



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:31 PM UTC

PDB ID : 2X3X / pdb_00002x3x
Title : structure of mouse syndapin I (crystal form 1)
Authors : Ma, Q.; Rao, Y.; Vahedi-Faridi, A.; Saenger, W.; Haucke, V.
Deposited on : 2010-01-28
Resolution : 3.35 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
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

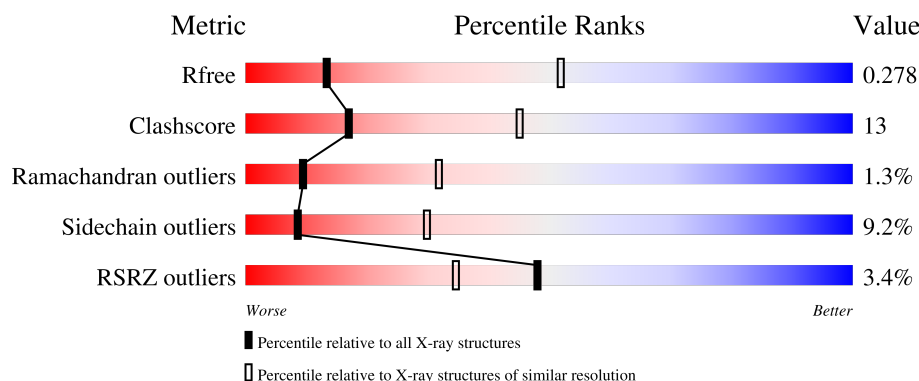
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	337	0% 57% 26% 14%
1	B	337	2% 56% 22% 19%
1	C	337	7% 61% 24% 14%
2	D	60	68% 20% 5% 7%
2	E	60	3% 67% 18% 8% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8006 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2418	1514	430	457	17			
1	B	274	Total	C	N	O	S	0	0	0
			2277	1431	403	427	16			
1	C	291	Total	C	N	O	S	0	0	0
			2417	1513	430	457	17			

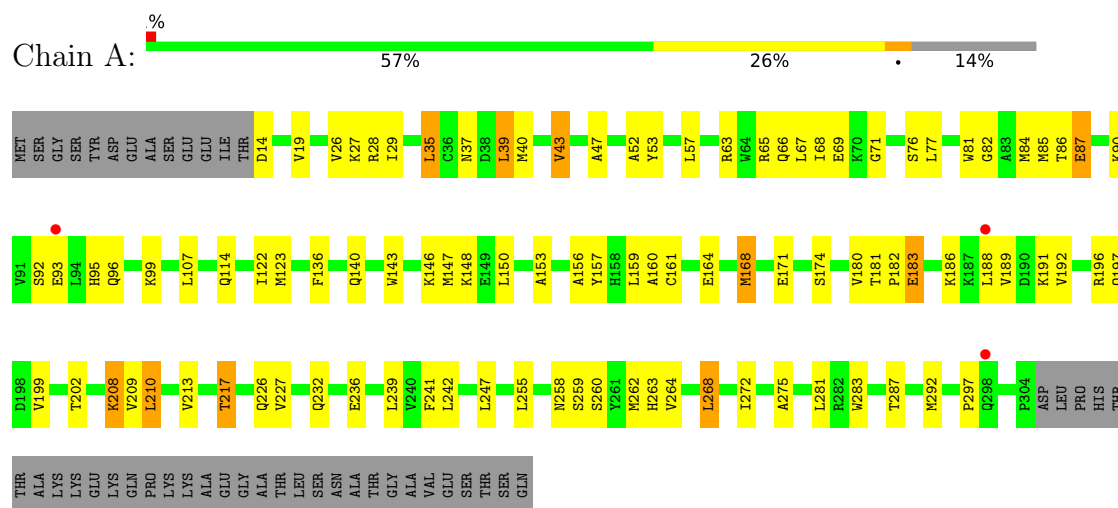
- Molecule 2 is a protein called PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	56	Total	C	N	O	S	0	0	0
			447	276	76	94	1			
2	E	56	Total	C	N	O	S	0	0	0
			447	276	76	94	1			

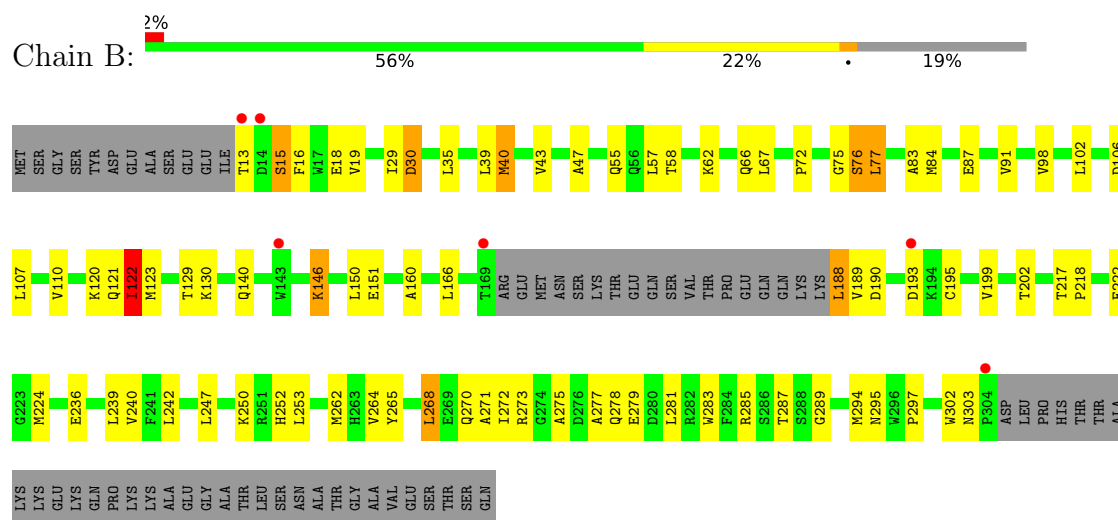
3 Residue-property plots

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.

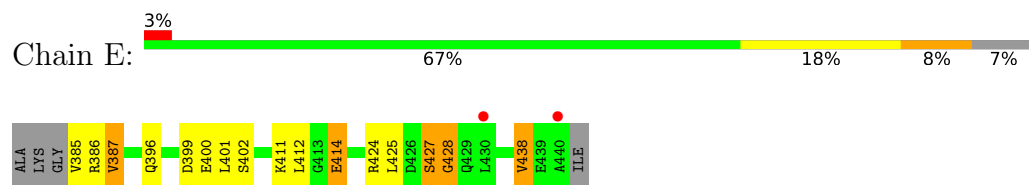
- Molecule 1: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1



- Molecule 1: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1



- Molecule 1: PROTEIN KINASE C AND CASEIN KINASE SUBSTRATE IN NEURONS PROTEIN 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.08Å 154.54Å 255.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.13 – 3.35 73.13 – 3.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.13-3.35) 98.5 (73.13-3.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.221 , 0.277 0.225 , 0.278	Depositor DCC
R_{free} test set	1192 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	1.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 109.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8006	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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 [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	0.52	0/2466	0.82	2/3305 (0.1%)
1	B	0.50	0/2323	0.79	2/3114 (0.1%)
1	C	0.47	0/2465	0.78	2/3304 (0.1%)
2	D	0.48	0/454	0.71	1/611 (0.2%)
2	E	0.55	0/454	0.68	0/611
All	All	0.50	0/8162	0.79	7/10945 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	GLY	CA-C-N	7.18	126.89	119.56
1	A	71	GLY	C-N-CA	7.18	126.89	119.56
2	D	427	SER	N-CA-C	6.24	120.22	111.30
1	C	289	GLY	CA-C-N	5.64	126.89	119.84
1	C	289	GLY	C-N-CA	5.64	126.89	119.84
1	B	289	GLY	CA-C-N	5.31	126.48	119.84
1	B	289	GLY	C-N-CA	5.31	126.48	119.84

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	2418	0	2377	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2277	0	2234	59	0
1	C	2417	0	2372	54	0
2	D	447	0	410	13	0
2	E	447	0	410	14	0
All	All	8006	0	7803	201	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 13.

All (201) 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:35:LEU:HD11	1:B:72:PRO:HD2	1.34	1.05
1:A:150:LEU:HD11	1:A:210:LEU:HD22	1.46	0.97
2:D:387:VAL:HG13	2:D:438:VAL:HG13	1.54	0.89
2:D:387:VAL:HG13	2:D:438:VAL:CG1	2.04	0.88
1:A:143:TRP:CZ3	1:A:217:THR:HG23	2.08	0.86
2:D:387:VAL:CG1	2:D:438:VAL:HG11	2.08	0.83
1:A:35:LEU:HD11	1:B:72:PRO:CD	2.09	0.81
2:D:387:VAL:CG1	2:D:438:VAL:CG1	2.61	0.79
1:C:26:VAL:HG21	1:C:133:GLU:HG2	1.65	0.78
2:D:387:VAL:HG11	2:D:438:VAL:HG11	1.63	0.78
1:A:160:ALA:HB1	1:A:199:VAL:HG22	1.67	0.77
1:C:47:ALA:HB1	1:C:103:LEU:HD11	1.66	0.77
1:B:57:LEU:HD13	1:B:91:VAL:CG2	2.18	0.73
1:B:188:LEU:HD13	1:B:189:VAL:HG23	1.68	0.73
1:B:57:LEU:HD13	1:B:91:VAL:HG23	1.70	0.72
1:B:39:LEU:CD2	1:B:110:VAL:HG21	2.20	0.71
2:E:401:LEU:HD11	2:E:425:LEU:HD13	1.69	0.71
1:A:143:TRP:HZ3	1:A:217:THR:HG23	1.55	0.71
1:C:64:TRP:HB2	1:C:85:MET:HE2	1.72	0.71
2:E:387:VAL:HG23	2:E:438:VAL:HG13	1.72	0.70
1:A:239:LEU:HD12	1:B:281:LEU:HD11	1.72	0.69
1:C:47:ALA:CB	1:C:103:LEU:HD11	2.23	0.69
1:A:95:HIS:NE2	1:A:255:LEU:HD11	2.08	0.68
1:B:217:THR:HG22	1:C:221:MET:HE1	1.73	0.68
1:A:180:VAL:HG23	1:A:180:VAL:O	1.94	0.67
1:A:68:ILE:HD12	1:A:85:MET:CE	2.25	0.67
1:A:247:LEU:HD21	1:B:273:ARG:NH1	2.10	0.66
1:C:294:MET:HE3	1:C:296:TRP:HA	1.77	0.66
1:C:150:LEU:HD21	1:C:210:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:CYS:O	1:C:199:VAL:HG23	1.96	0.65
1:A:160:ALA:CB	1:A:199:VAL:HG22	2.26	0.65
1:A:40:MET:HG2	1:A:107:LEU:HD22	1.80	0.64
1:B:122:ILE:HG23	1:B:122:ILE:O	1.97	0.63
1:A:199:VAL:HA	1:A:202:THR:HG22	1.80	0.63
1:A:82:GLY:HA2	1:A:85:MET:CE	2.31	0.60
1:A:147:MET:HE1	1:B:297:PRO:HG3	1.83	0.60
1:A:283:TRP:CE2	1:A:287:THR:HG21	2.36	0.60
1:A:150:LEU:HD11	1:A:210:LEU:CD2	2.27	0.60
1:B:16:PHE:CZ	1:B:224:MET:HE3	2.37	0.60
1:B:83:ALA:HB1	1:B:268:LEU:CD2	2.31	0.60
1:A:43:VAL:HG12	1:A:107:LEU:HD23	1.84	0.59
1:C:94:LEU:HD22	1:C:258:ASN:HD21	1.67	0.59
1:C:123:MET:HE2	1:C:123:MET:C	2.28	0.59
2:E:387:VAL:HG23	2:E:438:VAL:CG1	2.33	0.59
2:D:401:LEU:HD21	2:D:425:LEU:HD13	1.85	0.59
1:C:189:VAL:O	1:C:192:VAL:HG22	2.03	0.59
2:D:427:SER:N	2:D:428:GLY:HA2	2.18	0.59
1:B:123:MET:HE3	1:B:123:MET:HA	1.85	0.59
1:C:192:VAL:HA	1:C:195:CYS:HB3	1.84	0.57
1:B:146:LYS:O	1:B:150:LEU:N	2.38	0.57
1:A:122:ILE:HD12	1:A:123:MET:N	2.20	0.57
1:A:186:LYS:NZ	1:A:189:VAL:HG11	2.20	0.56
1:A:68:ILE:HD12	1:A:85:MET:HE3	1.89	0.55
1:A:77:LEU:HD22	1:A:275:ALA:HB1	1.88	0.55
1:A:82:GLY:HA2	1:A:85:MET:HE2	1.89	0.55
1:A:241:PHE:HD1	1:A:242:LEU:HD22	1.72	0.55
1:A:292:MET:CE	1:B:15:SER:HA	2.37	0.55
1:A:174:SER:HB3	1:A:180:VAL:HG11	1.90	0.54
1:A:160:ALA:HB1	1:A:199:VAL:CG2	2.37	0.54
1:A:65:ARG:O	1:A:69:GLU:HB2	2.09	0.53
1:B:83:ALA:HB1	1:B:268:LEU:HD22	1.91	0.53
1:A:43:VAL:CG1	1:A:107:LEU:HD23	2.38	0.53
1:B:188:LEU:CD1	1:B:189:VAL:HG23	2.36	0.53
1:C:150:LEU:HD21	1:C:210:LEU:CD1	2.39	0.52
1:C:172:MET:HE2	1:C:173:ASN:ND2	2.24	0.52
1:B:160:ALA:HB3	1:B:202:THR:HG21	1.90	0.52
2:E:387:VAL:CG2	2:E:438:VAL:CG1	2.86	0.52
1:A:146:LYS:HB3	1:A:213:VAL:HG22	1.91	0.52
1:B:83:ALA:C	1:B:268:LEU:HD21	2.34	0.52
1:C:159:LEU:HD23	1:C:160:ALA:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD12	1:A:85:MET:HE1	1.90	0.52
1:B:218:PRO:HG3	1:C:221:MET:HE3	1.92	0.52
1:A:239:LEU:CD1	1:B:281:LEU:HD11	2.39	0.51
1:A:150:LEU:HD13	1:A:209:VAL:HG12	1.92	0.51
1:A:37:ASN:HA	1:A:40:MET:HE3	1.93	0.51
1:A:86:THR:HG22	1:A:90:LYS:HD3	1.92	0.51
2:D:387:VAL:HG12	2:D:409:LEU:HD13	1.93	0.51
1:A:19:VAL:HG13	1:A:140:GLN:NE2	2.25	0.50
1:A:242:LEU:HB3	1:B:77:LEU:HD11	1.93	0.50
1:B:283:TRP:CE2	1:B:287:THR:HG21	2.46	0.50
1:C:174:SER:HB2	1:C:188:LEU:HD22	1.94	0.50
1:C:178:GLN:CG	1:C:180:VAL:HG23	2.42	0.50
1:A:87:GLU:OE2	1:B:253:LEU:HD13	2.12	0.50
1:A:160:ALA:HB3	1:A:202:THR:HG21	1.93	0.50
1:A:292:MET:HE1	1:B:15:SER:HA	1.94	0.50
1:A:52:ALA:O	1:A:53:TYR:C	2.55	0.50
1:A:208:LYS:HE3	2:D:436:ASN:HD22	1.76	0.50
1:B:76:SER:HB2	1:B:275:ALA:HA	1.94	0.50
1:B:278:GLN:O	1:B:279:GLU:C	2.53	0.50
2:E:412:LEU:HD11	2:E:424:ARG:HB2	1.94	0.50
1:C:76:SER:OG	1:C:275:ALA:HA	2.12	0.50
1:A:161:CYS:HB3	1:B:302:TRP:CE3	2.47	0.49
1:C:85:MET:HE3	1:C:85:MET:HA	1.93	0.49
1:C:153:ALA:HB1	1:C:206:TYR:HA	1.94	0.49
1:B:40:MET:O	1:B:43:VAL:HG22	2.13	0.49
1:C:254:ASN:HB3	1:C:257:GLU:HG3	1.93	0.49
1:A:26:VAL:HA	1:A:29:ILE:HD12	1.93	0.49
1:A:136:PHE:CZ	1:A:227:VAL:HG12	2.48	0.49
1:C:60:TRP:CZ3	1:C:85:MET:HE3	2.47	0.49
1:B:19:VAL:HG13	1:B:140:GLN:NE2	2.28	0.49
1:A:96:GLN:HE21	1:A:96:GLN:HA	1.78	0.49
1:A:143:TRP:CZ3	1:A:217:THR:CG2	2.90	0.49
1:C:283:TRP:NE1	1:C:287:THR:HG21	2.28	0.48
2:E:387:VAL:HG21	2:E:438:VAL:HG11	1.94	0.48
1:C:283:TRP:CE2	1:C:287:THR:HG21	2.48	0.48
1:A:272:ILE:HG21	1:B:247:LEU:HG	1.95	0.48
1:A:76:SER:HB2	1:A:275:ALA:HA	1.96	0.48
1:A:150:LEU:HA	1:A:209:VAL:HG11	1.96	0.48
1:B:270:GLN:O	1:B:271:ALA:C	2.55	0.48
1:C:76:SER:N	1:C:280:ASP:OD1	2.47	0.48
2:E:402:SER:O	2:E:425:LEU:HD21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:TRP:CH2	1:C:85:MET:HE1	2.49	0.48
1:A:84:MET:O	1:A:87:GLU:HG3	2.14	0.48
1:C:122:ILE:HD12	1:C:123:MET:N	2.29	0.47
2:E:411:LYS:NZ	2:E:414:GLU:OE2	2.34	0.47
1:B:98:VAL:O	1:B:102:LEU:HB2	2.14	0.47
1:B:29:ILE:HG22	1:B:129:THR:OG1	2.14	0.47
1:A:68:ILE:HD11	1:A:81:TRP:CE2	2.50	0.47
1:B:236:GLU:O	1:B:240:VAL:HG22	2.14	0.47
1:B:122:ILE:O	1:B:122:ILE:CD1	2.62	0.46
1:A:160:ALA:C	1:A:199:VAL:HG22	2.40	0.46
1:C:109:LYS:HD3	1:C:245:VAL:HG22	1.97	0.46
1:B:294:MET:HE3	1:B:295:ASN:N	2.29	0.46
1:C:194:LYS:O	1:C:198:ASP:N	2.45	0.46
1:C:135:GLY:C	1:C:227:VAL:HG21	2.41	0.46
1:B:75:GLY:O	1:B:76:SER:C	2.58	0.46
1:C:185:GLN:HG2	1:C:189:VAL:HG22	1.99	0.45
1:B:39:LEU:HD13	1:B:242:LEU:CD1	2.46	0.45
1:C:150:LEU:HD23	1:C:209:VAL:HG13	1.98	0.45
1:A:236:GLU:HB2	1:B:281:LEU:HD21	1.98	0.45
1:A:268:LEU:HD13	1:B:250:LYS:HG3	1.98	0.45
1:A:283:TRP:NE1	1:A:287:THR:HG21	2.31	0.45
2:E:401:LEU:HD21	2:E:425:LEU:CD1	2.46	0.45
1:A:186:LYS:HZ3	1:A:189:VAL:HG11	1.81	0.45
1:C:76:SER:O	1:C:79:ARG:N	2.50	0.45
1:C:209:VAL:O	1:C:213:VAL:HG23	2.17	0.45
1:B:190:ASP:HA	1:B:193:ASP:HB3	1.99	0.45
1:A:268:LEU:HD22	1:A:272:ILE:HD11	1.99	0.45
1:A:281:LEU:HD21	1:B:236:GLU:HB2	1.98	0.45
2:E:427:SER:N	2:E:428:GLY:CA	2.79	0.45
1:A:174:SER:CB	1:A:180:VAL:HG11	2.46	0.44
1:A:232:GLN:HE21	1:B:285:ARG:NH1	2.15	0.44
2:D:390:LEU:HD21	2:D:439:GLU:HB3	2.00	0.44
1:C:94:LEU:CD2	1:C:258:ASN:HD21	2.30	0.44
1:A:157:TYR:HA	1:A:202:THR:CG2	2.47	0.44
1:A:63:ARG:O	1:A:67:LEU:HD13	2.17	0.44
1:A:68:ILE:CD1	1:A:85:MET:HE1	2.47	0.44
1:C:185:GLN:NE2	1:C:189:VAL:HG11	2.33	0.44
1:B:30:ASP:OD1	1:B:129:THR:HG21	2.17	0.44
1:A:181:THR:O	1:A:183:GLU:N	2.51	0.43
1:C:99:LYS:O	1:C:103:LEU:HD12	2.18	0.43
1:C:17:TRP:CZ3	1:C:221:MET:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:386:ARG:C	2:E:387:VAL:HG12	2.42	0.43
1:A:66:GLN:OE1	2:E:385:VAL:HG23	2.18	0.43
1:C:39:LEU:HD23	1:C:110:VAL:HG21	2.01	0.43
1:C:98:VAL:O	1:C:102:LEU:HB2	2.17	0.43
2:D:421:CYS:HB2	2:D:433:TYR:CE2	2.53	0.43
1:C:182:PRO:HA	1:C:185:GLN:HB3	2.00	0.43
1:A:260:SER:O	1:A:264:VAL:HG23	2.18	0.43
1:B:47:ALA:HB2	1:B:102:LEU:HD23	2.00	0.43
1:C:85:MET:SD	1:C:85:MET:N	2.92	0.43
2:E:387:VAL:CG2	2:E:438:VAL:HG11	2.49	0.43
1:A:153:ALA:O	1:A:156:ALA:HB3	2.18	0.43
1:A:159:LEU:HD23	1:A:160:ALA:N	2.34	0.43
1:C:53:TYR:CE2	1:C:57:LEU:HD21	2.54	0.43
1:A:47:ALA:O	1:A:99:LYS:HG3	2.19	0.42
1:B:195:CYS:O	1:B:199:VAL:HG23	2.19	0.42
1:B:278:GLN:O	1:B:281:LEU:N	2.53	0.42
1:A:39:LEU:HD22	1:A:39:LEU:O	2.19	0.42
1:C:178:GLN:HG2	1:C:180:VAL:HG23	2.02	0.42
1:B:277:ALA:O	1:B:281:LEU:HD13	2.19	0.42
1:C:242:LEU:HD23	1:C:246:LEU:HD13	2.01	0.42
1:C:260:SER:O	1:C:264:VAL:HG23	2.19	0.42
1:B:107:LEU:C	1:B:107:LEU:HD23	2.44	0.42
1:A:57:LEU:HB2	1:A:92:SER:HB2	2.02	0.42
1:C:141:LYS:HB3	1:C:142:PRO:HD3	2.01	0.42
1:A:96:GLN:HA	1:A:96:GLN:NE2	2.35	0.42
2:E:385:VAL:HG13	2:E:411:LYS:HB2	2.01	0.42
1:A:247:LEU:HD13	1:B:272:ILE:CG2	2.50	0.41
1:B:294:MET:HE3	1:B:295:ASN:H	1.85	0.41
1:C:20:GLY:N	1:C:140:GLN:HE22	2.18	0.41
1:B:83:ALA:CB	1:B:268:LEU:CD2	2.97	0.41
1:B:264:VAL:HG12	1:B:265:TYR:CD2	2.55	0.41
1:C:150:LEU:CD2	1:C:209:VAL:HG13	2.50	0.41
1:A:157:TYR:HD2	1:A:202:THR:HG23	1.85	0.41
1:A:188:LEU:O	1:A:192:VAL:HG22	2.21	0.41
1:C:160:ALA:O	1:C:199:VAL:HG22	2.21	0.41
1:B:106:ASP:CG	1:B:252:HIS:HD1	2.28	0.41
1:B:277:ALA:HB3	1:B:278:GLN:HE21	1.85	0.41
1:C:129:THR:O	1:C:133:GLU:HB2	2.21	0.41
1:C:259:SER:O	1:C:262:MET:N	2.54	0.41
1:A:168:MET:HE1	1:A:196:ARG:HD3	2.03	0.41
1:B:40:MET:HE3	1:B:40:MET:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:O	1:A:160:ALA:C	2.63	0.41
1:A:199:VAL:CA	1:A:202:THR:HG22	2.49	0.41
1:B:121:GLN:C	1:B:123:MET:H	2.29	0.41
1:A:107:LEU:HD13	1:A:107:LEU:C	2.46	0.40
1:A:259:SER:HB3	1:A:263:HIS:CE1	2.56	0.40
2:D:401:LEU:CD2	2:D:425:LEU:HD13	2.50	0.40
1:C:181:THR:CG2	1:C:182:PRO:HD2	2.52	0.40
2:D:401:LEU:HD13	2:D:431:GLY:CA	2.51	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	289/337 (86%)	262 (91%)	22 (8%)	5 (2%)	7	27
1	B	270/337 (80%)	249 (92%)	18 (7%)	3 (1%)	11	36
1	C	289/337 (86%)	260 (90%)	26 (9%)	3 (1%)	12	38
2	D	54/60 (90%)	52 (96%)	2 (4%)	0	100	100
2	E	54/60 (90%)	48 (89%)	5 (9%)	1 (2%)	6	25
All	All	956/1131 (84%)	871 (91%)	73 (8%)	12 (1%)	9	32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	ASN
1	A	183	GLU
1	B	122	ILE
1	B	76	SER
1	C	178	GLN
1	A	182	PRO

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Mol	Chain	Res	Type
1	A	191	LYS
1	C	260	SER
1	A	258	ASN
2	E	428	GLY
1	A	297	PRO
1	C	180	VAL

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	258/295 (88%)	238 (92%)	20 (8%)	11	37
1	B	241/295 (82%)	216 (90%)	25 (10%)	7	24
1	C	257/295 (87%)	235 (91%)	22 (9%)	10	33
2	D	45/47 (96%)	41 (91%)	4 (9%)	9	31
2	E	45/47 (96%)	38 (84%)	7 (16%)	2	10
All	All	846/979 (86%)	768 (91%)	78 (9%)	8	30

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	27	LYS
1	A	28	ARG
1	A	35	LEU
1	A	39	LEU
1	A	43	VAL
1	A	87	GLU
1	A	93	GLU
1	A	114	GLN
1	A	148	LYS
1	A	164	GLU
1	A	168	MET
1	A	171	GLU

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	208	LYS
1	A	210	LEU
1	A	217	THR
1	A	226	GLN
1	A	262	MET
1	A	268	LEU
1	B	13	THR
1	B	15	SER
1	B	18	GLU
1	B	30	ASP
1	B	35	LEU
1	B	40	MET
1	B	55	GLN
1	B	58	THR
1	B	62	LYS
1	B	66	GLN
1	B	67	LEU
1	B	77	LEU
1	B	84	MET
1	B	87	GLU
1	B	120	LYS
1	B	122	ILE
1	B	130	LYS
1	B	146	LYS
1	B	151	GLU
1	B	166	LEU
1	B	188	LEU
1	B	222	GLU
1	B	239	LEU
1	B	262	MET
1	B	268	LEU
1	C	14	ASP
1	C	35	LEU
1	C	44	GLN
1	C	63	ARG
1	C	66	GLN
1	C	73	GLN
1	C	85	MET
1	C	86	THR
1	C	93	GLU
1	C	101	SER

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Mol	Chain	Res	Type
1	C	120	LYS
1	C	123	MET
1	C	129	THR
1	C	146	LYS
1	C	159	LEU
1	C	171	GLU
1	C	191	LYS
1	C	226	GLN
1	C	237	LYS
1	C	268	LEU
1	C	298	GLN
1	C	300	GLU
2	D	387	VAL
2	D	394	ASP
2	D	400	GLU
2	D	438	VAL
2	E	387	VAL
2	E	396	GLN
2	E	399	ASP
2	E	400	GLU
2	E	414	GLU
2	E	427	SER
2	E	438	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	55	GLN
1	A	96	GLN
1	A	112	ASN
1	A	114	GLN
1	A	121	GLN
1	A	197	GLN
1	A	203	GLN
1	A	230	GLN
1	A	270	GLN
1	B	33	HIS
1	B	44	GLN
1	B	96	GLN
1	B	121	GLN
1	B	140	GLN

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Mol	Chain	Res	Type
1	B	203	GLN
1	B	233	GLN
1	B	278	GLN
1	C	56	GLN
1	C	95	HIS
1	C	112	ASN
1	C	114	GLN
1	C	173	ASN
1	C	185	GLN
1	C	197	GLN
1	C	203	GLN
1	C	226	GLN
1	C	258	ASN
2	D	436	ASN
2	E	418	GLN
2	E	429	GLN

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 ⓘ

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	291/337 (86%)	-0.02	3 (1%) 79 66	87, 102, 115, 127	0
1	B	274/337 (81%)	0.04	6 (2%) 62 46	87, 102, 120, 136	0
1	C	291/337 (86%)	0.44	22 (7%) 20 16	86, 103, 121, 124	0
2	D	56/60 (93%)	0.31	0 100 100	96, 102, 111, 116	0
2	E	56/60 (93%)	0.31	2 (3%) 46 33	92, 102, 108, 113	0
All	All	968/1131 (85%)	0.17	33 (3%) 48 34	86, 102, 119, 136	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	TRP	4.1
1	B	169	THR	3.6
1	C	80	ALA	3.3
1	C	78	GLU	3.0
1	B	143	TRP	2.9
1	C	122	ILE	2.9
1	C	67	LEU	2.7
1	C	72	PRO	2.7
1	B	193	ASP	2.6
1	B	13	THR	2.6
1	C	81	TRP	2.5
1	A	188	LEU	2.4
1	C	82	GLY	2.4
1	C	280	ASP	2.3
1	C	167	ALA	2.3
1	C	74	TYR	2.3
1	B	14	ASP	2.3
1	C	57	LEU	2.3
1	C	287	THR	2.3
1	C	79	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	249	ILE	2.2
1	C	83	ALA	2.2
1	C	69	GLU	2.2
1	B	304	PRO	2.2
1	C	188	LEU	2.1
1	C	85	MET	2.1
1	C	70	LYS	2.1
1	A	298	GLN	2.1
1	C	73	GLN	2.1
2	E	430	LEU	2.1
2	E	440	ALA	2.1
1	A	93	GLU	2.1
1	C	192	VAL	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.