



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:25 am GMT

PDB ID : 1NUG  
Title : Role of Calcium Ions in the Activation and Activity of the Transglutaminase  
3 Enzyme (2 calciums, 1 Mg, inactive form)  
Authors : Ahvazi, B.  
Deposited on : 2003-01-31  
Resolution : 2.40 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](mailto: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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

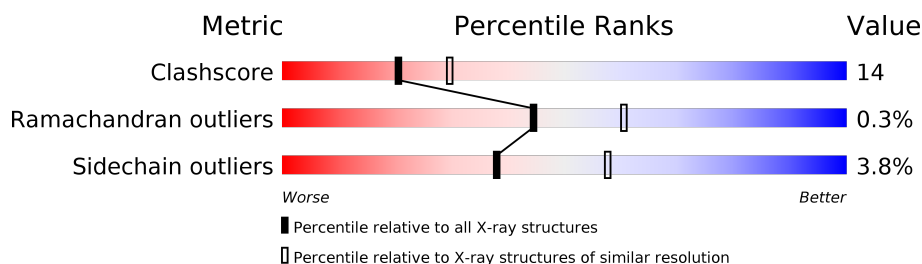
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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  $\geq 3$ , 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	
1	B	692	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11386 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			
1	B	679	Total	C	N	O	S	0	0	0
			5301	3342	919	1017	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

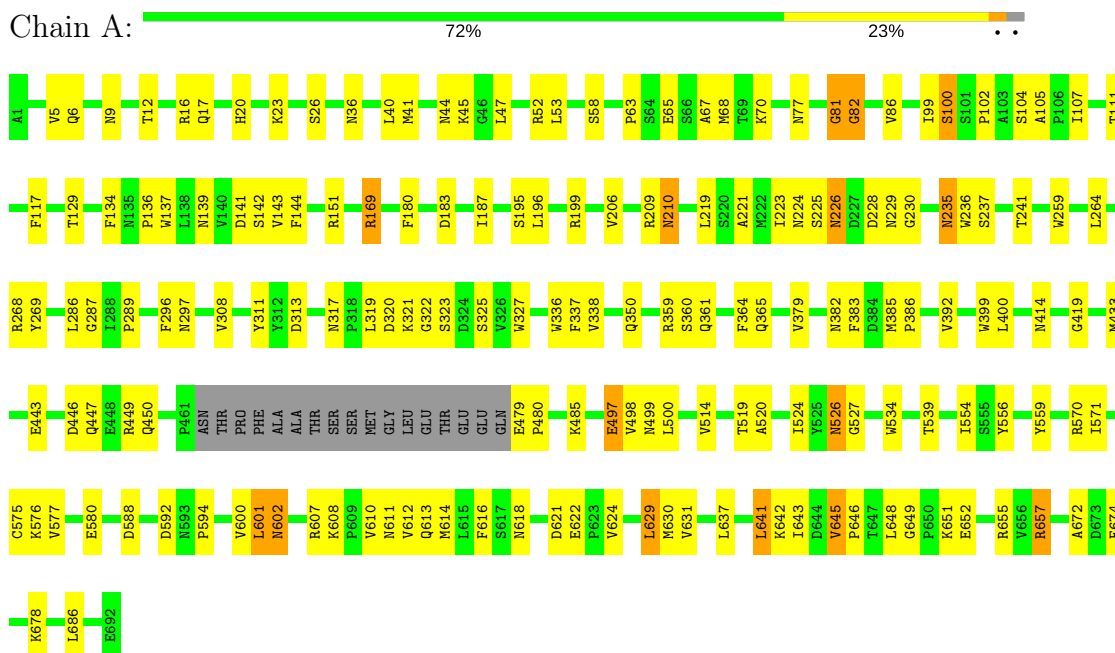
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	405	Total 405	O 405	0	0
5	B	404	Total 404	O 404	0	0

### 3 Residue-property plots

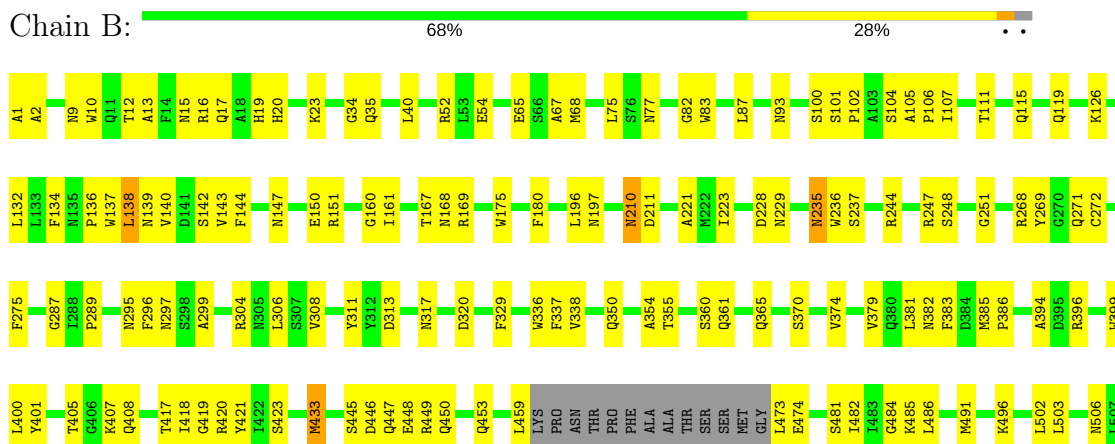
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: Protein-glutamine glutamyltransferase E



#### • Molecule 1: Protein-glutamine glutamyltransferase E



S508	R509	D510	T511	K512	T515	A520	I524	Y525	N526	W534	M540	E545	E546	E547	A548	E549	S555	Y556	A557	Q558	Y559	S565	V577	P578	D579	E580	V585	E586	P594	T595	L596	L601	R605	Y606	V610	N611	V612	Q613	N614	L615	F616	V624	R625	D626
G627	V628	L629	M630	G635	L636	L637	L641	K642	I643	D644	V645	P646	T647	L648	G649	P650	K651	E652	R653	S654	R655	V656	R657	I660	K668	Q669	A672	D673	C676	N677	K678	F679	A684	A691	E692									

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.51Å 66.81Å 116.53Å 97.24° 90.28° 98.36°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	10.2 (20.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.194 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 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, MG, 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	0.35	0/5377	0.62	0/7295
1	B	0.35	0/5411	0.61	1/7341 (0.0%)
All	All	0.35	0/10788	0.62	1/14636 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	637	LEU	CA-CB-CG	6.38	129.97	115.30

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	5266	0	5206	123	0
1	B	5301	0	5230	171	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	405	0	0	11	0
5	B	404	0	0	15	0
All	All	11386	0	10436	293	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 14.

All (293) 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:611:ASN:HB3	1:A:657:ARG:HH22	1.11	1.09
1:A:169:ARG:HB3	1:A:169:ARG:HH11	1.21	1.01
1:A:611:ASN:HB3	1:A:657:ARG:NH2	1.85	0.90
1:A:611:ASN:CB	1:A:657:ARG:HH22	1.93	0.80
1:B:275:PHE:CD2	1:B:355:THR:HG22	2.16	0.80
1:B:657:ARG:HH11	1:B:657:ARG:HG2	1.47	0.77
1:B:295:ASN:HD21	1:B:419:GLY:HA2	1.48	0.77
1:A:169:ARG:CB	1:A:169:ARG:HH11	1.98	0.75
1:B:577:VAL:HG12	1:B:580:GLU:HB2	1.67	0.75
1:B:289:PRO:HB2	1:B:336:TRP:HB3	1.68	0.75
1:B:453:GLN:HA	1:B:453:GLN:NE2	2.03	0.74
1:B:235:ASN:ND2	1:B:237:SER:H	1.86	0.74
1:A:570:ARG:HD3	1:A:588:ASP:OD1	1.88	0.74
1:B:272:CYS:HA	1:B:355:THR:HG21	1.69	0.73
1:A:169:ARG:NH1	1:A:169:ARG:HB3	2.00	0.73
1:B:526:ASN:HD22	1:B:526:ASN:H	1.37	0.72
1:A:6:GLN:NE2	1:A:44:ASN:HA	2.04	0.72
1:B:167:THR:HG21	1:B:420:ARG:NH1	2.05	0.72
1:B:75:LEU:HD11	1:B:87:LEU:HB2	1.72	0.71
1:B:453:GLN:HA	1:B:453:GLN:HE21	1.55	0.70
1:B:524:ILE:HB	1:B:526:ASN:ND2	2.06	0.69
1:A:44:ASN:OD1	1:A:45:LYS:HG2	1.93	0.69
1:B:272:CYS:HA	1:B:355:THR:CG2	2.24	0.68
1:B:167:THR:HG23	1:B:421:TYR:HE1	1.60	0.67
1:B:355:THR:HG23	5:B:831:HOH:O	1.96	0.66
1:A:111:THR:HG22	1:A:129:THR:HG22	1.78	0.66
1:B:235:ASN:C	1:B:235:ASN:HD22	1.99	0.65
1:B:611:ASN:HB3	1:B:657:ARG:NH2	2.12	0.65
1:B:235:ASN:HD22	1:B:236:TRP:N	1.94	0.65
1:B:657:ARG:HH11	1:B:657:ARG:CG	2.10	0.65
1:A:526:ASN:HD22	1:A:526:ASN:H	1.45	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:HB2	1:B:169:ARG:HH11	1.63	0.64
1:B:615:LEU:HD22	5:B:857:HOH:O	1.98	0.64
1:A:58:SER:HB2	1:A:63:PRO:HB3	1.78	0.64
1:A:102:PRO:HG2	1:A:105:ALA:HB2	1.80	0.64
1:B:524:ILE:HB	1:B:526:ASN:HD21	1.61	0.63
1:B:169:ARG:CB	1:B:169:ARG:HH11	2.11	0.63
1:B:385:MET:HB2	1:B:386:PRO:HD3	1.81	0.62
1:B:102:PRO:HG2	1:B:105:ALA:HB2	1.81	0.61
1:A:618:ASN:O	1:A:651:LYS:HA	2.01	0.61
1:B:137:TRP:CE2	1:B:151:ARG:HD3	2.35	0.61
1:B:555:SER:H	1:B:558:GLN:NE2	1.98	0.61
1:A:385:MET:HB2	1:A:386:PRO:HD3	1.83	0.61
1:B:433:MET:HG3	5:B:721:HOH:O	2.00	0.61
1:B:646:PRO:HG2	5:B:1020:HOH:O	2.02	0.60
1:B:167:THR:HG23	1:B:421:TYR:CE1	2.37	0.60
1:B:1:ALA:C	1:B:119:GLN:HE22	2.05	0.59
1:B:160:GLY:O	1:B:161:ILE:HD12	2.02	0.59
1:B:678:LYS:HA	1:B:678:LYS:HE2	1.85	0.59
1:A:289:PRO:HB2	1:A:336:TRP:HB3	1.83	0.59
1:A:195:SER:O	1:A:199:ARG:HD3	2.03	0.58
1:B:134:PHE:HB3	1:B:143:VAL:HG21	1.85	0.58
1:B:169:ARG:CB	1:B:169:ARG:NH1	2.66	0.58
1:A:524:ILE:HB	1:A:526:ASN:ND2	2.18	0.58
1:A:600:VAL:HG23	1:A:686:LEU:HD21	1.86	0.58
1:B:161:ILE:HD13	5:B:839:HOH:O	2.04	0.58
1:A:107:ILE:HD13	1:A:134:PHE:CE2	2.39	0.57
1:A:137:TRP:CE2	1:A:151:ARG:HD3	2.39	0.57
1:B:677:ASN:HD22	1:B:678:LYS:H	1.53	0.57
1:B:481:SER:OG	1:B:508:SER:HB3	2.04	0.57
1:A:142:SER:HB2	1:A:338:VAL:HG22	1.86	0.57
1:A:526:ASN:HD22	1:A:526:ASN:N	2.03	0.57
1:A:337:PHE:CE1	1:A:350:GLN:HG3	2.40	0.57
1:A:382:ASN:HB3	1:A:383:PHE:CG	2.40	0.57
1:B:169:ARG:NH1	1:B:169:ARG:HB3	2.19	0.56
1:B:526:ASN:HD22	1:B:526:ASN:N	2.03	0.56
1:B:520:ALA:HB3	1:B:534:TRP:HB3	1.87	0.56
1:B:20:HIS:HD2	5:B:814:HOH:O	1.86	0.56
1:B:606:VAL:HG23	1:B:691:ALA:O	2.04	0.56
1:A:228:ASP:O	1:A:229:ASN:HB2	2.06	0.56
1:B:555:SER:H	1:B:558:GLN:HE21	1.52	0.56
1:A:196:LEU:HG	1:A:228:ASP:HB3	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ILE:HB	1:A:526:ASN:HD21	1.70	0.56
1:A:414:ASN:HA	5:A:1007:HOH:O	2.05	0.55
1:B:197:ASN:HD22	1:B:197:ASN:H	1.54	0.55
1:A:226:ASN:H	1:A:226:ASN:HD22	1.55	0.55
1:B:142:SER:HB2	1:B:338:VAL:HG22	1.89	0.55
1:B:446:ASP:O	1:B:450:GLN:HG3	2.07	0.55
1:B:82:GLY:O	1:B:83:TRP:HB2	2.07	0.55
1:B:605:ARG:HG2	1:B:691:ALA:HB3	1.89	0.55
1:B:196:LEU:HG	1:B:228:ASP:HB3	1.89	0.55
1:A:221:ALA:HB2	1:A:365:GLN:HB3	1.88	0.54
1:B:221:ALA:HB2	1:B:365:GLN:HB3	1.89	0.54
1:B:677:ASN:ND2	1:B:678:LYS:H	2.05	0.54
5:A:914:HOH:O	1:B:496:LYS:HG3	2.07	0.54
1:B:677:ASN:ND2	1:B:678:LYS:N	2.55	0.54
1:A:23:LYS:HE3	1:A:180:PHE:CE2	2.43	0.54
1:A:630:MET:O	1:A:672:ALA:HA	2.07	0.54
1:A:169:ARG:NH2	1:A:592:ASP:OD1	2.38	0.54
1:B:236:TRP:NE1	1:B:271:GLN:HG2	2.23	0.54
1:A:136:PRO:HG3	1:A:287:GLY:O	2.08	0.54
1:B:82:GLY:CA	1:B:102:PRO:HB3	2.37	0.53
1:B:272:CYS:CA	1:B:355:THR:HG21	2.37	0.53
1:B:396:ARG:HE	1:B:417:THR:HG21	1.72	0.53
1:B:612:VAL:O	1:B:657:ARG:NH1	2.40	0.53
1:B:512:LYS:HB3	1:B:577:VAL:HG21	1.90	0.53
1:B:594:PRO:HB2	1:B:616:PHE:HE1	1.73	0.53
1:B:635:GLY:HA3	1:B:668:LYS:HE2	1.90	0.53
1:A:520:ALA:HB3	1:A:534:TRP:HB3	1.89	0.53
1:A:622:GLU:OE1	1:A:678:LYS:HE3	2.09	0.53
1:B:168:ASN:HB2	5:B:1049:HOH:O	2.09	0.53
1:A:479:GLU:HB3	1:A:480:PRO:HD3	1.90	0.53
1:B:197:ASN:ND2	1:B:197:ASN:H	2.07	0.52
1:B:485:LYS:HD3	1:B:486:LEU:N	2.25	0.52
1:A:379:VAL:HA	1:A:385:MET:HB3	1.91	0.52
1:B:630:MET:O	1:B:672:ALA:HA	2.09	0.52
1:B:210:ASN:H	1:B:210:ASN:HD22	1.57	0.52
1:B:594:PRO:HB2	1:B:616:PHE:CE1	2.45	0.52
1:B:657:ARG:CZ	1:B:657:ARG:HB3	2.40	0.52
1:B:677:ASN:ND2	1:B:678:LYS:HG2	2.24	0.52
1:A:577:VAL:HG23	1:A:580:GLU:HB2	1.92	0.52
1:B:299:ALA:HB2	1:B:418:ILE:HD13	1.91	0.51
1:B:482:ILE:HD13	1:B:506:ASN:HA	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:HB2	1:B:115:GLN:HB3	1.92	0.51
1:A:608:LYS:HD3	5:A:1095:HOH:O	2.10	0.51
1:B:613:GLN:OE1	1:B:655:ARG:HD3	2.11	0.51
1:A:313:ASP:OD2	1:A:317:ASN:HB2	2.10	0.51
1:B:445:SER:HB2	1:B:447:GLN:OE1	2.11	0.51
1:B:484:GLY:HA2	1:B:503:LEU:O	2.12	0.50
1:B:627:CYS:HB2	1:B:645:VAL:HB	1.93	0.50
1:A:52:ARG:HG2	1:A:53:LEU:N	2.27	0.50
1:A:514:VAL:O	1:A:539:THR:HA	2.11	0.49
1:A:6:GLN:HE21	1:A:44:ASN:HA	1.73	0.49
1:A:9:ASN:HB3	1:A:40:LEU:HB2	1.92	0.49
1:B:546:GLU:HG2	1:B:547:GLU:N	2.27	0.49
1:A:224:ASN:O	1:A:230:GLY:HA3	2.13	0.49
1:B:235:ASN:HD22	1:B:237:SER:H	1.58	0.49
1:A:514:VAL:HG22	1:A:577:VAL:CG1	2.43	0.49
1:B:502:LEU:O	1:B:549:GLU:HA	2.12	0.49
1:A:235:ASN:HD22	1:A:235:ASN:C	2.15	0.49
1:B:401:TYR:HD2	1:B:408:GLN:HB3	1.77	0.49
1:B:210:ASN:N	1:B:210:ASN:HD22	2.11	0.49
1:B:649:GLY:C	1:B:652:GLU:HG2	2.33	0.49
1:A:602:ASN:HB2	5:A:1036:HOH:O	2.13	0.49
1:B:630:MET:CE	1:B:642:LYS:HG3	2.43	0.49
1:B:93:ASN:ND2	5:B:1078:HOH:O	2.45	0.49
1:B:657:ARG:NH1	1:B:657:ARG:CG	2.71	0.48
1:B:136:PRO:HG3	1:B:287:GLY:O	2.13	0.48
1:B:139:ASN:HA	1:B:144:PHE:CG	2.49	0.48
1:B:247:ARG:HG3	1:B:565:SER:HB3	1.95	0.48
1:A:206:VAL:HA	1:A:209:ARG:HD2	1.96	0.48
1:A:311:TYR:CD2	1:A:399:TRP:HB2	2.48	0.48
1:A:602:ASN:N	1:A:602:ASN:HD22	2.11	0.48
1:A:629:LEU:HD22	1:A:631:VAL:HG23	1.95	0.48
1:B:379:VAL:HA	1:B:385:MET:HB3	1.94	0.48
1:A:36:ASN:HB2	1:A:99:ILE:O	2.13	0.48
1:B:611:ASN:HB3	1:B:657:ARG:HH22	1.78	0.48
1:B:9:ASN:HB3	1:B:40:LEU:HB2	1.94	0.48
1:B:491:MET:CG	1:B:496:LYS:HE2	2.43	0.48
1:A:169:ARG:NH1	5:A:982:HOH:O	2.39	0.48
1:A:641:LEU:HD23	1:A:642:LYS:N	2.29	0.47
1:B:138:LEU:HD13	1:B:140:VAL:HG23	1.96	0.47
1:B:624:VAL:CG2	1:B:648:LEU:HB3	2.43	0.47
1:B:394:ALA:O	1:B:418:ILE:HD12	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:GLU:OE1	1:B:449:ARG:HD2	2.14	0.47
1:B:630:MET:HE1	1:B:642:LYS:CG	2.45	0.47
1:B:641:LEU:HD22	1:B:643:ILE:HG13	1.96	0.47
1:B:337:PHE:CE1	1:B:350:GLN:HG3	2.48	0.47
1:B:82:GLY:HA3	1:B:102:PRO:HB3	1.94	0.47
1:A:556:TYR:HA	1:A:559:TYR:CE2	2.50	0.47
1:B:313:ASP:OD2	1:B:317:ASN:HB2	2.15	0.47
1:B:370:SER:O	1:B:374:VAL:HG23	2.15	0.47
1:B:139:ASN:HA	1:B:144:PHE:CD1	2.50	0.47
1:B:34:GLY:HA2	1:B:101:SER:O	2.15	0.47
1:B:615:LEU:HD23	1:B:653:ARG:NH2	2.30	0.47
1:A:206:VAL:HA	1:A:209:ARG:CD	2.45	0.47
1:A:308:VAL:HG13	1:A:325:SER:HB3	1.97	0.47
1:B:586:GLU:HB3	5:B:1047:HOH:O	2.13	0.47
1:B:138:LEU:HD22	1:B:140:VAL:HG22	1.96	0.47
1:A:317:ASN:OD1	1:A:519:THR:HG21	2.14	0.47
1:A:641:LEU:HD22	1:A:643:ILE:HG13	1.96	0.47
1:A:610:VAL:HG22	5:A:961:HOH:O	2.13	0.46
1:A:576:LYS:NZ	1:A:580:GLU:O	2.42	0.46
1:B:107:ILE:HD13	1:B:134:PHE:CE2	2.50	0.46
1:A:210:ASN:HD22	1:A:210:ASN:H	1.63	0.46
1:A:296:PHE:O	1:A:297:ASN:HB2	2.13	0.46
1:B:111:THR:HG23	1:B:126:LYS:HE3	1.98	0.46
1:B:175:TRP:CE2	1:B:251:GLY:HA2	2.51	0.46
1:B:382:ASN:HB3	1:B:383:PHE:CG	2.50	0.46
1:A:20:HIS:HD2	5:A:781:HOH:O	1.98	0.46
1:A:607:ARG:HB2	1:A:607:ARG:HH11	1.81	0.46
1:A:36:ASN:HB3	1:A:100:SER:CB	2.46	0.46
1:A:382:ASN:HB3	1:A:383:PHE:CD1	2.50	0.46
1:A:613:GLN:OE1	1:A:655:ARG:HD2	2.15	0.46
1:A:104:SER:O	1:A:210:ASN:HB2	2.15	0.46
1:A:446:ASP:O	1:A:450:GLN:HG3	2.16	0.46
1:B:299:ALA:HB1	1:B:308:VAL:HG11	1.98	0.46
1:B:473:LEU:HD13	1:B:473:LEU:C	2.35	0.46
1:A:498:VAL:HG12	1:A:500:LEU:CD1	2.46	0.46
1:A:67:ALA:O	1:A:68:MET:HB2	2.16	0.46
1:B:52:ARG:HG3	5:B:1055:HOH:O	2.16	0.46
1:B:610:VAL:HB	1:B:660:ILE:CG1	2.45	0.46
1:B:161:ILE:CD1	1:B:669:GLN:HE22	2.29	0.46
1:A:134:PHE:HB3	1:A:143:VAL:HG21	1.98	0.45
1:A:151:ARG:HD2	5:A:886:HOH:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:ND2	1:A:237:SER:H	2.14	0.45
1:B:503:LEU:HD23	1:B:549:GLU:HB3	1.98	0.45
1:A:183:ASP:O	1:A:187:ILE:HG13	2.16	0.45
1:A:228:ASP:O	1:A:229:ASN:CB	2.64	0.45
1:B:555:SER:OG	1:B:558:GLN:HG3	2.16	0.45
1:B:652:GLU:HG3	5:B:1092:HOH:O	2.15	0.45
1:A:65:GLU:HA	1:A:70:LYS:O	2.17	0.45
1:B:23:LYS:HE3	1:B:180:PHE:CE2	2.51	0.45
1:B:596:LEU:HD23	1:B:684:ALA:HB2	1.99	0.45
1:B:82:GLY:HA2	1:B:102:PRO:HB3	1.98	0.45
1:A:323:SER:O	1:A:527:GLY:HA3	2.17	0.45
1:B:13:ALA:O	1:B:17:GLN:HB2	2.17	0.45
1:A:219:LEU:O	1:A:223:ILE:HG12	2.17	0.45
1:A:359:ARG:CZ	1:A:364:PHE:CE1	2.99	0.45
1:B:360:SER:O	1:B:361:GLN:HB2	2.17	0.45
1:A:117:PHE:CD1	1:B:651:LYS:HG3	2.52	0.45
1:A:141:ASP:OD2	1:A:143:VAL:HG22	2.17	0.45
1:B:83:TRP:HA	1:B:100:SER:O	2.16	0.45
1:A:624:VAL:CG2	1:A:648:LEU:HB3	2.47	0.44
1:A:235:ASN:HD22	1:A:236:TRP:N	2.15	0.44
1:B:228:ASP:O	1:B:229:ASN:HB2	2.17	0.44
1:B:615:LEU:HD23	1:B:653:ARG:CZ	2.47	0.44
1:B:160:GLY:C	1:B:161:ILE:HD12	2.37	0.44
1:A:12:THR:HG22	1:A:16:ARG:HD3	2.00	0.44
1:A:500:LEU:HD21	1:A:571:ILE:HG13	1.98	0.44
1:A:594:PRO:HG2	1:A:616:PHE:HE1	1.81	0.44
1:A:621:ASP:OD1	1:A:651:LYS:NZ	2.43	0.44
1:B:210:ASN:HD22	1:B:211:ASP:N	2.15	0.44
1:A:601:LEU:HD21	1:A:613:GLN:HB2	2.00	0.44
1:B:295:ASN:O	1:B:329:PHE:HA	2.18	0.44
1:A:447:GLN:CD	1:A:447:GLN:H	2.21	0.44
1:B:12:THR:HG22	1:B:16:ARG:HD3	1.99	0.44
1:B:610:VAL:HB	1:B:660:ILE:HG12	1.99	0.44
1:A:392:VAL:O	1:A:419:GLY:HA3	2.18	0.43
1:B:510:ASP:HB2	1:B:512:LYS:HE3	1.99	0.43
1:A:602:ASN:HD21	1:A:610:VAL:HG13	1.82	0.43
1:B:447:GLN:H	1:B:447:GLN:CD	2.22	0.43
1:B:248:SER:HA	1:B:673:ASP:OD1	2.17	0.43
1:B:2:ALA:HA	1:B:119:GLN:NE2	2.33	0.43
1:A:320:ASP:O	1:A:322:GLY:N	2.51	0.43
1:A:498:VAL:HB	1:A:554:ILE:HB	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASN:OD1	1:B:150:GLU:HG3	2.17	0.43
1:A:443:GLU:HG2	5:A:972:HOH:O	2.17	0.43
1:A:81:GLY:O	1:A:82:GLY:O	2.36	0.43
1:B:235:ASN:HD21	1:B:237:SER:CB	2.32	0.43
1:B:311:TYR:CD2	1:B:399:TRP:HB2	2.53	0.43
1:A:210:ASN:N	1:A:210:ASN:HD22	2.17	0.43
1:A:5:VAL:CG2	1:A:41:MET:HE3	2.49	0.43
1:A:36:ASN:HB3	1:A:100:SER:OG	2.19	0.43
1:A:497:GLU:HG2	1:A:499:ASN:ND2	2.34	0.43
1:B:381:LEU:O	1:B:385:MET:CG	2.67	0.43
1:A:645:VAL:HA	1:A:646:PRO:HD3	1.92	0.42
1:B:486:LEU:HG	1:B:585:VAL:CG1	2.50	0.42
1:A:77:ASN:HA	1:A:86:VAL:HG13	2.00	0.42
1:A:360:SER:O	1:A:361:GLN:HB2	2.18	0.42
1:A:268:ARG:HA	1:A:269:TYR:HA	1.69	0.42
1:A:641:LEU:CD2	1:A:643:ILE:HG13	2.49	0.42
1:B:104:SER:O	1:B:210:ASN:HB2	2.19	0.42
1:A:139:ASN:HA	1:A:144:PHE:CD1	2.53	0.42
1:A:26:SER:HB2	5:A:763:HOH:O	2.19	0.42
1:A:485:LYS:HD2	5:A:797:HOH:O	2.18	0.42
1:A:612:VAL:HG12	1:A:613:GLN:N	2.35	0.42
1:B:10:TRP:O	1:B:15:ASN:ND2	2.53	0.42
1:A:327:TRP:N	1:A:327:TRP:CD1	2.88	0.42
1:B:244:ARG:HH21	1:B:248:SER:CB	2.33	0.42
1:B:65:GLU:HG2	5:B:939:HOH:O	2.19	0.42
1:B:67:ALA:O	1:B:68:MET:HB2	2.19	0.42
1:B:405:THR:CB	1:B:407:LYS:HG2	2.50	0.42
1:B:296:PHE:O	1:B:297:ASN:HB2	2.20	0.42
1:A:225:SER:HA	1:A:230:GLY:CA	2.50	0.41
1:A:649:GLY:HA3	1:A:652:GLU:OE2	2.20	0.41
1:B:268:ARG:HA	1:B:269:TYR:HA	1.69	0.41
1:B:615:LEU:HD13	5:B:857:HOH:O	2.20	0.41
1:B:400:LEU:O	1:B:408:GLN:HA	2.21	0.41
1:B:577:VAL:HG22	1:B:578:PRO:HD2	2.03	0.41
1:B:625:ARG:H	1:B:677:ASN:ND2	2.19	0.41
1:A:225:SER:HA	1:A:230:GLY:N	2.36	0.41
1:A:382:ASN:HA	1:A:383:PHE:HA	1.79	0.41
1:B:105:ALA:HA	1:B:106:PRO:HD3	1.93	0.41
1:B:515:THR:O	1:B:515:THR:HG23	2.21	0.41
1:B:677:ASN:HD22	1:B:678:LYS:N	2.15	0.41
1:A:400:LEU:HA	1:A:400:LEU:HD13	1.96	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:CD1	5:B:839:HOH:O	2.68	0.41
1:B:306:LEU:HG	1:B:459:LEU:HD11	2.03	0.41
1:B:624:VAL:HG22	1:B:648:LEU:HB3	2.03	0.41
1:A:602:ASN:ND2	1:A:610:VAL:HG13	2.36	0.41
1:B:556:TYR:HA	1:B:559:TYR:CE2	2.56	0.41
1:B:223:ILE:HB	1:B:354:ALA:HB1	2.03	0.40
1:A:259:TRP:CZ2	1:A:264:LEU:HD22	2.57	0.40
1:B:272:CYS:CB	1:B:355:THR:HG21	2.51	0.40
1:B:676:CYS:SG	1:B:679:PHE:HB2	2.61	0.40
1:A:645:VAL:HG11	1:A:674:PHE:HE1	1.86	0.40
1:B:19:HIS:CE1	1:B:35:GLN:HB3	2.56	0.40
1:B:612:VAL:HG12	1:B:613:GLN:N	2.36	0.40
1:A:82:GLY:HA2	1:A:102:PRO:HB3	2.02	0.40
1:B:405:THR:HB	1:B:407:LYS:HG2	2.03	0.40
1:B:169:ARG:NH1	5:B:954:HOH:O	2.51	0.40
1:B:630:MET:HE1	1:B:642:LYS:HB2	2.04	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%)	635 (95%)	33 (5%)	3 (0%)	38	54
1	B	675/692 (98%)	635 (94%)	39 (6%)	1 (0%)	55	72
All	All	1346/1384 (97%)	1270 (94%)	72 (5%)	4 (0%)	44	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLY
1	A	321	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	304	ARG
1	A	81	GLY

### 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%)	558 (96%)	23 (4%)	36	55
1	B	585/595 (98%)	564 (96%)	21 (4%)	40	60
All	All	1166/1190 (98%)	1122 (96%)	44 (4%)	38	58

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	47	LEU
1	A	100	SER
1	A	169	ARG
1	A	210	ASN
1	A	226	ASN
1	A	235	ASN
1	A	241	THR
1	A	286	LEU
1	A	319	LEU
1	A	433	MET
1	A	449	ARG
1	A	497	GLU
1	A	526	ASN
1	A	575	CYS
1	A	601	LEU
1	A	602	ASN
1	A	614	MET
1	A	629	LEU
1	A	637	LEU
1	A	641	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	645	VAL
1	A	657	ARG
1	B	77	ASN
1	B	132	LEU
1	B	138	LEU
1	B	210	ASN
1	B	235	ASN
1	B	320	ASP
1	B	423	SER
1	B	433	MET
1	B	474	GLU
1	B	526	ASN
1	B	540	MET
1	B	545	GLU
1	B	577	VAL
1	B	601	LEU
1	B	613	GLN
1	B	614	MET
1	B	629	LEU
1	B	637	LEU
1	B	641	LEU
1	B	657	ARG
1	B	677	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	17	GLN
1	A	20	HIS
1	A	91	ASN
1	A	210	ASN
1	A	226	ASN
1	A	229	ASN
1	A	235	ASN
1	A	280	ASN
1	A	450	GLN
1	A	526	ASN
1	A	567	ASN
1	A	602	ASN
1	A	669	GLN
1	B	20	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	36	ASN
1	B	50	ASN
1	B	77	ASN
1	B	91	ASN
1	B	119	GLN
1	B	197	ASN
1	B	210	ASN
1	B	235	ASN
1	B	280	ASN
1	B	295	ASN
1	B	357	GLN
1	B	382	ASN
1	B	430	ASN
1	B	453	GLN
1	B	517	ASN
1	B	526	ASN
1	B	558	GLN
1	B	669	GLN
1	B	677	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 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

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.