



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:26 AM UTC

PDB ID : 3TW8 / pdb_00003tw8
Title : GEF domain of DENND 1B in complex with Rab GTPase Rab35
Authors : Wu, X.D.; Kummel, D.; Reinisch, K.M.
Deposited on : 2011-09-21
Resolution : 2.10 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

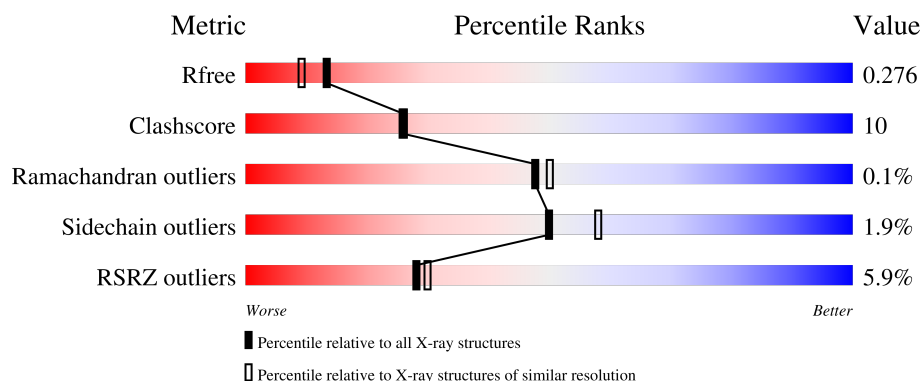
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	391	3% 69% 17% • 12%
1	C	391	5% 74% 17% • 7%
2	B	181	10% 78% 14% • 7%
2	D	181	8% 77% 17% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8573 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 DENN domain-containing protein 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	87	0	0
			2751	1772	458	504	17			
1	C	362	Total	C	N	O	S	115	0	0
			2893	1863	480	533	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q6P3S1-2
C	1	SER	-	expression tag	UNP Q6P3S1-2

- Molecule 2 is a protein called Ras-related protein Rab-35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	60	0	0
			1357	858	232	262	5			
2	D	173	Total	C	N	O	S	75	0	0
			1385	876	236	268	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q15286
D	0	SER	-	expression tag	UNP Q15286

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total	O	0	0
			80	80		
3	B	18	Total	O	0	0
			18	18		

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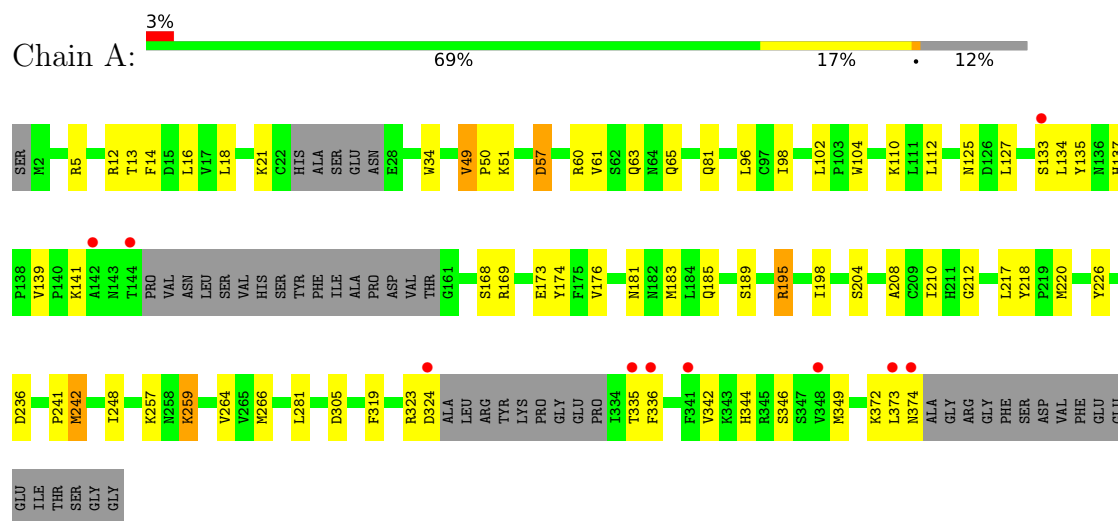
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	64	Total 64	O 64	0	0
3	D	25	Total 25	O 25	0	0

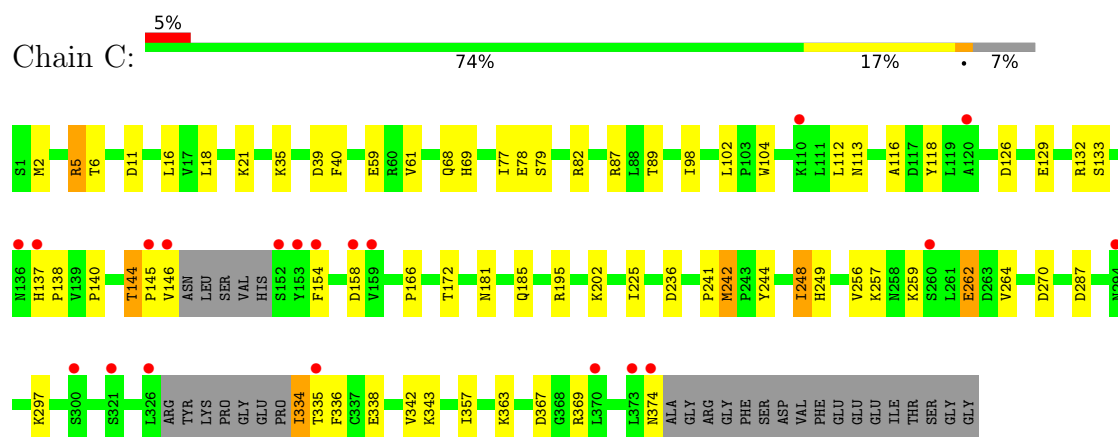
3 Residue-property plots

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.

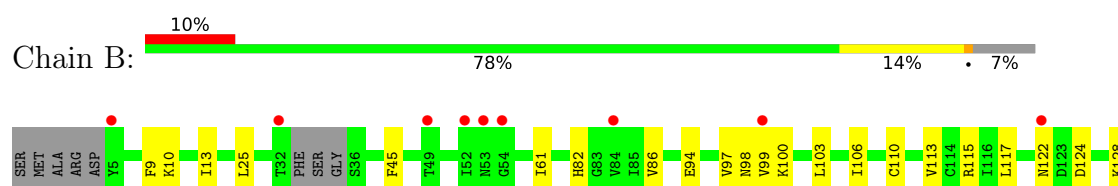
• Molecule 1: DENN domain-containing protein 1B

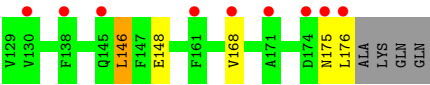


• Molecule 1: DENN domain-containing protein 1B

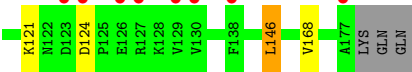
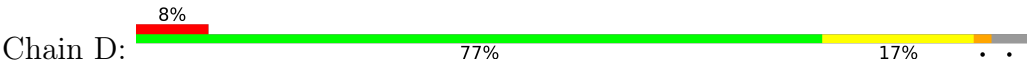


• Molecule 2: Ras-related protein Rab-35





● Molecule 2: Ras-related protein Rab-35



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.59Å 56.56Å 175.31Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	24.89 – 2.10 24.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.89-2.10) 91.1 (24.89-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.227 , 0.269 0.237 , 0.276	Depositor DCC
R_{free} test set	4502 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.7	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	0.94	EDS
Total number of atoms	8573	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	1.18	6/2812 (0.2%)	1.10	8/3813 (0.2%)
1	C	1.18	5/2960 (0.2%)	1.16	14/4020 (0.3%)
2	B	0.92	0/1377	0.98	2/1858 (0.1%)
2	D	1.06	1/1406 (0.1%)	1.04	1/1897 (0.1%)
All	All	1.12	12/8555 (0.1%)	1.09	25/11588 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	ARG	CZ-NH1	-10.05	1.18	1.32
1	C	195	ARG	CZ-NH2	-9.45	1.21	1.33
1	A	195	ARG	CZ-NH2	-9.29	1.21	1.33
1	A	195	ARG	CZ-NH1	-8.93	1.20	1.32
1	C	369	ARG	CD-NE	-8.45	1.34	1.46
1	A	204	SER	C-O	-6.16	1.17	1.24
1	A	212	GLY	N-CA	6.02	1.53	1.45
1	A	57	ASP	N-CA	5.59	1.53	1.46
1	A	208	ALA	C-O	5.54	1.30	1.24
1	C	249	HIS	C-O	-5.30	1.17	1.23
1	C	11	ASP	C-O	-5.25	1.17	1.24
2	D	124	ASP	CB-CG	-5.02	1.39	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	ARG	NE-CZ-NH2	12.62	130.56	119.20
1	C	195	ARG	NH1-CZ-NH2	-11.80	103.96	119.30
1	A	195	ARG	NH1-CZ-NH2	-11.33	104.58	119.30
1	C	144	THR	CA-C-N	10.20	130.61	119.90
1	C	144	THR	C-N-CA	10.20	130.61	119.90
1	A	195	ARG	NE-CZ-NH2	8.82	127.14	119.20
2	D	33	PHE	CA-CB-CG	-7.11	106.69	113.80
2	B	128	LYS	CG-CD-CE	-6.90	95.42	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	N-CA-C	6.87	118.92	111.77
1	A	195	ARG	NE-CZ-NH1	6.61	128.11	121.50
1	A	21	LYS	CB-CG-CD	6.33	125.87	111.30
1	C	59	GLU	CA-CB-CG	-6.26	101.58	114.10
1	C	59	GLU	CB-CG-CD	-6.01	102.39	112.60
1	A	141	LYS	CA-CB-CG	5.82	125.73	114.10
1	C	158	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	129	GLU	CB-CG-CD	-5.79	102.76	112.60
1	C	129	GLU	CA-CB-CG	-5.78	102.55	114.10
1	C	297	LYS	CB-CG-CD	5.70	124.41	111.30
1	A	169	ARG	CG-CD-NE	-5.56	99.76	112.00
2	B	124	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	132	ARG	CA-CB-CG	-5.27	103.56	114.10
1	C	297	LYS	CA-CB-CG	5.20	124.51	114.10
1	C	343	LYS	CG-CD-CE	5.19	123.23	111.30
1	A	49	VAL	O-C-N	5.09	123.68	120.07
1	C	257	LYS	N-CA-C	5.05	117.52	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2751	0	2760	56	1
1	C	2893	0	2896	51	2
2	B	1357	0	1348	19	0
2	D	1385	0	1369	29	2
3	A	80	0	0	3	0
3	B	18	0	0	1	0
3	C	64	0	0	7	0
3	D	25	0	0	1	0
All	All	8573	0	8373	152	3

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 10.

All (152) 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:257:LYS:NZ	1:A:266:MET:HE1	1.86	0.91
1:A:257:LYS:NZ	1:A:266:MET:CE	2.39	0.86
1:A:257:LYS:HZ1	1:A:266:MET:CE	1.91	0.83
1:C:262:GLU:O	1:C:264:VAL:HG23	1.85	0.76
2:D:94:GLU:O	2:D:97:VAL:HG22	1.85	0.76
2:B:122:ASN:HD22	2:B:148:GLU:HB3	1.54	0.72
2:B:106:ILE:HG21	2:B:115:ARG:HD2	1.72	0.71
2:D:106:ILE:HG21	2:D:115:ARG:HD2	1.72	0.71
1:C:146:VAL:HB	1:C:154:PHE:CZ	2.25	0.71
2:D:10:LYS:H	2:D:82:HIS:HD2	1.36	0.71
1:A:257:LYS:HZ3	1:A:266:MET:HE1	1.54	0.70
1:C:146:VAL:CB	1:C:154:PHE:CE2	2.74	0.69
1:C:241:PRO:HG2	1:C:242:MET:CE	2.22	0.69
2:D:117:LEU:HD23	2:D:146:LEU:HD13	1.74	0.69
1:A:241:PRO:HD2	1:A:242:MET:HE3	1.75	0.68
1:C:259:LYS:NZ	3:C:424:HOH:O	2.25	0.67
1:A:168:SER:HB2	3:A:433:HOH:O	1.94	0.66
1:A:257:LYS:HZ1	1:A:266:MET:HE1	1.53	0.66
1:A:189:SER:OG	3:A:441:HOH:O	2.13	0.66
1:C:363:LYS:HE3	2:D:72:THR:HB	1.77	0.66
1:A:63:GLN:H	1:A:63:GLN:CD	2.04	0.66
1:A:257:LYS:HZ1	1:A:266:MET:HE2	1.62	0.65
2:D:9:PHE:CD2	2:D:168:VAL:CG1	2.80	0.64
2:B:117:LEU:HD23	2:B:146:LEU:HD13	1.80	0.64
1:C:181:ASN:O	1:C:185:GLN:HG2	1.99	0.62
1:A:12:ARG:HD3	1:A:135:TYR:CE1	2.35	0.62
1:A:51:LYS:NZ	3:A:460:HOH:O	2.27	0.61
1:A:241:PRO:HG2	1:A:242:MET:CE	2.30	0.61
2:B:94:GLU:O	2:B:97:VAL:HG22	2.00	0.61
2:D:9:PHE:CD2	2:D:168:VAL:HG12	2.35	0.61
2:D:97:VAL:HG23	2:D:98:ASN:N	2.16	0.60
1:C:146:VAL:HB	1:C:154:PHE:CE2	2.34	0.60
1:C:334:ILE:CG2	1:C:374:ASN:HD21	2.13	0.60
2:B:106:ILE:HG21	2:B:115:ARG:CD	2.32	0.60
1:C:82:ARG:HD3	3:C:394:HOH:O	2.02	0.59
1:C:242:MET:CE	1:C:242:MET:H	2.14	0.59
1:C:87:ARG:NH1	1:C:89:THR:HG22	2.18	0.58
1:C:2:MET:HE1	1:C:367:ASP:HB3	1.85	0.58
1:C:242:MET:H	1:C:242:MET:HE3	1.68	0.58
1:A:102:LEU:HD13	1:A:104:TRP:CZ2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:GLU:O	2:D:97:VAL:CG2	2.53	0.56
1:C:236:ASP:OD1	1:C:259:LYS:HE3	2.06	0.56
1:C:335:THR:HG22	1:C:336:PHE:H	1.71	0.56
2:D:110:CYS:O	2:D:113:VAL:HG23	2.06	0.56
1:A:323:ARG:O	1:A:324:ASP:OD2	2.25	0.55
1:A:81:GLN:NE2	1:A:226:TYR:CD2	2.74	0.55
2:B:10:LYS:H	2:B:82:HIS:HD2	1.54	0.55
2:D:106:ILE:HG21	2:D:115:ARG:CD	2.37	0.55
1:A:241:PRO:HG2	1:A:242:MET:HE2	1.89	0.54
1:C:144:THR:HG22	1:C:145:PRO:N	2.23	0.54
1:A:195:ARG:O	1:A:264:VAL:HG13	2.09	0.53
1:C:241:PRO:HD2	1:C:242:MET:HE3	1.89	0.53
1:C:335:THR:HG22	1:C:336:PHE:N	2.23	0.53
1:C:342:VAL:CG1	1:C:342:VAL:O	2.56	0.53
1:A:34:TRP:CZ2	1:A:127:LEU:HD21	2.43	0.53
1:A:241:PRO:HD2	1:A:242:MET:CE	2.39	0.53
1:A:335:THR:HG22	1:A:336:PHE:N	2.24	0.52
2:D:99:VAL:HG11	2:D:117:LEU:CD1	2.39	0.52
1:A:335:THR:HG22	1:A:336:PHE:H	1.75	0.52
1:A:242:MET:CE	1:A:242:MET:H	2.23	0.51
1:A:236:ASP:OD1	1:A:259:LYS:HE2	2.11	0.51
2:D:86:VAL:HG21	2:D:103:LEU:HD21	1.93	0.51
1:A:241:PRO:CD	1:A:242:MET:HE3	2.40	0.50
1:C:68:GLN:HG2	3:C:396:HOH:O	2.11	0.50
2:D:5:TYR:CD1	2:D:5:TYR:C	2.90	0.50
2:D:9:PHE:CE2	2:D:168:VAL:HG12	2.47	0.50
2:B:100:LYS:HB2	3:B:181:HOH:O	2.12	0.50
1:C:77:ILE:HB	3:C:398:HOH:O	2.12	0.50
1:A:60:ARG:O	1:A:63:GLN:NE2	2.35	0.49
1:A:102:LEU:HD13	1:A:104:TRP:CH2	2.47	0.49
2:B:45:PHE:C	2:B:45:PHE:CD1	2.90	0.49
2:B:9:PHE:CD2	2:B:168:VAL:HG12	2.48	0.49
1:A:344:HIS:CE1	1:A:346:SER:OG	2.66	0.49
1:C:87:ARG:NH1	1:C:116:ALA:CB	2.76	0.48
1:A:185:GLN:NE2	1:A:281:LEU:CD2	2.76	0.48
2:B:97:VAL:HG23	2:B:98:ASN:N	2.29	0.48
1:A:181:ASN:O	1:A:185:GLN:HG2	2.14	0.48
2:B:175:ASN:O	2:B:176:LEU:C	2.57	0.48
1:C:2:MET:CE	1:C:367:ASP:HB3	2.43	0.48
1:C:102:LEU:HD13	1:C:104:TRP:CZ2	2.48	0.48
1:A:220:MET:HE1	1:A:319:PHE:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ILE:HB	2:B:61:ILE:HD11	1.95	0.47
1:A:185:GLN:NE2	1:A:281:LEU:HD22	2.29	0.47
2:D:36:SER:HB3	3:D:202:HOH:O	2.14	0.47
1:A:257:LYS:NZ	1:A:266:MET:HE2	2.23	0.47
2:B:9:PHE:CD2	2:B:168:VAL:CG1	2.97	0.47
1:C:16:LEU:HD11	1:C:18:LEU:HD21	1.96	0.47
2:D:4:ASP:OD1	2:D:4:ASP:N	2.48	0.47
1:A:195:ARG:HB2	1:A:264:VAL:HG22	1.97	0.46
1:C:241:PRO:CD	1:C:242:MET:HE3	2.46	0.46
1:C:118:TYR:CE1	1:C:126:ASP:HB3	2.50	0.46
1:A:102:LEU:HD11	1:A:139:VAL:HG13	1.98	0.46
2:B:45:PHE:HA	2:B:61:ILE:O	2.16	0.46
1:C:241:PRO:HD2	1:C:242:MET:CE	2.46	0.46
2:D:45:PHE:HA	2:D:61:ILE:O	2.16	0.46
1:A:13:THR:OG1	1:A:134:LEU:HD23	2.17	0.45
1:C:6:THR:CG2	3:C:397:HOH:O	2.64	0.45
1:A:16:LEU:HD11	1:A:18:LEU:HD21	1.98	0.45
2:D:9:PHE:CD2	2:D:168:VAL:HG11	2.50	0.45
2:B:86:VAL:HG21	2:B:103:LEU:HD21	1.98	0.45
1:A:134:LEU:HD23	1:A:134:LEU:O	2.16	0.45
1:C:241:PRO:HG2	1:C:242:MET:HE2	1.98	0.45
1:C:338:GLU:HG2	1:C:357:ILE:HD11	1.98	0.45
2:B:113:VAL:O	2:B:115:ARG:NH1	2.46	0.44
1:C:104:TRP:HH2	1:C:140:PRO:HG2	1.83	0.44
2:D:113:VAL:O	2:D:115:ARG:NH1	2.50	0.44
2:D:45:PHE:CD1	2:D:45:PHE:C	2.94	0.44
1:A:49:VAL:N	1:A:50:PRO:CD	2.81	0.44
1:A:198:ILE:HD12	1:A:210:ILE:HD13	1.99	0.44
1:A:257:LYS:HZ3	1:A:266:MET:CE	2.16	0.44
2:D:36:SER:OG	2:D:38:ILE:HG22	2.18	0.44
2:D:110:CYS:HB3	2:D:113:VAL:HG23	2.00	0.43
1:C:78:GLU:O	1:C:79:SER:OG	2.27	0.43
1:C:98:ILE:HG13	1:C:112:LEU:HD21	1.99	0.43
1:A:174:TYR:CE2	1:A:183:MET:HE3	2.53	0.43
1:A:305:ASP:OD1	1:A:305:ASP:C	2.60	0.43
1:C:18:LEU:HD22	1:C:35:LYS:HB3	2.00	0.43
1:C:39:ASP:O	1:C:40:PHE:C	2.62	0.43
1:C:241:PRO:CG	1:C:242:MET:CE	2.96	0.43
2:D:10:LYS:HE2	2:D:60:GLN:NE2	2.34	0.43
2:B:110:CYS:O	2:B:113:VAL:HG23	2.19	0.42
1:A:14:PHE:CE2	1:A:134:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLN:NE2	1:A:226:TYR:CE2	2.87	0.42
1:A:98:ILE:HG13	1:A:112:LEU:HD21	2.02	0.42
1:C:69:HIS:CE1	1:C:113:ASN:OD1	2.72	0.42
1:C:133:SER:O	1:C:137:HIS:HB2	2.19	0.42
1:A:65:GLN:O	1:C:21:LYS:NZ	2.49	0.42
1:A:57:ASP:C	1:A:57:ASP:OD1	2.62	0.42
1:A:12:ARG:HD3	1:A:135:TYR:CZ	2.54	0.41
1:C:87:ARG:NH1	1:C:116:ALA:HB1	2.35	0.41
1:C:342:VAL:O	1:C:342:VAL:HG12	2.18	0.41
1:C:225:ILE:HB	1:C:244:TYR:CB	2.50	0.41
1:A:344:HIS:CD2	1:A:349:MET:HG2	2.55	0.41
2:B:94:GLU:O	2:B:97:VAL:CG2	2.68	0.41
2:B:99:VAL:HG11	2:B:117:LEU:CD1	2.51	0.41
1:A:217:LEU:O	1:A:218:TYR:C	2.63	0.41
1:A:241:PRO:CD	1:A:242:MET:CE	2.99	0.41
1:A:372:LYS:C	1:A:374:ASN:N	2.78	0.41
1:C:5:ARG:HH11	1:C:5:ARG:HD3	1.71	0.41
2:D:9:PHE:HB2	2:D:59:LEU:HD12	2.03	0.41
1:A:133:SER:O	1:A:137:HIS:HB2	2.20	0.41
1:C:166:PRO:HA	1:C:172:THR:OG1	2.21	0.41
2:D:18:GLY:O	2:D:121:LYS:HE3	2.21	0.40
1:A:323:ARG:O	1:A:324:ASP:CG	2.65	0.40
1:C:137:HIS:HA	1:C:138:PRO:HD2	1.90	0.40
1:C:248:ILE:HD12	1:C:256:VAL:HG21	2.01	0.40
1:A:173:GLU:HA	1:A:176:VAL:HG22	2.04	0.40
1:C:202:LYS:HD2	3:C:430:HOH:O	2.20	0.40
1:C:270:ASP:OD1	3:C:439:HOH:O	2.22	0.40
1:C:363:LYS:CE	2:D:72:THR:HB	2.47	0.40
2:D:14:ILE:HA	2:D:67:GLN:OE1	2.22	0.40
2:D:8:LEU:HD12	2:D:9:PHE:H	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:CG	1:A:181:ASN:ND2[1_545]	2.15	0.05
1:C:287:ASP:OD2	2:D:33:PHE:CE1[1_565]	2.17	0.03
1:C:287:ASP:OD2	2:D:33:PHE:CZ[1_565]	2.18	0.02

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	335/391 (86%)	322 (96%)	12 (4%)	1 (0%)	36	36
1	C	356/391 (91%)	345 (97%)	11 (3%)	0	100	100
2	B	165/181 (91%)	158 (96%)	7 (4%)	0	100	100
2	D	169/181 (93%)	164 (97%)	5 (3%)	0	100	100
All	All	1025/1144 (90%)	989 (96%)	35 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	LEU

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	312/351 (89%)	305 (98%)	7 (2%)	45	53
1	C	328/351 (93%)	322 (98%)	6 (2%)	51	60
2	B	151/160 (94%)	149 (99%)	2 (1%)	61	69
2	D	153/160 (96%)	150 (98%)	3 (2%)	48	56
All	All	944/1022 (92%)	926 (98%)	18 (2%)	50	58

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	96	LEU
1	A	110	LYS
1	A	242	MET
1	A	248	ILE
1	A	259	LYS
1	A	342	VAL
2	B	25	LEU
2	B	146	LEU
1	C	5	ARG
1	C	61	VAL
1	C	242	MET
1	C	248	ILE
1	C	262	GLU
1	C	334	ILE
2	D	25	LEU
2	D	99	VAL
2	D	146	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	185	GLN
1	A	315	GLN
2	B	60	GLN
2	B	82	HIS
2	B	109	ASN
2	B	122	ASN
2	B	141	GLN
1	C	69	HIS
1	C	374	ASN
2	D	60	GLN
2	D	82	HIS
2	D	109	ASN
2	D	122	ASN
2	D	141	GLN

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 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	343/391 (87%)	0.28	10 (2%)	53	56	18, 44, 77, 104	22 (6%)
1	C	362/391 (92%)	0.43	20 (5%)	30	32	26, 47, 80, 120	33 (9%)
2	B	169/181 (93%)	0.91	18 (10%)	11	11	30, 61, 85, 99	16 (9%)
2	D	173/181 (95%)	0.57	14 (8%)	18	19	22, 49, 75, 98	19 (10%)
All	All	1047/1144 (91%)	0.48	62 (5%)	28	30	18, 48, 80, 120	90 (8%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	177	ALA	6.1
1	C	152	SER	4.6
1	C	146	VAL	4.5
2	B	53	ASN	4.3
1	C	326	LEU	4.1
1	C	154	PHE	4.0
2	B	52	ILE	3.8
1	A	335	THR	3.7
1	A	144	THR	3.6
1	A	336	PHE	3.4
2	D	33	PHE	3.4
1	C	145	PRO	3.3
2	B	5	TYR	3.3
2	B	176	LEU	3.3
1	C	158	ASP	3.3
2	B	145	GLN	3.2
2	D	32	THR	3.2
1	C	335	THR	3.1
1	C	153	TYR	3.1
2	B	32	THR	3.0
1	C	159	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	348	VAL	3.0
1	A	142	ALA	2.9
1	C	374	ASN	2.9
1	C	136	ASN	2.9
1	A	341	PHE	2.8
2	B	99	VAL	2.7
2	B	49	THR	2.6
2	B	174	ASP	2.6
1	C	120	ALA	2.6
2	D	124	ASP	2.6
2	D	129	VAL	2.5
2	B	122	ASN	2.5
2	D	126	GLU	2.5
2	D	130	VAL	2.4
1	A	373	LEU	2.4
2	D	138	PHE	2.4
1	A	324	ASP	2.4
2	D	93	ALA	2.4
1	A	374	ASN	2.3
2	B	161	PHE	2.3
2	B	168	VAL	2.3
2	D	4	ASP	2.3
1	C	110	LYS	2.3
1	C	300	SER	2.3
1	C	294	ASN	2.2
2	D	127	ARG	2.1
1	A	133	SER	2.1
2	D	23	SER	2.1
2	B	138	PHE	2.1
1	C	260	SER	2.1
2	B	175	ASN	2.1
2	D	123	ASP	2.1
2	B	54	GLY	2.1
2	B	84	VAL	2.1
1	C	370	LEU	2.1
2	D	112	ASP	2.1
1	C	137	HIS	2.1
2	B	171	ALA	2.1
2	B	130	VAL	2.0
1	C	321	SER	2.0
1	C	373	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.