



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:19 AM GMT

PDB ID : 3ACO  
Title : Crystal structure of the EFC/F-BAR domain of human PACSIN2/Syndapin II (2.7 Å)  
Authors : Shimada, A.; Shirouzu, M.; Hanawa-Suetsugu, K.; Terada, T.; Umehara, T.; Suetsugu, S.; Yamamoto, M.; Yokoyama, S.  
Deposited on : 2010-01-07  
Resolution : 2.70 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

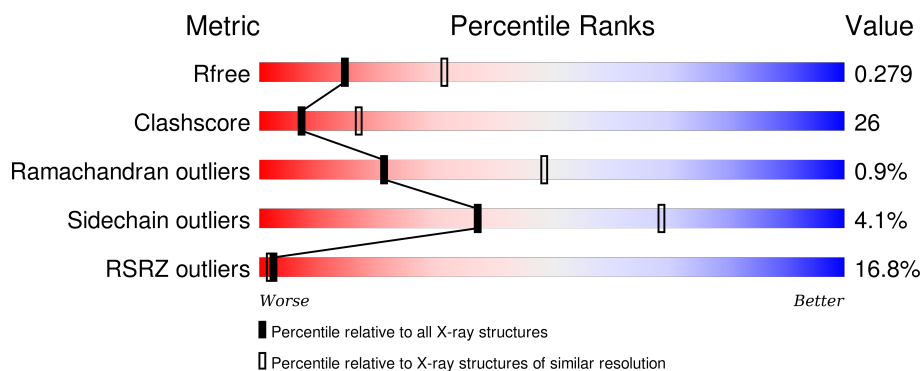
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	350	<div> <div>14%</div> <div>49%</div> <div>30%</div> <div>•</div> <div>19%</div> </div>
1	B	350	<div> <div>12%</div> <div>46%</div> <div>34%</div> <div>•</div> <div>19%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4983 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	284	Total	C	N	O	S	Se	0	0	0
			2354	1481	424	434	5	10			
1	B	284	Total	C	N	O	S	Se	0	0	0
			2354	1481	424	434	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

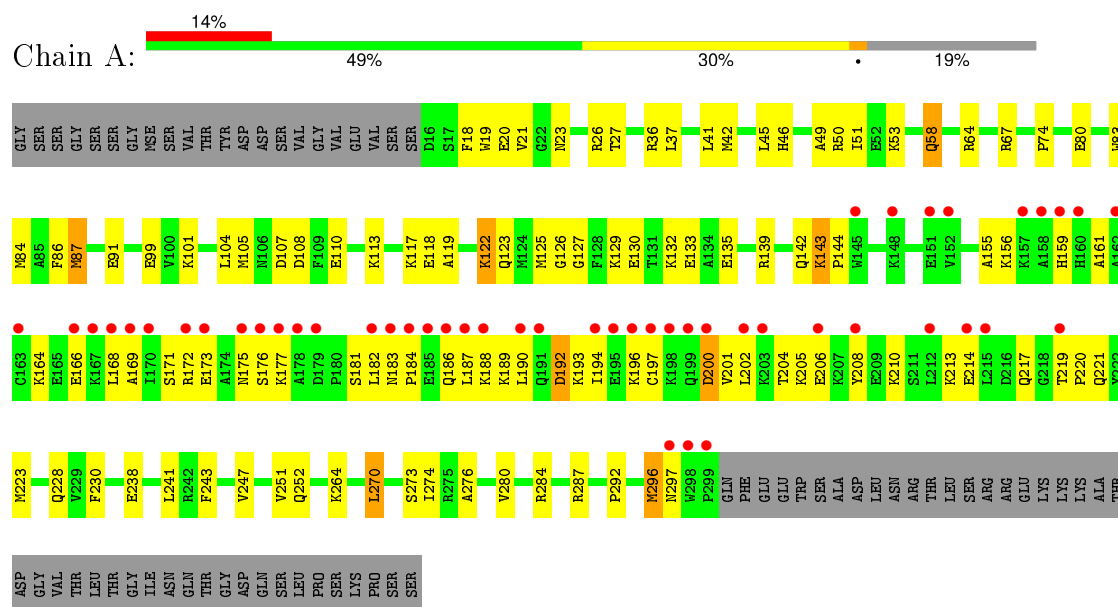
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total 122	O 122	0	0
3	B	151	Total 151	O 151	0	0

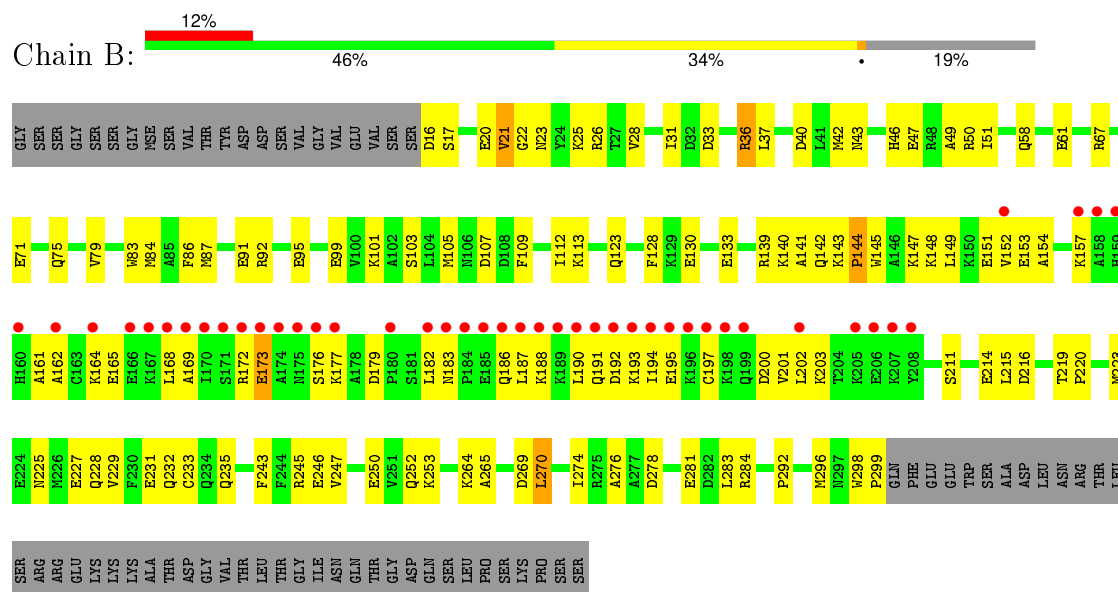
### 3 Residue-property plots

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: 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, $\alpha$ , $\beta$ , $\gamma$	31.61Å 84.65Å 357.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 2.70 48.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.88-2.70) 96.1 (48.71-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.63 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.279 0.226 , 0.279	Depositor DCC
$R_{free}$ test set	1303 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 82.5	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 27190 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4983	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.33	0/2393	0.51	0/3186
1	B	0.35	0/2393	0.51	0/3186
All	All	0.34	0/4786	0.51	0/6372

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

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	2354	0	2324	133	0
1	B	2354	0	2324	126	0
2	A	2	0	0	0	0
3	A	122	0	0	4	0
3	B	151	0	0	12	0
All	All	4983	0	4648	244	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 26.

All (244) 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:177:LYS:HA	1:A:182:LEU:HD21	1.49	0.94
1:B:211:SER:HA	1:B:214:GLU:HB2	1.55	0.88
1:A:143:LYS:H	1:A:144:PRO:HD2	1.37	0.88
1:A:58:GLN:HG2	1:B:51:ILE:HG12	1.56	0.86
1:B:152:VAL:HG22	1:B:211:SER:HB2	1.58	0.84
1:B:22:GLY:O	1:B:25:LYS:HG2	1.80	0.81
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.46	0.81
1:A:171:SER:HA	1:A:175:ASN:HD22	1.46	0.80
1:A:117:LYS:HG3	1:A:118:GLU:H	1.46	0.80
1:A:117:LYS:HG3	1:A:118:GLU:N	1.97	0.78
1:B:182:LEU:HD13	1:B:187:LEU:HD21	1.64	0.78
1:A:21:VAL:HA	1:A:142:GLN:NE2	2.00	0.76
1:A:135:GLU:HG3	1:A:139:ARG:HH12	1.52	0.74
1:A:184:PRO:O	1:A:188:LYS:HD3	1.87	0.74
1:A:177:LYS:O	1:A:182:LEU:HD11	1.88	0.73
1:A:20:GLU:HB2	1:A:23:ASN:ND2	2.05	0.71
1:A:135:GLU:HG3	1:A:139:ARG:NH1	2.05	0.71
1:A:166:GLU:HB3	1:A:197:CYS:HB3	1.71	0.71
1:B:243:PHE:O	1:B:247:VAL:HG23	1.90	0.71
1:B:86:PHE:HB2	1:B:87:MSE:HE2	1.72	0.70
1:A:213:LYS:O	1:A:217:GLN:HG2	1.90	0.70
1:A:270:LEU:HD13	1:B:252:GLN:HG2	1.73	0.70
1:A:122:LYS:HE3	1:A:127:GLY:H	1.55	0.70
1:B:223:MSE:O	1:B:227:GLU:HG2	1.93	0.69
1:B:219:THR:HG23	1:B:220:PRO:HD3	1.74	0.69
1:A:172:ARG:O	1:A:190:LEU:HD21	1.94	0.69
1:A:189:LYS:HA	1:A:192:ASP:OD1	1.95	0.66
1:A:241:LEU:HD22	1:B:79:VAL:HG21	1.77	0.66
1:A:190:LEU:HD12	1:A:193:LYS:HD3	1.76	0.66
1:A:280:VAL:HG12	1:A:284:ARG:NH1	2.12	0.65
1:A:200:ASP:O	1:A:204:THR:HG22	1.96	0.65
1:A:27:THR:HG1	1:A:230:PHE:HE1	1.43	0.65
1:A:177:LYS:HE2	1:A:187:LEU:HD11	1.77	0.65
1:B:225:ASN:O	1:B:228:GLN:HB3	1.97	0.65
1:B:95:GLU:HG2	3:B:468:HOH:O	1.96	0.64
1:B:278:ASP:CG	1:B:281:GLU:HG2	2.17	0.64
1:A:132:LYS:HA	1:A:135:GLU:HB3	1.80	0.64
1:A:84:MSE:O	1:A:87:MSE:HG2	2.00	0.62
1:B:173:GLU:O	1:B:177:LYS:HB2	1.99	0.62
1:A:122:LYS:HD3	1:A:122:LYS:C	2.20	0.62
1:A:53:LYS:HB2	1:A:101:LYS:HD2	1.81	0.62
1:B:172:ARG:NH2	1:B:193:LYS:HD3	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HA	1:A:204:THR:CG2	2.30	0.62
1:B:165:GLU:OE2	1:B:168:LEU:HD12	2.00	0.61
1:A:284:ARG:NH1	1:A:284:ARG:HG3	2.14	0.61
1:A:83:TRP:O	1:A:87:MSE:HE3	2.00	0.61
1:B:17:SER:H	1:B:20:GLU:CG	2.14	0.60
1:B:61:GLU:HG2	3:B:423:HOH:O	1.99	0.60
1:B:148:LYS:O	1:B:215:LEU:HD13	2.00	0.60
1:A:143:LYS:N	1:A:144:PRO:HD2	2.14	0.60
1:A:135:GLU:CG	1:A:139:ARG:HH12	2.14	0.60
1:A:201:VAL:HA	1:A:204:THR:HG22	1.82	0.60
1:B:148:LYS:HE2	1:B:214:GLU:HB3	1.84	0.60
1:B:270:LEU:HD22	1:B:274:ILE:HD11	1.84	0.60
1:B:154:ALA:O	1:B:157:LYS:HG2	2.01	0.60
1:B:202:LEU:HD23	1:B:202:LEU:O	2.02	0.60
1:B:148:LYS:HD2	1:B:151:GLU:OE1	2.01	0.59
1:A:200:ASP:C	1:A:202:LEU:H	2.03	0.59
1:A:156:LYS:HA	1:A:208:TYR:CD2	2.37	0.59
1:B:130:GLU:H	1:B:130:GLU:CD	2.06	0.59
1:A:21:VAL:HA	1:A:142:GLN:HE22	1.67	0.59
1:B:28:VAL:HA	1:B:31:ILE:HD13	1.85	0.59
1:A:164:LYS:O	1:A:164:LYS:HD3	2.03	0.58
1:B:195:GLU:C	1:B:197:CYS:H	2.06	0.58
1:A:67:ARG:HB2	1:A:67:ARG:NH1	2.17	0.58
1:B:31:ILE:H	1:B:31:ILE:HD12	1.68	0.58
1:A:243:PHE:O	1:A:247:VAL:HG12	2.03	0.58
1:A:168:LEU:O	1:A:168:LEU:HD23	2.02	0.58
1:B:17:SER:H	1:B:20:GLU:HG3	1.69	0.58
1:A:159:HIS:C	1:A:161:ALA:H	2.07	0.58
1:A:42:MSE:HE3	1:A:113:LYS:HB2	1.86	0.58
1:A:19:TRP:HZ3	1:A:223:MSE:HA	1.69	0.57
1:A:122:LYS:HD3	1:A:123:GLN:N	2.19	0.57
1:B:42:MSE:HE3	1:B:113:LYS:HB2	1.86	0.57
1:A:296:MSE:HE1	1:B:20:GLU:OE1	2.04	0.57
1:B:21:VAL:HA	1:B:142:GLN:NE2	2.20	0.57
1:B:112:ILE:HD11	1:B:247:VAL:HG11	1.86	0.57
1:B:101:LYS:NZ	3:B:404:HOH:O	2.36	0.57
1:A:296:MSE:HA	1:A:296:MSE:HE3	1.87	0.57
1:B:298:TRP:HB3	1:B:299:PRO:HD2	1.87	0.57
1:A:86:PHE:HB2	1:A:87:MSE:CE	2.33	0.56
1:B:188:LYS:HA	1:B:191:GLN:NE2	2.20	0.56
1:A:156:LYS:HA	1:A:208:TYR:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:TRP:CZ3	1:A:223:MSE:HA	2.40	0.56
1:B:83:TRP:O	1:B:87:MSE:HE3	2.06	0.55
1:A:201:VAL:O	1:A:201:VAL:HG12	2.07	0.55
1:A:187:LEU:O	1:A:187:LEU:HD23	2.06	0.55
1:B:183:ASN:HD22	1:B:186:GLN:NE2	2.05	0.55
1:A:204:THR:HG23	1:A:205:LYS:N	2.22	0.54
1:A:64:ARG:HD3	3:A:425:HOH:O	2.08	0.54
1:A:129:LYS:HD3	1:A:129:LYS:O	2.07	0.54
1:B:46:HIS:HA	1:B:105:MSE:HE1	1.89	0.54
1:A:51:ILE:HG12	1:B:58:GLN:HE21	1.72	0.54
1:B:246:GLU:O	1:B:250:GLU:HG3	2.07	0.54
1:A:296:MSE:HE2	1:A:297:ASN:H	1.73	0.53
1:B:31:ILE:HD12	1:B:31:ILE:N	2.23	0.53
1:B:183:ASN:HD22	1:B:186:GLN:HE21	1.56	0.53
1:B:188:LYS:HE3	1:B:192:ASP:OD2	2.07	0.53
1:B:187:LEU:O	1:B:191:GLN:HG3	2.09	0.53
1:A:122:LYS:HE2	1:A:126:GLY:HA2	1.89	0.53
1:B:219:THR:HG23	1:B:220:PRO:CD	2.39	0.53
1:A:182:LEU:HD12	1:A:182:LEU:N	2.24	0.52
1:B:42:MSE:HE1	1:B:113:LYS:HG3	1.90	0.52
1:B:169:ALA:HB1	1:B:194:ILE:HG12	1.92	0.52
1:B:46:HIS:HA	1:B:105:MSE:CE	2.39	0.52
1:B:92:ARG:NH2	1:B:269:ASP:OD2	2.43	0.52
1:B:284:ARG:HH11	1:B:284:ARG:HG2	1.75	0.52
1:A:51:ILE:HG12	1:B:58:GLN:NE2	2.25	0.52
1:B:145:TRP:CZ3	1:B:149:LEU:HD22	2.45	0.52
1:A:156:LYS:HG3	1:A:208:TYR:HE2	1.75	0.52
1:B:264:LYS:HB3	3:B:430:HOH:O	2.09	0.52
1:A:192:ASP:HB3	1:A:196:LYS:HE3	1.92	0.51
1:A:105:MSE:HE2	1:A:105:MSE:HA	1.91	0.51
1:A:192:ASP:O	1:A:196:LYS:HG3	2.10	0.51
1:B:49:ALA:HB2	1:B:105:MSE:HE3	1.91	0.51
1:B:36:ARG:NE	1:B:40:ASP:OD2	2.42	0.51
1:A:217:GLN:HA	1:A:217:GLN:HE21	1.75	0.51
1:B:95:GLU:O	1:B:99:GLU:HG3	2.11	0.51
1:A:219:THR:N	1:A:220:PRO:HD2	2.26	0.51
1:B:179:ASP:O	1:B:182:LEU:HG	2.10	0.51
1:A:270:LEU:HD22	1:A:274:ILE:HD11	1.92	0.51
1:B:123:GLN:HE21	1:B:128:PHE:N	2.08	0.51
1:B:161:ALA:O	1:B:165:GLU:HB2	2.11	0.51
1:B:194:ILE:O	1:B:194:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:HB2	1:B:87:MSE:CE	2.39	0.51
1:B:144:PRO:HG2	1:B:145:TRP:H	1.76	0.51
1:B:43:ASN:O	1:B:47:GLU:HG3	2.10	0.51
1:A:296:MSE:HE2	1:A:297:ASN:N	2.25	0.50
1:A:67:ARG:HH11	1:A:67:ARG:HB2	1.76	0.50
1:A:74:PRO:HG2	1:B:37:LEU:HD21	1.91	0.50
1:B:228:GLN:HE21	1:B:228:GLN:HA	1.76	0.50
1:A:210:LYS:O	1:A:214:GLU:HG3	2.12	0.50
1:B:36:ARG:HH11	1:B:36:ARG:HG3	1.76	0.50
1:B:148:LYS:HD3	3:B:412:HOH:O	2.11	0.50
1:B:219:THR:N	1:B:220:PRO:HD2	2.26	0.50
1:B:20:GLU:O	1:B:21:VAL:C	2.50	0.50
1:A:202:LEU:O	1:A:206:GLU:HG3	2.12	0.49
1:A:169:ALA:C	1:A:194:ILE:HG22	2.33	0.49
1:B:36:ARG:HD3	1:B:36:ARG:C	2.33	0.49
1:A:46:HIS:NE2	1:A:50:ARG:NH1	2.61	0.49
1:A:104:LEU:HD21	1:A:251:VAL:HG13	1.94	0.49
1:A:117:LYS:CG	1:A:118:GLU:N	2.73	0.49
1:B:200:ASP:O	1:B:203:LYS:HB3	2.13	0.49
1:A:200:ASP:C	1:A:202:LEU:N	2.66	0.49
1:B:182:LEU:HB3	1:B:187:LEU:HD21	1.95	0.48
1:A:238:GLU:HB2	1:B:283:LEU:HD11	1.93	0.48
1:A:217:GLN:HA	1:A:217:GLN:NE2	2.29	0.48
1:B:103:SER:O	1:B:107:ASP:HB2	2.14	0.48
1:A:87:MSE:N	1:A:87:MSE:HE2	2.29	0.48
1:A:110:GLU:OE1	1:A:113:LYS:HD3	2.14	0.48
1:A:270:LEU:O	1:A:274:ILE:HG13	2.14	0.48
1:B:143:LYS:N	1:B:144:PRO:HD2	2.29	0.48
1:A:125:MSE:HG3	1:A:126:GLY:N	2.30	0.47
1:B:147:LYS:C	1:B:149:LEU:H	2.17	0.47
1:A:247:VAL:O	1:A:251:VAL:HG23	2.15	0.47
1:A:143:LYS:H	1:A:144:PRO:CD	2.17	0.46
1:B:188:LYS:C	1:B:190:LEU:H	2.19	0.46
1:A:104:LEU:CD2	1:A:251:VAL:HG13	2.46	0.46
1:B:162:ALA:C	1:B:164:LYS:H	2.19	0.46
1:B:152:VAL:HG22	1:B:211:SER:CB	2.37	0.46
1:B:176:SER:O	1:B:182:LEU:HD21	2.15	0.46
1:A:125:MSE:HG3	1:A:126:GLY:H	1.81	0.46
1:A:49:ALA:HB1	1:A:101:LYS:HG3	1.97	0.46
1:B:71:GLU:HG3	1:B:84:MSE:HE1	1.97	0.46
1:A:189:LYS:O	1:A:192:ASP:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASP:OD1	1:B:281:GLU:HG2	2.16	0.46
1:B:141:ALA:HB1	1:B:225:ASN:HB3	1.98	0.46
1:B:195:GLU:C	1:B:197:CYS:N	2.68	0.46
1:B:197:CYS:O	1:B:201:VAL:HG23	2.15	0.46
1:A:171:SER:O	1:A:175:ASN:HB2	2.16	0.46
1:A:202:LEU:HD23	1:A:202:LEU:C	2.36	0.46
1:A:183:ASN:HB2	1:A:186:GLN:OE1	2.16	0.45
1:B:42:MSE:HB3	1:B:109:PHE:CE1	2.52	0.45
1:B:229:VAL:O	1:B:232:GLN:HB3	2.17	0.45
1:B:219:THR:CG2	1:B:220:PRO:HD3	2.44	0.45
1:A:86:PHE:HB2	1:A:87:MSE:HE3	1.97	0.45
1:A:159:HIS:C	1:A:161:ALA:N	2.70	0.45
1:B:33:ASP:O	1:B:37:LEU:HG	2.17	0.45
1:A:20:GLU:HB2	1:A:23:ASN:HD22	1.80	0.45
1:A:296:MSE:CE	1:A:297:ASN:H	2.30	0.45
1:B:20:GLU:HB2	1:B:23:ASN:OD1	2.17	0.45
1:B:50:ARG:NH1	3:B:379:HOH:O	2.50	0.45
1:A:58:GLN:NE2	3:A:421:HOH:O	2.49	0.44
1:B:188:LYS:HA	1:B:191:GLN:HE21	1.82	0.44
1:A:142:GLN:O	1:A:142:GLN:HG2	2.17	0.44
1:A:104:LEU:HA	1:A:108:ASP:OD2	2.17	0.44
1:B:33:ASP:HA	3:B:408:HOH:O	2.17	0.44
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.83	0.44
1:B:67:ARG:HD2	3:B:386:HOH:O	2.17	0.44
1:A:67:ARG:HH11	1:A:67:ARG:CB	2.30	0.44
1:B:16:ASP:HA	1:B:20:GLU:HG3	2.00	0.44
1:B:245:ARG:HG2	1:B:245:ARG:HH11	1.81	0.44
3:A:421:HOH:O	1:B:51:ILE:HA	2.18	0.43
1:A:117:LYS:CG	1:A:118:GLU:H	2.22	0.43
1:A:18:PHE:CE2	1:B:292:PRO:HG3	2.52	0.43
1:A:110:GLU:OE1	1:A:110:GLU:HA	2.19	0.43
1:B:49:ALA:CB	1:B:105:MSE:HE3	2.48	0.43
1:A:172:ARG:O	1:A:176:SER:HB2	2.19	0.43
1:A:177:LYS:HE2	1:A:187:LEU:CD1	2.47	0.43
1:A:143:LYS:N	1:A:144:PRO:CD	2.80	0.43
1:A:284:ARG:NH1	1:A:284:ARG:CG	2.80	0.43
1:B:87:MSE:O	1:B:91:GLU:HG3	2.19	0.43
1:A:155:ALA:O	1:A:208:TYR:HB2	2.19	0.43
1:A:287:ARG:CZ	1:A:292:PRO:HB2	2.49	0.43
1:A:41:LEU:O	1:A:45:LEU:HG	2.19	0.43
1:A:132:LYS:O	1:A:133:GLU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD22	1:B:274:ILE:CD1	2.49	0.42
1:A:37:LEU:HD13	1:B:75:GLN:OE1	2.18	0.42
1:A:182:LEU:H	1:A:182:LEU:CD1	2.31	0.42
1:A:182:LEU:H	1:A:182:LEU:HD12	1.84	0.42
1:A:252:GLN:CG	1:B:270:LEU:HD13	2.49	0.42
1:A:273:SER:O	1:A:276:ALA:HB3	2.19	0.42
1:A:19:TRP:CZ2	1:B:292:PRO:HB3	2.54	0.42
1:B:140:LYS:HB3	3:B:390:HOH:O	2.20	0.42
1:A:80:GLU:HG2	1:A:80:GLU:O	2.19	0.42
1:A:53:LYS:HD2	1:A:101:LYS:HE3	2.01	0.42
1:B:148:LYS:CE	1:B:214:GLU:HB3	2.49	0.42
1:B:228:GLN:NE2	1:B:228:GLN:HA	2.35	0.42
1:B:17:SER:N	1:B:20:GLU:HG3	2.33	0.42
1:B:105:MSE:O	1:B:109:PHE:HB3	2.20	0.42
1:A:20:GLU:OE2	1:B:296:MSE:SE	2.88	0.41
1:A:171:SER:HA	1:A:175:ASN:ND2	2.24	0.41
1:A:270:LEU:HD13	1:B:252:GLN:CG	2.46	0.41
1:A:87:MSE:O	1:A:91:GLU:HG3	2.20	0.41
1:A:264:LYS:NZ	3:A:441:HOH:O	2.53	0.41
1:B:152:VAL:HG12	1:B:152:VAL:O	2.21	0.41
1:A:172:ARG:HH11	1:A:193:LYS:CE	2.34	0.41
1:B:151:GLU:C	1:B:153:GLU:N	2.74	0.41
1:A:19:TRP:HB2	1:B:296:MSE:HE2	2.03	0.41
1:A:182:LEU:O	1:A:184:PRO:HD3	2.20	0.41
1:B:148:LYS:O	1:B:148:LYS:HG3	2.20	0.41
1:A:183:ASN:HB2	1:A:186:GLN:CD	2.42	0.41
1:B:231:GLU:HG3	1:B:235:GLN:HE21	1.85	0.41
1:B:233:CYS:HB3	3:B:349:HOH:O	2.22	0.40
1:B:265:ALA:HA	3:B:446:HOH:O	2.21	0.40
1:B:182:LEU:HD22	1:B:187:LEU:CD2	2.50	0.40
1:B:84:MSE:O	1:B:87:MSE:HG2	2.21	0.40
1:B:276:ALA:HB3	3:B:376:HOH:O	2.21	0.40
1:A:173:GLU:O	1:A:177:LYS:HE3	2.22	0.40
1:B:216:ASP:C	1:B:219:THR:HG22	2.42	0.40
1:A:166:GLU:C	1:A:168:LEU:H	2.24	0.40
1:A:122:LYS:CE	1:A:126:GLY:HA2	2.51	0.40
1:B:36:ARG:NH1	1:B:36:ARG:HG3	2.36	0.40
1:A:183:ASN:HB2	1:A:186:GLN:HG3	2.03	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	282/350 (81%)	253 (90%)	26 (9%)	3 (1%)	17	42
1	B	282/350 (81%)	256 (91%)	24 (8%)	2 (1%)	26	55
All	All	564/700 (81%)	509 (90%)	50 (9%)	5 (1%)	21	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	VAL
1	A	119	ALA
1	A	181	SER
1	A	143	LYS
1	B	144	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	246/292 (84%)	232 (94%)	14 (6%)	25	53
1	B	246/292 (84%)	240 (98%)	6 (2%)	57	85
All	All	492/584 (84%)	472 (96%)	20 (4%)	37	69

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	58	GLN
1	A	87	MSE
1	A	99	GLU
1	A	107	ASP
1	A	122	LYS
1	A	130	GLU
1	A	192	ASP
1	A	200	ASP
1	A	221	GLN
1	A	228	GLN
1	A	270	LEU
1	A	296	MSE
1	B	26	ARG
1	B	36	ARG
1	B	133	GLU
1	B	173	GLU
1	B	253	LYS
1	B	270	LEU

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	121	HIS
1	A	159	HIS
1	A	175	ASN
1	A	217	GLN
1	A	225	ASN
1	A	228	GLN
1	A	232	GLN
1	A	259	ASN
1	B	46	HIS
1	B	58	GLN
1	B	116	GLN
1	B	123	GLN
1	B	175	ASN
1	B	186	GLN
1	B	191	GLN
1	B	199	GLN
1	B	217	GLN
1	B	228	GLN
1	B	235	GLN

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Mol	Chain	Res	Type
1	B	297	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	274/350 (78%)	0.90	49 (17%) <b>2</b> <b>1</b>	10, 54, 166, 190	0
1	B	274/350 (78%)	0.82	43 (15%) <b>3</b> <b>2</b>	9, 42, 156, 196	0
All	All	548/700 (78%)	0.86	92 (16%) <b>2</b> <b>2</b>	9, 48, 159, 196	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	ALA	14.1
1	A	162	ALA	6.5
1	A	166	GLU	6.3
1	B	176	SER	5.9
1	B	170	ILE	5.7
1	A	194	ILE	5.6
1	B	177	LYS	5.3
1	A	202	LEU	5.3
1	B	182	LEU	5.3
1	B	172	ARG	5.1
1	B	166	GLU	4.9
1	A	187	LEU	4.8
1	A	170	ILE	4.8
1	A	176	SER	4.6
1	B	162	ALA	4.6
1	B	167	LYS	4.5
1	A	172	ARG	4.4
1	A	182	LEU	4.4
1	A	298	TRP	4.2
1	A	183	ASN	4.1
1	A	173	GLU	4.1
1	B	184	PRO	4.1
1	B	187	LEU	4.0
1	B	168	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	178	ALA	3.9
1	B	158	ALA	3.9
1	A	208	TYR	3.9
1	A	177	LYS	3.8
1	B	197	CYS	3.8
1	B	190	LEU	3.8
1	A	191	GLN	3.8
1	A	297	ASN	3.8
1	B	175	ASN	3.8
1	A	169	ALA	3.7
1	A	197	CYS	3.7
1	A	196	LYS	3.7
1	B	164	LYS	3.7
1	B	199	GLN	3.6
1	B	159	HIS	3.6
1	A	188	LYS	3.4
1	B	196	LYS	3.4
1	B	192	ASP	3.4
1	B	194	ILE	3.4
1	B	183	ASN	3.3
1	A	145	TRP	3.3
1	B	193	LYS	3.3
1	A	199	GLN	3.2
1	B	180	PRO	3.2
1	A	152	VAL	3.1
1	B	191	GLN	3.1
1	B	208	TYR	3.1
1	A	151	GLU	3.0
1	A	184	PRO	3.0
1	A	186	GLN	3.0
1	A	185	GLU	3.0
1	B	207	LYS	3.0
1	B	171	SER	3.0
1	B	160	HIS	2.9
1	A	168	LEU	2.9
1	A	206	GLU	2.9
1	A	198	LYS	2.9
1	A	214	GLU	2.8
1	A	167	LYS	2.8
1	A	159	HIS	2.8
1	B	157	LYS	2.7
1	A	195	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	174	ALA	2.7
1	A	203	LYS	2.7
1	A	157	LYS	2.6
1	B	173	GLU	2.6
1	B	186	GLN	2.6
1	B	205	LYS	2.6
1	A	158	ALA	2.5
1	A	148	LYS	2.5
1	A	175	ASN	2.5
1	B	195	GLU	2.5
1	A	215	LEU	2.4
1	B	198	LYS	2.4
1	A	190	LEU	2.4
1	A	179	ASP	2.3
1	B	202	LEU	2.3
1	B	189	LYS	2.3
1	B	152	VAL	2.3
1	B	206	GLU	2.3
1	A	219	THR	2.2
1	A	163	CYS	2.2
1	B	188	LYS	2.2
1	A	160	HIS	2.2
1	A	200	ASP	2.2
1	A	212	LEU	2.2
1	B	185	GLU	2.1
1	A	299	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	400	1/1	0.82	0.11	-7.43	57,57,57,57	0
2	CA	A	401	1/1	0.95	0.09	-10.14	58,58,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.