



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 02:51 PM EDT

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

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 : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

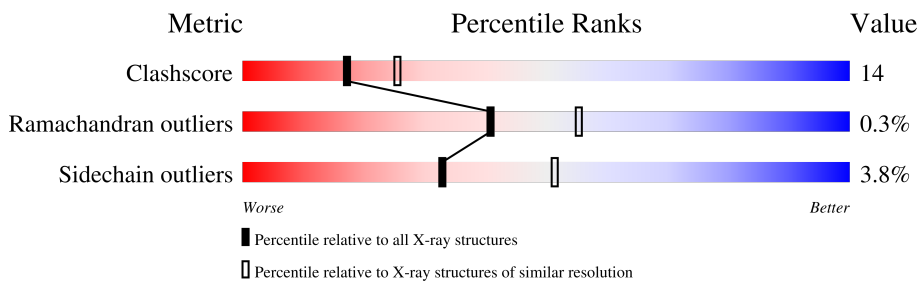
1 Overall quality at a glance

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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 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	
1	B	692	

2 Entry composition [i](#)

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
			Total	C	N	O	S			
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 mutation	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 mutation	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	A	2	Total	Cl	0	0
			2	2		
2	B	2	Total	Cl	0	0
			2	2		

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

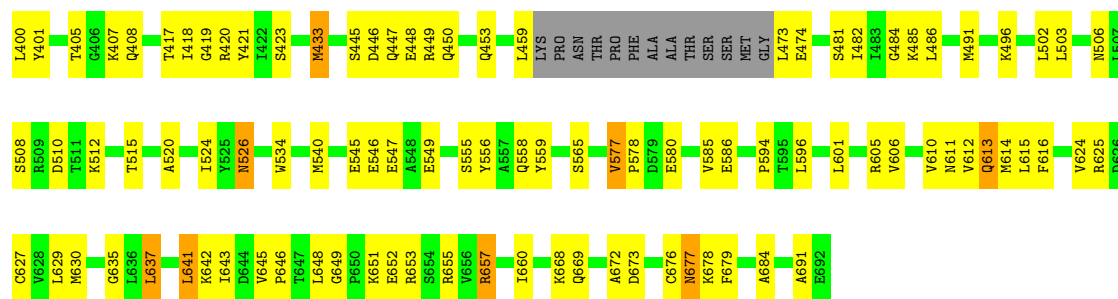
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

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

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



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	57.51Å 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.	Xtrriage
Total number of atoms	11386	wwPDB-VP
Average B, all atoms (Å ²)	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:HH11	1:A:169:ARG:HB3	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:HG2	1:B:657:ARG:HH11	1.47	0.77
1:B:295:ASN:HD21	1:B:419:GLY:HA2	1.48	0.77
1:A:169:ARG:HH11	1:A:169:ARG:CB	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:HB3	1:A:169:ARG:NH1	2.00	0.73
1:B:526:ASN:H	1:B:526:ASN:HD22	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:HH11	1:B:169:ARG:HB2	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:HH11	1:B:169:ARG:CB	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:82:GLY:O	1:B:83:TRP:HB2	2.07	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: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:H	1:B:197:ASN:ND2	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:C	1:A:235:ASN:HD22	2.15	0.49
1:B:401:TYR:HD2	1:B:408:GLN:HB3	1.77	0.49
1:B:210:ASN:HD22	1:B:210:ASN:N	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:93:ASN:ND2	5:B:1078:HOH:O	2.45	0.49
1:B:630:MET:CE	1:B:642:LYS:HG3	2.43	0.49
1:B:657:ARG:CG	1:B:657:ARG:NH1	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:82:GLY:HA3	1:B:102:PRO:HB3	1.94	0.47
1:B:337:PHE:CE1	1:B:350:GLN:HG3	2.48	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:34:GLY:HA2	1:B:101:SER:O	2.15	0.47
1:B:139:ASN:HA	1:B:144:PHE:CD1	2.50	0.47
1:B:370:SER:O	1:B:374:VAL:HG23	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:HH11	1:A:607:ARG:HB2	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:67:ALA:O	1:A:68:MET:HB2	2.16	0.46
1:A:498:VAL:HG12	1:A:500:LEU:CD1	2.46	0.46
1:B:52:ARG:HG3	5:B:1055:HOH:O	2.16	0.46
1:B:161:ILE:CD1	1:B:669:GLN:HE22	2.29	0.46
1:B:610:VAL:HB	1:B:660:ILE:CG1	2.45	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:H	1:A:447:GLN:CD	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:248:SER:HA	1:B:673:ASP:OD1	2.17	0.43
1:B:447:GLN:CD	1:B:447:GLN:H	2.22	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:81:GLY:O	1:A:82:GLY:O	2.36	0.43
1:A:443:GLU:HG2	5:A:972:HOH:O	2.17	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:HD22	1:A:210:ASN:N	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:26:SER:HB2	5:A:763:HOH:O	2.19	0.42
1:A:139:ASN:HA	1:A:144:PHE:CD1	2.53	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: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:244:ARG:HH21	1:B:248:SER:CB	2.33	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:HD13	1:A:400:LEU:HA	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 [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%)	635 (95%)	33 (5%)	3 (0%)	34	48
1	B	675/692 (98%)	635 (94%)	39 (6%)	1 (0%)	51	68
All	All	1346/1384 (97%)	1270 (94%)	72 (5%)	4 (0%)	41	55

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 [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%)	31	49
1	B	585/595 (98%)	564 (96%)	21 (4%)	35	54
All	All	1166/1190 (98%)	1122 (96%)	44 (4%)	33	51

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

Sometimes 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 [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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.