



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 3HAH / pdb_00003hah
Title : Crystal structure of human PACSIN1 F-BAR domain (C2 lattice)
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Deposited on : 2009-05-01
Resolution : 2.77 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

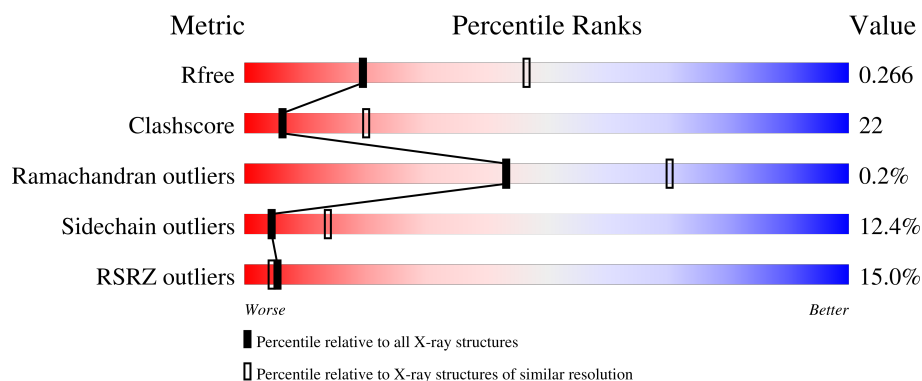
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	325	
1	B	325	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4511 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 human PACSIN1 F-BAR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	1	0
			2234	1405	396	418	15			
1	B	266	Total	C	N	O	S	0	0	0
			2215	1395	392	414	14			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	21	Total	O	0	0
			21	21		

- Molecule 1: human PACSIN1 F-BAR



GLY

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.01Å 85.46Å 88.39Å 90.00° 117.56° 90.00°	Depositor
Resolution (Å)	48.07 – 2.77 48.07 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.07-2.77) 98.1 (48.07-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.215 , 0.260 0.225 , 0.266	Depositor DCC
R_{free} test set	1328 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.973	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4511	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% 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](#)

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	0.52	0/2277	0.90	2/3050 (0.1%)
1	B	0.52	0/2260	0.89	2/3029 (0.1%)
All	All	0.52	0/4537	0.90	4/6079 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	GLY	CA-C-N	7.71	127.38	119.82
1	A	292	GLY	C-N-CA	7.71	127.38	119.82
1	B	123	LYS	N-CA-C	-7.28	100.72	110.55
1	B	269	ARG	N-CA-C	-6.95	103.78	111.36

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	2234	0	2193	123	0
1	B	2215	0	2171	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	39	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	0	1	0
All	All	4511	0	4364	196	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 22.

All (196) 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:B:31:ARG:HH22	1:B:235:GLN:HE22	1.06	0.99
1:A:31:ARG:HH22	1:A:235:GLN:HE22	1.13	0.96
1:A:54:LYS:HB2	1:A:102:LYS:HD3	1.54	0.90
1:A:75:PRO:HD2	1:B:38:LEU:HD21	1.51	0.90
1:B:304:GLU:O	1:B:305:TRP:HB2	1.76	0.85
1:B:261:ASN:HD22	1:B:263:SER:H	1.21	0.85
1:A:31:ARG:HH22	1:A:235:GLN:NE2	1.75	0.84
1:B:220:THR:HG22	1:B:221:PRO:HD3	1.62	0.82
1:A:31:ARG:NH2	1:A:235:GLN:HE22	1.79	0.81
1:A:150:MET:HE1	1:B:300:PRO:HG3	1.63	0.79
1:A:19:PHE:H	1:B:295:MET:HE3	1.49	0.78
1:B:297:MET:HE2	1:B:298:ASN:H	1.48	0.78
1:A:225:GLU:O	1:A:229:GLN:HG2	1.85	0.77
1:A:19:PHE:N	1:B:295:MET:HE3	2.00	0.75
1:A:90:GLU:OE2	1:B:49:ARG:NH2	2.20	0.75
1:A:90:GLU:HG2	1:A:271:LEU:HD22	1.67	0.75
1:B:201:ASP:HA	1:B:204:LYS:HD3	1.69	0.74
1:B:261:ASN:ND2	1:B:263:SER:H	1.84	0.74
1:A:224:MET:HE2	1:B:299:TRP:CZ2	2.21	0.74
1:A:43:MET:HG2	1:A:110:LEU:HG	1.69	0.73
1:A:64:ALA:HA	1:A:88:MET:HG3	1.71	0.73
1:A:146:TRP:CH2	1:A:220:THR:HG22	2.23	0.72
1:A:167:GLU:OE1	1:A:199:LYS:HD3	1.89	0.72
1:A:286:TRP:O	1:A:290:THR:HB	1.90	0.71
1:A:284:LEU:HD11	1:B:239:GLU:HB2	1.72	0.71
1:A:31:ARG:NH1	3:A:329:HOH:O	2.24	0.71
1:B:110:LEU:O	1:B:110:LEU:HD23	1.92	0.70
1:B:58:GLN:NE2	1:B:58:GLN:HA	2.07	0.69
1:B:31:ARG:HH22	1:B:235:GLN:NE2	1.86	0.69
1:A:278:ALA:HB3	1:B:246:LYS:HD2	1.77	0.67
1:A:58:GLN:HE21	1:A:58:GLN:HA	1.60	0.66
1:A:88:MET:HE2	1:A:88:MET:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLN:NE2	1:A:235:GLN:HA	2.11	0.65
1:A:216:VAL:O	1:A:220:THR:HG23	1.97	0.65
1:A:131:GLU:H	1:A:131:GLU:CD	2.04	0.64
1:A:144:LYS:HB3	1:A:145:PRO:HD3	1.80	0.64
1:B:291:SER:HA	1:B:295:MET:HE2	1.81	0.63
1:A:37:ARG:HG3	1:A:38:LEU:N	2.13	0.63
1:A:303:GLU:O	1:B:161:HIS:HE1	1.81	0.62
1:B:160:TYR:CE2	1:B:206:GLN:HB2	2.34	0.62
1:A:124:GLN:OE1	1:A:130:LYS:HB2	2.00	0.62
1:A:112:LYS:HD3	1:A:248:VAL:HG22	1.82	0.61
1:A:146:TRP:CZ3	1:A:220:THR:HG22	2.34	0.61
1:B:200:GLN:O	1:B:203:GLN:HG2	1.99	0.61
1:B:216:VAL:HA	1:B:219:THR:HG23	1.83	0.61
1:A:281:GLN:H	1:A:281:GLN:CD	2.09	0.61
1:B:126:MET:HA	1:B:126:MET:CE	2.32	0.60
1:B:144:LYS:HB3	1:B:145:PRO:HD3	1.83	0.60
1:A:246:LYS:HE3	1:B:278:ALA:O	2.00	0.60
1:A:263:SER:O	1:A:267:VAL:HG12	2.01	0.60
1:A:160:TYR:HA	1:A:205:THR:CG2	2.31	0.60
1:B:279:ASP:HB3	1:B:282:GLU:HB3	1.83	0.60
1:A:300:PRO:HG3	1:B:150:MET:HE1	1.83	0.60
1:B:160:TYR:HE2	1:B:206:GLN:HB2	1.67	0.60
1:A:38:LEU:HD21	1:B:75:PRO:HD2	1.82	0.59
1:A:44:ASN:O	1:A:48:GLU:HG3	2.01	0.59
1:B:220:THR:HG22	1:B:221:PRO:CD	2.31	0.59
1:B:258:LEU:O	1:B:261:ASN:HB3	2.03	0.59
1:A:206:GLN:O	1:A:210:GLU:HG3	2.02	0.59
1:A:23:GLY:H	1:A:143:GLN:HE22	1.50	0.59
1:B:297:MET:HA	1:B:297:MET:HE3	1.85	0.58
1:A:93:LYS:HE3	1:A:270:GLU:OE2	2.02	0.58
1:B:37:ARG:O	1:B:40:ASN:HB2	2.03	0.58
1:A:257:ASN:HD21	1:A:259:ALA:HB3	1.68	0.58
1:A:156:ALA:HB1	1:A:209:TYR:HA	1.85	0.58
1:A:216:VAL:HG11	1:B:300:PRO:HG2	1.84	0.57
1:A:257:ASN:HB3	1:A:260:GLU:CG	2.34	0.57
1:B:201:ASP:HA	1:B:204:LYS:CD	2.35	0.57
1:B:26:LYS:HG2	1:B:27:ARG:N	2.20	0.56
1:B:261:ASN:HD22	1:B:263:SER:N	1.96	0.56
1:B:297:MET:HE2	1:B:298:ASN:N	2.20	0.56
1:B:297:MET:CE	1:B:298:ASN:H	2.18	0.56
1:B:30:LYS:N	1:B:30:LYS:HD2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HG21	1:B:250:LEU:HD13	1.88	0.55
1:B:215:ASP:O	1:B:219:THR:HG22	2.06	0.55
1:A:160:TYR:CE1	1:A:206:GLN:HB2	2.42	0.55
1:A:282:GLU:HG2	1:A:285:ARG:NH2	2.21	0.55
1:A:160:TYR:HA	1:A:205:THR:HG21	1.89	0.55
1:B:31:ARG:NH2	1:B:235:GLN:HE22	1.90	0.55
1:A:212:VAL:O	1:A:213:LEU:C	2.50	0.55
1:B:31:ARG:HD2	3:B:326:HOH:O	2.07	0.55
1:B:64:ALA:HA	1:B:88:MET:HG3	1.87	0.55
1:B:124:GLN:HB2	1:B:127:GLY:O	2.07	0.54
1:A:146:TRP:O	1:A:150:MET:HB2	2.07	0.54
1:B:85:GLY:HA2	1:B:88:MET:CE	2.37	0.54
1:A:58:GLN:HE21	1:A:58:GLN:CA	2.21	0.54
1:A:214:GLU:HG2	1:A:218:LYS:HE2	1.90	0.54
1:A:80:LEU:CD2	1:B:245:LEU:HB3	2.38	0.54
1:B:87:ILE:O	1:B:90:GLU:HG3	2.07	0.53
1:B:88:MET:HE2	1:B:88:MET:H	1.74	0.53
1:A:303:GLU:O	1:B:161:HIS:CE1	2.60	0.53
1:B:142:ALA:HB1	1:B:226:ASN:HB3	1.90	0.53
1:A:68:ARG:HH21	1:A:68:ARG:HG3	1.74	0.53
1:B:85:GLY:HA2	1:B:88:MET:HE1	1.91	0.53
1:A:257:ASN:HB3	1:A:260:GLU:HG2	1.91	0.53
1:B:259:ALA:C	1:B:261:ASN:H	2.16	0.53
1:A:220:THR:O	1:A:221:PRO:C	2.52	0.52
1:A:284:LEU:CD1	1:B:239:GLU:HB2	2.40	0.52
1:B:291:SER:C	1:B:295:MET:HE2	2.33	0.52
1:A:31:ARG:HD3	1:B:287:PHE:CZ	2.45	0.52
1:B:212:VAL:O	1:B:216:VAL:HG13	2.10	0.52
1:A:160:TYR:CD1	1:A:206:GLN:HB2	2.46	0.51
1:A:54:LYS:HB2	1:A:102:LYS:CD	2.35	0.51
1:A:64:ALA:O	1:A:68:ARG:HB2	2.11	0.51
1:B:101:VAL:HG22	1:B:255:HIS:O	2.11	0.51
1:A:257:ASN:OD1	1:A:260:GLU:HG2	2.10	0.50
1:B:16:THR:HA	1:B:21:GLU:HG3	1.92	0.50
1:A:21:GLU:OE2	1:B:297:MET:HE1	2.12	0.50
1:B:162:LEU:O	1:B:166:GLU:HG2	2.12	0.50
1:B:259:ALA:C	1:B:261:ASN:N	2.68	0.50
1:A:80:LEU:HD22	1:B:245:LEU:HB3	1.94	0.50
1:A:220:THR:OG1	1:A:221:PRO:HD3	2.12	0.50
1:B:253:LYS:HD3	1:B:253:LYS:C	2.36	0.49
1:B:238:GLU:OE1	1:B:241:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HG3	1:A:68:ARG:NH2	2.26	0.49
1:A:139:PHE:CZ	1:A:230:VAL:HG12	2.47	0.49
1:A:19:PHE:CB	1:B:295:MET:HE3	2.43	0.49
1:A:43:MET:HG3	1:A:113:VAL:CG2	2.42	0.49
1:A:235:GLN:HA	1:A:235:GLN:HE21	1.78	0.49
1:A:264:TYR:O	1:A:267:VAL:HG13	2.13	0.49
1:A:153:LEU:HG	1:A:153:LEU:O	2.13	0.49
1:B:123:LYS:HG2	1:B:128:GLY:O	2.13	0.49
1:B:165:LYS:O	1:B:165:LYS:HG2	2.13	0.49
1:A:262:SER:O	1:A:266:HIS:HD2	1.96	0.48
1:B:126:MET:HA	1:B:126:MET:HE2	1.94	0.48
1:A:257:ASN:HB3	1:A:260:GLU:HG3	1.95	0.48
1:A:19:PHE:HB2	1:B:295:MET:HE3	1.95	0.48
1:B:102:LYS:HB3	1:B:102:LYS:HE2	1.64	0.48
1:A:295:MET:HE1	1:B:17:ASP:O	2.13	0.48
1:A:303:GLU:CB	1:B:157:LYS:HZ1	2.27	0.48
1:B:64:ALA:HA	1:B:88:MET:CG	2.44	0.48
1:B:207:GLU:HG2	1:B:211:LYS:NZ	2.29	0.48
1:A:212:VAL:O	1:A:215:ASP:N	2.47	0.47
1:A:52:ILE:HG12	1:B:59:GLN:HB3	1.95	0.47
1:A:76:GLN:OE1	1:B:241:ARG:NH1	2.47	0.47
1:A:87:ILE:O	1:A:90:GLU:HG3	2.15	0.47
1:B:216:VAL:O	1:B:220:THR:HB	2.13	0.47
1:B:267:VAL:HG22	1:B:268:TYR:CD2	2.49	0.47
1:A:30:LYS:HE2	3:A:341:HOH:O	2.14	0.47
1:A:17:ASP:O	1:A:27:ARG:NH2	2.47	0.47
1:B:88:MET:HE2	1:B:88:MET:HB2	1.62	0.47
1:A:235:GLN:NE2	1:A:235:GLN:CA	2.78	0.46
1:B:214:GLU:O	1:B:218:LYS:HG3	2.15	0.46
1:B:124:GLN:O	1:B:127:GLY:N	2.49	0.46
1:B:110:LEU:HD23	1:B:110:LEU:C	2.40	0.46
1:A:22:VAL:HA	1:A:143:GLN:NE2	2.30	0.46
1:B:291:SER:CA	1:B:295:MET:HE2	2.44	0.46
1:A:139:PHE:CE1	1:A:230:VAL:HG12	2.51	0.46
1:A:167:GLU:O	1:A:171:MET:HG2	2.16	0.46
1:A:224:MET:O	1:A:225:GLU:C	2.57	0.46
1:A:241:ARG:NH1	1:B:76:GLN:OE1	2.49	0.45
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.59	0.45
1:A:19:PHE:CA	1:B:295:MET:HE3	2.46	0.45
1:B:167:GLU:HA	1:B:198:CYS:SG	2.57	0.44
1:B:169:LEU:C	1:B:171:MET:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:HD11	1:A:84:TRP:CE2	2.52	0.44
1:A:205:THR:HG23	1:A:206:GLN:N	2.33	0.44
1:A:262:SER:O	1:A:266:HIS:CD2	2.70	0.44
1:A:140:ARG:O	1:A:141:LYS:C	2.61	0.44
1:A:80:LEU:CD2	1:B:245:LEU:HD13	2.48	0.43
1:B:148:LYS:O	1:B:151:LYS:HG2	2.18	0.43
1:A:154:GLU:HG3	1:A:158:LYS:HE2	2.00	0.43
1:A:195:VAL:O	1:A:199:LYS:HG2	2.18	0.43
1:B:146:TRP:O	1:B:150:MET:HB2	2.18	0.43
1:A:201:ASP:O	1:A:202:VAL:C	2.62	0.43
1:A:160:TYR:HA	1:A:205:THR:HG23	1.99	0.43
1:B:17:ASP:O	1:B:27:ARG:NH2	2.51	0.43
1:A:238:GLU:CD	1:A:241:ARG:NH2	2.76	0.43
1:B:121:TYR:N	1:B:121:TYR:CD2	2.85	0.43
1:B:125:ILE:H	1:B:125:ILE:HG12	1.68	0.43
1:B:130:LYS:HE2	1:B:134:GLU:OE2	2.19	0.43
1:A:235:GLN:HE21	1:A:235:GLN:CA	2.32	0.43
1:A:275:ILE:CG2	1:B:250:LEU:HD13	2.49	0.43
1:A:71:ILE:HD12	1:A:88:MET:HE3	1.99	0.42
1:B:126:MET:HA	1:B:126:MET:HE3	2.02	0.42
1:A:58:GLN:HA	1:A:58:GLN:NE2	2.33	0.42
1:A:215:ASP:O	1:A:216:VAL:C	2.63	0.42
1:A:250:LEU:HD13	1:A:250:LEU:HA	1.93	0.42
1:A:98:HIS:NE2	1:A:258:LEU:HD11	2.34	0.42
1:A:239:GLU:HB2	1:B:284:LEU:HD11	2.02	0.42
1:A:242:LEU:HB3	1:B:80:LEU:HD13	2.01	0.42
1:A:53:GLU:HG3	1:A:101:VAL:CG1	2.49	0.41
1:A:101:VAL:HG22	1:A:255:HIS:O	2.20	0.41
1:A:38:LEU:HD12	1:A:241:ARG:NH1	2.35	0.41
1:A:17:ASP:OD1	1:A:17:ASP:N	2.52	0.41
1:A:146:TRP:CH2	1:A:216:VAL:HG13	2.55	0.41
1:A:257:ASN:CG	1:A:260:GLU:HG2	2.46	0.41
1:A:66:ARG:HG2	1:A:67:TRP:CD1	2.55	0.41
1:A:212:VAL:C	1:A:214:GLU:N	2.79	0.41
1:B:124:GLN:HE22	1:B:133:LYS:HG3	1.85	0.41
1:A:146:TRP:HH2	1:A:220:THR:HG22	1.81	0.40
1:B:65:LYS:O	1:B:66:ARG:C	2.64	0.40
1:A:49:ARG:HB2	1:B:63:TRP:CZ2	2.56	0.40
1:A:250:LEU:HD22	1:B:275:ILE:CG2	2.52	0.40
1:A:76:GLN:HB2	1:B:38:LEU:HD13	2.02	0.40
1:B:215:ASP:O	1:B:218:LYS:N	2.54	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	266/325 (82%)	250 (94%)	15 (6%)	1 (0%)	30	57
1	B	262/325 (81%)	248 (95%)	14 (5%)	0	100	100
All	All	528/650 (81%)	498 (94%)	29 (6%)	1 (0%)	43	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	VAL

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	235/289 (81%)	208 (88%)	27 (12%)	5	16
1	B	233/289 (81%)	202 (87%)	31 (13%)	4	12
All	All	468/578 (81%)	410 (88%)	58 (12%)	4	14

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	31	ARG

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Mol	Chain	Res	Type
1	A	37	ARG
1	A	52	ILE
1	A	58	GLN
1	A	66	ARG
1	A	69	GLN
1	A	80	LEU
1	A	90	GLU
1	A	103	ASN
1	A	113	VAL
1	A	131	GLU
1	A	162	LEU
1	A	165	LYS
1	A	169	LEU
1	A	195	VAL
1	A	200	GLN
1	A	204	LYS
1	A	208	LYS
1	A	227	MET
1	A	229	GLN
1	A	235	GLN
1	A	243	VAL
1	A	250	LEU
1	A	267	VAL
1	A	281	GLN
1	A	290	THR
1	B	26	LYS
1	B	31	ARG
1	B	37	ARG
1	B	42	LEU
1	B	69	GLN
1	B	80	LEU
1	B	90	GLU
1	B	96	GLU
1	B	99	GLN
1	B	125	ILE
1	B	126	MET
1	B	133	LYS
1	B	149	LYS
1	B	158	LYS
1	B	161	HIS
1	B	167	GLU
1	B	198	CYS

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Mol	Chain	Res	Type
1	B	200	GLN
1	B	202	VAL
1	B	204	LYS
1	B	219	THR
1	B	220	THR
1	B	243	VAL
1	B	245	LEU
1	B	250	LEU
1	B	261	ASN
1	B	267	VAL
1	B	271	LEU
1	B	289	SER
1	B	297	MET
1	B	305	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	58	GLN
1	A	59	GLN
1	A	99	GLN
1	A	103	ASN
1	A	107	ASN
1	A	143	GLN
1	A	206	GLN
1	A	226	ASN
1	A	235	GLN
1	A	236	GLN
1	A	257	ASN
1	A	266	HIS
1	B	58	GLN
1	B	99	GLN
1	B	104	ASN
1	B	117	GLN
1	B	122	HIS
1	B	143	GLN
1	B	161	HIS
1	B	203	GLN
1	B	206	GLN
1	B	226	ASN
1	B	235	GLN

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Mol	Chain	Res	Type
1	B	236	GLN
1	B	261	ASN
1	B	266	HIS
1	B	281	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](#)

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, 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	269/325 (82%)	0.78	39 (14%) 6 5	29, 58, 108, 121	1 (0%)
1	B	266/325 (81%)	0.90	41 (15%) 5 4	43, 61, 121, 142	0
All	All	535/650 (82%)	0.84	80 (14%) 5 4	29, 60, 111, 142	1 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	ALA	6.5
1	A	126[A]	MET	6.3
1	B	305	TRP	5.5
1	A	304	GLU	5.4
1	A	192	GLN	5.1
1	B	165	LYS	4.8
1	B	125	ILE	4.4
1	A	170	ALA	4.4
1	A	169	LEU	4.4
1	B	197	LYS	4.4
1	A	195	VAL	4.1
1	B	169	LEU	4.1
1	B	171	MET	4.1
1	B	260	GLU	4.0
1	A	16	THR	3.8
1	B	199	LYS	3.7
1	A	303	GLU	3.7
1	A	204	LYS	3.7
1	B	196	ASP	3.6
1	B	127	GLY	3.6
1	B	198	CYS	3.6
1	B	124	GLN	3.5
1	A	199	LYS	3.2
1	B	266	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	LYS	3.2
1	A	261	ASN	3.1
1	B	202	VAL	3.1
1	A	165	LYS	3.1
1	B	208	LYS	3.1
1	B	166	GLU	3.0
1	A	171	MET	3.0
1	B	16	THR	3.0
1	B	122	HIS	3.0
1	A	281	GLN	3.0
1	B	204	LYS	3.0
1	A	201	ASP	2.9
1	A	196	ASP	2.9
1	A	158	LYS	2.9
1	A	302	PHE	2.9
1	A	162	LEU	2.9
1	B	159	ALA	2.9
1	B	168	LYS	2.8
1	A	163	ALA	2.8
1	A	215	ASP	2.8
1	B	304	GLU	2.8
1	B	30	LYS	2.7
1	B	162	LEU	2.7
1	B	153	LEU	2.7
1	A	266	HIS	2.6
1	A	301	GLN	2.6
1	A	156	ALA	2.6
1	B	269	ARG	2.6
1	B	215	ASP	2.5
1	B	164	CYS	2.5
1	B	119	ASP	2.4
1	A	220	THR	2.4
1	B	298	ASN	2.4
1	B	17	ASP	2.4
1	A	166	GLU	2.4
1	A	209	TYR	2.3
1	B	121	TYR	2.3
1	A	168	LYS	2.3
1	B	163	ALA	2.3
1	A	159	ALA	2.3
1	A	164	CYS	2.2
1	A	133	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	203	GLN	2.2
1	A	202	VAL	2.2
1	A	205	THR	2.1
1	B	157	LYS	2.1
1	B	167	GLU	2.1
1	B	303	GLU	2.1
1	B	200	GLN	2.1
1	A	160	TYR	2.1
1	B	265	ILE	2.1
1	A	282	GLU	2.1
1	B	154	GLU	2.1
1	A	200	GLN	2.1
1	A	140	ARG	2.0
1	B	161	HIS	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](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	400	1/1	0.98	0.06	49,49,49,49	0
2	CA	B	400	1/1	0.99	0.07	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.