



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:40 PM UTC

PDB ID : 3HAJ / pdb_00003haj
Title : Crystal structure of human PACSIN2 F-BAR domain (p212121 lattice)
Authors : Wang, Q.; Navarro, M.V.A.S.; Peng, G.; Rajashankar, K.R.; Sondermann, H.
Deposited on : 2009-05-01
Resolution : 2.78 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

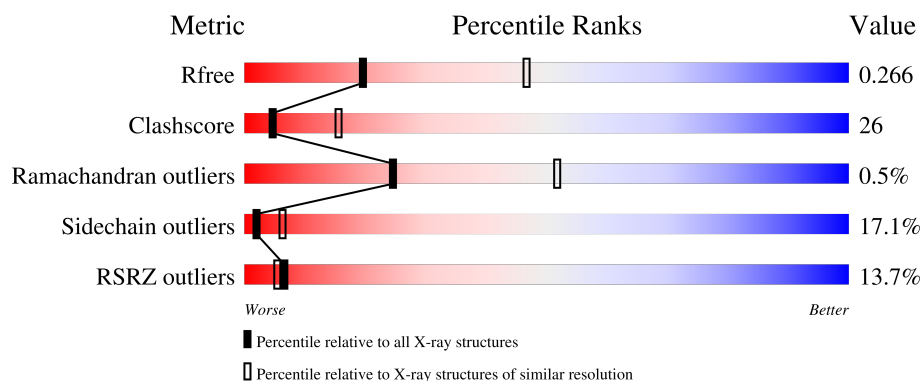
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	486	8% 33% 21% 5% 41%
1	B	486	8% 30% 20% 8% 42%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4753 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 PACSIN2 F-BAR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2368	1489	427	437	15			
1	B	284	Total	C	N	O	S	0	0	0
			2347	1475	424	433	15			

- 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		

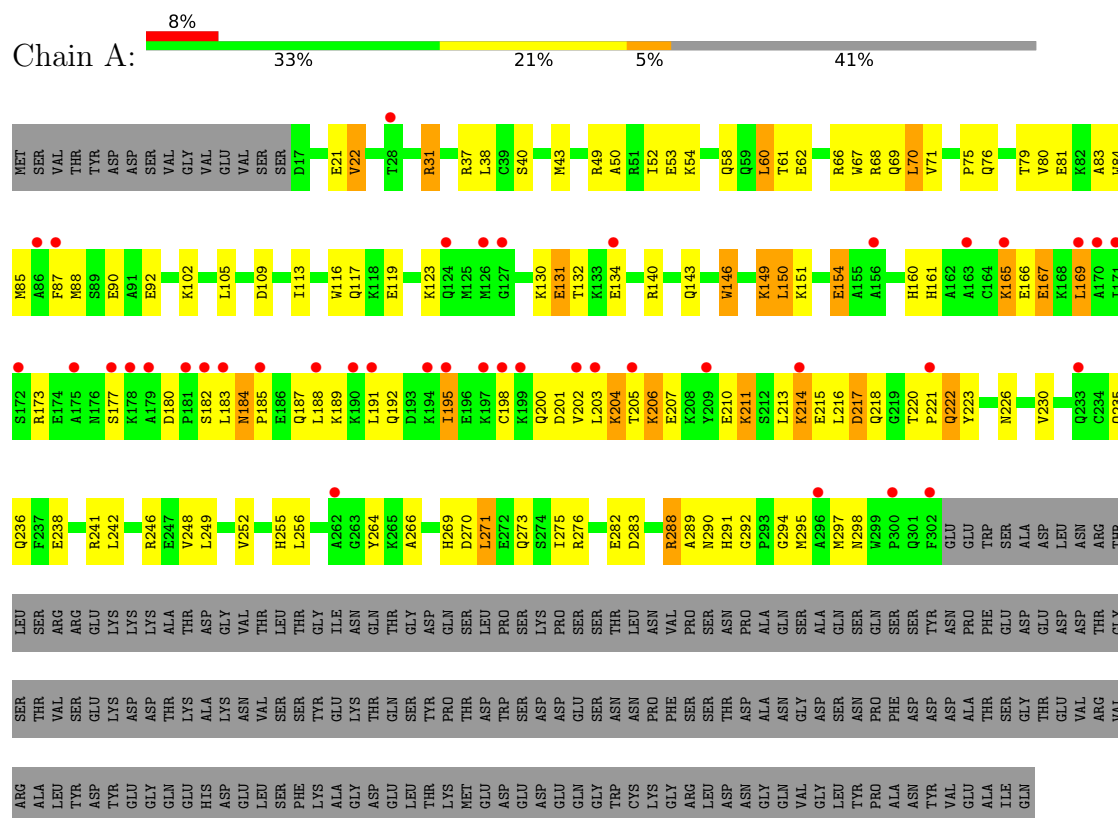
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	22	Total	O	0	0
			22	22		

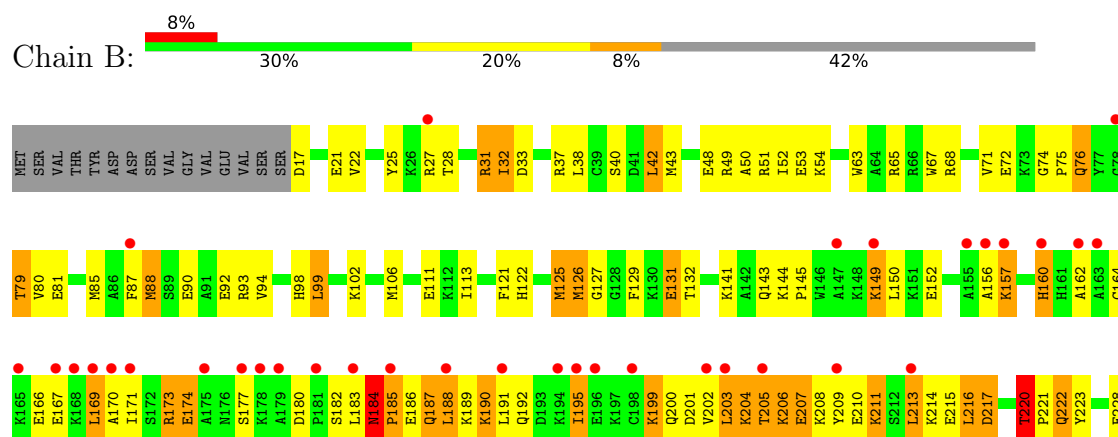
3 Residue-property plots

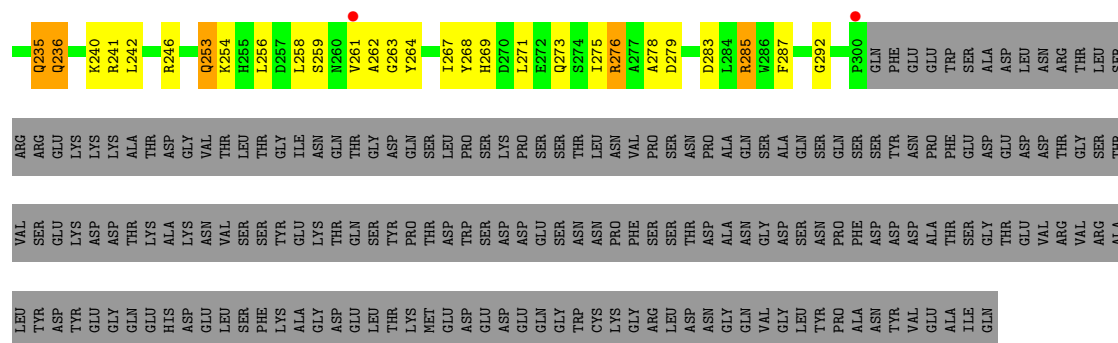
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: human PACSIN2 F-BAR



• Molecule 1: human PACSIN2 F-BAR





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	31.30Å 88.39Å 357.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.72 – 2.78 44.72 – 2.78	Depositor EDS
% Data completeness (in resolution range)	95.4 (44.72-2.78) 95.4 (44.72-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.224 , 0.274 0.216 , 0.266	Depositor DCC
R_{free} test set	1259 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4753	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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	0.28	0/2417	0.71	2/3235 (0.1%)
1	B	0.29	0/2395	0.74	3/3205 (0.1%)
All	All	0.28	0/4812	0.73	5/6440 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	GLY	CA-C-N	5.89	125.59	119.82
1	B	292	GLY	C-N-CA	5.89	125.59	119.82
1	A	292	GLY	CA-C-N	5.48	125.31	119.28
1	A	292	GLY	C-N-CA	5.48	125.31	119.28
1	B	182	SER	N-CA-C	5.16	117.72	110.14

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	2368	0	2334	123	0
1	B	2347	0	2317	148	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	0	0	0
3	B	22	0	0	4	0
All	All	4753	0	4651	243	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 (243) 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:192:GLN:HA	1:B:195:ILE:HD11	1.37	1.06
1:B:183:LEU:HB3	1:B:187:GLN:HG3	1.41	1.01
1:A:183:LEU:HB3	1:A:184:ASN:HB3	1.39	1.01
1:B:285:ARG:HG2	1:B:285:ARG:HH21	1.23	0.99
1:B:79:THR:HG21	1:B:279:ASP:H	1.27	0.97
1:A:288:ARG:HG2	1:A:288:ARG:HH21	1.33	0.94
1:A:222:GLN:HA	1:A:222:GLN:HE21	1.32	0.92
1:A:206:LYS:O	1:A:210:GLU:HG2	1.73	0.88
1:A:38:LEU:HD13	1:B:76:GLN:HG2	1.57	0.87
1:A:67:TRP:HB3	1:A:88:MET:HE2	1.56	0.86
1:B:269:HIS:O	1:B:273:GLN:HG2	1.76	0.86
1:B:37:ARG:HG2	1:B:37:ARG:HH21	1.41	0.85
1:A:183:LEU:HB3	1:A:184:ASN:CB	2.07	0.84
1:B:156:ALA:HB1	1:B:209:TYR:HA	1.62	0.79
1:A:37:ARG:HH11	1:B:75:PRO:HD3	1.48	0.78
1:B:228:GLU:OE1	3:B:508:HOH:O	2.03	0.77
1:B:235:GLN:HE21	1:B:235:GLN:HA	1.49	0.77
1:B:65:ARG:NH2	3:B:500:HOH:O	2.09	0.76
1:B:184:ASN:N	1:B:185:PRO:HD3	2.01	0.76
1:B:143:GLN:HG2	1:B:223:TYR:HE1	1.51	0.75
1:B:222:GLN:HA	1:B:222:GLN:HE21	1.48	0.75
1:A:184:ASN:HB2	1:A:185:PRO:HD2	1.68	0.74
1:B:192:GLN:CA	1:B:195:ILE:HD11	2.16	0.73
1:A:204:LYS:HG3	1:A:205:THR:N	2.03	0.73
1:A:184:ASN:N	1:A:184:ASN:HD22	1.89	0.71
1:B:285:ARG:HH21	1:B:285:ARG:CG	2.02	0.71
1:B:220:THR:H	1:B:221:PRO:HD2	1.54	0.71
1:B:170:ALA:HA	1:B:173:ARG:HB3	1.72	0.71
1:B:79:THR:HG21	1:B:279:ASP:N	2.03	0.70
1:B:126:MET:HE3	1:B:126:MET:HA	1.73	0.69
1:B:32:ILE:HG12	1:B:132:THR:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:SER:HA	1:B:43:MET:HE3	1.74	0.69
1:A:58:GLN:O	1:A:62:GLU:HG2	1.92	0.68
1:A:183:LEU:C	1:A:184:ASN:HD22	2.02	0.68
1:B:169:LEU:HD13	1:B:170:ALA:N	2.08	0.68
1:B:33:ASP:OD2	1:B:132:THR:HG21	1.94	0.68
1:B:211:LYS:O	1:B:214:LYS:HB2	1.95	0.67
1:A:252:VAL:CG1	1:B:87:PHE:HZ	2.10	0.65
1:B:166:GLU:O	1:B:169:LEU:HD12	1.97	0.64
1:B:170:ALA:CB	1:B:195:ILE:HG23	2.27	0.64
1:B:156:ALA:HB1	1:B:209:TYR:CA	2.27	0.64
1:B:210:GLU:HA	1:B:213:LEU:HG	1.79	0.64
1:B:177:SER:HA	1:B:180:ASP:OD1	1.97	0.63
1:A:87:PHE:O	1:A:90:GLU:HG3	1.97	0.63
1:B:31:ARG:HH11	1:B:31:ARG:HB3	1.64	0.63
1:B:285:ARG:HG2	1:B:285:ARG:NH2	2.04	0.63
1:A:204:LYS:HE3	1:A:204:LYS:C	2.23	0.63
1:A:38:LEU:HD21	1:B:75:PRO:HD2	1.81	0.62
1:A:189:LYS:HA	1:A:192:GLN:HE21	1.64	0.62
1:B:87:PHE:HB3	1:B:88:MET:HE3	1.80	0.62
1:B:220:THR:N	1:B:221:PRO:HD2	2.15	0.62
1:A:184:ASN:N	1:A:184:ASN:ND2	2.47	0.61
1:B:200:GLN:O	1:B:204:LYS:HB3	2.00	0.61
1:A:248:VAL:O	1:A:252:VAL:HG23	1.99	0.61
1:B:87:PHE:O	1:B:90:GLU:HG3	2.01	0.60
1:A:40:SER:HA	1:A:43:MET:HE3	1.83	0.60
1:B:48:GLU:HG3	1:B:51:ARG:NH1	2.17	0.60
1:A:143:GLN:HG3	1:A:223:TYR:HE1	1.66	0.60
1:B:129:PHE:HB2	1:B:132:THR:HG23	1.84	0.60
1:B:81:GLU:O	1:B:85:MET:HG2	2.02	0.60
1:A:204:LYS:HG3	1:A:205:THR:H	1.67	0.59
1:B:32:ILE:HD11	1:B:131:GLU:HB2	1.83	0.59
1:A:204:LYS:HB2	1:A:204:LYS:NZ	2.17	0.59
1:A:184:ASN:HB2	1:A:185:PRO:CD	2.32	0.59
1:B:220:THR:H	1:B:221:PRO:CD	2.15	0.59
1:B:32:ILE:CD1	1:B:131:GLU:HB2	2.33	0.59
1:A:288:ARG:HH21	1:A:288:ARG:CG	2.09	0.59
1:B:79:THR:CG2	1:B:279:ASP:H	2.09	0.59
1:B:208:LYS:HA	1:B:211:LYS:HB3	1.85	0.59
1:A:235:GLN:HE21	1:A:235:GLN:HA	1.69	0.58
1:B:160:HIS:C	1:B:160:HIS:CD2	2.82	0.58
1:B:144:LYS:HB3	1:B:145:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:GLU:OE2	1:B:199:LYS:HA	2.04	0.57
1:A:150:LEU:O	1:A:154:GLU:HB2	2.04	0.57
1:A:246:ARG:HH22	1:B:276:ARG:HH21	1.52	0.57
1:A:271:LEU:HD13	1:B:253:GLN:HB2	1.85	0.57
1:B:149:LYS:NZ	1:B:215:GLU:HB2	2.20	0.57
1:B:37:ARG:HG2	1:B:37:ARG:NH2	2.13	0.57
1:A:264:TYR:CD2	1:B:259:SER:HA	2.40	0.56
1:A:79:THR:HG23	1:A:283:ASP:OD1	2.05	0.56
1:A:161:HIS:O	1:A:165:LYS:HB2	2.05	0.56
1:A:288:ARG:HG2	1:A:288:ARG:NH2	2.12	0.56
1:B:202:VAL:O	1:B:206:LYS:HB3	2.06	0.56
1:B:222:GLN:HA	1:B:222:GLN:NE2	2.20	0.56
1:B:269:HIS:O	1:B:273:GLN:CG	2.52	0.56
1:B:169:LEU:O	1:B:173:ARG:HB3	2.06	0.56
1:A:22:VAL:HA	1:A:143:GLN:NE2	2.21	0.56
1:A:202:VAL:O	1:A:206:LYS:HB2	2.05	0.56
1:A:256:LEU:HD11	1:B:87:PHE:CZ	2.41	0.55
1:A:264:TYR:CE2	1:B:259:SER:HA	2.41	0.55
1:A:182:SER:HB2	1:A:183:LEU:HA	1.89	0.55
1:B:162:ALA:O	1:B:166:GLU:HB2	2.07	0.55
1:A:222:GLN:HE21	1:A:222:GLN:CA	2.10	0.55
1:B:79:THR:HG22	1:B:283:ASP:OD2	2.07	0.55
1:B:187:GLN:HA	1:B:190:LYS:HE2	1.89	0.55
1:A:67:TRP:O	1:A:71:VAL:HG23	2.07	0.55
1:A:154:GLU:OE1	1:A:154:GLU:HA	2.07	0.54
1:A:85:MET:C	1:A:87:PHE:H	2.15	0.54
1:A:85:MET:C	1:A:87:PHE:N	2.65	0.54
1:A:266:ALA:O	1:A:269:HIS:HB3	2.08	0.54
1:B:38:LEU:HD13	1:B:241:ARG:NH1	2.23	0.54
1:B:88:MET:HE3	1:B:88:MET:N	2.23	0.54
1:A:297:MET:HE1	1:B:21:GLU:HG3	1.88	0.53
1:A:31:ARG:HD3	1:A:238:GLU:CD	2.33	0.53
1:A:220:THR:N	1:A:221:PRO:HD2	2.23	0.53
1:A:84:TRP:HD1	1:A:84:TRP:O	1.92	0.53
1:A:290:ASN:O	1:A:295:MET:HE3	2.09	0.53
1:B:220:THR:N	1:B:221:PRO:CD	2.72	0.53
1:A:116:TRP:CH2	1:A:241:ARG:HG3	2.44	0.52
1:A:109:ASP:OD2	1:A:255:HIS:HD2	1.92	0.52
1:A:75:PRO:HD2	1:B:38:LEU:HD21	1.92	0.52
1:B:183:LEU:HD13	1:B:187:GLN:HE21	1.74	0.52
1:A:84:TRP:NE1	1:A:88:MET:HE1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:CYS:C	1:B:166:GLU:H	2.18	0.51
1:A:50:ALA:O	1:A:102:LYS:HG3	2.11	0.51
1:B:32:ILE:HG13	1:B:121:PHE:HE1	1.75	0.51
1:A:76:GLN:HE21	1:A:80:VAL:HB	1.76	0.51
1:A:105:LEU:CD2	1:A:252:VAL:HG13	2.39	0.51
1:B:186:GLU:O	1:B:189:LYS:HG2	2.10	0.51
1:B:81:GLU:HG2	1:B:85:MET:HE2	1.92	0.51
1:B:201:ASP:O	1:B:205:THR:HG23	2.09	0.51
1:B:170:ALA:HB3	1:B:195:ILE:HG23	1.93	0.51
1:B:211:LYS:O	1:B:211:LYS:HD3	2.11	0.51
1:B:157:LYS:NZ	1:B:157:LYS:HB3	2.25	0.51
1:B:106:MET:O	1:B:111:GLU:HG2	2.11	0.50
1:A:130:LYS:O	1:A:134:GLU:HB2	2.11	0.50
1:A:146:TRP:CD1	1:A:146:TRP:C	2.89	0.50
1:B:49:ARG:NH1	1:B:53:GLU:OE2	2.44	0.50
1:B:195:ILE:HD12	1:B:195:ILE:H	1.76	0.50
1:A:22:VAL:HA	1:A:143:GLN:HE22	1.76	0.50
1:B:160:HIS:CD2	1:B:160:HIS:O	2.65	0.50
1:B:149:LYS:HZ2	1:B:215:GLU:HB2	1.75	0.50
1:A:143:GLN:HG3	1:A:223:TYR:CE1	2.47	0.50
1:B:67:TRP:O	1:B:71:VAL:HG23	2.11	0.49
1:B:126:MET:N	1:B:127:GLY:HA3	2.27	0.49
1:A:109:ASP:O	1:A:113:ILE:HG13	2.11	0.49
1:A:117:GLN:HG2	1:A:117:GLN:O	2.12	0.49
1:A:183:LEU:CB	1:A:184:ASN:HB3	2.28	0.49
1:A:214:LYS:O	1:A:218:GLN:HG3	2.13	0.49
1:B:262:ALA:HB3	3:B:492:HOH:O	2.10	0.49
1:A:289:ALA:HA	1:A:294:GLY:HA3	1.95	0.49
1:B:184:ASN:N	1:B:185:PRO:CD	2.74	0.49
1:A:276:ARG:HA	1:B:246:ARG:NH1	2.28	0.49
1:B:184:ASN:O	1:B:188:LEU:HB2	2.12	0.49
1:A:76:GLN:NE2	1:A:80:VAL:HB	2.28	0.48
1:A:220:THR:N	1:A:221:PRO:CD	2.75	0.48
1:A:270:ASP:HA	1:A:273:GLN:HG2	1.94	0.48
1:B:235:GLN:HA	1:B:235:GLN:NE2	2.22	0.48
1:B:285:ARG:CG	1:B:285:ARG:NH2	2.67	0.48
1:A:288:ARG:CG	1:A:288:ARG:NH2	2.72	0.48
1:B:174:GLU:CG	1:B:191:LEU:HB3	2.43	0.48
1:B:203:LEU:O	1:B:207:GLU:HB3	2.14	0.48
1:B:122:HIS:N	1:B:131:GLU:OE2	2.38	0.47
1:A:177:SER:HA	1:A:180:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:HD3	1:A:288:ARG:C	2.39	0.47
1:B:42:LEU:HD13	1:B:113:ILE:HD13	1.96	0.47
1:A:83:ALA:HB1	1:A:275:ILE:HA	1.97	0.47
1:B:213:LEU:N	1:B:213:LEU:HD23	2.30	0.47
1:B:72:GLU:HG3	1:B:85:MET:CE	2.45	0.47
1:B:93:ARG:HA	1:B:93:ARG:HD3	1.65	0.46
1:A:177:SER:HA	1:A:180:ASP:CG	2.40	0.46
1:A:246:ARG:HG3	1:B:278:ALA:HB3	1.96	0.46
1:A:252:VAL:HG12	1:B:87:PHE:HZ	1.80	0.46
1:A:256:LEU:HD11	1:B:87:PHE:CE2	2.51	0.46
1:A:226:ASN:O	1:A:230:VAL:HG23	2.15	0.46
1:B:31:ARG:HB3	1:B:31:ARG:NH1	2.29	0.46
1:A:84:TRP:O	1:A:84:TRP:CD1	2.68	0.46
1:B:216:LEU:HD23	1:B:217:ASP:N	2.29	0.46
1:A:66:ARG:O	1:A:70:LEU:HD23	2.15	0.46
1:A:81:GLU:O	1:A:85:MET:HE2	2.16	0.46
1:A:68:ARG:HH22	1:A:92:GLU:CD	2.24	0.46
1:A:84:TRP:CD1	1:A:88:MET:HE1	2.51	0.45
1:A:217:ASP:HA	1:A:220:THR:HG22	1.98	0.45
1:A:49:ARG:NH1	1:A:53:GLU:OE2	2.47	0.45
1:A:188:LEU:O	1:A:192:GLN:HB2	2.16	0.45
1:A:242:LEU:HD22	1:B:80:VAL:HG21	1.98	0.45
1:A:235:GLN:HA	1:A:235:GLN:NE2	2.30	0.45
1:A:222:GLN:HA	1:A:222:GLN:NE2	2.16	0.45
1:A:150:LEU:O	1:A:150:LEU:HD13	2.16	0.45
1:B:48:GLU:HG3	1:B:51:ARG:HH12	1.80	0.45
1:B:149:LYS:HD2	1:B:149:LYS:HA	1.45	0.45
1:A:167:GLU:CG	1:A:198:CYS:HB3	2.47	0.45
1:A:252:VAL:HG11	1:B:87:PHE:HZ	1.80	0.45
1:A:249:LEU:HB3	1:B:275:ILE:HD13	1.97	0.44
1:A:291:HIS:ND1	1:B:27:ARG:HD3	2.32	0.44
1:B:164:CYS:C	1:B:166:GLU:N	2.74	0.44
1:A:195:ILE:HD13	1:A:195:ILE:C	2.42	0.44
1:B:72:GLU:HG3	1:B:85:MET:HE1	1.99	0.44
1:A:85:MET:HE2	1:A:85:MET:HB2	1.92	0.43
1:A:173:ARG:HD2	1:A:173:ARG:HA	1.71	0.43
1:B:79:THR:H	1:B:283:ASP:CG	2.26	0.43
1:B:170:ALA:HB1	1:B:195:ILE:HG23	2.00	0.43
1:A:37:ARG:HH11	1:B:74:GLY:HA2	1.84	0.43
1:A:146:TRP:HZ3	1:A:220:THR:HB	1.83	0.43
1:B:126:MET:HB2	3:B:493:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:HA	1:A:198:CYS:SG	2.59	0.43
1:B:31:ARG:NH2	1:B:235:GLN:NE2	2.67	0.43
1:B:85:MET:C	1:B:87:PHE:N	2.74	0.43
1:B:166:GLU:C	1:B:169:LEU:HD12	2.44	0.43
1:B:258:LEU:HA	1:B:261:VAL:HG21	2.01	0.43
1:A:201:ASP:HA	1:A:204:LYS:HG2	2.01	0.43
1:A:166:GLU:O	1:A:169:LEU:HB3	2.19	0.42
1:A:151:LYS:HD2	1:A:151:LYS:HA	1.79	0.42
1:B:264:TYR:CE1	1:B:268:TYR:HE2	2.38	0.42
1:B:48:GLU:O	1:B:52:ILE:HG13	2.19	0.42
1:B:50:ALA:HB1	1:B:102:LYS:CG	2.50	0.42
1:A:131:GLU:CD	1:A:131:GLU:H	2.28	0.42
1:B:254:LYS:HE3	1:B:254:LYS:HB2	1.64	0.42
1:B:37:ARG:NH2	1:B:37:ARG:CG	2.79	0.42
1:A:52:ILE:HD11	1:B:63:TRP:HB2	2.01	0.41
1:A:76:GLN:HB2	1:B:38:LEU:HD22	2.01	0.41
1:A:87:PHE:CZ	1:B:256:LEU:HD11	2.54	0.41
1:A:252:VAL:HG11	1:B:87:PHE:CZ	2.55	0.41
1:B:87:PHE:HB3	1:B:88:MET:CE	2.49	0.41
1:B:263:GLY:O	1:B:267:ILE:HG13	2.20	0.41
1:A:160:HIS:HD2	1:A:205:THR:HB	1.84	0.41
1:B:25:TYR:CD1	1:B:25:TYR:C	2.98	0.41
1:B:236:GLN:O	1:B:240:LYS:HD3	2.20	0.41
1:B:68:ARG:HH22	1:B:92:GLU:CD	2.28	0.41
1:B:207:GLU:HG2	1:B:208:LYS:N	2.34	0.41
1:B:192:GLN:C	1:B:195:ILE:HD11	2.45	0.41
1:A:217:ASP:HA	1:A:220:THR:CG2	2.50	0.41
1:B:143:GLN:HG2	1:B:223:TYR:CE1	2.42	0.41
1:B:222:GLN:HE21	1:B:222:GLN:CA	2.18	0.41
1:A:298:ASN:HD22	1:A:298:ASN:HA	1.65	0.41
1:B:94:VAL:O	1:B:98:HIS:HD2	2.03	0.41
1:A:182:SER:HA	1:A:183:LEU:C	2.46	0.41
1:A:211:LYS:HB3	1:A:211:LYS:HE3	1.80	0.41
1:A:252:VAL:CG1	1:B:87:PHE:CZ	2.97	0.41
1:A:149:LYS:HB3	1:A:216:LEU:HG	2.02	0.41
1:A:211:LYS:O	1:A:215:GLU:HB2	2.21	0.41
1:B:42:LEU:HD13	1:B:113:ILE:CD1	2.51	0.41
1:B:169:LEU:C	1:B:169:LEU:HD22	2.46	0.41
1:A:31:ARG:NH2	1:B:287:PHE:CD1	2.89	0.41
1:A:180:ASP:OD1	1:A:180:ASP:O	2.37	0.41
1:B:32:ILE:CG1	1:B:132:THR:HG22	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH2	1:A:235:GLN:NE2	2.69	0.40
1:B:125:MET:HE3	1:B:125:MET:O	2.21	0.40
1:B:126:MET:HB3	1:B:127:GLY:HA2	2.03	0.40
1:B:99:LEU:HD22	1:B:99:LEU:HA	1.93	0.40
1:A:60:LEU:HD22	1:B:52:ILE:HG21	2.02	0.40
1:A:80:VAL:HG21	1:B:242:LEU:HD22	2.04	0.40
1:A:184:ASN:OD1	1:A:187:GLN:HB2	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	284/486 (58%)	277 (98%)	7 (2%)	0	100	100
1	B	282/486 (58%)	268 (95%)	11 (4%)	3 (1%)	11	32
All	All	566/972 (58%)	545 (96%)	18 (3%)	3 (0%)	24	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	PRO
1	B	220	THR
1	B	184	ASN

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	247/424 (58%)	210 (85%)	37 (15%)	3	9
1	B	245/424 (58%)	198 (81%)	47 (19%)	1	4
All	All	492/848 (58%)	408 (83%)	84 (17%)	2	6

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	22	VAL
1	A	31	ARG
1	A	54	LYS
1	A	60	LEU
1	A	61	THR
1	A	69	GLN
1	A	70	LEU
1	A	119	GLU
1	A	123	LYS
1	A	131	GLU
1	A	132	THR
1	A	140	ARG
1	A	146	TRP
1	A	149	LYS
1	A	150	LEU
1	A	154	GLU
1	A	165	LYS
1	A	167	GLU
1	A	169	LEU
1	A	184	ASN
1	A	191	LEU
1	A	195	ILE
1	A	200	GLN
1	A	203	LEU
1	A	204	LYS
1	A	206	LYS
1	A	207	GLU
1	A	211	LYS
1	A	213	LEU
1	A	214	LYS
1	A	217	ASP
1	A	222	GLN
1	A	236	GLN

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	282	GLU
1	A	288	ARG
1	B	17	ASP
1	B	22	VAL
1	B	28	THR
1	B	31	ARG
1	B	32	ILE
1	B	42	LEU
1	B	54	LYS
1	B	76	GLN
1	B	79	THR
1	B	88	MET
1	B	99	LEU
1	B	125	MET
1	B	126	MET
1	B	131	GLU
1	B	141	LYS
1	B	149	LYS
1	B	150	LEU
1	B	152	GLU
1	B	157	LYS
1	B	160	HIS
1	B	169	LEU
1	B	171	ILE
1	B	173	ARG
1	B	174	GLU
1	B	184	ASN
1	B	187	GLN
1	B	188	LEU
1	B	190	LYS
1	B	195	ILE
1	B	199	LYS
1	B	203	LEU
1	B	204	LYS
1	B	205	THR
1	B	206	LYS
1	B	207	GLU
1	B	211	LYS
1	B	213	LEU
1	B	216	LEU
1	B	217	ASP

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Mol	Chain	Res	Type
1	B	220	THR
1	B	222	GLN
1	B	235	GLN
1	B	236	GLN
1	B	253	GLN
1	B	271	LEU
1	B	276	ARG
1	B	285	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	47	HIS
1	A	58	GLN
1	A	59	GLN
1	A	69	GLN
1	A	115	ASN
1	A	143	GLN
1	A	160	HIS
1	A	184	ASN
1	A	192	GLN
1	A	222	GLN
1	A	229	GLN
1	A	233	GLN
1	A	235	GLN
1	A	236	GLN
1	A	255	HIS
1	A	260	ASN
1	A	273	GLN
1	A	298	ASN
1	B	36	HIS
1	B	44	ASN
1	B	58	GLN
1	B	69	GLN
1	B	222	GLN
1	B	235	GLN
1	B	236	GLN
1	B	253	GLN
1	B	273	GLN
1	B	291	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](#)

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	286/486 (58%)	0.76	41 (14%)	6 5	27, 69, 159, 174	0
1	B	284/486 (58%)	0.62	37 (13%)	7 6	23, 63, 161, 177	0
All	All	570/972 (58%)	0.69	78 (13%)	6 5	23, 66, 160, 177	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	LEU	5.2
1	A	302	PHE	5.2
1	A	171	ILE	4.8
1	B	87	PHE	4.6
1	B	160	HIS	4.2
1	A	203	LEU	3.9
1	A	194	LYS	3.8
1	A	195	ILE	3.8
1	B	178	LYS	3.8
1	A	182	SER	3.8
1	A	175	ALA	3.8
1	A	185	PRO	3.8
1	A	198	CYS	3.7
1	A	205	THR	3.7
1	A	177	SER	3.6
1	B	205	THR	3.6
1	A	191	LEU	3.5
1	A	87	PHE	3.5
1	A	183	LEU	3.5
1	A	202	VAL	3.5
1	B	261	VAL	3.5
1	B	169	LEU	3.4
1	B	191	LEU	3.4
1	B	171	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	185	PRO	3.4
1	B	202	VAL	3.3
1	A	221	PRO	3.2
1	B	209	TYR	3.2
1	A	170	ALA	3.1
1	A	181	PRO	3.1
1	A	169	LEU	3.1
1	B	175	ALA	3.0
1	A	163	ALA	2.9
1	B	147	ALA	2.9
1	B	157	LYS	2.9
1	B	195	ILE	2.9
1	B	183	LEU	2.9
1	A	178	LYS	2.8
1	B	177	SER	2.8
1	A	188	LEU	2.8
1	B	170	ALA	2.8
1	A	86	ALA	2.7
1	B	181	PRO	2.7
1	A	197	LYS	2.7
1	B	155	ALA	2.7
1	B	156	ALA	2.7
1	A	262	ALA	2.7
1	A	127	GLY	2.6
1	B	168	LYS	2.6
1	A	179	ALA	2.6
1	B	300	PRO	2.6
1	A	190	LYS	2.5
1	A	209	TYR	2.5
1	B	149	LYS	2.5
1	B	163	ALA	2.5
1	A	156	ALA	2.4
1	B	179	ALA	2.4
1	A	28	THR	2.3
1	B	196	GLU	2.3
1	A	296	ALA	2.3
1	B	194	LYS	2.3
1	B	162	ALA	2.3
1	A	126	MET	2.3
1	A	300	PRO	2.3
1	B	203	LEU	2.3
1	B	167	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	199	LYS	2.2
1	B	198	CYS	2.2
1	A	233	GLN	2.2
1	B	165	LYS	2.2
1	B	213	LEU	2.2
1	A	172	SER	2.2
1	A	165	LYS	2.1
1	A	134	GLU	2.1
1	A	124	GLN	2.1
1	B	78	GLY	2.1
1	B	27	ARG	2.0
1	A	214	LYS	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(Å ²)	Q<0.9
2	CA	B	488	1/1	0.97	0.06	68,68,68,68	0
2	CA	A	488	1/1	0.98	0.06	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.