



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:26 AM GMT

PDB ID : 2D11
Title : Crystal structure of the Radixin FERM domain complexed with the NHERF-2 C-terminal tail peptide
Authors : Terawaki, S.; Maesaki, R.; Hakoshima, T.
Deposited on : 2005-08-11
Resolution : 2.81 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:

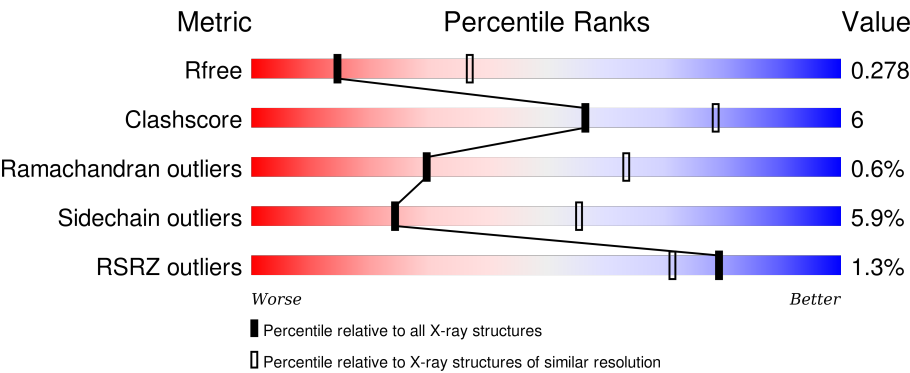
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	312	<div><div>75%18%6%</div><div></div></div>
1	B	312	<div><div>79%14%6%</div><div></div></div>
1	C	312	<div><div>71%22%6%</div><div></div></div>
1	D	312	<div><div>76%16%6%</div><div></div></div>
2	E	28	<div><div>4%50%11%36%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	28	<div><div></div><div>61%</div><div></div><div></div><div>36%</div></div>
2	G	28	<div><div>11%</div><div></div><div>46%</div><div>11%</div><div></div><div>39%</div></div>
2	H	28	<div><div>11%</div><div></div><div>54%</div><div></div><div></div><div>39%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10601 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	294	Total	C	N	O	S	0	0	0
			2453	1585	418	441	9			
1	B	294	Total	C	N	O	S	0	0	0
			2453	1585	418	441	9			
1	C	294	Total	C	N	O	S	0	0	0
			2449	1582	417	441	9			
1	D	294	Total	C	N	O	S	0	0	0
			2445	1579	416	441	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP P26043
A	0	SER	-	CLONING ARTIFACT	UNP P26043
B	-1	GLY	-	CLONING ARTIFACT	UNP P26043
B	0	SER	-	CLONING ARTIFACT	UNP P26043
C	-1	GLY	-	CLONING ARTIFACT	UNP P26043
C	0	SER	-	CLONING ARTIFACT	UNP P26043
D	-1	GLY	-	CLONING ARTIFACT	UNP P26043
D	0	SER	-	CLONING ARTIFACT	UNP P26043

- Molecule 2 is a protein called Na(+)/H(+) exchange regulatory cofactor NHE-RF2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	S	0	0	0
			164	103	33	27	1			
2	F	18	Total	C	N	O	S	0	0	0
			164	103	33	27	1			
2	G	17	Total	C	N	O	S	0	0	0
			155	97	31	26	1			
2	H	17	Total	C	N	O	S	0	0	0
			155	97	31	26	1			

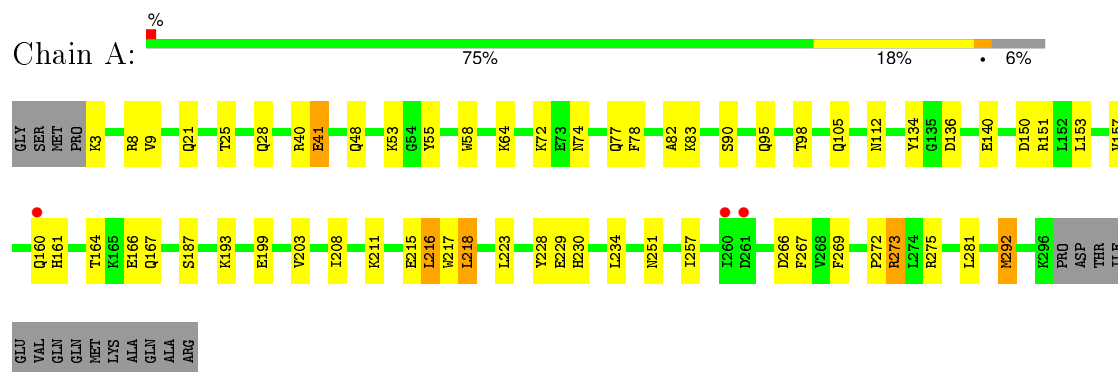
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0
3	B	60	Total 60	O 60	0	0
3	C	30	Total 30	O 30	0	0
3	D	40	Total 40	O 40	0	0
3	E	1	Total 1	O 1	0	0

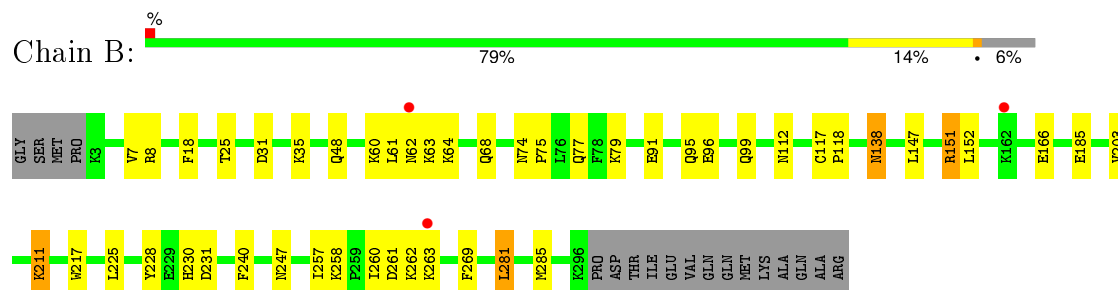
3 Residue-property plots

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.

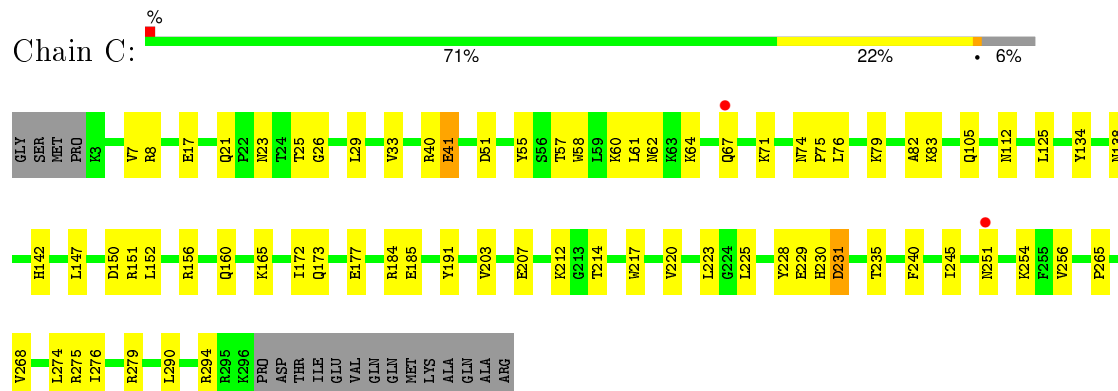
• Molecule 1: Radixin



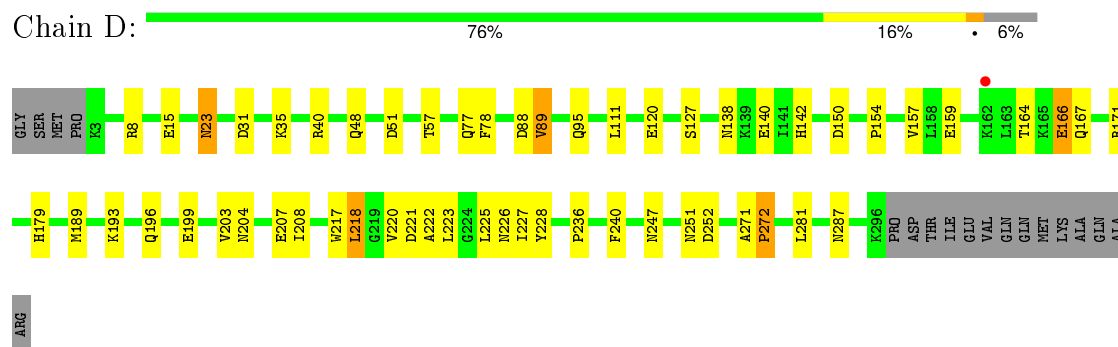
• Molecule 1: Radixin



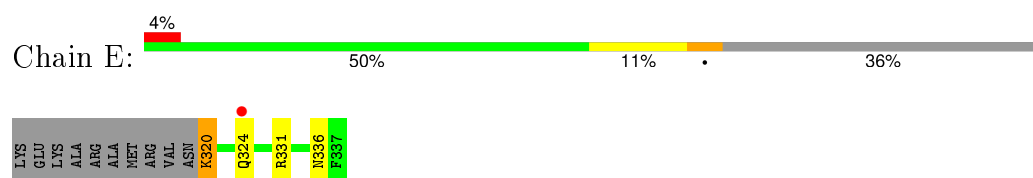
• Molecule 1: Radixin



• Molecule 1: Radixin



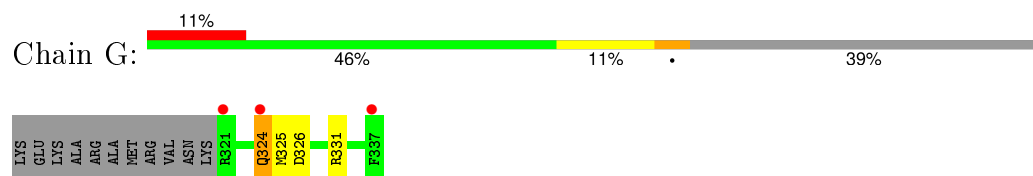
- Molecule 2: Na(+)/H(+) exchange regulatory cofactor NHE-RF2



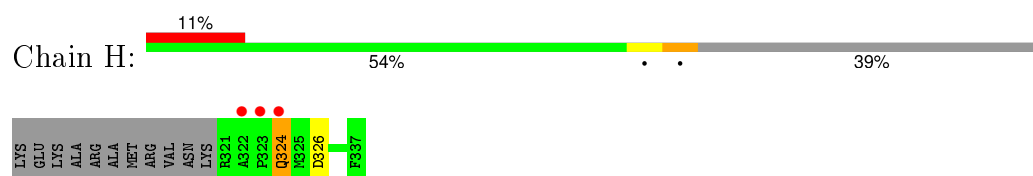
- Molecule 2: Na(+)/H(+) exchange regulatory cofactor NHE-RF2



- Molecule 2: Na(+)/H(+) exchange regulatory cofactor NHE-RF2



- Molecule 2: Na(+)/H(+) exchange regulatory cofactor NHE-RF2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.63Å 144.38Å 177.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.81 29.50 – 2.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.70-2.81) 95.0 (29.50-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.278 0.221 , 0.278	Depositor DCC
R_{free} test set	1081 reflections (2.65%)	DCC
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 41862 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	0.40	0/2512	0.53	0/3391
1	B	0.41	0/2512	0.53	0/3391
1	C	0.39	0/2508	0.52	0/3387
1	D	0.38	0/2504	0.53	0/3383
2	E	0.38	0/168	0.48	0/221
2	F	0.41	0/168	0.47	0/221
2	G	0.40	0/159	0.50	0/210
2	H	0.39	0/159	0.49	0/210
All	All	0.39	0/10690	0.52	0/14414

There are no bond length outliers.

There are no bond angle outliers.

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	2453	0	2447	36	0
1	B	2453	0	2447	25	0
1	C	2449	0	2436	36	0
1	D	2445	0	2425	28	0
2	E	164	0	159	2	0
2	F	164	0	159	0	0
2	G	155	0	146	2	0
2	H	155	0	146	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	0	2	0
3	B	60	0	0	0	0
3	C	30	0	0	3	0
3	D	40	0	0	0	0
3	E	1	0	0	0	0
All	All	10601	0	10365	126	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 6.

All (126) 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:82:ALA:H	1:A:105:GLN:HE22	1.05	0.98
1:D:40:ARG:H	1:D:95:GLN:HE22	1.14	0.95
1:C:138:ASN:H	1:C:142:HIS:HD1	1.18	0.90
1:B:211:LYS:HE2	1:B:211:LYS:H	1.35	0.89
1:A:40:ARG:H	1:A:95:GLN:HE22	1.23	0.84
1:B:60:LYS:H	1:B:68:GLN:HE22	1.27	0.83
1:B:247:ASN:HD22	1:B:258:LYS:HD3	1.44	0.79
1:D:164:THR:H	1:D:167:GLN:HE21	1.39	0.70
1:C:82:ALA:H	1:C:105:GLN:HE22	1.40	0.68
1:A:40:ARG:H	1:A:95:GLN:NE2	1.92	0.68
1:A:164:THR:H	1:A:167:GLN:HE21	1.40	0.67
1:A:48:GLN:NE2	3:A:341:HOH:O	2.23	0.67
1:A:199:GLU:HG3	1:A:234:LEU:HB3	1.78	0.65
1:D:154:PRO:HG2	1:D:157:VAL:HG23	1.78	0.65
1:D:127:SER:OG	1:D:179:HIS:HE1	1.80	0.65
1:A:136:ASP:O	1:D:35:LYS:NZ	2.30	0.64
1:A:217:TRP:HB2	1:A:228:TYR:HB2	1.80	0.64
1:B:185:GLU:H	1:B:185:GLU:CD	2.02	0.63
1:B:95:GLN:O	1:B:99:GLN:HG3	1.99	0.62
1:C:79:LYS:HE2	3:C:335:HOH:O	1.99	0.62
1:D:31:ASP:O	1:D:35:LYS:HG3	2.00	0.61
1:A:82:ALA:H	1:A:105:GLN:NE2	1.88	0.61
1:C:256:VAL:HG12	1:C:268:VAL:HG22	1.82	0.60
1:D:138:ASN:H	1:D:142:HIS:HD1	1.50	0.60
1:D:164:THR:H	1:D:167:GLN:NE2	2.01	0.59
1:A:166:GLU:H	1:A:166:GLU:CD	2.05	0.58
1:C:240:PHE:HB3	1:C:245:ILE:HD11	1.84	0.58
1:D:217:TRP:HB2	1:D:228:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:HE21	1:D:140:GLU:HG2	1.68	0.58
1:A:82:ALA:N	1:A:105:GLN:HE22	1.89	0.58
1:C:64:LYS:HB2	1:C:67:GLN:HB2	1.86	0.58
1:C:217:TRP:HB2	1:C:228:TYR:HB2	1.87	0.57
1:B:217:TRP:CD1	1:B:230:HIS:HA	2.40	0.57
1:B:31:ASP:O	1:B:35:LYS:HG3	2.04	0.57
1:A:3:LYS:HA	1:A:21:GLN:HE22	1.66	0.57
1:B:261:ASP:C	1:B:263:LYS:H	2.08	0.57
1:C:125:LEU:HB3	1:C:191:TYR:CE1	2.40	0.57
1:B:48:GLN:HG2	1:B:79:LYS:HB2	1.86	0.56
1:D:8:ARG:HE	1:D:15:GLU:CD	2.09	0.56
1:C:279:ARG:NH1	3:C:336:HOH:O	2.39	0.55
1:A:215:GLU:O	1:A:216:LEU:HD13	2.05	0.55
1:C:265:PRO:HG2	2:G:331:ARG:HD3	1.89	0.55
1:B:8:ARG:HE	1:B:77:GLN:HE22	1.55	0.54
1:C:8:ARG:HD2	3:C:337:HOH:O	2.07	0.54
1:B:211:LYS:CE	1:B:211:LYS:H	2.13	0.54
1:D:48:GLN:O	1:D:78:PHE:HA	2.08	0.54
1:C:229:GLU:O	1:C:231:ASP:N	2.42	0.53
1:A:40:ARG:N	1:A:95:GLN:HE22	1.98	0.53
1:C:276:ILE:O	1:C:279:ARG:HB3	2.10	0.52
1:A:8:ARG:HE	1:A:77:GLN:HE22	1.57	0.52
1:C:112:ASN:ND2	1:C:151:ARG:HH22	2.08	0.52
1:D:166:GLU:CD	1:D:166:GLU:H	2.13	0.52
1:C:112:ASN:HD22	1:C:151:ARG:HH22	1.56	0.52
1:B:257:ILE:HD11	1:B:269:PHE:HE1	1.74	0.51
1:C:26:GLY:HA3	1:C:61:LEU:HA	1.91	0.51
1:A:292:MET:CE	1:A:292:MET:HA	2.41	0.51
1:C:207:GLU:HG3	1:C:217:TRP:CZ3	2.46	0.50
1:D:208:ILE:HD13	1:D:218:LEU:HB2	1.92	0.50
1:B:260:ILE:O	1:B:260:ILE:HG22	2.10	0.50
1:A:273:ARG:HH12	1:A:275:ARG:HH22	1.59	0.50
1:D:40:ARG:N	1:D:95:GLN:HE22	1.96	0.50
1:D:40:ARG:H	1:D:95:GLN:NE2	1.95	0.49
1:D:8:ARG:NH1	1:D:77:GLN:OE1	2.45	0.49
1:C:7:VAL:HG12	1:C:76:LEU:HB2	1.94	0.49
1:C:147:LEU:HB3	1:C:152:LEU:HD11	1.94	0.49
2:E:320:LYS:O	2:E:320:LYS:HD2	2.12	0.49
1:D:226:ASN:HB3	1:D:236:PRO:HB3	1.95	0.48
1:C:274:LEU:HD21	1:C:275:ARG:HH21	1.79	0.48
1:D:88:ASP:HA	1:D:196:GLN:HE22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ARG:O	1:C:160:GLN:HB2	2.14	0.48
1:A:164:THR:H	1:A:167:GLN:NE2	2.10	0.48
1:B:63:LYS:HG3	1:B:64:LYS:N	2.28	0.48
1:A:112:ASN:ND2	1:A:151:ARG:HH22	2.12	0.48
1:A:292:MET:HE3	1:A:292:MET:HA	1.95	0.47
1:A:9:VAL:HG22	1:A:78:PHE:HB2	1.95	0.47
1:B:225:LEU:HB2	1:B:240:PHE:HB2	1.95	0.47
1:C:29:LEU:O	1:C:33:VAL:HG23	2.14	0.47
1:C:290:LEU:O	1:C:294:ARG:HG3	2.15	0.46
1:D:89:VAL:H	1:D:196:GLN:HE22	1.62	0.46
1:A:90:SER:OG	1:A:193:LYS:HE2	2.15	0.46
1:A:257:ILE:HD12	1:A:267:PHE:HD2	1.81	0.46
1:D:222:ALA:HA	1:D:287:ASN:HD22	1.81	0.45
1:A:257:ILE:HD11	1:A:269:PHE:HE1	1.81	0.45
1:B:112:ASN:ND2	1:B:151:ARG:NH2	2.65	0.45
1:A:266:ASP:O	2:E:331:ARG:HD2	2.16	0.45
3:A:342:HOH:O	1:D:35:LYS:HE2	2.17	0.45
1:C:251:ASN:HB2	1:C:254:LYS:HB3	1.97	0.45
1:C:58:TRP:CD1	1:C:83:LYS:HE3	2.52	0.45
1:B:185:GLU:N	1:B:185:GLU:CD	2.70	0.44
1:C:152:LEU:HD13	1:C:172:ILE:HD13	1.99	0.44
1:B:217:TRP:HB2	1:B:228:TYR:HB2	1.99	0.44
1:B:25:THR:HA	1:B:64:LYS:HA	2.00	0.44
2:G:324:GLN:HE21	2:G:325:MET:N	2.16	0.43
1:A:157:VAL:HA	1:A:160:GLN:HG2	2.00	0.43
1:A:25:THR:HA	1:A:64:LYS:HA	2.00	0.43
1:C:25:THR:HA	1:C:64:LYS:HA	1.99	0.43
1:C:23:ASN:HA	1:C:64:LYS:HD3	2.01	0.43
1:D:220:VAL:HG22	1:D:225:LEU:HD22	1.99	0.43
1:C:134:TYR:OH	1:C:150:ASP:OD2	2.28	0.43
1:B:281:LEU:O	1:B:285:MET:HG3	2.18	0.43
1:A:53:LYS:HE3	1:A:55:TYR:HE1	1.84	0.43
1:D:23:ASN:H	1:D:23:ASN:HD22	1.66	0.43
1:C:74:ASN:HA	1:C:75:PRO:HA	1.89	0.43
1:A:208:ILE:HD13	1:A:218:LEU:HB2	1.99	0.43
1:C:41:GLU:H	1:C:41:GLU:HG2	1.48	0.43
1:B:74:ASN:HA	1:B:75:PRO:HA	1.86	0.42
1:B:138:ASN:HD22	1:B:138:ASN:C	2.20	0.42
1:B:117:CYS:HA	1:B:118:PRO:HD3	1.94	0.42
1:D:189:MET:O	1:D:193:LYS:HG3	2.19	0.42
1:B:147:LEU:HB3	1:B:152:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:THR:HG23	1:C:279:ARG:HH22	1.85	0.42
1:A:41:GLU:HG3	1:A:98:THR:HG21	2.01	0.42
1:C:173:GLN:O	1:C:177:GLU:HG3	2.19	0.42
1:D:271:ALA:HA	1:D:272:PRO:HD3	1.87	0.42
1:C:220:VAL:HG22	1:C:225:LEU:HD22	2.01	0.42
1:D:120:GLU:OE1	1:D:171:ARG:NH2	2.50	0.41
1:C:51:ASP:OD1	1:C:55:TYR:HB2	2.20	0.41
1:A:217:TRP:CD1	1:A:230:HIS:HA	2.55	0.41
1:A:134:TYR:OH	1:A:150:ASP:OD1	2.33	0.41
2:H:324:GLN:HB3	2:H:324:GLN:HE21	1.64	0.41
1:A:160:GLN:HG3	1:A:161:HIS:HD2	1.85	0.40
1:B:7:VAL:CG2	1:B:18:PHE:HB2	2.51	0.40
1:C:185:GLU:H	1:C:185:GLU:CD	2.24	0.40
1:A:58:TRP:CD1	1:A:83:LYS:HE3	2.56	0.40
1:A:273:ARG:HH12	1:A:275:ARG:NH2	2.19	0.40
1:D:227:ILE:HD13	1:D:240:PHE:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/312 (94%)	284 (97%)	7 (2%)	1 (0%)	46	78
1	B	292/312 (94%)	285 (98%)	6 (2%)	1 (0%)	46	78
1	C	292/312 (94%)	280 (96%)	9 (3%)	3 (1%)	19	51
1	D	292/312 (94%)	280 (96%)	10 (3%)	2 (1%)	26	60
2	E	16/28 (57%)	16 (100%)	0	0	100	100
2	F	16/28 (57%)	16 (100%)	0	0	100	100
2	G	15/28 (54%)	15 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	15/28 (54%)	15 (100%)	0	0	100	100
All	All	1230/1360 (90%)	1191 (97%)	32 (3%)	7 (1%)	30	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	231	ASP
1	D	272	PRO
1	C	230	HIS
1	B	262	LYS
1	C	71	LYS
1	D	252	ASP
1	A	272	PRO

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	264/282 (94%)	248 (94%)	16 (6%)	23	54
1	B	264/282 (94%)	253 (96%)	11 (4%)	36	70
1	C	263/282 (93%)	250 (95%)	13 (5%)	31	64
1	D	262/282 (93%)	244 (93%)	18 (7%)	19	47
2	E	17/25 (68%)	14 (82%)	3 (18%)	2	6
2	F	17/25 (68%)	16 (94%)	1 (6%)	24	55
2	G	16/25 (64%)	14 (88%)	2 (12%)	6	17
2	H	16/25 (64%)	14 (88%)	2 (12%)	6	17
All	All	1119/1228 (91%)	1053 (94%)	66 (6%)	24	55

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU

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Mol	Chain	Res	Type
1	A	72	LYS
1	A	74	ASN
1	A	140	GLU
1	A	153	LEU
1	A	187	SER
1	A	203	VAL
1	A	211	LYS
1	A	216	LEU
1	A	218	LEU
1	A	223	LEU
1	A	229	GLU
1	A	251	ASN
1	A	273	ARG
1	A	281	LEU
1	A	292	MET
1	B	61	LEU
1	B	62	ASN
1	B	91	GLU
1	B	96	GLU
1	B	138	ASN
1	B	151	ARG
1	B	166	GLU
1	B	203	VAL
1	B	211	LYS
1	B	231	ASP
1	B	281	LEU
1	C	17	GLU
1	C	21	GLN
1	C	40	ARG
1	C	41	GLU
1	C	60	LYS
1	C	62	ASN
1	C	165	LYS
1	C	184	ARG
1	C	203	VAL
1	C	212	LYS
1	C	214	THR
1	C	223	LEU
1	C	235	THR
1	D	23	ASN
1	D	51	ASP
1	D	57	THR

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Mol	Chain	Res	Type
1	D	89	VAL
1	D	111	LEU
1	D	150	ASP
1	D	159	GLU
1	D	166	GLU
1	D	199	GLU
1	D	203	VAL
1	D	204	ASN
1	D	207	GLU
1	D	218	LEU
1	D	221	ASP
1	D	223	LEU
1	D	247	ASN
1	D	251	ASN
1	D	281	LEU
2	E	320	LYS
2	E	324	GLN
2	E	336	ASN
2	F	326	ASP
2	G	324	GLN
2	G	326	ASP
2	H	324	GLN
2	H	326	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	32	GLN
1	A	74	ASN
1	A	77	GLN
1	A	95	GLN
1	A	99	GLN
1	A	105	GLN
1	A	112	ASN
1	A	131	GLN
1	A	161	HIS
1	A	167	GLN
1	A	204	ASN
1	A	287	ASN
1	B	6	ASN
1	B	28	GLN

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Mol	Chain	Res	Type
1	B	32	GLN
1	B	68	GLN
1	B	77	GLN
1	B	112	ASN
1	B	131	GLN
1	B	138	ASN
1	B	167	GLN
1	B	174	ASN
1	B	247	ASN
1	C	48	GLN
1	C	77	GLN
1	C	99	GLN
1	C	105	GLN
1	C	112	ASN
1	C	173	GLN
1	C	179	HIS
1	C	226	ASN
1	D	23	ASN
1	D	48	GLN
1	D	95	GLN
1	D	99	GLN
1	D	160	GLN
1	D	167	GLN
1	D	173	GLN
1	D	174	ASN
1	D	179	HIS
1	D	196	GLN
1	D	251	ASN
1	D	287	ASN
2	E	336	ASN
2	F	336	ASN
2	G	324	GLN
2	G	328	ASN
2	H	324	GLN
2	H	336	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 ⓘ

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	294/312 (94%)	-0.28	3 (1%) 84 77	20, 34, 46, 53	0
1	B	294/312 (94%)	-0.26	3 (1%) 84 77	18, 33, 49, 56	0
1	C	294/312 (94%)	-0.05	2 (0%) 89 84	20, 39, 55, 60	0
1	D	294/312 (94%)	-0.33	1 (0%) 94 92	20, 33, 45, 57	0
2	E	18/28 (64%)	0.34	1 (5%) 28 18	53, 59, 71, 72	0
2	F	18/28 (64%)	0.34	0 100 100	44, 58, 71, 71	0
2	G	17/28 (60%)	0.78	3 (17%) 2 1	63, 66, 76, 77	0
2	H	17/28 (60%)	0.51	3 (17%) 2 1	44, 49, 62, 64	0
All	All	1246/1360 (91%)	-0.19	16 (1%) 79 71	18, 35, 56, 77	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	321	ARG	3.0
1	A	260	ILE	2.9
1	A	160	GLN	2.7
2	G	324	GLN	2.7
2	H	322	ALA	2.6
2	G	337	PHE	2.6
1	C	67	GLN	2.5
1	C	251	ASN	2.4
2	E	324	GLN	2.3
2	H	324	GLN	2.3
1	D	162	LYS	2.2
1	B	162	LYS	2.2
1	A	261	ASP	2.2
1	B	263	LYS	2.2
2	H	323	PRO	2.1
1	B	62	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.