



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:38 PM GMT

PDB ID : 1L9M
Title : Three-dimensional structure of the human transglutaminase 3 enzyme: binding of calcium ions change structure for activation
Authors : Ahvazi, B.
Deposited on : 2002-03-26
Resolution : 2.10 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

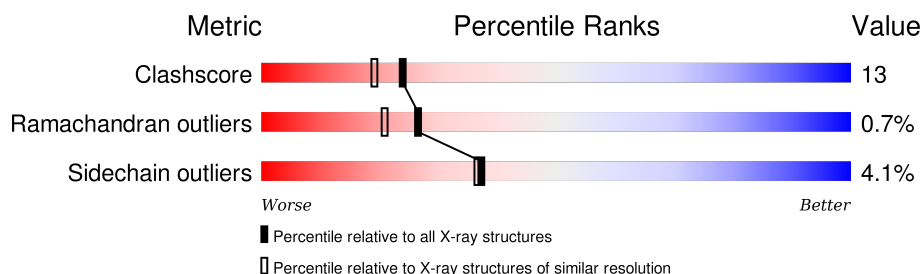
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	692	 76% 19% . .
1	B	692	 72% 24% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11487 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 Protein-glutamine glutamyltransferase E3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total	C	N	O	S	0	0	0
			5266	3323	915	1005	23			
1	B	681	Total	C	N	O	S	0	0	0
			5314	3350	922	1019	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ASP	ASN	SEE REMARK 999	UNP Q08188
A	264	LEU	PHE	ENGINEERED	UNP Q08188
A	561	ARG	LYS	SEE REMARK 999	UNP Q08188
A	653	ARG	GLY	SEE REMARK 999	UNP Q08188
B	250	ASP	ASN	SEE REMARK 999	UNP Q08188
B	264	LEU	PHE	ENGINEERED	UNP Q08188
B	561	ARG	LYS	SEE REMARK 999	UNP Q08188
B	653	ARG	GLY	SEE REMARK 999	UNP Q08188

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Br	0	0
			1	1		
2	A	1	Total	Br	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

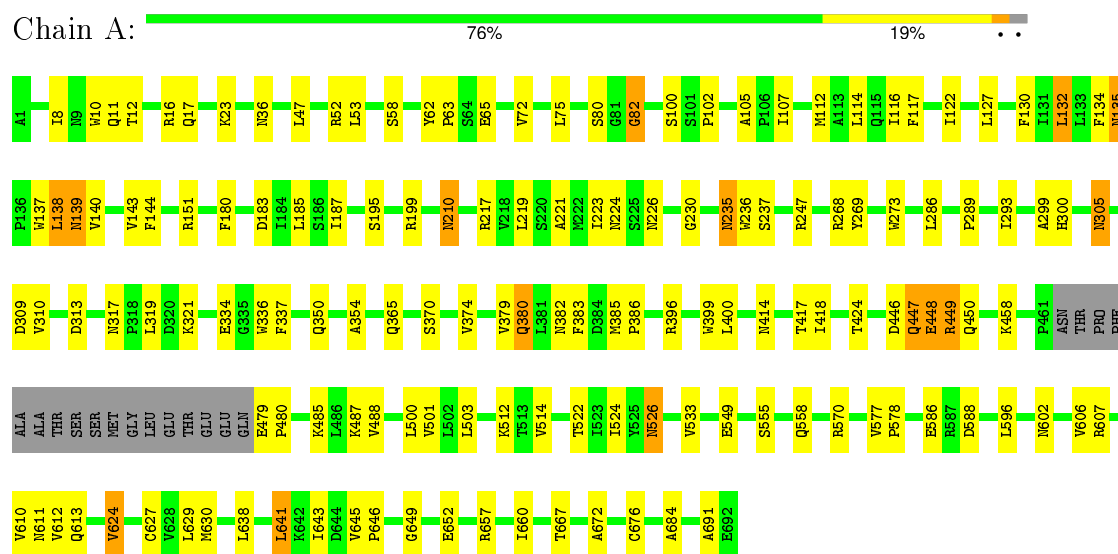
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	458	Total 458	O 458	0	0
5	B	443	Total 443	O 443	0	0

3 Residue-property plots

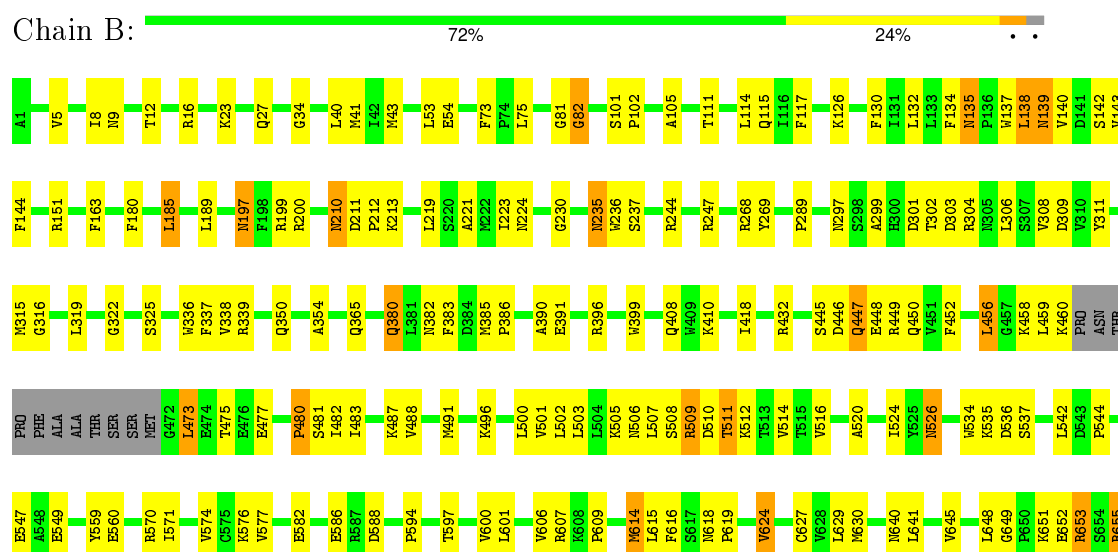
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

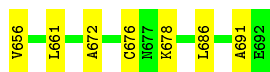
Note EDS was not executed.

• Molecule 1: Protein-glutamine glutamyltransferase E3



• Molecule 1: Protein-glutamine glutamyltransferase E3





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	57.71Å 67.52Å 116.21Å 97.24° 90.15° 98.67°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.182 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11487	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.34	0/5377	0.61	0/7295
1	B	0.33	0/5424	0.59	0/7357
All	All	0.33	0/10801	0.60	0/14652

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5266	0	5206	120	0
1	B	5314	0	5246	162	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	458	0	0	9	0
5	B	443	0	0	10	0
All	All	11487	0	10452	275	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 13.

All (275) 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:B:447:GLN:H	1:B:447:GLN:HE21	1.00	0.96
1:B:302:THR:HB	1:B:308:VAL:HG13	1.48	0.95
1:B:597:THR:HG23	1:B:615:LEU:HB2	1.55	0.87
1:A:512:LYS:HD2	1:A:577:VAL:HG11	1.57	0.86
1:B:447:GLN:H	1:B:447:GLN:NE2	1.73	0.83
1:A:447:GLN:HE21	1:A:447:GLN:H	1.25	0.82
1:B:509:ARG:HA	1:B:544:PRO:HB3	1.64	0.80
1:B:655:ARG:HB3	1:B:655:ARG:HH11	1.48	0.79
1:B:304:ARG:HH21	1:B:309:ASP:H	1.32	0.78
1:B:447:GLN:N	1:B:447:GLN:HE21	1.81	0.78
1:A:487:LYS:HE2	1:A:503:LEU:HD11	1.66	0.78
1:B:570:ARG:HD3	1:B:588:ASP:OD1	1.87	0.75
1:B:139:ASN:HD22	1:B:140:VAL:H	1.34	0.73
1:B:487:LYS:HE2	1:B:503:LEU:HD11	1.70	0.73
1:A:210:ASN:HD22	1:A:210:ASN:H	1.37	0.73
1:B:304:ARG:NH2	1:B:309:ASP:H	1.87	0.72
1:B:139:ASN:HD22	1:B:140:VAL:N	1.87	0.72
1:B:197:ASN:HD22	1:B:197:ASN:H	1.39	0.71
1:B:526:ASN:HD22	1:B:526:ASN:H	1.39	0.71
1:A:447:GLN:NE2	1:A:447:GLN:H	1.88	0.70
1:B:213:LYS:HD3	1:B:339:ARG:HE	1.55	0.70
1:A:570:ARG:HD3	1:A:588:ASP:OD1	1.91	0.69
1:B:449:ARG:HE	1:B:449:ARG:HA	1.56	0.69
1:B:648:LEU:HD23	1:B:652:GLU:HB3	1.75	0.68
1:B:655:ARG:HA	5:B:859:HOH:O	1.94	0.68
1:A:102:PRO:HG2	1:A:105:ALA:HB2	1.75	0.67
1:A:224:ASN:O	1:A:230:GLY:HA3	1.94	0.67
1:A:135:ASN:HD21	1:A:137:TRP:HB2	1.60	0.67
1:B:449:ARG:HA	1:B:449:ARG:NE	2.09	0.67
1:B:606:VAL:HG12	1:B:607:ARG:HG3	1.76	0.66
1:B:459:LEU:O	1:B:460:LYS:HD2	1.96	0.66
1:A:221:ALA:HB2	1:A:365:GLN:HB3	1.78	0.65
1:A:300:HIS:HB2	5:A:1030:HOH:O	1.97	0.65
1:B:138:LEU:HD22	1:B:140:VAL:HG22	1.80	0.64
1:B:235:ASN:ND2	1:B:237:SER:H	1.96	0.64
1:A:414:ASN:CG	1:A:417:THR:HG23	2.18	0.63
1:B:200:ARG:HD3	5:B:802:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ASN:HD22	1:A:526:ASN:H	1.47	0.63
1:B:235:ASN:C	1:B:235:ASN:HD22	2.03	0.62
1:A:313:ASP:OD2	1:A:317:ASN:HB2	2.00	0.62
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.63	0.62
1:A:293:ILE:HG13	1:A:334:GLU:HG3	1.81	0.61
1:B:500:LEU:CD1	1:B:571:ILE:HG12	2.30	0.61
1:B:82:GLY:HA2	1:B:102:PRO:HB3	1.82	0.61
1:B:102:PRO:HG2	1:B:105:ALA:HB2	1.82	0.61
1:B:302:THR:H	1:B:308:VAL:HG12	1.65	0.61
1:B:609:PRO:HG3	1:B:661:LEU:HD13	1.82	0.61
1:A:82:GLY:HA2	1:A:102:PRO:HB3	1.83	0.60
1:B:27:GLN:HA	1:B:27:GLN:HE21	1.65	0.60
1:B:509:ARG:HA	1:B:544:PRO:CB	2.32	0.60
1:A:310:VAL:HG21	1:A:396:ARG:NH1	2.17	0.60
1:B:23:LYS:HE3	1:B:180:PHE:CE2	2.36	0.59
1:A:65:GLU:HB2	1:B:655:ARG:HE	1.67	0.59
1:B:224:ASN:O	1:B:230:GLY:HA3	2.02	0.59
1:B:655:ARG:HB3	1:B:655:ARG:NH1	2.15	0.59
1:A:117:PHE:CD1	1:B:651:LYS:HD2	2.37	0.59
1:A:337:PHE:CE1	1:A:350:GLN:HG3	2.37	0.59
1:A:210:ASN:N	1:A:210:ASN:HD22	1.98	0.59
1:B:219:LEU:O	1:B:223:ILE:HG12	2.03	0.59
1:A:638:LEU:HD22	5:A:972:HOH:O	2.03	0.59
1:A:58:SER:HB2	1:A:63:PRO:HB3	1.85	0.58
1:A:219:LEU:O	1:A:223:ILE:HG12	2.03	0.58
1:A:526:ASN:HD22	1:A:526:ASN:N	2.02	0.58
1:B:473:LEU:HD13	1:B:473:LEU:O	2.03	0.57
1:B:600:VAL:HG23	1:B:686:LEU:HD21	1.86	0.57
1:A:235:ASN:ND2	1:A:237:SER:H	2.02	0.57
1:B:678:LYS:HA	1:B:678:LYS:HE2	1.86	0.57
1:B:306:LEU:HD12	1:B:456:LEU:HD23	1.85	0.57
1:A:602:ASN:OD1	1:A:610:VAL:HG23	2.04	0.57
1:B:618:ASN:HB2	1:B:648:LEU:HD22	1.86	0.57
1:B:630:MET:HE3	1:B:640:ASN:OD1	2.03	0.57
1:B:244:ARG:NH1	1:B:630:MET:HE1	2.20	0.57
1:B:139:ASN:ND2	1:B:140:VAL:N	2.52	0.57
1:A:72:VAL:HB	1:B:653:ARG:NH1	2.20	0.57
1:B:480:PRO:HA	5:B:1027:HOH:O	2.05	0.57
1:B:520:ALA:HB3	1:B:534:TRP:HB3	1.87	0.57
1:A:138:LEU:HD22	1:A:140:VAL:HG22	1.87	0.56
1:A:447:GLN:HE21	1:A:447:GLN:N	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ASN:ND2	1:B:197:ASN:H	2.03	0.56
1:A:117:PHE:HB3	1:B:651:LYS:HD2	1.87	0.56
1:B:380:GLN:HG3	1:B:458:LYS:HD3	1.86	0.56
1:B:244:ARG:HH12	1:B:630:MET:HE1	1.70	0.56
1:B:526:ASN:HD22	1:B:526:ASN:N	2.03	0.56
1:B:210:ASN:H	1:B:210:ASN:HD22	1.52	0.56
1:B:221:ALA:HB2	1:B:365:GLN:HB3	1.88	0.56
1:B:399:TRP:CH2	1:B:410:LYS:HG3	2.41	0.56
1:B:648:LEU:CD2	1:B:652:GLU:HB3	2.36	0.55
1:A:235:ASN:HD22	1:A:235:ASN:C	2.09	0.55
1:B:473:LEU:HD11	1:B:475:THR:OG1	2.06	0.55
1:B:382:ASN:HB3	1:B:383:PHE:CG	2.42	0.55
1:A:479:GLU:N	1:A:480:PRO:CD	2.70	0.55
1:B:210:ASN:N	1:B:210:ASN:HD22	2.06	0.54
1:B:480:PRO:O	1:B:481:SER:HB3	2.08	0.54
1:B:491:MET:HG2	1:B:496:LYS:NZ	2.22	0.54
1:B:111:THR:HG23	1:B:126:LYS:HE3	1.90	0.54
1:B:311:TYR:HB3	1:B:319:LEU:HD12	1.89	0.54
1:A:555:SER:H	1:A:558:GLN:HE21	1.55	0.54
1:B:213:LYS:HD3	1:B:339:ARG:NE	2.23	0.54
1:B:235:ASN:HD22	1:B:237:SER:H	1.55	0.53
1:A:122:ILE:HG13	1:B:619:PRO:HB3	1.89	0.53
1:A:52:ARG:HG2	1:A:53:LEU:N	2.21	0.53
1:B:142:SER:HB2	1:B:338:VAL:HG22	1.90	0.53
1:A:382:ASN:HB3	1:A:383:PHE:CD1	2.44	0.53
1:A:667:THR:HG22	5:A:821:HOH:O	2.07	0.53
1:A:667:THR:HG23	1:A:667:THR:O	2.09	0.53
1:B:34:GLY:HA2	1:B:101:SER:O	2.09	0.53
1:B:487:LYS:HE2	1:B:503:LEU:CD1	2.37	0.53
1:A:139:ASN:N	1:A:139:ASN:HD22	2.06	0.52
1:B:137:TRP:CE2	1:B:151:ARG:HD3	2.44	0.52
1:A:23:LYS:HE3	1:A:180:PHE:CE2	2.44	0.52
1:A:247:ARG:HD2	5:A:720:HOH:O	2.08	0.52
1:B:9:ASN:HB3	1:B:40:LEU:HB2	1.91	0.52
1:B:511:THR:OG1	1:B:544:PRO:HD3	2.10	0.52
1:A:53:LEU:HB3	1:A:114:LEU:HD11	1.92	0.52
1:B:27:GLN:HA	1:B:27:GLN:NE2	2.25	0.52
1:A:210:ASN:H	1:A:210:ASN:ND2	2.07	0.52
1:A:414:ASN:OD1	1:A:417:THR:HG23	2.10	0.52
1:B:289:PRO:HB2	1:B:336:TRP:HB3	1.91	0.52
1:B:54:GLU:HG3	1:B:117:PHE:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ASP:HB2	1:B:512:LYS:HE3	1.91	0.52
1:B:505:LYS:HG3	1:B:547:GLU:HG2	1.91	0.52
1:B:139:ASN:HA	1:B:144:PHE:CG	2.45	0.51
1:A:555:SER:H	1:A:558:GLN:NE2	2.08	0.51
1:B:502:LEU:O	1:B:549:GLU:HA	2.10	0.51
1:B:571:ILE:HD12	1:B:571:ILE:N	2.24	0.51
1:A:606:VAL:HG23	1:A:691:ALA:O	2.10	0.51
1:B:456:LEU:HD13	1:B:456:LEU:O	2.10	0.51
1:A:612:VAL:HG12	1:A:613:GLN:N	2.26	0.51
1:A:135:ASN:C	1:A:135:ASN:HD22	2.14	0.51
1:A:293:ILE:CG1	1:A:334:GLU:HG3	2.41	0.51
1:A:610:VAL:HG13	1:A:660:ILE:CG1	2.41	0.51
1:B:12:THR:HG22	1:B:16:ARG:HD3	1.92	0.51
1:B:302:THR:HG21	1:B:390:ALA:HB1	1.93	0.51
1:B:514:VAL:HG22	1:B:577:VAL:CG2	2.41	0.51
1:B:54:GLU:HB2	1:B:115:GLN:HB3	1.92	0.50
1:B:163:PHE:CE2	1:B:432:ARG:HB2	2.46	0.50
1:A:646:PRO:HG2	5:A:1065:HOH:O	2.11	0.50
1:A:137:TRP:CE2	1:A:151:ARG:HD3	2.46	0.50
1:B:624:VAL:HG12	1:B:648:LEU:HB3	1.94	0.50
1:A:596:LEU:HD23	1:A:684:ALA:HB2	1.94	0.50
1:A:289:PRO:HB2	1:A:336:TRP:HB3	1.93	0.50
1:A:107:ILE:HD13	1:A:134:PHE:CE2	2.47	0.49
1:A:446:ASP:O	1:A:450:GLN:HG3	2.13	0.49
1:B:396:ARG:NH2	1:B:586:GLU:OE1	2.46	0.49
1:A:114:LEU:HB2	1:A:127:LEU:HD11	1.94	0.49
1:B:535:LYS:O	1:B:536:ASP:HB2	2.12	0.49
1:A:382:ASN:HB3	1:A:383:PHE:CG	2.47	0.49
1:B:297:ASN:O	1:B:418:ILE:HG23	2.13	0.48
1:B:653:ARG:HB2	5:B:796:HOH:O	2.13	0.48
1:A:135:ASN:HD22	1:A:137:TRP:H	1.61	0.48
1:B:223:ILE:HB	1:B:354:ALA:HB1	1.95	0.48
1:B:316:GLY:HA2	1:B:574:VAL:HG23	1.95	0.48
1:A:624:VAL:HG13	1:A:676:CYS:HB2	1.96	0.48
1:B:130:PHE:HE2	1:B:132:LEU:HG	1.79	0.48
1:B:524:ILE:HB	1:B:526:ASN:ND2	2.28	0.47
1:B:576:LYS:HB2	1:B:582:GLU:HG3	1.96	0.47
1:A:36:ASN:OD1	1:A:100:SER:HB2	2.15	0.47
1:A:247:ARG:HG2	1:A:273:TRP:CH2	2.49	0.47
1:B:618:ASN:CB	1:B:648:LEU:HD22	2.44	0.47
1:B:235:ASN:HD22	1:B:236:TRP:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.30	0.47
1:A:235:ASN:HD22	1:A:237:SER:H	1.61	0.47
1:A:223:ILE:HB	1:A:354:ALA:HB1	1.97	0.47
1:B:473:LEU:HD13	1:B:473:LEU:C	2.35	0.47
1:B:483:ILE:HG13	1:B:507:LEU:HD11	1.97	0.46
1:B:501:VAL:CG1	1:B:549:GLU:HB2	2.45	0.46
1:B:655:ARG:HD2	5:B:859:HOH:O	2.14	0.46
1:A:649:GLY:O	1:A:652:GLU:HB2	2.16	0.46
1:A:183:ASP:O	1:A:187:ILE:HG13	2.15	0.46
1:A:217:ARG:NH2	1:A:365:GLN:NE2	2.63	0.46
1:B:597:THR:CG2	1:B:615:LEU:HB2	2.36	0.46
1:A:135:ASN:ND2	1:A:137:TRP:HB2	2.30	0.46
1:B:134:PHE:HB3	1:B:143:VAL:HG21	1.98	0.46
1:B:135:ASN:HD21	1:B:137:TRP:HB2	1.81	0.46
1:B:514:VAL:HG22	1:B:577:VAL:HG22	1.98	0.46
1:A:624:VAL:HG12	1:A:627:CYS:SG	2.56	0.46
1:A:226:ASN:HD22	1:A:226:ASN:H	1.64	0.46
1:B:491:MET:HG2	1:B:496:LYS:HZ3	1.81	0.45
1:A:446:ASP:HB3	1:A:450:GLN:HE21	1.80	0.45
1:B:27:GLN:HE21	1:B:27:GLN:CA	2.25	0.45
1:B:268:ARG:HA	1:B:269:TYR:HA	1.68	0.45
1:B:199:ARG:NE	5:B:768:HOH:O	2.50	0.45
1:B:382:ASN:HB3	1:B:383:PHE:CD1	2.52	0.45
1:B:247:ARG:HD2	5:B:708:HOH:O	2.17	0.45
1:A:268:ARG:HA	1:A:269:TYR:HA	1.74	0.45
1:B:53:LEU:HB3	1:B:114:LEU:HD11	1.99	0.45
1:A:299:ALA:HB2	1:A:418:ILE:HD13	1.98	0.45
1:A:485:LYS:HE3	1:A:487:LYS:HG2	1.98	0.45
1:B:306:LEU:HG	1:B:459:LEU:CD1	2.47	0.45
1:A:577:VAL:HG13	1:A:578:PRO:HD2	1.98	0.45
1:B:481:SER:C	1:B:482:ILE:HD12	2.36	0.45
1:B:516:VAL:O	1:B:537:SER:HA	2.17	0.45
1:B:648:LEU:HD23	1:B:649:GLY:O	2.17	0.44
1:A:134:PHE:HB3	1:A:143:VAL:HG21	1.98	0.44
1:A:235:ASN:HD22	1:A:236:TRP:N	2.15	0.44
1:B:322:GLY:HA2	1:B:325:SER:OG	2.18	0.44
1:A:641:LEU:HD22	1:A:643:ILE:HG13	2.00	0.44
1:B:396:ARG:HH22	1:B:586:GLU:CD	2.21	0.44
1:A:385:MET:HB2	1:A:386:PRO:HD3	2.00	0.44
1:A:611:ASN:OD1	1:A:657:ARG:HD2	2.17	0.44
1:B:385:MET:N	1:B:386:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:HE2	1:A:132:LEU:HG	1.83	0.44
1:A:449:ARG:NH2	5:A:1050:HOH:O	2.51	0.44
1:B:488:VAL:HG22	1:B:500:LEU:CD2	2.47	0.44
1:A:117:PHE:CG	1:B:651:LYS:HD2	2.53	0.44
1:A:602:ASN:HB2	5:A:1081:HOH:O	2.18	0.44
1:A:448:GLU:OE2	1:A:449:ARG:NH1	2.50	0.44
1:A:602:ASN:CG	1:A:610:VAL:HG23	2.37	0.43
1:A:610:VAL:CG1	1:A:660:ILE:HG13	2.48	0.43
1:A:62:TYR:N	1:A:63:PRO:HD3	2.33	0.43
1:B:606:VAL:HG23	1:B:691:ALA:O	2.18	0.43
1:A:139:ASN:HA	1:A:144:PHE:CD1	2.53	0.43
1:A:607:ARG:NH1	1:A:607:ARG:HB2	2.34	0.43
1:B:594:PRO:HB2	1:B:616:PHE:HE1	1.83	0.43
1:B:511:THR:HA	1:B:542:LEU:O	2.18	0.43
1:A:448:GLU:HG3	1:A:449:ARG:N	2.33	0.43
1:B:211:ASP:HA	1:B:212:PRO:HD2	1.94	0.43
1:B:210:ASN:H	1:B:210:ASN:ND2	2.16	0.43
1:A:112:MET:HG2	1:A:127:LEU:HD12	2.00	0.43
1:A:382:ASN:HA	1:A:383:PHE:HA	1.74	0.43
1:B:197:ASN:N	1:B:197:ASN:ND2	2.67	0.43
1:A:52:ARG:HG3	5:A:1155:HOH:O	2.19	0.43
1:A:488:VAL:HA	1:A:500:LEU:HD23	2.01	0.43
1:B:337:PHE:CE1	1:B:350:GLN:HG3	2.53	0.42
1:B:380:GLN:H	1:B:380:GLN:CD	2.22	0.42
1:A:309:ASP:HB3	1:A:399:TRP:CD1	2.54	0.42
1:A:501:VAL:CG1	1:A:549:GLU:HB3	2.49	0.42
1:A:305:ASN:HD22	1:A:305:ASN:C	2.22	0.42
1:A:65:GLU:OE1	1:B:653:ARG:NH1	2.53	0.42
1:B:82:GLY:CA	1:B:102:PRO:HB3	2.50	0.42
1:A:396:ARG:NH2	1:A:586:GLU:OE2	2.51	0.42
1:B:73:PHE:N	1:B:73:PHE:CD1	2.86	0.42
1:A:293:ILE:HD13	1:A:424:THR:HB	2.02	0.42
1:B:594:PRO:HB2	1:B:616:PHE:CE1	2.55	0.42
1:B:8:ILE:HD13	1:B:41:MET:HE3	2.02	0.42
1:B:5:VAL:HG22	1:B:43:MET:SD	2.60	0.42
1:A:370:SER:O	1:A:374:VAL:HG23	2.20	0.42
1:B:302:THR:CB	1:B:308:VAL:HG13	2.35	0.42
1:B:627:CYS:HB2	1:B:645:VAL:HB	2.00	0.42
1:B:303:ASP:N	5:B:949:HOH:O	2.53	0.41
1:B:653:ARG:HE	1:B:653:ARG:HB3	1.41	0.41
1:A:524:ILE:HB	1:A:526:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:MET:O	1:A:672:ALA:HA	2.20	0.41
1:B:559:TYR:CD1	1:B:560:GLU:N	2.88	0.41
1:B:185:LEU:HD22	1:B:189:LEU:CD1	2.51	0.41
1:A:10:TRP:O	1:A:11:GLN:C	2.58	0.41
1:A:522:THR:HG23	1:A:533:VAL:HG11	2.02	0.41
1:B:138:LEU:O	1:B:144:PHE:HB2	2.21	0.41
1:B:213:LYS:HE3	5:B:749:HOH:O	2.21	0.41
1:B:491:MET:CG	1:B:496:LYS:HZ2	2.33	0.41
1:A:12:THR:HG22	1:A:16:ARG:HD3	2.02	0.41
1:B:524:ILE:HB	1:B:526:ASN:HD21	1.84	0.41
1:B:614:MET:HB3	1:B:656:VAL:HB	2.02	0.41
1:B:139:ASN:N	1:B:139:ASN:HD22	2.17	0.41
1:B:624:VAL:HG22	1:B:676:CYS:SG	2.61	0.41
1:A:195:SER:O	1:A:199:ARG:HG3	2.21	0.41
1:A:53:LEU:HD22	1:A:116:ILE:HG12	2.02	0.41
1:A:627:CYS:HB2	1:A:645:VAL:O	2.21	0.41
1:B:299:ALA:HB3	1:B:391:GLU:HA	2.02	0.41
1:A:137:TRP:CD2	1:A:151:ARG:HD3	2.56	0.41
1:B:139:ASN:HA	1:B:144:PHE:CD1	2.55	0.40
1:A:379:VAL:HA	1:A:385:MET:HB3	2.03	0.40
5:A:1071:HOH:O	1:B:615:LEU:HD22	2.21	0.40
1:A:135:ASN:ND2	1:A:137:TRP:H	2.19	0.40
1:A:524:ILE:HB	1:A:526:ASN:HD21	1.87	0.40
1:B:630:MET:O	1:B:672:ALA:HA	2.22	0.40
1:B:235:ASN:C	1:B:235:ASN:ND2	2.72	0.40
1:A:479:GLU:N	1:A:480:PRO:HD3	2.35	0.40
1:A:514:VAL:HG22	1:A:577:VAL:CG2	2.52	0.40
1:B:449:ARG:HH21	1:B:452:PHE:CB	2.34	0.40
1:B:8:ILE:HG13	1:B:9:ASN:N	2.37	0.40
1:A:380:GLN:HG3	1:A:458:LYS:HD3	2.03	0.40
1:B:445:SER:HB2	1:B:447:GLN:NE2	2.36	0.40
1:B:199:ARG:NH2	5:B:987:HOH:O	2.49	0.40
1:B:446:ASP:O	1:B:450:GLN:HG3	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	671/692 (97%)	644 (96%)	24 (4%)	3 (0%)	39	37
1	B	677/692 (98%)	635 (94%)	35 (5%)	7 (1%)	19	13
All	All	1348/1384 (97%)	1279 (95%)	59 (4%)	10 (1%)	26	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	LYS
1	B	81	GLY
1	B	82	GLY
1	B	508	SER
1	B	509	ARG
1	A	80	SER
1	B	477	GLU
1	B	511	THR
1	A	82	GLY
1	B	480	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	581/595 (98%)	558 (96%)	23 (4%)	38	38
1	B	586/595 (98%)	561 (96%)	25 (4%)	35	34
All	All	1167/1190 (98%)	1119 (96%)	48 (4%)	37	36

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	17	GLN
1	A	47	LEU
1	A	75	LEU
1	A	132	LEU
1	A	135	ASN
1	A	138	LEU
1	A	139	ASN
1	A	185	LEU
1	A	210	ASN
1	A	235	ASN
1	A	286	LEU
1	A	305	ASN
1	A	319	LEU
1	A	380	GLN
1	A	400	LEU
1	A	447	GLN
1	A	448	GLU
1	A	449	ARG
1	A	526	ASN
1	A	624	VAL
1	A	629	LEU
1	A	641	LEU
1	B	75	LEU
1	B	135	ASN
1	B	138	LEU
1	B	139	ASN
1	B	185	LEU
1	B	197	ASN
1	B	210	ASN
1	B	235	ASN
1	B	301	ASP
1	B	315	MET
1	B	380	GLN
1	B	408	GLN
1	B	447	GLN
1	B	448	GLU
1	B	456	LEU
1	B	473	LEU
1	B	506	ASN
1	B	526	ASN
1	B	601	LEU

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Mol	Chain	Res	Type
1	B	614	MET
1	B	624	VAL
1	B	629	LEU
1	B	641	LEU
1	B	653	ARG
1	B	655	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	20	HIS
1	A	77	ASN
1	A	91	ASN
1	A	119	GLN
1	A	135	ASN
1	A	139	ASN
1	A	210	ASN
1	A	226	ASN
1	A	235	ASN
1	A	280	ASN
1	A	305	ASN
1	A	365	GLN
1	A	408	GLN
1	A	447	GLN
1	A	450	GLN
1	A	526	ASN
1	A	558	GLN
1	A	567	ASN
1	A	669	GLN
1	B	20	HIS
1	B	27	GLN
1	B	77	ASN
1	B	91	ASN
1	B	115	GLN
1	B	135	ASN
1	B	139	ASN
1	B	197	ASN
1	B	210	ASN
1	B	226	ASN
1	B	235	ASN
1	B	280	ASN

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Mol	Chain	Res	Type
1	B	403	ASN
1	B	408	GLN
1	B	411	ASN
1	B	447	GLN
1	B	506	ASN
1	B	526	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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 ⓘ

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 ⓘ

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.