



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:57 AM GMT

PDB ID : 2YVC
Title : Crystal structure of the Radixin FERM domain complexed with the NEP cytoplasmic tail
Authors : Terawaki, S.; Kitano, K.; Hakoshima, T.
Deposited on : 2007-04-11
Resolution : 3.20 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

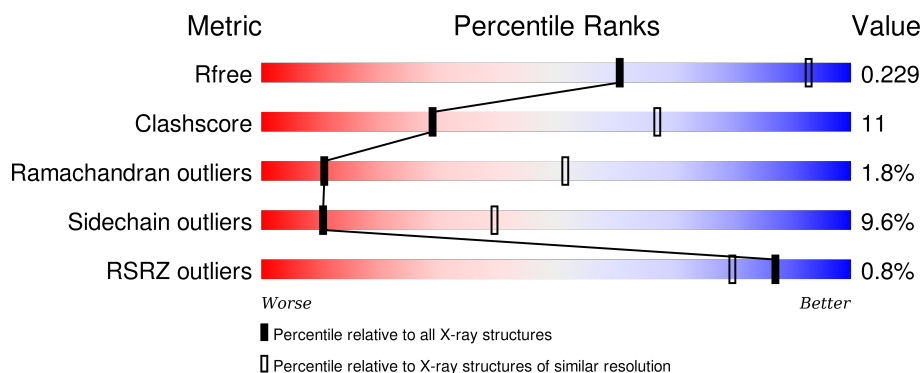
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



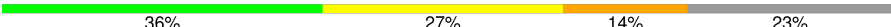
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	312	<div> <div style="width: 64%;"></div> <div style="width: 26%;"></div> <div style="width: 5%;"></div> </div> <div> <div style="width: 64%;"></div> <div style="width: 26%;"></div> <div style="width: 5%;"></div> </div>
1	B	312	<div> <div style="width: 63%;"></div> <div style="width: 29%;"></div> <div style="width: 5%;"></div> </div> <div> <div style="width: 63%;"></div> <div style="width: 29%;"></div> <div style="width: 5%;"></div> </div>
1	C	312	<div> <div style="width: 67%;"></div> <div style="width: 24%;"></div> <div style="width: 6%;"></div> </div> <div> <div style="width: 67%;"></div> <div style="width: 24%;"></div> <div style="width: 6%;"></div> </div>
2	D	22	<div> <div style="width: 27%;"></div> <div style="width: 5%;"></div> <div style="width: 68%;"></div> </div> <div> <div style="width: 27%;"></div> <div style="width: 5%;"></div> <div style="width: 68%;"></div> </div>
2	E	22	<div> <div style="width: 23%;"></div> <div style="width: 77%;"></div> </div> <div> <div style="width: 23%;"></div> <div style="width: 77%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	F	22	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (36%), yellow (27%), orange (14%), and grey (23%).

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7607 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 Radixin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2472	1599	422	442	9			
1	B	297	Total	C	N	O	S	0	0	0
			2486	1607	424	445	10			
1	C	292	Total	C	N	O	S	0	0	0
			2449	1583	418	439	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P26043
A	0	SER	-	EXPRESSION TAG	UNP P26043
B	-1	GLY	-	EXPRESSION TAG	UNP P26043
B	0	SER	-	EXPRESSION TAG	UNP P26043
C	-1	GLY	-	EXPRESSION TAG	UNP P26043
C	0	SER	-	EXPRESSION TAG	UNP P26043

- Molecule 2 is a protein called Neprilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O		0	0	0
			35	21	7	7				
2	E	5	Total	C	N	O		0	0	0
			25	15	5	5				
2	F	17	Total	C	N	O	S	0	0	0
			140	86	27	26	1			



- Molecule 2: Neprilysin



- Molecule 2: Neprilysin



- Molecule 2: Neprilysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.79Å 116.84Å 141.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 3.20 49.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.71-3.20) 99.6 (49.31-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.267 0.222 , 0.229	Depositor DCC
R_{free} test set	1522 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 30481 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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	0.45	0/2532	0.63	1/3415 (0.0%)
1	B	0.46	0/2546	0.60	0/3433
1	C	0.42	0/2507	0.55	0/3380
2	D	0.58	0/34	0.39	0/46
2	E	0.70	0/24	0.53	0/32
2	F	0.44	0/141	0.66	0/185
All	All	0.45	0/7784	0.60	1/10491 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	LEU	CA-CB-CG	5.48	127.91	115.30

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	2472	0	2487	57	0
1	B	2486	0	2504	68	0
1	C	2449	0	2460	46	0
2	D	35	0	13	0	0
2	E	25	0	9	0	0
2	F	140	0	151	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7607	0	7624	174	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 11.

All (174) 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:A:5:ILE:HB	1:A:20:ILE:HG22	1.40	1.02
1:B:138:ASN:H	1:B:142:HIS:HD2	1.10	0.92
1:A:256:VAL:HG12	1:A:268:VAL:HG22	1.54	0.90
1:B:138:ASN:H	1:B:142:HIS:CD2	1.91	0.89
1:A:60:LYS:H	1:A:68:GLN:HE22	1.12	0.88
1:C:7:VAL:HG12	1:C:76:LEU:HB2	1.58	0.85
1:B:123:VAL:HG13	1:B:172:ILE:HD13	1.61	0.82
1:C:222:ALA:HA	1:C:287:ASN:HD22	1.46	0.79
1:B:116:TYR:H	1:B:200:MET:HG3	1.47	0.79
1:A:5:ILE:HB	1:A:20:ILE:CG2	2.13	0.76
1:C:74:ASN:HB3	1:C:75:PRO:HD3	1.67	0.75
1:C:138:ASN:H	1:C:142:HIS:HD2	1.34	0.75
1:A:222:ALA:HA	1:A:287:ASN:HD21	1.52	0.74
1:A:56:SER:O	1:A:279:ARG:NH2	2.22	0.73
1:B:112:ASN:OD1	1:B:151:ARG:NH2	2.21	0.72
1:A:222:ALA:HA	1:A:287:ASN:ND2	2.05	0.72
1:B:89:VAL:HG23	1:B:93:LEU:HD12	1.70	0.72
1:B:132:ALA:HB2	1:B:187:SER:HB2	1.72	0.71
1:A:240:PHE:HB3	1:A:245:ILE:HD11	1.72	0.71
1:C:138:ASN:H	1:C:142:HIS:CD2	2.09	0.70
1:B:190:GLU:OE1	1:B:190:GLU:HA	1.93	0.68
1:B:7:VAL:HG22	1:B:18:PHE:HB2	1.74	0.68
1:C:245:ILE:HB	2:F:12:ILE:HG21	1.75	0.68
1:A:257:ILE:O	1:A:266:ASP:HB2	1.94	0.68
1:A:138:ASN:H	1:A:142:HIS:HD2	1.42	0.68
1:A:8:ARG:HG3	1:A:17:GLU:HG2	1.74	0.68
1:B:20:ILE:HG23	1:B:24:THR:OG1	1.96	0.65
1:B:222:ALA:HA	1:B:287:ASN:ND2	2.12	0.65
1:A:60:LYS:H	1:A:68:GLN:NE2	1.92	0.64
1:C:171:ARG:HA	1:C:174:ASN:HD22	1.63	0.64
1:B:146:TYR:HE2	1:B:173:GLN:HE21	1.47	0.63
1:B:168:TRP:O	1:B:172:ILE:HG12	1.99	0.62
1:B:18:PHE:CE2	1:B:32:GLN:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:CG2	1:B:18:PHE:HB2	2.30	0.61
1:B:113:ASP:HA	1:B:156:ARG:HH21	1.66	0.61
1:C:33:VAL:O	1:C:37:VAL:HG23	2.02	0.60
1:A:15:GLU:C	1:A:16:LEU:HD12	2.22	0.59
1:B:276:ILE:O	1:B:280:ILE:HG12	2.03	0.59
1:B:215:GLU:O	1:B:230:HIS:HB2	2.02	0.59
1:B:32:GLN:O	1:B:36:THR:HG23	2.03	0.58
1:C:137:TYR:CD2	1:C:177:GLU:HG2	2.38	0.58
1:C:162:LYS:HE3	1:C:162:LYS:HA	1.85	0.58
1:C:222:ALA:HA	1:C:287:ASN:ND2	2.16	0.57
1:A:34:VAL:HG13	1:A:39:LEU:O	2.04	0.57
1:B:117:CYS:O	1:B:156:ARG:NH1	2.38	0.56
1:C:217:TRP:HB2	1:C:228:TYR:HB2	1.88	0.55
1:B:40:ARG:O	1:B:42:VAL:HG13	2.06	0.55
1:B:192:LEU:O	1:B:196:GLN:HG2	2.07	0.54
1:A:217:TRP:CD1	1:A:230:HIS:HA	2.43	0.54
1:B:146:TYR:HE2	1:B:173:GLN:NE2	2.06	0.54
1:A:256:VAL:CG1	1:A:268:VAL:HG22	2.34	0.54
1:C:251:ASN:HD22	1:C:252:ASP:N	2.05	0.53
1:B:290:LEU:O	1:B:294:ARG:HG2	2.08	0.53
1:A:147:LEU:HD22	1:A:152:LEU:HD11	1.90	0.53
1:A:126:ALA:O	1:A:130:VAL:HG13	2.08	0.53
1:A:142:HIS:HB3	1:A:146:TYR:CD1	2.44	0.53
1:A:8:ARG:HG3	1:A:17:GLU:CG	2.38	0.53
1:B:289:GLU:O	1:B:293:ARG:HB2	2.09	0.53
1:C:7:VAL:HG23	1:C:18:PHE:HB2	1.90	0.52
1:C:196:GLN:HA	1:C:201:TYR:CD2	2.45	0.52
1:A:124:LEU:HD13	1:A:194:ILE:HD13	1.92	0.52
1:C:247:ASN:HD22	2:F:9:ILE:HD11	1.75	0.52
1:B:142:HIS:HB3	1:B:146:TYR:CG	2.45	0.52
1:B:34:VAL:HG11	1:B:42:VAL:HG11	1.92	0.52
1:A:23:ASN:N	1:A:23:ASN:HD22	2.08	0.52
1:A:29:LEU:HD22	1:A:65:VAL:HG21	1.91	0.51
1:A:24:THR:HG23	1:A:28:GLN:HE21	1.75	0.51
1:B:18:PHE:CE2	1:B:32:GLN:CG	2.94	0.50
1:B:164:THR:HG23	1:B:167:GLN:OE1	2.12	0.50
1:A:240:PHE:CB	1:A:245:ILE:HD11	2.41	0.50
1:B:127:SER:CB	1:B:175:TRP:HB3	2.42	0.50
1:C:273:ARG:HG2	1:C:276:ILE:HG12	1.94	0.50
1:B:7:VAL:HG12	1:B:76:LEU:HB2	1.94	0.50
1:C:251:ASN:O	1:C:253:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:VAL:HG11	1:C:42:VAL:HG11	1.94	0.49
1:B:117:CYS:H	1:B:156:ARG:NH1	2.09	0.49
1:C:205:TYR:CD2	1:C:233:LYS:HE2	2.47	0.49
1:A:252:ASP:CG	1:A:253:LYS:H	2.14	0.49
2:F:22:ARG:HG2	2:F:22:ARG:HH21	1.77	0.49
1:B:18:PHE:CE2	2:F:17:PRO:HB3	2.48	0.49
1:B:34:VAL:HG22	1:B:39:LEU:HD23	1.93	0.49
1:A:196:GLN:HA	1:A:201:TYR:CG	2.47	0.49
1:A:74:ASN:HB3	1:A:75:PRO:CD	2.42	0.49
1:C:138:ASN:HB3	1:C:141:ILE:HB	1.95	0.49
1:A:160:GLN:HE22	1:C:262:LYS:H	1.60	0.49
1:C:250:PHE:O	1:C:250:PHE:CD1	2.66	0.49
1:B:288:HIS:O	1:B:291:TYR:HB3	2.12	0.49
1:A:23:ASN:H	1:A:23:ASN:HD22	1.59	0.49
1:B:79:LYS:HG2	1:B:81:ARG:NE	2.27	0.48
1:B:185:GLU:HA	1:B:188:MET:CE	2.42	0.48
1:A:211:LYS:HE3	1:A:268:VAL:HG11	1.94	0.48
1:A:15:GLU:O	1:A:16:LEU:HD12	2.14	0.48
1:B:240:PHE:HB3	1:B:245:ILE:HD11	1.96	0.48
1:B:20:ILE:HG23	1:B:24:THR:HG1	1.78	0.48
1:C:217:TRP:CE2	1:C:233:LYS:HE3	2.49	0.48
1:A:226:ASN:HD22	1:A:236:PRO:HB3	1.78	0.48
1:B:95:GLN:O	1:B:99:GLN:HG3	2.14	0.48
1:C:250:PHE:HB3	1:C:255:PHE:CD1	2.49	0.47
1:B:217:TRP:HB2	1:B:228:TYR:HB2	1.96	0.47
1:A:166:GLU:H	1:A:166:GLU:CD	2.18	0.47
1:A:6:ASN:O	1:A:76:LEU:N	2.39	0.47
1:B:115:ILE:HG23	1:B:200:MET:HB2	1.97	0.47
1:B:132:ALA:HB2	1:B:187:SER:CB	2.43	0.47
1:B:215:GLU:HB3	1:B:230:HIS:CD2	2.50	0.47
1:C:173:GLN:O	1:C:177:GLU:HG3	2.15	0.46
1:C:123:VAL:HG13	1:C:172:ILE:HD13	1.97	0.46
2:F:12:ILE:HA	2:F:12:ILE:HD13	1.84	0.46
1:B:153:LEU:HD21	1:B:172:ILE:HD11	1.96	0.46
1:C:168:TRP:O	1:C:172:ILE:HG12	2.16	0.46
1:B:247:ASN:HD22	1:B:258:LYS:HD2	1.81	0.46
1:A:94:ILE:HG13	1:A:94:ILE:H	1.58	0.46
1:A:10:THR:HG22	1:A:15:GLU:HB2	1.97	0.46
1:C:63:LYS:HB3	1:C:67:GLN:OE1	2.16	0.46
1:A:138:ASN:N	1:A:142:HIS:HD2	2.11	0.45
1:A:49:TYR:HB3	1:A:78:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ASP:HA	1:B:156:ARG:NH2	2.31	0.45
1:B:242:TRP:C	1:B:244:GLU:H	2.20	0.45
1:A:127:SER:CB	1:A:175:TRP:HB3	2.47	0.45
1:B:21:GLN:HB2	1:B:24:THR:HG23	1.99	0.45
1:C:256:VAL:HG23	1:C:268:VAL:HG22	1.98	0.45
1:A:34:VAL:HG11	1:A:42:VAL:HG11	2.00	0.44
1:A:75:PRO:HG2	1:A:77:GLN:HE21	1.83	0.44
1:C:41:GLU:HG3	1:C:98:THR:OG1	2.18	0.44
1:C:215:GLU:O	1:C:230:HIS:HB2	2.17	0.44
1:B:277:ASN:HD22	1:B:277:ASN:HA	1.63	0.44
1:C:247:ASN:HA	2:F:12:ILE:H	1.81	0.44
1:C:235:THR:HA	1:C:236:PRO:HD3	1.88	0.44
1:B:255:PHE:HD1	1:B:277:ASN:ND2	2.15	0.44
1:C:34:VAL:HG13	1:C:39:LEU:O	2.18	0.44
1:C:96:GLU:OE1	1:C:100:ARG:NH1	2.51	0.44
1:B:246:ARG:HB3	1:B:258:LYS:O	2.18	0.43
1:B:74:ASN:HB3	1:B:75:PRO:CD	2.48	0.43
1:B:219:GLY:O	1:B:225:LEU:HA	2.18	0.43
1:C:74:ASN:CB	1:C:75:PRO:HD3	2.43	0.43
1:A:41:GLU:HG3	1:A:98:THR:OG1	2.18	0.43
1:A:74:ASN:HB3	1:A:75:PRO:HD3	1.99	0.43
1:A:21:GLN:HA	1:A:22:PRO:HD3	1.91	0.43
1:B:12:MET:HE1	1:B:108:GLU:HG2	2.00	0.43
1:B:174:ASN:O	1:B:178:GLU:HG3	2.18	0.43
1:C:50:VAL:HG23	1:C:54:GLY:HA2	2.00	0.43
1:A:20:ILE:HD11	1:A:24:THR:HG21	2.01	0.43
1:B:138:ASN:N	1:B:142:HIS:CD2	2.74	0.42
2:F:19:LYS:O	2:F:19:LYS:HG3	2.18	0.42
1:A:217:TRP:HB2	1:A:228:TYR:HB2	2.01	0.42
1:B:185:GLU:HA	1:B:188:MET:HE2	2.00	0.42
1:B:55:TYR:CD2	1:B:55:TYR:N	2.87	0.42
1:A:155:GLN:OE1	2:F:16:LYS:HG3	2.19	0.42
1:C:190:GLU:O	1:C:194:ILE:HG12	2.19	0.42
1:B:57:THR:HG23	1:B:279:ARG:HH12	1.84	0.42
1:C:168:TRP:C	1:C:170:GLU:H	2.23	0.42
1:C:125:LEU:HD21	1:C:194:ILE:HB	2.02	0.42
1:A:111:LEU:HA	1:A:111:LEU:HD12	1.64	0.42
1:B:140:GLU:HB2	1:B:141:ILE:HD12	2.02	0.42
1:C:138:ASN:N	1:C:142:HIS:HD2	2.10	0.42
1:A:22:PRO:O	1:A:66:THR:HG21	2.18	0.42
1:A:143:LYS:HD3	1:A:144:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:HA	1:A:15:GLU:HA	2.02	0.42
1:B:133:LYS:HD3	1:B:134:TYR:CE1	2.55	0.42
1:B:234:LEU:O	1:B:236:PRO:HD3	2.20	0.42
1:C:67:GLN:HB2	1:C:67:GLN:HE21	1.73	0.41
1:A:89:VAL:HG13	1:A:93:LEU:HD12	2.02	0.41
1:A:95:GLN:HB3	1:A:97:ILE:HG12	2.02	0.41
1:A:258:LYS:HA	1:A:259:PRO:HD3	1.70	0.41
1:C:74:ASN:HB3	1:C:75:PRO:CD	2.44	0.41
2:F:22:ARG:NH2	2:F:22:ARG:HG2	2.36	0.41
1:C:127:SER:OG	1:C:179:HIS:HE1	2.04	0.41
1:B:196:GLN:HA	1:B:201:TYR:CD2	2.56	0.41
1:B:252:ASP:HA	1:B:274:LEU:HD13	2.03	0.40
1:A:3:LYS:HA	1:A:4:PRO:HD3	1.97	0.40
1:B:89:VAL:HG23	1:B:93:LEU:CD1	2.45	0.40
1:C:196:GLN:HA	1:C:201:TYR:CG	2.56	0.40
1:B:55:TYR:N	1:B:55:TYR:HD2	2.18	0.40
1:B:18:PHE:HE2	1:B:32:GLN:CG	2.34	0.40
1:A:252:ASP:CG	1:A:253:LYS:N	2.75	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	293/312 (94%)	265 (90%)	24 (8%)	4 (1%)	14	57
1	B	295/312 (95%)	274 (93%)	18 (6%)	3 (1%)	19	65
1	C	290/312 (93%)	255 (88%)	27 (9%)	8 (3%)	6	37
2	D	5/22 (23%)	4 (80%)	0	1 (20%)	0	0
2	E	3/22 (14%)	1 (33%)	2 (67%)	0	100	100
2	F	15/22 (68%)	12 (80%)	3 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	901/1002 (90%)	811 (90%)	74 (8%)	16 (2%)	11	51

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	252	ASP
1	A	222	ALA
1	B	253	LYS
1	C	148	ALA
1	A	144	PRO
1	A	296	LYS
1	C	243	SER
1	C	183	LEU
1	C	272	PRO
1	C	275	ARG
1	A	22	PRO
1	B	74	ASN
1	C	244	GLU
2	D	12	ILE
1	B	243	SER
1	C	56	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 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	268/282 (95%)	238 (89%)	30 (11%)	7	32
1	B	270/282 (96%)	251 (93%)	19 (7%)	19	58
1	C	265/282 (94%)	241 (91%)	24 (9%)	12	42
2	F	16/20 (80%)	10 (62%)	6 (38%)	0	0
All	All	819/866 (95%)	740 (90%)	79 (10%)	10	39

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	18	PHE
1	A	21	GLN
1	A	23	ASN
1	A	27	LYS
1	A	35	LYS
1	A	41	GLU
1	A	47	LEU
1	A	50	VAL
1	A	53	LYS
1	A	63	LYS
1	A	66	THR
1	A	70	VAL
1	A	71	LYS
1	A	94	ILE
1	A	97	ILE
1	A	111	LEU
1	A	124	LEU
1	A	130	VAL
1	A	187	SER
1	A	203	VAL
1	A	204	ASN
1	A	210	ASN
1	A	218	LEU
1	A	223	LEU
1	A	225	LEU
1	A	260	ILE
1	A	261	ASP
1	A	281	LEU
1	A	287	ASN
1	B	10	THR
1	B	17	GLU
1	B	20	ILE
1	B	35	LYS
1	B	36	THR
1	B	55	TYR
1	B	59	LEU
1	B	77	GLN
1	B	79	LYS
1	B	94	ILE
1	B	96	GLU
1	B	108	GLU
1	B	111	LEU

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Mol	Chain	Res	Type
1	B	151	ARG
1	B	156	ARG
1	B	214	THR
1	B	218	LEU
1	B	248	ILE
1	B	277	ASN
1	C	10	THR
1	C	11	THR
1	C	35	LYS
1	C	37	VAL
1	C	39	LEU
1	C	41	GLU
1	C	59	LEU
1	C	67	GLN
1	C	79	LYS
1	C	89	VAL
1	C	108	GLU
1	C	111	LEU
1	C	161	HIS
1	C	162	LYS
1	C	199	GLU
1	C	214	THR
1	C	218	LEU
1	C	227	ILE
1	C	246	ARG
1	C	248	ILE
1	C	251	ASN
1	C	262	LYS
1	C	266	ASP
1	C	295	ARG
2	F	7	MET
2	F	10	THR
2	F	12	ILE
2	F	18	LYS
2	F	19	LYS
2	F	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	23	ASN

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Mol	Chain	Res	Type
1	A	28	GLN
1	A	67	GLN
1	A	68	GLN
1	A	142	HIS
1	A	149	ASN
1	A	160	GLN
1	A	174	ASN
1	A	179	HIS
1	A	210	ASN
1	A	226	ASN
1	A	247	ASN
1	A	277	ASN
1	A	287	ASN
1	B	6	ASN
1	B	67	GLN
1	B	74	ASN
1	B	131	GLN
1	B	142	HIS
1	B	173	GLN
1	B	247	ASN
1	B	277	ASN
1	B	287	ASN
1	C	6	ASN
1	C	142	HIS
1	C	173	GLN
1	C	174	ASN
1	C	179	HIS
1	C	251	ASN
1	C	277	ASN
1	C	287	ASN
2	F	21	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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(Å ²)	Q<0.9
1	A	295/312 (94%)	-0.23	0 100 100	29, 54, 83, 110	0
1	B	297/312 (95%)	-0.09	2 (0%) 89 83	27, 55, 98, 121	0
1	C	292/312 (93%)	-0.07	5 (1%) 73 60	44, 72, 118, 133	0
2	D	7/22 (31%)	0.11	0 100 100	73, 73, 74, 77	0
2	E	5/22 (22%)	0.68	0 100 100	87, 87, 88, 88	0
2	F	17/22 (77%)	-0.41	0 100 100	45, 54, 68, 71	0
All	All	913/1002 (91%)	-0.13	7 (0%) 87 80	27, 60, 107, 133	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72	LYS	3.2
1	C	22	PRO	3.0
1	B	261	ASP	2.7
1	C	67	GLN	2.5
1	C	71	LYS	2.2
1	B	262	LYS	2.2
1	C	74	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.