



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:59 AM UTC

PDB ID : 1NUF / pdb_00001nuf
Title : Role of Calcium Ions in the Activation and Activity of the Transglutaminase
3 Enzyme
Authors : Ahvazi, B.
Deposited on : 2003-01-31
Resolution : 2.70 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
Xtriage (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

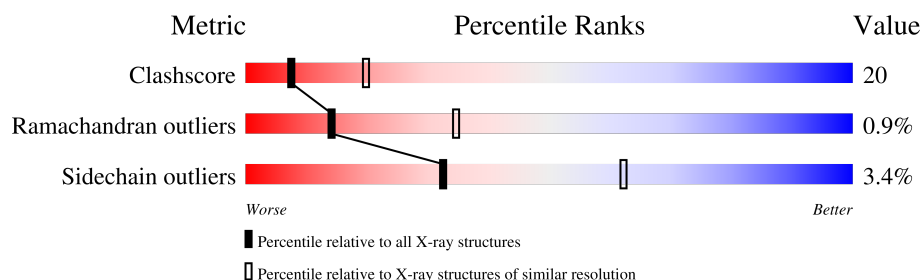
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	692	 60% 34% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5473 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 E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total	C	N	O	S	0	0	0
			5266	3323	915	1005	23			

There are 4 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 mutation	UNP Q08188
A	561	ARG	LYS	SEE REMARK 999	UNP Q08188
A	653	ARG	GLY	SEE REMARK 999	UNP Q08188

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cl	0	0
			4	4		

- Molecule 3 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Br	0	0
			4	4		

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

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

- Molecule 5 is water.

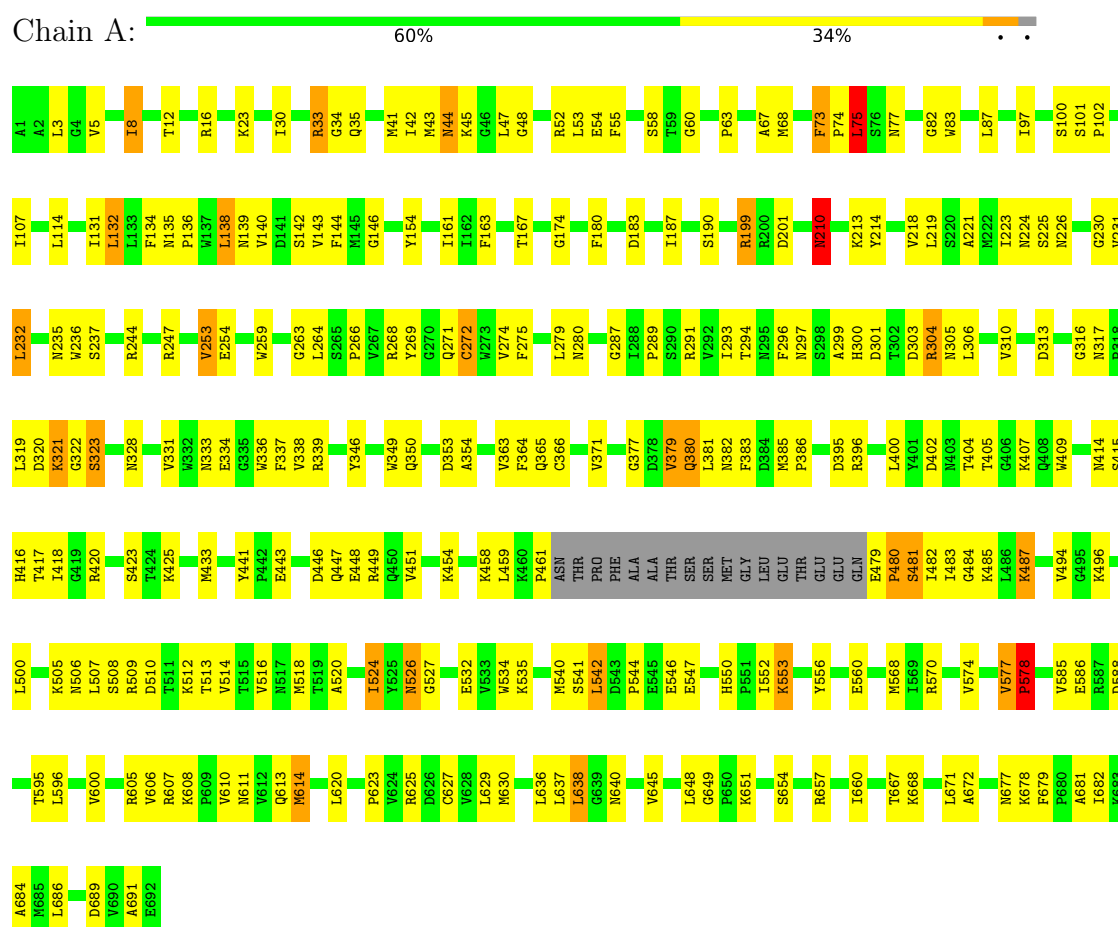
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	198	Total 198	O 198	0	0

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 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. 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 E



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.74Å 115.84Å 61.96Å 90.00° 94.14° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.186 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5473	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: BR, CA, 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	0.42	0/5377	0.94	25/7295 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	681	ALA	N-CA-C	8.06	121.10	111.02
1	A	73	PHE	CA-C-N	6.47	126.69	119.90
1	A	73	PHE	C-N-CA	6.47	126.69	119.90
1	A	33	ARG	N-CA-C	6.42	119.08	110.35
1	A	75	LEU	N-CA-C	-6.13	100.32	109.15
1	A	524	ILE	N-CA-C	-6.12	99.74	109.17
1	A	595	THR	N-CA-C	6.07	119.27	110.28
1	A	232	LEU	N-CA-C	6.01	119.03	109.24
1	A	253	VAL	N-CA-C	6.00	116.12	110.30
1	A	379	VAL	N-CA-C	5.78	120.10	112.76
1	A	97	ILE	N-CA-C	5.62	116.57	108.48
1	A	146	GLY	N-CA-C	5.57	119.90	112.77
1	A	409	TRP	N-CA-C	5.48	118.39	108.69
1	A	346	TYR	N-CA-C	5.46	118.94	112.72
1	A	423	SER	N-CA-C	5.42	118.41	109.85
1	A	77	ASN	N-CA-C	-5.34	106.78	113.72
1	A	577	VAL	CA-C-N	5.32	126.49	119.84
1	A	577	VAL	C-N-CA	5.32	126.49	119.84
1	A	210	ASN	N-CA-C	-5.21	106.51	112.92
1	A	516	VAL	N-CA-C	5.17	115.31	107.75
1	A	305	ASN	N-CA-C	-5.16	105.99	113.21
1	A	272	CYS	N-CA-C	5.14	121.75	110.80
1	A	514	VAL	N-CA-C	5.11	115.20	107.75
1	A	323	SER	N-CA-C	-5.05	105.92	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	620	LEU	N-CA-C	5.03	116.60	110.41

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	213	0
2	A	4	0	0	0	0
3	A	4	0	0	1	0
4	A	1	0	0	0	0
5	A	198	0	0	12	0
All	All	5473	0	5206	213	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 20.

All (213) 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:380:GLN:HG3	1:A:458:LYS:HD3	1.25	1.17
1:A:630:MET:HG3	1:A:640:ASN:HD21	1.19	1.04
1:A:304:ARG:HD3	1:A:459:LEU:HD11	1.40	1.01
1:A:606:VAL:HG12	1:A:607:ARG:HG3	1.45	0.96
1:A:395:ASP:OD1	1:A:415:SER:HB3	1.67	0.92
1:A:605:ARG:HG2	1:A:691:ALA:HB3	1.51	0.92
1:A:82:GLY:HA2	1:A:102:PRO:HB3	1.53	0.89
1:A:380:GLN:CG	1:A:458:LYS:HD3	2.05	0.86
1:A:577:VAL:HG13	1:A:578:PRO:HD2	1.57	0.85
1:A:44:ASN:HD22	1:A:45:LYS:N	1.77	0.82
1:A:506:ASN:HD22	1:A:507:LEU:N	1.77	0.81
1:A:44:ASN:ND2	1:A:45:LYS:HG2	1.95	0.81
1:A:506:ASN:HD22	1:A:507:LEU:H	1.30	0.79
1:A:380:GLN:HG3	1:A:458:LYS:CD	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HB3	1:A:114:LEU:HD11	1.67	0.75
1:A:505:LYS:HG3	1:A:547:GLU:HG3	1.69	0.73
1:A:542:LEU:HB3	1:A:546:GLU:HB3	1.70	0.72
1:A:570:ARG:HD3	1:A:588:ASP:OD1	1.91	0.71
1:A:479:GLU:N	1:A:480:PRO:HD3	2.06	0.71
1:A:225:SER:OG	1:A:266:PRO:HB3	1.91	0.71
1:A:304:ARG:HB3	1:A:459:LEU:HD21	1.76	0.67
1:A:526:ASN:HD22	1:A:526:ASN:H	1.42	0.67
1:A:446:ASP:HA	1:A:449:ARG:NH1	2.10	0.66
1:A:300:HIS:ND1	5:A:848:HOH:O	2.28	0.66
1:A:33:ARG:HB3	1:A:132:LEU:HD11	1.78	0.65
1:A:510:ASP:N	1:A:544:PRO:HG3	2.11	0.65
1:A:510:ASP:H	1:A:544:PRO:HG3	1.61	0.65
1:A:58:SER:HB2	1:A:63:PRO:HB3	1.78	0.64
1:A:481:SER:HB3	1:A:482:ILE:HD12	1.78	0.64
1:A:30:ILE:HD12	1:A:131:ILE:HD12	1.80	0.63
1:A:75:LEU:HD21	1:A:87:LEU:HB2	1.79	0.63
1:A:316:GLY:HA2	1:A:574:VAL:HG23	1.80	0.63
1:A:605:ARG:HB2	1:A:608:LYS:HD2	1.80	0.63
1:A:44:ASN:HD21	1:A:45:LYS:HG2	1.64	0.63
1:A:414:ASN:HD22	1:A:415:SER:N	1.96	0.62
1:A:667:THR:HG22	1:A:689:ASP:OD1	1.99	0.62
1:A:542:LEU:HA	1:A:546:GLU:OE2	1.99	0.62
1:A:33:ARG:HB3	1:A:132:LEU:CD1	2.29	0.62
1:A:479:GLU:N	1:A:480:PRO:CD	2.62	0.62
1:A:483:ILE:HD11	1:A:505:LYS:HE2	1.80	0.62
1:A:433:MET:HE2	5:A:901:HOH:O	1.99	0.62
1:A:480:PRO:O	1:A:481:SER:HB2	2.00	0.62
1:A:35:GLN:HE21	1:A:135:ASN:HD21	1.48	0.61
1:A:321:LYS:HE3	5:A:808:HOH:O	2.01	0.61
1:A:459:LEU:O	1:A:461:PRO:HD3	2.00	0.61
1:A:107:ILE:HD13	1:A:134:PHE:CE2	2.36	0.60
1:A:334:GLU:HA	1:A:350:GLN:O	2.02	0.60
1:A:630:MET:HG3	1:A:640:ASN:ND2	2.04	0.60
1:A:235:ASN:C	1:A:235:ASN:HD22	2.09	0.60
1:A:526:ASN:HD22	1:A:526:ASN:N	1.99	0.60
1:A:414:ASN:ND2	1:A:416:HIS:H	2.00	0.60
1:A:67:ALA:O	1:A:68:MET:HB2	2.02	0.60
1:A:385:MET:HB2	1:A:386:PRO:HD3	1.84	0.60
1:A:518:MET:HE1	1:A:550:HIS:CE1	2.36	0.59
1:A:614:MET:C	1:A:614:MET:HE2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LYS:HD3	1:A:339:ARG:HE	1.67	0.59
1:A:235:ASN:ND2	1:A:237:SER:H	2.00	0.59
1:A:44:ASN:HD22	1:A:44:ASN:C	2.07	0.58
1:A:414:ASN:HD22	1:A:414:ASN:C	2.11	0.58
1:A:600:VAL:HG23	1:A:686:LEU:HD21	1.84	0.58
1:A:553:LYS:HB2	1:A:553:LYS:NZ	2.19	0.58
1:A:293:ILE:HG13	1:A:334:GLU:HG3	1.86	0.58
1:A:482:ILE:HD12	1:A:482:ILE:N	2.18	0.58
1:A:396:ARG:HH22	1:A:586:GLU:CD	2.11	0.57
1:A:139:ASN:HA	1:A:144:PHE:CG	2.40	0.57
1:A:5:VAL:CG2	1:A:114:LEU:HD23	2.34	0.57
1:A:235:ASN:HD22	1:A:236:TRP:N	2.03	0.57
1:A:482:ILE:HD11	1:A:577:VAL:HG21	1.87	0.56
1:A:636:LEU:HD21	1:A:668:LYS:HB2	1.86	0.56
1:A:232:LEU:CD1	1:A:274:VAL:HG12	2.35	0.56
1:A:35:GLN:NE2	1:A:135:ASN:HD21	2.03	0.56
1:A:483:ILE:HD11	1:A:505:LYS:HB3	1.87	0.56
1:A:337:PHE:CE1	1:A:350:GLN:HG3	2.42	0.55
1:A:416:HIS:HB3	1:A:443:GLU:OE1	2.07	0.55
1:A:638:LEU:HB2	3:A:709:BR:BR	2.62	0.55
1:A:139:ASN:HA	1:A:144:PHE:CD1	2.42	0.55
1:A:381:LEU:O	1:A:385:MET:HG3	2.07	0.55
1:A:47:LEU:HD23	1:A:48:GLY:N	2.22	0.54
1:A:613:GLN:HG2	1:A:657:ARG:HG2	1.88	0.54
1:A:201:ASP:OD2	1:A:201:ASP:C	2.52	0.53
1:A:614:MET:HE2	1:A:614:MET:O	2.08	0.53
1:A:596:LEU:HD23	1:A:684:ALA:HB2	1.90	0.53
1:A:625:ARG:HH11	1:A:625:ARG:HG2	1.72	0.53
1:A:232:LEU:HD11	1:A:274:VAL:HG12	1.90	0.53
1:A:506:ASN:ND2	1:A:507:LEU:N	2.53	0.53
1:A:224:ASN:O	1:A:230:GLY:HA3	2.09	0.53
1:A:154:TYR:O	1:A:289:PRO:HA	2.09	0.52
1:A:520:ALA:HB3	1:A:534:TRP:HB3	1.92	0.52
1:A:75:LEU:CD2	1:A:87:LEU:HB2	2.40	0.52
1:A:23:LYS:HE3	1:A:180:PHE:CE2	2.45	0.52
1:A:183:ASP:O	1:A:187:ILE:HG13	2.10	0.52
1:A:382:ASN:HB3	1:A:383:PHE:CG	2.44	0.52
1:A:506:ASN:ND2	1:A:508:SER:H	2.08	0.52
1:A:524:ILE:HB	1:A:526:ASN:ND2	2.25	0.51
1:A:42:ILE:N	1:A:42:ILE:HD12	2.26	0.51
1:A:677:ASN:ND2	1:A:678:LYS:HD3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASN:HD22	1:A:210:ASN:H	1.56	0.51
1:A:136:PRO:HG3	1:A:287:GLY:O	2.10	0.51
1:A:319:LEU:O	1:A:323:SER:HB3	2.10	0.51
1:A:138:LEU:HD22	1:A:140:VAL:HG22	1.92	0.51
1:A:414:ASN:OD1	1:A:417:THR:HG23	2.11	0.51
1:A:610:VAL:HG13	1:A:660:ILE:CG1	2.41	0.51
1:A:280:ASN:HD22	1:A:333:ASN:HD22	1.58	0.50
1:A:41:MET:HE1	1:A:55:PHE:CZ	2.46	0.50
1:A:679:PHE:HB3	1:A:682:ILE:HD11	1.94	0.50
1:A:377:GLY:C	1:A:379:VAL:H	2.20	0.49
1:A:253:VAL:HG12	1:A:254:GLU:OE1	2.12	0.49
1:A:134:PHE:HB3	1:A:143:VAL:HG21	1.95	0.49
1:A:505:LYS:CG	1:A:547:GLU:HG3	2.40	0.49
1:A:512:LYS:O	1:A:541:SER:HA	2.13	0.49
1:A:30:ILE:CD1	1:A:131:ILE:HD12	2.42	0.48
1:A:231:VAL:HG22	1:A:259:TRP:CE2	2.48	0.48
1:A:363:VAL:HG12	1:A:364:PHE:N	2.28	0.48
1:A:41:MET:HE1	1:A:55:PHE:CE2	2.48	0.48
1:A:272:CYS:HA	1:A:275:PHE:HD2	1.78	0.48
1:A:279:LEU:HD22	1:A:354:ALA:HB2	1.95	0.48
1:A:320:ASP:O	1:A:322:GLY:N	2.47	0.48
1:A:494:VAL:HG12	1:A:679:PHE:HE2	1.77	0.48
1:A:415:SER:C	1:A:416:HIS:HD2	2.22	0.48
1:A:484:GLY:HA3	1:A:585:VAL:HG21	1.95	0.48
1:A:524:ILE:HB	1:A:526:ASN:HD21	1.79	0.48
1:A:323:SER:O	1:A:527:GLY:HA3	2.13	0.48
1:A:363:VAL:CG1	1:A:364:PHE:N	2.76	0.48
1:A:610:VAL:HG13	1:A:660:ILE:HG12	1.96	0.48
1:A:637:LEU:HD21	1:A:660:ILE:HG22	1.96	0.48
1:A:349:TRP:O	1:A:371:VAL:HG23	2.13	0.48
1:A:221:ALA:HB2	1:A:365:GLN:HB3	1.95	0.47
1:A:247:ARG:HD2	5:A:716:HOH:O	2.13	0.47
1:A:214:TYR:O	1:A:218:VAL:HG23	2.14	0.47
1:A:509:ARG:O	1:A:510:ASP:HB2	2.14	0.47
1:A:577:VAL:CG1	1:A:578:PRO:HD2	2.36	0.47
1:A:268:ARG:HB3	1:A:269:TYR:CG	2.50	0.47
1:A:605:ARG:NH1	1:A:608:LYS:HZ1	2.13	0.47
1:A:623:PRO:HB3	1:A:649:GLY:HA2	1.97	0.47
1:A:611:ASN:HB2	5:A:872:HOH:O	2.15	0.47
1:A:289:PRO:HB2	1:A:336:TRP:HB3	1.95	0.47
1:A:163:PHE:O	1:A:294:THR:HG21	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASN:ND2	1:A:44:ASN:C	2.74	0.46
1:A:73:PHE:CD1	1:A:73:PHE:N	2.84	0.46
1:A:448:GLU:HG3	1:A:449:ARG:N	2.31	0.46
1:A:187:ILE:O	1:A:190:SER:HB2	2.15	0.46
1:A:174:GLY:HA3	1:A:671:LEU:HD21	1.97	0.46
1:A:542:LEU:HD12	1:A:542:LEU:N	2.31	0.46
1:A:52:ARG:NH1	1:A:54:GLU:OE2	2.49	0.45
1:A:414:ASN:HD22	1:A:416:HIS:H	1.63	0.45
1:A:23:LYS:HE3	1:A:180:PHE:CZ	2.51	0.45
1:A:235:ASN:HD22	1:A:237:SER:H	1.62	0.45
1:A:236:TRP:NE1	1:A:271:GLN:HG2	2.31	0.45
1:A:60:GLY:HA3	5:A:759:HOH:O	2.15	0.45
1:A:263:GLY:O	1:A:264:LEU:HB2	2.16	0.45
1:A:416:HIS:CD2	5:A:840:HOH:O	2.69	0.45
1:A:487:LYS:NZ	1:A:487:LYS:CB	2.79	0.45
1:A:605:ARG:NH1	1:A:608:LYS:NZ	2.64	0.45
1:A:570:ARG:HD2	5:A:712:HOH:O	2.16	0.45
1:A:219:LEU:O	1:A:223:ILE:HG12	2.17	0.45
1:A:299:ALA:HB2	1:A:418:ILE:HD13	1.99	0.45
1:A:416:HIS:CD2	1:A:416:HIS:N	2.84	0.45
1:A:8:ILE:HG12	1:A:41:MET:HG3	1.99	0.45
1:A:199:ARG:NH1	1:A:199:ARG:HG2	2.31	0.45
1:A:231:VAL:HG22	1:A:259:TRP:CD2	2.51	0.45
1:A:313:ASP:OD2	1:A:317:ASN:HB2	2.16	0.45
1:A:484:GLY:HA3	1:A:585:VAL:CG2	2.47	0.45
1:A:500:LEU:HB2	1:A:552:ILE:HB	1.97	0.45
1:A:73:PHE:HA	1:A:74:PRO:HD3	1.72	0.45
1:A:210:ASN:HD22	1:A:210:ASN:N	2.15	0.45
1:A:301:ASP:OD2	1:A:303:ASP:O	2.35	0.45
1:A:481:SER:C	1:A:482:ILE:HD12	2.42	0.44
1:A:532:GLU:OE1	1:A:535:LYS:HD3	2.17	0.44
1:A:447:GLN:N	1:A:447:GLN:OE1	2.50	0.44
1:A:441:TYR:CG	1:A:447:GLN:HB3	2.52	0.44
1:A:53:LEU:HD12	1:A:75:LEU:HD12	1.98	0.44
1:A:142:SER:CB	1:A:338:VAL:HG22	2.47	0.44
1:A:484:GLY:O	1:A:485:LYS:HG3	2.18	0.44
1:A:625:ARG:HG2	1:A:625:ARG:NH1	2.33	0.44
1:A:161:ILE:HB	1:A:425:LYS:HD2	1.99	0.44
1:A:415:SER:HB2	5:A:795:HOH:O	2.18	0.44
1:A:494:VAL:CG1	1:A:679:PHE:HE2	2.31	0.43
1:A:296:PHE:HB2	1:A:420:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ASN:HB3	1:A:383:PHE:CD1	2.53	0.43
1:A:68:MET:HB2	5:A:745:HOH:O	2.18	0.43
1:A:405:THR:C	1:A:407:LYS:H	2.27	0.43
1:A:496:LYS:HE2	1:A:496:LYS:HB3	1.85	0.43
1:A:3:LEU:HG	1:A:43:MET:HE3	2.00	0.43
1:A:223:ILE:O	1:A:223:ILE:HG22	2.19	0.43
1:A:651:LYS:HE3	5:A:821:HOH:O	2.19	0.43
1:A:244:ARG:NH2	1:A:630:MET:HE3	2.34	0.43
1:A:5:VAL:HG21	1:A:114:LEU:HD23	2.01	0.43
1:A:167:THR:HG21	1:A:297:ASN:ND2	2.33	0.42
1:A:627:CYS:HB2	1:A:645:VAL:HB	2.01	0.42
1:A:154:TYR:CD1	1:A:291:ARG:HB3	2.54	0.42
1:A:414:ASN:CG	1:A:417:THR:HG23	2.44	0.42
1:A:420:ARG:NH1	5:A:746:HOH:O	2.52	0.42
1:A:402:ASP:CG	1:A:405:THR:HG23	2.45	0.42
1:A:268:ARG:HA	1:A:269:TYR:HA	1.61	0.42
1:A:540:MET:HE1	1:A:550:HIS:HB2	2.01	0.42
1:A:404:THR:OG1	1:A:405:THR:N	2.53	0.42
1:A:447:GLN:O	1:A:451:VAL:HG23	2.19	0.42
1:A:672:ALA:HB3	1:A:684:ALA:HB3	2.01	0.41
1:A:34:GLY:HA2	1:A:101:SER:O	2.20	0.41
1:A:304:ARG:HB3	1:A:459:LEU:CD2	2.48	0.41
1:A:316:GLY:HA2	1:A:574:VAL:CG2	2.49	0.41
1:A:328:ASN:OD1	1:A:568:MET:HE1	2.21	0.41
1:A:382:ASN:HA	1:A:383:PHE:HA	1.72	0.41
1:A:293:ILE:O	1:A:331:VAL:HG13	2.21	0.41
1:A:454:LYS:HE3	1:A:458:LYS:HZ1	1.85	0.41
1:A:638:LEU:HA	1:A:638:LEU:HD12	1.78	0.41
1:A:648:LEU:HD22	1:A:654:SER:HB2	2.03	0.41
1:A:12:THR:HG22	1:A:16:ARG:HD3	2.03	0.41
1:A:83:TRP:HA	1:A:100:SER:O	2.21	0.41
1:A:480:PRO:O	1:A:481:SER:CB	2.67	0.41
1:A:199:ARG:HH11	1:A:199:ARG:CG	2.34	0.40
1:A:556:TYR:CE1	1:A:560:GLU:HB3	2.55	0.40
1:A:353:ASP:O	1:A:366:CYS:HB3	2.22	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	671/692 (97%)	628 (94%)	37 (6%)	6 (1%)	14	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	PRO
1	A	321	LYS
1	A	481	SER
1	A	304	ARG
1	A	226	ASN
1	A	578	PRO

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	581/595 (98%)	561 (97%)	20 (3%)	32	62

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	44	ASN
1	A	75	LEU
1	A	132	LEU
1	A	138	LEU

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Mol	Chain	Res	Type
1	A	199	ARG
1	A	210	ASN
1	A	306	LEU
1	A	310	VAL
1	A	380	GLN
1	A	400	LEU
1	A	487	LYS
1	A	513	THR
1	A	526	ASN
1	A	542	LEU
1	A	553	LYS
1	A	578	PRO
1	A	614	MET
1	A	629	LEU
1	A	638	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	17	GLN
1	A	35	GLN
1	A	44	ASN
1	A	148	HIS
1	A	210	ASN
1	A	235	ASN
1	A	280	ASN
1	A	365	GLN
1	A	380	GLN
1	A	382	ASN
1	A	393	ASN
1	A	414	ASN
1	A	416	HIS
1	A	506	ASN
1	A	526	ASN
1	A	567	ASN
1	A	613	GLN
1	A	640	ASN
1	A	669	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 9 ligands modelled in this entry, 9 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

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.