



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:49 am BST

PDB ID : 5WQD  
Title : Crystal structure of TRF2 TRFH in complex with an NBS1 peptide  
Authors : Hu, C.; Chen, Y.; Lei, M.  
Deposited on : 2016-11-26  
Resolution : 3.00 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

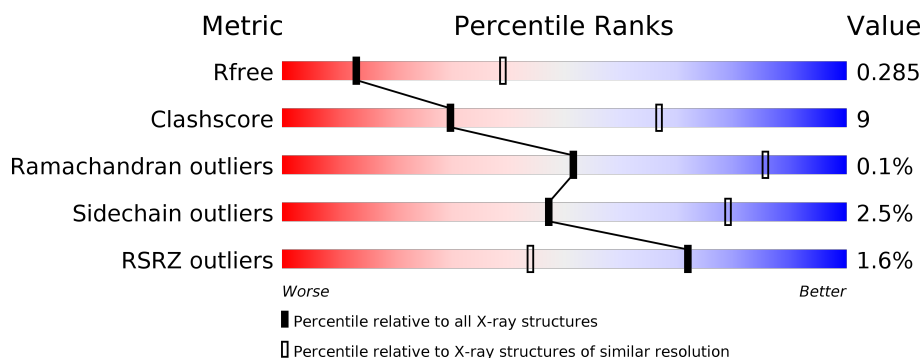
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	204	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	204	<div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	C	204	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>22%</div> <div>.</div> </div> </div>
1	D	204	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>22%</div> </div> </div>
1	E	204	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>..</div> </div> </div>
1	F	204	<div> <div></div> <div>68%</div> <div>27%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	204	<div><div>%</div><div><div></div><div>66%</div><div>27%</div><div></div><div></div></div></div>
2	H	16	<div><div>19%</div><div><div></div><div>50%</div><div>25%</div><div>25%</div></div></div>
2	I	16	<div><div>6%</div><div><div></div><div>56%</div><div>25%</div><div>19%</div></div></div>
2	J	16	<div><div>6%</div><div><div></div><div>50%</div><div>13%</div><div>38%</div></div></div>
2	K	16	<div><div></div><div><div></div><div>56%</div><div>6%</div><div>38%</div></div></div>
2	L	16	<div><div>13%</div><div><div></div><div>50%</div><div>13%</div><div>38%</div></div></div>
2	M	16	<div><div></div><div><div></div><div>31%</div><div>13%</div><div>56%</div></div></div>
2	N	16	<div><div>6%</div><div><div></div><div>56%</div><div>44%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11619 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 Telomeric repeat-binding factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1605	1020	275	300	10			
1	B	202	Total	C	N	O	S	0	0	0
			1632	1036	287	299	10			
1	C	204	Total	C	N	O	S	0	0	0
			1634	1037	288	300	9			
1	D	203	Total	C	N	O	S	0	0	0
			1625	1034	286	296	9			
1	E	198	Total	C	N	O	S	0	0	0
			1562	992	271	289	10			
1	F	195	Total	C	N	O	S	0	0	0
			1498	957	257	276	8			
1	G	195	Total	C	N	O	S	0	0	0
			1489	946	258	277	8			

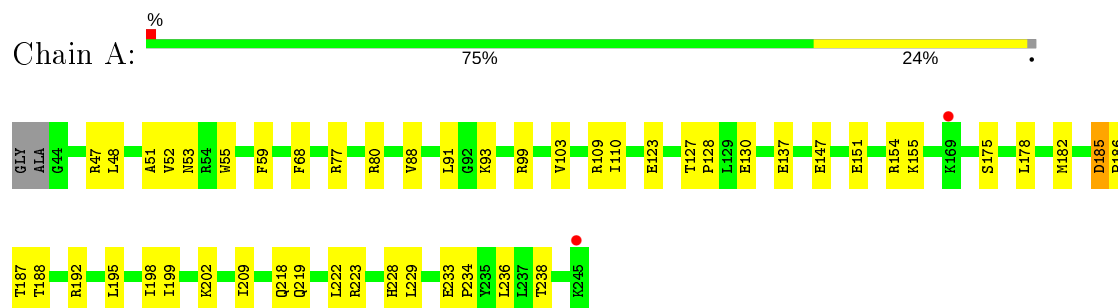
- Molecule 2 is a protein called Nibrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	12	Total	C	N	O		0	0	0
			100	65	18	17				
2	I	13	Total	C	N	O	S	0	0	0
			108	70	19	18	1			
2	J	10	Total	C	N	O		0	0	0
			81	53	13	15				
2	K	10	Total	C	N	O		0	0	0
			81	53	13	15				
2	L	10	Total	C	N	O		0	0	0
			81	53	13	15				
2	M	7	Total	C	N	O		0	0	0
			54	35	8	11				
2	N	9	Total	C	N	O		0	0	0
			69	44	11	14				

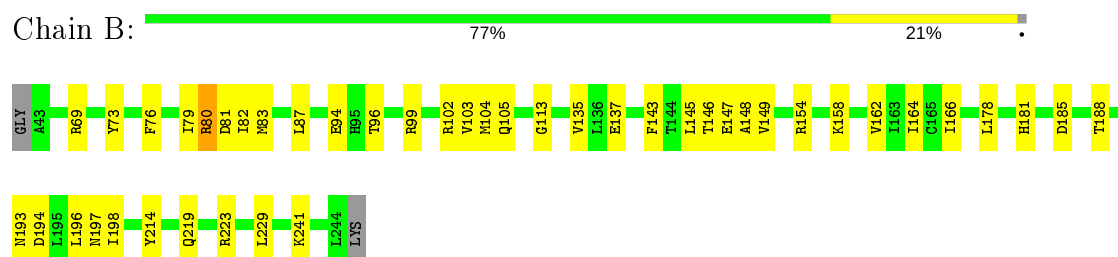
### 3 Residue-property plots [i](#)

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.

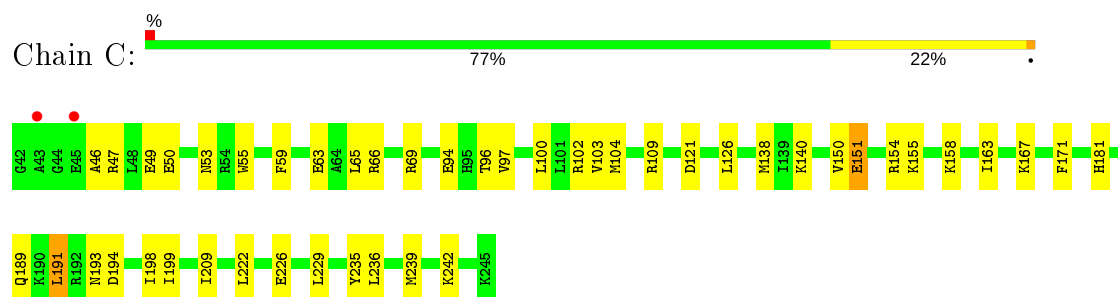
#### • Molecule 1: Telomeric repeat-binding factor 2



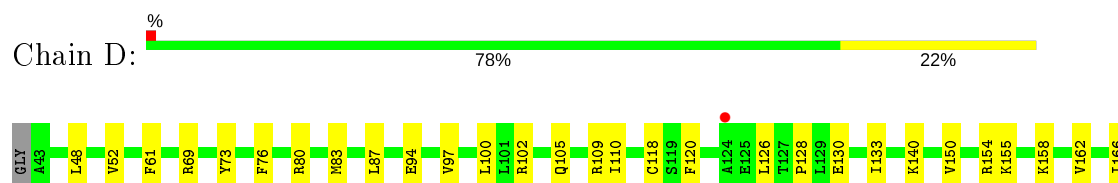
#### • Molecule 1: Telomeric repeat-binding factor 2



#### • Molecule 1: Telomeric repeat-binding factor 2

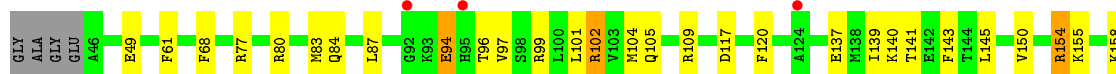
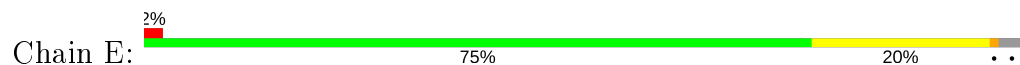


#### • Molecule 1: Telomeric repeat-binding factor 2





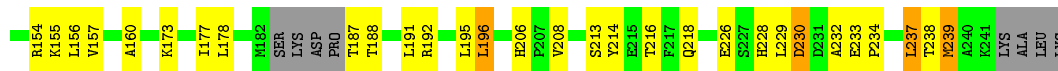
• Molecule 1: Telomeric repeat-binding factor 2



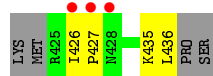
• Molecule 1: Telomeric repeat-binding factor 2



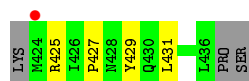
• Molecule 1: Telomeric repeat-binding factor 2



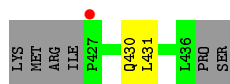
• Molecule 2: Nibrin



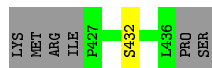
• Molecule 2: Nibrin



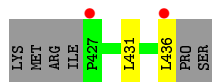
## ● Molecule 2: Nibrin



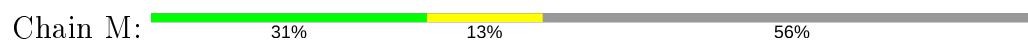
## ● Molecule 2: Nibrin



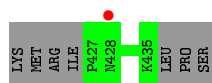
## ● Molecule 2: Nibrin



## ● Molecule 2: Nibrin



## ● Molecule 2: Nibrin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.62Å 153.27Å 108.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 3.00 48.17 – 2.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.17-3.00) 96.1 (48.17-2.98)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.233 , 0.284 0.232 , 0.285	Depositor DCC
$R_{free}$ test set	2304 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.2	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 72.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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	0/1629	0.41	0/2194
1	B	0.23	0/1657	0.37	0/2228
1	C	0.24	0/1659	0.41	0/2232
1	D	0.24	0/1649	0.39	0/2216
1	E	0.24	0/1587	0.42	0/2145
1	F	0.24	0/1519	0.41	0/2056
1	G	0.25	0/1511	0.47	0/2046
2	H	0.23	0/102	0.43	0/138
2	I	0.23	0/110	0.44	0/148
2	J	0.24	0/83	0.41	0/112
2	K	0.26	0/83	0.44	0/112
2	L	0.26	0/83	0.68	0/112
2	M	0.21	0/55	0.37	0/75
2	N	0.21	0/71	0.43	0/97
All	All	0.24	0/11798	0.42	0/15911

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	1605	0	1602	30	0
1	B	1632	0	1660	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1634	0	1652	24	0
1	D	1625	0	1658	27	0
1	E	1562	0	1535	29	0
1	F	1498	0	1463	40	0
1	G	1489	0	1423	36	0
2	H	100	0	107	3	0
2	I	108	0	116	3	0
2	J	81	0	84	2	0
2	K	81	0	84	1	0
2	L	81	0	84	1	0
2	M	54	0	48	2	0
2	N	69	0	62	0	0
All	All	11619	0	11578	217	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 9.

All (217) 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:D:158:LYS:HE2	1:D:181:HIS:HB3	1.60	0.84
1:F:102:ARG:NH2	1:F:138:MET:SD	2.50	0.84
1:E:233:GLU:HG2	1:E:237:LEU:HD21	1.66	0.78
1:A:55:TRP:HB3	1:A:236:LEU:HD11	1.66	0.78
1:E:94:GLU:OE2	1:E:97:VAL:N	2.20	0.73
1:G:143:PHE:HB3	1:G:145:LEU:HD13	1.71	0.72
1:G:97:VAL:HA	1:G:100:LEU:HB3	1.71	0.71
1:B:146:THR:HG22	1:B:148:ALA:H	1.55	0.71
1:C:97:VAL:HA	1:C:100:LEU:HB3	1.71	0.70
1:F:59:PHE:HB2	1:F:236:LEU:HD13	1.73	0.70
1:F:61:PHE:CE2	1:F:65:LEU:HD11	2.28	0.68
1:F:171:PHE:HB3	1:F:199:ILE:HG23	1.74	0.68
1:C:102:ARG:NH1	1:C:138:MET:SD	2.67	0.67
1:A:99:ARG:NH2	1:A:228:HIS:O	2.28	0.67
1:F:206:HIS:HD2	1:F:208:VAL:HG12	1.58	0.67
1:F:129:LEU:HD23	1:F:164:ILE:HG21	1.76	0.67
1:A:185:ASP:OD1	1:A:187:THR:OG1	2.13	0.65
1:F:192:ARG:HA	1:F:195:LEU:HD12	1.78	0.65
1:E:77:ARG:HG3	1:E:80:ARG:HH21	1.61	0.65
1:F:102:ARG:HA	1:F:105:GLN:HB2	1.76	0.65
1:C:158:LYS:HE3	1:C:181:HIS:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ARG:HG2	1:B:158:LYS:HE2	1.80	0.64
1:C:140:LYS:HG2	1:C:150:VAL:HG21	1.79	0.63
1:F:55:TRP:HB3	1:F:236:LEU:HD11	1.80	0.63
1:F:130:GLU:HA	1:F:133:ILE:HD12	1.79	0.63
1:F:208:VAL:HG13	1:F:209:ILE:HD12	1.81	0.63
1:D:130:GLU:HA	1:D:133:ILE:HD12	1.81	0.63
1:G:47:ARG:HA	1:G:50:GLU:HB2	1.81	0.62
1:G:102:ARG:HG2	1:G:139:ILE:HG13	1.81	0.62
1:A:233:GLU:OE2	1:A:238:THR:HG22	2.00	0.62
1:B:80:ARG:NH1	1:B:81:ASP:OD1	2.33	0.62
1:F:103:VAL:HG21	1:F:229:LEU:HD11	1.80	0.62
1:C:189:GLN:O	1:C:193:ASN:ND2	2.24	0.62
1:B:103:VAL:HG11	1:B:229:LEU:HD11	1.82	0.61
1:G:45:GLU:HG2	1:G:48:LEU:HD21	1.81	0.61
1:A:137:GLU:OE1	1:A:154:ARG:NH1	2.34	0.61
1:F:73:TYR:HA	1:F:76:PHE:HB3	1.83	0.60
1:A:236:LEU:HD12	1:A:236:LEU:H	1.66	0.60
1:F:165:CYS:HB2	1:F:174:ALA:HB2	1.84	0.59
1:C:109:ARG:NH2	2:J:430:GLN:O	2.35	0.59
1:E:207:PRO:O	1:E:211:ASN:N	2.34	0.59
1:E:68:PHE:O	1:E:219:GLN:NE2	2.36	0.59
1:B:105:GLN:HB3	2:I:431:LEU:HD23	1.85	0.59
1:C:94:GLU:HG2	1:C:96:THR:HG22	1.85	0.59
2:H:426:ILE:HB	2:H:427:PRO:HD3	1.84	0.59
1:A:88:VAL:HG12	2:H:426:ILE:HG12	1.84	0.59
1:E:99:ARG:HB3	1:E:143:PHE:CZ	2.38	0.58
1:C:63:GLU:OE1	1:C:66:ARG:NH2	2.34	0.58
1:G:178:LEU:HD21	1:G:196:LEU:HG	1.86	0.58
1:G:69:ARG:NH1	1:G:226:GLU:OE1	2.36	0.58
1:E:178:LEU:HD21	1:E:196:LEU:HG	1.86	0.58
1:A:147:GLU:OE1	1:A:154:ARG:NH2	2.36	0.58
1:G:130:GLU:HA	1:G:133:ILE:HD12	1.85	0.58
1:B:104:MET:HG3	2:I:431:LEU:HD22	1.86	0.57
1:E:171:PHE:HB3	1:E:199:ILE:HG23	1.84	0.57
1:A:48:LEU:HD22	1:B:241:LYS:HG2	1.86	0.57
1:B:193:ASN:HA	1:B:196:LEU:HD12	1.87	0.57
1:D:94:GLU:HB3	1:D:97:VAL:HG12	1.86	0.57
1:F:187:THR:N	1:F:189:GLN:OE1	2.38	0.57
1:E:101:LEU:O	1:E:105:GLN:N	2.29	0.56
1:F:191:LEU:HD21	1:F:208:VAL:HG21	1.86	0.56
1:E:102:ARG:NH1	1:E:105:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:NH1	1:B:105:GLN:OE1	2.33	0.56
1:G:61:PHE:HE2	1:G:229:LEU:HD11	1.71	0.56
1:B:94:GLU:OE2	1:B:96:THR:N	2.39	0.56
1:C:191:LEU:HA	1:C:194:ASP:HB2	1.86	0.56
1:D:120:PHE:HE1	1:D:128:PRO:HB3	1.71	0.56
1:D:110:ILE:O	1:D:214:TYR:OH	2.19	0.56
1:G:61:PHE:CE2	1:G:229:LEU:HD11	2.42	0.55
1:F:113:GLY:HA2	1:F:128:PRO:HB2	1.87	0.55
1:C:103:VAL:HG21	1:C:229:LEU:HD11	1.88	0.55
1:A:53:ASN:HB3	1:A:91:LEU:HD23	1.88	0.55
1:G:206:HIS:CD2	1:G:208:VAL:HG12	2.42	0.54
1:C:104:MET:HG2	2:J:431:LEU:HG	1.90	0.54
1:G:145:LEU:HD21	1:G:228:HIS:CE1	2.43	0.54
1:G:145:LEU:HD21	1:G:228:HIS:ND1	2.22	0.54
1:F:189:GLN:N	1:F:189:GLN:OE1	2.41	0.54
1:C:151:GLU:HA	1:C:154:ARG:HB3	1.90	0.54
1:C:171:PHE:HB3	1:C:199:ILE:HG23	1.89	0.53
1:F:236:LEU:H	1:F:236:LEU:HD12	1.73	0.53
1:C:69:ARG:NH2	1:C:226:GLU:OE2	2.41	0.53
1:D:69:ARG:NH2	1:D:226:GLU:OE2	2.41	0.53
1:E:109:ARG:HA	1:E:120:PHE:HE2	1.74	0.53
1:B:143:PHE:HB3	1:B:145:LEU:HD13	1.91	0.53
1:E:140:LYS:HA	1:E:145:LEU:HD21	1.91	0.53
1:C:65:LEU:HD22	1:C:222:LEU:HD11	1.91	0.53
1:A:195:LEU:O	1:A:199:ILE:HG13	2.09	0.53
1:A:198:ILE:HD13	1:A:209:ILE:HD13	1.91	0.52
1:F:61:PHE:CD2	1:F:100:LEU:HD11	2.44	0.52
1:A:103:VAL:HG21	1:A:229:LEU:HD11	1.91	0.52
1:B:158:LYS:HD3	1:B:181:HIS:HB3	1.91	0.51
1:E:87:LEU:HD11	2:L:431:LEU:HD13	1.91	0.51
1:F:80:ARG:NH1	1:F:81:ASP:OD1	2.44	0.51
1:D:155:LYS:NZ	1:D:187:THR:OG1	2.42	0.50
1:D:162:VAL:O	1:D:166:ILE:HG13	2.12	0.50
1:G:94:GLU:OE2	1:G:96:THR:HG23	2.12	0.50
1:D:126:LEU:HB3	1:D:130:GLU:HG3	1.94	0.50
1:B:185:ASP:OD1	1:B:188:THR:OG1	2.28	0.50
1:D:73:TYR:HA	1:D:76:PHE:HB3	1.94	0.49
1:D:80:ARG:NH1	2:K:432:SER:OG	2.46	0.49
1:A:68:PHE:HD1	1:A:222:LEU:HD22	1.78	0.49
1:A:185:ASP:HB2	1:A:186:PRO:HD2	1.94	0.49
1:B:194:ASP:O	1:B:198:ILE:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:PHE:HB2	1:E:145:LEU:HD22	1.94	0.49
1:C:121:ASP:HB2	1:C:126:LEU:HD21	1.95	0.48
1:D:140:LYS:HD2	1:D:150:VAL:HG21	1.95	0.48
1:G:173:LYS:O	1:G:177:ILE:HD12	2.12	0.48
1:B:103:VAL:HG21	1:B:229:LEU:HD21	1.95	0.48
1:E:109:ARG:HA	1:E:120:PHE:CE2	2.49	0.48
1:B:147:GLU:OE1	1:B:154:ARG:NH2	2.46	0.48
1:D:154:ARG:HG2	1:D:158:LYS:HD2	1.96	0.48
1:B:162:VAL:O	1:B:166:ILE:HG13	2.15	0.47
1:D:171:PHE:HB3	1:D:199:ILE:HG23	1.96	0.47
1:F:84:GLN:HE21	2:M:432:SER:H	1.62	0.47
1:A:175:SER:HA	1:A:178:LEU:HB3	1.96	0.47
1:B:193:ASN:O	1:B:197:ASN:ND2	2.39	0.47
1:C:59:PHE:CZ	1:D:52:VAL:HG11	2.49	0.47
1:E:163:ILE:HD11	1:E:212:PHE:CG	2.50	0.47
1:C:198:ILE:HD13	1:C:209:ILE:HG12	1.97	0.47
1:D:102:ARG:NH1	1:D:105:GLN:OE1	2.47	0.47
1:E:139:ILE:HG23	1:E:143:PHE:CD1	2.49	0.47
1:G:228:HIS:N	1:G:228:HIS:CD2	2.81	0.47
1:D:48:LEU:O	1:D:52:VAL:HG12	2.15	0.47
2:H:435:LYS:NZ	2:H:436:LEU:O	2.46	0.47
1:B:162:VAL:HG11	1:B:178:LEU:HD12	1.95	0.47
1:E:162:VAL:HG13	1:E:163:ILE:HG23	1.96	0.47
1:G:120:PHE:HE1	1:G:128:PRO:HB3	1.80	0.47
1:F:84:GLN:NE2	2:M:430:GLN:OE1	2.46	0.47
1:A:127:THR:HG23	1:A:130:GLU:H	1.79	0.47
1:D:61:PHE:CD2	1:D:100:LEU:HD21	2.50	0.47
1:F:79:ILE:HG22	1:F:83:MET:HE2	1.95	0.47
2:I:427:PRO:HB2	2:I:429:TYR:CE1	2.50	0.47
1:A:59:PHE:HB2	1:A:236:LEU:HD13	1.97	0.46
1:B:219:GLN:O	1:B:223:ARG:HG2	2.14	0.46
1:E:194:ASP:O	1:E:198:ILE:HG13	2.15	0.46
1:E:77:ARG:HG3	1:E:80:ARG:NH2	2.29	0.46
1:E:150:VAL:HG12	1:E:154:ARG:HG3	1.98	0.46
1:F:61:PHE:CE2	1:F:100:LEU:HD11	2.51	0.46
1:G:61:PHE:CE2	1:G:65:LEU:HD11	2.51	0.46
1:G:229:LEU:HD23	1:G:230:ASP:O	2.15	0.46
1:F:110:ILE:O	1:F:214:TYR:OH	2.26	0.46
1:B:69:ARG:HD3	1:B:223:ARG:HH12	1.80	0.45
1:D:61:PHE:CG	1:D:100:LEU:HD21	2.51	0.45
1:D:120:PHE:CE1	1:D:128:PRO:HB3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLU:HA	1:C:53:ASN:HB2	1.98	0.45
1:D:178:LEU:HD12	1:D:182:MET:HB2	1.99	0.45
1:A:178:LEU:O	1:A:182:MET:HB2	2.17	0.45
1:F:69:ARG:HG3	1:F:222:LEU:HD21	1.99	0.45
1:G:191:LEU:O	1:G:195:LEU:HD12	2.17	0.45
1:G:105:GLN:O	1:G:109:ARG:HD3	2.17	0.45
1:G:234:PRO:HD2	1:G:237:LEU:HD21	1.99	0.45
1:C:163:ILE:O	1:C:167:LYS:HG3	2.17	0.44
1:B:105:GLN:HG3	1:B:135:VAL:HG11	2.00	0.44
1:E:49:GLU:OE2	1:E:49:GLU:N	2.46	0.44
1:F:162:VAL:HG12	1:F:177:ILE:HB	2.00	0.44
1:B:137:GLU:OE2	1:B:154:ARG:NH1	2.46	0.44
1:G:156:LEU:O	1:G:160:ALA:N	2.45	0.44
1:F:61:PHE:O	1:F:65:LEU:HD12	2.18	0.44
1:G:233:GLU:HB3	1:G:237:LEU:HD11	1.99	0.44
1:F:206:HIS:CD2	1:F:208:VAL:HG12	2.45	0.44
1:A:198:ILE:O	1:A:202:LYS:N	2.51	0.43
1:G:214:TYR:O	1:G:218:GLN:HG3	2.17	0.43
1:D:204:LEU:HA	1:D:209:ILE:HD11	2.00	0.43
1:G:136:LEU:HA	1:G:139:ILE:HD12	1.99	0.43
1:C:55:TRP:HB3	1:C:236:LEU:HD13	2.00	0.43
1:E:94:GLU:OE2	1:E:96:THR:N	2.52	0.43
1:D:69:ARG:NH1	1:D:226:GLU:OE1	2.52	0.43
1:C:155:LYS:HE2	1:C:155:LYS:HB2	1.82	0.43
1:G:213:SER:OG	1:G:216:THR:OG1	2.35	0.43
1:F:57:LEU:HD21	1:F:101:LEU:HD21	2.00	0.42
1:B:113:GLY:HA3	1:B:214:TYR:OH	2.19	0.42
1:B:73:TYR:HA	1:B:76:PHE:HB3	2.00	0.42
1:F:101:LEU:O	1:F:105:GLN:N	2.51	0.42
1:G:238:THR:HG23	1:G:239:MET:SD	2.60	0.42
1:B:83:MET:O	1:B:87:LEU:HG	2.20	0.42
1:D:172:GLU:H	1:D:172:GLU:CD	2.23	0.42
1:E:158:LYS:HD2	1:E:181:HIS:HB3	2.01	0.42
1:F:222:LEU:O	1:F:226:GLU:HG2	2.19	0.42
1:D:214:TYR:O	1:D:218:GLN:HG3	2.19	0.42
1:E:154:ARG:HB3	1:E:154:ARG:HH11	1.85	0.42
1:G:230:ASP:C	1:G:232:ALA:H	2.23	0.42
1:F:159:GLU:O	1:F:163:ILE:HG23	2.18	0.42
1:A:77:ARG:HG3	1:A:80:ARG:HH21	1.84	0.42
1:F:94:GLU:HG2	1:F:97:VAL:H	1.85	0.42
1:F:220:LYS:HG2	1:F:223:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:GLU:HA	1:G:150:VAL:HB	2.02	0.42
1:B:79:ILE:HA	1:B:82:ILE:HD12	2.02	0.42
1:D:222:LEU:O	1:D:226:GLU:HG3	2.19	0.42
1:E:61:PHE:CD1	1:E:104:MET:HB2	2.55	0.42
1:G:151:GLU:O	1:G:155:LYS:HG2	2.20	0.42
1:B:99:ARG:HB3	1:B:143:PHE:CZ	2.55	0.41
1:E:137:GLU:O	1:E:141:THR:HG23	2.19	0.41
1:E:83:MET:HE2	1:E:83:MET:HB3	1.94	0.41
1:A:109:ARG:HB3	1:A:128:PRO:O	2.20	0.41
1:A:234:PRO:O	1:A:238:THR:HG23	2.21	0.41
1:G:187:THR:OG1	1:G:188:THR:N	2.53	0.41
1:A:110:ILE:HG22	1:A:218:GLN:HG2	2.02	0.41
1:B:146:THR:O	1:B:149:VAL:HG22	2.21	0.41
1:A:219:GLN:O	1:A:223:ARG:HG2	2.21	0.41
1:A:123:GLU:CD	1:A:123:GLU:H	2.24	0.41
1:A:151:GLU:O	1:A:155:LYS:HG2	2.20	0.41
1:B:164:ILE:HA	1:B:164:ILE:HD13	1.91	0.41
1:E:105:GLN:HG2	1:E:109:ARG:NH1	2.35	0.41
1:F:61:PHE:CZ	1:F:65:LEU:HD11	2.56	0.41
1:A:47:ARG:O	1:A:51:ALA:N	2.50	0.41
1:G:192:ARG:O	1:G:196:LEU:HD12	2.21	0.41
1:F:150:VAL:O	1:F:154:ARG:N	2.54	0.41
1:D:83:MET:O	1:D:87:LEU:HD22	2.20	0.40
1:A:188:THR:O	1:A:192:ARG:N	2.28	0.40
1:A:48:LEU:O	1:A:52:VAL:HG23	2.21	0.40
1:C:46:ALA:HA	1:C:49:GLU:HG2	2.02	0.40
1:F:225:LEU:HD23	1:F:225:LEU:HA	1.93	0.40
1:C:239:MET:HA	1:C:242:LYS:HG2	2.04	0.40
1:F:57:LEU:HD12	1:F:83:MET:HG2	2.02	0.40
1:G:129:LEU:HA	1:G:129:LEU:HD23	1.90	0.40
1:G:154:ARG:HA	1:G:157:VAL:HG23	2.04	0.40
1:G:52:VAL:O	1:G:56:VAL:HG12	2.22	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	200/204 (98%)	194 (97%)	5 (2%)	1 (0%)	29	68
1	B	200/204 (98%)	192 (96%)	8 (4%)	0	100	100
1	C	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
1	D	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
1	E	196/204 (96%)	186 (95%)	10 (5%)	0	100	100
1	F	191/204 (94%)	182 (95%)	9 (5%)	0	100	100
1	G	191/204 (94%)	183 (96%)	8 (4%)	0	100	100
2	H	10/16 (62%)	8 (80%)	2 (20%)	0	100	100
2	I	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	J	8/16 (50%)	6 (75%)	2 (25%)	0	100	100
2	K	8/16 (50%)	8 (100%)	0	0	100	100
2	L	8/16 (50%)	8 (100%)	0	0	100	100
2	M	5/16 (31%)	4 (80%)	1 (20%)	0	100	100
2	N	7/16 (44%)	5 (71%)	2 (29%)	0	100	100
All	All	1438/1540 (93%)	1373 (96%)	64 (4%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	LYS

### 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	171/182 (94%)	170 (99%)	1 (1%)	86	95
1	B	177/182 (97%)	176 (99%)	1 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	175/182 (96%)	171 (98%)	4 (2%)	50	80
1	D	174/182 (96%)	170 (98%)	4 (2%)	50	80
1	E	164/182 (90%)	158 (96%)	6 (4%)	34	70
1	F	152/182 (84%)	147 (97%)	5 (3%)	38	73
1	G	149/182 (82%)	141 (95%)	8 (5%)	22	57
2	H	12/16 (75%)	12 (100%)	0	100	100
2	I	13/16 (81%)	12 (92%)	1 (8%)	13	42
2	J	10/16 (62%)	10 (100%)	0	100	100
2	K	10/16 (62%)	10 (100%)	0	100	100
2	L	10/16 (62%)	9 (90%)	1 (10%)	7	29
2	M	6/16 (38%)	6 (100%)	0	100	100
2	N	8/16 (50%)	8 (100%)	0	100	100
All	All	1231/1386 (89%)	1200 (98%)	31 (2%)	47	79

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
1	B	80	ARG
1	C	47	ARG
1	C	151	GLU
1	C	191	LEU
1	C	235	TYR
1	D	109	ARG
1	D	118	CYS
1	D	190	LYS
1	D	200	ARG
1	E	84	GLN
1	E	94	GLU
1	E	102	ARG
1	E	117	ASP
1	E	154	ARG
1	E	155	LYS
1	F	109	ARG
1	F	126	LEU
1	F	151	GLU
1	F	191	LEU
1	F	195	LEU

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Mol	Chain	Res	Type
1	G	47	ARG
1	G	63	GLU
1	G	66	ARG
1	G	107	LEU
1	G	196	LEU
1	G	230	ASP
1	G	237	LEU
1	G	239	MET
2	I	425	ARG
2	L	436	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	206	HIS
1	G	206	HIS
1	G	228	HIS

### 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<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	202/204 (99%)	-0.14	2 (0%) 82 59	36, 78, 133, 164	0
1	B	202/204 (99%)	-0.31	0 100 100	34, 61, 114, 133	0
1	C	204/204 (100%)	-0.15	2 (0%) 82 59	43, 71, 136, 197	0
1	D	203/204 (99%)	-0.12	2 (0%) 82 59	50, 78, 121, 150	0
1	E	198/204 (97%)	0.04	5 (2%) 57 29	56, 97, 150, 185	0
1	F	195/204 (95%)	0.05	1 (0%) 91 75	63, 102, 148, 184	0
1	G	195/204 (95%)	-0.11	3 (1%) 73 46	49, 95, 162, 204	0
2	H	12/16 (75%)	0.76	3 (25%) 0 0	55, 100, 167, 175	0
2	I	13/16 (81%)	0.03	1 (7%) 13 4	46, 75, 146, 146	0
2	J	10/16 (62%)	0.10	1 (10%) 7 2	64, 81, 112, 130	0
2	K	10/16 (62%)	-0.07	0 100 100	56, 79, 118, 136	0
2	L	10/16 (62%)	0.92	2 (20%) 1 0	89, 117, 157, 167	0
2	M	7/16 (43%)	0.98	0 100 100	98, 110, 134, 134	0
2	N	9/16 (56%)	0.81	1 (11%) 5 1	80, 116, 154, 172	0
All	All	1470/1540 (95%)	-0.08	23 (1%) 72 44	34, 84, 143, 204	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	426	ILE	4.4
1	C	45	GLU	3.6
1	C	43	ALA	3.5
1	G	146	THR	3.3
1	D	124	ALA	3.0
1	E	124	ALA	2.9
1	G	43	ALA	2.9
2	L	436	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	L	427	PRO	2.7
2	N	428	ASN	2.7
1	D	232	ALA	2.6
2	J	427	PRO	2.3
1	G	122	MET	2.3
1	A	169	LYS	2.3
2	H	428	ASN	2.3
1	E	95	HIS	2.3
1	E	227	SER	2.3
1	E	92	GLY	2.2
1	A	245	LYS	2.2
1	E	177	ILE	2.1
1	F	238	THR	2.1
2	I	424	MET	2.1
2	H	427	PRO	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.