



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:47 AM UTC

PDB ID : 1DF0 / pdb_00001df0
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

<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

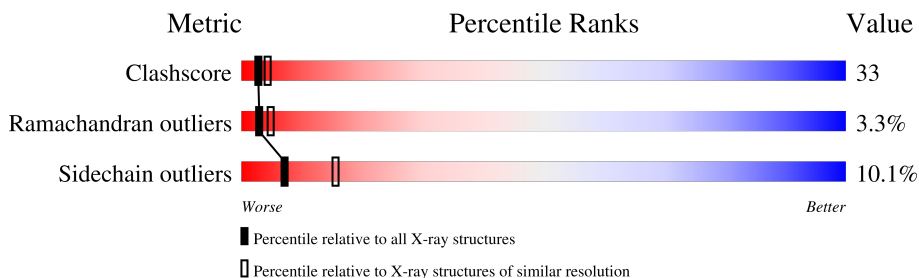
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	700	 39% 40% 9% • 11%
2	B	184	 54% 32% 10% •

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
			Total	C	N	O	S			
1	A	624	4964	3169	833	939	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called CALPAIN.

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

- Molecule 3 is water.

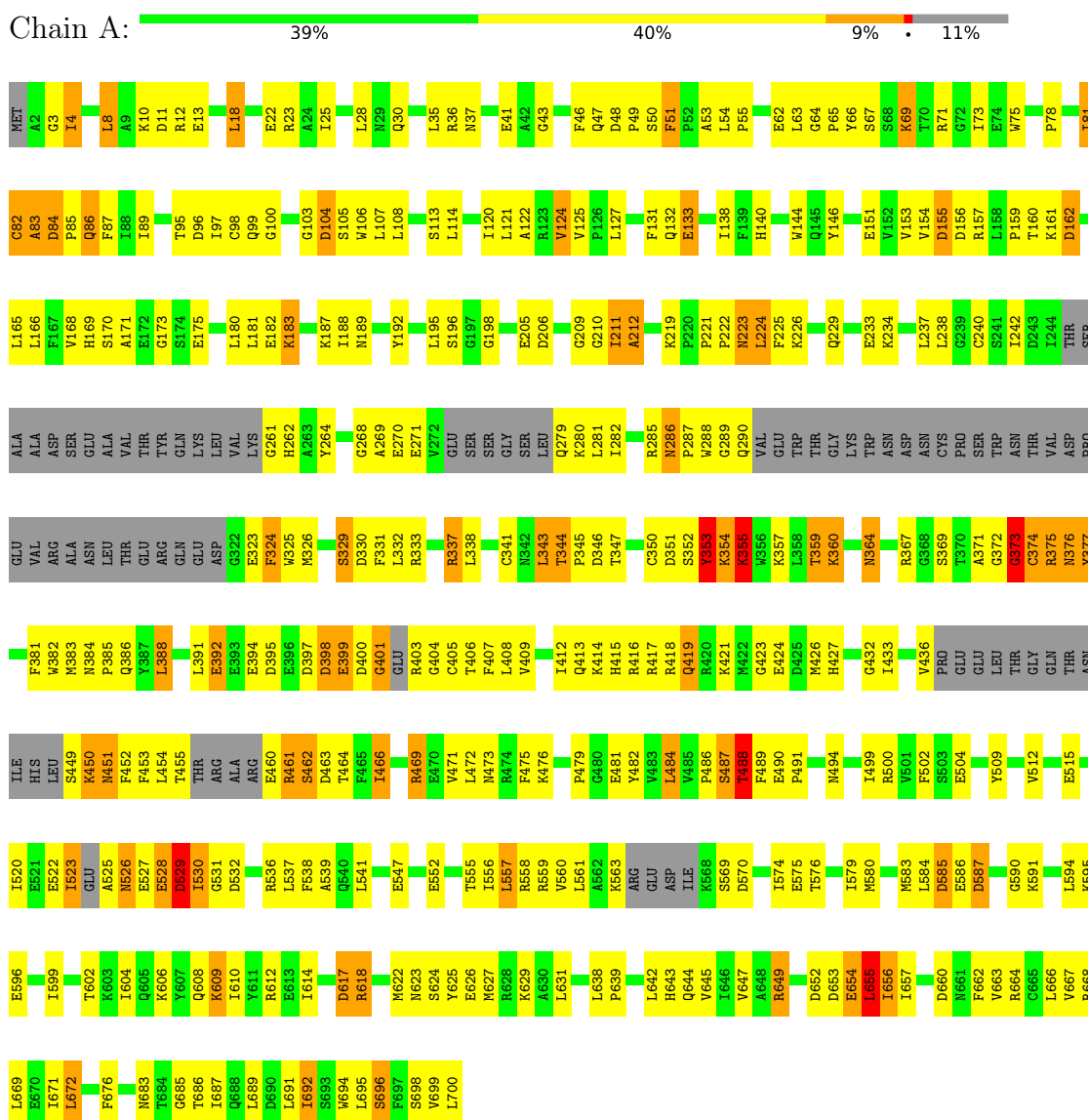
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	300	Total 300	O 300	0	0
3	B	58	Total 58	O 58	0	0

3 Residue-property plots

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. Residues are color-coded 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. 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.

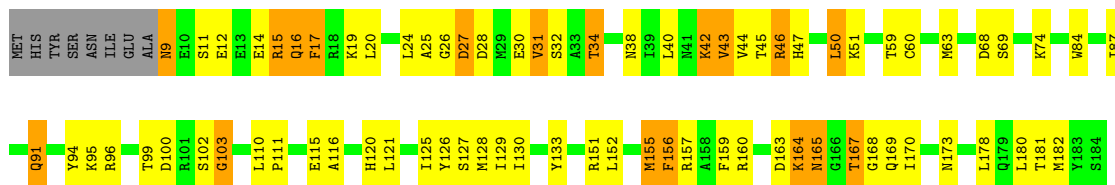
Note EDS was not executed.

- Molecule 1: M-CALPAIN



- Molecule 2: CALPAIN





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.70Å 80.18Å 80.72Å 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.	Xtrriage
Total number of atoms	6749	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

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	0.56	1/5070 (0.0%)	1.06	37/6841 (0.5%)
2	B	0.65	2/1454 (0.1%)	1.12	16/1955 (0.8%)
All	All	0.58	3/6524 (0.0%)	1.08	53/8796 (0.6%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	157	ARG	CA-C	6.07	1.60	1.52
2	B	156	PHE	CA-CB	5.55	1.62	1.53
1	A	645	VAL	CA-CB	-5.18	1.48	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	GLN	N-CA-C	-9.67	100.34	113.30
1	A	353	TYR	N-CA-C	-8.55	100.84	114.09
1	A	529	ASP	N-CA-C	-8.05	93.64	110.80
2	B	42	LYS	N-CA-C	-7.98	103.57	113.38
1	A	531	GLY	N-CA-C	7.86	122.78	112.25
1	A	451	ASN	N-CA-C	7.67	121.53	110.10
1	A	155	ASP	N-CA-C	-7.29	99.72	110.52
2	B	43	VAL	N-CA-C	7.13	117.69	111.56
1	A	570	ASP	N-CA-C	7.12	119.22	109.11
1	A	289	GLY	N-CA-C	-6.93	100.58	112.64
1	A	373	GLY	N-CA-C	6.74	129.16	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	ALA	N-CA-C	-6.73	104.33	112.54
1	A	377	TYR	CA-C-N	6.31	126.79	119.47
1	A	377	TYR	C-N-CA	6.31	126.79	119.47
1	A	649	ARG	N-CA-C	6.29	119.43	111.69
2	B	157	ARG	N-CA-C	6.15	118.49	111.11
1	A	371	ALA	N-CA-C	6.14	118.39	110.65
2	B	47	HIS	CA-C-N	6.13	125.82	119.82
2	B	47	HIS	C-N-CA	6.13	125.82	119.82
1	A	653	ASP	N-CA-C	-6.06	102.49	110.43
1	A	488	THR	N-CA-C	-6.04	101.53	110.46
1	A	397	ASP	N-CA-C	6.01	118.46	110.53
1	A	357	LYS	N-CA-C	-5.95	99.49	109.07
2	B	167	THR	N-CA-C	-5.95	101.04	109.96
1	A	100	GLY	N-CA-C	-5.88	104.69	112.81
1	A	87	PHE	N-CA-C	-5.88	103.65	111.24
1	A	138	ILE	N-CA-C	5.87	116.75	108.17
1	A	212	ALA	N-CA-C	5.78	118.14	108.02
2	B	165	ASN	N-CA-C	5.74	119.90	113.01
1	A	385	PRO	N-CA-C	-5.71	102.84	111.41
1	A	344	THR	N-CA-C	-5.66	102.05	110.20
2	B	133	TYR	N-CA-C	5.63	120.84	113.30
2	B	91	GLN	N-CA-C	-5.44	105.26	111.14
1	A	569	SER	N-CA-C	-5.41	101.07	109.72
2	B	103	GLY	N-CA-C	-5.38	107.59	114.37
1	A	645	VAL	CB-CA-C	-5.36	105.02	111.88
1	A	515	GLU	N-CA-C	-5.34	103.34	110.55
1	A	69	LYS	N-CA-C	-5.34	107.14	113.97
2	B	16	GLN	N-CA-C	-5.32	105.48	111.28
1	A	221	PRO	N-CA-C	-5.29	104.24	110.70
2	B	11	SER	N-CA-C	5.28	117.43	109.41
1	A	590	GLY	N-CA-C	-5.27	108.04	115.32
1	A	51	PHE	CA-C-N	5.27	125.21	119.78
1	A	51	PHE	C-N-CA	5.27	125.21	119.78
1	A	587	ASP	N-CA-C	-5.20	106.78	113.02
1	A	83	ALA	N-CA-C	5.18	121.83	110.80
2	B	127	SER	N-CA-C	-5.13	107.31	113.21
1	A	270	GLU	N-CA-C	5.12	117.16	109.23
1	A	242	ILE	N-CA-C	-5.10	100.23	107.77
1	A	691	LEU	N-CA-C	5.08	116.50	111.07
2	B	12	GLU	N-CA-C	5.07	117.54	111.71
2	B	155	MET	N-CA-C	5.04	117.67	111.82
1	A	355	LYS	N-CA-C	5.03	117.50	109.81

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	358	0
2	B	1427	0	1375	82	0
3	A	300	0	0	20	0
3	B	58	0	0	6	0
All	All	6749	0	6182	414	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 33.

All (414) 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:HD12	1:A:523:ILE:H	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:HD3	1:A:375:ARG:O	1.74	0.88
1:A:281:LEU:HD21	1:A:326:MET:N	1.90	0.86
1:A:375:ARG:HD3	1:A:375:ARG:C	2.01	0.86
2:B:110:LEU:HD13	2:B:130:ILE:HD12	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:GLN:O	1:A:233:GLU:HG3	1.81	0.81
1:A:466:ILE:HD13	1:A:466:ILE:N	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
1:A:286:ASN:C	1:A:286:ASN:HD22	1.92	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
2:B:60:CYS:HA	2:B:63:MET:HE3	1.68	0.74
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: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
1:A:627:MET:HE3	1:A:631:LEU:HG	1.72	0.71
1:A:452:PHE:C	1:A:454:LEU:H	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:689:LEU:HD12	1:A:694:TRP:HE3	1.61	0.65
2:B:125:ILE:O	2:B:129:ILE:HG13	1.97	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:18:LEU:CD1	1:A:25:ILE:HG12	2.30	0.62
1:A:281:LEU:CD2	1:A:325:TRP:HB3	2.30	0.62
1:A:388:LEU:HD13	1:A:388:LEU:C	2.24	0.61
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:64:GLY:O	1:A:67:SER:HB3	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:699:VAL:C	1:A:700:LEU:HG	2.26	0.61
2:B:38:ASN:O	2:B:42:LYS:HG3	2.00	0.61
1:A:700:LEU:HD13	2:B:128:MET:HE3	1.82	0.60
1:A:285:ARG:C	1:A:285:ARG:HD3	2.25	0.60
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:155:ASP:OD2	1:A:157:ARG:HB2	2.01	0.60
1:A:452:PHE:O	1:A:454:LEU:N	2.35	0.60
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
1:A:285:ARG:HD3	1:A:286:ASN:N	2.18	0.59
1:A:375:ARG:C	1:A:375:ARG:CD	2.70	0.59
1:A:624:SER:OG	1:A:655:LEU:HB3	2.02	0.59
1:A:472:LEU:HD13	1:A:472:LEU:C	2.28	0.59
1:A:672:LEU:CD2	2:B:182:MET:HE2	2.33	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:525:ALA:O	1:A:526:ASN:C	2.46	0.58
1:A:83:ALA:O	1:A:84:ASP:HB2	2.04	0.58
1:A:374:CYS:N	1:A:381:PHE:HD1	2.01	0.58
1:A:219:LYS:O	1:A:219:LYS:HG3	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:527:GLU:C	1:A:528:GLU:O	2.42	0.57
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:421:LYS:HD2	1:A:424:GLU:OE2	2.04	0.57
1:A:523:ILE:HD13	1:A:599:ILE:HG23	1.85	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
2:B:125:ILE:HA	2:B:128:MET:HE2	1.86	0.57
1:A:576:THR:O	1:A:579:ILE:HG13	2.05	0.57
2:B:126:TYR:C	2:B:128:MET:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:165:LEU:H	1:A:165:LEU:HD22	1.70	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:386:GLN:HE22	1:A:451:ASN:H	1.53	0.56
1:A:699:VAL:HG13	3:A:975:HOH:O	2.06	0.56
1:A:386:GLN:HB2	1:A:512:VAL:CG1	2.35	0.56
1:A:326:MET:HE2	1:A:331:PHE:N	2.21	0.56
1:A:452:PHE:C	1:A:454:LEU:N	2.64	0.56
1:A:47:GLN:HB3	1:A:157:ARG:HH12	1.71	0.56
1:A:3:GLY:C	2:B:69:SER:HB3	2.31	0.56
1:A:386:GLN:HE21	1:A:512:VAL:HG13	1.72	0.55
1:A:585:ASP:C	1:A:587:ASP:H	2.14	0.55
1:A:105:SER:HA	1:A:108:LEU:HD23	1.88	0.55
1:A:73:ILE:HG12	1:A:166:LEU:CD1	2.36	0.55
1:A:412:ILE:HG13	1:A:469:ARG:O	2.06	0.55
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:672:LEU:HD23	2:B:182:MET:HE2	1.89	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:583:MET:HE3	1:A:584:LEU:HD21	1.89	0.54
1:A:144:TRP:CG	1:A:209:GLY:HA2	2.42	0.54
1:A:282:ILE:HD11	1:A:331:PHE:HB2	1.88	0.54
1:A:466:ILE:N	1:A:466:ILE:CD1	2.68	0.54
1:A:579:ILE:HD11	1:A:664:ARG:HD3	1.89	0.54
2:B:163:ASP:OD1	2:B:167:THR:O	2.24	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: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
1:A:84:ASP:H	1:A:85:PRO:CD	2.21	0.54
1:A:286:ASN:ND2	1:A:286:ASN:C	2.62	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	2:B:96:ARG:HH11	1.73	0.53
1:A:667:VAL:HG12	1:A:671:ILE:CD1	2.39	0.53
1:A:161:LYS:HB3	1:A:166:LEU:HD21	1.91	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:140:HIS:HD2	1:A:151:GLU:OE2	1.91	0.53
1:A:372:GLY:O	1:A:491:PRO:HB3	2.08	0.52
1:A:427:HIS:HE1	1:A:494:ASN:O	1.92	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:HA	1:A:354:LYS:HE2	1.90	0.52
1:A:18:LEU:HD13	1:A:25:ILE:HG12	1.91	0.52
1:A:399:GLU:CG	1:A:400:ASP:N	2.72	0.52
2:B:45:THR:O	2:B:46:ARG:HB2	2.09	0.52
1:A:132:GLN:O	1:A:133:GLU:O	2.28	0.52
1:A:373:GLY:H	1:A:384:ASN:CG	2.18	0.52
1:A:672:LEU:HG	2:B:181:THR:OG1	2.10	0.52
1:A:62:GLU:C	1:A:63:LEU:HD12	2.35	0.51
1:A:240:CYS:HA	1:A:337:ARG:O	2.10	0.51
1:A:574:ILE:HG22	3:A:730:HOH:O	2.09	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:107:LEU:HD13	1:A:182:GLU:HG3	1.93	0.51
1:A:234:LYS:HA	1:A:354:LYS:O	2.10	0.51
1:A:408:LEU:CD2	1:A:472:LEU:HD11	2.40	0.51
1:A:75:TRP:CZ3	1:A:159:PRO:HD3	2.46	0.51
1:A:520:ILE:N	1:A:520:ILE:HD12	2.25	0.51
1:A:114:LEU:HB3	1:A:121:LEU:HD13	1.92	0.51
1:A:367:ARG:CZ	1:A:655:LEU:HD21	2.41	0.51
1:A:609:LYS:HZ2	1:A:609:LYS:HB3	1.75	0.51
1:A:563:LYS:C	3:A:1000:HOH:O	2.53	0.50
2:B:167:THR:C	2:B:169:GLN:H	2.19	0.50
1:A:472:LEU:HD13	1:A:473:ASN:N	2.26	0.50
1:A:617:ASP:O	1:A:618:ARG:C	2.54	0.50
1:A:124:VAL:HG22	1:A:124:VAL:O	2.11	0.50
1:A:395:ASP:OD2	1:A:406:THR:HB	2.12	0.50
2:B:27:ASP:OD2	2:B:27:ASP:N	2.44	0.50
1:A:51:PHE:HB2	1:A:187:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:CB	1:A:157:ARG:HH21	2.24	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:127:LEU:N	1:A:127:LEU:HD22	2.28	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
2:B:110:LEU:HB2	2:B:111:PRO:HD3	1.94	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
1:A:654:GLU:O	1:A:656:ILE:HG22	2.11	0.49
1:A:237:LEU:HB2	1:A:341:CYS:HB3	1.95	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: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
1:A:69:LYS:HD2	3:A:778:HOH:O	2.12	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:692:ILE:HD12	1:A:692:ILE:N	2.12	0.49
1:A:694:TRP:CE2	1:A:698:SER:OG	2.65	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:187:LYS:C	1:A:189:ASN:H	2.22	0.48
1:A:285:ARG:HD3	1:A:286:ASN:C	2.39	0.48
1:A:359:THR:CG2	1:A:509:TYR:HB3	2.38	0.48
1:A:373:GLY:HA3	1:A:487:SER:CB	2.42	0.48
1:A:373:GLY:O	1:A:374:CYS:CB	2.60	0.48
1:A:668:ARG:HG2	2:B:182:MET:CE	2.44	0.48
1:A:668:ARG:HG2	2:B:182:MET:HE2	1.96	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
1:A:614:ILE:HG21	1:A:622:MET:HE2	1.94	0.48
1:A:415:HIS:CE1	1:A:419:GLN:HB2	2.49	0.48
2:B:125:ILE:O	2:B:128:MET:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:669:LEU:HA	2:B:182:MET:HE3	1.96	0.47
1:A:171:ALA:C	1:A:173:GLY:H	2.22	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:460:GLU:O	1:A:461:ARG:CB	2.63	0.47
1:A:579:ILE:CD1	1:A:664:ARG:HD3	2.45	0.47
2:B:159:PHE:CE1	2:B:170:ILE:HG23	2.49	0.47
1:A:364:ASN:HB3	3:A:985:HOH:O	2.15	0.47
1:A:382:TRP:HE3	1:A:451:ASN:O	1.98	0.47
1:A:65:PRO:C	1:A:67:SER:H	2.23	0.47
1:A:187:LYS:C	1:A:189:ASN:N	2.72	0.47
1:A:386:GLN:C	1:A:512:VAL:HG12	2.40	0.47
1:A:455:THR:HA	3:A:903:HOH:O	2.14	0.47
1:A:585:ASP:O	1:A:586:GLU:HB2	2.15	0.47
1:A:595:LYS:O	1:A:599:ILE:HG13	2.14	0.47
1:A:3:GLY:O	2:B:69:SER:HB3	2.14	0.47
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:689:LEU:HD13	1:A:694:TRP:HA	1.96	0.47
2:B:51:LYS:HB3	2:B:103:GLY:HA2	1.97	0.47
2:B:20:LEU:O	2:B:24:LEU:HG	2.16	0.47
2:B:164:LYS:HG3	2:B:165:ASN:N	2.24	0.47
1:A:106:TRP:CE2	1:A:198:GLY:HA3	2.50	0.46
1:A:654:GLU:OE2	1:A:656:ILE:HG21	2.15	0.46
1:A:124:VAL:O	1:A:124:VAL:CG2	2.63	0.46
1:A:13:GLU:OE2	1:A:13:GLU:HA	2.16	0.46
1:A:486:PRO:HB3	1:A:499:ILE:HD11	1.97	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:30:GLN:NE2	1:A:50:SER:OG	2.48	0.46
1:A:30:GLN:HE22	1:A:187:LYS:NZ	2.14	0.46
1:A:696:SER:O	1:A:700:LEU:HB2	2.15	0.46
1:A:700:LEU:CD1	2:B:128:MET:HE3	2.45	0.46
2:B:110:LEU:HD13	2:B:130:ILE:CD1	2.39	0.46
1:A:386:GLN:CB	1:A:512:VAL:CG1	2.94	0.46
1:A:323:GLU:O	1:A:324:PHE:HB3	2.16	0.46
1:A:369:SER:HB3	1:A:647:VAL:CG1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:CYS:O	1:A:476:LYS:HA	2.15	0.46
1:A:527:GLU:O	1:A:528:GLU:O	2.34	0.46
1:A:672:LEU:HD23	2:B:182:MET:CE	2.45	0.46
2:B:128:MET:HG3	3:B:198:HOH:O	2.16	0.46
1:A:211:ILE:HG21	1:A:502:PHE:CD2	2.51	0.45
1:A:609:LYS:HB3	1:A:609:LYS:NZ	2.32	0.45
1:A:261:GLY:N	3:A:886:HOH:O	2.49	0.45
1:A:686:THR:HG22	2:B:173:ASN:CA	2.46	0.45
2:B:14:GLU:O	2:B:17:PHE:HB2	2.16	0.45
1:A:37:ASN:N	1:A:37:ASN:HD22	2.13	0.45
1:A:373:GLY:CA	1:A:384:ASN:ND2	2.71	0.45
1:A:54:LEU:HB3	1:A:55:PRO:HD2	1.98	0.45
1:A:78:PRO:HG2	1:A:131:PHE:CZ	2.51	0.45
1:A:400:ASP:O	1:A:401:GLY:O	2.34	0.45
2:B:43:VAL:HG11	2:B:84:TRP:HH2	1.79	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
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
2:B:163:ASP:O	2:B:164:LYS:C	2.59	0.44
1:A:532:ASP:O	1:A:536:ARG:HG3	2.17	0.44
1:A:538:PHE:CD2	1:A:594:LEU:HD23	2.53	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
3:A:975:HOH:O	2:B:155:MET:HG3	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:539:ALA:C	1:A:541:LEU:H	2.25	0.44
1:A:95:THR:OG1	1:A:97:ILE:HG12	2.18	0.44
1:A:360:LYS:HA	1:A:499:ILE:O	2.18	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:82:CYS:SG	1:A:85:PRO:HD3	2.58	0.43
1:A:375:ARG:C	1:A:377:TYR:N	2.76	0.43
1:A:122:ALA:HA	1:A:127:LEU:HD21	1.99	0.43
1:A:183:LYS:HG2	1:A:192:TYR:OH	2.18	0.43
1:A:432:GLY:HA2	1:A:462:SER:HA	2.00	0.43
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.82	0.43
1:A:692:ILE:HD11	3:A:764:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:O	1:A:81:ILE:HG22	2.18	0.43
1:A:394:GLU:OE2	1:A:403:ARG:CB	2.66	0.43
1:A:463:ASP:O	1:A:464:THR:OG1	2.34	0.43
1:A:4:ILE:CD1	2:B:180:LEU:HA	2.46	0.43
1:A:373:GLY:CA	1:A:487:SER:HB2	2.48	0.43
1:A:512:VAL:O	1:A:512:VAL:CG1	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:N	1:A:391:LEU:HD22	2.34	0.43
1:A:462:SER:O	1:A:463:ASP:HB2	2.19	0.43
1:A:282:ILE:HD12	1:A:282:ILE:C	2.43	0.43
1:A:400:ASP:CG	1:A:401:GLY:N	2.77	0.43
1:A:700:LEU:CD1	2:B:128:MET:HG2	2.45	0.43
1:A:8:LEU:O	1:A:12:ARG:HG3	2.18	0.42
1:A:520:ILE:HD12	1:A:520:ILE:H	1.84	0.42
2:B:31:VAL:HG12	2:B:32:SER:O	2.18	0.42
1:A:326:MET:HE2	1:A:330:ASP:C	2.44	0.42
1:A:344:THR:OG1	1:A:346:ASP:OD2	2.28	0.42
1:A:686:THR:HG22	2:B:173:ASN:HA	2.01	0.42
1:A:30:GLN:NE2	1:A:187:LYS:NZ	2.68	0.42
1:A:97:ILE:HG22	1:A:98:CYS:N	2.34	0.42
1:A:374:CYS:O	1:A:375:ARG:C	2.62	0.42
1:A:375:ARG:C	1:A:377:TYR:H	2.27	0.42
1:A:576:THR:OG1	1:A:660:ASP:OD1	2.30	0.42
2:B:28:ASP:O	2:B:30:GLU:HG3	2.20	0.42
1:A:160:THR:HG22	1:A:165:LEU:HD13	2.01	0.42
1:A:700:LEU:CD2	2:B:128:MET:HG2	2.45	0.42
1:A:345:PRO:O	1:A:355:LYS:HE2	2.20	0.42
1:A:78:PRO:HD3	1:A:156:ASP:O	2.20	0.42
1:A:104:ASP:OD1	1:A:196:SER:HA	2.20	0.42
1:A:125:VAL:O	1:A:125:VAL:HG12	2.19	0.42
1:A:383:MET:HE1	1:A:625:TYR:O	2.20	0.42
1:A:409:VAL:O	1:A:472:LEU:HA	2.19	0.42
1:A:585:ASP:C	1:A:587:ASP:N	2.78	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:426:MET:CE	1:A:469:ARG:HB3	2.49	0.42
1:A:205:GLU:OE1	1:A:211:ILE:HD12	2.20	0.41
1:A:262:HIS:HD2	1:A:264:TYR:CZ	2.38	0.41
1:A:407:PHE:CD2	1:A:409:VAL:HG23	2.55	0.41
1:A:671:ILE:HG12	3:A:976:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ALA:O	2:B:26:GLY:C	2.62	0.41
1:A:398:ASP:CG	1:A:399:GLU:N	2.77	0.41
1:A:585:ASP:O	1:A:596:GLU:OE2	2.39	0.41
1:A:692:ILE:CD1	1:A:692:ILE:N	2.79	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:376:ASN:N	1:A:376:ASN:ND2	2.67	0.41
1:A:412:ILE:HA	1:A:469:ARG:O	2.20	0.41
2:B:99:THR:HG22	2:B:100:ASP:N	2.34	0.41
1:A:539:ALA:CB	3:A:727:HOH:O	2.69	0.41
1:A:30:GLN:HE22	1:A:187:LYS:HZ1	1.68	0.41
1:A:41:GLU:C	1:A:43:GLY:H	2.28	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:662:PHE:CZ	1:A:666:LEU:HD11	2.56	0.41
1:A:672:LEU:HD12	1:A:672:LEU:HA	1.94	0.41
1:A:86:GLN:HG2	1:A:89:ILE:CD1	2.51	0.41
1:A:105:SER:C	1:A:107:LEU:N	2.78	0.41
1:A:547:GLU:C	1:A:591:LYS:HE2	2.46	0.41
2:B:100:ASP:CG	2:B:102:SER:HB3	2.46	0.41
1:A:237:LEU:C	1:A:238:LEU:HD12	2.46	0.40
1:A:398:ASP:CG	1:A:399:GLU:H	2.29	0.40
1:A:400:ASP:OD1	1:A:401:GLY:N	2.54	0.40
1:A:10:LYS:O	1:A:11:ASP:C	2.64	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:576:THR:HG22	1:A:580:MET:HE3	2.03	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 [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	612/700 (87%)	528 (86%)	61 (10%)	23 (4%)	2	3
2	B	174/184 (95%)	162 (93%)	9 (5%)	3 (2%)	7	15
All	All	786/884 (89%)	690 (88%)	70 (9%)	26 (3%)	3	5

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
2	B	164	LYS

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	520/603 (86%)	464 (89%)	56 (11%)	6	13
2	B	155/162 (96%)	143 (92%)	12 (8%)	12	27
All	All	675/765 (88%)	607 (90%)	68 (10%)	7	15

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	8	LEU
1	A	18	LEU
1	A	22	GLU
1	A	23	ARG
1	A	28	LEU
1	A	81	ILE
1	A	82	CYS
1	A	86	GLN
1	A	104	ASP
1	A	113	SER
1	A	124	VAL
1	A	170	SER
1	A	180	LEU
1	A	183	LYS
1	A	195	LEU
1	A	211	ILE
1	A	224	LEU
1	A	286	ASN
1	A	329	SER
1	A	332	LEU
1	A	337	ARG
1	A	338	LEU
1	A	343	LEU
1	A	353	TYR
1	A	355	LYS
1	A	359	THR
1	A	360	LYS
1	A	364	ASN
1	A	375	ARG
1	A	388	LEU
1	A	392	GLU
1	A	399	GLU
1	A	418	ARG
1	A	419	GLN

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Mol	Chain	Res	Type
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	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	663	VAL
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	31	VAL
2	B	34	THR
2	B	50	LEU
2	B	68	ASP
2	B	115	GLU
2	B	120	HIS
2	B	121	LEU
2	B	152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	140	HIS

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Mol	Chain	Res	Type
1	A	142	GLN
1	A	169	HIS
1	A	286	ASN
1	A	334	HIS
1	A	342	ASN
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	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	139	ASN

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](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.