Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:25 PM GMT

PDB ID	:	3TW8
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

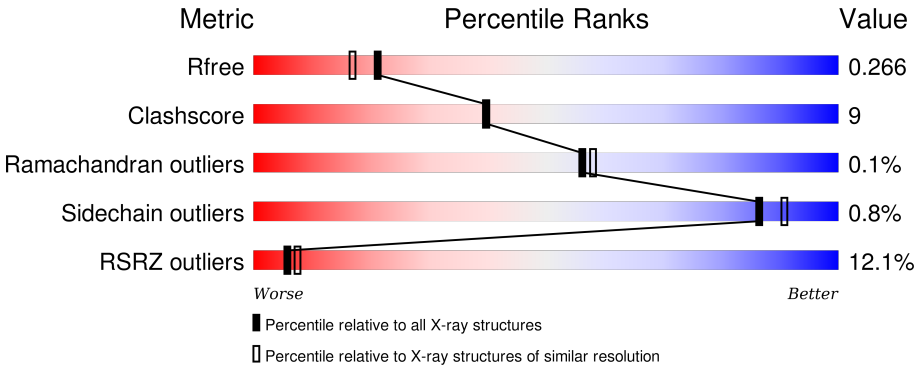
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 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 <=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	7% 73% 14% • 12%
1	C	391	11% 75% 16% • 7%
2	B	181	17% 78% 14% • 7%
2	D	181	15% 76% 19% • •

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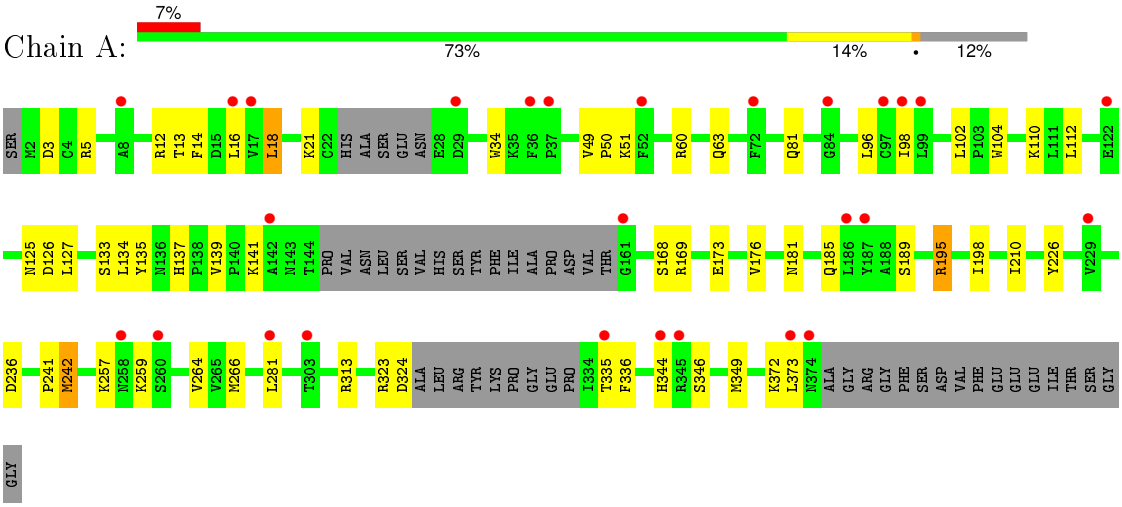
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	64	Total O 64 64	0	0
3	D	25	Total O 25 25	0	0

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.

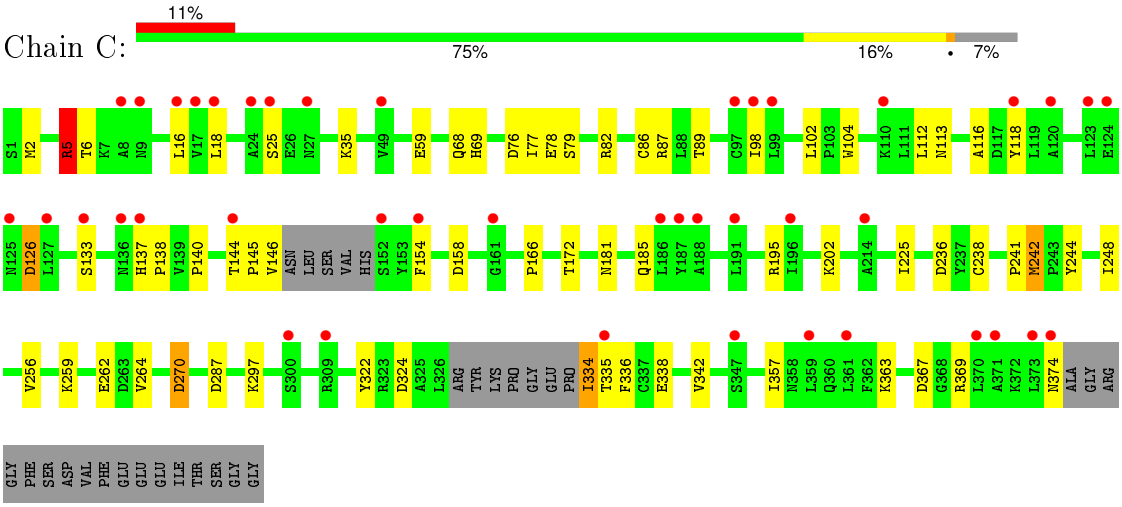
- Molecule 1: DENN domain-containing protein 1B

Chain A:



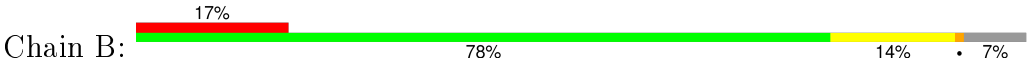
- Molecule 1: DENN domain-containing protein 1B

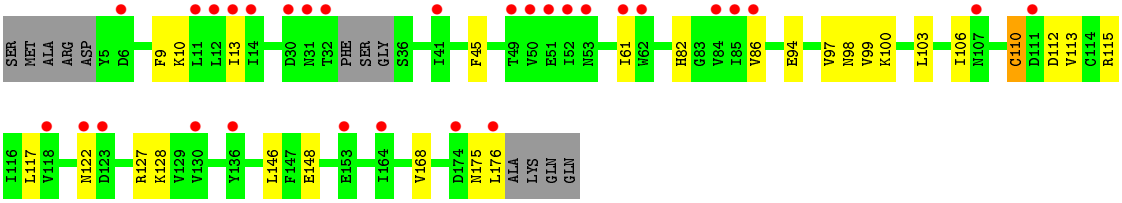
Chain C:



- Molecule 2: Ras-related protein Rab-35

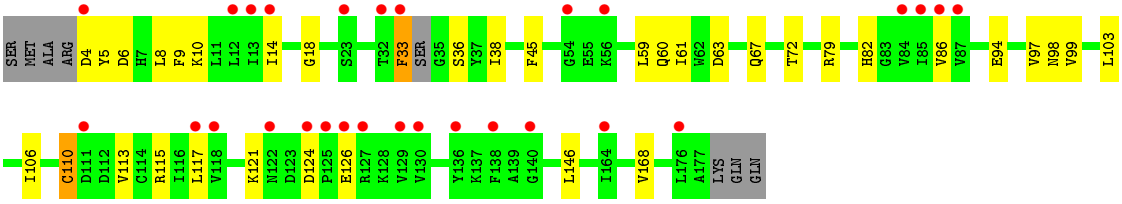
Chain B:





- Molecule 2: Ras-related protein Rab-35

Chain D:



4 Data and refinement statistics (i)

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) 91.2 (24.89-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.227 , 0.269 0.226 , 0.266	Depositor DCC
R_{free} test set	4502 reflections (7.56%)	DCC
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 64040 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.97	3/2812 (0.1%)	1.00	13/3813 (0.3%)
1	C	1.00	8/2960 (0.3%)	0.99	12/4020 (0.3%)
2	B	0.79	2/1377 (0.1%)	0.82	3/1858 (0.2%)
2	D	0.92	3/1406 (0.2%)	0.89	6/1897 (0.3%)
All	All	0.94	16/8555 (0.2%)	0.95	34/11588 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	ARG	CZ-NH1	-11.05	1.18	1.33
1	A	195	ARG	CZ-NH1	-9.84	1.20	1.33
1	C	195	ARG	CZ-NH2	-9.14	1.21	1.33
1	A	195	ARG	CZ-NH2	-8.98	1.21	1.33
1	C	238	CYS	CB-SG	-8.88	1.67	1.82
1	C	369	ARG	CD-NE	-7.08	1.34	1.46
1	C	25	SER	CB-OG	-6.50	1.33	1.42
2	D	110	CYS	CB-SG	-6.47	1.71	1.82
2	D	124	ASP	CB-CG	-5.83	1.39	1.51
1	C	158	ASP	CB-CG	-5.80	1.39	1.51
2	D	126	GLU	CB-CG	-5.66	1.41	1.52
2	B	127	ARG	CB-CG	5.33	1.67	1.52
1	C	86	CYS	CB-SG	-5.24	1.73	1.81
1	A	372	LYS	CB-CG	-5.18	1.38	1.52
2	B	110	CYS	CB-SG	-5.07	1.73	1.81
1	C	59	GLU	CB-CG	5.06	1.61	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	ARG	NE-CZ-NH2	20.52	130.56	120.30
1	A	195	ARG	NE-CZ-NH1	15.61	128.11	120.30
1	C	195	ARG	NH1-CZ-NH2	-14.04	103.96	119.40
1	A	195	ARG	NE-CZ-NH2	13.68	127.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	ARG	NH1-CZ-NH2	-13.48	104.58	119.40
1	C	195	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	C	126	ASP	CB-CG-OD2	-9.18	110.04	118.30
2	B	112	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	3	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	313	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	3	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	D	63	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	126	ASP	CB-CG-OD1	6.05	123.75	118.30
2	D	33	PHE	CB-CG-CD1	-5.96	116.63	120.80
2	B	128	LYS	CD-CE-NZ	-5.94	98.03	111.70
1	A	126	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	76	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	76	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	313	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	169	ARG	CG-CD-NE	-5.73	99.76	111.80
1	C	270	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	141	LYS	CA-CB-CG	5.61	125.73	113.40
1	C	324	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	128	LYS	CG-CD-CE	-5.49	95.42	111.90
1	A	21	LYS	CB-CG-CD	5.49	125.87	111.60
1	C	59	GLU	CA-CB-CG	-5.37	101.58	113.40
2	D	79	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	D	33	PHE	CB-CG-CD2	5.25	124.47	120.80
1	C	5	ARG	CG-CD-NE	5.19	122.69	111.80
1	A	18	LEU	CA-CB-CG	5.16	127.16	115.30
2	D	6	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	D	63	ASP	CB-CG-OD1	5.12	122.90	118.30
1	C	297	LYS	CA-CB-CG	5.05	124.51	113.40
1	A	126	ASP	CB-CG-OD1	5.00	122.80	118.30

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	2751	0	2760	49	1
1	C	2893	0	2896	47	2
2	B	1357	0	1348	19	0
2	D	1385	0	1369	28	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	141	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 9.

All (141) 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	1.80	0.96
1:A:257:LYS:NZ	1:A:266:MET:CE	2.39	0.85
1:A:257:LYS:HZ1	1:A:266:MET:CE	1.91	0.83
1:C:242:MET:H	1:C:242:MET:HE3	1.47	0.77
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
1:A:257:LYS:HZ3	1:A:266:MET:HE1	1.49	0.73
2:B:122:ASN:HD22	2:B:148:GLU:HB3	1.54	0.72
1:A:257:LYS:HZ1	1:A:266:MET:HE1	1.47	0.71
2:D:106:ILE:HG21	2:D:115:ARG:HD2	1.72	0.71
2:B:106:ILE:HG21	2:B: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: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:51:LYS:NZ	3:A:460:HOH:O	2.27	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: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
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:241:PRO:HD2	1:A:242:MET:HE3	1.81	0.62
1:A:12:ARG:HD3	1:A:135:TYR:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:63:GLN:H	1:A:63:GLN:CD	2.04	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:A:257:LYS:HZ1	1:A:266:MET:HE2	1.67	0.59
1:C:82:ARG:HD3	3:C:394:HOH:O	2.02	0.59
1:C:242:MET:H	1:C:242:MET:CE	2.14	0.59
1:C:87:ARG:NH1	1:C:89:THR:HG22	2.18	0.58
1:A:241:PRO:HG2	1:A:242:MET:HE2	1.87	0.57
1:A:102:LEU:HD13	1:A:104:TRP:CZ2	2.40	0.56
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
2:B:10:LYS:H	2:B:82:HIS:HD2	1.54	0.55
1:A:81:GLN:NE2	1:A:226:TYR:CD2	2.74	0.55
2:D:106:ILE:HG21	2:D:115:ARG:CD	2.37	0.55
1:C:144:THR:HG22	1:C:145:PRO:N	2.23	0.54
1:C:335:THR:HG22	1:C:336:PHE:N	2.23	0.53
1:A:195:ARG:O	1:A:264:VAL:HG13	2.09	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
2:D:99:VAL:HG11	2:D:117:LEU:CD1	2.39	0.52
1:A:335:THR:HG22	1:A:336:PHE:N	2.24	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:C:78:GLU:O	1:C:79:SER:OG	2.27	0.51
2:D:86:VAL:HG21	2:D:103:LEU:HD21	1.93	0.51
1:A:236:ASP:OD1	1:A:259:LYS:HE2	2.11	0.51
1:C:68:GLN:HG2	3:C:396:HOH:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:241:PRO:HG2	1:C:242:MET:HE2	1.93	0.48
2:B:97:VAL:HG23	2:B:98:ASN:N	2.29	0.48
1:A:241:PRO:CD	1:A:242:MET:HE3	2.42	0.48
1:A:181:ASN:O	1:A:185:GLN:HG2	2.14	0.48
1:A:242:MET:H	1:A:242:MET:HE3	1.78	0.48
1:C:102:LEU:HD13	1:C:104:TRP:CZ2	2.48	0.48
1:C:2:MET:CE	1:C:367:ASP:HB3	2.43	0.48
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
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:N	2:D:4:ASP:OD1	2.48	0.47
1:A:195:ARG:HB2	1:A:264:VAL:HG22	1.97	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
1:C:241:PRO:HD2	1:C:242:MET:CE	2.46	0.46
2:B:45:PHE:HA	2:B:61:ILE:O	2.16	0.46
2:D:45:PHE:HA	2:D:61:ILE:O	2.16	0.46
1:C:6:THR:CG2	3:C:397:HOH:O	2.64	0.45
1:A:13:THR:OG1	1:A:134:LEU:HD23	2.17	0.45
2:D:5:TYR:CD1	2:D:5:TYR:C	2.90	0.45
2:D:9:PHE:CD2	2:D:168:VAL:HG11	2.50	0.45
1:A:16:LEU:HD11	1:A:18:LEU:HD21	1.98	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:338:GLU:HG2	1:C:357:ILE:HD11	1.98	0.45
2:D:113:VAL:O	2:D:115:ARG:NH1	2.50	0.44
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:B:45:PHE:C	2:B:45:PHE:CD1	2.90	0.44
1:A:49:VAL:N	1:A:50:PRO:CD	2.81	0.44
1:A:257:LYS:HZ3	1:A:266:MET:CE	2.16	0.44
1:A:198:ILE:HD12	1:A:210:ILE:HD13	1.99	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:98:ILE:HG13	1:C:112:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:O	2:B:176:LEU:C	2.57	0.43
1:C:2:MET:HE1	1:C:367:ASP:HB3	1.99	0.43
1:C:241:PRO:CG	1:C:242:MET:CE	2.96	0.43
1:C:18:LEU:HD22	1:C:35:LYS:HB3	2.00	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:81:GLN:NE2	1:A:226:TYR:CE2	2.87	0.42
1:A:14:PHE:CE2	1:A:134:LEU:HD22	2.54	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: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:HG12	1:C:342:VAL:O	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:99:VAL:HG11	2:B:117:LEU:CD1	2.51	0.41
2:B:94:GLU:O	2:B:97:VAL:CG2	2.68	0.41
1:A:241:PRO:CD	1:A:242:MET:CE	2.99	0.41
2:D:9:PHE:HB2	2:D:59:LEU:HD12	2.03	0.41
1:C:5:ARG:HH11	1:C:5:ARG:HD3	1.71	0.41
1:A:257:LYS:NZ	1:A:266:MET:HE2	2.30	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: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:C:363:LYS:CE	2:D:72:THR:HB	2.47	0.40
1:C:202:LYS:HD2	3:C:430:HOH:O	2.20	0.40
1:A:173:GLU:HA	1:A:176:VAL:HG22	2.04	0.40
2:D:14:ILE:HA	2:D:67:GLN:OE1	2.22	0.40
1:C:270:ASP:OD1	3:C:439:HOH:O	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 (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	335/391 (86%)	322 (96%)	12 (4%)	1 (0%)	46 45
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%)	56 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	LEU

5.3.2 Protein sidechains (i)

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%)	308 (99%)	4 (1%)	76 82
1	C	328/351 (93%)	324 (99%)	4 (1%)	78 84
2	B	151/160 (94%)	151 (100%)	0	100 100
2	D	153/160 (96%)	153 (100%)	0	100 100
All	All	944/1022 (92%)	936 (99%)	8 (1%)	86 91

All (8) 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	C	5	ARG
1	C	242	MET
1	C	322	TYR
1	C	334	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

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

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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, 95^{th} 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%)	0.47	27 (7%) 15 21	26, 45, 83, 104	22 (6%)
1	C	362/391 (92%)	0.61	42 (11%) 6 9	26, 50, 84, 120	33 (9%)
2	B	169/181 (93%)	1.05	30 (17%) 2 2	36, 62, 86, 99	16 (9%)
2	D	173/181 (95%)	0.68	28 (16%) 3 3	31, 52, 80, 98	19 (10%)
All	All	1047/1144 (91%)	0.65	127 (12%) 6 7	26, 51, 85, 120	90 (8%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	31	ASN	5.5
2	B	52	ILE	5.4
2	D	176	LEU	5.1
1	C	8	ALA	5.0
2	B	85	ILE	4.9
2	B	12	LEU	4.9
2	B	53	ASN	4.7
2	B	13	ILE	4.7
1	C	123	LEU	4.7
1	C	152	SER	4.7
2	B	174	ASP	4.7
2	D	14	ILE	4.6
2	B	50	VAL	4.2
1	C	99	LEU	4.2
1	A	187	TYR	4.1
1	C	136	ASN	4.0
2	D	124	ASP	3.9
2	D	84	VAL	3.9
1	C	98	ILE	3.9
1	A	335	THR	3.9
2	D	33	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	123	ASP	3.8
2	D	85	ILE	3.8
1	C	125	ASN	3.7
2	B	84	VAL	3.7
2	D	125	PRO	3.7
1	A	29	ASP	3.7
2	B	136	TYR	3.6
2	B	122	ASN	3.6
1	C	16	LEU	3.6
2	D	136	TYR	3.6
2	D	86	VAL	3.6
1	A	373	LEU	3.5
2	B	30	ASP	3.5
2	B	32	THR	3.5
2	B	6	ASP	3.4
1	C	373	LEU	3.4
2	B	111	ASP	3.4
1	C	370	LEU	3.3
1	A	8	ALA	3.3
1	A	98	ILE	3.3
2	D	13	ILE	3.2
2	D	138	PHE	3.2
2	B	107	ASN	3.1
2	D	12	LEU	3.1
1	A	260	SER	3.1
1	C	110	LYS	3.1
1	C	186	LEU	3.1
2	B	164	ILE	3.1
2	D	32	THR	3.0
1	A	17	VAL	3.0
1	A	142	ALA	3.0
1	A	99	LEU	3.0
1	C	27	ASN	3.0
2	B	153	GLU	2.9
2	B	11	LEU	2.9
1	A	374	ASN	2.9
2	D	140	GLY	2.9
2	B	51	GLU	2.9
1	A	72	PHE	2.8
1	C	188	ALA	2.8
2	B	49	THR	2.8
1	A	52	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	97	CYS	2.8
2	D	54	GLY	2.8
2	D	111	ASP	2.8
1	A	161	GLY	2.7
2	B	86	VAL	2.7
2	D	87	VAL	2.7
1	C	300	SER	2.7
2	B	176	LEU	2.7
1	C	118	TYR	2.7
1	C	347	SER	2.7
1	C	371	ALA	2.6
1	C	374	ASN	2.6
1	C	124	GLU	2.6
1	C	191	LEU	2.6
1	C	154	PHE	2.6
1	C	359	LEU	2.6
1	C	335	THR	2.5
2	D	122	ASN	2.5
1	A	122	GLU	2.5
1	A	344	HIS	2.5
1	C	127	LEU	2.5
2	B	61	ILE	2.5
2	D	130	VAL	2.5
2	B	14	ILE	2.5
2	B	62	TRP	2.5
2	D	127	ARG	2.5
2	D	56	LYS	2.4
1	C	9	ASN	2.4
2	B	41	ILE	2.4
2	D	164	ILE	2.4
1	A	16	LEU	2.4
1	A	36	PHE	2.3
1	C	18	LEU	2.3
1	C	361	LEU	2.3
1	A	229	VAL	2.3
2	D	129	VAL	2.3
1	C	17	VAL	2.3
1	A	37	PRO	2.3
1	C	309	ARG	2.3
2	D	4	ASP	2.3
2	D	117	LEU	2.3
2	B	118	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	214	ALA	2.2
1	A	345	ARG	2.2
1	C	196	ILE	2.2
2	D	126	GLU	2.2
1	C	144	THR	2.2
1	C	187	TYR	2.2
2	D	118	VAL	2.2
1	A	97	CYS	2.1
1	A	84	GLY	2.1
1	C	25	SER	2.1
2	D	23	SER	2.1
1	C	120	ALA	2.1
1	C	161	GLY	2.1
1	C	137	HIS	2.1
1	A	303	THR	2.1
1	A	281	LEU	2.1
2	B	130	VAL	2.1
1	A	258	ASN	2.0
1	A	186	LEU	2.0
1	C	24	ALA	2.0
1	C	49	VAL	2.0
1	C	133	SER	2.0

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.