



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:11 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

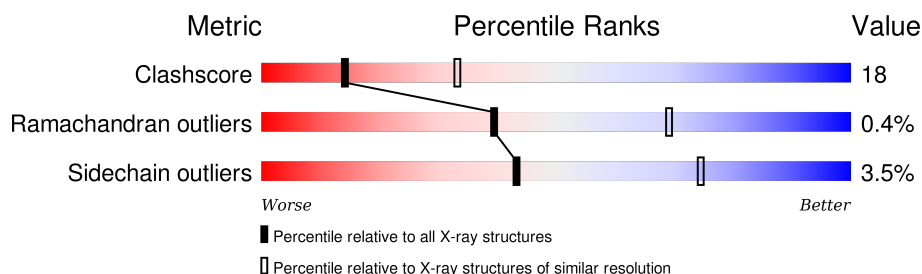
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	692	 66% 30% . .
1	B	692	 63% 32% . .

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	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	B	4	Total	Cl	0	0
			4	4		
3	A	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	B	5	Total 5	Br 5	0	0
4	A	4	Total 4	Br 4	0	0

- Molecule 5 is water.

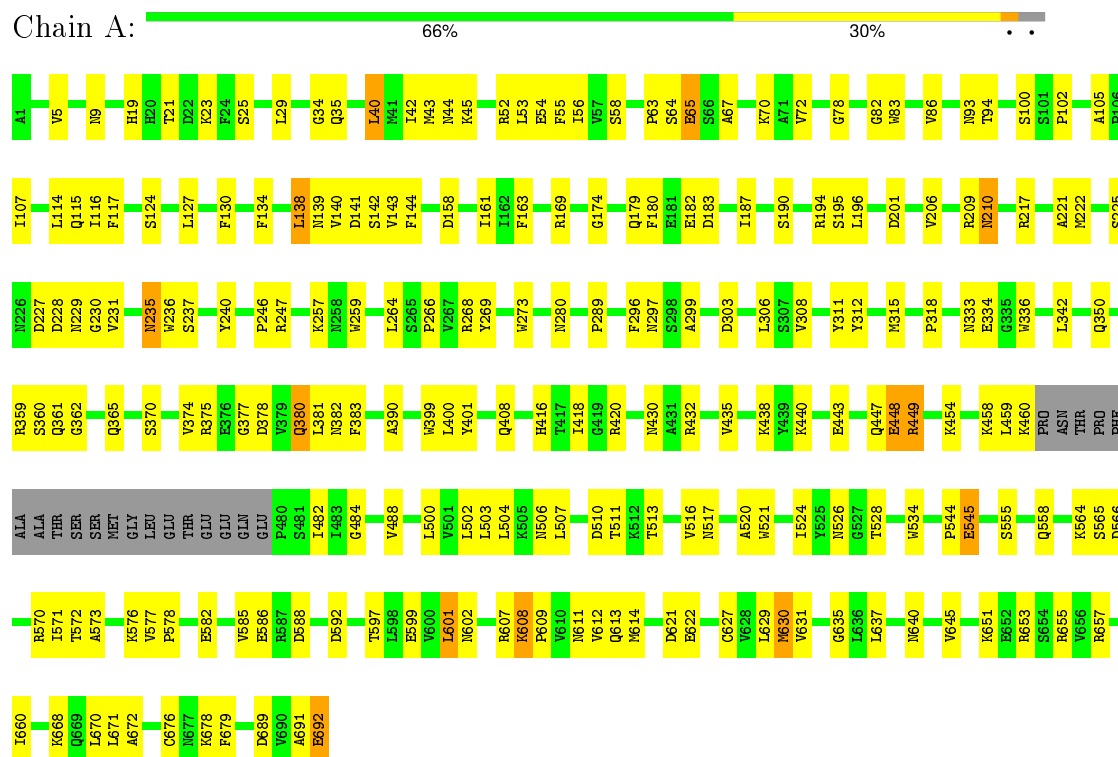
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total 193	O 193	0	0
5	B	205	Total 205	O 205	0	0

3 Residue-property plots

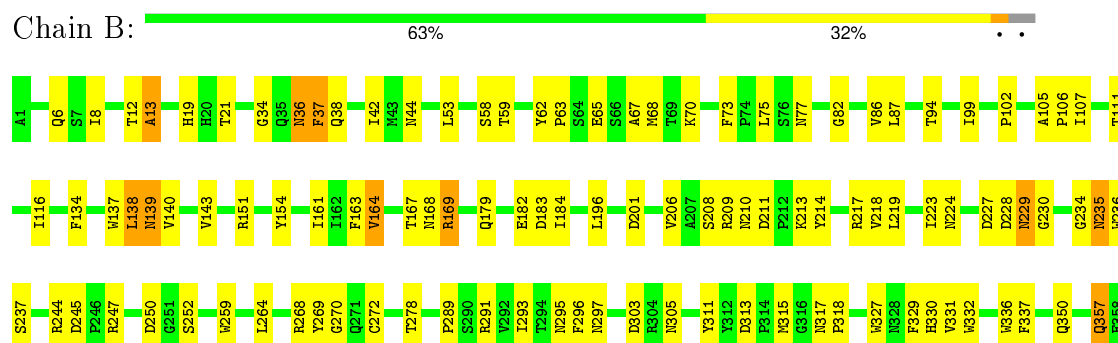
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Protein-glutamine glutamyltransferase E



• Molecule 1: Protein-glutamine glutamyltransferase E



L629	L630	V631	E632	L637	V645	P646	G649	P650	K651	R655	V656	R657	I660	R664	S665	K668	D673	K678	F679	I682	K683	A691	E692																											
L542	D543	P544	E545	E546	E547	A548	E549	E560	R561	V562	L563	R564	S565	D566	N567	R570	L571	E580	S581	E582	E586	R587	D588	I589	I590	T597	L598	E599	V600	L601	R602	V606	R607	V610	I611	V612	Q613	R614	L615	F616	S617	R618	P619	E622	P623	V624	R625	D626	C627	V628
ALA	THR	SER	SER	MET	GLY	LEU	GLU	THR	GLU	GLU	GLN	GLU	P460	I483	G484	V488	M491	L492	K496	E497	K498	N499	L500	V501	L502	L503	L504	R505	N506	L507	R509	D510	T511	K512	T515	T519	A520	W521	I524	Y525	W526	G527	T528	E532	W533	W534	K535	D536	T539	
R359	G362	V363	F364	Q365	Q380	L381	N382	F383	D384	K385	F386	R396	W399	D402	W403	T404	T405	G406	K407	S415	H416	T417	I418	S423	T424	K425	R432	K440	E443	G444	S445	D446	Q447	E448	R449	Q450	Y451	F452	Q453	K458	L459	K460	PRO	ASN	THR	PRO	PHE	ALA		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.54 Å 115.37 Å 121.39 Å 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 ²)	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: CA, BR, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	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:NH1	1:A:657:ARG:HB3	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:HB2	1:A:607:ARG:HH11	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:342:LEU:HD22	1:A:381:LEU:HD13	1.76	0.66
1:A:280:ASN:HB2	1:A:333:ASN:ND2	2.10	0.66
1:B:657:ARG:HH11	1:B:657:ARG:HG2	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:B:611:ASN:ND2	1:B:657:ARG:HH22	1.94	0.63
1:A:629:LEU:HD22	1:A:631:VAL:HG23	1.80	0.63
1:A:196:LEU:HG	1:A:228:ASP:HB3	1.79	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:H	1:A:210:ASN:HD22	1.47	0.62
1:B:542:LEU:HD21	1:B:548:ALA:HB2	1.81	0.61
1:A:334:GLU:HA	1:A:350:GLN:O	2.00	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:B:235:ASN:HD22	1:B:237:SER:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:ND2	1:A:237:SER:H	2.00	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:576:LYS:CD	1:A:582:GLU:HG3	2.22	0.58
1:A:58:SER:HB2	1:A:63:PRO:HB3	1.86	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:627:CYS:HB2	1:B:645:VAL:HB	1.86	0.57
1:B:484:GLY:HA2	1:B:503:LEU:O	2.04	0.57
1:A:42:ILE:HG12	1:A:94:THR:OG1	2.04	0.57
1:A:502:LEU:HD11	1:A:504:LEU:HD21	1.84	0.57
1:A:78:GLY:O	1:A:86:VAL:HG22	2.05	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:259:TRP:CZ2	1:B:264:LEU:HD22	2.40	0.56
1:B:211:ASP:CG	1:B:213:LYS:HZ2	2.09	0.56
1:A:657:ARG:HB3	1:A:657:ARG:CZ	2.35	0.56
1:A:482:ILE:HD13	1:A:577:VAL:HG21	1.87	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:630:MET:O	1:A:672:ALA:HA	2.06	0.55
1:A:259:TRP:CH2	1:A:264:LEU:HD22	2.40	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:B:169:ARG:HD2	1:B:590:ILE:HB	1.88	0.55
1:A:524:ILE:HB	1:A:526:ASN:OD1	2.06	0.55
1:A:607:ARG:CB	1:A:607:ARG:HH11	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:417:THR:HG23	1:B:418:ILE:HD12	1.89	0.54
1:B:206:VAL:HA	1:B:209:ARG:HD2	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:HH11	1:A:657:ARG:HB3	1.69	0.54
1:A:9:ASN:HB3	1:A:40:LEU:HB2	1.90	0.53
1:B:520:ALA:CB	1:B:534:TRP:HB3	2.36	0.53
1:A:44:ASN:OD1	1:A:45:LYS:HG2	2.08	0.53
1:B:37:PHE:N	1:B:37:PHE:CD1	2.76	0.53
1:A:622:GLU:OE1	1:A:678:LYS:HE2	2.08	0.53
1:B:610:VAL:HG13	1:B:660:ILE:CG1	2.39	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: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:B:560:GLU:HG3	1:B:561:ARG:N	2.25	0.51
1:A:174:GLY:HA3	1:A:671:LEU:HD21	1.92	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:B:657:ARG:HH11	1:B:657:ARG:CG	2.23	0.51
1:A:83:TRP:HA	1:A:100:SER:O	2.10	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:B:268:ARG:HB3	1:B:269:TYR:CE2	2.46	0.50
1:A:296:PHE:O	1:A:297:ASN:HB2	2.11	0.50
1:B:252:SER:HB3	1:B:278:THR:HA	1.94	0.50
1:A:163:PHE:CZ	1:A:432:ARG:HA	2.47	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:B:610:VAL:HG13	1:B:660:ILE:HG12	1.94	0.49
1:A:380:GLN:HE21	1:A:380:GLN:C	2.15	0.49
1:A:342:LEU:HD22	1:A:381:LEU:HD22	1.95	0.49
1:A:23:LYS:NZ	5:A:738:HOH:O	2.46	0.49
1:B:629:LEU:CD2	1:B:631:VAL:HG23	2.43	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:217:ARG:NH2	1:B:365:GLN:NE2	2.61	0.49
1:A:601:LEU:HD11	1:A:613:GLN:NE2	2.28	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:B:106:PRO:HG3	1:B:210:ASN:HB3	1.95	0.48
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: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:599:GLU:O	1:B:612:VAL:HG13	2.14	0.48
1:B:405:THR:OG1	1:B:407:LYS:HB2	2.14	0.48
1:B:196:LEU:HG	1:B:228:ASP:HB3	1.96	0.47
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:289:PRO:HB2	1:B:336:TRP:HB3	1.95	0.47
1:B:77:ASN:HA	1:B:86:VAL:HG13	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:543:ASP:O	1:B:546:GLU:HB3	2.14	0.47
1:B:359:ARG:NH1	1:B:362:GLY:O	2.46	0.47
1:B:330:HIS:CD2	1:B:332:TRP:HE3	2.32	0.47
1:B:163:PHE:CZ	1:B:432:ARG:HA	2.49	0.47
1:A:544:PRO:O	1:A:545:GLU:CB	2.62	0.47
1:B:503:LEU:HD23	1:B:549:GLU:HG2	1.96	0.47
1:A:635:GLY:HA3	1:A:668:LYS:HE2	1.97	0.47
1:A:315:MET:O	1:A:517:ASN:HB3	2.13	0.47
1:B:235:ASN:C	1:B:235:ASN:HD22	2.17	0.47
1:B:151:ARG:HH11	1:B:151:ARG:HG2	1.79	0.47
1:A:138:LEU:HD22	1:A:140:VAL:H	1.80	0.47
1:B:607:ARG:HB2	1:B:607:ARG:NH1	2.30	0.47
4:A:711:BR:BR	1:B:38:GLN:HB2	2.70	0.47
1:A:266:PRO:HB2	5:A:797:HOH:O	2.13	0.47
1:A:482:ILE:HD12	1:A:482:ILE:N	2.29	0.47
1:B:615:LEU:HD21	1:B:655:ARG:HG2	1.96	0.47
1:A:206:VAL:HA	1:A:209:ARG:HD2	1.97	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:B:317:ASN:OD1	1:B:519:THR:HG21	2.15	0.46
1:A:312:TYR:CE2	1:A:572:THR:HG21	2.50	0.46
1:B:664:ARG:HD2	1:B:668:LYS:HZ3	1.80	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:A:268:ARG:HA	1:A:269:TYR:HA	1.69	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:B:382:ASN:HA	1:B:383:PHE:HA	1.69	0.46
1:A:447:GLN:CD	1:A:447:GLN:H	2.17	0.46
1:A:247:ARG:HG2	1:A:273:TRP:CH2	2.51	0.46
1:B:303:ASP:CB	1:B:305:ASN:ND2	2.79	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:570:ARG:HA	1:B:588:ASP:OD1	2.16	0.45
1:B:492:LEU:HD13	1:B:589:ILE:HB	1.98	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:B:247:ARG:NH1	1:B:566:ASP:OD1	2.50	0.45
1:A:43:MET:O	1:A:93:ASN:HB3	2.15	0.45
1:B:492:LEU:CD1	1:B:589:ILE:HB	2.46	0.45
1:B:563:LEU:CD1	1:B:567:ASN:HA	2.42	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:415:SER:HB2	1:B:449:ARG:NH1	2.31	0.45
1:B:36:ASN:CB	1:B:99:ILE:O	2.64	0.45
1:A:502:LEU:CD2	1:A:516:VAL:HG11	2.47	0.45
1:B:206:VAL:HA	1:B:209:ARG:CD	2.46	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:500:LEU:HD22	1:B:571:ILE:HG13	1.99	0.44
1:B:268:ARG:HA	1:B:269:TYR:HA	1.66	0.44
1:B:491:MET:CG	1:B:496:LYS:HE2	2.46	0.44
1:B:405:THR:C	1:B:407:LYS:H	2.20	0.44
1:B:385:MET:O	1:B:386:PRO:C	2.54	0.44
1:B:645:VAL:HG12	5:B:875:HOH:O	2.16	0.44
1:A:42:ILE:HA	1:A:94:THR:HA	1.99	0.44
1:B:213:LYS:NZ	1:B:213:LYS:HB2	2.32	0.44
1:B:535:LYS:O	1:B:536:ASP:HB2	2.17	0.44
1:A:420:ARG:HG2	5:A:735:HOH:O	2.17	0.44
1:B:563:LEU:HD11	1:B:567:ASN:CA	2.43	0.44
1:A:55:PHE:O	1:A:72:VAL:HA	2.17	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:B:34:GLY:HA3	1:B:138:LEU:CD1	2.47	0.44
1:A:228:ASP:O	1:A:229:ASN:HB2	2.18	0.44
1:B:229:ASN:HD22	1:B:229:ASN:HA	1.58	0.44
1:A:158:ASP:HA	1:A:179:GLN:OE1	2.17	0.44
1:B:213:LYS:HZ2	1:B:213:LYS:HB2	1.81	0.44
1:A:564:LYS:O	1:A:566:ASP:N	2.50	0.44
1:B:402:ASP:OD1	1:B:404:THR:N	2.51	0.44
1:A:448:GLU:OE2	1:A:449:ARG:NE	2.47	0.44
1:B:544:PRO:C	1:B:546:GLU:H	2.20	0.44
1:A:370:SER:O	1:A:374:VAL:HG23	2.18	0.44
1:A:25:SER:OG	1:A:182:GLU:HG2	2.18	0.44
1:B:646:PRO:HG2	5:B:875:HOH:O	2.17	0.43
1:B:417:THR:HG23	1:B:418:ILE:CD1	2.46	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:396:ARG:HH22	1:B:586:GLU:CD	2.21	0.43
1:B:224:ASN:O	1:B:230:GLY:HA3	2.17	0.43
1:B:526:ASN:HD22	1:B:526:ASN:N	2.16	0.43
1:B:524:ILE:HB	1:B:526:ASN:ND2	2.32	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:259:TRP:CH2	1:B:264:LEU:HD22	2.53	0.43
1:B:62:TYR:O	1:B:63:PRO:C	2.57	0.43
1:A:382:ASN:HB3	1:A:383:PHE:CD2	2.53	0.43
1:A:377:GLY:O	1:A:454: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:A:182:GLU:O	1:A:257:LYS:HE2	2.19	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:601:LEU:N	1:B:601:LEU:HD22	2.34	0.42
1:B:296:PHE:O	1:B:297:ASN:HB2	2.19	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:520:ALA:HB3	1:A:534:TRP:HB3	2.02	0.42
1:A:161:ILE:HG13	1:A:430:ASN:OD1	2.20	0.42
1:B:179:GLN:HA	1:B:184:ILE:HG21	2.01	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:313:ASP:C	1:B:313:ASP:OD1	2.58	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:A:225:SER:HA	1:A:230:GLY:CA	2.50	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: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: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:208:SER:C	1:B:210:ASN:H	2.24	0.41
1:B:36:ASN:N	1:B:36:ASN:HD22	2.17	0.41
1:B:36:ASN:N	1:B:36:ASN:ND2	2.67	0.41
1:B:295:ASN:O	1:B:329:PHE:HA	2.21	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:512:LYS:NZ	1:B:580:GLU:OE2	2.54	0.41
1:B:602:ASN:ND2	1:B:611:ASN:H	2.13	0.41
1:B:510:ASP:C	1:B:544:PRO:HG3	2.40	0.41
1:B:137:TRP:CD2	1:B:151:ARG:HD2	2.56	0.41
1:A:311:TYR:CD2	1:A:399:TRP:HB2	2.56	0.41
1:B:357:GLN:HB2	1:B:357:GLN:HE21	1.67	0.41
1:A:528:THR:HA	5:A:870:HOH:O	2.20	0.41
1:A:630:MET:HB3	1:A:640:ASN:HD21	1.85	0.41
1:B:168:ASN:HA	1:B:168:ASN:HD22	1.63	0.41
1:A:359:ARG:HD3	1:A:362:GLY:O	2.20	0.41
1:B:611:ASN:ND2	1:B:657:ARG:NH2	2.63	0.41
1:A:195:SER:HA	1:A:222:MET:SD	2.61	0.41
1:B:327:TRP:N	1:B:327:TRP:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:111:THR:HG22	5:B:864:HOH:O	2.21	0.41
1:A:240:TYR:CG	1:A:246:PRO:HD3	2.56	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: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:A:573:ALA:HB3	1:A:585:VAL:HB	2.04	0.40
1:B:182:GLU:HA	1:B:182:GLU:OE2	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%)	39	69
1	B	669/692 (97%)	619 (92%)	47 (7%)	3 (0%)	39	69
All	All	1338/1384 (97%)	1246 (93%)	86 (6%)	6 (0%)	39	69

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%)	42	73
1	B	579/595 (97%)	559 (96%)	20 (4%)	43	74
All	All	1158/1190 (97%)	1117 (96%)	41 (4%)	43	74

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

Some 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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.