



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 08:12 PM EDT

PDB ID : 1NUD  
Title : Role of Calcium Ions in the Activation and Activity of the Transglutaminase  
3 Enzyme (3 calciums, active form)  
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](mailto: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.

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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 : 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) : 2.23.2

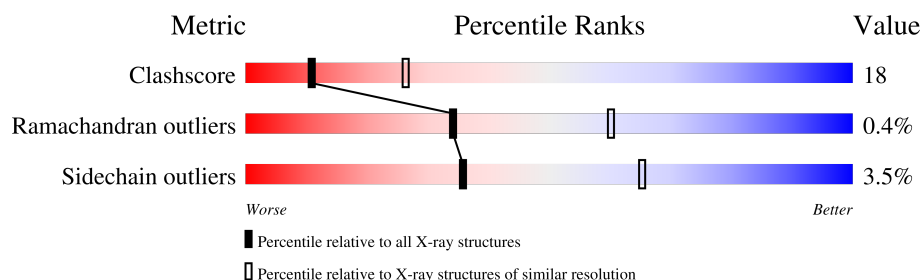
# 1 Overall quality at a glance

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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  $\geq 3$ , 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

There are 5 unique types of molecules in this entry. The entry contains 10921 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	673	Total	C	N	O	S	0	0	0
			5250	3313	913	1001	23			
1	B	673	Total	C	N	O	S	0	0	0
			5250	3313	913	1001	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	B	4	Total	Cl	0	0
			4	4		

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	Br 4	0	0
4	B	5	Total 5	Br 5	0	0

- Molecule 5 is water.

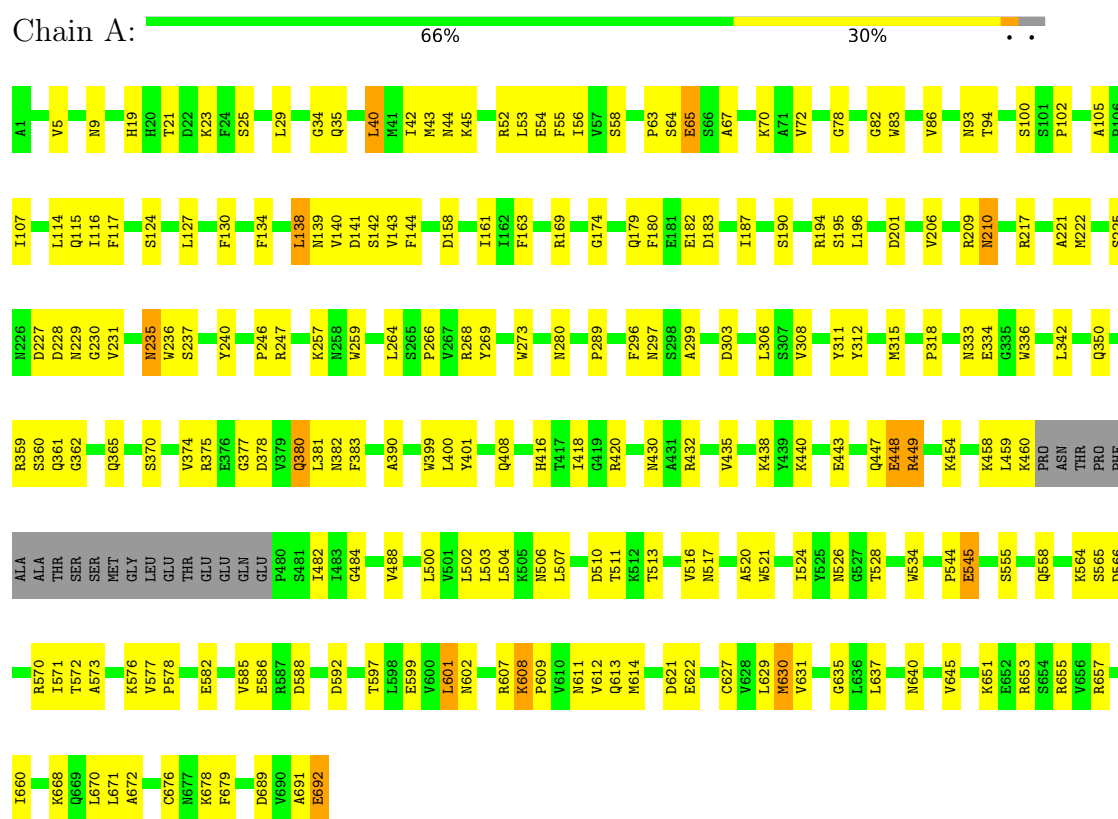
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total 193	O 193	0	0
5	B	205	Total 205	O 205	0	0

### 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



L629	L542	ALA	R359	S237
M630	D543	THR	G362	R244
V631	P544	SER	V363	D245
E632	E545	MET	F364	P246
L637	E546	GLY	Q365	R247
V645	E547	LEU	Q380	D250
P646	A548	GLU	L381	G251
G649	E549	THR	N382	S252
P650	E560	GLU	F383	W259
K651	R561	GLN	D384	L264
R655	Y562	GLU	M385	R268
V656	L563	P480	P386	Y269
R657	S565	I483	R396	G270
I660	D566	G484	W399	G271
R664	N567	V488	D402	C272
S665	R570	M491	N403	T278
K668	I571	L492	T404	P289
D673	E580	K496	T405	S290
K678	S581	E497	K407	R291
F679	E582	V498	V498	V292
I682	E586	M499	S415	I293
K683	R587	L500	H416	T294
A691	D588	V501	T417	N295
E692	I589	L502	I418	F296
	L590	L503	L504	N297
	T597	S505	S423	D303
	L598	N506	T424	R304
	E599	L507	K425	N305
	V600	S508	R432	Y311
	L601	R509	K440	T312
	N602	D510		D313
	V606	T511		P314
	R607	K512	E443	M315
	V610	T515	G444	G316
	N611	T519	S445	N317
	V612	A520	D446	P318
	Q613	W521	Q447	W327
	M614	I524	E448	N328
	F616	Y525	R449	F329
	S617	N526	Q450	H330
	N618	G527	V451	V331
	P619	T528	Q453	W332
	E622	E532	K458	W336
	P623	W533	L459	F337
	V624	V534	K460	Q350
	R625	K535	ASN	
	D626	D536	THR	
	C627		PRO	
	V628	T539	PHE	
			ALA	
				E358

## 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, $\alpha$ , $\beta$ , $\gamma$	57.54Å 115.37Å 121.39Å 90.00° 92.66° 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, $R_{free}$	0.199 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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	0.37	0/5360	0.62	0/7270
1	B	0.35	0/5360	0.62	0/7270
All	All	0.36	0/10720	0.62	0/14540

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	5250	0	5194	169	0
1	B	5250	0	5194	212	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
4	A	4	0	0	1	0
4	B	5	0	0	2	0
5	A	193	0	0	9	0
5	B	205	0	0	11	0
All	All	10921	0	10388	381	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 18.

All (381) 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:576:LYS:HD3	1:A:582:GLU:HG3	1.35	1.08
1:B:448:GLU:HG3	1:B:449:ARG:HD2	1.47	0.94
1:A:611:ASN:HB3	1:A:657:ARG:NH2	1.82	0.92
1:B:611:ASN:HD22	1:B:657:ARG:HH22	1.21	0.89
1:A:82:GLY:HA2	1:A:102:PRO:HB3	1.54	0.88
1:A:138:LEU:HD22	1:A:140:VAL:HG22	1.55	0.88
1:B:75:LEU:HD11	1:B:87:LEU:HB2	1.56	0.85
1:A:141:ASP:OD2	1:A:143:VAL:HG22	1.76	0.84
1:A:586:GLU:HB2	4:B:712:BR:BR	2.33	0.84
1:B:82:GLY:HA2	1:B:102:PRO:HB3	1.58	0.84
1:A:555:SER:H	1:A:558:GLN:HE21	1.22	0.83
1:B:459:LEU:O	1:B:460:LYS:HD2	1.78	0.83
1:B:623:PRO:HB3	1:B:649:GLY:HA2	1.59	0.83
1:B:570:ARG:HD3	1:B:588:ASP:OD1	1.79	0.82
1:A:657:ARG:HB3	1:A:657:ARG:NH1	1.95	0.81
1:B:563:LEU:HD11	1:B:567:ASN:HA	1.62	0.81
1:B:440:LYS:HE2	1:B:443:GLU:OE2	1.80	0.81
1:A:611:ASN:HB3	1:A:657:ARG:HH21	1.44	0.80
1:B:235:ASN:ND2	1:B:237:SER:H	1.80	0.80
1:B:611:ASN:HB3	1:B:657:ARG:HH12	1.47	0.78
1:A:629:LEU:HD23	1:A:630:MET:N	2.00	0.77
1:B:139:ASN:HD22	1:B:140:VAL:N	1.83	0.77
1:B:380:GLN:HG2	5:B:849:HOH:O	1.84	0.77
1:B:520:ALA:HB3	1:B:534:TRP:HB3	1.68	0.76
1:A:139:ASN:OD1	1:A:140:VAL:HG13	1.86	0.75
1:A:65:GLU:OE1	1:A:70:LYS:HD3	1.86	0.75
1:A:289:PRO:HB2	1:A:336:TRP:HB3	1.69	0.75
1:B:363:VAL:HG12	1:B:365:GLN:HG2	1.70	0.74
1:A:637:LEU:HD21	1:A:660:ILE:HG22	1.71	0.73
1:B:606:VAL:HG23	1:B:691:ALA:O	1.87	0.73
1:A:607:ARG:HH11	1:A:607:ARG:HB2	1.54	0.72
1:A:380:GLN:HG3	1:A:458:LYS:HD3	1.71	0.71
1:B:214:TYR:O	1:B:218:VAL:HG23	1.91	0.71
1:A:691:ALA:O	1:A:692:GLU:HB2	1.91	0.71
1:B:102:PRO:HG2	1:B:105:ALA:HB2	1.73	0.70
1:B:449:ARG:O	1:B:453:GLN:HG2	1.91	0.70
1:B:138:LEU:HD22	1:B:140:VAL:HG22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ARG:HD3	1:A:588:ASP:OD1	1.92	0.70
1:A:23:LYS:HE3	1:A:180:PHE:CE2	2.27	0.69
1:B:446:ASP:O	1:B:450:GLN:HB2	1.91	0.69
1:B:606:VAL:CG2	1:B:665:SER:HB3	2.22	0.69
1:B:68:MET:HB2	5:B:737:HOH:O	1.92	0.68
1:A:114:LEU:HB2	1:A:127:LEU:HD11	1.74	0.68
1:A:280:ASN:HB2	1:A:333:ASN:HD21	1.57	0.68
1:B:12:THR:O	1:B:13:ALA:HB2	1.94	0.68
1:B:6:GLN:HE21	1:B:44:ASN:HA	1.60	0.67
1:A:299:ALA:HB1	1:A:308:VAL:HG11	1.75	0.67
1:A:602:ASN:HD21	1:A:611:ASN:H	1.43	0.66
1:A:280:ASN:HB2	1:A:333:ASN:ND2	2.10	0.66
1:A:342:LEU:HD22	1:A:381:LEU:HD13	1.76	0.66
1:B:657:ARG:HG2	1:B:657:ARG:HH11	1.58	0.66
1:A:607:ARG:HB2	1:A:607:ARG:NH1	2.11	0.66
1:A:56:ILE:HG12	1:A:72:VAL:HG22	1.77	0.65
1:A:138:LEU:CD2	1:A:140:VAL:HG22	2.26	0.65
1:B:602:ASN:HD21	1:B:611:ASN:H	1.43	0.65
1:A:375:ARG:HG3	1:A:440:LYS:HA	1.78	0.65
1:A:19:HIS:O	1:A:21:THR:HG23	1.98	0.64
1:B:139:ASN:HD22	1:B:140:VAL:H	1.43	0.64
1:B:313:ASP:OD2	1:B:317:ASN:HB2	1.96	0.64
1:B:611:ASN:HB3	1:B:657:ARG:NH1	2.12	0.64
1:A:613:GLN:OE1	1:A:655:ARG:HD3	1.98	0.64
1:B:36:ASN:HB2	1:B:99:ILE:O	1.98	0.64
1:B:244:ARG:HD2	5:B:839:HOH:O	1.98	0.64
1:A:196:LEU:HG	1:A:228:ASP:HB3	1.79	0.63
1:A:629:LEU:HD22	1:A:631:VAL:HG23	1.80	0.63
1:B:611:ASN:ND2	1:B:657:ARG:HH22	1.94	0.63
1:A:29:LEU:HD23	1:A:130:PHE:HB3	1.80	0.63
1:B:629:LEU:HD22	1:B:631:VAL:HG23	1.81	0.63
1:A:555:SER:H	1:A:558:GLN:NE2	1.96	0.62
1:A:210:ASN:HD22	1:A:210:ASN:H	1.47	0.62
1:A:334:GLU:HA	1:A:350:GLN:O	2.00	0.61
1:B:542:LEU:HD21	1:B:548:ALA:HB2	1.81	0.61
1:B:134:PHE:HB3	1:B:143:VAL:HG21	1.82	0.61
1:B:107:ILE:HD13	1:B:134:PHE:CE2	2.36	0.61
1:A:299:ALA:HB2	1:A:418:ILE:HD13	1.83	0.60
1:A:378:ASP:HB3	5:A:806:HOH:O	2.01	0.60
1:B:637:LEU:HD21	1:B:660:ILE:HG22	1.83	0.60
1:A:235:ASN:ND2	1:A:237:SER:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASN:HD22	1:B:237:SER:H	1.49	0.59
1:B:611:ASN:HD22	1:B:657:ARG:NH2	1.96	0.59
1:A:484:GLY:HA2	1:A:503:LEU:O	2.02	0.59
1:B:12:THR:O	1:B:13:ALA:CB	2.49	0.59
1:B:601:LEU:HD21	1:B:613:GLN:HG2	1.83	0.59
1:A:102:PRO:HG2	1:A:105:ALA:HB2	1.84	0.59
1:A:416:HIS:HA	1:A:443:GLU:OE1	2.03	0.59
1:A:54:GLU:HB2	1:A:115:GLN:HB3	1.84	0.58
1:A:599:GLU:O	1:A:612:VAL:HG13	2.03	0.58
1:A:382:ASN:HB3	1:A:383:PHE:CG	2.38	0.58
1:B:488:VAL:HG22	1:B:500:LEU:HD11	1.85	0.58
1:A:58:SER:HB2	1:A:63:PRO:HB3	1.86	0.58
1:A:576:LYS:CD	1:A:582:GLU:HG3	2.22	0.58
1:B:382:ASN:HB3	1:B:383:PHE:CG	2.39	0.58
1:A:602:ASN:ND2	1:A:611:ASN:H	2.02	0.58
1:B:235:ASN:HD22	1:B:236:TRP:N	2.02	0.57
1:B:606:VAL:HG21	1:B:665:SER:HB3	1.84	0.57
1:A:459:LEU:O	1:A:460:LYS:HD2	2.04	0.57
1:B:42:ILE:HG12	1:B:94:THR:OG1	2.03	0.57
1:A:513:THR:O	1:A:578:PRO:HD3	2.05	0.57
1:A:488:VAL:HA	1:A:500:LEU:HD23	1.87	0.57
1:B:484:GLY:HA2	1:B:503:LEU:O	2.04	0.57
1:B:627:CYS:HB2	1:B:645:VAL:HB	1.86	0.57
1:A:42:ILE:HG12	1:A:94:THR:OG1	2.04	0.57
1:A:78:GLY:O	1:A:86:VAL:HG22	2.05	0.57
1:A:502:LEU:HD11	1:A:504:LEU:HD21	1.84	0.57
1:A:676:CYS:SG	1:A:679:PHE:HB2	2.44	0.56
1:B:228:ASP:O	1:B:229:ASN:HB2	2.04	0.56
1:B:211:ASP:CG	1:B:213:LYS:HZ2	2.09	0.56
1:B:259:TRP:CZ2	1:B:264:LEU:HD22	2.40	0.56
1:A:482:ILE:HD13	1:A:577:VAL:HG21	1.87	0.56
1:A:657:ARG:HB3	1:A:657:ARG:CZ	2.35	0.56
1:A:544:PRO:O	1:A:545:GLU:HB2	2.06	0.56
1:B:526:ASN:ND2	1:B:528:THR:H	2.03	0.56
1:A:259:TRP:CH2	1:A:264:LEU:HD22	2.40	0.55
1:A:630:MET:O	1:A:672:ALA:HA	2.06	0.55
1:B:586:GLU:HB3	5:B:858:HOH:O	2.05	0.55
1:A:459:LEU:C	1:A:460:LYS:HD2	2.25	0.55
1:B:488:VAL:HA	1:B:500:LEU:HD12	1.89	0.55
1:B:613:GLN:HA	1:B:656:VAL:O	2.06	0.55
1:A:306:LEU:HD13	1:A:459:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ILE:HB	1:A:526:ASN:OD1	2.06	0.55
1:B:169:ARG:HD2	1:B:590:ILE:HB	1.88	0.55
1:A:607:ARG:HH11	1:A:607:ARG:CB	2.20	0.55
1:B:268:ARG:HB3	1:B:269:TYR:CD2	2.42	0.55
1:A:629:LEU:HD23	1:A:630:MET:H	1.72	0.55
1:B:617:SER:O	1:B:619:PRO:HD3	2.07	0.55
1:A:52:ARG:HB3	1:A:117:PHE:HB2	1.88	0.54
1:A:217:ARG:NH2	1:A:365:GLN:NE2	2.55	0.54
1:B:532:GLU:OE1	1:B:535:LYS:HE3	2.08	0.54
1:A:19:HIS:CE1	1:A:35:GLN:HB3	2.41	0.54
1:A:54:GLU:HB2	1:A:115:GLN:HE21	1.72	0.54
1:B:615:LEU:CD2	1:B:655:ARG:HG2	2.37	0.54
1:A:629:LEU:CD2	1:A:631:VAL:HG23	2.37	0.54
1:B:206:VAL:HA	1:B:209:ARG:HD2	1.89	0.54
1:B:417:THR:HG23	1:B:418:ILE:HD12	1.89	0.54
1:A:657:ARG:HD3	5:A:841:HOH:O	2.07	0.54
1:B:65:GLU:HA	1:B:70:LYS:O	2.07	0.54
1:A:657:ARG:HB3	1:A:657:ARG:HH11	1.69	0.54
1:A:9:ASN:HB3	1:A:40:LEU:HB2	1.90	0.53
1:A:44:ASN:OD1	1:A:45:LYS:HG2	2.08	0.53
1:B:520:ALA:CB	1:B:534:TRP:HB3	2.36	0.53
1:B:37:PHE:CD1	1:B:37:PHE:N	2.76	0.53
1:A:622:GLU:OE1	1:A:678:LYS:HE2	2.08	0.53
1:A:183:ASP:O	1:A:187:ILE:HG13	2.09	0.53
1:B:53:LEU:CD2	1:B:116:ILE:HG12	2.38	0.53
1:B:610:VAL:HG13	1:B:660:ILE:CG1	2.39	0.53
1:A:447:GLN:OE1	1:A:447:GLN:N	2.30	0.53
1:A:64:SER:HB3	1:A:67:ALA:HB3	1.90	0.53
1:B:169:ARG:HH11	1:B:590:ILE:HB	1.74	0.53
1:B:235:ASN:HD21	1:B:237:SER:CB	2.22	0.52
1:B:139:ASN:ND2	1:B:140:VAL:HG13	2.25	0.52
1:B:524:ILE:HA	1:B:566:ASP:OD2	2.09	0.52
1:A:612:VAL:HG12	1:A:613:GLN:N	2.24	0.52
1:B:382:ASN:HB3	1:B:383:PHE:CD2	2.45	0.52
1:B:664:ARG:HD2	1:B:668:LYS:NZ	2.25	0.52
1:B:451:VAL:HB	5:B:746:HOH:O	2.09	0.52
1:B:497:GLU:HG3	1:B:499:ASN:ND2	2.24	0.52
1:B:139:ASN:ND2	1:B:140:VAL:N	2.56	0.52
1:B:497:GLU:HG3	1:B:499:ASN:HD21	1.75	0.52
1:A:318:PRO:HG2	1:A:570:ARG:HG2	1.91	0.52
1:B:515:THR:HG22	1:B:539:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLY:HA3	1:A:671:LEU:HD21	1.92	0.51
1:B:560:GLU:HG3	1:B:561:ARG:N	2.25	0.51
1:A:235:ASN:HD22	1:A:236:TRP:N	2.09	0.51
1:A:360:SER:HB3	1:A:365:GLN:HG3	1.92	0.51
1:A:627:CYS:CB	1:A:645:VAL:HB	2.40	0.51
1:A:83:TRP:HA	1:A:100:SER:O	2.10	0.51
1:B:657:ARG:HH11	1:B:657:ARG:CG	2.23	0.51
1:B:491:MET:HG2	1:B:496:LYS:HE2	1.93	0.51
1:B:36:ASN:H	1:B:36:ASN:ND2	2.08	0.51
1:A:631:VAL:CG1	1:A:670:LEU:HD11	2.41	0.51
1:B:19:HIS:O	1:B:21:THR:HG23	2.11	0.50
1:B:167:THR:HG21	1:B:297:ASN:ND2	2.25	0.50
1:B:679:PHE:HB3	1:B:682:ILE:HD11	1.94	0.50
1:B:169:ARG:HG2	4:B:708:BR:BR	2.66	0.50
1:B:303:ASP:HB3	1:B:305:ASN:ND2	2.26	0.50
3:B:706:CL:CL	5:B:824:HOH:O	2.57	0.50
1:B:34:GLY:HA3	1:B:138:LEU:HD12	1.94	0.50
1:B:164:VAL:HG12	1:B:329:PHE:CZ	2.47	0.50
1:A:296:PHE:O	1:A:297:ASN:HB2	2.11	0.50
1:B:268:ARG:HB3	1:B:269:TYR:CE2	2.46	0.50
1:A:163:PHE:CZ	1:A:432:ARG:HA	2.47	0.50
1:B:252:SER:HB3	1:B:278:THR:HA	1.94	0.50
1:B:511:THR:O	1:B:512:LYS:HD3	2.12	0.50
1:A:259:TRP:CZ2	1:A:264:LEU:HD22	2.47	0.50
1:B:67:ALA:O	1:B:68:MET:HB2	2.12	0.49
1:B:313:ASP:OD1	1:B:315:MET:N	2.45	0.49
1:B:488:VAL:HA	1:B:500:LEU:CD1	2.42	0.49
1:A:380:GLN:HE22	1:A:381:LEU:HG	1.77	0.49
1:A:627:CYS:HB2	1:A:645:VAL:HB	1.94	0.49
1:A:612:VAL:HG12	1:A:613:GLN:H	1.78	0.49
1:B:161:ILE:HB	1:B:425:LYS:HD2	1.94	0.49
1:A:342:LEU:HD22	1:A:381:LEU:HD22	1.95	0.49
1:A:380:GLN:HE21	1:A:380:GLN:C	2.15	0.49
1:B:610:VAL:HG13	1:B:660:ILE:HG12	1.94	0.49
1:A:23:LYS:NZ	5:A:738:HOH:O	2.46	0.49
1:A:231:VAL:HA	1:A:259:TRP:CD1	2.48	0.49
1:A:511:THR:HB	1:B:607:ARG:NH2	2.28	0.49
1:B:629:LEU:CD2	1:B:631:VAL:HG23	2.43	0.49
1:A:601:LEU:HD11	1:A:613:GLN:NE2	2.28	0.49
1:B:217:ARG:NH2	1:B:365:GLN:NE2	2.61	0.49
1:A:576:LYS:HD3	1:A:582:GLU:CG	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:CG2	1:A:114:LEU:HD23	2.42	0.48
1:A:564:LYS:C	1:A:566:ASP:H	2.17	0.48
1:B:106:PRO:HG3	1:B:210:ASN:HB3	1.95	0.48
1:A:247:ARG:HG2	1:A:273:TRP:CZ2	2.48	0.48
1:B:673:ASP:OD1	1:B:683:LYS:HE3	2.14	0.48
1:B:6:GLN:NE2	1:B:44:ASN:HA	2.27	0.48
1:B:506:ASN:O	1:B:545:GLU:HA	2.13	0.48
1:A:107:ILE:HD13	1:A:134:PHE:CE2	2.49	0.48
1:A:210:ASN:H	1:A:210:ASN:ND2	2.11	0.48
1:B:405:THR:OG1	1:B:407:LYS:HB2	2.14	0.48
1:B:599:GLU:O	1:B:612:VAL:HG13	2.14	0.48
1:A:361:GLN:NE2	5:A:747:HOH:O	2.46	0.47
1:B:63:PRO:HB3	1:B:70:LYS:HB2	1.96	0.47
1:B:77:ASN:HA	1:B:86:VAL:HG13	1.95	0.47
1:B:196:LEU:HG	1:B:228:ASP:HB3	1.96	0.47
1:B:289:PRO:HB2	1:B:336:TRP:HB3	1.95	0.47
1:A:360:SER:O	1:A:361:GLN:HB2	2.15	0.47
1:B:59:THR:HA	5:B:853:HOH:O	2.13	0.47
1:B:163:PHE:CZ	1:B:432:ARG:HA	2.49	0.47
1:B:330:HIS:CD2	1:B:332:TRP:HE3	2.32	0.47
1:B:359:ARG:NH1	1:B:362:GLY:O	2.46	0.47
1:B:543:ASP:O	1:B:546:GLU:HB3	2.14	0.47
1:A:544:PRO:O	1:A:545:GLU:CB	2.62	0.47
1:A:315:MET:O	1:A:517:ASN:HB3	2.13	0.47
1:A:635:GLY:HA3	1:A:668:LYS:HE2	1.97	0.47
1:B:503:LEU:HD23	1:B:549:GLU:HG2	1.96	0.47
1:B:235:ASN:HD22	1:B:235:ASN:C	2.17	0.47
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.79	0.47
1:A:138:LEU:HD22	1:A:140:VAL:H	1.80	0.47
1:A:266:PRO:HB2	5:A:797:HOH:O	2.13	0.47
4:A:711:BR:BR	1:B:38:GLN:HB2	2.70	0.47
1:B:607:ARG:NH1	1:B:607:ARG:HB2	2.30	0.47
1:A:206:VAL:HA	1:A:209:ARG:HD2	1.97	0.47
1:A:482:ILE:N	1:A:482:ILE:HD12	2.29	0.47
1:B:615:LEU:HD21	1:B:655:ARG:HG2	1.96	0.47
1:A:382:ASN:HA	1:A:383:PHE:HA	1.67	0.46
1:B:396:ARG:HB2	1:B:418:ILE:HD13	1.97	0.46
1:A:312:TYR:CE2	1:A:572:THR:HG21	2.50	0.46
1:B:317:ASN:OD1	1:B:519:THR:HG21	2.15	0.46
1:A:268:ARG:HA	1:A:269:TYR:HA	1.69	0.46
1:B:154:TYR:CE1	1:B:291:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ARG:HD2	1:B:668:LYS:HZ3	1.80	0.46
1:B:252:SER:CB	1:B:278:THR:HA	2.45	0.46
1:A:500:LEU:HD13	1:A:571:ILE:HG13	1.97	0.46
1:A:447:GLN:H	1:A:447:GLN:CD	2.17	0.46
1:B:382:ASN:HA	1:B:383:PHE:HA	1.69	0.46
1:A:247:ARG:HG2	1:A:273:TRP:CH2	2.51	0.46
1:A:53:LEU:HD22	1:A:116:ILE:HG12	1.96	0.46
1:A:435:VAL:O	1:A:438:LYS:HB2	2.16	0.46
1:B:303:ASP:CB	1:B:305:ASN:ND2	2.79	0.46
1:B:492:LEU:HD13	1:B:589:ILE:HB	1.98	0.45
1:B:570:ARG:HA	1:B:588:ASP:OD1	2.16	0.45
1:B:597:THR:HG22	1:B:598:LEU:N	2.30	0.45
1:A:139:ASN:HA	1:A:144:PHE:CG	2.51	0.45
1:B:250:ASP:HB2	1:B:632:GLU:OE2	2.15	0.45
1:A:139:ASN:HA	1:A:144:PHE:CD1	2.52	0.45
1:A:169:ARG:NH2	1:A:592:ASP:OD1	2.50	0.45
1:A:43:MET:O	1:A:93:ASN:HB3	2.15	0.45
1:B:247:ARG:NH1	1:B:566:ASP:OD1	2.50	0.45
1:B:492:LEU:CD1	1:B:589:ILE:HB	2.46	0.45
1:A:570:ARG:NH2	1:A:588:ASP:OD2	2.50	0.45
1:B:234:GLY:HA2	1:B:270:GLY:O	2.16	0.45
1:B:563:LEU:CD1	1:B:567:ASN:HA	2.42	0.45
1:A:502:LEU:CD2	1:A:516:VAL:HG11	2.47	0.45
1:B:36:ASN:CB	1:B:99:ILE:O	2.64	0.45
1:B:206:VAL:HA	1:B:209:ARG:CD	2.46	0.45
1:B:415:SER:HB2	1:B:449:ARG:NH1	2.31	0.45
1:A:653:ARG:NE	5:A:792:HOH:O	2.50	0.45
1:B:58:SER:HB2	1:B:63:PRO:CG	2.47	0.44
1:B:318:PRO:HD2	1:B:521:TRP:CD1	2.52	0.44
1:B:268:ARG:HA	1:B:269:TYR:HA	1.66	0.44
1:B:385:MET:O	1:B:386:PRO:C	2.54	0.44
1:B:405:THR:C	1:B:407:LYS:H	2.20	0.44
1:B:491:MET:CG	1:B:496:LYS:HE2	2.46	0.44
1:B:500:LEU:HD22	1:B:571:ILE:HG13	1.99	0.44
1:A:42:ILE:HA	1:A:94:THR:HA	1.99	0.44
1:A:420:ARG:HG2	5:A:735:HOH:O	2.17	0.44
1:B:213:LYS:HB2	1:B:213:LYS:NZ	2.32	0.44
1:B:535:LYS:O	1:B:536:ASP:HB2	2.17	0.44
1:B:645:VAL:HG12	5:B:875:HOH:O	2.16	0.44
1:A:55:PHE:O	1:A:72:VAL:HA	2.17	0.44
1:B:563:LEU:HD11	1:B:567:ASN:CA	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:VAL:HG12	1:B:613:GLN:N	2.31	0.44
1:A:158:ASP:HA	1:A:179:GLN:OE1	2.17	0.44
1:A:228:ASP:O	1:A:229:ASN:HB2	2.18	0.44
1:B:34:GLY:HA3	1:B:138:LEU:CD1	2.47	0.44
1:B:229:ASN:HD22	1:B:229:ASN:HA	1.58	0.44
1:A:448:GLU:OE2	1:A:449:ARG:NE	2.47	0.44
1:A:564:LYS:O	1:A:566:ASP:N	2.50	0.44
1:B:213:LYS:HZ2	1:B:213:LYS:HB2	1.81	0.44
1:B:402:ASP:OD1	1:B:404:THR:N	2.51	0.44
1:A:370:SER:O	1:A:374:VAL:HG23	2.18	0.44
1:B:544:PRO:C	1:B:546:GLU:H	2.20	0.44
1:A:25:SER:OG	1:A:182:GLU:HG2	2.18	0.44
1:B:417:THR:HG23	1:B:418:ILE:CD1	2.46	0.43
1:B:646:PRO:HG2	5:B:875:HOH:O	2.17	0.43
1:B:53:LEU:HD22	1:B:116:ILE:HG12	2.00	0.43
1:B:679:PHE:CB	1:B:682:ILE:HD11	2.48	0.43
1:A:235:ASN:HD22	1:A:235:ASN:C	2.20	0.43
1:B:224:ASN:O	1:B:230:GLY:HA3	2.17	0.43
1:B:396:ARG:HH22	1:B:586:GLU:CD	2.21	0.43
1:B:524:ILE:HB	1:B:526:ASN:ND2	2.32	0.43
1:B:526:ASN:N	1:B:526:ASN:HD22	2.16	0.43
1:B:73:PHE:CD1	1:B:73:PHE:N	2.86	0.43
1:B:363:VAL:CG1	1:B:364:PHE:N	2.81	0.43
1:B:502:LEU:HG	1:B:504:LEU:HD13	1.99	0.43
1:B:62:TYR:O	1:B:63:PRO:C	2.57	0.43
1:B:259:TRP:CH2	1:B:264:LEU:HD22	2.53	0.43
1:A:377:GLY:O	1:A:454:LYS:HE2	2.19	0.43
1:A:382:ASN:HB3	1:A:383:PHE:CD2	2.53	0.43
1:A:182:GLU:O	1:A:257:LYS:HE2	2.19	0.43
1:A:221:ALA:HB2	1:A:365:GLN:HB3	2.00	0.43
1:A:564:LYS:C	1:A:566:ASP:N	2.72	0.43
1:B:245:ASP:OD1	1:B:565:SER:HB3	2.19	0.43
1:B:154:TYR:CD1	1:B:291:ARG:HB3	2.54	0.43
1:A:306:LEU:CD1	1:A:459:LEU:HD12	2.49	0.42
1:B:296:PHE:O	1:B:297:ASN:HB2	2.19	0.42
1:B:601:LEU:N	1:B:601:LEU:HD22	2.34	0.42
1:A:190:SER:O	1:A:194:ARG:HG2	2.18	0.42
1:B:651:LYS:HE3	5:B:790:HOH:O	2.20	0.42
1:B:380:GLN:HG3	1:B:458:LYS:HD3	2.00	0.42
1:B:503:LEU:O	1:B:504:LEU:HD12	2.19	0.42
1:B:526:ASN:HD21	1:B:528:THR:HB	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:TYR:CD2	1:B:399:TRP:HB2	2.54	0.42
1:B:622:GLU:OE1	1:B:678:LYS:HD2	2.20	0.42
1:B:138:LEU:CD2	1:B:140:VAL:HG22	2.45	0.42
1:A:161:ILE:HG13	1:A:430:ASN:OD1	2.20	0.42
1:A:520:ALA:HB3	1:A:534:TRP:HB3	2.02	0.42
1:A:401:TYR:HD2	1:A:408:GLN:HB2	1.84	0.42
1:A:621:ASP:OD1	1:A:651:LYS:NZ	2.53	0.42
1:B:179:GLN:HA	1:B:184:ILE:HG21	2.01	0.42
1:A:225:SER:HA	1:A:230:GLY:CA	2.50	0.42
1:A:416:HIS:HD1	1:A:443:GLU:HB3	1.84	0.42
1:A:448:GLU:HG3	1:A:449:ARG:N	2.35	0.42
1:B:313:ASP:OD1	1:B:313:ASP:C	2.58	0.42
1:A:34:GLY:HA3	1:A:138:LEU:CD1	2.50	0.42
1:B:602:ASN:HD21	1:B:610:VAL:HA	1.84	0.41
1:A:53:LEU:CD2	1:A:116:ILE:HG12	2.50	0.41
1:B:105:ALA:HA	1:B:106:PRO:HD3	1.93	0.41
1:B:582:GLU:N	1:B:582:GLU:OE1	2.54	0.41
1:A:318:PRO:HD2	1:A:521:TRP:CD1	2.56	0.41
1:A:510:ASP:C	1:A:544:PRO:HG3	2.41	0.41
1:B:337:PHE:CE1	1:B:350:GLN:HG3	2.55	0.41
1:B:448:GLU:OE1	1:B:449:ARG:NH1	2.54	0.41
1:B:657:ARG:NH1	1:B:657:ARG:CG	2.83	0.41
1:B:36:ASN:ND2	1:B:36:ASN:N	2.67	0.41
1:B:36:ASN:N	1:B:36:ASN:HD22	2.17	0.41
1:B:208:SER:C	1:B:210:ASN:H	2.24	0.41
1:B:272:CYS:HG	1:B:525:TYR:HH	1.62	0.41
1:B:293:ILE:O	1:B:331:VAL:HG13	2.21	0.41
1:B:295:ASN:O	1:B:329:PHE:HA	2.21	0.41
1:B:512:LYS:NZ	1:B:580:GLU:OE2	2.54	0.41
1:A:311:TYR:CD2	1:A:399:TRP:HB2	2.56	0.41
1:A:528:THR:HA	5:A:870:HOH:O	2.20	0.41
1:B:137:TRP:CD2	1:B:151:ARG:HD2	2.56	0.41
1:B:357:GLN:HE21	1:B:357:GLN:HB2	1.67	0.41
1:B:510:ASP:C	1:B:544:PRO:HG3	2.40	0.41
1:B:602:ASN:ND2	1:B:611:ASN:H	2.13	0.41
1:A:359:ARG:HD3	1:A:362:GLY:O	2.20	0.41
1:A:630:MET:HB3	1:A:640:ASN:HD21	1.85	0.41
1:B:168:ASN:HD22	1:B:168:ASN:HA	1.63	0.41
1:A:195:SER:HA	1:A:222:MET:SD	2.61	0.41
1:B:327:TRP:CD1	1:B:327:TRP:N	2.89	0.41
1:B:611:ASN:ND2	1:B:657:ARG:NH2	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:TYR:CG	1:A:246:PRO:HD3	2.56	0.41
1:B:111:THR:HG22	5:B:864:HOH:O	2.21	0.41
1:B:448:GLU:HG3	1:B:449:ARG:N	2.35	0.41
1:B:625:ARG:O	1:B:626:ASP:HB2	2.20	0.41
1:B:515:THR:HG22	1:B:539:THR:HG23	2.03	0.40
1:A:114:LEU:O	1:A:124:SER:HA	2.20	0.40
1:A:577:VAL:HG12	1:A:578:PRO:HD2	2.04	0.40
1:B:423:SER:HB3	1:B:432:ARG:HG3	2.03	0.40
1:B:445:SER:O	1:B:448:GLU:HB3	2.21	0.40
1:A:573:ALA:HB3	1:A:585:VAL:HB	2.04	0.40
1:A:607:ARG:C	1:A:608:LYS:HD2	2.41	0.40
1:A:608:LYS:HA	1:A:609:PRO:HD3	1.99	0.40
1:B:182:GLU:OE2	1:B:182:GLU:HA	2.21	0.40
1:B:219:LEU:O	1:B:223:ILE:HG12	2.21	0.40
1:B:483:ILE:HD13	1:B:507:LEU:HD21	2.04	0.40
1:A:390:ALA:HB3	5:A:849:HOH:O	2.20	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	669/692 (97%)	627 (94%)	39 (6%)	3 (0%)	34	60
1	B	669/692 (97%)	619 (92%)	47 (7%)	3 (0%)	34	60
All	All	1338/1384 (97%)	1246 (93%)	86 (6%)	6 (0%)	34	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	ALA
1	A	565	SER

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Mol	Chain	Res	Type
1	B	201	ASP
1	A	201	ASP
1	B	227	ASP
1	A	227	ASP

### 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	579/595 (97%)	558 (96%)	21 (4%)	35	64
1	B	579/595 (97%)	559 (96%)	20 (4%)	36	65
All	All	1158/1190 (97%)	1117 (96%)	41 (4%)	36	65

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	65	GLU
1	A	138	LEU
1	A	142	SER
1	A	210	ASN
1	A	235	ASN
1	A	303	ASP
1	A	380	GLN
1	A	400	LEU
1	A	448	GLU
1	A	449	ARG
1	A	506	ASN
1	A	507	LEU
1	A	545	GLU
1	A	597	THR
1	A	601	LEU
1	A	608	LYS
1	A	614	MET
1	A	630	MET

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Mol	Chain	Res	Type
1	A	689	ASP
1	A	692	GLU
1	B	8	ILE
1	B	36	ASN
1	B	37	PHE
1	B	138	LEU
1	B	139	ASN
1	B	164	VAL
1	B	169	ARG
1	B	183	ASP
1	B	229	ASN
1	B	235	ASN
1	B	357	GLN
1	B	380	GLN
1	B	507	LEU
1	B	509	ARG
1	B	526	ASN
1	B	560	GLU
1	B	586	GLU
1	B	614	MET
1	B	629	LEU
1	B	655	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	115	GLN
1	A	210	ASN
1	A	229	ASN
1	A	235	ASN
1	A	271	GLN
1	A	280	ASN
1	A	361	GLN
1	A	365	GLN
1	A	408	GLN
1	A	506	ASN
1	A	550	HIS
1	A	558	GLN
1	A	602	ASN
1	A	611	ASN
1	B	6	GLN

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Mol	Chain	Res	Type
1	B	20	HIS
1	B	36	ASN
1	B	38	GLN
1	B	77	ASN
1	B	119	GLN
1	B	139	ASN
1	B	226	ASN
1	B	229	ASN
1	B	235	ASN
1	B	357	GLN
1	B	361	GLN
1	B	365	GLN
1	B	408	GLN
1	B	450	GLN
1	B	526	ASN
1	B	602	ASN
1	B	611	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 23 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 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.