



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID : 3HAJ
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

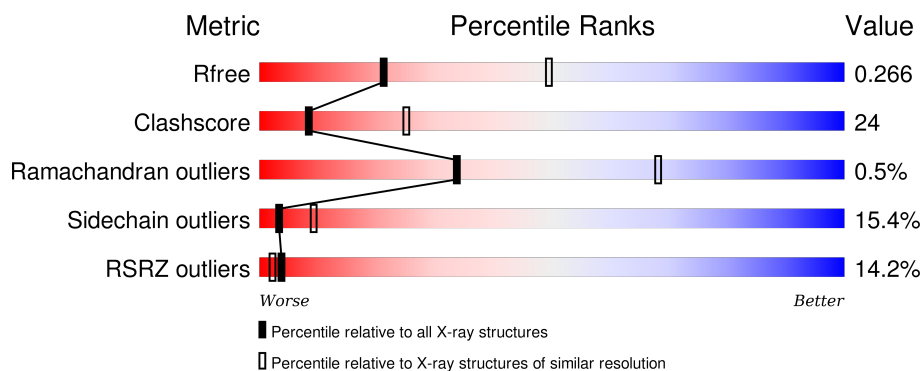
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	
1	B	486	

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 (three-letter code: CA) (formula: Ca).

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

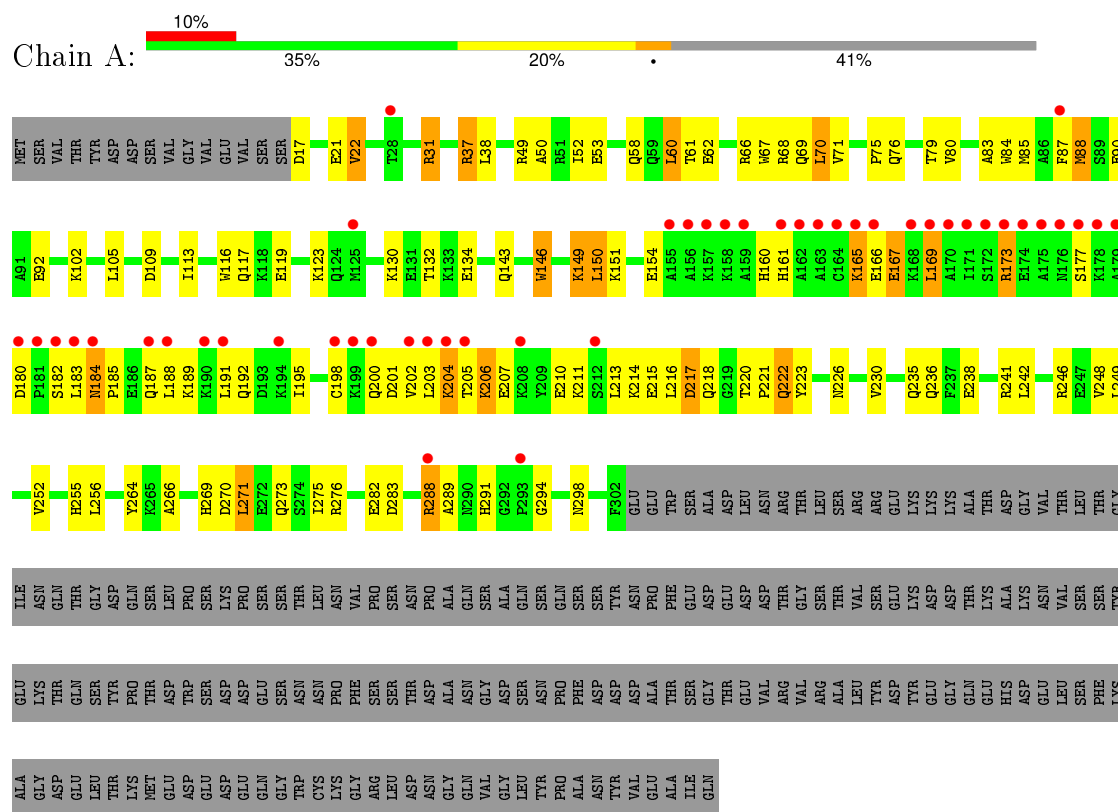
- Molecule 3 is water.

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

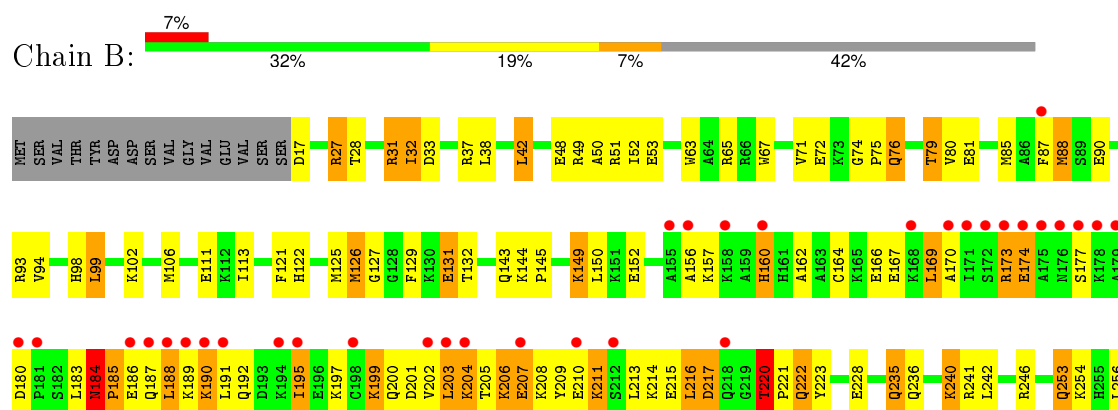
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: human PACSIN2 F-BAR



• Molecule 1: human PACSIN2 F-BAR



	LYS	ASN	D257
GLY	THR	GLN	L258
ASP	GLN	THR	S259
LEU	SER	GLY	N260
THR	TYR	ASP	Y261
LYS	PRO	GLN	A262
MET	THR	SER	G263
GLU	ASP	LEU	Y264
ASP	TRP	PRO	I267
GLU	ASP	SER	L267
ASP	ASP	LYS	Y268
GLU	ASP	PRO	H269
GLN	GLU	SER	D270
GLY	SER	THR	L271
TRP	ASN	THR	E272
CYS	ASN	LEU	S273
LYS	PRO	ASN	S274
GLY	PHE	VAL	I275
ARG	SER	PRO	R276
LEU	SER	SER	A277
ASP	THR	ASN	Z278
ASN	ASP	PRO	D279
GLY	ALA	ALA	I283
GLN	ASN	GLN	L284
VAL	GLY	SER	G284
GLY	ASP	ALA	R285
LEU	SER	GLN	N286
TYR	ASN	SER	F287
PRO	PRO	GLN	P300
ALA	PHE	SER	GLN
ASN	ASP	SER	GLN
TYR	ASP	TYR	PHE
VAL	ASP	ASN	GLU
GLU	ALA	PRO	GLU
ILE	THR	PHE	TRP
ALA	SER	GLU	SER
GLN	GLY	ASP	ALA
	THR	GLU	ASP
	THR	ASP	LEU
	VAL	ASP	ASN
	ARG	THR	ARG
	VAL	GLY	THR
	ARG	SER	LEU
	ALA	THR	SER
	LEU	VAL	ARG
	TYR	SER	ARG
	ASP	GLU	GLU
	TYR	LYS	LYS
	GLU	ASP	LYS
	GLY	ASP	LYS
	GLN	THR	ALA
	GLU	LYS	THR
	HIS	ALA	ASP
	ASP	LYS	GLY
	LEU	ASN	VAL
	GLU	SER	THR
	PHE	SER	LEU
	SER	THR	THR
	LYS	TYR	GLY
	ALA	GLU	ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	31.30 Å 88.39 Å 357.72 Å 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 2.77 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.224 , 0.274 0.218 , 0.266	Depositor DCC
R_{free} test set	1258 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 77.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 25179 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/2417	0.37	0/3235
1	B	0.24	0/2395	0.41	0/3205
All	All	0.24	0/4812	0.39	0/6440

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2368	0	2334	114	0
1	B	2347	0	2317	139	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	14	0	0	0	0
3	B	22	0	0	4	0
All	All	4753	0	4651	226	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 24.

All (226) 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:HE21	1:A:222:GLN:HA	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: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:HA	1:B:235:GLN:HE21	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:HE21	1:B:222:GLN:HA	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:CG	1:B:285:ARG:HH21	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:32:ILE:HG12	1:B:132:THR:HG22	1.75	0.69
1:A:58:GLN:O	1:A:62:GLU:HG2	1.92	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:A:183:LEU:C	1:A:184:ASN:HD22	2.02	0.63
1:B:177:SER:HA	1:B:180:ASP:OD1	1.97	0.63
1:B:31:ARG:HB3	1:B:31:ARG:HH11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:O	1:A:90:GLU:HG3	1.97	0.63
1:B:285:ARG:HG2	1:B:285:ARG:NH2	2.04	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:220:THR:N	1:B:221:PRO:HD2	2.15	0.62
1:A:184:ASN:ND2	1:A:184:ASN:N	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: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:NZ	1:A:204:LYS:HB2	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:B:79:THR:CG2	1:B:279:ASP:H	2.09	0.59
1:A:288:ARG:CG	1:A:288:ARG:HH21	2.09	0.59
1:A:204:LYS:C	1:A:204:LYS:HE3	2.23	0.59
1:B:208:LYS:HA	1:B:211:LYS:HB3	1.85	0.59
1:A:235:GLN:HA	1:A:235:GLN:HE21	1.69	0.58
1:B:144:LYS:HB3	1:B:145:PRO:HD3	1.86	0.57
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:288:ARG:HG2	1:A:288:ARG:NH2	2.12	0.56
1:A:161:HIS:O	1:A:165:LYS:HB2	2.05	0.56
1:A:79:THR:HG23	1:A:283:ASP:OD1	2.05	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:202:VAL:O	1:A:206:LYS:HB2	2.05	0.56
1:A:22:VAL:HA	1:A:143:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:149:LYS:HZ2	1:B:215:GLU:HB2	1.70	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:B:187:GLN:HA	1:B:190:LYS:HE2	1.89	0.55
1:B:79:THR:HG22	1:B:283:ASP:OD2	2.07	0.55
1:A:222:GLN:HE21	1:A:222:GLN:CA	2.10	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: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:A:220:THR:N	1:A:221:PRO:HD2	2.23	0.53
1:B:160:HIS:C	1:B:160:HIS:CD2	2.82	0.53
1:A:84:TRP:O	1:A:84:TRP:HD1	1.92	0.53
1:B:220:THR:N	1:B:221:PRO:CD	2.72	0.53
1:B:87:PHE:HB3	1:B:88:MET:HE1	1.91	0.52
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:B:183:LEU:HD13	1:B:187:GLN:HE21	1.74	0.52
1:A:75:PRO:HD2	1:B:38:LEU:HD21	1.92	0.52
1:B:32:ILE:HG13	1:B:121:PHE:HE1	1.75	0.51
1:A:50:ALA:O	1:A:102:LYS:HG3	2.11	0.51
1:A:105:LEU:CD2	1:A:252:VAL:HG13	2.39	0.51
1:A:76:GLN:HE21	1:A:80:VAL:HB	1.76	0.51
1:B:186:GLU:O	1:B:189:LYS:HG2	2.10	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:B:195:ILE:HD12	1:B:195:ILE:H	1.76	0.50
1:B:49:ARG:NH1	1:B:53:GLU:OE2	2.44	0.50
1:A:22:VAL:HA	1:A:143:GLN:HE22	1.76	0.50
1:B:160:HIS:O	1:B:160:HIS:CD2	2.65	0.50
1:A:143:GLN:HG3	1:A:223:TYR:CE1	2.47	0.50
1:B:81:GLU:HG2	1:B:85:MET:HE2	1.93	0.49
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:183:LEU:CB	1:A:184:ASN:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:MET:C	1:A:87:PHE:H	2.15	0.49
1:A:85:MET:C	1:A:87:PHE:N	2.65	0.49
1:A:109:ASP:O	1:A:113:ILE:HG13	2.11	0.49
1:A:117:GLN:O	1:A:117:GLN:HG2	2.12	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:B:184:ASN:O	1:B:188:LEU:HB2	2.12	0.49
1:A:276:ARG:HA	1:B:246:ARG:NH1	2.28	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:285:ARG:NH2	1:B:285:ARG:CG	2.67	0.48
1:B:235:GLN:NE2	1:B:235:GLN:HA	2.22	0.48
1:A:31:ARG:HD3	1:A:238:GLU:CD	2.33	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
1:B:42:LEU:HD13	1:B:113:ILE:HD13	1.96	0.47
1:B:72:GLU:HG3	1:B:85:MET:HE1	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:HD3	1:B:93:ARG:HA	1.65	0.46
1:A:246:ARG:HG3	1:B:278:ALA:HB3	1.96	0.46
1:B:164:CYS:C	1:B:166:GLU:H	2.18	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:B:31:ARG:HB3	1:B:31:ARG:NH1	2.29	0.46
1:A:226:ASN:O	1:A:230:VAL:HG23	2.15	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:146:TRP:C	1:A:146:TRP:CD1	2.89	0.46
1:A:67:TRP:HB3	1:A:88:MET:CE	2.46	0.45
1:A:217:ASP:HA	1:A:220:THR:HG22	1.98	0.45
1:A:188:LEU:O	1:A:192:GLN:HB2	2.16	0.45
1:A:67:TRP:HB3	1:A:88:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HD22	1:B:80:VAL:HG21	1.98	0.45
1:A:49:ARG:NH1	1:A:53:GLU:OE2	2.47	0.45
1:A:235:GLN:HA	1:A:235:GLN:NE2	2.30	0.45
1:A:222:GLN:NE2	1:A:222:GLN:HA	2.16	0.45
1:B:48:GLU:HG3	1:B:51:ARG:HH12	1.80	0.45
1:A:150:LEU:HD13	1:A:150:LEU:O	2.16	0.45
1:B:149:LYS:HD2	1:B:149:LYS:HA	1.45	0.45
1:A:252:VAL:HG11	1:B:87:PHE:HZ	1.80	0.45
1:A:167:GLU:CG	1:A:198:CYS:HB3	2.47	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:170:ALA:HB1	1:B:195:ILE:HG23	2.00	0.43
1:A:173:ARG:HA	1:A:173:ARG:HD2	1.71	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
1:B:31:ARG:NH2	1:B:235:GLN:NE2	2.67	0.43
1:A:167:GLU:HA	1:A:198:CYS:SG	2.59	0.43
1:B:258:LEU:HA	1:B:261:VAL:HG21	2.01	0.43
1:A:288:ARG:C	1:A:288:ARG:HD3	2.39	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:B:264:TYR:CE1	1:B:268:TYR:HE2	2.38	0.42
1:A:151:LYS:HD2	1:A:151:LYS:HA	1.79	0.42
1:B:87:PHE:HB3	1:B:88:MET:CE	2.49	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:B:254:LYS:HB2	1:B:254:LYS:HE3	1.64	0.42
1:B:37:ARG:CG	1:B:37:ARG:NH2	2.79	0.42
1:A:177:SER:HA	1:A:180:ASP:CG	2.40	0.42
1:A:252:VAL:HG11	1:B:87:PHE:CZ	2.55	0.41
1:A:87:PHE:CZ	1:B:256:LEU:HD11	2.54	0.41
1:A:76:GLN:HB2	1:B:38:LEU:HD22	2.01	0.41
1:B:263:GLY:O	1:B:267:ILE:HG13	2.20	0.41
1:A:52:ILE:HD11	1:B:63:TRP:HB2	2.01	0.41
1:A:160:HIS:HD2	1:A:205:THR:HB	1.84	0.41
1:B:236:GLN:O	1:B:240:LYS:HD3	2.20	0.41
1:B:207:GLU:HG2	1:B:208:LYS:N	2.34	0.41
1:B:126:MET:HA	1:B:126:MET:CE	2.50	0.41
1:B:143:GLN:HG2	1:B:223:TYR:CE1	2.42	0.41
1:A:217:ASP:HA	1:A:220:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLN:HE21	1:B:222:GLN:CA	2.18	0.41
1:B:94:VAL:O	1:B:98:HIS:HD2	2.03	0.41
1:A:298:ASN:HD22	1:A:298:ASN:HA	1.65	0.41
1:A:252:VAL:CG1	1:B:87:PHE:CZ	2.97	0.41
1:A:211:LYS:HB3	1:A:211:LYS:HE3	1.80	0.41
1:B:164:CYS:C	1:B:166:GLU:N	2.74	0.41
1:B:85:MET:C	1:B:87:PHE:N	2.74	0.41
1:B:42:LEU:HD13	1:B:113:ILE:CD1	2.51	0.41
1:A:211:LYS:O	1:A:215:GLU:HB2	2.21	0.41
1:A:149:LYS:HB3	1:A:216:LEU:HG	2.02	0.41
1:B:32:ILE:CG1	1:B:132:THR:HG22	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:A:31:ARG:NH2	1:A:235:GLN:NE2	2.69	0.40
1:B:126:MET:HB3	1:B:127:GLY:HA2	2.03	0.40
1:A:68:ARG:HH22	1:A:92:GLU:CD	2.24	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:184:ASN:OD1	1:A:187:GLN:HB2	2.21	0.40
1:A:80:VAL:HG21	1:B:242:LEU:HD22	2.04	0.40
1:B:106:MET:HB3	1:B:106:MET:HE3	1.94	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%)	17	47
All	All	566/972 (58%)	545 (96%)	18 (3%)	3 (0%)	34	68

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 ⓘ

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%)	212 (86%)	35 (14%)	4	11
1	B	245/424 (58%)	204 (83%)	41 (17%)	3	7
All	All	492/848 (58%)	416 (85%)	76 (15%)	3	9

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	21	GLU
1	A	22	VAL
1	A	31	ARG
1	A	37	ARG
1	A	60	LEU
1	A	61	THR
1	A	69	GLN
1	A	70	LEU
1	A	88	MET
1	A	119	GLU
1	A	123	LYS
1	A	132	THR
1	A	146	TRP
1	A	149	LYS
1	A	150	LEU
1	A	165	LYS
1	A	167	GLU
1	A	169	LEU
1	A	173	ARG

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Mol	Chain	Res	Type
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	213	LEU
1	A	217	ASP
1	A	222	GLN
1	A	236	GLN
1	A	271	LEU
1	A	282	GLU
1	A	288	ARG
1	B	17	ASP
1	B	27	ARG
1	B	28	THR
1	B	31	ARG
1	B	32	ILE
1	B	42	LEU
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	149	LYS
1	B	150	LEU
1	B	152	GLU
1	B	160	HIS
1	B	169	LEU
1	B	173	ARG
1	B	174	GLU
1	B	184	ASN
1	B	188	LEU
1	B	190	LYS
1	B	195	ILE
1	B	197	LYS
1	B	199	LYS
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	204	LYS
1	B	206	LYS
1	B	207	GLU
1	B	211	LYS
1	B	216	LEU
1	B	217	ASP
1	B	220	THR
1	B	222	GLN
1	B	235	GLN
1	B	240	LYS
1	B	253	GLN
1	B	269	HIS
1	B	271	LEU
1	B	276	ARG

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

Mol	Chain	Res	Type
1	A	47	HIS
1	A	58	GLN
1	A	69	GLN
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	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	269	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.99	47 (16%)	2 1	27, 69, 159, 174	0
1	B	284/486 (58%)	0.82	34 (11%)	6 3	23, 63, 161, 177	0
All	All	570/972 (58%)	0.90	81 (14%)	4 2	23, 66, 160, 177	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	7.2
1	B	188	LEU	7.1
1	B	178	LYS	6.9
1	A	171	ILE	6.5
1	A	182	SER	6.5
1	B	171	ILE	6.4
1	A	203	LEU	6.1
1	B	179	ALA	6.1
1	A	198	CYS	6.0
1	B	187	GLN	5.9
1	A	170	ALA	5.9
1	B	191	LEU	5.8
1	A	179	ALA	5.8
1	B	195	ILE	5.6
1	B	172	SER	5.5
1	A	165	LYS	5.4
1	A	202	VAL	5.3
1	B	190	LYS	5.2
1	A	175	ALA	5.1
1	B	168	LYS	5.0
1	B	181	PRO	4.7
1	B	194	LYS	4.6
1	B	180	ASP	4.6
1	A	181	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	187	GLN	4.6
1	A	178	LYS	4.5
1	A	161	HIS	4.3
1	A	169	LEU	4.3
1	A	191	LEU	3.9
1	A	159	ALA	3.9
1	A	166	GLU	3.9
1	B	156	ALA	3.8
1	B	204	LYS	3.8
1	A	205	THR	3.7
1	A	188	LEU	3.7
1	A	177	SER	3.7
1	A	172	SER	3.6
1	B	176	ASN	3.5
1	A	157	LYS	3.5
1	B	177	SER	3.5
1	A	176	ASN	3.4
1	A	194	LYS	3.4
1	A	173	ARG	3.4
1	A	199	LYS	3.3
1	B	155	ALA	3.1
1	A	162	ALA	3.1
1	A	288	ARG	3.1
1	B	174	GLU	3.1
1	B	87	PHE	3.0
1	A	208	LYS	3.0
1	A	168	LYS	3.0
1	B	158	LYS	2.9
1	A	155	ALA	2.8
1	B	203	LEU	2.8
1	A	174	GLU	2.8
1	B	160	HIS	2.8
1	B	186	GLU	2.7
1	B	173	ARG	2.7
1	A	184	ASN	2.5
1	A	293	PRO	2.5
1	A	180	ASP	2.5
1	A	183	LEU	2.5
1	A	158	LYS	2.4
1	B	218	GLN	2.4
1	A	87	PHE	2.3
1	A	156	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	210	GLU	2.3
1	A	125	MET	2.3
1	A	204	LYS	2.3
1	B	175	ALA	2.2
1	B	202	VAL	2.2
1	B	198	CYS	2.2
1	A	212	SER	2.1
1	B	189	LYS	2.1
1	A	190	LYS	2.1
1	B	170	ALA	2.1
1	B	212	SER	2.1
1	A	164	CYS	2.1
1	A	28	THR	2.1
1	A	200	GLN	2.1
1	B	207	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	CA	A	488	1/1	0.98	0.17	-1.10	69,69,69,69	0
2	CA	B	488	1/1	0.94	0.10	-3.88	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.