



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:06 PM UTC

PDB ID : 3DF0 / pdb_00003df0
Title : Calcium-dependent complex between m-calpain and calpastatin
Authors : Moldoveanu, T.; Gehring, K.; Green, D.R.
Deposited on : 2008-06-11
Resolution : 2.95 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
Xtrriage (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

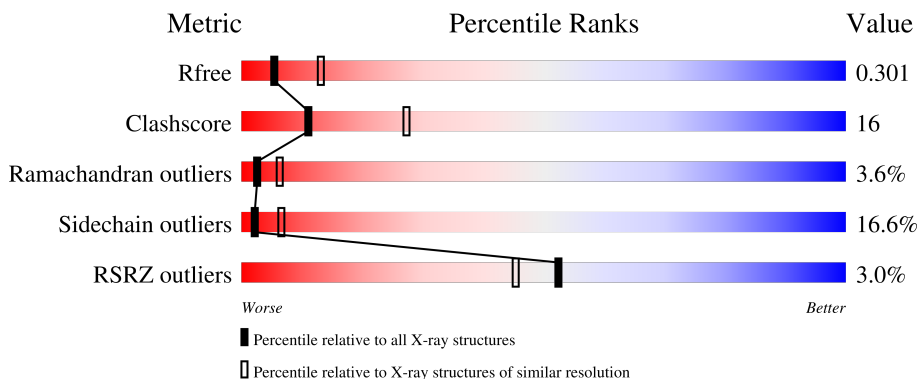
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	714	
2	B	184	
3	C	86	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7300 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 Calpain-2 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	676	5453	3468	915	1047	23	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	engineered mutation	UNP Q07009
A	701	GLY	-	expression tag	UNP Q07009
A	702	LYS	-	expression tag	UNP Q07009
A	703	LEU	-	expression tag	UNP Q07009
A	704	ALA	-	expression tag	UNP Q07009
A	705	ALA	-	expression tag	UNP Q07009
A	706	ALA	-	expression tag	UNP Q07009
A	707	LEU	-	expression tag	UNP Q07009
A	708	GLU	-	expression tag	UNP Q07009
A	709	HIS	-	expression tag	UNP Q07009
A	710	HIS	-	expression tag	UNP Q07009
A	711	HIS	-	expression tag	UNP Q07009
A	712	HIS	-	expression tag	UNP Q07009
A	713	HIS	-	expression tag	UNP Q07009
A	714	HIS	-	expression tag	UNP Q07009

- Molecule 2 is a protein called Calpain small subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	174	1411	888	243	270	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	MET	SER	variant	UNP Q64537

- Molecule 3 is a protein called Calpastatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	56	426	270	64	90	2	0	0	0

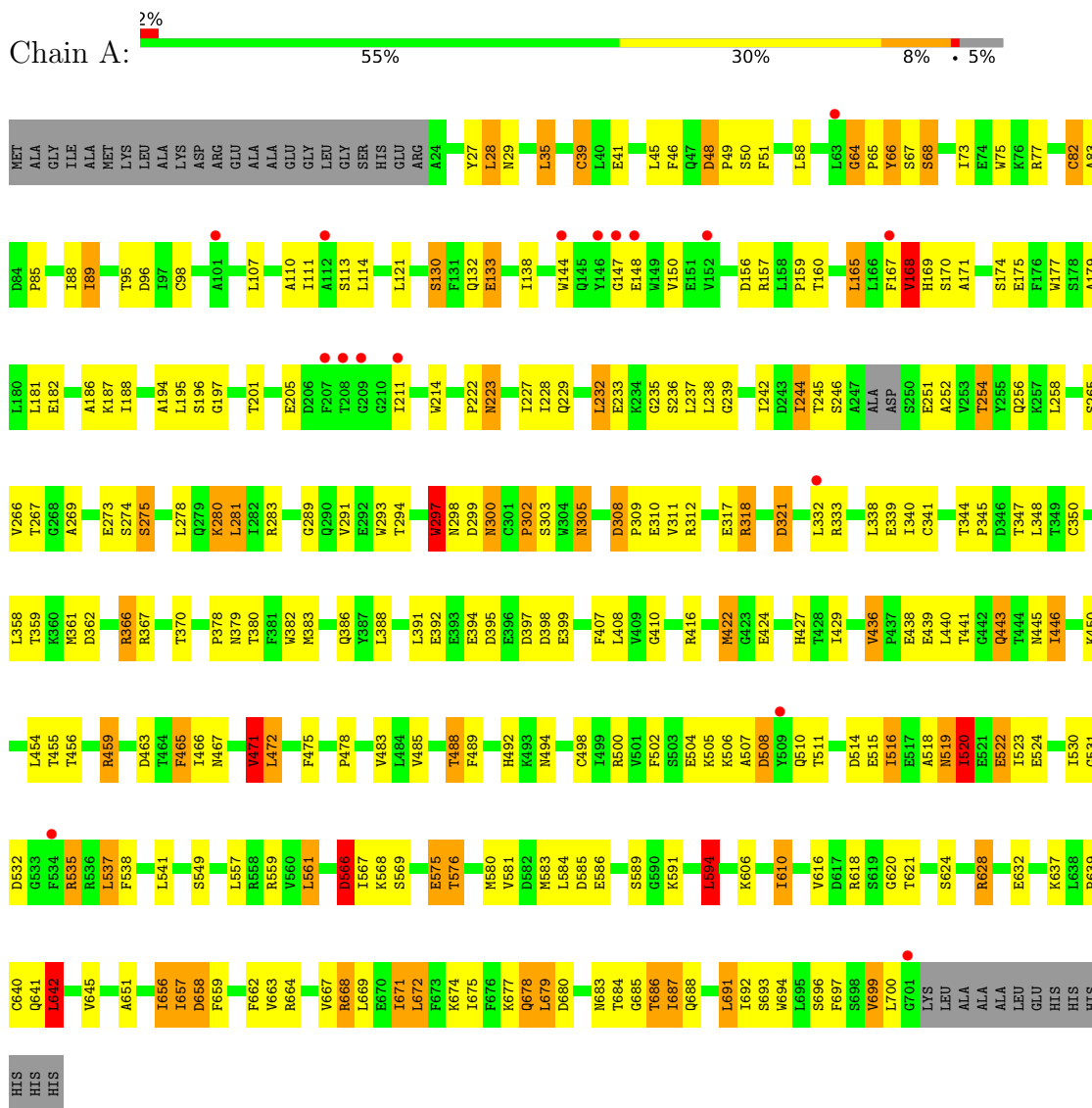
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	Ca	0	0
			6	6		
4	B	4	Total	Ca	0	0
			4	4		

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: Calpain-2 catalytic subunit

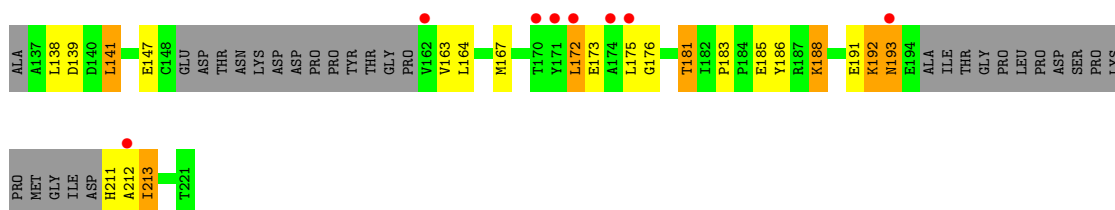


- Molecule 2: Calpain small subunit 1





- Molecule 3: Calpastatin



4 Data and refinement statistics i

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	147.39Å 147.39Å 47.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.95 49.15 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.95) 99.9 (49.15-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.299 0.223 , 0.301	Depositor DCC
R_{free} test set	1164 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 84.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7300	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.87	7/5575 (0.1%)	1.07	18/7536 (0.2%)
2	B	0.71	0/1438	1.02	3/1932 (0.2%)
3	C	0.84	1/430 (0.2%)	1.09	2/580 (0.3%)
All	All	0.84	8/7443 (0.1%)	1.06	23/10048 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	ASN	CG-OD1	17.84	1.57	1.23
1	A	305	ASN	CG-ND2	16.41	1.67	1.33
1	A	310	GLU	CD-OE1	12.36	1.48	1.25
3	C	188	LYS	CE-NZ	6.70	1.69	1.49
1	A	478	PRO	CA-C	6.54	1.55	1.51
1	A	300	ASN	C-O	5.20	1.31	1.23
1	A	471	VAL	CA-CB	5.14	1.60	1.54
1	A	520	ILE	CA-CB	5.02	1.61	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	GLN	N-CA-C	8.52	122.35	108.55
3	C	163	VAL	N-CA-C	7.94	119.34	107.75
1	A	64	GLY	CA-C-N	7.32	128.98	119.84
1	A	64	GLY	C-N-CA	7.32	128.98	119.84
3	C	213	ILE	N-CA-C	7.31	119.15	112.43
1	A	620	GLY	N-CA-C	-6.98	104.99	115.32
1	A	485	VAL	N-CA-C	6.80	114.88	108.15
2	B	114	ASP	N-CA-C	-6.67	104.72	112.92
1	A	671	ILE	N-CA-C	-6.33	105.53	111.48
1	A	488	THR	N-CA-C	-6.04	101.52	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ASN	CB-CG-ND2	-6.04	107.35	116.40
1	A	308	ASP	CA-C-N	6.02	125.90	119.28
1	A	308	ASP	C-N-CA	6.02	125.90	119.28
1	A	46	PHE	N-CA-C	5.94	118.93	109.24
2	B	156	ASP	N-CA-C	-5.81	105.95	113.16
1	A	305	ASN	CB-CG-OD1	5.77	132.34	120.80
1	A	642	LEU	N-CA-C	5.41	116.98	111.14
1	A	303	SER	N-CA-C	-5.35	106.60	113.23
1	A	297	TRP	N-CA-C	5.26	121.99	110.80
1	A	424	GLU	N-CA-C	5.14	117.17	110.43
1	A	688	GLN	N-CA-C	5.10	117.71	108.69
2	B	125	ILE	CB-CA-C	-5.06	105.22	111.70
1	A	658	ASP	N-CA-C	-5.01	104.06	110.53

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	5453	0	5294	189	0
2	B	1411	0	1362	48	0
3	C	426	0	413	14	0
4	A	6	0	0	0	0
4	B	4	0	0	0	0
All	All	7300	0	7069	235	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 16.

All (235) 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)
3:C:188:LYS:NZ	3:C:188:LYS:CE	1.69	1.55
1:A:305:ASN:CG	1:A:305:ASN:ND2	1.67	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ARG:HG3	1:A:668:ARG:HH11	1.15	1.08
1:A:679:LEU:HD23	1:A:687:ILE:HD11	1.07	1.06
2:B:268:MET:CE	2:B:268:MET:HA	1.88	1.01
3:C:176:GLY:HA2	3:C:181:THR:HG21	1.38	1.01
1:A:679:LEU:CD2	1:A:687:ILE:HD11	1.93	0.99
2:B:268:MET:HA	2:B:268:MET:HE2	1.46	0.98
1:A:679:LEU:HD23	1:A:687:ILE:CD1	1.96	0.94
1:A:168:VAL:HB	1:A:182:GLU:OE1	1.67	0.94
1:A:668:ARG:HG3	1:A:668:ARG:NH1	1.85	0.89
1:A:668:ARG:HH21	2:B:270:SER:HB3	1.38	0.86
1:A:516:ILE:H	1:A:516:ILE:HD12	1.42	0.85
1:A:621:THR:HB	1:A:656:ILE:HD12	1.57	0.85
1:A:317:GLU:HG2	1:A:318:ARG:H	1.43	0.83
1:A:675:ILE:HD13	1:A:697:PHE:CD2	2.18	0.79
2:B:149:MET:HE3	2:B:236:VAL:HG21	1.66	0.79
1:A:523:ILE:HG13	1:A:524:GLU:H	1.49	0.78
1:A:651:ALA:HB2	1:A:657:ILE:HD11	1.68	0.74
1:A:144:TRP:CH2	1:A:147:GLY:HA2	2.23	0.73
1:A:82:CYS:SG	1:A:174:SER:HB2	2.27	0.73
1:A:621:THR:CB	1:A:656:ILE:HD12	2.19	0.73
1:A:559:ARG:HG2	3:C:138:LEU:HD22	1.72	0.72
1:A:668:ARG:NH2	2:B:270:SER:HB3	2.05	0.72
1:A:566:ASP:OD1	1:A:566:ASP:N	2.23	0.72
3:C:176:GLY:CA	3:C:181:THR:HG21	2.19	0.72
1:A:197:GLY:HA2	3:C:175:LEU:O	1.89	0.71
1:A:168:VAL:CG1	1:A:179:ALA:HA	2.22	0.70
2:B:259:ASN:ND2	2:B:262:GLU:OE1	2.25	0.70
1:A:668:ARG:HH11	1:A:668:ARG:CG	2.00	0.68
1:A:532:ASP:HA	1:A:535:ARG:HB2	1.75	0.68
2:B:268:MET:HA	2:B:268:MET:HE3	1.74	0.68
1:A:96:ASP:O	1:A:170:SER:HA	1.94	0.68
1:A:510:GLN:O	1:A:511:THR:HB	1.93	0.67
1:A:397:ASP:OD2	1:A:399:GLU:HB2	1.95	0.67
1:A:523:ILE:HG23	1:A:524:GLU:HG3	1.77	0.66
1:A:201:THR:HG23	1:A:339:GLU:HB3	1.77	0.66
1:A:549:SER:HA	1:A:591:LYS:HG2	1.77	0.66
2:B:268:MET:HE2	2:B:268:MET:CA	2.24	0.65
1:A:684:THR:C	1:A:686:THR:H	2.03	0.65
1:A:488:THR:HG22	1:A:489:PHE:N	2.11	0.65
1:A:201:THR:CG2	1:A:339:GLU:HB3	2.26	0.65
1:A:167:PHE:O	1:A:168:VAL:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLY:O	1:A:338:LEU:HD12	1.99	0.63
1:A:567:ILE:O	1:A:567:ILE:HG22	1.97	0.63
2:B:150:VAL:HA	2:B:161:LEU:HD21	1.80	0.63
2:B:201:GLU:HA	2:B:205:PHE:O	1.98	0.62
1:A:668:ARG:HD3	2:B:268:MET:HE1	1.80	0.62
2:B:171:ASN:O	2:B:174:LYS:HG2	2.00	0.62
2:B:121:GLU:O	2:B:125:ILE:HG12	2.00	0.62
1:A:691:LEU:HD23	2:B:245:PHE:CD2	2.35	0.62
1:A:201:THR:HG21	1:A:214:TRP:HE1	1.65	0.61
1:A:107:LEU:O	1:A:110:ALA:HB3	2.00	0.61
1:A:302:PRO:HA	1:A:305:ASN:OD1	2.00	0.61
1:A:228:ILE:HG22	1:A:232:LEU:HD12	1.83	0.61
2:B:221:ASP:O	2:B:223:THR:N	2.33	0.61
1:A:407:PHE:C	1:A:408:LEU:HD12	2.25	0.60
2:B:196:LEU:HB3	2:B:197:PRO:HD3	1.83	0.60
1:A:684:THR:O	1:A:686:THR:N	2.34	0.60
1:A:305:ASN:ND2	1:A:305:ASN:CB	2.61	0.60
1:A:668:ARG:HE	2:B:270:SER:C	2.09	0.60
1:A:436:VAL:HG12	1:A:483:VAL:HG23	1.82	0.60
1:A:201:THR:O	1:A:205:GLU:HG3	2.02	0.59
1:A:422:MET:HG3	1:A:422:MET:O	1.97	0.59
1:A:581:VAL:O	1:A:583:MET:N	2.30	0.59
1:A:641:GLN:O	1:A:645:VAL:HG23	2.03	0.59
1:A:516:ILE:HD12	1:A:516:ILE:N	2.16	0.58
1:A:317:GLU:CG	1:A:318:ARG:H	2.14	0.58
1:A:651:ALA:HB2	1:A:657:ILE:CD1	2.33	0.58
1:A:111:ILE:HD13	1:A:181:LEU:HD23	1.86	0.57
1:A:516:ILE:HG21	2:B:260:ILE:HG13	1.86	0.57
1:A:113:SER:HB3	1:A:265:SER:OG	2.05	0.57
1:A:317:GLU:HG2	1:A:318:ARG:N	2.16	0.57
1:A:114:LEU:HD23	1:A:121:LEU:HD12	1.86	0.57
1:A:358:LEU:HD13	1:A:502:PHE:CE1	2.40	0.57
2:B:154:ASP:HA	2:B:165:GLU:OE1	2.05	0.56
1:A:488:THR:HG22	1:A:489:PHE:H	1.69	0.55
2:B:207:LEU:HD12	2:B:212:TYR:CE1	2.42	0.55
1:A:699:VAL:HG13	1:A:700:LEU:HG	1.88	0.54
2:B:153:MET:O	2:B:165:GLU:HG2	2.06	0.54
2:B:260:ILE:HG23	2:B:261:GLN:N	2.22	0.54
1:A:541:LEU:HD21	3:C:138:LEU:HG	1.90	0.54
1:A:606:LYS:O	1:A:610:ILE:HG12	2.07	0.54
1:A:75:TRP:CZ3	1:A:159:PRO:HD3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASP:OD2	1:A:505:LYS:HD2	2.08	0.53
1:A:130:SER:HB3	1:A:132:GLN:H	1.72	0.53
1:A:523:ILE:HG13	1:A:524:GLU:N	2.19	0.53
1:A:576:THR:HG23	1:A:664:ARG:HD3	1.91	0.53
1:A:309:PRO:HA	1:A:312:ARG:HB3	1.91	0.53
1:A:382:TRP:CE3	1:A:382:TRP:O	2.62	0.53
1:A:366:ARG:HA	1:A:494:ASN:OD1	2.09	0.53
2:B:157:THR:C	2:B:159:GLY:H	2.16	0.53
1:A:585:ASP:OD2	1:A:589:SER:O	2.26	0.53
1:A:347:THR:HG23	1:A:350:CYS:HB3	1.90	0.53
2:B:268:MET:O	2:B:269:TYR:HD2	1.92	0.52
1:A:144:TRP:CZ2	1:A:147:GLY:HA2	2.44	0.52
1:A:692:ILE:HD12	1:A:693:SER:N	2.25	0.52
1:A:699:VAL:CG1	1:A:700:LEU:HG	2.38	0.52
1:A:659:PHE:O	1:A:662:PHE:HB3	2.10	0.52
1:A:82:CYS:SG	1:A:174:SER:CB	2.98	0.51
1:A:274:SER:O	1:A:275:SER:C	2.53	0.51
2:B:260:ILE:HG23	2:B:261:GLN:H	1.74	0.51
1:A:96:ASP:OD1	1:A:175:GLU:OE1	2.28	0.51
1:A:236:SER:C	1:A:237:LEU:HD23	2.35	0.51
1:A:510:GLN:O	1:A:511:THR:CB	2.59	0.51
1:A:280:LYS:HE2	1:A:280:LYS:H	1.75	0.51
1:A:675:ILE:HD13	1:A:697:PHE:HD2	1.72	0.51
3:C:192:LYS:O	3:C:193:ASN:CB	2.59	0.51
2:B:158:THR:C	2:B:160:LYS:H	2.19	0.51
1:A:380:THR:O	1:A:383:MET:HG2	2.11	0.50
1:A:229:GLN:HG3	1:A:269:ALA:HB1	1.93	0.50
1:A:561:LEU:HD11	1:A:569:SER:HB2	1.94	0.50
1:A:114:LEU:CD2	1:A:121:LEU:HD12	2.42	0.50
1:A:440:LEU:HD13	1:A:446:ILE:HG13	1.93	0.50
1:A:523:ILE:CG1	1:A:524:GLU:H	2.22	0.50
1:A:167:PHE:HB3	1:A:182:GLU:OE2	2.11	0.50
1:A:83:ALA:O	1:A:85:PRO:HD3	2.12	0.49
1:A:680:ASP:CG	1:A:680:ASP:O	2.54	0.49
1:A:379:ASN:HA	1:A:450:LYS:HE3	1.94	0.49
1:A:677:LYS:O	1:A:678:GLN:HB2	2.12	0.49
1:A:466:ILE:HD11	3:C:172:LEU:HD23	1.94	0.49
1:A:691:LEU:HD23	2:B:245:PHE:CG	2.48	0.49
1:A:168:VAL:HB	1:A:182:GLU:CD	2.36	0.49
1:A:186:ALA:HA	1:A:195:LEU:HD21	1.95	0.49
2:B:216:ILE:O	2:B:220:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLY:HA2	1:A:321:ASP:O	2.12	0.48
1:A:186:ALA:HB2	1:A:195:LEU:HD11	1.95	0.48
1:A:358:LEU:HD13	1:A:502:PHE:CZ	2.48	0.48
1:A:663:VAL:O	1:A:664:ARG:C	2.57	0.48
1:A:77:ARG:NE	1:A:156:ASP:OD2	2.47	0.48
1:A:201:THR:HG23	1:A:339:GLU:OE2	2.14	0.48
2:B:205:PHE:CE1	2:B:238:LEU:HB3	2.48	0.48
1:A:410:GLY:HA2	1:A:472:LEU:HB2	1.95	0.48
1:A:668:ARG:HD3	2:B:268:MET:CE	2.42	0.48
1:A:581:VAL:C	1:A:583:MET:N	2.71	0.47
1:A:159:PRO:CG	1:A:167:PHE:HD2	2.27	0.47
1:A:472:LEU:C	1:A:472:LEU:HD12	2.39	0.47
1:A:160:THR:HG22	1:A:165:LEU:HA	1.95	0.47
1:A:516:ILE:HG13	1:A:639:PRO:HD3	1.97	0.47
2:B:148:SER:O	2:B:152:VAL:HG22	2.14	0.47
1:A:159:PRO:HG2	1:A:167:PHE:HD2	1.80	0.47
3:C:188:LYS:NZ	3:C:188:LYS:CD	2.70	0.47
1:A:244:ILE:HG22	3:C:173:GLU:HG2	1.95	0.47
2:B:154:ASP:OD2	2:B:157:THR:HA	2.15	0.47
2:B:248:LEU:HD12	2:B:256:ILE:HD12	1.96	0.47
1:A:537:LEU:HD23	3:C:141:LEU:HD22	1.95	0.47
1:A:628:ARG:O	1:A:632:GLU:HG3	2.15	0.47
1:A:27:TYR:C	1:A:29:ASN:N	2.71	0.47
1:A:515:GLU:O	1:A:516:ILE:C	2.58	0.47
1:A:642:LEU:HD12	1:A:642:LEU:HA	1.57	0.47
1:A:693:SER:HA	1:A:696:SER:OG	2.15	0.46
1:A:27:TYR:C	1:A:29:ASN:H	2.24	0.46
1:A:168:VAL:HG11	1:A:179:ALA:HA	1.97	0.46
1:A:35:LEU:O	1:A:39:CYS:SG	2.74	0.46
1:A:367:ARG:HG3	1:A:492:HIS:HB3	1.98	0.46
1:A:581:VAL:C	1:A:583:MET:H	2.21	0.46
1:A:211:ILE:HG13	1:A:345:PRO:HA	1.97	0.45
1:A:77:ARG:HG3	1:A:157:ARG:HG2	1.99	0.45
1:A:67:SER:O	1:A:68:SER:C	2.59	0.45
1:A:232:LEU:HG	1:A:238:LEU:HD13	1.99	0.45
1:A:538:PHE:CD2	1:A:594:LEU:HD12	2.51	0.45
1:A:561:LEU:HD11	1:A:569:SER:CB	2.46	0.45
1:A:488:THR:CG2	1:A:489:PHE:N	2.79	0.45
2:B:100:GLU:OE2	2:B:167:LYS:HD2	2.17	0.45
1:A:256:GLN:O	1:A:294:THR:N	2.37	0.44
1:A:429:ILE:HG13	1:A:471:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:NH1	1:A:333:ARG:HB2	2.32	0.44
1:A:465:PHE:N	1:A:465:PHE:CD2	2.84	0.44
1:A:362:ASP:HB3	1:A:498:CYS:HB3	1.99	0.44
1:A:370:THR:HA	1:A:383:MET:O	2.17	0.44
1:A:386:GLN:HB3	1:A:483:VAL:CG1	2.47	0.44
2:B:116:GLU:OE1	2:B:158:THR:OG1	2.35	0.44
2:B:118:SER:OG	2:B:121:GLU:HB2	2.17	0.44
2:B:172:ASN:O	2:B:173:ILE:C	2.60	0.44
2:B:208:ASN:OD1	2:B:211:ILE:HG12	2.18	0.44
1:A:518:ALA:O	1:A:519:ASN:OD1	2.35	0.44
1:A:378:PRO:HB2	1:A:454:LEU:HD21	2.00	0.44
1:A:530:ILE:HG22	1:A:531:GLY:N	2.33	0.44
1:A:175:GLU:HG2	1:A:177:TRP:CD1	2.53	0.43
1:A:362:ASP:HA	1:A:498:CYS:HA	1.99	0.43
1:A:658:ASP:OD2	1:A:658:ASP:C	2.60	0.43
2:B:176:TRP:HZ3	2:B:236:VAL:CG2	2.31	0.43
1:A:28:LEU:HD13	1:A:50:SER:HB2	2.00	0.43
1:A:238:LEU:HG	1:A:340:ILE:HG12	2.01	0.43
2:B:261:GLN:O	2:B:262:GLU:C	2.60	0.43
2:B:260:ILE:CG2	2:B:261:GLN:H	2.32	0.43
1:A:254:THR:HG23	1:A:258:LEU:O	2.19	0.43
2:B:156:ASP:OD1	2:B:156:ASP:N	2.47	0.43
1:A:201:THR:HG21	1:A:214:TRP:NE1	2.33	0.43
1:A:95:THR:O	1:A:171:ALA:HB2	2.19	0.42
1:A:267:THR:OG1	1:A:283:ARG:HG2	2.19	0.42
1:A:39:CYS:C	1:A:41:GLU:N	2.74	0.42
1:A:386:GLN:HB3	1:A:483:VAL:HG11	2.01	0.42
1:A:51:PHE:HB2	1:A:187:LYS:HE3	2.01	0.42
1:A:169:HIS:NE2	3:C:186:TYR:CZ	2.88	0.42
1:A:238:LEU:HB3	1:A:266:VAL:HB	2.01	0.42
1:A:48:ASP:HA	1:A:49:PRO:HD2	1.92	0.42
1:A:640:CYS:O	1:A:641:GLN:C	2.62	0.42
2:B:268:MET:C	2:B:269:TYR:HD2	2.26	0.42
1:A:427:HIS:O	1:A:467:ASN:HA	2.19	0.42
1:A:677:LYS:O	1:A:678:GLN:CB	2.67	0.41
2:B:108:VAL:HG13	2:B:115:MET:SD	2.60	0.41
1:A:194:ALA:C	1:A:196:SER:H	2.28	0.41
1:A:236:SER:HB3	1:A:341:CYS:O	2.21	0.41
2:B:158:THR:O	2:B:160:LYS:N	2.53	0.41
1:A:223:ASN:O	1:A:227:ILE:N	2.52	0.41
1:A:233:GLU:C	1:A:235:GLY:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:LEU:O	1:A:561:LEU:HB2	2.20	0.41
3:C:183:PRO:HB2	3:C:186:TYR:HB2	2.03	0.41
1:A:27:TYR:HB2	1:A:150:VAL:HG13	2.02	0.41
2:B:251:ASN:C	2:B:253:THR:H	2.27	0.41
1:A:321:ASP:OD1	1:A:321:ASP:N	2.53	0.41
2:B:180:TYR:CE2	2:B:191:ILE:HG12	2.55	0.41
1:A:175:GLU:HG2	1:A:177:TRP:HD1	1.84	0.41
3:C:191:GLU:HB3	3:C:192:LYS:H	1.66	0.41
1:A:459:ARG:HA	1:A:459:ARG:HD2	1.76	0.41
1:A:672:LEU:HD12	1:A:672:LEU:HA	1.82	0.41
1:A:398:ASP:OD2	1:A:398:ASP:N	2.51	0.41
1:A:407:PHE:CE1	1:A:475:PHE:HB2	2.55	0.41
1:A:504:GLU:OE1	1:A:506:LYS:NZ	2.54	0.41
1:A:516:ILE:HA	1:A:637:LYS:O	2.21	0.41
1:A:567:ILE:O	1:A:567:ILE:CG2	2.67	0.41
1:A:575:GLU:H	1:A:575:GLU:HG2	1.59	0.41
1:A:576:THR:HG23	1:A:664:ARG:CD	2.50	0.41
1:A:668:ARG:CD	2:B:268:MET:HE1	2.48	0.41
1:A:281:LEU:HD11	1:A:297:TRP:CZ3	2.56	0.41
1:A:465:PHE:N	1:A:465:PHE:HD2	2.19	0.41
1:A:64:GLY:O	1:A:66:TYR:N	2.54	0.40
1:A:669:LEU:C	1:A:671:ILE:H	2.29	0.40
1:A:308:ASP:HA	1:A:309:PRO:HD3	1.83	0.40
1:A:408:LEU:HB2	1:A:502:PHE:HB2	2.03	0.40
1:A:89:ILE:C	1:A:89:ILE:HD13	2.46	0.40
1:A:506:LYS:O	1:A:508:ASP:N	2.54	0.40
1:A:576:THR:CG2	1:A:664:ARG:HD3	2.51	0.40
1:A:699:VAL:O	1:A:700:LEU:HD23	2.22	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	672/714 (94%)	565 (84%)	84 (12%)	23 (3%)	3	7
2	B	172/184 (94%)	155 (90%)	10 (6%)	7 (4%)	2	5
3	C	50/86 (58%)	38 (76%)	10 (20%)	2 (4%)	2	5
All	All	894/984 (91%)	758 (85%)	104 (12%)	32 (4%)	2	6

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	PRO
1	A	168	VAL
1	A	252	ALA
1	A	298	ASN
1	A	441	THR
1	A	507	ALA
1	A	516	ILE
1	A	566	ASP
1	A	618	ARG
2	B	222	GLU
3	C	193	ASN
3	C	212	ALA
1	A	297	TRP
1	A	685	GLY
2	B	247	SER
2	B	261	GLN
1	A	275	SER
1	A	445	ASN
2	B	227	ASP
1	A	28	LEU
1	A	133	GLU
1	A	522	GLU
1	A	594	LEU
2	B	123	MET
2	B	159	GLY
1	A	68	SER
1	A	291	VAL
1	A	519	ASN
2	B	115	MET
1	A	520	ILE
1	A	222	PRO
1	A	302	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	587/613 (96%)	492 (84%)	95 (16%)	2	7
2	B	153/162 (94%)	128 (84%)	25 (16%)	2	7
3	C	47/74 (64%)	36 (77%)	11 (23%)	1	2
All	All	787/849 (93%)	656 (83%)	131 (17%)	2	6

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	39	CYS
1	A	45	LEU
1	A	48	ASP
1	A	58	LEU
1	A	66	TYR
1	A	73	ILE
1	A	82	CYS
1	A	88	ILE
1	A	89	ILE
1	A	98	CYS
1	A	130	SER
1	A	133	GLU
1	A	138	ILE
1	A	148	GLU
1	A	165	LEU
1	A	168	VAL
1	A	188	ILE
1	A	223	ASN
1	A	232	LEU
1	A	242	ILE
1	A	244	ILE
1	A	245	THR
1	A	246	SER
1	A	251	GLU
1	A	254	THR

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Mol	Chain	Res	Type
1	A	273	GLU
1	A	278	LEU
1	A	280	LYS
1	A	281	LEU
1	A	293	TRP
1	A	299	ASP
1	A	300	ASN
1	A	311	VAL
1	A	318	ARG
1	A	321	ASP
1	A	332	LEU
1	A	344	THR
1	A	348	LEU
1	A	359	THR
1	A	361	MET
1	A	366	ARG
1	A	388	LEU
1	A	391	LEU
1	A	392	GLU
1	A	394	GLU
1	A	416	ARG
1	A	422	MET
1	A	436	VAL
1	A	438	GLU
1	A	439	GLU
1	A	443	GLN
1	A	446	ILE
1	A	455	THR
1	A	456	THR
1	A	459	ARG
1	A	463	ASP
1	A	465	PHE
1	A	471	VAL
1	A	472	LEU
1	A	500	ARG
1	A	508	ASP
1	A	514	ASP
1	A	520	ILE
1	A	522	GLU
1	A	535	ARG
1	A	537	LEU
1	A	561	LEU

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Mol	Chain	Res	Type
1	A	566	ASP
1	A	568	LYS
1	A	575	GLU
1	A	576	THR
1	A	580	MET
1	A	584	LEU
1	A	586	GLU
1	A	594	LEU
1	A	610	ILE
1	A	616	VAL
1	A	624	SER
1	A	628	ARG
1	A	642	LEU
1	A	656	ILE
1	A	657	ILE
1	A	667	VAL
1	A	668	ARG
1	A	672	LEU
1	A	674	LYS
1	A	678	GLN
1	A	679	LEU
1	A	683	ASN
1	A	686	THR
1	A	687	ILE
1	A	691	LEU
1	A	694	TRP
1	A	699	VAL
2	B	98	GLU
2	B	109	GLN
2	B	110	LEU
2	B	120	THR
2	B	130	VAL
2	B	131	THR
2	B	136	LEU
2	B	144	ASP
2	B	156	ASP
2	B	165	GLU
2	B	179	ILE
2	B	187	ARG
2	B	193	SER
2	B	196	LEU
2	B	206	HIS

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Mol	Chain	Res	Type
2	B	209	GLN
2	B	221	ASP
2	B	232	ILE
2	B	238	LEU
2	B	257	GLN
2	B	261	GLN
2	B	264	LEU
2	B	265	GLN
2	B	266	LEU
2	B	268	MET
3	C	139	ASP
3	C	141	LEU
3	C	147	GLU
3	C	164	LEU
3	C	167	MET
3	C	172	LEU
3	C	181	THR
3	C	185	GLU
3	C	192	LYS
3	C	211	HIS
3	C	213	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	262	HIS
1	A	290	GLN
1	A	319	GLN
1	A	415	HIS
1	A	443	GLN
1	A	510	GLN
1	A	540	GLN
1	A	608	GLN
2	B	124	ASN
2	B	210	HIS
2	B	251	ASN
2	B	265	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 10 ligands modelled in this entry, 10 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	676/714 (94%)	0.38	17 (2%) 58 50	75, 97, 108, 127	0
2	B	174/184 (94%)	0.06	2 (1%) 78 73	73, 94, 106, 112	0
3	C	56/86 (65%)	0.87	8 (14%) 6 6	92, 103, 110, 117	0
All	All	906/984 (92%)	0.35	27 (2%) 52 45	73, 97, 108, 127	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	172	LEU	3.6
1	A	534	PHE	3.4
3	C	193	ASN	3.2
3	C	212	ALA	3.1
1	A	207	PHE	3.1
1	A	509	TYR	3.0
1	A	211	ILE	3.0
1	A	701	GLY	2.9
3	C	162	VAL	2.9
2	B	270	SER	2.7
1	A	209	GLY	2.7
1	A	146	TYR	2.6
2	B	269	TYR	2.5
1	A	208	THR	2.5
3	C	175	LEU	2.4
1	A	101	ALA	2.3
1	A	144	TRP	2.3
1	A	332	LEU	2.3
3	C	170	THR	2.3
1	A	167	PHE	2.2
1	A	147	GLY	2.2
1	A	112	ALA	2.2
3	C	171	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	148	GLU	2.1
3	C	174	ALA	2.1
1	A	152	VAL	2.0
1	A	63	LEU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
4	CA	A	720	1/1	0.95	0.12	72,72,72,72	0
4	CA	B	601	1/1	0.95	0.06	105,105,105,105	0
4	CA	A	716	1/1	0.96	0.06	119,119,119,119	0
4	CA	A	718	1/1	0.97	0.06	103,103,103,103	0
4	CA	A	719	1/1	0.97	0.12	71,71,71,71	0
4	CA	B	602	1/1	0.97	0.09	94,94,94,94	0
4	CA	B	603	1/1	0.98	0.08	79,79,79,79	0
4	CA	B	604	1/1	0.98	0.08	87,87,87,87	0
4	CA	A	717	1/1	0.99	0.06	130,130,130,130	0
4	CA	A	715	1/1	0.99	0.06	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.