



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:18 AM GMT

PDB ID : 3ABH  
Title : Crystal structure of the EFC/F-BAR domain of human PACSIN2/Syndapin II (2.0 Å)  
Authors : Shimada, A.; Shirouzu, M.; Hanawa-Suetsugu, K.; Terada, T.; Umehara, T.; Suetsugu, S.; Yamamoto, M.; Yokoyama, S.  
Deposited on : 2009-12-11  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/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  
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

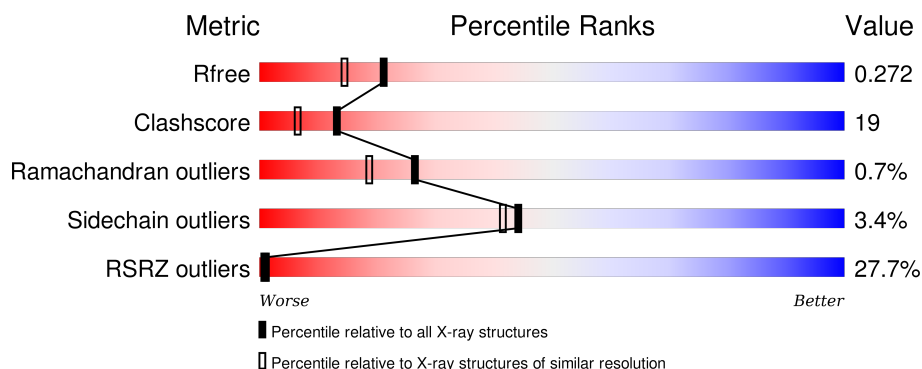
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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>24%</div> <div>66%</div> <div>24%</div> <div>8%</div> </div>
1	B	312	<div> <div>25%</div> <div>62%</div> <div>28%</div> <div>8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5335 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 Protein kinase C and casein kinase substrate in neurons protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	Se	0	0	0
			2392	1505	429	443	5	10			
1	B	288	Total	C	N	O	S	Se	0	0	0
			2392	1505	429	443	5	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q9UNF0
A	-5	SER	-	EXPRESSION TAG	UNP Q9UNF0
A	-4	SER	-	EXPRESSION TAG	UNP Q9UNF0
A	-3	GLY	-	EXPRESSION TAG	UNP Q9UNF0
A	-2	SER	-	EXPRESSION TAG	UNP Q9UNF0
A	-1	SER	-	EXPRESSION TAG	UNP Q9UNF0
A	0	GLY	-	EXPRESSION TAG	UNP Q9UNF0
B	-6	GLY	-	EXPRESSION TAG	UNP Q9UNF0
B	-5	SER	-	EXPRESSION TAG	UNP Q9UNF0
B	-4	SER	-	EXPRESSION TAG	UNP Q9UNF0
B	-3	GLY	-	EXPRESSION TAG	UNP Q9UNF0
B	-2	SER	-	EXPRESSION TAG	UNP Q9UNF0
B	-1	SER	-	EXPRESSION TAG	UNP Q9UNF0
B	0	GLY	-	EXPRESSION TAG	UNP Q9UNF0

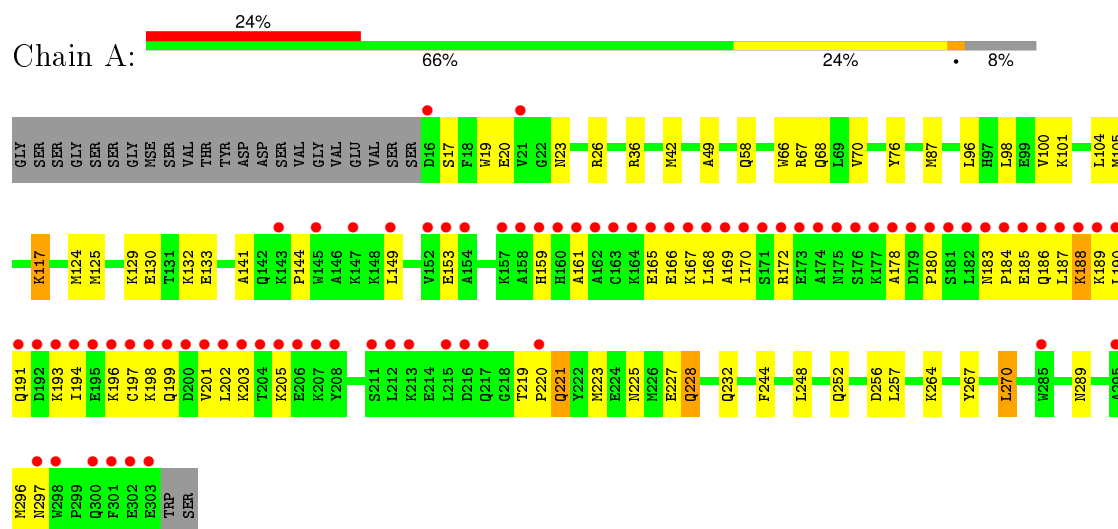
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	276	Total	O	0	0
			276	276		
2	B	275	Total	O	0	0
			275	275		

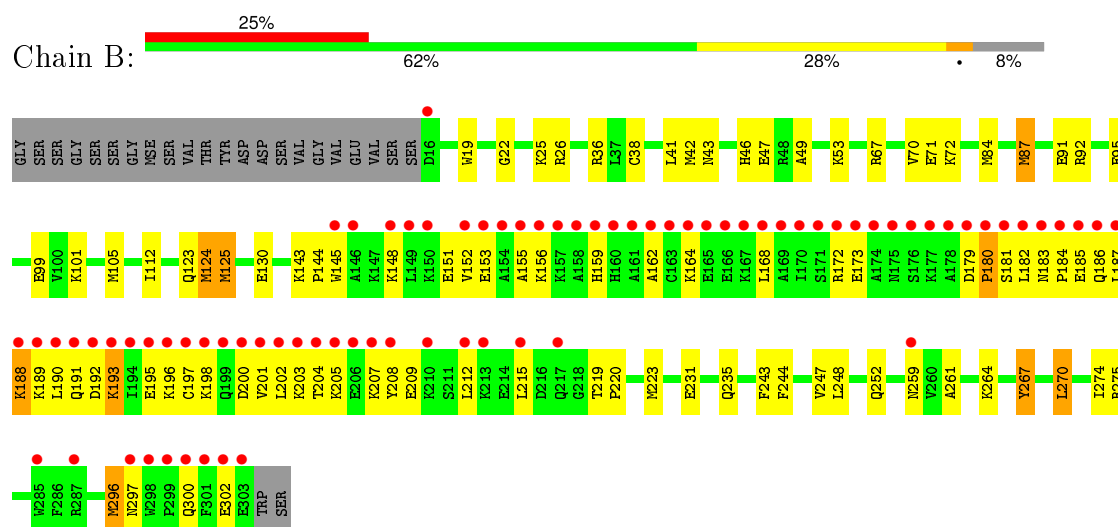
### 3 Residue-property plots [i](#)

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: Protein kinase C and casein kinase substrate in neurons protein 2



- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	31.52Å 86.14Å 353.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.00 48.59 – 1.99	Depositor EDS
% Data completeness (in resolution range)	93.5 (48.59-2.00) 93.3 (48.59-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.97 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.234 , 0.271 0.234 , 0.272	Depositor DCC
$R_{free}$ test set	3166 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 72.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 64312 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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, 0.375 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	0.32	0/2432	0.48	0/3238
1	B	0.33	0/2432	0.47	0/3238
All	All	0.32	0/4864	0.47	0/6476

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	TYR	Sidechain
1	B	267	TYR	Sidechain

### 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	2392	0	2353	89	0
1	B	2392	0	2353	102	0
2	A	276	0	0	14	0
2	B	275	0	0	9	0
All	All	5335	0	4706	179	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 19.

All (179) 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:19:TRP:HB2	1:B:296:MSE:HG3	1.40	1.04
1:A:185:GLU:HA	1:A:188:LYS:HD3	1.50	0.94
1:B:46:HIS:ND1	1:B:105:MSE:HE1	1.83	0.93
1:B:188:LYS:HA	1:B:188:LYS:HE3	1.54	0.89
1:B:179:ASP:HB3	1:B:182:LEU:HD21	1.60	0.84
1:B:84:MSE:O	1:B:87:MSE:HG2	1.85	0.76
1:B:46:HIS:CG	1:B:105:MSE:HE1	2.21	0.75
1:B:123:GLN:HB2	1:B:125:MSE:HE3	1.68	0.74
1:B:296:MSE:HE2	1:B:297:ASN:H	1.54	0.73
1:B:53:LYS:HB2	1:B:101:LYS:HD2	1.70	0.72
1:B:67:ARG:O	1:B:71:GLU:HG3	1.89	0.72
1:B:70:VAL:HG21	1:B:87:MSE:HE1	1.72	0.71
1:B:219:THR:N	1:B:220:PRO:HD2	2.06	0.71
1:B:84:MSE:SE	1:B:87:MSE:HE2	2.40	0.71
1:B:70:VAL:CG2	1:B:87:MSE:HE1	2.23	0.68
1:B:145:TRP:HE1	1:B:219:THR:HG22	1.58	0.67
1:A:100:VAL:HA	2:A:461:HOH:O	1.94	0.66
1:A:17:SER:HB3	1:B:296:MSE:HE3	1.77	0.66
1:B:172:ARG:NH1	1:B:193:LYS:HG2	2.10	0.66
1:A:19:TRP:CB	1:B:296:MSE:HG3	2.24	0.65
1:B:172:ARG:HH12	1:B:193:LYS:HG2	1.62	0.65
1:B:172:ARG:HD3	1:B:190:LEU:HD22	1.80	0.64
1:A:270:LEU:HD13	1:B:252:GLN:HG2	1.80	0.64
1:A:19:TRP:HB2	1:B:296:MSE:CG	2.22	0.63
1:A:219:THR:N	1:A:220:PRO:HD2	2.13	0.63
1:B:72:LYS:HD2	2:B:532:HOH:O	1.99	0.62
1:A:189:LYS:HE3	1:A:193:LYS:NZ	2.15	0.61
1:A:297:ASN:HA	2:A:362:HOH:O	2.00	0.61
1:B:187:LEU:HD23	1:B:191:GLN:HE21	1.66	0.60
1:B:189:LYS:HA	1:B:192:ASP:OD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LYS:O	1:A:199:GLN:HB3	2.00	0.60
1:A:149:LEU:O	1:A:153:GLU:HG2	2.02	0.59
1:A:170:ILE:HG12	1:A:194:ILE:HG13	1.84	0.58
1:B:67:ARG:HA	1:B:87:MSE:HE3	1.85	0.58
1:B:300:GLN:O	1:B:302:GLU:HG3	2.03	0.58
1:A:188:LYS:HD2	1:A:188:LYS:N	2.19	0.57
1:B:124:MSE:HE3	1:B:125:MSE:N	2.18	0.57
1:A:104:LEU:C	1:A:105:MSE:HE2	2.25	0.57
1:A:132:LYS:HG3	2:A:524:HOH:O	2.03	0.57
1:A:129:LYS:O	1:A:133:GLU:HG3	2.04	0.57
1:A:17:SER:OG	1:B:296:MSE:HG2	2.05	0.56
1:A:168:LEU:O	1:A:172:ARG:HG3	2.05	0.56
1:B:183:ASN:HB2	1:B:186:GLN:HB2	1.85	0.56
1:B:91:GLU:O	1:B:95:GLU:HG3	2.06	0.56
1:B:25:LYS:HE2	2:B:526:HOH:O	2.05	0.56
1:A:244:PHE:O	1:A:248:LEU:HG	2.04	0.56
1:A:168:LEU:HD23	1:A:168:LEU:O	2.06	0.55
1:A:202:LEU:HD23	1:A:202:LEU:O	2.06	0.55
1:B:261:ALA:HA	1:B:264:LYS:HE2	1.88	0.55
1:B:190:LEU:HA	1:B:193:LYS:HD3	1.89	0.55
1:A:130:GLU:H	1:A:130:GLU:CD	2.09	0.55
1:B:192:ASP:O	1:B:196:LYS:HG2	2.06	0.54
1:A:166:GLU:OE1	1:A:198:LYS:HD3	2.08	0.54
1:A:197:CYS:O	1:A:201:VAL:HG23	2.07	0.54
1:B:205:LYS:O	1:B:209:GLU:HG3	2.08	0.54
1:A:178:ALA:O	1:A:180:PRO:HD3	2.07	0.54
1:A:166:GLU:HG3	1:A:167:LYS:N	2.22	0.54
1:A:289:ASN:HB3	2:A:484:HOH:O	2.07	0.54
1:B:180:PRO:HG2	1:B:181:SER:H	1.73	0.53
1:B:197:CYS:O	1:B:201:VAL:HG23	2.09	0.53
1:B:43:ASN:O	1:B:47:GLU:HG3	2.08	0.53
1:A:188:LYS:HD2	1:A:188:LYS:H	1.72	0.53
1:B:259:ASN:HB3	2:B:487:HOH:O	2.09	0.53
1:A:223:MSE:O	1:A:227:GLU:HG3	2.08	0.52
1:A:228:GLN:O	1:A:232:GLN:HG2	2.10	0.52
1:A:187:LEU:HD23	1:A:187:LEU:C	2.30	0.52
1:B:148:LYS:O	1:B:151:GLU:HG2	2.10	0.51
1:A:188:LYS:H	1:A:188:LYS:CD	2.22	0.51
1:B:185:GLU:O	1:B:189:LYS:HG2	2.11	0.51
1:A:252:GLN:HE21	1:B:267:TYR:HB3	1.74	0.51
1:B:193:LYS:HD2	1:B:193:LYS:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:O	1:A:105:MSE:HE2	2.11	0.51
1:B:202:LEU:HD23	1:B:202:LEU:O	2.11	0.51
1:A:96:LEU:HD13	1:A:257:LEU:HD13	1.91	0.50
1:A:76:TYR:HB3	2:A:483:HOH:O	2.10	0.50
1:B:130:GLU:CD	1:B:130:GLU:H	2.13	0.50
1:B:22:GLY:O	1:B:25:LYS:HG3	2.12	0.50
1:A:183:ASN:CB	1:A:186:GLN:HB2	2.42	0.50
1:B:212:LEU:HD23	1:B:212:LEU:C	2.32	0.50
1:B:187:LEU:O	1:B:187:LEU:HD23	2.12	0.50
1:A:125:MSE:HE3	2:A:313:HOH:O	2.11	0.50
1:A:296:MSE:HE3	1:A:297:ASN:O	2.11	0.50
1:B:148:LYS:O	1:B:152:VAL:HG23	2.13	0.49
1:A:199:GLN:HG2	1:A:203:LYS:HE2	1.94	0.49
1:A:166:GLU:HG3	1:A:167:LYS:H	1.77	0.49
1:B:95:GLU:O	1:B:99:GLU:HG3	2.12	0.49
1:A:67:ARG:NH1	2:A:408:HOH:O	2.44	0.49
1:A:191:GLN:C	1:A:194:ILE:HG22	2.32	0.49
1:B:219:THR:N	1:B:220:PRO:CD	2.76	0.48
1:B:159:HIS:HA	1:B:204:THR:OG1	2.13	0.48
1:B:46:HIS:CE1	1:B:105:MSE:HE1	2.46	0.48
1:A:199:GLN:HE21	1:A:203:LYS:CE	2.25	0.48
1:A:124:MSE:HA	1:A:124:MSE:HE3	1.95	0.48
1:A:20:GLU:HB2	1:A:23:ASN:ND2	2.29	0.48
1:B:164:LYS:O	1:B:168:LEU:HG	2.14	0.48
1:B:41:LEU:HD23	1:B:112:ILE:HD12	1.96	0.48
1:B:84:MSE:SE	1:B:87:MSE:CE	3.10	0.48
1:B:203:LYS:HE3	1:B:207:LYS:HE2	1.95	0.48
1:B:193:LYS:N	1:B:193:LYS:HD2	2.29	0.47
1:A:68:GLN:HG2	2:A:427:HOH:O	2.12	0.47
1:A:49:ALA:HB1	1:A:101:LYS:HG2	1.97	0.47
1:A:129:LYS:NZ	2:A:449:HOH:O	2.47	0.47
1:B:124:MSE:C	1:B:124:MSE:HE3	2.34	0.47
1:A:188:LYS:HA	1:A:191:GLN:OE1	2.14	0.47
1:B:244:PHE:O	1:B:248:LEU:HG	2.14	0.47
1:B:153:GLU:HG2	2:B:486:HOH:O	2.13	0.47
1:B:19:TRP:HZ3	1:B:223:MSE:HA	1.80	0.47
1:A:270:LEU:HD13	1:B:252:GLN:CG	2.44	0.47
1:B:185:GLU:HA	2:B:426:HOH:O	2.14	0.47
1:A:296:MSE:HE3	1:A:297:ASN:C	2.34	0.47
1:A:117:LYS:NZ	1:A:117:LYS:HB3	2.29	0.47
1:A:17:SER:CB	1:B:296:MSE:HE3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:HG22	2:B:525:HOH:O	2.14	0.46
1:A:19:TRP:CZ3	1:A:223:MSE:HA	2.50	0.46
1:A:172:ARG:HB2	1:A:190:LEU:HD11	1.98	0.46
1:A:105:MSE:HE2	1:A:105:MSE:HA	1.96	0.46
1:A:232:GLN:NE2	1:A:232:GLN:HA	2.30	0.46
1:A:252:GLN:NE2	1:B:267:TYR:HB3	2.31	0.46
1:A:96:LEU:HD23	2:A:444:HOH:O	2.16	0.46
1:B:143:LYS:HB3	1:B:144:PRO:CD	2.46	0.46
1:A:264:LYS:HG3	2:A:557:HOH:O	2.16	0.46
1:B:183:ASN:HB3	1:B:184:PRO:HD2	1.97	0.46
1:B:46:HIS:ND1	1:B:105:MSE:CE	2.68	0.45
1:B:188:LYS:HA	1:B:188:LYS:CE	2.38	0.45
1:A:144:PRO:HG2	2:A:361:HOH:O	2.15	0.45
1:A:199:GLN:HE21	1:A:203:LYS:HE2	1.81	0.45
1:A:166:GLU:O	1:A:170:ILE:HG13	2.16	0.45
1:B:179:ASP:O	1:B:182:LEU:HG	2.16	0.45
1:B:123:GLN:HE21	1:B:125:MSE:HG3	1.80	0.45
1:B:219:THR:O	1:B:223:MSE:HG3	2.16	0.45
1:A:191:GLN:O	1:A:194:ILE:HG22	2.17	0.45
1:B:49:ALA:HB3	1:B:105:MSE:HE2	1.98	0.45
1:A:141:ALA:HB1	1:A:225:ASN:HB3	1.99	0.45
1:A:166:GLU:OE2	1:A:201:VAL:HG21	2.17	0.45
1:A:159:HIS:CD2	1:A:205:LYS:HA	2.52	0.45
1:B:275:ARG:HA	2:B:525:HOH:O	2.17	0.45
1:B:196:LYS:O	1:B:200:ASP:HB2	2.16	0.44
1:A:172:ARG:C	1:A:190:LEU:HD21	2.38	0.44
1:A:183:ASN:HB3	1:A:186:GLN:HB2	1.99	0.44
1:B:92:ARG:HD2	2:B:394:HOH:O	2.17	0.44
1:B:42:MSE:HG3	1:B:112:ILE:HD13	1.99	0.44
1:B:42:MSE:HG2	1:B:112:ILE:HG23	2.00	0.43
1:A:42:MSE:HB3	2:A:576:HOH:O	2.18	0.43
1:B:195:GLU:O	1:B:198:LYS:HB3	2.18	0.43
1:A:202:LEU:HD23	1:A:202:LEU:C	2.38	0.43
1:B:124:MSE:O	1:B:125:MSE:HB3	2.18	0.43
1:B:155:ALA:HB1	1:B:208:TYR:HA	2.00	0.43
1:B:202:LEU:HD23	1:B:202:LEU:C	2.38	0.42
1:B:187:LEU:C	1:B:187:LEU:HD23	2.40	0.42
1:B:243:PHE:CZ	1:B:247:VAL:HG21	2.55	0.42
1:A:232:GLN:HE21	1:A:232:GLN:HA	1.84	0.42
1:A:19:TRP:HZ3	1:A:223:MSE:HA	1.82	0.42
1:B:162:ALA:HB1	1:B:201:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLN:HE22	1:A:225:ASN:HD21	1.68	0.42
1:B:19:TRP:CZ3	1:B:223:MSE:HA	2.55	0.42
1:A:58:GLN:NE2	2:A:327:HOH:O	2.52	0.42
1:B:148:LYS:CD	1:B:215:LEU:HA	2.50	0.41
1:A:49:ALA:HB2	1:A:105:MSE:HE3	2.02	0.41
1:A:188:LYS:CD	1:A:188:LYS:N	2.79	0.41
1:A:187:LEU:HD23	1:A:187:LEU:O	2.20	0.41
1:A:221:GLN:CA	1:A:221:GLN:HE21	2.32	0.41
1:A:183:ASN:HB2	1:A:186:GLN:HB2	2.01	0.41
1:A:159:HIS:HD2	1:A:205:LYS:HA	1.86	0.41
1:B:38:CYS:O	1:B:112:ILE:HD11	2.19	0.41
1:B:231:GLU:HG3	1:B:235:GLN:HE21	1.86	0.41
1:B:215:LEU:O	1:B:219:THR:HG23	2.20	0.41
1:A:256:ASP:HB2	1:B:267:TYR:CD2	2.56	0.41
1:B:38:CYS:HA	1:B:112:ILE:HD11	2.03	0.41
1:B:193:LYS:CD	1:B:193:LYS:H	2.32	0.41
1:B:197:CYS:HA	1:B:200:ASP:HB3	2.02	0.41
1:A:165:GLU:OE1	1:A:168:LEU:HD13	2.21	0.41
1:A:252:GLN:HG2	1:B:270:LEU:HD13	2.02	0.41
1:B:153:GLU:O	1:B:156:LYS:HB3	2.21	0.41
1:B:243:PHE:O	1:B:247:VAL:HG23	2.21	0.41
1:B:71:GLU:CG	1:B:84:MSE:HE1	2.51	0.40
1:A:161:ALA:O	1:A:165:GLU:HB2	2.22	0.40
1:A:169:ALA:HA	1:A:172:ARG:HD2	2.03	0.40
1:B:264:LYS:HE3	2:B:564:HOH:O	2.21	0.40
1:A:66:TRP:O	1:A:70:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 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	286/312 (92%)	278 (97%)	7 (2%)	1 (0%)	46	41
1	B	286/312 (92%)	270 (94%)	13 (4%)	3 (1%)	19	11
All	All	572/624 (92%)	548 (96%)	20 (4%)	4 (1%)	26	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PRO
1	B	125	MSE
1	B	124	MSE
1	B	180	PRO

### 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	250/259 (96%)	241 (96%)	9 (4%)	42	39
1	B	250/259 (96%)	242 (97%)	8 (3%)	46	44
All	All	500/518 (96%)	483 (97%)	17 (3%)	44	41

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	36	ARG
1	A	87	MSE
1	A	98	LEU
1	A	117	LYS
1	A	188	LYS
1	A	221	GLN
1	A	228	GLN
1	A	270	LEU
1	B	26	ARG
1	B	36	ARG
1	B	87	MSE

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Mol	Chain	Res	Type
1	B	173	GLU
1	B	188	LYS
1	B	193	LYS
1	B	270	LEU
1	B	296	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	58	GLN
1	A	116	GLN
1	A	199	GLN
1	A	221	GLN
1	A	225	ASN
1	A	232	GLN
1	A	235	GLN
1	A	259	ASN
1	A	289	ASN
1	A	297	ASN
1	B	23	ASN
1	B	58	GLN
1	B	68	GLN
1	B	175	ASN
1	B	186	GLN
1	B	191	GLN
1	B	225	ASN
1	B	228	GLN
1	B	235	GLN

### 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 [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	278/312 (89%)	1.71	76 (27%) ⓘ ⓘ	11, 26, 114, 129	0
1	B	278/312 (89%)	1.71	78 (28%) ⓘ ⓘ	9, 26, 110, 124	0
All	All	556/624 (89%)	1.71	154 (27%) ⓘ ⓘ	9, 26, 111, 129	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	LEU	12.0
1	A	182	LEU	11.1
1	A	187	LEU	11.0
1	B	187	LEU	11.0
1	A	194	ILE	10.7
1	A	168	LEU	9.9
1	A	176	SER	9.9
1	B	170	ILE	9.4
1	A	169	ALA	8.6
1	B	169	ALA	8.4
1	A	208	TYR	8.4
1	B	176	SER	8.3
1	B	172	ARG	8.0
1	A	178	ALA	7.9
1	B	186	GLN	7.9
1	B	194	ILE	7.8
1	A	158	ALA	7.7
1	A	183	ASN	7.7
1	B	208	TYR	7.7
1	B	184	PRO	7.5
1	A	170	ILE	7.4
1	A	180	PRO	7.4
1	B	168	LEU	7.4
1	A	175	ASN	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	193	LYS	7.3
1	A	184	PRO	7.3
1	A	172	ARG	7.2
1	B	181	SER	7.1
1	B	188	LYS	7.1
1	A	174	ALA	6.7
1	B	183	ASN	6.6
1	A	186	GLN	6.5
1	A	181	SER	6.5
1	B	201	VAL	6.4
1	A	202	LEU	6.4
1	B	212	LEU	6.3
1	B	197	CYS	6.3
1	B	162	ALA	6.3
1	B	180	PRO	6.3
1	B	199	GLN	6.2
1	B	192	ASP	6.1
1	B	167	LYS	6.1
1	A	201	VAL	6.1
1	B	301	PHE	6.0
1	B	174	ALA	6.0
1	A	197	CYS	5.9
1	A	199	GLN	5.9
1	A	190	LEU	5.8
1	B	182	LEU	5.8
1	A	301	PHE	5.8
1	B	178	ALA	5.8
1	B	185	GLU	5.8
1	A	160	HIS	5.7
1	A	193	LYS	5.6
1	A	163	CYS	5.6
1	A	185	GLU	5.5
1	A	192	ASP	5.5
1	A	162	ALA	5.4
1	A	200	ASP	5.4
1	B	175	ASN	5.2
1	B	196	LYS	5.1
1	B	198	LYS	5.1
1	B	159	HIS	5.1
1	A	203	LYS	5.0
1	B	173	GLU	5.0
1	A	189	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	163	CYS	4.9
1	A	171	SER	4.8
1	B	200	ASP	4.8
1	B	203	LYS	4.6
1	B	204	THR	4.6
1	A	165	GLU	4.6
1	A	188	LYS	4.6
1	B	189	LYS	4.5
1	A	196	LYS	4.5
1	A	167	LYS	4.4
1	A	198	LYS	4.4
1	B	191	GLN	4.3
1	B	160	HIS	4.3
1	A	161	ALA	4.3
1	B	179	ASP	4.2
1	A	191	GLN	4.2
1	B	213	LYS	4.1
1	A	173	GLU	4.1
1	A	157	LYS	4.0
1	B	285	TRP	3.8
1	A	300	GLN	3.8
1	A	166	GLU	3.8
1	A	216	ASP	3.7
1	A	206	GLU	3.7
1	B	202	LEU	3.7
1	B	161	ALA	3.7
1	A	211	SER	3.6
1	A	177	LYS	3.6
1	A	204	THR	3.6
1	A	285	TRP	3.6
1	B	157	LYS	3.6
1	B	152	VAL	3.6
1	A	205	LYS	3.6
1	B	298	TRP	3.6
1	B	303	GLU	3.6
1	A	159	HIS	3.5
1	B	207	LYS	3.5
1	A	302	GLU	3.4
1	A	303	GLU	3.4
1	A	164	LYS	3.4
1	B	166	GLU	3.3
1	A	179	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	164	LYS	3.3
1	B	158	ALA	3.3
1	B	148	LYS	3.3
1	B	171	SER	3.3
1	A	154	ALA	3.2
1	A	212	LEU	3.2
1	B	302	GLU	3.1
1	A	195	GLU	3.0
1	A	207	LYS	3.0
1	B	165	GLU	3.0
1	B	153	GLU	2.9
1	A	152	VAL	2.9
1	A	153	GLU	2.9
1	B	155	ALA	2.8
1	B	300	GLN	2.8
1	B	297	ASN	2.8
1	B	210	LYS	2.8
1	A	217	GLN	2.8
1	B	215	LEU	2.8
1	B	177	LYS	2.7
1	A	149	LEU	2.6
1	B	16	ASP	2.6
1	A	145	TRP	2.5
1	A	298	TRP	2.5
1	B	154	ALA	2.5
1	A	215	LEU	2.4
1	A	213	LYS	2.4
1	B	156	LYS	2.4
1	B	195	GLU	2.4
1	B	149	LEU	2.3
1	B	146	ALA	2.3
1	B	299	PRO	2.3
1	B	217	GLN	2.3
1	B	145	TRP	2.3
1	A	21	VAL	2.2
1	A	297	ASN	2.2
1	A	295	ALA	2.2
1	B	150	LYS	2.2
1	B	287	ARG	2.2
1	A	220	PRO	2.2
1	B	205	LYS	2.1
1	A	147	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	LYS	2.1
1	B	259	ASN	2.1
1	A	16	ASP	2.0
1	B	206	GLU	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.