



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:35 PM UTC

PDB ID : 3ABH / pdb_00003abh
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

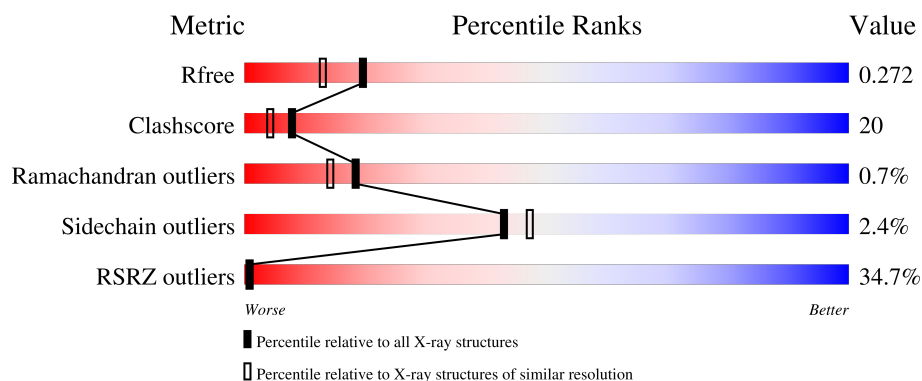
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	312	30% 66% 23% 8%
1	B	312	31% 61% 29% 8%

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

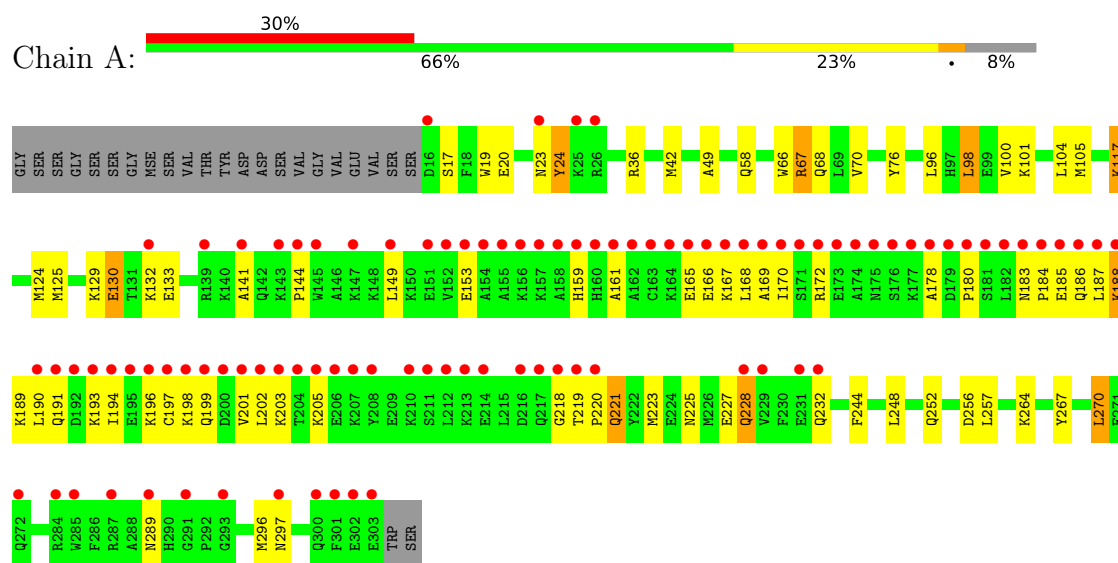
- Molecule 2 is water.

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

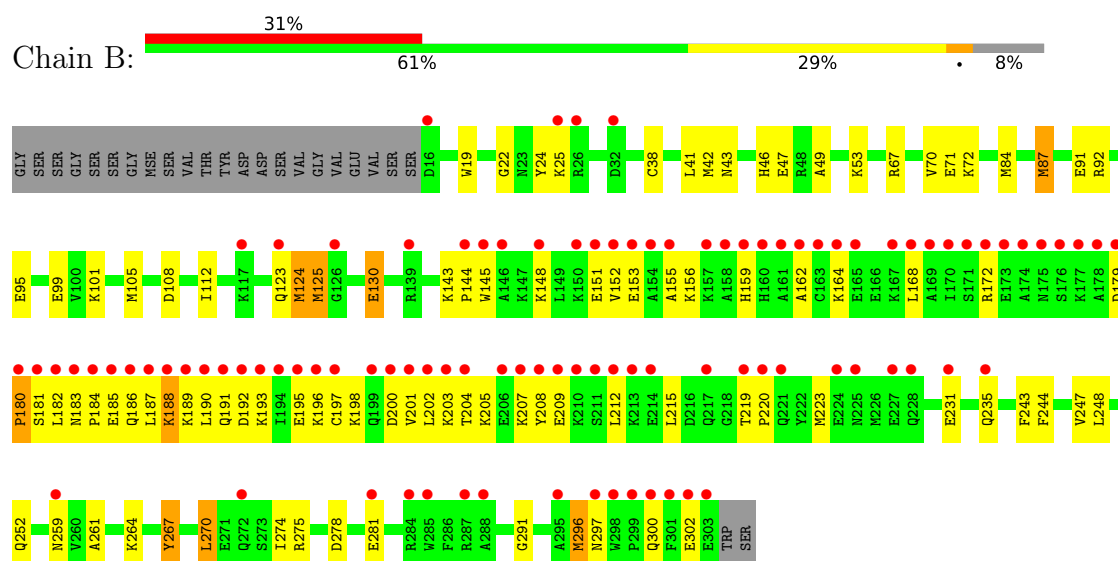
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 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, α , β , γ	31.52Å 86.14Å 353.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.00 48.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (48.59-2.00) 93.5 (48.59-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.271 0.234 , 0.272	Depositor DCC
R_{free} test set	3231 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5335	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.36	0/2432	0.81	3/3238 (0.1%)
1	B	0.37	0/2432	0.79	3/3238 (0.1%)
All	All	0.37	0/4864	0.80	6/6476 (0.1%)

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.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	LEU	N-CA-C	-6.39	104.39	111.36
1	B	291	GLY	CA-C-N	5.88	126.30	119.47
1	B	291	GLY	C-N-CA	5.88	126.30	119.47
1	B	108	ASP	N-CA-C	5.64	117.12	110.97
1	A	67	ARG	N-CA-C	-5.22	105.48	111.07
1	A	24	TYR	N-CA-C	-5.01	107.12	113.18

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

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	95	0
1	B	2392	0	2353	105	0
2	A	276	0	0	14	0
2	B	275	0	0	9	0
All	All	5335	0	4706	188	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 20.

All (188) 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:HE3	1:B:188:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:104:LEU:C	1:A:105:MSE:HE2	2.25	0.62
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
1:A:196:LYS:O	1:A:199:GLN:HB3	2.00	0.60
1:A:130:GLU:H	1:A:130:GLU:CD	2.09	0.59
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:N	1:A:188:LYS:HD2	2.19	0.57
1:B:124:MSE:HE3	1:B:125:MSE:N	2.18	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:187:LEU:HD23	1:A:187:LEU:C	2.30	0.56
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:25:LYS:HE2	2:B:526:HOH:O	2.05	0.56
1:B:91:GLU:O	1:B:95:GLU:HG3	2.06	0.56
1:A:244:PHE:O	1:A:248:LEU:HG	2.04	0.56
1:A:168:LEU:O	1:A:168:LEU:HD23	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:130:GLU:H	1:B:130:GLU:CD	2.13	0.55
1:B:212:LEU:C	1:B:212:LEU:HD23	2.32	0.55
1:B:190:LEU:HA	1:B:193:LYS:HD3	1.89	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:A:191:GLN:C	1:A:194:ILE:HG22	2.32	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:124:MSE:HE3	1:B:124:MSE:C	2.34	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:A:296:MSE:HE3	1:A:297:ASN:C	2.34	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:H	1:B:193:LYS:HD2	1.76	0.51
1:A:104:LEU:O	1:A:105:MSE:HE2	2.11	0.51
1:B:202:LEU:O	1:B:202:LEU:HD23	2.11	0.51
1:A:76:TYR:HB3	2:A:483:HOH:O	2.10	0.50
1:A:96:LEU:HD13	1:A:257:LEU:HD13	1.91	0.50
1:A:183:ASN:CB	1:A:186:GLN:HB2	2.42	0.50
1:B:22:GLY:O	1:B:25:LYS:HG3	2.12	0.50
1:A:125:MSE:HE3	2:A:313:HOH:O	2.11	0.50
1:B:187:LEU:HD23	1:B:187:LEU:O	2.12	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:172:ARG:C	1:A:190:LEU:HD21	2.38	0.49
1:B:159:HIS:HA	1:B:204:THR:OG1	2.13	0.48
1:B:219:THR:N	1:B:220:PRO:CD	2.76	0.48
1:B:46:HIS:CE1	1:B:105:MSE:HE1	2.46	0.48
1:A:124:MSE:HE3	1:A:124:MSE:HA	1.95	0.48
1:A:199:GLN:HE21	1:A:203:LYS:CE	2.25	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:A:202:LEU:HD23	1:A:202:LEU:C	2.38	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:A:68:GLN:HG2	2:A:427:HOH:O	2.12	0.47
1:B:193:LYS:HD2	1:B:193:LYS:N	2.29	0.47
1:A:49:ALA:HB1	1:A:101:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:NZ	2:A:449:HOH:O	2.47	0.47
1:B:187:LEU:HD23	1:B:187:LEU:C	2.40	0.47
1:B:202:LEU:HD23	1:B:202:LEU:C	2.38	0.47
1:A:188:LYS:HA	1:A:191:GLN:OE1	2.14	0.47
1:B:153:GLU:HG2	2:B:486:HOH:O	2.13	0.47
1:B:244:PHE:O	1:B:248:LEU:HG	2.14	0.47
1:A:270:LEU:HD13	1:B:252:GLN:CG	2.44	0.47
1:B:19:TRP:HZ3	1:B:223:MSE:HA	1.80	0.47
1:B:185:GLU:HA	2:B:426:HOH:O	2.14	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
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:A:264:LYS:HG3	2:A:557:HOH:O	2.16	0.46
1:B:143:LYS:HB3	1:B:144:PRO:CD	2.46	0.46
1:B:183:ASN:HB3	1:B:184:PRO:HD2	1.97	0.46
1:A:144:PRO:HG2	2:A:361:HOH:O	2.15	0.45
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: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:123:GLN:HE21	1:B:125:MSE:HG3	1.80	0.45
1:B:179:ASP:O	1:B:182:LEU:HG	2.16	0.45
1:B:219:THR:O	1:B:223:MSE:HG3	2.16	0.45
1:A:168:LEU:HD23	1:A:168:LEU:C	2.42	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:159:HIS:CD2	1:A:205:LYS:HA	2.52	0.45
1:A:166:GLU:C	1:A:168:LEU:H	2.25	0.45
1:A:166:GLU:OE2	1:A:201:VAL:HG21	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:ARG:C	1:A:36:ARG:HD3	2.43	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:243:PHE:CZ	1:B:247:VAL:HG21	2.55	0.42
1:A:232:GLN:HA	1:A:232:GLN:HE21	1.84	0.42
1:B:130:GLU:CD	1:B:130:GLU:N	2.77	0.42
1:A:19:TRP:HZ3	1:A:223:MSE:HA	1.82	0.42
1:A:221:GLN:HE22	1:A:225:ASN:HD21	1.68	0.42
1:B:162:ALA:HB1	1:B:201:VAL:HG22	2.02	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:A:49:ALA:HB2	1:A:105:MSE:HE3	2.02	0.41
1:A:130:GLU:CD	1:A:130:GLU:N	2.78	0.41
1:B:148:LYS:CD	1:B:215:LEU:HA	2.50	0.41
1:A:24:TYR:CD1	1:A:24:TYR:C	2.97	0.41
1:B:24:TYR:C	1:B:24:TYR:CD1	2.98	0.41
1:A:187:LEU:HD23	1:A:187:LEU:O	2.20	0.41
1:A:188:LYS:N	1:A:188:LYS:CD	2.79	0.41
1:A:221:GLN:CA	1:A:221:GLN:HE21	2.32	0.41
1:A:159:HIS:HD2	1:A:205:LYS:HA	1.86	0.41
1:A:183:ASN:HB2	1:A:186:GLN:HB2	2.01	0.41
1:A:218:GLY:C	1:A:220:PRO:HD2	2.46	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: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:215:LEU:O	1:B:219:THR:HG23	2.20	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:193:LYS:H	1:B:193:LYS:CD	2.32	0.41
1:B:197:CYS:HA	1:B:200:ASP:HB3	2.02	0.41
1:B:243:PHE:O	1:B:247:VAL:HG23	2.21	0.41
1:B:278:ASP:CG	1:B:281:GLU:HG2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	35
1	B	286/312 (92%)	270 (94%)	13 (4%)	3 (1%)	12	8
All	All	572/624 (92%)	548 (96%)	20 (4%)	4 (1%)	18	14

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 [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	250/259 (96%)	243 (97%)	7 (3%)	38	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	250/259 (96%)	245 (98%)	5 (2%)	48	54
All	All	500/518 (96%)	488 (98%)	12 (2%)	43	47

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LEU
1	A	117	LYS
1	A	130	GLU
1	A	188	LYS
1	A	221	GLN
1	A	228	GLN
1	A	270	LEU
1	B	87	MSE
1	B	130	GLU
1	B	188	LYS
1	B	270	LEU
1	B	296	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	57	GLN
1	A	58	GLN
1	A	68	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	268	HIS
1	A	272	GLN
1	A	297	ASN
1	B	23	ASN
1	B	123	GLN
1	B	159	HIS
1	B	186	GLN
1	B	191	GLN

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Mol	Chain	Res	Type
1	B	225	ASN
1	B	228	GLN
1	B	235	GLN
1	B	289	ASN
1	B	290	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	278/312 (89%)	1.46	95 (34%)  	11, 26, 114, 129	0
1	B	278/312 (89%)	1.48	98 (35%)  	9, 26, 110, 124	0
All	All	556/624 (89%)	1.47	193 (34%)  	9, 26, 111, 129	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PRO	8.7
1	A	201	VAL	6.8
1	B	301	PHE	6.4
1	B	188	LYS	6.1
1	A	182	LEU	6.1
1	B	168	LEU	6.1
1	B	184	PRO	6.1
1	A	285	TRP	6.0
1	A	162	ALA	5.8
1	A	187	LEU	5.8
1	A	169	ALA	5.6
1	B	208	TYR	5.6
1	B	285	TRP	5.5
1	B	178	ALA	5.4
1	B	197	CYS	5.3
1	A	208	TYR	5.3
1	B	201	VAL	5.3
1	A	168	LEU	5.2
1	B	193	LYS	5.2
1	B	177	LYS	5.2
1	B	212	LEU	5.1
1	A	163	CYS	5.1
1	B	169	ALA	4.9
1	A	143	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	188	LYS	4.9
1	A	198	LYS	4.9
1	B	259	ASN	4.9
1	A	174	ALA	4.8
1	B	170	ILE	4.8
1	B	199	GLN	4.8
1	A	180	PRO	4.7
1	B	220	PRO	4.7
1	A	160	HIS	4.6
1	B	190	LEU	4.6
1	A	170	ILE	4.6
1	A	178	ALA	4.6
1	A	16	ASP	4.6
1	A	167	LYS	4.6
1	A	202	LEU	4.5
1	B	192	ASP	4.4
1	B	303	GLU	4.4
1	B	196	LYS	4.3
1	B	297	ASN	4.3
1	B	200	ASP	4.3
1	B	219	THR	4.2
1	B	176	SER	4.2
1	B	174	ALA	4.2
1	B	300	GLN	4.2
1	A	203	LYS	4.2
1	B	158	ALA	4.2
1	A	301	PHE	4.1
1	A	204	THR	4.1
1	B	194	ILE	4.1
1	B	187	LEU	4.1
1	A	152	VAL	4.1
1	B	157	LYS	4.1
1	B	298	TRP	4.0
1	B	180	PRO	4.0
1	A	190	LEU	4.0
1	B	183	ASN	4.0
1	B	213	LYS	4.0
1	A	195	GLU	4.0
1	B	228	GLN	4.0
1	A	197	CYS	3.9
1	A	157	LYS	3.9
1	A	213	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	148	LYS	3.9
1	B	186	GLN	3.9
1	A	158	ALA	3.8
1	B	202	LEU	3.8
1	A	144	PRO	3.8
1	A	211	SER	3.8
1	B	16	ASP	3.8
1	B	287	ARG	3.8
1	B	159	HIS	3.7
1	B	204	THR	3.7
1	B	172	ARG	3.7
1	A	303	GLU	3.7
1	A	232	GLN	3.7
1	A	191	GLN	3.7
1	B	123	GLN	3.6
1	B	155	ALA	3.6
1	B	181	SER	3.6
1	A	219	THR	3.6
1	A	155	ALA	3.6
1	A	25	LYS	3.6
1	B	25	LYS	3.5
1	B	163	CYS	3.5
1	B	189	LYS	3.5
1	A	291	GLY	3.5
1	A	173	GLU	3.5
1	A	300	GLN	3.5
1	A	161	ALA	3.4
1	B	182	LEU	3.4
1	A	132	LYS	3.4
1	B	175	ASN	3.4
1	A	166	GLU	3.4
1	B	150	LYS	3.4
1	A	199	GLN	3.4
1	A	217	GLN	3.4
1	A	181	SER	3.4
1	A	165	GLU	3.3
1	B	173	GLU	3.3
1	A	185	GLU	3.3
1	A	200	ASP	3.3
1	A	176	SER	3.3
1	A	220	PRO	3.3
1	A	293	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	141	ALA	3.3
1	A	284	ARG	3.3
1	B	152	VAL	3.2
1	B	295	ALA	3.2
1	A	147	LYS	3.2
1	A	177	LYS	3.1
1	A	206	GLU	3.1
1	A	145	TRP	3.1
1	B	203	LYS	3.1
1	B	217	GLN	3.1
1	A	297	ASN	3.1
1	B	284	ARG	3.1
1	B	231	GLU	3.1
1	B	160	HIS	3.0
1	A	171	SER	3.0
1	A	175	ASN	3.0
1	B	165	GLU	3.0
1	A	192	ASP	3.0
1	B	161	ALA	3.0
1	A	172	ARG	3.0
1	B	209	GLU	3.0
1	B	167	LYS	3.0
1	B	146	ALA	3.0
1	B	195	GLU	2.9
1	A	159	HIS	2.9
1	A	154	ALA	2.9
1	B	225	ASN	2.9
1	B	207	LYS	2.9
1	B	272	GLN	2.9
1	A	179	ASP	2.9
1	A	194	ILE	2.9
1	B	191	GLN	2.8
1	B	179	ASP	2.8
1	B	151	GLU	2.8
1	A	302	GLU	2.8
1	B	227	GLU	2.8
1	A	212	LEU	2.8
1	A	216	ASP	2.7
1	A	26	ARG	2.7
1	B	139	ARG	2.7
1	B	153	GLU	2.7
1	A	228	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	183	ASN	2.6
1	A	205	LYS	2.6
1	A	139	ARG	2.6
1	A	193	LYS	2.5
1	A	151	GLU	2.5
1	A	153	GLU	2.5
1	B	164	LYS	2.5
1	B	224	GLU	2.5
1	A	207	LYS	2.5
1	B	210	LYS	2.4
1	A	231	GLU	2.4
1	B	154	ALA	2.4
1	B	281	GLU	2.4
1	A	196	LYS	2.4
1	A	149	LEU	2.4
1	A	214	GLU	2.4
1	B	235	GLN	2.4
1	B	145	TRP	2.4
1	B	162	ALA	2.3
1	B	185	GLU	2.3
1	B	206	GLU	2.3
1	A	23	ASN	2.3
1	A	156	LYS	2.3
1	A	164	LYS	2.3
1	B	211	SER	2.3
1	B	26	ARG	2.3
1	B	302	GLU	2.2
1	A	186	GLN	2.2
1	B	221	GLN	2.2
1	B	299	PRO	2.2
1	B	171	SER	2.1
1	A	210	LYS	2.1
1	B	32	ASP	2.1
1	A	218	GLY	2.1
1	B	214	GLU	2.1
1	A	272	GLN	2.1
1	A	287	ARG	2.1
1	B	144	PRO	2.1
1	B	126	GLY	2.1
1	A	229	VAL	2.1
1	B	288	ALA	2.1
1	B	117	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	289	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.