Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 10:25 AM JST

PDB ID	:	6LNM
Title	:	Crystal structure of CASK-CaMK in complex with Mint1-CID
Authors	:	Cai, Q.; Zhang, M.
Deposited on	:	2019-12-31
Resolution	:	2.40 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:

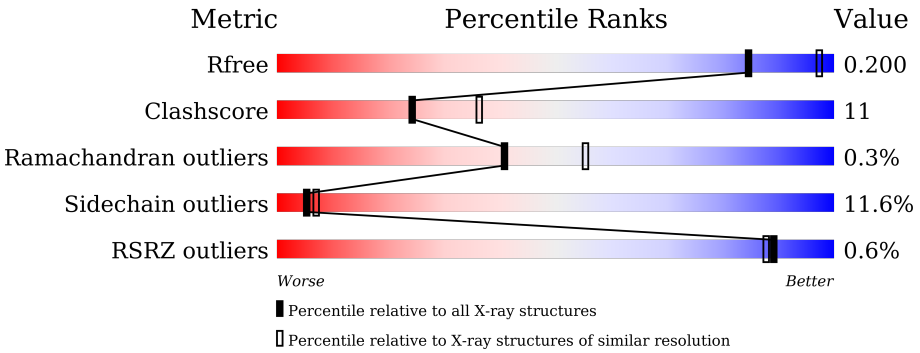
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	351	73% 17% • 7%
1	C	351	% 67% 21% • 8%
1	E	351	% 70% 18% • 8%
2	B	50	54% 26% • 16%
2	D	50	2% 48% 22% 14% 16%
2	F	50	2% 52% 24% 10% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8985 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 Peripheral plasma membrane protein CASK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	1	0
			2602	1670	448	467	17			
1	C	322	Total	C	N	O	S	0	0	0
			2580	1656	445	462	17			
1	E	322	Total	C	N	O	S	0	1	0
			2589	1664	445	463	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q62915
A	-4	PRO	-	expression tag	UNP Q62915
A	-3	GLY	-	expression tag	UNP Q62915
A	-2	SER	-	expression tag	UNP Q62915
A	-1	GLU	-	expression tag	UNP Q62915
A	0	PHE	-	expression tag	UNP Q62915
C	-5	GLY	-	expression tag	UNP Q62915
C	-4	PRO	-	expression tag	UNP Q62915
C	-3	GLY	-	expression tag	UNP Q62915
C	-2	SER	-	expression tag	UNP Q62915
C	-1	GLU	-	expression tag	UNP Q62915
C	0	PHE	-	expression tag	UNP Q62915
E	-5	GLY	-	expression tag	UNP Q62915
E	-4	PRO	-	expression tag	UNP Q62915
E	-3	GLY	-	expression tag	UNP Q62915
E	-2	SER	-	expression tag	UNP Q62915
E	-1	GLU	-	expression tag	UNP Q62915
E	0	PHE	-	expression tag	UNP Q62915

- Molecule 2 is a protein called Amyloid-beta A4 precursor protein-binding family A member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	42	Total	C	N	O	S	0	1	0
			352	225	60	66	1			
2	D	42	Total	C	N	O	S	0	0	0
			344	220	57	66	1			
2	F	43	Total	C	N	O	S	0	0	0
			351	225	58	67	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	345	GLY	-	expression tag	UNP B2RUJ5
B	346	PRO	-	expression tag	UNP B2RUJ5
B	347	GLY	-	expression tag	UNP B2RUJ5
B	348	SER	-	expression tag	UNP B2RUJ5
B	349	GLU	-	expression tag	UNP B2RUJ5
B	350	PHE	-	expression tag	UNP B2RUJ5
D	345	GLY	-	expression tag	UNP B2RUJ5
D	346	PRO	-	expression tag	UNP B2RUJ5
D	347	GLY	-	expression tag	UNP B2RUJ5
D	348	SER	-	expression tag	UNP B2RUJ5
D	349	GLU	-	expression tag	UNP B2RUJ5
D	350	PHE	-	expression tag	UNP B2RUJ5
F	345	GLY	-	expression tag	UNP B2RUJ5
F	346	PRO	-	expression tag	UNP B2RUJ5
F	347	GLY	-	expression tag	UNP B2RUJ5
F	348	SER	-	expression tag	UNP B2RUJ5
F	349	GLU	-	expression tag	UNP B2RUJ5
F	350	PHE	-	expression tag	UNP B2RUJ5

- Molecule 3 is water.

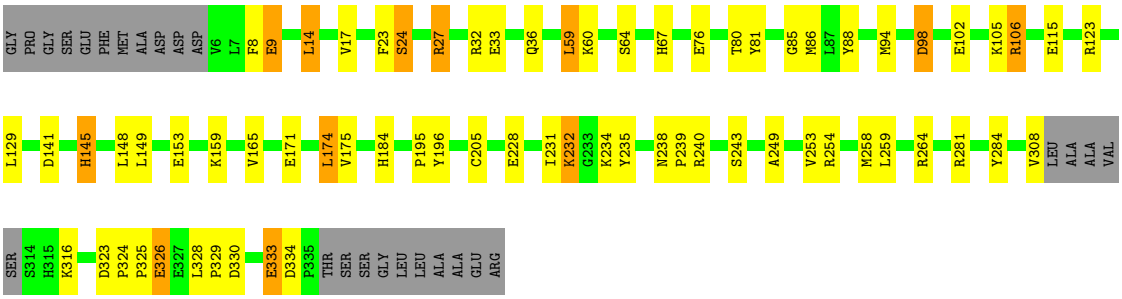
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		
3	B	5	Total	O	0	0
			5	5		
3	C	64	Total	O	0	0
			64	64		
3	D	5	Total	O	0	0
			5	5		
3	E	44	Total	O	0	0
			44	44		
3	F	6	Total	O	0	0
			6	6		

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.

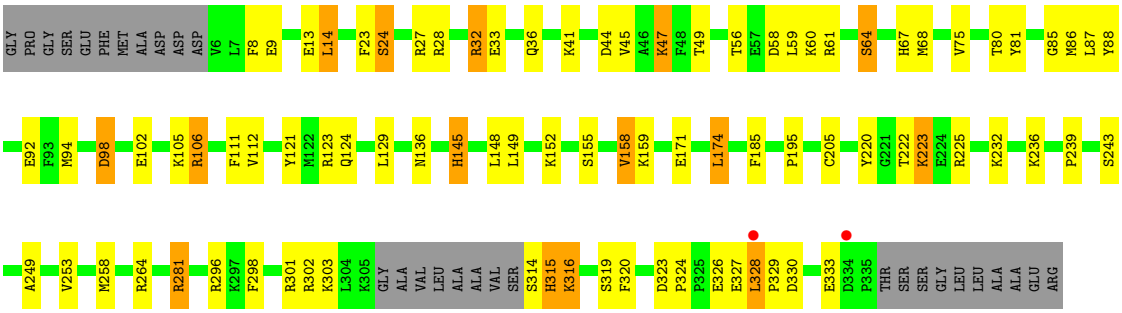
• Molecule 1: Peripheral plasma membrane protein CASK

Chain A:



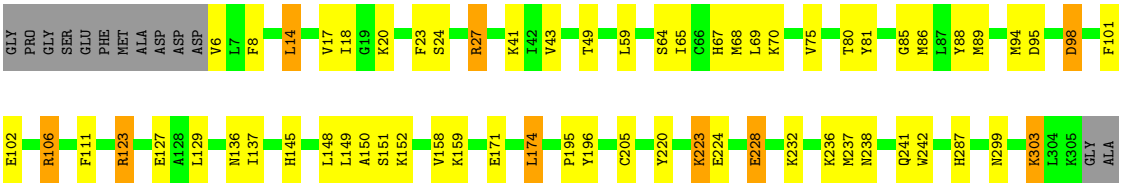
• Molecule 1: Peripheral plasma membrane protein CASK

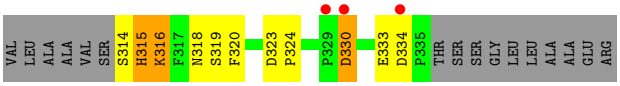
Chain C:



• Molecule 1: Peripheral plasma membrane protein CASK

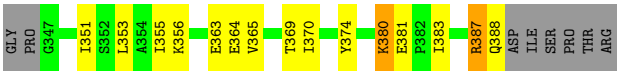
Chain E:





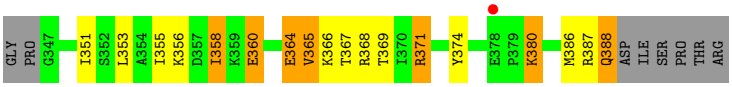
• Molecule 2: Amyloid-beta A4 precursor protein-binding family A member 1

Chain B:



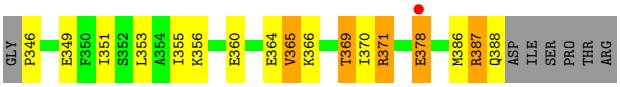
• Molecule 2: Amyloid-beta A4 precursor protein-binding family A member 1

Chain D:



• Molecule 2: Amyloid-beta A4 precursor protein-binding family A member 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	151.42Å 151.42Å 49.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.40 – 2.40 41.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.40-2.40) 99.5 (41.40-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.171 , 0.213 0.160 , 0.200	Depositor DCC
R_{free} test set	2384 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 9.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.127 for -h,-k,l 0.129 for h,-h-k,-l 0.416 for -k,-h,-l	Xtriage
Reported twinning fraction	0.570 for H, K, L 0.430 for -K, -H, -L	Depositor
Outliers	0 of 49551 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8985	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.71	1/2669 (0.0%)	0.86	0/3602
1	C	0.71	1/2644 (0.0%)	0.88	2/3568 (0.1%)
1	E	0.70	0/2657	0.87	0/3586
2	B	0.70	0/362	0.99	0/488
2	D	0.74	0/351	0.94	0/474
2	F	0.67	0/359	0.98	0/485
All	All	0.71	2/9042 (0.0%)	0.88	2/12203 (0.0%)

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	A	0	1
1	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	GLU	CD-OE2	-5.72	1.19	1.25
1	C	92	GLU	CD-OE2	-5.03	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	28	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	C	32	ARG	CG-CD-NE	5.41	123.17	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ASP	Peptide
1	E	334	ASP	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	2602	0	2595	44	1
1	C	2580	0	2572	64	0
1	E	2589	0	2581	62	0
2	B	352	0	364	9	0
2	D	344	0	351	22	0
2	F	351	0	359	13	0
3	A	43	0	0	5	0
3	B	5	0	0	0	0
3	C	64	0	0	9	0
3	D	5	0	0	3	0
3	E	44	0	0	4	0
3	F	6	0	0	3	0
All	All	8985	0	8822	194	1

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 11.

All (194) 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:E:228:GLU:OE1	1:E:232:LYS:HE2	1.48	1.12
1:E:174:LEU:HD12	1:E:195:PRO:HB2	1.45	0.99
1:E:95:ASP:HB3	1:E:151:SER:HA	1.46	0.96
1:A:174:LEU:HD12	1:A:195:PRO:HB2	1.48	0.94
1:C:155:SER:HB2	3:C:423:HOH:O	1.69	0.92
1:E:228:GLU:OE1	1:E:232:LYS:CE	2.21	0.87
1:E:238:ASN:OD1	3:E:401:HOH:O	1.92	0.87
1:C:328:LEU:HD23	1:C:329:PRO:HD2	1.53	0.87
1:E:174:LEU:CD1	1:E:195:PRO:HB2	2.05	0.86
1:C:174:LEU:HD12	1:C:195:PRO:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLU:O	1:E:106:ARG:HG2	1.83	0.79
1:C:47:LYS:NZ	1:C:47:LYS:HB3	1.98	0.79
2:B:380:LYS:HE2	2:B:380:LYS:H	1.48	0.78
1:C:75:VAL:HG21	1:C:320:PHE:CZ	2.19	0.78
1:E:75:VAL:HG21	1:E:320:PHE:CZ	2.19	0.78
1:C:102:GLU:O	1:C:106:ARG:HG2	1.84	0.77
2:B:380:LYS:H	2:B:380:LYS:CE	1.98	0.76
1:C:60:LYS:HG3	2:D:358:ILE:HG13	1.67	0.76
1:C:316:LYS:HE2	3:C:457:HOH:O	1.84	0.76
1:C:174:LEU:CD1	1:C:195:PRO:HB2	2.17	0.75
1:C:23:PHE:CD2	1:C:324:PRO:HG2	2.22	0.75
1:A:23:PHE:CD2	1:A:324:PRO:HG2	2.22	0.74
1:A:174:LEU:CD1	1:A:195:PRO:HB2	2.17	0.74
1:E:23:PHE:CD2	1:E:324:PRO:HG2	2.23	0.73
1:A:102:GLU:O	1:A:106:ARG:HG2	1.87	0.73
1:A:94:MET:CE	1:A:159:LYS:HB2	2.19	0.72
2:F:349:GLU:HG2	3:F:401:HOH:O	1.89	0.72
1:C:112:VAL:HG22	2:D:388:GLN:HA	1.72	0.71
1:E:43:VAL:HG21	1:E:89:MET:HE2	1.71	0.71
1:C:64:SER:CB	3:D:403:HOH:O	2.38	0.70
1:C:75:VAL:CG2	1:C:320:PHE:CZ	2.74	0.70
1:C:145:HIS:H	1:C:145:HIS:CD2	2.10	0.70
1:E:127:GLU:OE1	3:E:402:HOH:O	2.10	0.70
1:E:43:VAL:CG2	1:E:89:MET:HE2	2.21	0.69
1:E:94:MET:HE2	1:E:159:LYS:HB2	1.74	0.69
1:E:75:VAL:CG2	1:E:320:PHE:CZ	2.75	0.69
1:E:314:SER:HB3	1:E:316:LYS:NZ	2.07	0.69
1:A:94:MET:HE2	1:A:159:LYS:HB2	1.74	0.69
1:E:94:MET:CE	1:E:159:LYS:HB2	2.23	0.69
1:C:102:GLU:OE2	1:C:152:LYS:NZ	2.27	0.68
1:C:67:HIS:NE2	1:C:80:THR:HG23	2.10	0.67
1:E:67:HIS:NE2	1:E:80:THR:HG23	2.10	0.66
1:A:129:LEU:CD1	1:A:205:CYS:SG	2.84	0.66
2:F:365:VAL:O	2:F:369:THR:HG22	1.96	0.66
1:A:67:HIS:NE2	1:A:80:THR:HG23	2.11	0.66
2:D:365:VAL:O	2:D:369:THR:HG23	1.96	0.66
1:C:94:MET:HE2	1:C:159:LYS:HB2	1.77	0.66
1:E:43:VAL:HG21	1:E:89:MET:CE	2.26	0.66
1:A:281:ARG:HD2	2:D:360:GLU:HG2	1.77	0.65
1:E:75:VAL:HG21	1:E:320:PHE:CE2	2.31	0.65
2:D:364:GLU:OE1	2:D:368:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:SER:HB2	3:D:403:HOH:O	1.96	0.64
1:C:281:ARG:HG2	3:C:445:HOH:O	1.96	0.64
1:C:296:ARG:O	3:C:401:HOH:O	2.14	0.64
1:C:315:HIS:HD2	1:C:326:GLU:OE1	1.81	0.63
1:C:75:VAL:HG21	1:C:320:PHE:CE2	2.34	0.63
1:C:222:THR:HB	3:C:452:HOH:O	1.99	0.62
1:C:94:MET:CE	1:C:159:LYS:HB2	2.30	0.62
2:B:365:VAL:O	2:B:369:THR:HG23	2.01	0.61
2:F:346:PRO:CD	3:F:402:HOH:O	2.47	0.61
2:B:387[B]:ARG:HH11	2:B:387[B]:ARG:HB3	1.67	0.60
1:C:314:SER:N	1:C:316:LYS:HZ3	1.98	0.60
1:C:24:SER:HB3	1:C:323:ASP:OD2	2.03	0.59
1:A:9:GLU:O	1:A:32:ARG:NH2	2.36	0.59
1:E:333:GLU:N	1:E:333:GLU:OE2	2.36	0.58
1:E:101:PHE:CE1	1:E:303:LYS:HD3	2.39	0.58
1:C:281:ARG:CG	3:C:445:HOH:O	2.51	0.58
1:E:129:LEU:CD1	1:E:205:CYS:SG	2.92	0.58
1:C:45:VAL:HG21	2:D:355:ILE:CD1	2.34	0.57
1:C:47:LYS:HB3	1:C:47:LYS:HZ1	1.66	0.57
1:A:115:GLU:OE2	3:A:401:HOH:O	2.17	0.56
1:E:238:ASN:HA	3:E:401:HOH:O	2.05	0.56
1:E:314:SER:HB3	1:E:316:LYS:HZ3	1.71	0.56
1:E:24:SER:HB3	1:E:323:ASP:OD2	2.06	0.56
1:C:315:HIS:CD2	1:C:326:GLU:OE1	2.58	0.56
1:E:333:GLU:H	1:E:333:GLU:CD	2.09	0.56
1:C:129:LEU:CD1	1:C:205:CYS:SG	2.94	0.56
1:C:58:ASP:OD1	1:C:61:ARG:NH1	2.39	0.55
1:C:223:LYS:HE3	1:C:330:ASP:HB2	1.89	0.55
1:A:232:LYS:HE2	1:A:234:LYS:HG3	1.87	0.55
1:A:24:SER:HB3	1:A:323:ASP:OD2	2.07	0.54
1:C:123:ARG:HH22	2:D:374:TYR:HH	1.54	0.54
2:F:366:LYS:HA	2:F:369:THR:CG2	2.38	0.54
1:A:80:THR:HA	1:A:88:TYR:O	2.08	0.54
1:E:43:VAL:CG2	1:E:89:MET:CE	2.85	0.54
1:E:80:THR:HA	1:E:88:TYR:O	2.07	0.54
1:E:287:HIS:CE1	2:F:388:GLN:HE21	2.26	0.54
1:A:102:GLU:HG3	1:A:149:LEU:HD12	1.89	0.53
1:A:281:ARG:HD2	2:D:360:GLU:CG	2.38	0.53
2:D:380:LYS:H	2:D:380:LYS:CD	2.22	0.53
1:C:64:SER:HB3	3:D:403:HOH:O	2.07	0.52
1:C:80:THR:HA	1:C:88:TYR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:GLY:HA2	2:F:351:ILE:HD13	1.90	0.52
1:E:314:SER:HB3	1:E:316:LYS:HZ1	1.74	0.52
1:E:228:GLU:OE1	1:E:232:LYS:CD	2.58	0.52
2:D:371:ARG:HH11	2:D:371:ARG:HB3	1.75	0.51
1:E:95:ASP:HB2	1:E:150:ALA:O	2.11	0.51
1:C:85:GLY:HA2	2:D:351:ILE:HD13	1.93	0.51
1:E:102:GLU:HG3	1:E:149:LEU:HD12	1.92	0.51
1:E:111:PHE:O	2:F:388:GLN:NE2	2.45	0.50
1:C:123:ARG:NH2	2:D:374:TYR:OH	2.32	0.50
1:E:81:TYR:HB2	1:E:88:TYR:HB2	1.93	0.50
1:A:123:ARG:NH2	2:B:374:TYR:OH	2.43	0.50
1:E:68:MET:SD	1:E:137:ILE:HD11	2.51	0.50
1:C:145:HIS:H	1:C:145:HIS:HD2	1.56	0.50
1:C:145:HIS:CD2	1:C:145:HIS:N	2.77	0.50
2:D:387:ARG:O	2:D:387:ARG:HG3	2.12	0.49
1:E:6:VAL:HG12	1:E:6:VAL:O	2.11	0.49
1:E:316:LYS:H	1:E:316:LYS:HE2	1.77	0.49
2:B:351:ILE:O	2:B:355:ILE:HG12	2.12	0.49
1:C:85:GLY:HA2	2:D:351:ILE:CD1	2.43	0.49
1:C:328:LEU:CD2	1:C:329:PRO:HD2	2.34	0.49
2:D:351:ILE:O	2:D:355:ILE:HG12	2.12	0.49
1:E:67:HIS:O	1:E:70:LYS:HE2	2.13	0.49
1:E:129:LEU:HD12	1:E:205:CYS:SG	2.52	0.49
1:A:81:TYR:HB2	1:A:88:TYR:HB2	1.95	0.48
1:A:235:TYR:OH	1:A:254:ARG:HG2	2.13	0.48
1:C:81:TYR:HB2	1:C:88:TYR:HB2	1.95	0.48
1:A:328:LEU:CD2	3:A:436:HOH:O	2.60	0.48
1:A:98:ASP:HA	1:A:148:LEU:HD23	1.96	0.48
1:A:326[A]:GLU:OE2	1:A:326[A]:GLU:HA	2.14	0.48
1:C:155:SER:CB	3:C:423:HOH:O	2.40	0.48
1:C:129:LEU:HD12	1:C:205:CYS:SG	2.54	0.48
1:C:121:TYR:CE1	1:C:149:LEU:HD21	2.48	0.48
1:A:141:ASP:HB2	1:A:165:VAL:CG2	2.44	0.48
1:E:123:ARG:HH11	1:E:123:ARG:HG3	1.79	0.48
1:A:284:TYR:HA	2:D:367:THR:HB	1.96	0.47
1:C:24:SER:OG	1:C:41:LYS:HG3	2.13	0.47
1:A:174:LEU:HD13	1:A:196:TYR:N	2.30	0.47
1:C:102:GLU:HG3	1:C:149:LEU:HD12	1.97	0.47
1:E:43:VAL:HG23	1:E:89:MET:HE2	1.96	0.47
1:E:228:GLU:CD	1:E:232:LYS:HD3	2.35	0.47
1:E:287:HIS:CE1	2:F:388:GLN:NE2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:HIS:H	1:E:145:HIS:CD2	2.33	0.47
1:E:65:ILE:O	1:E:69:LEU:HG	2.14	0.46
1:E:151:SER:OG	3:E:403:HOH:O	2.21	0.46
2:B:380:LYS:HE2	2:B:380:LYS:N	2.26	0.46
1:A:129:LEU:HD12	1:A:205:CYS:SG	2.56	0.46
2:D:356:LYS:HZ2	2:D:360:GLU:CD	2.19	0.45
2:F:378:GLU:H	2:F:378:GLU:CD	2.18	0.45
1:C:111:PHE:CE2	2:D:386:MET:HG2	2.52	0.45
1:C:124:GLN:OE1	1:C:158:VAL:HG13	2.17	0.45
2:F:371:ARG:NH1	2:F:371:ARG:HG2	2.31	0.45
1:E:95:ASP:CB	1:E:150:ALA:O	2.65	0.45
1:A:238:ASN:ND2	1:A:240:ARG:HB3	2.32	0.45
1:C:249:ALA:O	1:C:253:VAL:HG23	2.17	0.45
1:A:239:PRO:O	1:A:243:SER:HB3	2.16	0.44
1:A:231:ILE:O	1:A:259:LEU:HD11	2.17	0.44
1:C:239:PRO:O	1:C:243:SER:HB3	2.16	0.44
1:E:41:LYS:HE3	1:E:89:MET:HE1	2.00	0.44
1:E:223:LYS:HB2	1:E:330:ASP:OD2	2.17	0.44
1:A:258:MET:HB2	1:A:264:ARG:HA	1.99	0.44
1:A:8:PHE:HE2	1:A:14:LEU:HD12	1.83	0.43
1:E:41:LYS:HE3	1:E:89:MET:CE	2.48	0.43
1:E:174:LEU:HD13	1:E:196:TYR:N	2.33	0.43
1:A:85:GLY:HA2	2:B:351:ILE:HD13	2.01	0.43
1:A:184:HIS:HE1	3:A:431:HOH:O	2.00	0.43
1:A:281:ARG:NE	2:D:360:GLU:HG3	2.32	0.43
1:C:185:PHE:HB2	3:C:430:HOH:O	2.18	0.43
1:A:328:LEU:HD23	3:A:436:HOH:O	2.19	0.43
1:C:98:ASP:HA	1:C:148:LEU:HD23	2.00	0.43
1:C:44:ASP:HB3	1:C:47:LYS:HB2	2.00	0.43
1:A:145:HIS:ND1	1:A:145:HIS:N	2.67	0.43
1:A:165:VAL:HG13	1:A:325:PRO:HD3	2.01	0.43
1:E:228:GLU:OE1	1:E:232:LYS:HD3	2.18	0.43
1:A:249:ALA:O	1:A:253:VAL:HG23	2.18	0.43
1:A:94:MET:HE1	1:A:159:LYS:HB2	1.97	0.43
1:C:49:THR:HG22	3:C:436:HOH:O	2.19	0.42
2:F:356:LYS:O	2:F:360:GLU:HG3	2.20	0.42
1:E:174:LEU:HD13	1:E:195:PRO:C	2.40	0.42
1:C:298:PHE:O	1:C:302:ARG:HG3	2.19	0.42
1:E:24:SER:OG	1:E:41:LYS:HG3	2.19	0.42
1:C:68:MET:HA	2:D:369:THR:CG2	2.50	0.42
1:E:17:VAL:HG22	1:E:27:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLU:OE2	1:A:333:GLU:N	2.53	0.41
2:F:371:ARG:HG2	2:F:371:ARG:HH11	1.85	0.41
1:C:68:MET:HB2	2:D:369:THR:HG22	2.02	0.41
1:E:315:HIS:HA	1:E:318:ASN:HD22	1.85	0.41
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.92	0.41
1:A:8:PHE:HE2	1:A:14:LEU:CD1	2.34	0.41
1:C:8:PHE:HE2	1:C:14:LEU:CD1	2.34	0.41
1:C:258:MET:HB2	1:C:264:ARG:HA	2.02	0.41
1:E:8:PHE:HE2	1:E:14:LEU:CD1	2.34	0.41
1:E:299:ASN:O	1:E:303:LYS:HE2	2.21	0.41
1:A:17:VAL:HG22	1:A:27:ARG:HD2	2.03	0.40
1:C:303:LYS:HE3	1:C:303:LYS:HB2	1.92	0.40
1:E:98:ASP:HA	1:E:148:LEU:HD23	2.03	0.40
1:E:237:MET:HB3	1:E:242:TRP:CG	2.56	0.40
2:B:380:LYS:HE3	2:B:383:ILE:HD11	2.04	0.40
1:C:60:LYS:O	1:C:64:SER:HB3	2.21	0.40
1:A:328:LEU:HD21	3:A:436:HOH:O	2.20	0.40
1:C:94:MET:HG3	1:C:320:PHE:CE2	2.57	0.40
2:D:356:LYS:O	2:D:360:GLU:HB2	2.22	0.40
2:F:364:GLU:HB3	3:F:403:HOH:O	2.21	0.40

All (1) 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:A:153:GLU:OE2	1:A:228:GLU:OE2[1_554]	2.12	0.08

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	322/351 (92%)	317 (98%)	4 (1%)	1 (0%)	41 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	318/351 (91%)	312 (98%)	6 (2%)	0	100 100
1	E	319/351 (91%)	313 (98%)	6 (2%)	0	100 100
2	B	41/50 (82%)	38 (93%)	1 (2%)	2 (5%)	2 1
2	D	40/50 (80%)	37 (92%)	3 (8%)	0	100 100
2	F	41/50 (82%)	39 (95%)	1 (2%)	1 (2%)	6 6
All	All	1081/1203 (90%)	1056 (98%)	21 (2%)	4 (0%)	41 48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	387[A]	ARG
2	B	387[B]	ARG
2	F	387	ARG
1	A	329	PRO

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	282/299 (94%)	258 (92%)	24 (8%)	10 16
1	C	280/299 (94%)	245 (88%)	35 (12%)	4 5
1	E	281/299 (94%)	254 (90%)	27 (10%)	8 12
2	B	40/46 (87%)	32 (80%)	8 (20%)	1 1
2	D	39/46 (85%)	30 (77%)	9 (23%)	1 1
2	F	40/46 (87%)	31 (78%)	9 (22%)	1 1
All	All	962/1035 (93%)	850 (88%)	112 (12%)	5 7

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	14	LEU

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Mol	Chain	Res	Type
1	A	24	SER
1	A	27	ARG
1	A	33	GLU
1	A	36	GLN
1	A	59	LEU
1	A	60	LYS
1	A	64	SER
1	A	86	MET
1	A	98	ASP
1	A	105	LYS
1	A	106	ARG
1	A	145	HIS
1	A	171	GLU
1	A	174	LEU
1	A	175	VAL
1	A	232	LYS
1	A	308	VAL
1	A	316	LYS
1	A	326[A]	GLU
1	A	326[B]	GLU
1	A	330	ASP
1	A	333	GLU
2	B	353	LEU
2	B	356	LYS
2	B	363	GLU
2	B	364	GLU
2	B	370	ILE
2	B	380	LYS
2	B	381	GLU
2	B	388	GLN
1	C	9	GLU
1	C	13	GLU
1	C	14	LEU
1	C	24	SER
1	C	27	ARG
1	C	32	ARG
1	C	33	GLU
1	C	36	GLN
1	C	47	LYS
1	C	56	THR
1	C	59	LEU
1	C	64	SER

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Mol	Chain	Res	Type
1	C	86	MET
1	C	87	LEU
1	C	98	ASP
1	C	105	LYS
1	C	106	ARG
1	C	136	ASN
1	C	145	HIS
1	C	158	VAL
1	C	171	GLU
1	C	174	LEU
1	C	220	TYR
1	C	223	LYS
1	C	225	ARG
1	C	232	LYS
1	C	236	LYS
1	C	281	ARG
1	C	301	ARG
1	C	315	HIS
1	C	316	LYS
1	C	319	SER
1	C	327	GLU
1	C	328	LEU
1	C	333	GLU
2	D	353	LEU
2	D	358	ILE
2	D	360	GLU
2	D	364	GLU
2	D	365	VAL
2	D	366	LYS
2	D	371	ARG
2	D	380	LYS
2	D	388	GLN
1	E	14	LEU
1	E	18	ILE
1	E	20	LYS
1	E	27	ARG
1	E	49	THR
1	E	59	LEU
1	E	64	SER
1	E	86	MET
1	E	98	ASP
1	E	106	ARG

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Mol	Chain	Res	Type
1	E	123	ARG
1	E	136	ASN
1	E	152	LYS
1	E	158	VAL
1	E	171	GLU
1	E	174	LEU
1	E	220	TYR
1	E	223	LYS
1	E	224	GLU
1	E	228	GLU
1	E	236	LYS
1	E	241	GLN
1	E	303	LYS
1	E	315	HIS
1	E	316	LYS
1	E	319	SER
1	E	330	ASP
2	F	353	LEU
2	F	355	ILE
2	F	365	VAL
2	F	369	THR
2	F	370	ILE
2	F	371	ARG
2	F	378	GLU
2	F	386	MET
2	F	387	ARG

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	184	HIS
1	A	241	GLN
1	A	294	GLN
1	A	318	ASN
1	C	136	ASN
1	C	145	HIS
1	C	241	GLN
1	C	294	GLN
1	C	315	HIS
1	C	318	ASN
2	D	388	GLN
1	E	145	HIS

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Mol	Chain	Res	Type
1	E	238	ASN
1	E	241	GLN
1	E	318	ASN
2	F	388	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 monosaccharides 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, 95^{th} 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	325/351 (92%)	-0.67	0 100 100	15, 28, 55, 72	4 (1%)
1	C	322/351 (91%)	-0.74	2 (0%) 89 88	15, 29, 53, 88	4 (1%)
1	E	322/351 (91%)	-0.71	3 (0%) 84 82	18, 29, 50, 87	4 (1%)
2	B	42/50 (84%)	-0.36	0 100 100	19, 37, 70, 101	0
2	D	42/50 (84%)	-0.35	1 (2%) 59 57	19, 34, 89, 125	0
2	F	43/50 (86%)	-0.24	1 (2%) 60 58	23, 41, 88, 117	0
All	All	1096/1203 (91%)	-0.66	7 (0%) 89 88	15, 30, 56, 125	12 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	378	GLU	4.0
1	C	334	ASP	3.0
1	C	328	LEU	3.0
2	F	378	GLU	2.9
1	E	329	PRO	2.6
1	E	334	ASP	2.1
1	E	330	ASP	2.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.