



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:58 PM GMT

PDB ID : 1DF0
Title : Crystal structure of M-Calpain
Authors : Hosfield, C.M.; Elce, J.S.; Davies, P.L.; Jia, Z.
Deposited on : 1999-11-16
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

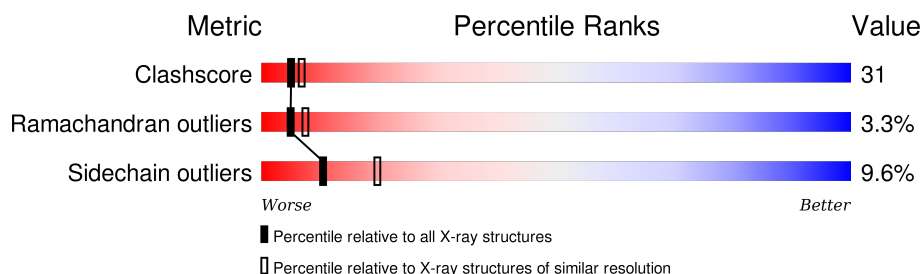
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	700	
2	B	184	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6749 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 M-CALPAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			4964	3169	833	939	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	ENGINEERED	UNP Q07009

- Molecule 2 is a protein called CALPAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1427	897	246	274	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	300	Total	O	0	0
			300	300		
3	B	58	Total	O	0	0
			58	58		

K95	R96		T99	D100	R101	S102	G103		L110	P111		E116		H120		I125	Y126	S127	M128	I129	I130	R131		R151	L152		M155	F156		F159	R160		D163	K164	M165	G166	T167	G168	Q169	I170		M173	I174	Q175		L178	Q179	L180	T181	M182	Y183	S184
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.70 Å 80.18 Å 80.72 Å 60.37° 70.85° 79.49°	Depositor
Resolution (Å)	25.00 – 2.60	Depositor
% Data completeness (in resolution range)	96.6 (25.00-2.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6749	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

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	0.48	0/5070	0.72	3/6841 (0.0%)
2	B	0.54	0/1454	0.73	2/1955 (0.1%)
All	All	0.49	0/6524	0.72	5/8796 (0.1%)

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
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	529	ASP	N-CA-C	-6.43	93.64	111.00
1	A	373	GLY	N-CA-C	6.43	129.16	113.10
2	B	156	PHE	CB-CG-CD1	-5.46	116.98	120.80
2	B	152	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	289	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
2	B	156	PHE	Sidechain

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	4964	0	4807	337	0
2	B	1427	0	1375	77	0
3	A	300	0	0	20	0
3	B	58	0	0	6	0
All	All	6749	0	6182	390	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 31.

All (390) 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:A:281:LEU:HD21	1:A:326:MET:H	1.16	1.08
1:A:281:LEU:HD22	1:A:325:TRP:HE3	1.12	1.06
1:A:523:ILE:H	1:A:523:ILE:HD12	1.23	1.01
1:A:692:ILE:HD12	1:A:692:ILE:H	1.27	0.97
1:A:281:LEU:HD22	1:A:325:TRP:CE3	1.99	0.95
1:A:466:ILE:HD13	1:A:466:ILE:H	1.30	0.94
1:A:373:GLY:H	1:A:384:ASN:HD21	1.16	0.92
1:A:286:ASN:ND2	1:A:288:TRP:H	1.68	0.92
1:A:413:GLN:HE22	1:A:427:HIS:H	0.95	0.92
1:A:281:LEU:HD23	1:A:282:ILE:N	1.86	0.91
1:A:373:GLY:N	1:A:384:ASN:HD21	1.70	0.89
1:A:654:GLU:HG2	1:A:656:ILE:HG22	1.55	0.88
1:A:375:ARG:O	1:A:375:ARG:HD3	1.74	0.88
1:A:281:LEU:HD21	1:A:326:MET:N	1.90	0.86
2:B:110:LEU:HD13	2:B:130:ILE:HD12	1.57	0.85
1:A:652:ASP:OD1	1:A:656:ILE:HG23	1.77	0.84
1:A:413:GLN:HE22	1:A:427:HIS:N	1.75	0.84
1:A:413:GLN:NE2	1:A:427:HIS:H	1.76	0.83
2:B:15:ARG:HD3	2:B:16:GLN:N	1.93	0.83
1:A:373:GLY:H	1:A:384:ASN:ND2	1.75	0.83
1:A:359:THR:HG21	1:A:509:TYR:HB3	1.62	0.82
1:A:375:ARG:HD3	1:A:375:ARG:C	2.01	0.81
1:A:229:GLN:O	1:A:233:GLU:HG3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ILE:N	1:A:466:ILE:HD13	1.96	0.80
1:A:367:ARG:H	1:A:494:ASN:HD21	1.29	0.79
1:A:367:ARG:H	1:A:494:ASN:ND2	1.80	0.79
1:A:373:GLY:CA	1:A:384:ASN:HD21	1.96	0.78
1:A:287:PRO:HG2	1:A:288:TRP:CE3	2.20	0.77
1:A:369:SER:HB3	1:A:647:VAL:HG11	1.66	0.77
1:A:699:VAL:O	1:A:700:LEU:HG	1.85	0.77
2:B:178:LEU:O	2:B:182:MET:HB2	1.85	0.76
1:A:417:ARG:HG2	3:A:761:HOH:O	1.85	0.76
1:A:373:GLY:HA2	1:A:384:ASN:HD21	1.50	0.75
1:A:36:ARG:HH21	1:A:37:ASN:HD21	1.35	0.74
1:A:4:ILE:HD11	2:B:180:LEU:HA	1.70	0.73
1:A:286:ASN:HD22	1:A:286:ASN:C	1.92	0.72
1:A:225:PHE:CE1	1:A:280:LYS:HG3	2.24	0.72
1:A:700:LEU:HD13	2:B:128:MET:HG2	1.72	0.71
1:A:700:LEU:HD22	2:B:128:MET:HG2	1.72	0.71
1:A:469:ARG:HD2	3:A:980:HOH:O	1.90	0.71
2:B:164:LYS:HG3	2:B:165:ASN:H	1.54	0.71
1:A:282:ILE:HD12	1:A:282:ILE:O	1.90	0.70
2:B:9:ASN:HA	3:B:233:HOH:O	1.91	0.70
1:A:388:LEU:HD22	1:A:482:TYR:O	1.92	0.70
1:A:399:GLU:HG2	1:A:400:ASP:N	2.07	0.70
1:A:466:ILE:HD11	1:A:471:VAL:HG12	1.73	0.69
1:A:500:ARG:HD3	3:A:988:HOH:O	1.92	0.69
2:B:110:LEU:CD1	2:B:130:ILE:HD12	2.23	0.69
1:A:343:LEU:HG	1:A:347:THR:HG21	1.75	0.69
1:A:281:LEU:CD1	1:A:325:TRP:HB3	2.23	0.68
1:A:529:ASP:O	1:A:530:ILE:HB	1.94	0.68
1:A:667:VAL:HG12	1:A:671:ILE:HD11	1.74	0.68
2:B:60:CYS:HA	2:B:63:MET:CE	2.24	0.68
1:A:286:ASN:HD22	1:A:288:TRP:H	1.41	0.68
1:A:392:GLU:O	1:A:479:PRO:HB3	1.94	0.68
1:A:654:GLU:HG2	1:A:654:GLU:O	1.93	0.68
1:A:120:ILE:HD11	1:A:343:LEU:HD21	1.75	0.67
1:A:614:ILE:CD1	1:A:629:LYS:HD2	2.24	0.67
1:A:89:ILE:HG12	1:A:175:GLU:HG3	1.77	0.67
1:A:269:ALA:HA	1:A:281:LEU:O	1.95	0.67
1:A:394:GLU:HA	1:A:405:CYS:SG	2.35	0.67
1:A:408:LEU:HD22	1:A:472:LEU:HD11	1.77	0.67
1:A:281:LEU:HD11	1:A:325:TRP:HB3	1.76	0.67
1:A:281:LEU:CD2	1:A:326:MET:H	2.01	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:CD1	2:B:180:LEU:HD23	2.25	0.66
1:A:512:VAL:O	1:A:512:VAL:HG13	1.96	0.66
1:A:359:THR:HG21	1:A:509:TYR:CB	2.26	0.66
1:A:452:PHE:C	1:A:454:LEU:H	1.99	0.66
1:A:281:LEU:HG	1:A:326:MET:O	1.96	0.66
1:A:699:VAL:HG12	2:B:151:ARG:NH1	2.10	0.66
2:B:125:ILE:O	2:B:129:ILE:HG13	1.97	0.65
1:A:668:ARG:HG2	2:B:182:MET:HE2	1.78	0.65
1:A:689:LEU:HD12	1:A:694:TRP:HE3	1.61	0.65
1:A:281:LEU:HD23	1:A:282:ILE:H	1.60	0.65
1:A:528:GLU:O	1:A:529:ASP:CB	2.45	0.64
2:B:16:GLN:O	2:B:19:LYS:HB3	1.96	0.64
1:A:614:ILE:HD12	1:A:629:LYS:HD2	1.78	0.64
1:A:449:SER:N	3:A:900:HOH:O	2.30	0.64
1:A:73:ILE:HG12	1:A:166:LEU:HD11	1.79	0.64
1:A:373:GLY:HA2	1:A:384:ASN:ND2	2.13	0.63
1:A:604:ILE:O	1:A:608:GLN:HG3	1.98	0.63
1:A:53:ALA:HB3	1:A:157:ARG:HH21	1.63	0.63
2:B:34:THR:HG22	3:B:189:HOH:O	1.99	0.63
1:A:78:PRO:HA	1:A:81:ILE:HG22	1.81	0.63
1:A:649:ARG:HH21	1:A:668:ARG:HH12	1.47	0.62
1:A:654:GLU:HG2	1:A:656:ILE:CG2	2.29	0.62
1:A:281:LEU:CD2	1:A:325:TRP:HB3	2.30	0.62
1:A:18:LEU:CD1	1:A:25:ILE:HG12	2.30	0.62
1:A:699:VAL:HG22	3:A:975:HOH:O	1.99	0.61
1:A:488:THR:HG22	1:A:490:GLU:O	2.01	0.61
1:A:523:ILE:H	1:A:523:ILE:CD1	1.95	0.61
2:B:43:VAL:HG11	2:B:84:TRP:CH2	2.36	0.61
1:A:64:GLY:O	1:A:67:SER:HB3	2.00	0.61
1:A:286:ASN:HD22	1:A:287:PRO:N	1.99	0.61
1:A:386:GLN:HB2	1:A:512:VAL:HG13	1.82	0.61
1:A:436:VAL:CG2	1:A:481:GLU:HB2	2.31	0.61
1:A:4:ILE:HD12	2:B:180:LEU:HD23	1.82	0.61
1:A:99:GLN:NE2	1:A:168:VAL:HG23	2.16	0.61
2:B:38:ASN:O	2:B:42:LYS:HG3	2.00	0.61
1:A:433:ILE:HG12	1:A:484:LEU:HD22	1.82	0.60
1:A:373:GLY:HA3	1:A:487:SER:HB2	1.82	0.60
1:A:233:GLU:O	1:A:353:TYR:O	2.19	0.60
2:B:59:THR:O	2:B:63:MET:HG3	2.00	0.60
1:A:452:PHE:O	1:A:454:LEU:N	2.35	0.60
1:A:155:ASP:OD2	1:A:157:ARG:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:HB2	1:A:169:HIS:CD2	2.37	0.60
1:A:552:GLU:O	1:A:555:THR:HG22	2.00	0.60
2:B:60:CYS:HA	2:B:63:MET:HE3	1.83	0.59
1:A:285:ARG:HD3	1:A:286:ASN:N	2.18	0.59
1:A:624:SER:OG	1:A:655:LEU:HB3	2.02	0.59
1:A:65:PRO:O	1:A:66:TYR:HB2	2.03	0.59
1:A:523:ILE:HD12	1:A:523:ILE:N	2.06	0.58
1:A:374:CYS:N	1:A:381:PHE:HD1	2.01	0.58
1:A:83:ALA:O	1:A:84:ASP:HB2	2.04	0.58
1:A:219:LYS:HG3	1:A:219:LYS:O	2.03	0.58
1:A:695:LEU:O	1:A:699:VAL:HG22	2.04	0.58
2:B:160:ARG:HG3	2:B:160:ARG:HH11	1.68	0.58
2:B:163:ASP:HA	3:B:242:HOH:O	2.03	0.58
1:A:78:PRO:HA	1:A:81:ILE:CG2	2.33	0.57
1:A:181:LEU:HD12	1:A:181:LEU:O	2.03	0.57
1:A:523:ILE:HD13	1:A:599:ILE:HG23	1.85	0.57
1:A:421:LYS:HD2	1:A:424:GLU:OE2	2.04	0.57
1:A:436:VAL:HG22	1:A:481:GLU:HB2	1.86	0.57
1:A:375:ARG:O	1:A:377:TYR:N	2.38	0.57
1:A:238:LEU:HD12	1:A:238:LEU:N	2.20	0.57
1:A:612:ARG:HG3	1:A:618:ARG:NH1	2.20	0.57
1:A:281:LEU:HD21	1:A:325:TRP:HB3	1.87	0.57
1:A:527:GLU:C	1:A:528:GLU:O	2.42	0.57
1:A:576:THR:O	1:A:579:ILE:HG13	2.05	0.57
1:A:388:LEU:C	1:A:388:LEU:HD13	2.24	0.56
1:A:286:ASN:HD21	1:A:288:TRP:HB2	1.71	0.56
1:A:376:ASN:N	1:A:376:ASN:HD22	2.03	0.56
1:A:654:GLU:O	1:A:654:GLU:CG	2.53	0.56
1:A:700:LEU:HD13	2:B:128:MET:CG	2.35	0.56
2:B:9:ASN:N	2:B:9:ASN:HD22	2.04	0.56
1:A:165:LEU:H	1:A:165:LEU:HD22	1.70	0.56
1:A:699:VAL:HG13	3:A:975:HOH:O	2.06	0.56
1:A:386:GLN:HE22	1:A:451:ASN:H	1.53	0.56
1:A:699:VAL:C	1:A:700:LEU:HG	2.26	0.56
1:A:285:ARG:HD3	1:A:285:ARG:C	2.25	0.56
1:A:386:GLN:HB2	1:A:512:VAL:CG1	2.35	0.56
1:A:47:GLN:HB3	1:A:157:ARG:HH12	1.71	0.56
1:A:386:GLN:HE21	1:A:512:VAL:HG13	1.72	0.55
1:A:105:SER:HA	1:A:108:LEU:HD23	1.88	0.55
1:A:412:ILE:HG13	1:A:469:ARG:O	2.06	0.55
1:A:73:ILE:HG12	1:A:166:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ILE:O	1:A:560:VAL:HG23	2.06	0.55
1:A:205:GLU:HG2	1:A:210:GLY:O	2.07	0.55
1:A:375:ARG:C	1:A:375:ARG:CD	2.70	0.55
2:B:87:ILE:O	2:B:91:GLN:HB2	2.07	0.55
1:A:287:PRO:HG2	1:A:288:TRP:CZ3	2.42	0.55
1:A:406:THR:HA	1:A:475:PHE:O	2.06	0.55
2:B:45:THR:HG23	2:B:45:THR:O	2.07	0.55
1:A:81:ILE:HG12	1:A:81:ILE:O	2.07	0.55
1:A:282:ILE:HD11	1:A:331:PHE:HB2	1.88	0.54
1:A:466:ILE:CD1	1:A:466:ILE:N	2.68	0.54
2:B:163:ASP:OD1	2:B:167:THR:O	2.24	0.54
1:A:579:ILE:HD11	1:A:664:ARG:HD3	1.89	0.54
1:A:144:TRP:CG	1:A:209:GLY:HA2	2.42	0.54
1:A:377:TYR:CD2	1:A:491:PRO:HD3	2.42	0.54
1:A:610:ILE:O	1:A:614:ILE:HG12	2.07	0.54
1:A:472:LEU:HD13	1:A:472:LEU:C	2.28	0.54
1:A:575:GLU:O	1:A:579:ILE:HG12	2.08	0.54
1:A:639:PRO:HD2	1:A:642:LEU:HD12	1.88	0.54
2:B:60:CYS:HA	2:B:63:MET:HE2	1.88	0.54
1:A:84:ASP:H	1:A:85:PRO:CD	2.21	0.54
1:A:525:ALA:O	1:A:526:ASN:C	2.46	0.54
1:A:211:ILE:HD12	1:A:212:ALA:H	1.72	0.53
1:A:268:GLY:O	1:A:282:ILE:HA	2.08	0.53
2:B:167:THR:O	2:B:169:GLN:N	2.42	0.53
1:A:409:VAL:O	1:A:472:LEU:HD22	2.08	0.53
1:A:643:HIS:O	1:A:647:VAL:HG12	2.08	0.53
2:B:96:ARG:HH11	2:B:96:ARG:HG2	1.73	0.53
1:A:667:VAL:HG12	1:A:671:ILE:CD1	2.39	0.53
1:A:374:CYS:N	1:A:381:PHE:CD1	2.77	0.53
1:A:529:ASP:O	1:A:530:ILE:O	2.27	0.53
1:A:161:LYS:HB3	1:A:166:LEU:HD21	1.91	0.53
1:A:140:HIS:HD2	1:A:151:GLU:OE2	1.91	0.53
1:A:427:HIS:HE1	1:A:494:ASN:O	1.92	0.52
1:A:372:GLY:O	1:A:491:PRO:HB3	2.08	0.52
1:A:18:LEU:HD11	1:A:25:ILE:HG12	1.91	0.52
1:A:234:LYS:HD3	1:A:354:LYS:O	2.09	0.52
1:A:354:LYS:HE2	1:A:354:LYS:HA	1.90	0.52
1:A:399:GLU:CG	1:A:400:ASP:N	2.72	0.52
1:A:18:LEU:HD13	1:A:25:ILE:HG12	1.91	0.52
2:B:45:THR:O	2:B:46:ARG:HB2	2.09	0.52
1:A:672:LEU:HG	2:B:181:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLN:O	1:A:133:GLU:O	2.28	0.52
1:A:700:LEU:HD13	2:B:128:MET:HE3	1.92	0.52
1:A:574:ILE:HG22	3:A:730:HOH:O	2.09	0.51
1:A:240:CYS:HA	1:A:337:ARG:O	2.10	0.51
1:A:30:GLN:HB3	1:A:35:LEU:HD11	1.93	0.51
1:A:488:THR:CG2	1:A:490:GLU:O	2.59	0.51
1:A:557:LEU:O	1:A:561:LEU:HG	2.11	0.51
1:A:452:PHE:C	1:A:454:LEU:N	2.64	0.51
1:A:234:LYS:HA	1:A:354:LYS:O	2.10	0.51
1:A:107:LEU:HD13	1:A:182:GLU:HG3	1.93	0.51
1:A:408:LEU:CD2	1:A:472:LEU:HD11	2.40	0.51
2:B:126:TYR:C	2:B:128:MET:H	2.13	0.51
1:A:3:GLY:C	2:B:69:SER:HB3	2.31	0.51
1:A:75:TRP:CZ3	1:A:159:PRO:HD3	2.46	0.51
1:A:585:ASP:C	1:A:587:ASP:H	2.14	0.51
1:A:520:ILE:HD12	1:A:520:ILE:N	2.25	0.51
1:A:367:ARG:CZ	1:A:655:LEU:HD21	2.41	0.51
1:A:609:LYS:HB3	1:A:609:LYS:HZ2	1.75	0.51
1:A:114:LEU:HB3	1:A:121:LEU:HD13	1.92	0.51
1:A:472:LEU:HD13	1:A:473:ASN:N	2.26	0.50
1:A:395:ASP:OD2	1:A:406:THR:HB	2.12	0.50
1:A:124:VAL:O	1:A:124:VAL:HG22	2.11	0.50
2:B:27:ASP:OD2	2:B:27:ASP:N	2.44	0.50
1:A:53:ALA:CB	1:A:157:ARG:HH21	2.24	0.50
1:A:51:PHE:HB2	1:A:187:LYS:HE3	1.94	0.50
1:A:350:CYS:HB3	1:A:353:TYR:HD2	1.75	0.50
2:B:126:TYR:O	2:B:130:ILE:HG12	2.11	0.50
1:A:692:ILE:H	1:A:692:ILE:CD1	2.03	0.50
1:A:286:ASN:ND2	1:A:286:ASN:C	2.62	0.50
1:A:127:LEU:N	1:A:127:LEU:HD22	2.28	0.49
2:B:110:LEU:HB2	2:B:111:PRO:HD3	1.94	0.49
1:A:223:ASN:HD22	1:A:226:LYS:HE2	1.77	0.49
2:B:50:LEU:HD23	2:B:95:LYS:HG3	1.94	0.49
1:A:654:GLU:O	1:A:656:ILE:HG22	2.11	0.49
1:A:522:GLU:OE1	1:A:522:GLU:HA	2.12	0.49
1:A:622:MET:HG2	1:A:623:ASN:N	2.27	0.49
2:B:15:ARG:NH1	2:B:16:GLN:OE1	2.45	0.49
2:B:160:ARG:HG3	2:B:160:ARG:NH1	2.27	0.49
1:A:237:LEU:HB2	1:A:341:CYS:HB3	1.95	0.49
1:A:187:LYS:O	1:A:189:ASN:N	2.45	0.49
2:B:50:LEU:HD21	2:B:94:TYR:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LYS:HD2	3:A:778:HOH:O	2.12	0.49
1:A:692:ILE:N	1:A:692:ILE:HD12	2.12	0.49
1:A:694:TRP:CE2	1:A:698:SER:OG	2.65	0.49
1:A:161:LYS:O	1:A:162:ASP:HB2	2.13	0.49
1:A:222:PRO:O	1:A:224:LEU:N	2.45	0.49
1:A:271:GLU:HA	1:A:279:GLN:O	2.13	0.49
1:A:364:ASN:HD21	1:A:644:GLN:HE22	1.61	0.49
1:A:627:MET:HG2	1:A:657:ILE:HD12	1.94	0.49
1:A:78:PRO:HG2	1:A:131:PHE:HZ	1.78	0.48
1:A:105:SER:HA	1:A:108:LEU:CD2	2.43	0.48
2:B:40:LEU:O	2:B:44:VAL:HG22	2.13	0.48
2:B:44:VAL:HG23	2:B:45:THR:N	2.28	0.48
1:A:699:VAL:O	1:A:700:LEU:CG	2.60	0.48
1:A:359:THR:CG2	1:A:509:TYR:HB3	2.38	0.48
1:A:373:GLY:O	1:A:374:CYS:CB	2.60	0.48
1:A:373:GLY:HA3	1:A:487:SER:CB	2.42	0.48
2:B:34:THR:CG2	3:B:189:HOH:O	2.61	0.48
1:A:211:ILE:HB	1:A:502:PHE:CE2	2.49	0.48
2:B:125:ILE:O	2:B:128:MET:HB3	2.14	0.48
1:A:415:HIS:CE1	1:A:419:GLN:HB2	2.49	0.48
1:A:46:PHE:HD1	1:A:155:ASP:HB3	1.79	0.48
1:A:84:ASP:N	1:A:85:PRO:CD	2.76	0.48
1:A:369:SER:CB	1:A:647:VAL:HG11	2.41	0.48
1:A:373:GLY:N	1:A:384:ASN:ND2	2.45	0.47
1:A:488:THR:CG2	1:A:489:PHE:N	2.78	0.47
1:A:618:ARG:NH2	3:A:916:HOH:O	2.47	0.47
1:A:373:GLY:H	1:A:384:ASN:CG	2.18	0.47
1:A:668:ARG:HG2	2:B:182:MET:CE	2.44	0.47
1:A:579:ILE:CD1	1:A:664:ARG:HD3	2.45	0.47
1:A:627:MET:HE3	1:A:631:LEU:HG	1.95	0.47
2:B:159:PHE:CE1	2:B:170:ILE:HG23	2.49	0.47
1:A:460:GLU:O	1:A:461:ARG:CB	2.63	0.47
1:A:382:TRP:HE3	1:A:451:ASN:O	1.98	0.47
1:A:364:ASN:HB3	3:A:985:HOH:O	2.15	0.47
1:A:595:LYS:O	1:A:599:ILE:HG13	2.14	0.47
1:A:585:ASP:O	1:A:586:GLU:HB2	2.15	0.47
1:A:455:THR:HA	3:A:903:HOH:O	2.14	0.47
1:A:689:LEU:HD13	1:A:694:TRP:HA	1.96	0.47
1:A:3:GLY:O	2:B:69:SER:HB3	2.14	0.47
1:A:62:GLU:C	1:A:63:LEU:HD12	2.35	0.47
2:B:51:LYS:HB3	2:B:103:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:NE	3:A:978:HOH:O	2.46	0.47
1:A:685:GLY:O	2:B:173:ASN:HA	2.14	0.47
1:A:672:LEU:HD23	2:B:182:MET:CE	2.45	0.47
2:B:164:LYS:HG3	2:B:165:ASN:N	2.24	0.47
2:B:20:LEU:O	2:B:24:LEU:HG	2.16	0.47
1:A:654:GLU:OE2	1:A:656:ILE:HG21	2.15	0.46
1:A:106:TRP:CE2	1:A:198:GLY:HA3	2.50	0.46
1:A:124:VAL:CG2	1:A:124:VAL:O	2.63	0.46
1:A:486:PRO:HB3	1:A:499:ILE:HD11	1.97	0.46
1:A:13:GLU:OE2	1:A:13:GLU:HA	2.16	0.46
1:A:351:ASP:OD2	1:A:351:ASP:N	2.48	0.46
1:A:676:PHE:CZ	1:A:687:ILE:HG23	2.51	0.46
1:A:696:SER:O	1:A:700:LEU:HB2	2.15	0.46
2:B:110:LEU:HD13	2:B:130:ILE:CD1	2.39	0.46
1:A:30:GLN:HE22	1:A:187:LYS:NZ	2.14	0.46
1:A:30:GLN:NE2	1:A:50:SER:OG	2.48	0.46
1:A:386:GLN:CB	1:A:512:VAL:CG1	2.94	0.46
1:A:576:THR:OG1	1:A:660:ASP:OD1	2.30	0.46
1:A:369:SER:HB3	1:A:647:VAL:CG1	2.43	0.46
1:A:527:GLU:O	1:A:528:GLU:O	2.34	0.46
1:A:323:GLU:O	1:A:324:PHE:HB3	2.16	0.46
1:A:405:CYS:O	1:A:476:LYS:HA	2.15	0.46
2:B:128:MET:HG3	3:B:198:HOH:O	2.16	0.46
2:B:167:THR:C	2:B:169:GLN:H	2.19	0.46
1:A:617:ASP:O	1:A:618:ARG:C	2.54	0.46
1:A:211:ILE:HG21	1:A:502:PHE:CD2	2.51	0.45
1:A:609:LYS:NZ	1:A:609:LYS:HB3	2.32	0.45
1:A:686:THR:HG22	2:B:173:ASN:CA	2.46	0.45
1:A:261:GLY:N	3:A:886:HOH:O	2.49	0.45
1:A:326:MET:HE2	1:A:330:ASP:HB3	1.99	0.45
1:A:672:LEU:CD2	2:B:182:MET:HE2	2.47	0.45
2:B:14:GLU:O	2:B:17:PHE:HB2	2.16	0.45
1:A:563:LYS:C	3:A:1000:HOH:O	2.53	0.45
1:A:373:GLY:CA	1:A:384:ASN:ND2	2.71	0.45
1:A:37:ASN:N	1:A:37:ASN:HD22	2.13	0.45
1:A:400:ASP:O	1:A:401:GLY:O	2.34	0.45
1:A:78:PRO:HG2	1:A:131:PHE:CZ	2.51	0.45
2:B:43:VAL:HG11	2:B:84:TRP:HH2	1.79	0.45
1:A:54:LEU:HB3	1:A:55:PRO:HD2	1.98	0.45
1:A:329:SER:O	1:A:333:ARG:HG3	2.16	0.45
2:B:30:GLU:HB3	2:B:74:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ILE:HG21	1:A:602:THR:HG21	1.99	0.45
1:A:206:ASP:OD2	1:A:469:ARG:NH2	2.42	0.44
1:A:538:PHE:CD2	1:A:594:LEU:HD23	2.53	0.44
1:A:532:ASP:O	1:A:536:ARG:HG3	2.17	0.44
3:A:975:HOH:O	2:B:155:MET:HG3	2.17	0.44
1:A:153:VAL:O	1:A:154:VAL:HG13	2.17	0.44
1:A:539:ALA:HB2	3:A:727:HOH:O	2.17	0.44
1:A:558:ARG:HH12	1:A:559:ARG:NH1	2.16	0.44
1:A:99:GLN:OE1	1:A:103:GLY:HA3	2.17	0.44
1:A:146:TYR:CD2	1:A:414:LYS:HA	2.53	0.44
1:A:96:ASP:HB2	1:A:171:ALA:HB3	1.99	0.44
1:A:699:VAL:HG12	2:B:151:ARG:CZ	2.48	0.44
2:B:9:ASN:CA	3:B:233:HOH:O	2.59	0.44
1:A:360:LYS:HA	1:A:499:ILE:O	2.18	0.44
1:A:95:THR:OG1	1:A:97:ILE:HG12	2.18	0.44
1:A:82:CYS:SG	1:A:85:PRO:HD3	2.58	0.43
1:A:187:LYS:C	1:A:189:ASN:H	2.22	0.43
1:A:627:MET:CE	1:A:631:LEU:HG	2.48	0.43
1:A:122:ALA:HA	1:A:127:LEU:HD21	1.99	0.43
1:A:432:GLY:HA2	1:A:462:SER:HA	2.00	0.43
1:A:183:LYS:HG2	1:A:192:TYR:OH	2.18	0.43
1:A:692:ILE:HD11	3:A:764:HOH:O	2.18	0.43
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.82	0.43
1:A:394:GLU:OE2	1:A:403:ARG:CB	2.66	0.43
1:A:78:PRO:O	1:A:81:ILE:HG22	2.18	0.43
1:A:463:ASP:O	1:A:464:THR:OG1	2.34	0.43
1:A:373:GLY:CA	1:A:487:SER:HB2	2.48	0.43
1:A:4:ILE:CD1	2:B:180:LEU:HA	2.46	0.43
1:A:512:VAL:CG1	1:A:512:VAL:O	2.65	0.43
2:B:25:ALA:O	2:B:28:ASP:HB2	2.18	0.43
1:A:473:ASN:HB3	1:A:475:PHE:CE1	2.54	0.43
1:A:391:LEU:HD22	1:A:391:LEU:N	2.34	0.43
1:A:462:SER:O	1:A:463:ASP:HB2	2.19	0.43
1:A:171:ALA:C	1:A:173:GLY:H	2.22	0.43
1:A:285:ARG:HD3	1:A:286:ASN:C	2.39	0.43
1:A:700:LEU:CD1	2:B:128:MET:HG2	2.45	0.43
1:A:520:ILE:HD12	1:A:520:ILE:H	1.84	0.42
1:A:8:LEU:O	1:A:12:ARG:HG3	2.18	0.42
2:B:31:VAL:HG12	2:B:32:SER:O	2.18	0.42
1:A:386:GLN:C	1:A:512:VAL:HG12	2.40	0.42
1:A:65:PRO:C	1:A:67:SER:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:C	1:A:189:ASN:N	2.72	0.42
1:A:686:THR:HG22	2:B:173:ASN:HA	2.01	0.42
1:A:672:LEU:HD23	2:B:182:MET:HE3	2.02	0.42
1:A:30:GLN:NE2	1:A:187:LYS:NZ	2.68	0.42
2:B:28:ASP:O	2:B:30:GLU:HG3	2.20	0.42
1:A:97:ILE:HG22	1:A:98:CYS:N	2.34	0.42
1:A:700:LEU:CD2	2:B:128:MET:HG2	2.45	0.42
1:A:160:THR:HG22	1:A:165:LEU:HD13	2.01	0.42
1:A:345:PRO:O	1:A:355:LYS:HE2	2.20	0.42
1:A:409:VAL:O	1:A:472:LEU:HA	2.19	0.42
1:A:78:PRO:HD3	1:A:156:ASP:O	2.20	0.42
1:A:125:VAL:O	1:A:125:VAL:HG12	2.19	0.42
1:A:104:ASP:OD1	1:A:196:SER:HA	2.20	0.42
1:A:426:MET:CE	1:A:469:ARG:HB3	2.49	0.42
1:A:382:TRP:O	1:A:450:LYS:HE3	2.20	0.42
1:A:423:GLY:N	3:A:704:HOH:O	2.47	0.42
1:A:205:GLU:OE1	1:A:211:ILE:HD12	2.20	0.41
1:A:671:ILE:HG12	3:A:976:HOH:O	2.20	0.41
1:A:407:PHE:CD2	1:A:409:VAL:HG23	2.55	0.41
2:B:99:THR:HG22	2:B:100:ASP:N	2.34	0.41
1:A:262:HIS:HD2	1:A:264:TYR:CZ	2.38	0.41
1:A:692:ILE:N	1:A:692:ILE:CD1	2.79	0.41
1:A:585:ASP:O	1:A:596:GLU:OE2	2.39	0.41
2:B:25:ALA:HB1	2:B:28:ASP:HB2	2.02	0.41
1:A:4:ILE:HD11	2:B:180:LEU:HD23	2.02	0.41
1:A:412:ILE:HA	1:A:469:ARG:O	2.20	0.41
1:A:376:ASN:ND2	1:A:376:ASN:N	2.67	0.41
1:A:539:ALA:CB	3:A:727:HOH:O	2.69	0.41
1:A:672:LEU:HD12	1:A:672:LEU:HA	1.94	0.41
1:A:394:GLU:HB3	1:A:404:GLY:O	2.21	0.41
1:A:638:LEU:HD22	1:A:642:LEU:HD13	2.03	0.41
1:A:30:GLN:HE22	1:A:187:LYS:HZ1	1.68	0.41
1:A:662:PHE:CZ	1:A:666:LEU:HD11	2.56	0.41
1:A:86:GLN:HG2	1:A:89:ILE:CD1	2.51	0.41
1:A:400:ASP:OD1	1:A:401:GLY:N	2.54	0.40
1:A:350:CYS:HB3	1:A:353:TYR:CD2	2.56	0.40
1:A:416:ARG:H	1:A:419:GLN:HG3	1.86	0.40
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.93	0.40
1:A:395:ASP:OD2	1:A:504:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

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	612/700 (87%)	528 (86%)	61 (10%)	23 (4%)	4	5
2	B	174/184 (95%)	162 (93%)	9 (5%)	3 (2%)	11	22
All	All	786/884 (89%)	690 (88%)	70 (9%)	26 (3%)	5	7

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	A	133	GLU
1	A	223	ASN
1	A	352	SER
1	A	354	LYS
1	A	373	GLY
1	A	453	PHE
1	A	461	ARG
1	A	526	ASN
1	A	528	GLU
1	A	655	LEU
2	B	46	ARG
1	A	376	ASN
1	A	398	ASP
1	A	401	GLY
1	A	462	SER
1	A	529	ASP
1	A	585	ASP
1	A	188	ILE
1	A	324	PHE
1	A	374	CYS
1	A	618	ARG
1	A	162	ASP
1	A	530	ILE
2	B	168	GLY

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Mol	Chain	Res	Type
2	B	164	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	520/603 (86%)	470 (90%)	50 (10%)	10	20
2	B	155/162 (96%)	140 (90%)	15 (10%)	10	19
All	All	675/765 (88%)	610 (90%)	65 (10%)	10	20

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	22	GLU
1	A	23	ARG
1	A	28	LEU
1	A	82	CYS
1	A	86	GLN
1	A	104	ASP
1	A	113	SER
1	A	170	SER
1	A	180	LEU
1	A	183	LYS
1	A	195	LEU
1	A	218	ARG
1	A	224	LEU
1	A	280	LYS
1	A	285	ARG
1	A	286	ASN
1	A	329	SER
1	A	337	ARG
1	A	343	LEU
1	A	353	TYR
1	A	355	LYS

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Mol	Chain	Res	Type
1	A	360	LYS
1	A	364	ASN
1	A	375	ARG
1	A	392	GLU
1	A	399	GLU
1	A	418	ARG
1	A	419	GLN
1	A	450	LYS
1	A	466	ILE
1	A	469	ARG
1	A	484	LEU
1	A	487	SER
1	A	488	THR
1	A	509	TYR
1	A	523	ILE
1	A	537	LEU
1	A	557	LEU
1	A	606	LYS
1	A	609	LYS
1	A	617	ASP
1	A	626	GLU
1	A	654	GLU
1	A	655	LEU
1	A	656	ILE
1	A	672	LEU
1	A	683	ASN
1	A	692	ILE
1	A	696	SER
2	B	9	ASN
2	B	15	ARG
2	B	17	PHE
2	B	27	ASP
2	B	34	THR
2	B	46	ARG
2	B	50	LEU
2	B	68	ASP
2	B	96	ARG
2	B	101	ARG
2	B	115	GLU
2	B	120	HIS
2	B	131	ARG
2	B	152	LEU

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Mol	Chain	Res	Type
2	B	175	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	37	ASN
1	A	47	GLN
1	A	129	GLN
1	A	169	HIS
1	A	286	ASN
1	A	334	HIS
1	A	364	ASN
1	A	376	ASN
1	A	379	ASN
1	A	384	ASN
1	A	386	GLN
1	A	413	GLN
1	A	419	GLN
1	A	427	HIS
1	A	451	ASN
1	A	492	HIS
1	A	494	ASN
1	A	608	GLN
1	A	644	GLN
1	A	683	ASN
2	B	23	GLN
2	B	47	HIS
2	B	91	GLN
2	B	139	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.