



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:13 AM GMT

PDB ID : 2ZXX
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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

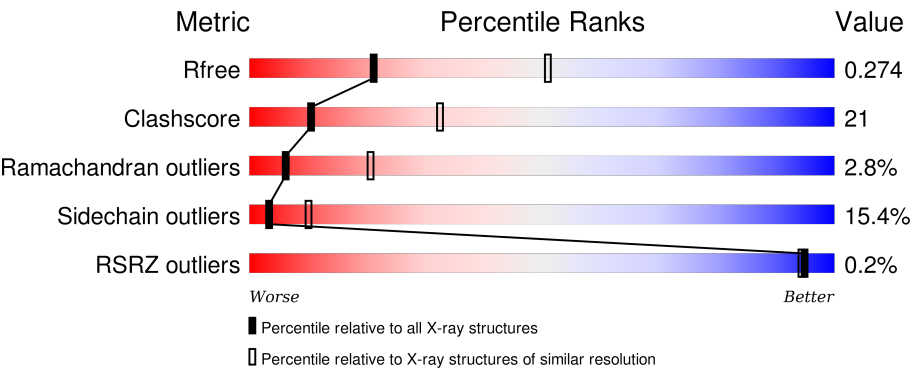
1 Overall quality at a glance i

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	79	<div><div></div><div><div>47%</div><div>34%</div><div>6%</div><div>•</div><div>11%</div></div></div>
1	B	79	<div><div></div><div><div>63%</div><div>30%</div><div>5%</div><div>•</div></div></div>
1	D	79	<div><div></div><div><div>51%</div><div>28%</div><div>•</div><div>18%</div></div></div>
1	E	79	<div><div></div><div><div>%</div><div>61%</div><div>35%</div><div>•</div><div>•</div></div></div>
2	C	197	<div><div></div><div><div>47%</div><div>37%</div><div>10%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	197	<div><div></div><div>47%</div><div>38%</div><div>8%</div><div>• 7%</div></div>

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 [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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Geminin

Chain A: 



• Molecule 1: Geminin

Chain B: 



• Molecule 1: Geminin

Chain D: 



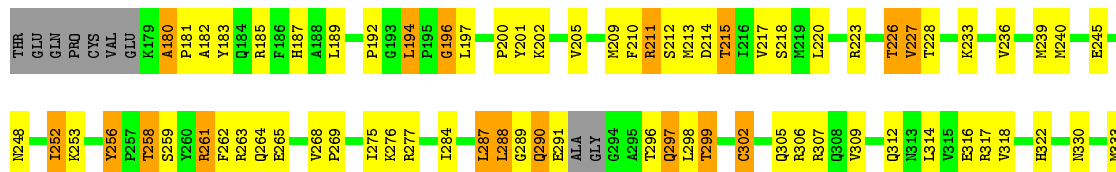
• Molecule 1: Geminin

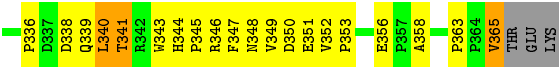
Chain E: 



• Molecule 2: DNA replication factor Cdt1

Chain C: 





● 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 37.43 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.00-2.80) 94.5 (37.43-2.79)	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 , 0.274	Depositor DCC
R_{free} test set	1434 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 28179 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.92	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.66	0/596	0.71	0/794
1	B	0.71	0/660	0.70	0/881
1	D	0.70	0/556	0.71	0/740
1	E	0.71	0/660	0.71	0/881
2	C	0.72	0/1541	0.77	0/2078
2	F	0.70	0/1537	0.77	0/2073
All	All	0.70	0/5550	0.74	0/7447

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.

There are no bond angle outliers.

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 [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	590	0	586	29	0
1	B	653	0	646	23	0
1	D	551	0	549	26	0
1	E	653	0	646	26	0
2	C	1512	0	1526	90	0
2	F	1508	0	1523	80	0
3	C	6	0	0	2	0
3	F	3	0	0	0	0
All	All	5476	0	5476	234	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 21.

All (234) 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
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:HG3	2:C:317:ARG:HH11	1.39	0.87
2:C:302:CYS:O	2:C:306:ARG:HG3	1.75	0.86
2:C:194:LEU:HD12	2:C:194:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:261:ARG:HG3	2:C:261:ARG:HH11	1.55	0.71
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:B:143:GLU:CD	2:F:307:ARG:HH22	1.97	0.67
1:A:104:ARG:NH2	2:C:192:PRO:HB3	2.09	0.67
1:A:90:ASN:HD22	1:A:90:ASN:C	1.99	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:CG	2:C:261:ARG:HH11	2.10	0.64
2:C:197:LEU:HA	2:C:343:TRP:CE2	2.33	0.63
1:E:82:ALA:HB2	2:F:333:MSE:HE3	1.80	0.62
1:A:115:GLU:HG3	2:C:183:TYR:CE1	2.34	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
2:C:317:ARG:NH1	2:C:317:ARG:HG3	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: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
2:C:180:ALA:O	2:C:185:ARG:HD3	2.01	0.60
2:F:305:GLN:O	2:F:309:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:HG3	2:C:183:TYR:CD1	2.36	0.59
1:B:127:GLU:HG3	1:B:130:ARG:NH1	2.17	0.59
2:F:200:PRO:HG3	2:F:352:VAL:HG21	1.83	0.58
1:D:109:GLU:HA	1:D:109:GLU:OE1	2.02	0.58
2:F:261:ARG:HB2	2:F:287:LEU:HD11	1.85	0.58
1:A:124:LYS:HE3	1:B:125:ASP:OD1	2.02	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
1:E:133:LYS:O	1:E:135:ASN:N	2.37	0.57
2:C:200:PRO:HB3	2:C:350:ASP:HA	1.86	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
1:D:147:TYR:CD1	1:D:148:MSE:CE	2.81	0.57
2:C:262:PHE:CE1	2:C:284:ILE:HG23	2.40	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
1:B:80:GLN:O	1:B:81:GLU:C	2.44	0.56
1:A:109:GLU:OE1	1:A:109:GLU:CA	2.54	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
2:C:287:LEU:C	2:C:288:LEU:HD23	2.28	0.54
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: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:239:MSE:O	2:F:241:ARG:NH1	2.41	0.53
2:F:202:LYS:NZ	2:F:352:VAL:O	2.40	0.53
1:E:79:THR:HG21	2:F:346:ARG:HH22	1.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:321:GLN:NE2	2:F:321:GLN:HA	2.25	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:210:PHE:C	2:F:212:SER:H	2.12	0.51
2:C:290:GLN:CG	2:C:291:GLU:N	2.63	0.51
1:E:81:GLU:HA	1:E:81:GLU:OE2	2.10	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:F:209:MSE:HG3	2:F:240:MSE:HE1	1.89	0.49
2:C:196:GLY:O	2:C:197:LEU:CB	2.59	0.49
2:C:252:ILE:C	2:C:252:ILE:HD13	2.33	0.49
2:F:347:PHE:O	2:F:348:ASN:CB	2.59	0.49
2:C:305:GLN:O	2:C:309:VAL:HG23	2.11	0.49
2:C:317:ARG:NH1	2:C:317:ARG:CG	2.74	0.49
1:A:127:GLU:OE2	1:A:127:GLU:HA	2.12	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
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
2:F:256:TYR:CG	2:F:259:SER:HB3	2.47	0.48
1:E:150:GLU:O	1:E:153:GLU:HB3	2.13	0.48
2:C:287:LEU:HB3	3:C:2:HOH:O	2.12	0.48
1:B:143:GLU:CD	2:F:307:ARG:NH2	2.64	0.48
2:C:277:ARG:HD2	2:C:365:VAL:HG23	1.90	0.48
2:C:197:LEU:HA	2:C:343:TRP:CZ2	2.49	0.48
2:F:200:PRO:HG3	2:F:352:VAL:CG2	2.43	0.48
2:C:217:VAL:HB	2:C:227:VAL:HG21	1.96	0.48
2:F:324:VAL:O	2:F:327:ALA:HB3	2.14	0.48
1:E:104:ARG:HG2	1:E:104:ARG:HH11	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
1:D:148:MSE:HA	1:D:148:MSE:HE2	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:B:96:TRP:O	1:B:97:LYS:C	2.52	0.47
2:F:218:SER:HA	2:F:298:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:330:ASN:CG	2:F:331:PRO:HD3	2.35	0.47
1:E:85:LEU:O	2:F:341:THR:HB	2.15	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:F:225:GLU:OE2	2:F:231:LYS:NZ	2.44	0.47
2:C:268:VAL:CG1	2:C:269:PRO:HD2	2.42	0.46
2:C:347:PHE:O	2:C:348:ASN:HB3	2.15	0.46
2:F:330:ASN:CB	2:F:331:PRO:CD	2.93	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
1:A:88:LYS:C	1:A:90:ASN:H	2.19	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:B:143:GLU:OE1	2:F:307:ARG:NH2	2.48	0.46
1:A:148:MSE:HA	1:A:151:VAL:HG13	1.96	0.46
1:B:94:GLN:HB3	1:B:94:GLN:HE21	1.54	0.45
2:C:277:ARG:HH11	2:C:365:VAL:HG23	1.81	0.45
2:C:233:LYS:NZ	2:C:245:GLU:OE1	2.50	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:D:147:TYR:HD1	1:D:148:MSE:HE3	1.72	0.45
2:C:349:VAL:C	2:C:351:GLU:H	2.19	0.45
1:D:127:GLU:HA	1:D:127:GLU:OE2	2.17	0.45
1:B:120:GLU:HA	1:B:123:GLN:NE2	2.32	0.45
2:F:330:ASN:HB3	2:F:331:PRO:CD	2.46	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:NH1	2:C:261:ARG:CG	2.74	0.45
2:C:215:THR:HG21	2:C:239:MSE:HE1	1.98	0.45
2:F:263:ARG:HD2	2:F:265:GLU:OE1	2.17	0.44
1:A:114:ASN:ND2	2:C:182:ALA:HB3	2.32	0.44
2:F:245:GLU:H	2:F:248:ASN:HD22	1.64	0.44
2:F:227:VAL:HG22	2:F:227:VAL:O	2.18	0.44
1:D:139:ALA:O	1:D:142:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:133:LYS:O	1:A:134:GLU:C	2.55	0.44
1:E:137:ASP:O	1:E:138:LEU:C	2.57	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
2:F:202:LYS:CE	2:F:352:VAL:O	2.66	0.43
2:F:290:GLN:CD	2:F:291:GLU:H	2.22	0.43
1:E:104:ARG:HG2	1:E:104:ARG:NH1	2.33	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:B:92:SER:O	1:B:95:TYR:HB3	2.18	0.43
1:D:131:LEU:CD2	1:E:132:ARG:HG3	2.37	0.43
1:D:103:ARG:HH21	1:E:104:ARG:HB2	1.84	0.43
2:C:210:PHE:CD2	2:C:210:PHE:C	2.92	0.43
1:A:90:ASN:ND2	1:A:90:ASN:C	2.69	0.43
2:F:220:LEU:O	2:F:223:ARG:HG3	2.18	0.43
2:F:222:ASN:HD22	2:F:222:ASN:HA	1.60	0.43
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:210:PHE:C	2:F:212:SER:N	2.73	0.42
2:F:245:GLU:OE1	2:F:245:GLU:HA	2.19	0.42
2:F:232:VAL:O	2:F:236:VAL:HG12	2.19	0.42
1:A:111:LEU:HD22	2:C:183:TYR:HA	2.01	0.42
1:E:98:GLU:CD	2:F:346:ARG:HH11	2.22	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:203:TYR:HD1	2:F:203:TYR:N	2.19	0.41
2:C:211:ARG:NH1	1:E:143:GLU:OE1	2.54	0.41
2:F:330:ASN:ND2	2:F:331:PRO:HD3	2.35	0.41
1:A:124:LYS:HE2	1:B:121:ILE:HG23	2.03	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:C:312:GLN:NE2	2:C:316:GLU:HG3	2.36	0.41
2:F:182:ALA:C	2:F:184:GLN:N	2.75	0.41
2:C:180:ALA:HA	2:C:181:PRO:HD3	1.89	0.40
1:B:81:GLU:C	1:B:83:PHE:N	2.74	0.40
2:F:265:GLU:HB2	2:F:283:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:HIS:HA	2:C:345:PRO:HD2	1.85	0.40
1:E:103:ARG:O	1:E:104:ARG:C	2.59	0.40
2:F:336:PRO:HB2	2:F:339:GLN:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	6	19
1	B	76/79 (96%)	61 (80%)	13 (17%)	2 (3%)	7	22
1	D	63/79 (80%)	55 (87%)	8 (13%)	0	100	100
1	E	76/79 (96%)	63 (83%)	11 (14%)	2 (3%)	7	22
2	C	181/197 (92%)	160 (88%)	17 (9%)	4 (2%)	8	28
2	F	180/197 (91%)	148 (82%)	24 (13%)	8 (4%)	3	10
All	All	644/710 (91%)	543 (84%)	83 (13%)	18 (3%)	6	21

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

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Mol	Chain	Res	Type
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%)	50 (79%)	13 (21%)	1	4
1	B	70/70 (100%)	62 (89%)	8 (11%)	7	21
1	D	58/70 (83%)	49 (84%)	9 (16%)	3	10
1	E	70/70 (100%)	63 (90%)	7 (10%)	9	27
2	C	169/173 (98%)	143 (85%)	26 (15%)	3	10
2	F	169/173 (98%)	140 (83%)	29 (17%)	2	7
All	All	599/626 (96%)	507 (85%)	92 (15%)	3	10

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	94	GLN
1	A	104	ARG
1	A	109	GLU
1	A	112	LYS
1	A	113	GLU
1	A	131	LEU
1	A	134	GLU
1	A	141	VAL

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Mol	Chain	Res	Type
1	A	143	GLU
1	A	151	VAL
1	A	155	LEU
1	A	157	ASN
1	B	88	LYS
1	B	89	GLU
1	B	94	GLN
1	B	111	LEU
1	B	126	SER
1	B	130	ARG
1	B	146	GLN
1	B	147	TYR
2	C	189	LEU
2	C	194	LEU
2	C	202	LYS
2	C	211	ARG
2	C	215	THR
2	C	218	SER
2	C	226	THR
2	C	227	VAL
2	C	236	VAL
2	C	252	ILE
2	C	256	TYR
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	314	LEU
2	C	340	LEU
2	C	341	THR
2	C	356	GLU
2	C	365	VAL
1	D	94	GLN
1	D	109	GLU
1	D	122	GLU
1	D	132	ARG

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Mol	Chain	Res	Type
1	D	141	VAL
1	D	145	VAL
1	D	150	GLU
1	D	151	VAL
1	D	155	LEU
1	E	79	THR
1	E	86	ILE
1	E	105	LYS
1	E	108	TYR
1	E	112	LYS
1	E	126	SER
1	E	148	MSE
2	F	179	LYS
2	F	189	LEU
2	F	191	GLN
2	F	198	VAL
2	F	205	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	256	TYR
2	F	258	THR
2	F	266	CYS
2	F	270	THR
2	F	276	LYS
2	F	282	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
2	F	338	ASP
2	F	359	GLU
2	F	365	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	94	GLN
1	A	135	ASN
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	297	GLN
2	C	312	GLN
2	C	330	ASN
1	D	102	GLN
1	D	135	ASN
1	D	157	ASN
1	E	80	GLN
1	E	94	GLN
1	E	135	ASN
1	E	144	HIS
2	F	184	GLN
2	F	204	GLN
2	F	222	ASN
2	F	248	ASN
2	F	264	GLN
2	F	267	ASN
2	F	297	GLN
2	F	305	GLN
2	F	308	GLN
2	F	313	ASN
2	F	321	GLN
2	F	348	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	69/79 (87%)	-0.30	0	100100	44, 61, 83, 90	0
1	B	77/79 (97%)	-0.29	0	100100	41, 54, 74, 82	0
1	D	64/79 (81%)	-0.35	0	100100	40, 63, 89, 93	0
1	E	77/79 (97%)	-0.26	1 (1%)	7971	35, 59, 76, 85	0
2	C	179/197 (90%)	-0.29	0	100100	38, 54, 75, 90	0
2	F	178/197 (90%)	-0.33	0	100100	40, 55, 73, 84	0
All	All	644/710 (90%)	-0.30	1 (0%)	9594	35, 56, 78, 93	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	79	THR	5.3

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

There are no such residues in this entry.