WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 09:42 PM EDT

PDB ID	:	3QE6
Title	:	Mouse PACSIN 3 F-BAR domain structure
Authors	:	Meng, G.; Bai, X.; Zheng, X.
Deposited on	:	2011-01-19
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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.

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
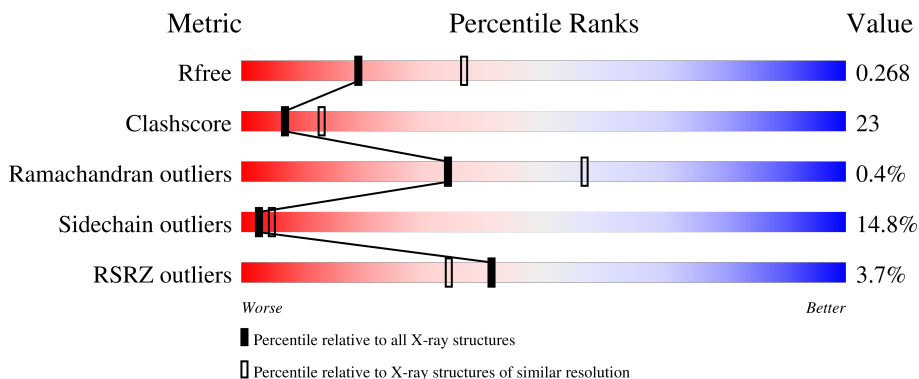
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	304	2% / 55% / 29% / 9% / 7%
1	B	304	5% / 59% / 29% / 5% · / 6%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4635 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 II substrate protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total 2312	C 1439	N 438	O 426	S 9	0	0	0
1	B	286	Total 2287	C 1429	N 428	O 422	S 8	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total 16	O 16	0	0
3	B	18	Total 18	O 18	0	0

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 II substrate protein 3

Chain A:

• Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain B:
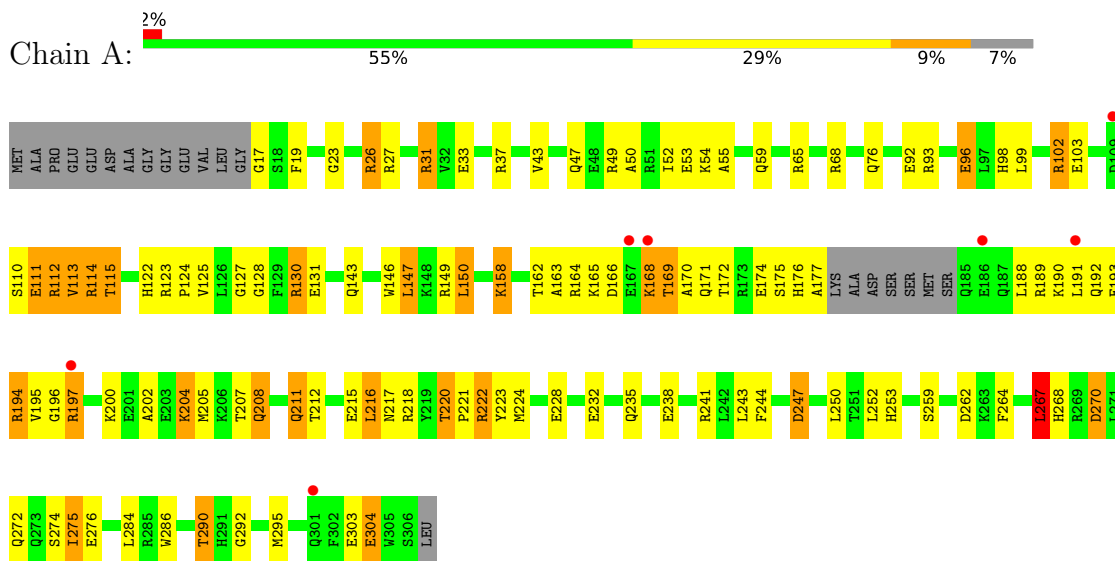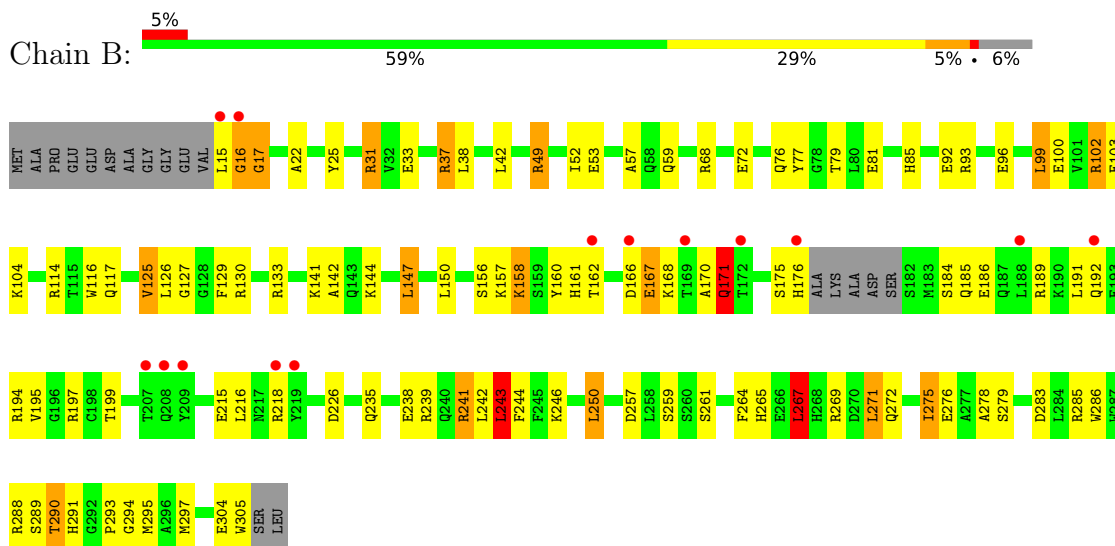
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.85Å 54.65Å 193.66Å 90.00° 96.92° 90.00°	Depositor
Resolution (Å)	28.01 – 2.60 28.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.01-2.60) 97.8 (28.01-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.79 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.227 , 0.274 0.228 , 0.268	Depositor DCC
R_{free} test set	1492 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	63.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.0	EDS
L-test for twinning[2]	$<|L|> = 0.51$, $<L^2> = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4635	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: MG

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	1.06	4/2366 (0.2%)	1.03	10/3181 (0.3%)
1	B	1.02	2/2342 (0.1%)	1.10	18/3158 (0.6%)
All	All	1.04	6/4708 (0.1%)	1.07	28/6339 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	GLU	CD-OE2	6.24	1.32	1.25
1	A	232	GLU	CG-CD	6.20	1.61	1.51
1	B	96	GLU	CG-CD	5.85	1.60	1.51
1	A	232	GLU	CB-CG	5.82	1.63	1.52
1	A	33	GLU	CG-CD	5.79	1.60	1.51
1	A	96	GLU	CG-CD	5.55	1.60	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	CB-CG-OD1	-11.95	107.54	118.30
1	B	68	ARG	NE-CZ-NH1	-10.75	114.92	120.30
1	B	171	GLN	CB-CA-C	-10.31	89.78	110.40
1	B	127	GLY	N-CA-C	-9.35	89.73	113.10
1	A	247	ASP	CB-CG-OD1	-8.67	110.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	GLY	N-CA-C	-8.46	91.96	113.10
1	B	49	ARG	NE-CZ-NH1	-8.29	116.16	120.30
1	B	17	GLY	N-CA-C	-7.50	94.35	113.10
1	A	194	ARG	N-CA-C	-6.95	92.25	111.00
1	B	192	GLN	N-CA-C	-6.48	93.50	111.00
1	B	37	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	267	LEU	CA-CB-CG	6.35	129.90	115.30
1	B	189	ARG	N-CA-C	-6.23	94.17	111.00
1	A	222	ARG	N-CA-C	-6.10	94.53	111.00
1	B	52	ILE	CG1-CB-CG2	-6.00	98.19	111.40
1	A	47	GLN	CB-CA-C	-5.86	98.68	110.40
1	B	267	LEU	CB-CG-CD2	5.78	120.83	111.00
1	B	216	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	125	VAL	N-CA-C	5.73	126.47	111.00
1	A	267	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	47	GLN	CA-CB-CG	5.45	125.40	113.40
1	B	171	GLN	N-CA-C	5.39	125.55	111.00
1	B	241	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	270	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	243	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	B	166	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	188	LEU	CB-CA-C	5.08	119.86	110.20
1	A	128	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	GLU	Peptide

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	2312	0	2184	115	0
1	B	2287	0	2102	96	2
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	16	0	0	2	0
3	B	18	0	0	1	0
All	All	4635	0	4286	201	2

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 23.

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:B:191:LEU:O	1:B:194:ARG:N	1.57	1.35
1:B:79:THR:CG2	1:B:278:ALA:HA	1.59	1.29
1:A:190:LYS:HA	1:A:191:LEU:CB	1.59	1.28
1:B:191:LEU:O	1:B:194:ARG:CA	1.94	1.15
1:A:164:ARG:NH2	1:A:202:ALA:HB1	1.66	1.11
1:B:257:ASP:OD1	1:B:259:SER:HB2	1.53	1.06
1:A:211:GLN:HE21	1:A:211:GLN:HA	1.19	1.05
1:B:191:LEU:O	1:B:194:ARG:CB	2.07	1.03
1:B:79:THR:HG21	1:B:279:SER:H	1.23	1.02
1:B:79:THR:HG21	1:B:279:SER:N	1.79	0.97
1:A:164:ARG:HH21	1:A:202:ALA:CB	1.76	0.97
1:A:220:THR:O	1:A:224:MET:HG3	1.64	0.97
1:B:79:THR:HG22	1:B:278:ALA:HA	1.44	0.97
1:B:184:SER:CB	1:B:186:GLU:CB	2.44	0.96
1:A:164:ARG:NH2	1:A:202:ALA:CB	2.29	0.94
1:A:190:LYS:CA	1:A:191:LEU:CB	2.45	0.94
1:A:93:ARG:NH2	3:A:319:HOH:O	1.99	0.93
1:B:238:GLU:CD	1:B:241:ARG:HH22	1.70	0.93
1:A:164:ARG:HH21	1:A:202:ALA:HB1	1.18	0.93
1:B:171:GLN:O	1:B:176:HIS:CB	2.18	0.92
1:A:204:LYS:NZ	1:A:208:GLN:HE22	1.68	0.91
1:B:171:GLN:HB3	1:B:175:SER:O	1.75	0.87
1:B:170:ALA:HB3	1:B:171:GLN:OE1	1.75	0.87
1:A:304:GLU:OE1	1:A:304:GLU:HA	1.75	0.86
1:A:207:THR:O	1:A:211:GLN:HG2	1.77	0.85
1:B:79:THR:CG2	1:B:278:ALA:CA	2.51	0.85
1:B:243:LEU:H	1:B:243:LEU:HD22	1.41	0.84
1:A:169:THR:C	1:A:171:GLN:H	1.79	0.84
1:A:146:TRP:HZ3	1:A:220:THR:HG22	1.45	0.80
1:B:158:LYS:O	1:B:162:THR:HG23	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HE21	1:A:211:GLN:CA	1.94	0.80
1:B:31:ARG:HH22	1:B:235:GLN:HE22	1.29	0.80
1:B:238:GLU:OE2	1:B:241:ARG:NH2	2.15	0.79
1:A:31:ARG:HG2	1:A:31:ARG:HH11	1.48	0.79
1:B:79:THR:HG23	1:B:278:ALA:HA	1.59	0.79
1:B:31:ARG:HH22	1:B:235:GLN:NE2	1.81	0.78
1:A:54:LYS:HD3	1:A:99:LEU:CD2	2.13	0.77
1:A:54:LYS:HD3	1:A:99:LEU:HD21	1.67	0.76
1:A:31:ARG:HH11	1:A:31:ARG:CG	2.00	0.74
1:A:54:LYS:CD	1:A:99:LEU:HD21	2.17	0.74
1:A:204:LYS:HZ2	1:A:208:GLN:HE22	1.33	0.74
1:A:169:THR:C	1:A:171:GLN:N	2.42	0.73
1:B:114:ARG:HH11	1:B:117:GLN:HE22	1.35	0.73
1:B:238:GLU:CD	1:B:241:ARG:NH2	2.41	0.73
1:B:79:THR:CG2	1:B:279:SER:H	2.01	0.71
1:B:79:THR:HG21	1:B:278:ALA:HA	1.66	0.71
1:B:15:LEU:O	1:B:16:GLY:C	2.27	0.69
1:A:222:ARG:O	1:A:223:TYR:HB3	1.92	0.69
1:B:125:VAL:HG13	1:B:126:LEU:N	2.08	0.69
1:A:31:ARG:NH2	1:A:235:GLN:NE2	2.41	0.69
1:A:247:ASP:OD1	1:A:247:ASP:N	2.24	0.68
1:B:191:LEU:O	1:B:195:VAL:N	2.27	0.67
1:B:22:ALA:HB2	1:B:147:LEU:HD11	1.77	0.66
1:A:211:GLN:HA	1:A:211:GLN:NE2	2.04	0.66
1:B:15:LEU:O	1:B:17:GLY:N	2.29	0.66
1:A:222:ARG:HG3	1:A:223:TYR:H	1.59	0.66
1:B:171:GLN:OE1	1:B:171:GLN:N	2.29	0.65
1:A:158:LYS:O	1:A:162:THR:HG23	1.97	0.64
1:B:79:THR:HG22	1:B:278:ALA:CA	2.22	0.64
1:B:126:LEU:HD12	1:B:133:ARG:CZ	2.27	0.64
1:B:243:LEU:H	1:B:243:LEU:CD2	2.12	0.63
1:A:195:VAL:O	1:A:195:VAL:HG23	1.99	0.62
1:A:204:LYS:HZ3	1:A:208:GLN:HE22	1.46	0.62
1:B:243:LEU:CD2	1:B:243:LEU:N	2.62	0.62
1:A:31:ARG:NH2	1:A:235:GLN:HE22	1.97	0.62
1:A:99:LEU:O	1:A:103:GLU:HG2	1.99	0.62
1:B:142:ALA:HB1	1:B:226:ASP:HB3	1.81	0.62
1:A:208:GLN:O	1:A:212:THR:HG23	1.99	0.61
1:A:189:ARG:O	1:A:191:LEU:CB	2.48	0.61
1:A:27:ARG:NH1	1:B:291:HIS:ND1	2.49	0.61
1:B:291:HIS:HA	1:B:295:MET:HE1	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:C	1:A:150:LEU:HD23	2.22	0.60
1:A:286:TRP:CE2	1:A:290:THR:HG21	2.37	0.59
1:B:271:LEU:HD22	1:B:275:ILE:HD11	1.85	0.58
1:A:23:GLY:O	1:A:26:ARG:HD2	2.03	0.58
1:B:191:LEU:C	1:B:194:ARG:N	2.51	0.58
1:A:31:ARG:HH21	1:A:235:GLN:HE22	1.51	0.58
1:B:239:ARG:O	1:B:243:LEU:HD22	2.03	0.58
1:B:235:GLN:HE21	1:B:235:GLN:HA	1.69	0.57
1:A:286:TRP:O	1:A:290:THR:HG23	2.04	0.57
1:A:31:ARG:HG2	1:A:31:ARG:NH1	2.11	0.57
1:A:264:PHE:O	1:A:268:HIS:HD2	1.88	0.57
1:B:102:ARG:NH1	1:B:103:GLU:OE2	2.35	0.57
1:B:271:LEU:O	1:B:275:ILE:HG12	2.04	0.56
1:B:33:GLU:HG2	1:B:129:PHE:HE1	1.71	0.56
1:A:253:HIS:ND1	1:B:271:LEU:HD13	2.21	0.56
1:B:116:TRP:CH2	1:B:241:ARG:HG3	2.39	0.56
1:A:65:ARG:HD3	3:A:309:HOH:O	2.06	0.56
1:A:123:ARG:HH11	1:A:123:ARG:HG2	1.71	0.56
1:B:170:ALA:CB	1:B:171:GLN:OE1	2.52	0.55
1:A:220:THR:O	1:A:222:ARG:O	2.25	0.55
1:B:49:ARG:NH1	1:B:53:GLU:OE2	2.39	0.55
1:A:19:PHE:HB2	1:B:295:MET:HE2	1.89	0.55
1:B:243:LEU:HD22	1:B:243:LEU:N	2.10	0.55
1:A:222:ARG:HG3	1:A:223:TYR:N	2.21	0.54
1:A:146:TRP:HZ3	1:A:220:THR:CG2	2.18	0.54
1:A:204:LYS:NZ	1:A:208:GLN:NE2	2.49	0.54
1:B:171:GLN:N	1:B:171:GLN:CD	2.60	0.54
1:B:184:SER:C	1:B:186:GLU:CB	2.77	0.53
1:A:163:ALA:C	1:A:165:LYS:H	2.11	0.53
1:A:146:TRP:HD1	1:A:147:LEU:HD13	1.74	0.53
1:B:171:GLN:O	1:B:175:SER:O	2.27	0.53
1:B:185:GLN:N	1:B:186:GLU:CB	2.72	0.53
1:A:284:LEU:HD11	1:B:239:ARG:HB2	1.92	0.52
1:B:286:TRP:CE2	1:B:290:THR:HG21	2.44	0.52
1:A:31:ARG:HH11	1:A:31:ARG:HB3	1.75	0.52
1:A:31:ARG:HH22	1:A:235:GLN:NE2	2.06	0.52
1:A:112:ARG:O	1:A:112:ARG:HG3	2.10	0.52
1:A:143:GLN:HG2	1:A:147:LEU:HD22	1.92	0.52
1:A:238:GLU:OE2	1:A:241:ARG:NH2	2.43	0.52
1:A:31:ARG:HH11	1:A:31:ARG:CB	2.23	0.51
1:A:93:ARG:HD3	1:A:96:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LEU:O	1:B:194:ARG:C	2.47	0.51
1:B:171:GLN:CD	1:B:171:GLN:H	2.14	0.51
1:A:192:GLN:O	1:A:193:GLU:CB	2.58	0.51
1:B:125:VAL:CG1	1:B:126:LEU:N	2.72	0.51
1:B:243:LEU:HD23	1:B:244:PHE:N	2.26	0.51
1:B:175:SER:O	1:B:176:HIS:CB	2.59	0.51
1:A:111:GLU:O	1:A:115:THR:HG23	2.11	0.50
1:B:31:ARG:NH2	1:B:235:GLN:HE22	2.04	0.50
1:A:286:TRP:O	1:A:290:THR:CG2	2.59	0.50
1:A:228:GLU:OE1	1:B:288:ARG:NH2	2.36	0.50
1:A:264:PHE:O	1:A:268:HIS:CD2	2.66	0.49
1:A:68:ARG:NH1	1:A:92:GLU:OE1	2.45	0.49
1:B:79:THR:HG21	1:B:278:ALA:CA	2.36	0.49
1:A:292:GLY:O	1:A:295:MET:HG3	2.13	0.49
1:B:72:GLU:HG2	1:B:85:HIS:CE1	2.48	0.49
1:A:304:GLU:OE1	1:A:304:GLU:CA	2.49	0.49
1:B:167:GLU:O	1:B:171:GLN:NE2	2.27	0.48
1:A:217:ASN:HA	1:A:220:THR:HG23	1.96	0.48
1:A:163:ALA:O	1:A:165:LYS:N	2.47	0.47
1:A:54:LYS:HB2	1:A:102:ARG:HG3	1.96	0.47
1:A:168:LYS:HB2	1:A:168:LYS:NZ	2.29	0.47
1:B:76:GLN:HG3	1:B:81:GLU:HB2	1.97	0.47
1:B:235:GLN:NE2	1:B:235:GLN:HA	2.28	0.47
1:B:130:ARG:HH11	1:B:130:ARG:HG2	1.79	0.47
1:B:197:ARG:C	1:B:199:THR:H	2.17	0.47
1:A:164:ARG:NH2	1:A:202:ALA:HB3	2.22	0.47
1:B:93:ARG:HB2	1:B:267:LEU:HG	1.96	0.47
1:B:126:LEU:HD13	3:B:312:HOH:O	2.15	0.47
1:A:194:ARG:C	1:A:196:GLY:N	2.67	0.47
1:A:176:HIS:O	1:A:177:ALA:HB3	2.15	0.47
1:A:17:GLY:O	1:A:27:ARG:NH2	2.49	0.46
1:B:76:GLN:HE21	1:B:77:TYR:H	1.63	0.46
1:B:93:ARG:HA	1:B:93:ARG:HE	1.79	0.46
1:A:270:ASP:O	1:A:274:SER:HB3	2.16	0.46
1:A:31:ARG:HH22	1:A:235:GLN:HE21	1.64	0.45
1:B:286:TRP:O	1:B:290:THR:HG23	2.17	0.45
1:A:93:ARG:O	1:A:96:GLU:HG2	2.16	0.45
1:A:220:THR:N	1:A:221:PRO:CD	2.79	0.45
1:B:79:THR:HB	1:B:283:ASP:OD1	2.16	0.45
1:B:114:ARG:NH1	1:B:117:GLN:HE22	2.10	0.45
1:B:243:LEU:HD23	1:B:243:LEU:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:HB2	1:A:130:ARG:HD3	1.98	0.44
1:A:43:VAL:HG23	1:A:113:VAL:CG2	2.48	0.44
1:A:50:ALA:HB1	1:A:102:ARG:HG2	1.99	0.44
1:A:190:LYS:C	1:A:192:GLN:H	2.21	0.44
1:B:126:LEU:HD12	1:B:133:ARG:NH2	2.33	0.44
1:A:222:ARG:O	1:A:224:MET:N	2.49	0.44
1:B:100:GLU:OE1	1:B:104:LYS:NZ	2.50	0.44
1:A:53:GLU:OE1	1:A:98:HIS:ND1	2.45	0.44
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.81	0.44
1:B:171:GLN:CB	1:B:175:SER:O	2.55	0.44
1:A:220:THR:C	1:A:222:ARG:O	2.56	0.44
1:A:272:GLN:O	1:A:276:GLU:HG3	2.18	0.44
1:B:286:TRP:O	1:B:290:THR:CG2	2.65	0.44
1:A:259:SER:HB3	1:B:264:PHE:CE2	2.53	0.43
1:A:162:THR:O	1:A:165:LYS:HG3	2.18	0.43
1:A:76:GLN:OE1	1:B:38:LEU:HD13	2.18	0.43
1:B:272:GLN:HG2	1:B:276:GLU:OE1	2.18	0.43
1:A:238:GLU:CD	1:A:241:ARG:NH2	2.72	0.43
1:A:216:LEU:O	1:A:220:THR:CG2	2.66	0.43
1:A:150:LEU:HD23	1:A:150:LEU:O	2.18	0.43
1:A:211:GLN:CA	1:A:211:GLN:NE2	2.68	0.43
1:A:55:ALA:O	1:A:59:GLN:HG3	2.17	0.43
1:A:166:ASP:O	1:A:169:THR:OG1	2.31	0.42
1:A:238:GLU:OE1	1:A:241:ARG:NH2	2.50	0.42
1:A:216:LEU:O	1:A:220:THR:HG22	2.20	0.42
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.84	0.42
1:A:259:SER:HB2	1:B:265:HIS:ND1	2.34	0.42
1:B:126:LEU:HD12	1:B:133:ARG:NH1	2.34	0.42
1:B:76:GLN:NE2	1:B:77:TYR:H	2.17	0.42
1:A:49:ARG:HA	1:A:49:ARG:HD2	1.87	0.42
1:A:110:SER:O	1:A:114:ARG:HB2	2.20	0.42
1:A:275:ILE:O	1:B:246:LYS:HE3	2.20	0.42
1:A:43:VAL:CG2	1:A:113:VAL:HG22	2.50	0.41
1:A:267:LEU:HD22	1:A:268:HIS:N	2.35	0.41
1:A:200:LYS:O	1:A:204:LYS:HB3	2.20	0.41
1:A:244:PHE:O	1:A:247:ASP:OD1	2.38	0.41
1:B:156:SER:O	1:B:160:TYR:N	2.52	0.41
1:A:124:PRO:HD2	1:A:127:GLY:O	2.20	0.41
1:A:174:GLU:O	1:A:175:SER:C	2.59	0.41
1:B:291:HIS:C	1:B:295:MET:HE2	2.41	0.41
1:A:158:LYS:HB3	1:A:158:LYS:HE3	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:O	1:A:197:ARG:N	2.54	0.41
1:B:57:ALA:HB1	1:B:99:LEU:HD22	2.03	0.41
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.77	0.41
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.84	0.40
1:A:52:ILE:HG12	1:B:59:GLN:HB3	2.03	0.40
1:A:194:ARG:O	1:A:195:VAL:C	2.58	0.40
1:B:25:TYR:CD1	1:B:25:TYR:C	2.94	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:VAL:O	1:B:293:PRO:O[2_656]	1.34	0.86
1:B:126:LEU:O	1:B:294:GLY:O[2_656]	2.03	0.17

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	279/304 (92%)	262 (94%)	15 (5%)	2 (1%)	22	43
1	B	282/304 (93%)	267 (95%)	15 (5%)	0	100	100
All	All	561/608 (92%)	529 (94%)	30 (5%)	2 (0%)	34	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ALA
1	A	169	THR

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	229/256 (90%)	193 (84%)	36 (16%)	2	4
1	B	217/256 (85%)	187 (86%)	30 (14%)	3	6
All	All	446/512 (87%)	380 (85%)	66 (15%)	3	5

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	31	ARG
1	A	37	ARG
1	A	102	ARG
1	A	111	GLU
1	A	112	ARG
1	A	113	VAL
1	A	114	ARG
1	A	115	THR
1	A	125	VAL
1	A	130	ARG
1	A	131	GLU
1	A	147	LEU
1	A	149	ARG
1	A	150	LEU
1	A	158	LYS
1	A	168	LYS
1	A	172	THR
1	A	197	ARG
1	A	204	LYS
1	A	205	MET
1	A	208	GLN
1	A	211	GLN
1	A	215	GLU
1	A	216	LEU
1	A	218	ARG
1	A	220	THR

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	250	LEU
1	A	252	LEU
1	A	262	ASP
1	A	267	LEU
1	A	275	ILE
1	A	290	THR
1	A	303	GLU
1	A	304	GLU
1	B	31	ARG
1	B	37	ARG
1	B	42	LEU
1	B	99	LEU
1	B	102	ARG
1	B	141	LYS
1	B	144	LYS
1	B	147	LEU
1	B	150	LEU
1	B	157	LYS
1	B	158	LYS
1	B	161	HIS
1	B	167	GLU
1	B	168	LYS
1	B	171	GLN
1	B	215	GLU
1	B	218	ARG
1	B	242	LEU
1	B	243	LEU
1	B	250	LEU
1	B	261	SER
1	B	267	LEU
1	B	269	ARG
1	B	271	LEU
1	B	275	ILE
1	B	285	ARG
1	B	289	SER
1	B	290	THR
1	B	297	MET
1	B	305	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	85	HIS
1	A	117	GLN
1	A	208	GLN
1	A	211	GLN
1	A	235	GLN
1	A	254	GLN
1	A	265	HIS
1	A	268	HIS
1	A	301	GLN
1	B	85	HIS
1	B	117	GLN
1	B	208	GLN
1	B	235	GLN
1	B	253	HIS
1	B	268	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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	283/304 (93%)	0.08	7 (2%)	57	51	40, 68, 196, 291	0
1	B	286/304 (94%)	0.13	14 (4%)	29	23	34, 64, 268, 370	0
All	All	569/608 (93%)	0.11	21 (3%)	41	34	34, 67, 238, 370	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	LEU	9.3
1	B	16	GLY	5.5
1	B	166	ASP	5.2
1	A	197	ARG	4.3
1	A	186	GLU	3.4
1	B	169	THR	3.4
1	B	188	LEU	3.1
1	B	192	GLN	3.0
1	A	168	LYS	2.9
1	B	172	THR	2.7
1	B	176	HIS	2.6
1	B	218	ARG	2.5
1	A	167	GLU	2.5
1	A	301	GLN	2.5
1	B	207	THR	2.4
1	A	109	ASP	2.3
1	B	162	THR	2.3
1	B	219	TYR	2.3
1	B	209	TYR	2.3
1	B	208	GLN	2.2
1	A	191	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	MG	B	1	1/1	0.94	0.07	26,26,26,26	0
2	MG	A	2	1/1	0.98	0.05	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.