179/197 (90%)	-0.10	3 (1%) 69 60	38, 54, 75, 90	0
2	F	178/197 (90%)	-0.14	2 (1%) 78 70	40, 55, 73, 84	0
All	All	644/710 (90%)	-0.13	11 (1%) 69 60	35, 56, 78, 93	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	79	THR	4.9
1	B	79	THR	4.4
1	B	80	GLN	3.7
1	E	80	GLN	3.5
1	A	88	LYS	3.5
2	F	295	ALA	3.2
2	F	365	VAL	3.1
2	C	365	VAL	3.0
2	C	295	ALA	2.4
1	E	136	LYS	2.4
2	C	294	GLY	2.3

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 [i](#)

There are no oligosaccharides 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.