



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 09:49 PM UTC

PDB ID : 3QE6 / pdb_00003qe6
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)

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

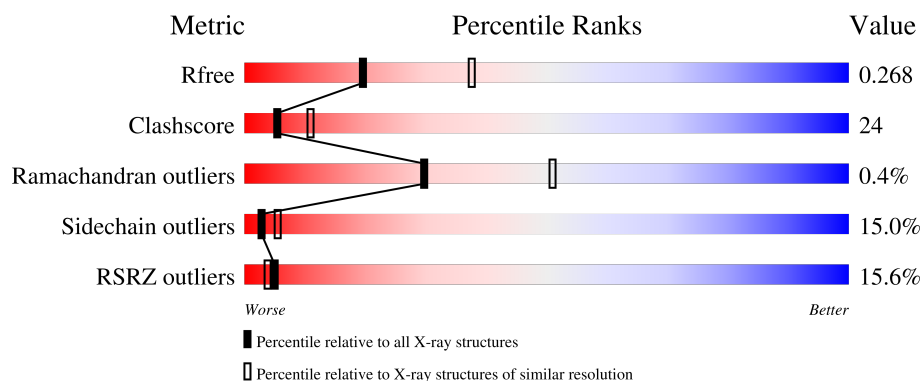
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	304	13% 51% 33% 9% • 7%
1	B	304	16% 59% 27% 7% • 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	C	N	O	S	0	0	0
			2312	1439	438	426	9			
1	B	286	Total	C	N	O	S	0	0	0
			2287	1429	428	422	8			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

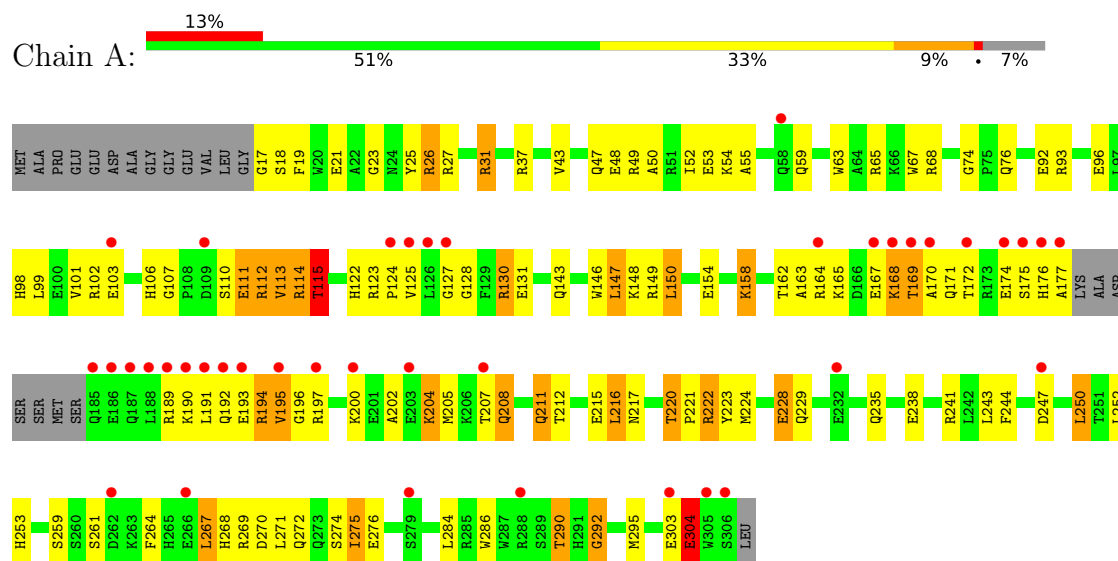
- Molecule 3 is water.

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

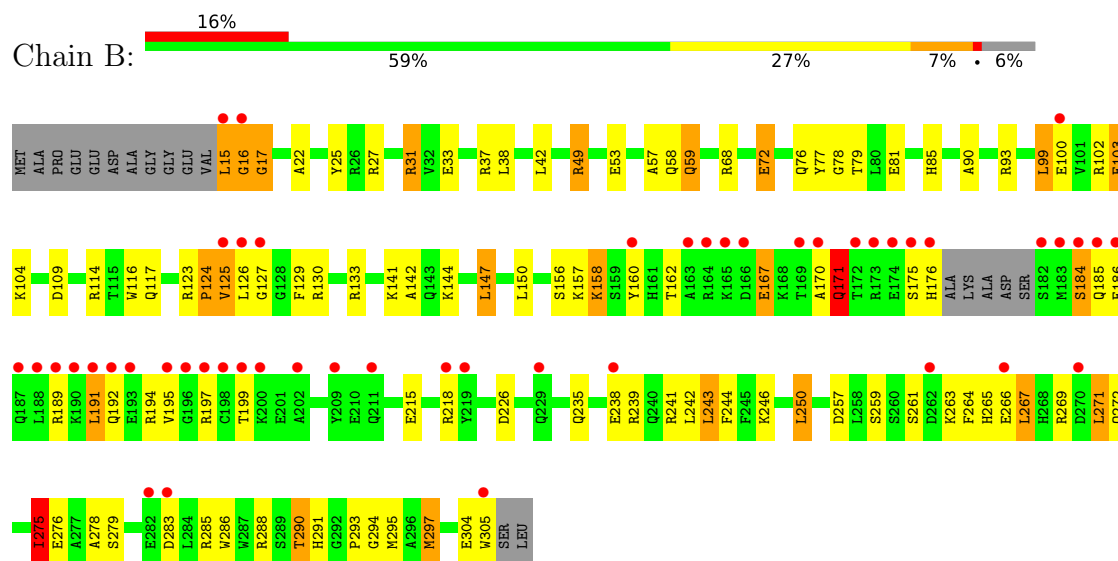
3 Residue-property plots [i](#)

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



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



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
$\langle I/\sigma(I) \rangle$ 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 (4.92%)	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)	0.28 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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

5.1 Standard geometry

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	1.25	5/2366 (0.2%)	1.39	21/3181 (0.7%)
1	B	1.19	3/2342 (0.1%)	1.42	25/3158 (0.8%)
All	All	1.22	8/4708 (0.2%)	1.41	46/6339 (0.7%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	VAL	CA-CB	7.87	1.63	1.54
1	B	59	GLN	N-CA	-6.98	1.38	1.46
1	A	304	GLU	N-CA	5.58	1.52	1.45
1	A	63	TRP	N-CA	-5.49	1.39	1.46
1	A	261	SER	CA-C	-5.44	1.45	1.52
1	B	59	GLN	C-O	-5.23	1.18	1.24
1	A	115	THR	CA-CB	5.22	1.61	1.53
1	B	90	ALA	CA-CB	5.20	1.61	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	VAL	N-CA-C	18.80	126.47	111.62
1	A	194	ARG	N-CA-C	-15.36	92.25	112.68
1	B	171	GLN	CB-CA-C	-13.98	89.78	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	GLN	N-CA-C	11.87	125.55	112.97
1	A	222	ARG	N-CA-C	-11.46	94.53	110.35
1	B	189	ARG	N-CA-C	-10.52	94.17	109.11
1	B	127	GLY	N-CA-C	-9.89	89.73	113.18
1	B	192	GLN	N-CA-C	-9.35	93.50	108.73
1	B	16	GLY	N-CA-C	-8.95	91.96	113.18
1	A	107	GLY	CA-C-N	8.68	128.27	119.24
1	A	107	GLY	C-N-CA	8.68	128.27	119.24
1	B	17	GLY	N-CA-C	-8.63	94.35	110.83
1	B	109	ASP	N-CA-C	8.19	120.21	111.28
1	A	304	GLU	N-CA-C	8.17	122.50	110.17
1	B	275	ILE	CB-CA-C	-7.57	102.28	111.97
1	A	271	LEU	N-CA-C	-7.53	103.01	111.07
1	A	292	GLY	CA-C-N	7.46	128.12	119.47
1	A	292	GLY	C-N-CA	7.46	128.12	119.47
1	A	47	GLN	CB-CA-C	-7.30	98.68	110.79
1	B	191	LEU	N-CA-C	-7.05	103.53	111.07
1	A	74	GLY	CA-C-N	6.82	127.41	120.04
1	A	74	GLY	C-N-CA	6.82	127.41	120.04
1	B	68	ARG	NE-CZ-NH1	-6.58	114.92	121.50
1	B	78	GLY	CA-C-N	6.38	129.13	120.38
1	B	78	GLY	C-N-CA	6.38	129.13	120.38
1	B	124	PRO	CA-C-N	-6.35	116.43	123.16
1	B	124	PRO	C-N-CA	-6.35	116.43	123.16
1	B	72	GLU	N-CA-C	6.24	117.88	111.14
1	A	148	LYS	N-CA-C	-6.20	104.43	111.07
1	A	106	HIS	N-CA-C	-6.18	105.90	113.50
1	B	171	GLN	CA-C-N	5.92	128.47	120.65
1	B	171	GLN	C-N-CA	5.92	128.47	120.65
1	A	250	LEU	N-CA-C	-5.77	105.13	111.82
1	B	266	GLU	N-CA-CB	5.76	118.69	110.16
1	A	128	GLY	N-CA-C	-5.65	100.58	112.45
1	A	47	GLN	CA-CB-CG	5.65	125.40	114.10
1	A	269	ARG	CA-C-N	-5.54	113.40	122.54
1	A	269	ARG	C-N-CA	-5.54	113.40	122.54
1	B	49	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	A	229	GLN	N-CA-CB	5.33	118.04	110.16
1	B	68	ARG	CA-C-N	5.32	126.01	119.99
1	B	68	ARG	C-N-CA	5.32	126.01	119.99
1	B	58	GLN	CA-CB-CG	-5.12	103.87	114.10
1	B	184	SER	N-CA-C	5.07	117.72	109.86
1	A	25	TYR	N-CA-C	-5.01	107.00	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	N-CA-CB	-5.00	101.93	110.33

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 [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	2312	0	2184	123	0
1	B	2287	0	2102	103	2
2	A	1	0	0	0	0
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	212	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 24.

All (212) 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:HA	1:A:211:GLN:HE21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:GLU:CD	1:B:241:ARG:HH22	1.70	0.98
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:93:ARG:NH2	3:A:319:HOH:O	1.99	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:A:169:THR:C	1:A:171:GLN:H	1.79	0.88
1:A:190:LYS:CA	1:A:191:LEU:CB	2.45	0.87
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:HA	1:A:304:GLU:OE1	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:HD22	1:B:243:LEU:H	1.41	0.84
1:B:291:HIS:HA	1:B:295:MET:HE2	1.62	0.82
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
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:B:238:GLU:CD	1:B:241:ARG:NH2	2.41	0.77
1:A:54:LYS:HD3	1:A:99:LEU:HD21	1.67	0.76
1:A:19:PHE:HB2	1:B:295:MET:HE3	1.67	0.75
1:A:31:ARG:HH11	1:A:31:ARG:CG	2.00	0.74
1:A:169:THR:C	1:A:171:GLN:N	2.42	0.74
1:A:54:LYS:CD	1:A:99:LEU:HD21	2.17	0.74
1:B:15:LEU:O	1:B:16:GLY:C	2.27	0.74
1:A:204:LYS:HZ2	1:A:208:GLN:HE22	1.33	0.74
1:B:114:ARG:HH11	1:B:117:GLN:HE22	1.35	0.73
1:A:27:ARG:NH2	1:B:295:MET:HE1	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HH22	1:B:295:MET:HE1	1.55	0.71
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: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:A:247:ASP:N	1:A:247:ASP:OD1	2.24	0.66
1:B:291:HIS:C	1:B:295:MET:HE2	2.22	0.65
1:B:171:GLN:OE1	1:B:171:GLN:N	2.29	0.65
1:A:150:LEU:C	1:A:150:LEU:HD23	2.22	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:B:191:LEU:C	1:B:194:ARG:N	2.51	0.63
1:B:291:HIS:CA	1:B:295:MET:HE2	2.27	0.62
1:A:195:VAL:HG23	1:A:195:VAL:O	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:171:GLN:N	1:B:171:GLN:CD	2.60	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:A:31:ARG:HH21	1:A:235:GLN:HE22	1.51	0.58
1:A:163:ALA:C	1:A:165:LYS:H	2.11	0.58
1:B:184:SER:C	1:B:186:GLU:CB	2.77	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:19:PHE:CB	1:B:295:MET:HE3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:LEU:O	1:B:194:ARG:C	2.47	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:B:171:GLN:CD	1:B:171:GLN:H	2.14	0.56
1:A:123:ARG:HG2	1:A:123:ARG:HH11	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:B:243:LEU:HD22	1:B:243:LEU:N	2.10	0.55
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:A:222:ARG:HG3	1:A:223:TYR:N	2.21	0.54
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:B:197:ARG:C	1:B:199:THR:H	2.17	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
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:A:21:GLU:CG	1:B:297:MET:HE1	2.40	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:243:LEU:HD23	1:B:243:LEU:C	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:190:LYS:C	1:A:192:GLN:H	2.21	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:A:194:ARG:C	1:A:196:GLY:N	2.67	0.48
1:A:220:THR:C	1:A:222:ARG:O	2.56	0.48
1:B:167:GLU:O	1:B:171:GLN:NE2	2.27	0.48
1:A:238:GLU:CD	1:A:241:ARG:NH2	2.72	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:HG2	1:B:130:ARG:HH11	1.79	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: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:A:174:GLU:O	1:A:175:SER:C	2.59	0.46
1:B:76:GLN:HE21	1:B:77:TYR:H	1.63	0.46
1:B:93:ARG:HE	1:B:93:ARG:HA	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:A:194:ARG:O	1:A:195:VAL:C	2.58	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:25:TYR:CD1	1:B:25:TYR:C	2.94	0.45
1:A:17:GLY:O	1:A:18:SER:C	2.60	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:163:ALA:C	1:A:165:LYS:N	2.77	0.43
1:B:272:GLN:HG2	1:B:276:GLU:OE1	2.18	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:55:ALA:O	1:A:59:GLN:HG3	2.17	0.43
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:222:ARG:C	1:A:224:MET:N	2.78	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:194:ARG:C	1:A:196:GLY:H	2.27	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:67:TRP:O	1:A:68:ARG:C	2.62	0.41
1:A:158:LYS:HB3	1:A:158:LYS:HE3	1.78	0.41
1:A:194:ARG:O	1:A:197:ARG:N	2.54	0.41
1:A:211:GLN:CA	1:A:211:GLN:NE2	2.68	0.41
1:B:57:ALA:HB1	1:B:99:LEU:HD22	2.03	0.41
1:B:79:THR:HG21	1:B:278:ALA:C	2.42	0.41
1:B:123:ARG:O	1:B:124:PRO:C	2.63	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

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 [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	279/304 (92%)	262 (94%)	15 (5%)	2 (1%)	18	38
1	B	282/304 (93%)	267 (95%)	15 (5%)	0	100	100
All	All	561/608 (92%)	529 (94%)	30 (5%)	2 (0%)	30	51

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%)	192 (84%)	37 (16%)	2	4
1	B	217/256 (85%)	187 (86%)	30 (14%)	3	7
All	All	446/512 (87%)	379 (85%)	67 (15%)	3	5

All (67) 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	48	GLU
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	154	GLU
1	A	158	LYS
1	A	167	GLU
1	A	168	LYS
1	A	172	THR
1	A	195	VAL
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	220	THR
1	A	228	GLU
1	A	243	LEU
1	A	250	LEU
1	A	252	LEU
1	A	267	LEU
1	A	275	ILE
1	A	290	THR
1	A	303	GLU
1	A	304	GLU
1	B	15	LEU
1	B	27	ARG
1	B	31	ARG
1	B	37	ARG
1	B	42	LEU
1	B	99	LEU

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Mol	Chain	Res	Type
1	B	103	GLU
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	167	GLU
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	263	LYS
1	B	267	LEU
1	B	269	ARG
1	B	271	LEU
1	B	275	ILE
1	B	285	ARG
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	117	GLN
1	A	208	GLN
1	A	211	GLN
1	A	229	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	208	GLN
1	B	235	GLN
1	B	253	HIS

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Mol	Chain	Res	Type
1	B	268	HIS
1	B	272	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	283/304 (93%)	0.81	40 (14%) 6 5	40, 68, 196, 291	0
1	B	286/304 (94%)	0.88	49 (17%) 4 3	34, 64, 268, 370	0
All	All	569/608 (93%)	0.85	89 (15%) 5 4	34, 67, 238, 370	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	SER	10.1
1	A	306	SER	8.6
1	B	186	GLU	7.9
1	B	166	ASP	7.4
1	A	177	ALA	7.3
1	A	188	LEU	7.1
1	B	188	LEU	6.8
1	A	191	LEU	6.7
1	B	183	MET	6.5
1	A	189	ARG	6.5
1	B	198	CYS	6.5
1	B	174	GLU	6.4
1	B	190	LYS	6.2
1	A	185	GLN	6.2
1	B	175	SER	5.9
1	B	187	GLN	5.7
1	B	170	ALA	5.2
1	A	190	LYS	5.2
1	A	193	GLU	5.2
1	B	185	GLN	5.0
1	B	165	LYS	4.8
1	A	186	GLU	4.7
1	B	305	TRP	4.6
1	B	184	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	127	GLY	4.5
1	B	15	LEU	4.3
1	A	195	VAL	4.2
1	A	305	TRP	4.0
1	B	196	GLY	3.9
1	A	170	ALA	3.9
1	A	175	SER	3.9
1	B	189	ARG	3.8
1	A	187	GLN	3.8
1	A	109	ASP	3.8
1	A	192	GLN	3.8
1	A	169	THR	3.7
1	B	169	THR	3.7
1	B	262	ASP	3.7
1	B	193	GLU	3.7
1	B	172	THR	3.6
1	A	197	ARG	3.5
1	A	126	LEU	3.5
1	B	218	ARG	3.4
1	A	200	LYS	3.3
1	A	172	THR	3.2
1	A	232	GLU	3.2
1	A	176	HIS	3.2
1	B	16	GLY	3.1
1	B	173	ARG	3.1
1	A	58	GLN	3.0
1	A	174	GLU	3.0
1	B	195	VAL	3.0
1	B	266	GLU	2.9
1	B	197	ARG	2.9
1	B	270	ASP	2.9
1	B	191	LEU	2.9
1	B	127	GLY	2.8
1	A	167	GLU	2.8
1	B	199	THR	2.8
1	A	164	ARG	2.8
1	B	163	ALA	2.8
1	B	125	VAL	2.7
1	B	176	HIS	2.7
1	A	247	ASP	2.7
1	B	192	GLN	2.7
1	B	200	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	288	ARG	2.7
1	B	126	LEU	2.6
1	A	262	ASP	2.6
1	B	202	ALA	2.6
1	A	207	THR	2.6
1	A	266	GLU	2.6
1	A	303	GLU	2.6
1	B	211	GLN	2.6
1	B	164	ARG	2.5
1	B	100	GLU	2.4
1	A	103	GLU	2.4
1	B	229	GLN	2.4
1	A	203	GLU	2.3
1	A	168	LYS	2.3
1	A	125	VAL	2.3
1	B	160	TYR	2.2
1	B	238	GLU	2.1
1	B	283	ASP	2.0
1	A	279	SER	2.0
1	A	124	PRO	2.0
1	B	282	GLU	2.0
1	B	209	TYR	2.0
1	B	219	TYR	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	1	1/1	0.97	0.03	26,26,26,26	0
2	MG	A	2	1/1	0.98	0.03	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.