



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 06:08 am BST

PDB ID : 6DJL  
Title : Crystal structure of the Rab11 GEF SH3BP5 bound to nucleotide free Rab11A  
Authors : Burke, J.E.; Jenkins, M.L.; Boulanger, M.J.  
Deposited on : 2018-05-25  
Resolution : 3.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

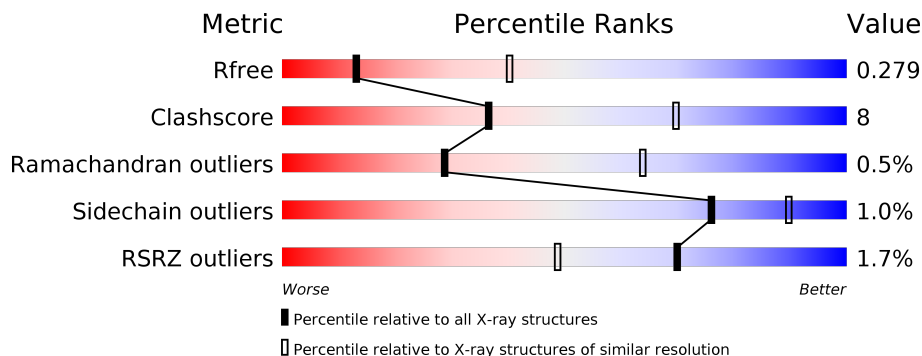
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	219	 3% 62% 18% 20%
1	F	219	 % 60% 20% 19%
1	G	219	 2% 62% 16% 21%
1	H	219	 6% 66% 15% 19%
2	B	266	 69% 14% 17%
2	C	266	 70% 14% 16%

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Mol	Chain	Length	Quality of chain			
2	D	266		70%	14%	16%
2	E	266		70%	15%	15%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 12888 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 Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	176	1390	880	236	272	2	0	0	0
1	F	177	1396	883	241	270	2	0	0	0
1	G	172	1353	857	230	264	2	0	0	0
1	H	177	1409	891	244	272	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P62491
A	-1	SER	-	expression tag	UNP P62491
A	0	HIS	-	expression tag	UNP P62491
A	70	LEU	GLN	engineered mutation	UNP P62491
F	-2	GLY	-	expression tag	UNP P62491
F	-1	SER	-	expression tag	UNP P62491
F	0	HIS	-	expression tag	UNP P62491
F	70	LEU	GLN	engineered mutation	UNP P62491
G	-2	GLY	-	expression tag	UNP P62491
G	-1	SER	-	expression tag	UNP P62491
G	0	HIS	-	expression tag	UNP P62491
G	70	LEU	GLN	engineered mutation	UNP P62491
H	-2	GLY	-	expression tag	UNP P62491
H	-1	SER	-	expression tag	UNP P62491
H	0	HIS	-	expression tag	UNP P62491
H	70	LEU	GLN	engineered mutation	UNP P62491

- Molecule 2 is a protein called SH3 domain-binding protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	221	Total 1798	C 1117	N 329	O 346	S 6	0	0	0
2	C	224	Total 1841	C 1140	N 343	O 352	S 6	0	0	0
2	D	224	Total 1841	C 1140	N 343	O 352	S 6	0	0	0
2	E	226	Total 1860	C 1150	N 345	O 359	S 6	0	0	0

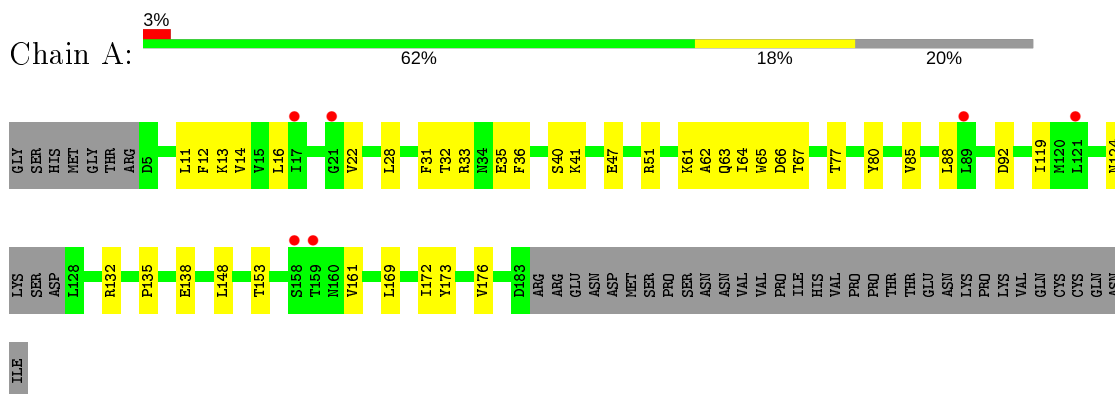
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP O60239
C	0	GLY	-	expression tag	UNP O60239
D	0	GLY	-	expression tag	UNP O60239
E	0	GLY	-	expression tag	UNP O60239

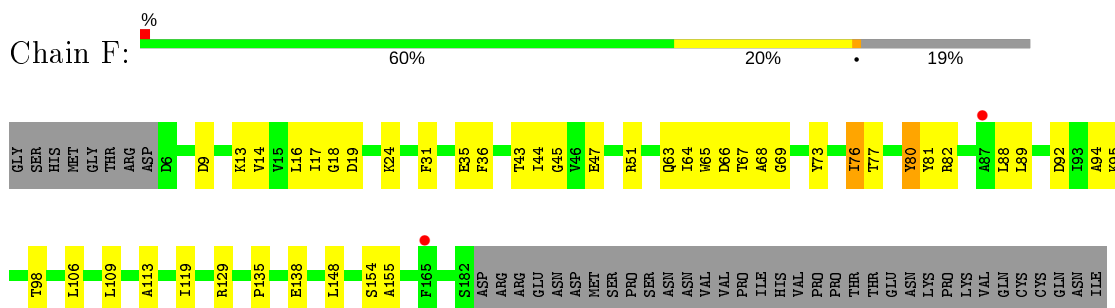
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

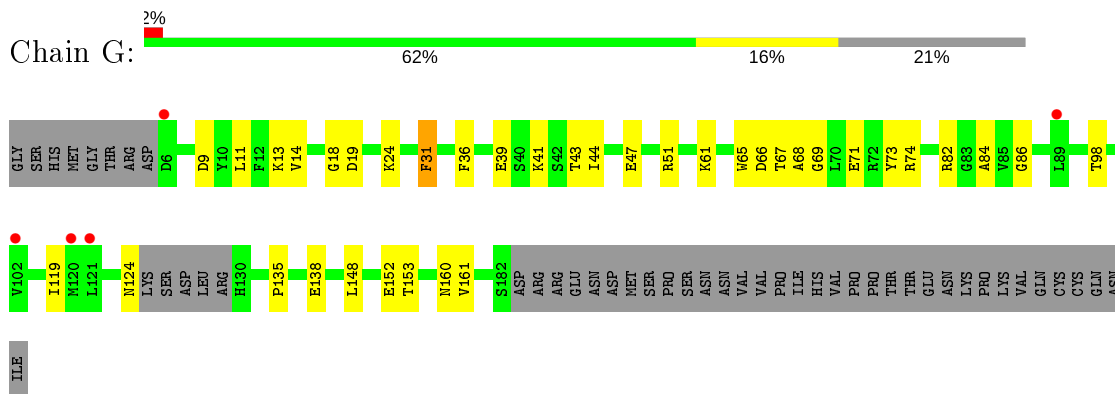
- Molecule 1: Ras-related protein Rab-11A



- Molecule 1: Ras-related protein Rab-11A



- Molecule 1: Ras-related protein Rab-11A



- Molecule 1: Ras-related protein Rab-11A



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.85Å 197.04Å 304.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 3.10 49.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.61-3.10) 99.8 (49.61-3.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 3.12Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.235 , 0.278 0.235 , 0.279	Depositor DCC
$R_{free}$ test set	3146 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	114.7	Xtrriage
Anisotropy	0.231	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 72.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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	0.24	0/1411	0.44	0/1908
1	F	0.26	0/1418	0.44	0/1917
1	G	0.25	0/1373	0.44	0/1856
1	H	0.25	0/1431	0.43	0/1933
2	B	0.27	0/1816	0.46	1/2431 (0.0%)
2	C	0.26	0/1860	0.41	0/2487
2	D	0.26	0/1860	0.41	0/2487
2	E	0.27	0/1879	0.41	0/2512
All	All	0.26	0/13048	0.43	1/17531 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	236	LEU	CA-CB-CG	5.20	127.25	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	1390	0	1370	24	0
1	F	1396	0	1383	37	1
1	G	1353	0	1335	33	0
1	H	1409	0	1407	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1798	0	1833	21	0
2	C	1841	0	1884	27	0
2	D	1841	0	1884	28	0
2	E	1860	0	1899	36	0
All	All	12888	0	12995	204	1

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 8.

All (204) 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)
2:C:61:ARG:NH1	2:C:62:ARG:HH12	1.48	1.10
2:D:51:LYS:HE3	2:E:195:ARG:HH21	1.42	0.83
1:G:47:GLU:HB3	1:G:66:ASP:HB3	1.64	0.79
2:C:133:LYS:NZ	2:C:145:GLU:OE1	2.14	0.76
1:H:71:GLU:HB2	1:H:74:ARG:HD3	1.66	0.75
2:E:247:LEU:HD11	1:F:63:GLN:HE22	1.50	0.75
2:C:147:ASP:HB2	2:C:149:ARG:HG2	1.70	0.74
2:E:50:GLU:HG2	1:F:82:ARG:HH12	1.52	0.73
2:E:62:ARG:NH1	2:E:235:LYS:HB3	2.04	0.73
2:D:103:GLU:HG3	2:D:106:ARG:HH12	1.54	0.71
1:H:47:GLU:HB3	1:H:66:ASP:HB3	1.73	0.70
1:F:18:GLY:O	1:F:24:LYS:NZ	2.23	0.70
2:D:147:ASP:O	2:D:149:ARG:N	2.24	0.69
2:D:118:ALA:HB3	2:D:183:THR:HG21	1.74	0.69
1:H:92:ASP:OD1	1:H:126:SER:OG	2.10	0.69
1:H:24:LYS:HE2	1:H:67:THR:HB	1.77	0.67
1:A:66:ASP:OD2	1:A:67:THR:HG23	1.95	0.67
2:D:160:ASN:O	2:D:164:GLN:NE2	2.29	0.66
2:D:98:SER:HA	2:D:201:LEU:HD23	1.78	0.65
2:C:74:ARG:HG2	2:E:160:ASN:HD21	1.60	0.65
2:C:61:ARG:NH1	2:C:62:ARG:NH1	2.33	0.64
2:E:50:GLU:HG2	1:F:82:ARG:NH1	2.13	0.64
1:G:119:ILE:HB	1:G:148:LEU:HD22	1.80	0.64
2:C:129:LEU:HD22	2:C:173:LYS:HD3	1.81	0.63
1:F:119:ILE:HB	1:F:148:LEU:HD22	1.79	0.62
2:C:44:ARG:HH21	2:C:253:ILE:HG12	1.62	0.62
1:A:35:GLU:OE1	1:A:63:GLN:NE2	2.33	0.62
1:G:152:GLU:O	1:G:160:ASN:ND2	2.31	0.61
2:B:109:ARG:HD2	2:C:235:LYS:NZ	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:THR:HG22	2:C:180:HIS:CD2	2.36	0.60
2:E:118:ALA:HB3	2:E:183:THR:HG21	1.82	0.60
2:E:126:THR:HG22	2:E:173:LYS:HE2	1.85	0.59
2:D:51:LYS:HE3	2:E:195:ARG:NH2	2.16	0.59
2:D:42:ASP:N	2:D:42:ASP:OD1	2.36	0.58
1:H:14:VAL:O	1:H:64:ILE:HA	2.02	0.58
2:B:142:ARG:HB3	2:B:149:ARG:NH1	2.17	0.58
1:A:47:GLU:HB3	1:A:66:ASP:HB3	1.85	0.58
1:A:31:PHE:HB3	1:A:51:ARG:NH1	2.18	0.58
2:E:99:LYS:HG2	2:E:100:PRO:HD3	1.85	0.58
1:G:153:THR:HG21	1:G:161:VAL:HB	1.85	0.58
2:D:184:ALA:O	2:D:188:ASN:ND2	2.38	0.57
2:C:61:ARG:HH11	2:C:62:ARG:HH12	1.46	0.56
1:F:16:LEU:HD12	1:F:88:LEU:HB2	1.86	0.56
1:A:119:ILE:HB	1:A:148:LEU:HD22	1.87	0.56
1:F:47:GLU:O	1:F:66:ASP:HB2	2.06	0.56
1:G:31:PHE:HB2	1:G:51:ARG:HH12	1.70	0.56
2:C:118:ALA:HB3	2:C:183:THR:HG21	1.87	0.56
1:F:14:VAL:O	1:F:64:ILE:HA	2.05	0.56
2:E:42:ASP:OD2	2:E:44:ARG:NE	2.38	0.55
2:E:45:ILE:HD12	1:F:44:ILE:HG23	1.88	0.55
2:E:119:THR:HG22	2:E:180:HIS:CD2	2.42	0.55
2:B:251:GLU:O	2:B:255:ASP:HB2	2.07	0.54
1:H:66:ASP:OD2	1:H:67:THR:HG22	2.07	0.54
2:C:74:ARG:HG2	2:E:160:ASN:ND2	2.23	0.54
2:C:87:LEU:O	2:C:91:ILE:HB	2.08	0.54
1:F:13:LYS:NZ	1:F:80:TYR:O	2.39	0.54
1:H:67:THR:OG1	1:H:69:GLY:N	2.37	0.54
1:G:31:PHE:HB2	1:G:51:ARG:NH1	2.24	0.53
1:F:47:GLU:O	1:F:66:ASP:CB	2.57	0.52
2:E:55:SER:O	2:E:59:ILE:HG12	2.10	0.52
1:G:67:THR:HG23	1:G:68:ALA:H	1.75	0.52
1:G:19:ASP:OD2	1:G:98:THR:HA	2.09	0.52
1:A:14:VAL:O	1:A:64:ILE:HA	2.10	0.51
1:H:93:ILE:HD11	1:H:125:LYS:HD3	1.92	0.51
2:C:98:SER:HA	2:C:201:LEU:HD23	1.93	0.51
2:B:122:PHE:CE1	2:B:177:GLU:HG3	2.46	0.51
1:H:119:ILE:HB	1:H:148:LEU:HD22	1.93	0.51
1:G:39:GLU:HG2	1:G:41:LYS:H	1.76	0.51
2:D:63:GLU:HG2	1:G:9:ASP:O	2.10	0.51
1:G:41:LYS:HD2	1:G:67:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:65:GLU:HB3	2:E:232:LEU:HD21	1.94	0.50
2:E:251:GLU:HB2	1:F:36:PHE:CE1	2.46	0.50
2:B:87:LEU:HD23	2:B:211:TYR:HA	1.94	0.50
1:F:18:GLY:C	1:F:24:LYS:HZ3	2.16	0.49
2:D:45:ILE:HG21	1:G:44:ILE:HG23	1.94	0.49
2:C:87:LEU:HD23	2:C:211:TYR:HA	1.95	0.49
1:F:129:ARG:HH11	1:F:129:ARG:HB2	1.77	0.49
1:A:11:LEU:HA	1:A:61:LYS:O	2.12	0.49
1:G:68:ALA:O	1:G:71:GLU:HG3	2.13	0.49
2:B:96:GLU:HG3	2:B:97:ASP:N	2.27	0.49
1:H:160:ASN:N	1:H:160:ASN:OD1	2.42	0.49
1:A:85:VAL:HG23	1:A:172:ILE:HD13	1.96	0.48
2:D:165:ARG:HA	2:D:168:GLU:HG2	1.95	0.48
2:E:59:ILE:HD12	2:E:240:LYS:HG3	1.96	0.48
2:D:105:ARG:NH1	2:E:238:LEU:HD22	2.28	0.48
1:A:77:THR:HA	1:A:80:TYR:HB3	1.95	0.48
2:D:85:ASP:O	2:D:89:LYS:HG2	2.13	0.48
1:F:35:GLU:OE1	1:F:63:GLN:NE2	2.47	0.48
1:H:67:THR:HG23	1:H:68:ALA:H	1.78	0.48
2:B:46:GLN:HG2	1:H:76:ILE:HG13	1.95	0.48
1:G:67:THR:OG1	1:G:69:GLY:N	2.42	0.47
2:B:109:ARG:HD2	2:C:235:LYS:HZ3	1.80	0.47
2:D:195:ARG:NH1	2:E:51:LYS:HD3	2.28	0.47
1:F:154:SER:OG	1:F:155:ALA:N	2.48	0.47
1:F:43:THR:OG1	1:F:44:ILE:N	2.47	0.47
1:F:66:ASP:OD1	1:F:67:THR:N	2.44	0.47
1:H:16:LEU:HD12	1:H:88:LEU:HB2	1.96	0.47
1:A:12:PHE:O	1:A:62:ALA:HA	2.15	0.47
1:F:31:PHE:CE2	1:F:51:ARG:HG2	2.50	0.47
2:B:136:ILE:HD11	2:B:163:THR:HA	1.97	0.47
2:E:115:ALA:O	2:E:119:THR:HG23	2.15	0.47
1:G:18:GLY:O	1:G:24:LYS:NZ	2.31	0.46
1:G:124:ASN:HA	1:G:153:THR:O	2.15	0.46
1:H:24:LYS:HA	1:H:27:LEU:HD23	1.97	0.46
2:B:44:ARG:NH1	2:B:256:GLU:OE2	2.49	0.46
2:C:99:LYS:N	2:C:100:PRO:HD2	2.30	0.46
2:E:195:ARG:HH12	2:E:198:GLU:CG	2.29	0.46
2:E:257:ILE:HG21	1:F:43:THR:HB	1.98	0.46
2:D:85:ASP:HA	2:D:88:VAL:HG12	1.97	0.46
1:F:19:ASP:OD2	1:F:98:THR:HA	2.15	0.46
1:F:81:TYR:HB3	1:F:113:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ASP:HB3	2:B:149:ARG:HE	1.81	0.46
2:C:43:PRO:HB2	2:C:44:ARG:HG3	1.99	0.45
1:F:129:ARG:NH1	1:F:129:ARG:HB2	2.31	0.45
1:G:41:LYS:HG2	1:G:47:GLU:HB2	1.98	0.45
2:C:196:GLN:HA	2:C:199:LYS:HG2	1.99	0.45
2:D:51:LYS:HE3	2:E:195:ARG:HE	1.81	0.45
2:B:85:ASP:O	2:B:88:VAL:HG22	2.16	0.45
1:F:17:ILE:HG13	1:F:89:LEU:HA	1.98	0.45
2:C:123:GLN:O	2:C:126:THR:OG1	2.28	0.45
2:D:45:ILE:HD13	1:G:44:ILE:HG23	1.98	0.45
1:A:28:LEU:HG	1:A:32:THR:HG21	1.99	0.45
2:D:50:GLU:HG2	1:G:82:ARG:HH12	1.81	0.45
2:D:51:LYS:CE	2:E:195:ARG:HH21	2.23	0.44
2:E:82:VAL:HA	2:E:85:ASP:OD2	2.17	0.44
1:A:36:PHE:CE1	2:C:251:GLU:HB3	2.52	0.44
2:B:85:ASP:O	2:B:89:LYS:HG2	2.17	0.44
1:F:106:LEU:HD11	1:F:148:LEU:HD11	1.98	0.44
1:F:135:PRO:HD2	1:F:138:GLU:OE2	2.18	0.44
1:G:41:LYS:HD2	1:G:67:THR:CG2	2.48	0.44
1:G:66:ASP:OD2	1:G:67:THR:HG22	2.18	0.44
1:A:41:LYS:HD2	1:A:67:THR:OG1	2.17	0.44
2:D:202:LYS:O	2:D:206:ASN:ND2	2.47	0.44
2:C:43:PRO:HD2	2:C:45:ILE:HD13	1.99	0.44
2:D:251:GLU:HB2	1:G:36:PHE:CE1	2.52	0.44
1:A:135:PRO:HG2	1:A:138:GLU:HB3	2.00	0.44
1:A:153:THR:HB	1:A:161:VAL:HG13	2.00	0.44
2:D:87:LEU:HD23	2:D:211:TYR:HA	1.99	0.44
1:F:92:ASP:HB3	1:F:95:LYS:HB2	2.00	0.44
1:G:43:THR:OG1	1:G:44:ILE:N	2.50	0.44
1:G:11:LEU:HA	1:G:61:LYS:O	2.18	0.44
1:G:71:GLU:HG2	1:G:74:ARG:HB2	2.00	0.44
1:F:67:THR:HG22	1:F:69:GLY:H	1.83	0.43
1:H:67:THR:OG1	1:H:68:ALA:N	2.49	0.43
1:G:13:LYS:HB3	1:G:84:ALA:HA	2.00	0.43
1:G:67:THR:OG1	1:G:68:ALA:N	2.49	0.43
2:B:66:LEU:HA	2:B:232:LEU:HD23	2.00	0.43
2:C:135:THR:HG21	2:C:162:ALA:HB3	2.00	0.43
2:E:62:ARG:HH11	2:E:235:LYS:HB3	1.79	0.43
2:E:87:LEU:HD23	2:E:211:TYR:HA	1.99	0.43
2:E:119:THR:HG22	2:E:180:HIS:NE2	2.33	0.43
1:G:13:LYS:HE3	1:G:65:TRP:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:67:GLU:O	2:E:71:GLN:HG2	2.18	0.43
2:D:47:GLY:O	2:D:51:LYS:HG3	2.19	0.43
1:A:47:GLU:O	1:A:66:ASP:HB2	2.19	0.43
1:H:154:SER:OG	1:H:155:ALA:N	2.52	0.43
1:A:41:LYS:NZ	1:A:67:THR:HG21	2.34	0.43
1:G:135:PRO:HG2	1:G:138:GLU:HB3	2.00	0.42
2:E:101:TYR:CE1	2:E:198:GLU:HB2	2.54	0.42
1:F:13:LYS:HE3	1:F:65:TRP:CD2	2.54	0.42
1:G:14:VAL:HA	1:G:86:GLY:O	2.20	0.42
1:H:41:LYS:HD2	1:H:67:THR:CG2	2.50	0.42
1:H:153:THR:HG21	1:H:161:VAL:HG22	2.01	0.42
2:C:41:VAL:HB	2:C:42:ASP:H	1.70	0.42
1:F:45:GLY:O	1:F:68:ALA:HA	2.19	0.42
2:B:50:GLU:HA	2:B:53:ASN:HD21	1.85	0.42
2:C:126:THR:HA	2:C:173:LYS:HD2	2.02	0.42
2:D:156:GLN:O	2:D:160:ASN:ND2	2.53	0.42
1:H:77:THR:HA	1:H:80:TYR:HB3	2.02	0.42
2:E:84:LEU:HA	2:E:84:LEU:HD23	1.90	0.42
1:A:124:ASN:HA	1:A:153:THR:O	2.20	0.42
2:B:50:GLU:HA	2:B:53:ASN:ND2	2.34	0.42
1:F:73:TYR:HB3	1:F:76:ILE:HG12	2.01	0.42
1:H:11:LEU:HD13	1:H:61:LYS:HD3	2.02	0.42
2:E:63:GLU:HG2	1:F:9:ASP:O	2.19	0.41
1:F:24:LYS:HG2	1:F:24:LYS:H	1.73	0.41
1:A:16:LEU:HD12	1:A:88:LEU:HB2	2.01	0.41
1:G:73:TYR:CD1	1:G:74:ARG:NH1	2.88	0.41
1:F:17:ILE:HD13	1:F:109:LEU:HD11	2.02	0.41
1:F:92:ASP:OD2	1:F:94:ALA:N	2.39	0.41
1:H:122:VAL:HG22	1:H:151:ILE:HD11	2.02	0.41
2:E:253:ILE:O	2:E:257:ILE:HG22	2.20	0.41
1:G:31:PHE:O	1:G:51:ARG:NH1	2.54	0.41
2:D:50:GLU:HG2	1:G:82:ARG:NH1	2.36	0.41
2:B:221:GLN:O	2:B:224:GLN:HG2	2.20	0.41
1:H:7:GLU:OE1	1:H:7:GLU:N	2.54	0.41
1:A:173:TYR:HA	1:A:176:VAL:HG22	2.03	0.41
2:C:156:GLN:NE2	2:C:160:ASN:O	2.54	0.41
1:H:41:LYS:HD2	1:H:67:THR:HG21	2.02	0.41
2:B:84:LEU:HB3	2:B:211:TYR:HE1	1.86	0.41
2:C:134:GLU:C	2:C:136:ILE:H	2.25	0.41
1:A:22:VAL:HG12	1:A:92:ASP:HB2	2.02	0.40
1:F:19:ASP:HB2	1:F:98:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:HE3	1:A:65:TRP:CD2	2.57	0.40
2:E:220:VAL:HA	2:E:223:GLU:HG2	2.02	0.40
1:A:47:GLU:O	1:A:66:ASP:CB	2.70	0.40
2:D:136:ILE:HD11	2:D:162:ALA:O	2.21	0.40
2:D:88:VAL:HG23	2:D:95:VAL:HG21	2.03	0.40
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.89	0.40
2:B:135:THR:HA	2:B:138:LEU:HD23	2.04	0.40
2:B:224:GLN:HA	2:B:227:LYS:HG2	2.03	0.40
2:B:83:LYS:O	2:B:86:GLU:HG2	2.20	0.40
1:F:76:ILE:HG13	1:F:77:THR:N	2.36	0.40
2:E:195:ARG:NH1	2:E:198:GLU:CD	2.75	0.40

All (1) 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:F:47:GLU:OE2	1:F:129:ARG:NH1[3_556]	2.09	0.11

## 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	172/219 (78%)	159 (92%)	11 (6%)	2 (1%)	13	44
1	F	175/219 (80%)	170 (97%)	5 (3%)	0	100	100
1	G	168/219 (77%)	155 (92%)	13 (8%)	0	100	100
1	H	175/219 (80%)	167 (95%)	7 (4%)	1 (1%)	25	59
2	B	219/266 (82%)	218 (100%)	1 (0%)	0	100	100
2	C	222/266 (84%)	214 (96%)	5 (2%)	3 (1%)	11	40
2	D	222/266 (84%)	216 (97%)	4 (2%)	2 (1%)	17	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	224/266 (84%)	224 (100%)	0	0	100	100
All	All	1577/1940 (81%)	1523 (97%)	46 (3%)	8 (0%)	29	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	43	PRO
1	A	132	ARG
2	C	152	ASP
2	C	136	ILE
2	D	43	PRO
1	A	33	ARG
1	H	67	THR
2	D	148	LYS

### 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	148/191 (78%)	147 (99%)	1 (1%)	84	93
1	F	148/191 (78%)	146 (99%)	2 (1%)	67	86
1	G	143/191 (75%)	142 (99%)	1 (1%)	84	93
1	H	151/191 (79%)	151 (100%)	0	100	100
2	B	189/230 (82%)	184 (97%)	5 (3%)	46	74
2	C	195/230 (85%)	195 (100%)	0	100	100
2	D	195/230 (85%)	192 (98%)	3 (2%)	65	85
2	E	198/230 (86%)	197 (100%)	1 (0%)	88	94
All	All	1367/1684 (81%)	1354 (99%)	13 (1%)	76	90

All (13) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	40	SER
2	B	91	ILE
2	B	95	VAL
2	B	102	TRP
2	B	138	LEU
2	B	250	LEU
2	D	42	ASP
2	D	159	LEU
2	D	171	GLN
2	E	121	ASP
1	F	76	ILE
1	F	80	TYR
1	G	31	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	164	GLN
2	C	180	HIS
2	C	196	GLN
2	D	188	ASN
2	E	160	ASN

### 5.3.3 RNA [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	176/219 (80%)	0.31	6 (3%) 45 24	96, 160, 225, 265	0
1	F	177/219 (80%)	0.17	2 (1%) 80 64	105, 150, 196, 229	0
1	G	172/219 (78%)	0.28	5 (2%) 51 28	87, 167, 227, 264	0
1	H	177/219 (80%)	0.37	13 (7%) 15 6	106, 169, 220, 251	0
2	B	221/266 (83%)	-0.31	0 100 100	76, 101, 149, 187	0
2	C	224/266 (84%)	-0.20	1 (0%) 92 84	70, 110, 159, 217	0
2	D	224/266 (84%)	-0.35	0 100 100	65, 103, 146, 164	0
2	E	226/266 (84%)	-0.24	0 100 100	66, 99, 140, 215	0
All	All	1597/1940 (82%)	-0.03	27 (1%) 70 49	65, 125, 209, 265	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	GLY	6.9
1	H	22	VAL	4.3
1	G	6	ASP	3.4
1	G	89	LEU	3.3
1	H	115	SER	3.0
1	H	93	ILE	2.9
1	A	17	ILE	2.7
2	C	156	GLN	2.7
1	G	102	VAL	2.6
1	F	165	PHE	2.6
1	A	89	LEU	2.6
1	H	80	TYR	2.5
1	H	17	ILE	2.4
1	G	121	LEU	2.4
1	A	158	SER	2.4
1	G	120	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	89	LEU	2.3
1	H	130	HIS	2.3
1	H	18	GLY	2.3
1	A	159	THR	2.2
1	H	150	PHE	2.2
1	H	88	LEU	2.1
1	H	136	THR	2.1
1	H	19	ASP	2.1
1	H	102	VAL	2.1
1	A	121	LEU	2.1
1	F	87	ALA	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.