



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:17 PM UTC

PDB ID : 5IG3 / pdb_00005ig3
Title : Crystal structure of the human CaMKII-alpha hub
Authors : McSpadden, E.; Cao, Y.M.; Bhattacharyya, M.; Gee, C.L.; Barros, T.; Kuriyan, J.
Deposited on : 2016-02-26
Resolution : 2.75 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:

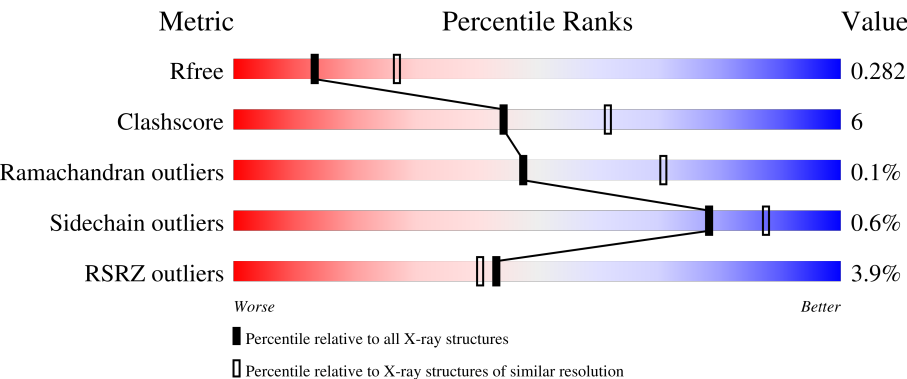
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	153	2% 80%14%• 6%
1	B	153	2% 72%11%17%
1	C	153	3% 71%15%• 14%
1	D	153	2% 71%12%• 17%
1	E	153	5% 67%15%18%

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Mol	Chain	Length	Quality of chain
1	F	153	6% 67% 13% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6312 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 Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1168	738	212	212	6			
1	B	127	Total	C	N	O	S	0	0	0
			1031	655	182	188	6			
1	C	132	Total	C	N	O	S	0	0	0
			1066	673	191	196	6			
1	D	127	Total	C	N	O	S	0	0	0
			1024	647	182	189	6			
1	E	125	Total	C	N	O	S	0	0	0
			1012	641	180	185	6			
1	F	123	Total	C	N	O	S	0	0	0
			996	630	177	183	6			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	GLY	-	expression tag	UNP Q9UQM7
A	324	SER	-	expression tag	UNP Q9UQM7
A	325	SER	-	expression tag	UNP Q9UQM7
A	326	HIS	-	expression tag	UNP Q9UQM7
A	327	HIS	-	expression tag	UNP Q9UQM7
A	328	HIS	-	expression tag	UNP Q9UQM7
A	329	HIS	-	expression tag	UNP Q9UQM7
A	330	HIS	-	expression tag	UNP Q9UQM7
A	331	HIS	-	expression tag	UNP Q9UQM7
A	332	SER	-	expression tag	UNP Q9UQM7
A	333	SER	-	expression tag	UNP Q9UQM7
A	334	GLY	-	expression tag	UNP Q9UQM7
A	335	LEU	-	expression tag	UNP Q9UQM7
A	336	GLU	-	expression tag	UNP Q9UQM7
A	337	VAL	-	expression tag	UNP Q9UQM7
A	338	LEU	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	339	PHE	-	expression tag	UNP Q9UQM7
A	340	GLN	-	expression tag	UNP Q9UQM7
A	341	GLY	-	expression tag	UNP Q9UQM7
A	342	PRO	-	expression tag	UNP Q9UQM7
A	343	HIS	-	expression tag	UNP Q9UQM7
A	344	MET	-	expression tag	UNP Q9UQM7
B	323	GLY	-	expression tag	UNP Q9UQM7
B	324	SER	-	expression tag	UNP Q9UQM7
B	325	SER	-	expression tag	UNP Q9UQM7
B	326	HIS	-	expression tag	UNP Q9UQM7
B	327	HIS	-	expression tag	UNP Q9UQM7
B	328	HIS	-	expression tag	UNP Q9UQM7
B	329	HIS	-	expression tag	UNP Q9UQM7
B	330	HIS	-	expression tag	UNP Q9UQM7
B	331	HIS	-	expression tag	UNP Q9UQM7
B	332	SER	-	expression tag	UNP Q9UQM7
B	333	SER	-	expression tag	UNP Q9UQM7
B	334	GLY	-	expression tag	UNP Q9UQM7
B	335	LEU	-	expression tag	UNP Q9UQM7
B	336	GLU	-	expression tag	UNP Q9UQM7
B	337	VAL	-	expression tag	UNP Q9UQM7
B	338	LEU	-	expression tag	UNP Q9UQM7
B	339	PHE	-	expression tag	UNP Q9UQM7
B	340	GLN	-	expression tag	UNP Q9UQM7
B	341	GLY	-	expression tag	UNP Q9UQM7
B	342	PRO	-	expression tag	UNP Q9UQM7
B	343	HIS	-	expression tag	UNP Q9UQM7
B	344	MET	-	expression tag	UNP Q9UQM7
C	323	GLY	-	expression tag	UNP Q9UQM7
C	324	SER	-	expression tag	UNP Q9UQM7
C	325	SER	-	expression tag	UNP Q9UQM7
C	326	HIS	-	expression tag	UNP Q9UQM7
C	327	HIS	-	expression tag	UNP Q9UQM7
C	328	HIS	-	expression tag	UNP Q9UQM7
C	329	HIS	-	expression tag	UNP Q9UQM7
C	330	HIS	-	expression tag	UNP Q9UQM7
C	331	HIS	-	expression tag	UNP Q9UQM7
C	332	SER	-	expression tag	UNP Q9UQM7
C	333	SER	-	expression tag	UNP Q9UQM7
C	334	GLY	-	expression tag	UNP Q9UQM7
C	335	LEU	-	expression tag	UNP Q9UQM7
C	336	GLU	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	337	VAL	-	expression tag	UNP Q9UQM7
C	338	LEU	-	expression tag	UNP Q9UQM7
C	339	PHE	-	expression tag	UNP Q9UQM7
C	340	GLN	-	expression tag	UNP Q9UQM7
C	341	GLY	-	expression tag	UNP Q9UQM7
C	342	PRO	-	expression tag	UNP Q9UQM7
C	343	HIS	-	expression tag	UNP Q9UQM7
C	344	MET	-	expression tag	UNP Q9UQM7
D	323	GLY	-	expression tag	UNP Q9UQM7
D	324	SER	-	expression tag	UNP Q9UQM7
D	325	SER	-	expression tag	UNP Q9UQM7
D	326	HIS	-	expression tag	UNP Q9UQM7
D	327	HIS	-	expression tag	UNP Q9UQM7
D	328	HIS	-	expression tag	UNP Q9UQM7
D	329	HIS	-	expression tag	UNP Q9UQM7
D	330	HIS	-	expression tag	UNP Q9UQM7
D	331	HIS	-	expression tag	UNP Q9UQM7
D	332	SER	-	expression tag	UNP Q9UQM7
D	333	SER	-	expression tag	UNP Q9UQM7
D	334	GLY	-	expression tag	UNP Q9UQM7
D	335	LEU	-	expression tag	UNP Q9UQM7
D	336	GLU	-	expression tag	UNP Q9UQM7
D	337	VAL	-	expression tag	UNP Q9UQM7
D	338	LEU	-	expression tag	UNP Q9UQM7
D	339	PHE	-	expression tag	UNP Q9UQM7
D	340	GLN	-	expression tag	UNP Q9UQM7
D	341	GLY	-	expression tag	UNP Q9UQM7
D	342	PRO	-	expression tag	UNP Q9UQM7
D	343	HIS	-	expression tag	UNP Q9UQM7
D	344	MET	-	expression tag	UNP Q9UQM7
E	323	GLY	-	expression tag	UNP Q9UQM7
E	324	SER	-	expression tag	UNP Q9UQM7
E	325	SER	-	expression tag	UNP Q9UQM7
E	326	HIS	-	expression tag	UNP Q9UQM7
E	327	HIS	-	expression tag	UNP Q9UQM7
E	328	HIS	-	expression tag	UNP Q9UQM7
E	329	HIS	-	expression tag	UNP Q9UQM7
E	330	HIS	-	expression tag	UNP Q9UQM7
E	331	HIS	-	expression tag	UNP Q9UQM7
E	332	SER	-	expression tag	UNP Q9UQM7
E	333	SER	-	expression tag	UNP Q9UQM7
E	334	GLY	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	335	LEU	-	expression tag	UNP Q9UQM7
E	336	GLU	-	expression tag	UNP Q9UQM7
E	337	VAL	-	expression tag	UNP Q9UQM7
E	338	LEU	-	expression tag	UNP Q9UQM7
E	339	PHE	-	expression tag	UNP Q9UQM7
E	340	GLN	-	expression tag	UNP Q9UQM7
E	341	GLY	-	expression tag	UNP Q9UQM7
E	342	PRO	-	expression tag	UNP Q9UQM7
E	343	HIS	-	expression tag	UNP Q9UQM7
E	344	MET	-	expression tag	UNP Q9UQM7
F	323	GLY	-	expression tag	UNP Q9UQM7
F	324	SER	-	expression tag	UNP Q9UQM7
F	325	SER	-	expression tag	UNP Q9UQM7
F	326	HIS	-	expression tag	UNP Q9UQM7
F	327	HIS	-	expression tag	UNP Q9UQM7
F	328	HIS	-	expression tag	UNP Q9UQM7
F	329	HIS	-	expression tag	UNP Q9UQM7
F	330	HIS	-	expression tag	UNP Q9UQM7
F	331	HIS	-	expression tag	UNP Q9UQM7
F	332	SER	-	expression tag	UNP Q9UQM7
F	333	SER	-	expression tag	UNP Q9UQM7
F	334	GLY	-	expression tag	UNP Q9UQM7
F	335	LEU	-	expression tag	UNP Q9UQM7
F	336	GLU	-	expression tag	UNP Q9UQM7
F	337	VAL	-	expression tag	UNP Q9UQM7
F	338	LEU	-	expression tag	UNP Q9UQM7
F	339	PHE	-	expression tag	UNP Q9UQM7
F	340	GLN	-	expression tag	UNP Q9UQM7
F	341	GLY	-	expression tag	UNP Q9UQM7
F	342	PRO	-	expression tag	UNP Q9UQM7
F	343	HIS	-	expression tag	UNP Q9UQM7
F	344	MET	-	expression tag	UNP Q9UQM7

- Molecule 2 is water.

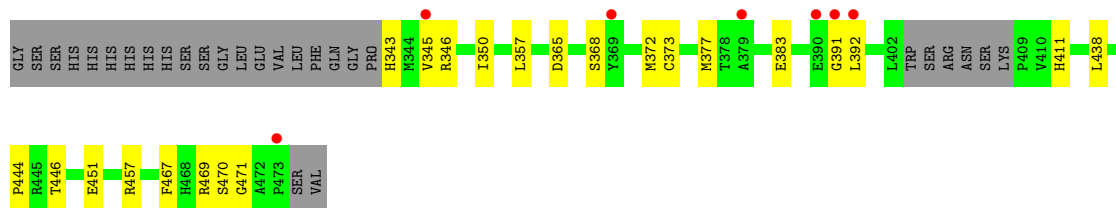
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	6	Total O 6 6	0	0
2	C	2	Total O 2 2	0	0

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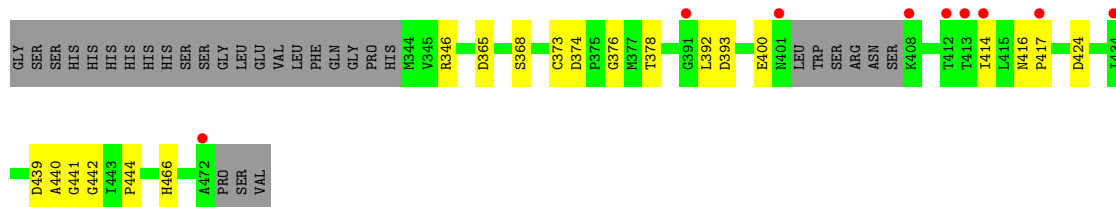
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	O	0	0
			2	2		
2	E	1	Total	O	0	0
			1	1		
2	F	1	Total	O	0	0
			1	1		

- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha



- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.89Å 89.89Å 226.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 2.75 48.63 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.63-2.75) 99.9 (48.63-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.220 , 0.268 0.235 , 0.282	Depositor DCC
R_{free} test set	1186 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6312	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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](#)

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	0.13	0/1201	0.32	0/1625
1	B	0.12	0/1058	0.34	0/1431
1	C	0.14	0/1093	0.37	0/1475
1	D	0.12	0/1049	0.33	0/1416
1	E	0.15	0/1038	0.30	0/1403
1	F	0.13	0/1020	0.34	0/1377
All	All	0.13	0/6459	0.34	0/8727

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 [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	1168	0	1117	17	0
1	B	1031	0	994	12	0
1	C	1066	0	1018	14	0
1	D	1024	0	983	10	0
1	E	1012	0	974	16	0
1	F	996	0	961	12	0
2	A	3	0	0	0	0
2	B	6	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1	0	0	0	0
2	F	1	0	0	0	0
All	All	6312	0	6047	74	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 6.

All (74) 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:C:374:ASP:OD2	1:C:458:ARG:NH1	1.90	1.03
1:B:374:ASP:OD1	1:B:458:ARG:NH1	1.93	1.01
1:A:331:HIS:HA	1:A:412:THR:O	1.73	0.88
1:B:393:ASP:OD2	1:E:411:HIS:NE2	2.20	0.74
1:C:346:ARG:NH1	1:C:424:ASP:O	2.24	0.70
1:F:374:ASP:OD2	1:F:376:GLY:N	2.23	0.69
1:A:346:ARG:NH1	1:A:424:ASP:O	2.25	0.69
1:F:439:ASP:O	1:F:441:GLY:N	2.31	0.64
1:B:378:THR:O	1:B:466:HIS:HA	1.99	0.63
1:A:408:LYS:NZ	1:A:439:ASP:O	2.33	0.62
1:B:402:LEU:HD22	1:E:444:PRO:HG3	1.82	0.61
1:F:346:ARG:NH2	1:F:424:ASP:OD1	2.34	0.61
1:E:365:ASP:OD2	1:E:368:SER:OG	2.15	0.61
1:F:378:THR:O	1:F:466:HIS:HA	2.00	0.60
1:E:377:MET:O	1:E:391:GLY:N	2.33	0.58
1:C:346:ARG:NH1	1:C:424:ASP:HA	2.18	0.58
1:A:335:LEU:HD22	1:A:351:ILE:HD13	1.86	0.57
1:A:338:LEU:HD23	1:A:351:ILE:HD11	1.86	0.57
1:D:411:HIS:NE2	1:F:393:ASP:OD2	2.37	0.56
1:E:383:GLU:OE1	1:E:469:ARG:NH2	2.38	0.56
1:C:344:MET:SD	1:C:344:MET:N	2.79	0.55
1:B:373:CYS:HB2	1:B:392:LEU:HD21	1.88	0.55
1:C:393:ASP:OD1	1:C:396:ARG:NH1	2.41	0.55
1:A:346:ARG:NH1	1:A:424:ASP:HA	2.23	0.54
1:B:346:ARG:HD2	1:B:421:LEU:HD13	1.89	0.54
1:C:333:SER:HA	1:C:414:ILE:HB	1.89	0.54
1:B:401:ASN:HB3	1:E:438:LEU:HD11	1.88	0.54
1:C:378:THR:O	1:C:466:HIS:HA	2.08	0.54
1:A:365:ASP:OD2	1:A:368:SER:OG	2.23	0.53
1:C:442:GLY:HA2	1:C:443:ILE:HB	1.91	0.52
1:C:382:PRO:HG2	1:C:472:ALA:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:CYS:HB2	1:D:392:LEU:HD21	1.92	0.51
1:A:346:ARG:NH2	1:A:457:ARG:HH22	2.09	0.50
1:F:400:GLU:N	1:F:400:GLU:OE1	2.44	0.50
1:A:402:LEU:HD22	1:F:444:PRO:HG3	1.92	0.50
1:A:344:MET:HE2	1:A:348:GLN:HE21	1.77	0.49
1:A:449:SER:HA	1:A:470:SER:O	2.11	0.49
1:D:347:LYS:HB3	1:D:419:ILE:HD12	1.95	0.49
1:B:347:LYS:HB3	1:B:419:ILE:HD12	1.95	0.49
1:E:373:CYS:HB2	1:E:392:LEU:HD21	1.95	0.48
1:D:361:ILE:HA	1:D:399:PHE:HE1	1.78	0.48
1:E:346:ARG:HE	1:E:457:ARG:HH22	1.62	0.47
1:F:439:ASP:O	1:F:442:GLY:N	2.39	0.47
1:D:379:ALA:HB3	1:D:389:VAL:HG23	1.97	0.47
1:F:373:CYS:HB2	1:F:392:LEU:HD21	1.96	0.47
1:E:451:GLU:HG2	1:E:469:ARG:HG3	1.97	0.47
1:C:373:CYS:HB2	1:C:392:LEU:HD21	1.97	0.46
1:E:357:LEU:HA	1:E:372:MET:HE1	1.98	0.45
1:B:370:THR:HG22	1:B:392:LEU:HD22	1.98	0.45
1:D:377:MET:HA	1:D:465:VAL:O	2.17	0.45
1:A:344:MET:HE2	1:A:348:GLN:NE2	2.32	0.45
1:D:357:LEU:HA	1:D:372:MET:HE1	1.99	0.44
1:D:378:THR:O	1:D:466:HIS:HA	2.16	0.44
1:F:365:ASP:OD2	1:F:368:SER:OG	2.34	0.44
1:C:456:HIS:CD2	1:C:458:ARG:HE	2.36	0.44
1:C:438:LEU:HD23	1:C:444:PRO:HA	1.99	0.43
1:E:346:ARG:O	1:E:350:ILE:HG12	2.18	0.43
1:E:467:PHE:CZ	1:E:469:ARG:HB2	2.54	0.43
1:B:393:ASP:OD2	1:E:411:HIS:CE1	2.72	0.43
1:A:346:ARG:HH12	1:A:424:ASP:HA	1.84	0.43
1:B:381:GLU:OE2	1:B:469:ARG:NH2	2.52	0.43
1:A:338:LEU:HD21	1:A:419:ILE:HG13	2.02	0.42
1:D:415:LEU:HB2	1:D:432:ILE:HB	2.02	0.42
1:A:333:SER:HA	1:A:414:ILE:O	2.20	0.42
1:C:453:ARG:HD3	1:C:467:PHE:HB2	2.02	0.41
1:D:467:PHE:CE2	1:D:469:ARG:NH1	2.88	0.41
1:C:449:SER:HB3	1:C:472:ALA:HB2	2.02	0.41
1:A:358:ILE:HD12	1:A:414:ILE:HD11	2.03	0.41
1:E:343:HIS:ND1	1:E:345:VAL:HG22	2.35	0.41
1:F:414:ILE:HG22	1:F:417:PRO:HG3	2.03	0.41
1:E:470:SER:HA	1:E:471:GLY:HA2	1.66	0.41
1:B:383:GLU:O	1:E:446:THR:HG21	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD22	1:A:417:PRO:HB2	2.04	0.40
1:F:416:ASN:N	1:F:417:PRO:HD3	2.36	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	142/153 (93%)	136 (96%)	6 (4%)	0	100	100
1	B	123/153 (80%)	120 (98%)	3 (2%)	0	100	100
1	C	126/153 (82%)	120 (95%)	6 (5%)	0	100	100
1	D	121/153 (79%)	118 (98%)	3 (2%)	0	100	100
1	E	121/153 (79%)	118 (98%)	3 (2%)	0	100	100
1	F	119/153 (78%)	118 (99%)	0	1 (1%)	16	30
All	All	752/918 (82%)	730 (97%)	21 (3%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	440	ALA

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	125/133 (94%)	124 (99%)	1 (1%)	73	84
1	B	110/133 (83%)	110 (100%)	0	100	100
1	C	114/133 (86%)	112 (98%)	2 (2%)	51	71
1	D	110/133 (83%)	109 (99%)	1 (1%)	70	82
1	E	108/133 (81%)	108 (100%)	0	100	100
1	F	106/133 (80%)	106 (100%)	0	100	100
All	All	673/798 (84%)	669 (99%)	4 (1%)	78	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	457	ARG
1	C	343	HIS
1	C	344	MET
1	D	467	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	387	ASN
1	B	356	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	144/153 (94%)	0.04	3 (2%) 63 61	52, 78, 140, 186	0
1	B	127/153 (83%)	-0.07	3 (2%) 59 57	52, 76, 134, 150	0
1	C	132/153 (86%)	0.19	5 (3%) 44 41	50, 91, 144, 173	0
1	D	127/153 (83%)	0.13	3 (2%) 59 57	53, 94, 136, 164	0
1	E	125/153 (81%)	0.45	7 (5%) 30 30	57, 101, 164, 214	0
1	F	123/153 (80%)	0.35	9 (7%) 21 21	58, 100, 155, 193	0
All	All	778/918 (84%)	0.18	30 (3%) 43 40	50, 91, 149, 214	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	ALA	4.6
1	C	472	ALA	3.9
1	E	379	ALA	3.8
1	E	345	VAL	3.5
1	D	402	LEU	3.3
1	E	369	TYR	3.3
1	D	409	PRO	3.3
1	F	412	THR	3.2
1	E	391	GLY	3.0
1	E	390	GLU	2.9
1	C	390	GLU	2.8
1	F	408	LYS	2.8
1	C	343	HIS	2.8
1	F	434	ILE	2.7
1	E	473	PRO	2.7
1	F	472	ALA	2.6
1	B	472	ALA	2.6
1	F	413	THR	2.4
1	F	414	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	345	VAL	2.3
1	F	391	GLY	2.3
1	C	345	VAL	2.3
1	B	403	TRP	2.3
1	E	392	LEU	2.2
1	C	344	MET	2.1
1	A	334	GLY	2.1
1	F	401	ASN	2.1
1	D	376	GLY	2.1
1	A	337	VAL	2.1
1	F	417	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.