



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:59 AM UTC

PDB ID : 1ZN3 / pdb_00001zn3
Title : Crystal structure of Glu335Ala mutant of Clostridium botulinum neurotoxin type E
Authors : Agarwal, R.; Binz, T.; Swaminathan, S.
Deposited on : 2005-05-11
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

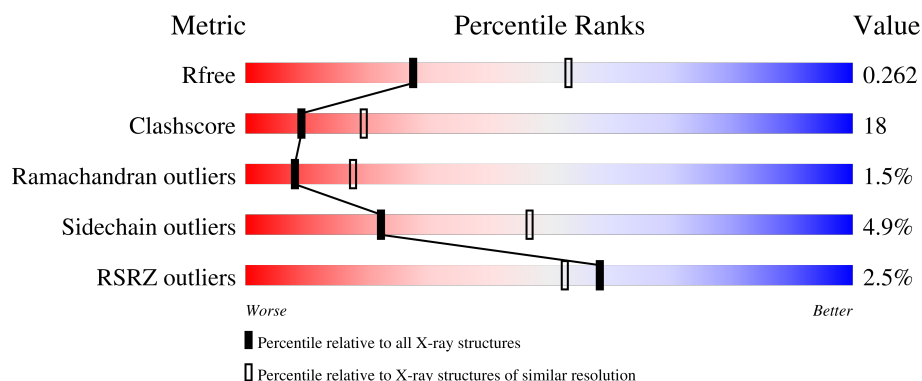
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	420	3% 66% 27% 5%
1	B	420	2% 58% 29% 5% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6756 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 botulinum neurotoxin type E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3295	2107	552	628	8			
1	B	387	Total	C	N	O	S	0	0	0
			3106	1990	516	593	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	GLU	engineered mutation	GB 40398
B	335	ALA	GLU	engineered mutation	GB 40398

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	199	Total	O	0	0
			199	199		

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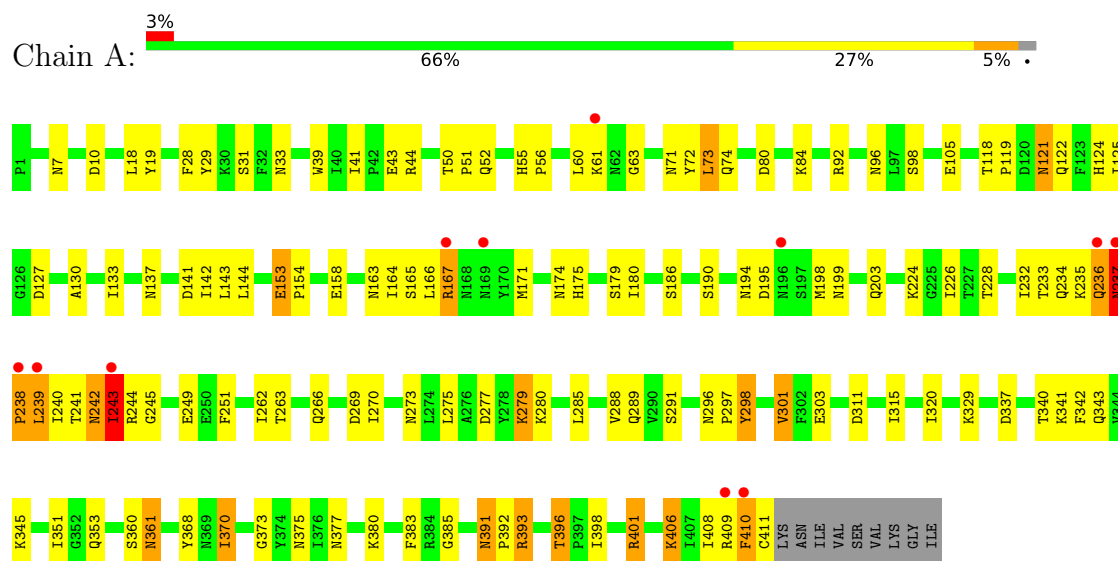
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	149	Total 149	O 149	0	0

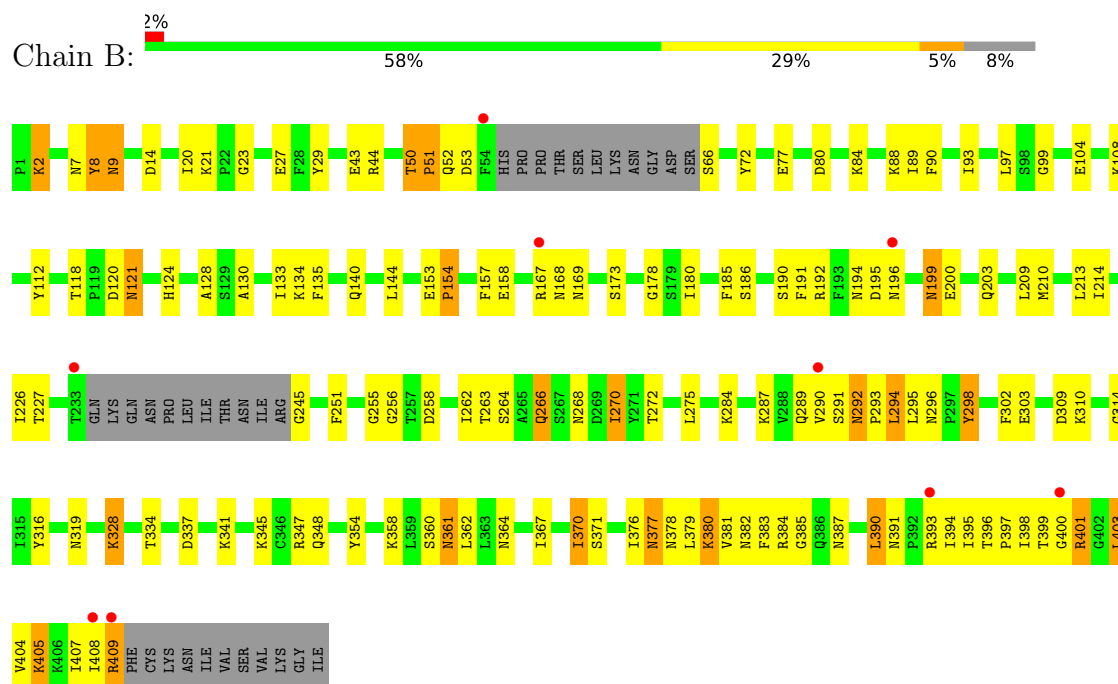
3 Residue-property plots

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 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.

• Molecule 1: botulinum neurotoxin type E



• Molecule 1: botulinum neurotoxin type E



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.09Å 144.72Å 83.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.57 – 2.60 42.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (42.57-2.60) 95.7 (42.57-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.259 0.221 , 0.262	Depositor DCC
R_{free} test set	643 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6756	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.51	1/3369 (0.0%)	1.05	19/4564 (0.4%)
1	B	0.50	2/3173 (0.1%)	1.00	15/4294 (0.3%)
All	All	0.51	3/6542 (0.0%)	1.02	34/8858 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	ASN	CA-C	-7.94	1.42	1.52
1	B	167	ARG	N-CA	6.21	1.53	1.46
1	A	243	ILE	CA-CB	5.54	1.61	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ASN	N-CA-C	11.73	125.43	110.65
1	B	23	GLY	N-CA-C	-8.83	101.24	112.54
1	A	56	PRO	N-CA-C	8.45	121.01	110.70
1	A	370	ILE	N-CA-C	7.63	117.74	110.42
1	B	303	GLU	N-CA-C	-7.38	103.17	111.14
1	B	186	SER	CA-C-N	6.84	126.80	119.28
1	B	186	SER	C-N-CA	6.84	126.80	119.28
1	B	370	ILE	N-CA-C	6.66	116.68	110.42
1	A	320	ILE	N-CA-C	6.63	118.18	110.62
1	A	239	LEU	N-CA-C	-6.43	105.54	113.19
1	B	270	ILE	N-CA-C	-6.24	104.43	110.42
1	A	186	SER	CA-C-N	6.09	125.77	119.56
1	A	186	SER	C-N-CA	6.09	125.77	119.56
1	B	399	THR	N-CA-C	6.08	120.73	112.88
1	A	391	ASN	CA-C-N	6.07	127.43	119.84
1	A	391	ASN	C-N-CA	6.07	127.43	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	CA-C-N	6.04	125.76	119.05
1	A	56	PRO	C-N-CA	6.04	125.76	119.05
1	A	55	HIS	CA-C-N	6.00	126.56	120.38
1	A	55	HIS	C-N-CA	6.00	126.56	120.38
1	A	377	ASN	CB-CA-C	-5.83	109.84	116.54
1	A	7	ASN	N-CA-C	-5.73	100.94	110.17
1	B	377	ASN	CB-CA-C	-5.67	109.52	117.23
1	A	303	GLU	N-CA-C	-5.58	105.10	111.07
1	A	158	GLU	N-CA-C	5.48	118.86	110.20
1	B	199	ASN	N-CA-C	-5.46	102.40	110.48
1	B	401	ARG	N-CA-C	-5.31	105.57	111.36
1	A	279	LYS	N-CA-C	-5.28	105.69	111.82
1	A	249	GLU	N-CA-C	-5.25	105.67	111.71
1	B	121	ASN	N-CA-C	5.17	120.51	113.37
1	B	376	ILE	N-CA-C	5.13	115.97	108.58
1	B	158	GLU	N-CA-C	5.13	117.67	110.23
1	B	398	ILE	N-CA-C	-5.11	102.04	109.29
1	B	185	PHE	N-CA-C	5.02	116.59	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3295	0	3259	125	0
1	B	3106	0	3067	112	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	2	0
3	B	1	0	0	0	0
4	A	199	0	0	10	0
4	B	149	0	0	11	0
All	All	6756	0	6326	232	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 (232) 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:236:GLN:O	1:A:238:PRO:HD2	1.40	1.20
1:A:235:LYS:C	1:A:237:ASN:H	1.69	0.99
1:A:401:ARG:NH1	3:A:501:CL:CL	2.32	0.98
1:B:263:THR:H	1:B:266:GLN:HE21	0.99	0.94
1:A:236:GLN:C	1:A:238:PRO:HD2	1.96	0.90
1:A:242:ASN:O	1:A:243:ILE:HG23	1.72	0.89
1:B:358:LYS:HE2	4:B:876:HOH:O	1.76	0.86
1:A:236:GLN:O	1:A:238:PRO:CD	2.23	0.86
1:A:198:MET:HE2	1:A:198:MET:HA	1.59	0.84
1:A:235:LYS:O	1:A:237:ASN:N	2.12	0.83
1:B:409:ARG:HH11	1:B:409:ARG:HA	1.44	0.83
1:B:384:ARG:HG3	1:B:390:LEU:HD13	1.60	0.83
1:B:379:LEU:HD23	1:B:384:ARG:HD2	1.60	0.82
1:A:234:GLN:HE22	1:A:243:ILE:HA	1.44	0.80
1:A:171:MET:HE3	4:A:565:HOH:O	1.82	0.80
1:B:263:THR:N	1:B:266:GLN:HE21	1.80	0.78
1:A:142:ILE:HG13	1:B:293:PRO:HG2	1.66	0.77
1:A:234:GLN:NE2	1:A:243:ILE:HA	2.01	0.76
1:B:409:ARG:HD2	1:B:409:ARG:N	2.00	0.75
1:B:345:LYS:HB2	1:B:383:PHE:CD2	2.23	0.74
1:B:347:ARG:HD2	1:B:354:TYR:OH	1.89	0.72
1:A:153:GLU:HB2	1:A:154:PRO:CD	2.20	0.71
1:B:385:GLY:HA2	1:B:391:ASN:HD22	1.58	0.69
1:A:166:LEU:HB3	1:A:167:ARG:NH1	2.08	0.68
1:B:130:ALA:HB2	1:B:144:LEU:HD22	1.74	0.68
1:B:275:LEU:HB3	4:B:953:HOH:O	1.92	0.67
1:A:119:PRO:HG2	1:A:122:GLN:HG2	1.76	0.67
1:B:284:LYS:HB3	4:B:884:HOH:O	1.93	0.67
1:B:401:ARG:HG3	4:B:856:HOH:O	1.95	0.66
1:B:130:ALA:HB2	1:B:144:LEU:CD2	2.26	0.64
1:B:310:LYS:HE2	1:B:314:GLY:HA2	1.78	0.64
1:A:174:ASN:ND2	1:A:224:LYS:HB2	2.12	0.64
1:A:289:GLN:HG3	1:A:291:SER:H	1.63	0.64
1:A:251:PHE:CZ	1:A:351:ILE:HD11	2.33	0.64
1:A:19:TYR:HB3	1:A:28:PHE:HB3	1.78	0.63
1:A:235:LYS:C	1:A:237:ASN:N	2.43	0.63
1:B:378:ASN:ND2	1:B:384:ARG:HH12	1.96	0.62
1:B:88:LYS:HA	4:B:941:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ILE:HG12	1:B:133:ILE:HG22	1.82	0.62
1:A:198:MET:HE2	1:A:198:MET:CA	2.31	0.61
1:B:120:ASP:OD1	1:B:284:LYS:HG2	2.01	0.61
1:A:298:TYR:O	1:A:301:VAL:HG13	2.00	0.61
1:B:190:SER:OG	1:B:203:GLN:HB3	2.01	0.60
1:B:292:ASN:HD22	1:B:294:LEU:H	1.48	0.60
1:B:272:THR:HA	4:B:953:HOH:O	1.99	0.60
1:B:387:ASN:HB3	1:B:390:LEU:HB2	1.84	0.59
1:A:121:ASN:C	1:A:121:ASN:HD22	2.09	0.59
1:B:262:ILE:HD12	1:B:262:ILE:H	1.66	0.58
1:A:105:GLU:CD	1:A:329:LYS:HD2	2.29	0.58
1:A:60:LEU:HB2	4:A:554:HOH:O	2.03	0.58
1:B:153:GLU:HB2	1:B:154:PRO:HD2	1.85	0.58
1:A:198:MET:HA	1:A:198:MET:CE	2.33	0.57
1:A:311:ASP:OD2	1:A:315:ILE:HB	2.05	0.57
1:A:238:PRO:C	1:A:240:ILE:H	2.10	0.57
1:B:403:LEU:O	1:B:407:ILE:HG13	2.04	0.57
1:B:403:LEU:O	1:B:403:LEU:HD22	2.05	0.57
1:A:262:ILE:HG23	1:A:266:GLN:HE21	1.70	0.57
1:B:290:VAL:CG1	1:B:296:ASN:HD21	2.18	0.57
1:B:14:ASP:OD1	1:B:135:PHE:HB3	2.05	0.56
1:B:191:PHE:CE2	1:B:203:GLN:HG2	2.40	0.56
1:B:377:ASN:O	1:B:380:LYS:HG3	2.05	0.56
1:B:245:GLY:HA3	4:B:894:HOH:O	2.06	0.56
1:B:290:VAL:HG12	1:B:296:ASN:HD21	1.70	0.56
1:B:407:ILE:O	1:B:409:ARG:N	2.40	0.55
1:A:165:SER:HB3	1:A:171:MET:HE3	1.90	0.54
1:A:224:LYS:HB3	1:A:228:THR:CG2	2.37	0.54
1:B:292:ASN:HD22	1:B:292:ASN:C	2.15	0.54
1:B:400:GLY:O	1:B:404:VAL:HG23	2.07	0.54
1:A:238:PRO:C	1:A:240:ILE:N	2.65	0.53
1:B:153:GLU:HB2	1:B:154:PRO:CD	2.38	0.53
1:A:142:ILE:HG13	1:B:293:PRO:CG	2.38	0.53
1:A:242:ASN:C	1:A:243:ILE:HG23	2.33	0.53
1:A:298:TYR:HA	1:A:301:VAL:CG1	2.39	0.53
1:B:263:THR:H	1:B:266:GLN:NE2	1.84	0.53
1:A:375:ASN:HD22	1:A:385:GLY:HA3	1.74	0.53
1:A:243:ILE:C	1:A:245:GLY:H	2.16	0.53
1:B:194:ASN:HA	1:B:199:ASN:O	2.08	0.52
1:A:237:ASN:O	1:A:239:LEU:N	2.43	0.52
1:B:409:ARG:HH11	1:B:409:ARG:CA	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:OG	1:A:41:ILE:HG12	2.09	0.52
1:A:92:ARG:HA	1:A:370:ILE:HG23	1.90	0.52
1:A:61:LYS:HD2	4:A:554:HOH:O	2.09	0.52
1:A:226:ILE:HD11	1:A:273:ASN:CG	2.35	0.52
1:A:275:LEU:O	1:A:279:LYS:HG3	2.10	0.52
1:B:192:ARG:HD2	1:B:200:GLU:HB3	1.92	0.52
1:B:347:ARG:HD2	1:B:354:TYR:CZ	2.45	0.52
1:A:80:ASP:O	1:A:84:LYS:HG2	2.11	0.51
1:A:153:GLU:HB2	1:A:154:PRO:HD2	1.89	0.51
1:A:285:LEU:HD12	1:A:288:VAL:HG21	1.92	0.51
1:B:134:LYS:HE2	1:B:140:GLN:HG3	1.92	0.51
1:B:210:MET:O	1:B:214:ILE:HG13	2.09	0.51
1:B:121:ASN:HA	1:B:287:LYS:O	2.11	0.51
1:B:168:ASN:N	1:B:168:ASN:HD22	2.09	0.51
1:A:226:ILE:HB	1:A:270:ILE:HD13	1.94	0.50
1:A:121:ASN:C	1:A:121:ASN:ND2	2.69	0.50
1:B:80:ASP:O	1:B:84:LYS:HD3	2.12	0.50
1:A:167:ARG:NH2	3:A:502:CL:CL	2.82	0.50
1:A:137:ASN:OD1	1:A:137:ASN:C	2.54	0.50
1:A:195:ASP:CG	1:A:199:ASN:HB2	2.37	0.50
1:A:368:TYR:HA	1:A:373:GLY:O	2.12	0.50
1:B:292:ASN:ND2	1:B:294:LEU:H	2.10	0.50
1:A:285:LEU:HA	1:A:288:VAL:HG23	1.93	0.49
1:B:2:LYS:HD3	1:B:2:LYS:N	2.26	0.49
1:B:263:THR:HG23	1:B:266:GLN:NE2	2.27	0.49
1:A:125:ILE:HD11	1:B:294:LEU:CD1	2.42	0.49
1:B:195:ASP:OD1	1:B:195:ASP:C	2.55	0.49
1:A:236:GLN:C	1:A:238:PRO:CD	2.80	0.49
1:A:240:ILE:O	1:A:240:ILE:HG22	2.13	0.49
1:A:297:PRO:O	1:A:301:VAL:HG12	2.12	0.49
1:B:266:GLN:O	1:B:270:ILE:HG12	2.12	0.49
1:A:194:ASN:HA	1:A:199:ASN:O	2.13	0.49
1:B:226:ILE:CG2	1:B:270:ILE:HD13	2.43	0.49
1:A:269:ASP:O	1:A:273:ASN:HB2	2.12	0.49
1:B:405:LYS:NZ	1:B:405:LYS:HB3	2.28	0.49
1:A:224:LYS:HB3	1:A:228:THR:HG23	1.94	0.48
1:A:345:LYS:HD3	1:A:383:PHE:CD2	2.48	0.48
1:A:251:PHE:HZ	1:A:351:ILE:HD11	1.76	0.48
1:A:406:LYS:O	1:A:410:PHE:HB2	2.14	0.48
1:B:7:ASN:O	1:B:9:ASN:N	2.46	0.48
1:B:262:ILE:HA	1:B:266:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:THR:OG1	1:B:337:ASP:HB2	2.13	0.48
1:A:242:ASN:C	1:A:243:ILE:CG2	2.87	0.48
1:B:118:THR:HG21	1:B:124:HIS:CG	2.49	0.48
1:B:264:SER:O	1:B:268:ASN:HB2	2.13	0.48
1:A:29:TYR:CD1	1:A:43:GLU:HG3	2.48	0.47
1:B:50:THR:O	1:B:52:GLN:N	2.47	0.47
1:B:364:ASN:HB3	1:B:367:ILE:HD12	1.95	0.47
1:A:166:LEU:HB3	1:A:167:ARG:HH12	1.77	0.47
1:B:2:LYS:CD	1:B:2:LYS:H	2.28	0.47
1:A:130:ALA:HB2	1:A:144:LEU:CD2	2.44	0.47
1:A:44:ARG:NH1	1:A:72:TYR:HB3	2.30	0.47
1:B:405:LYS:HG2	4:B:955:HOH:O	2.15	0.47
1:B:21:LYS:HG3	1:B:27:GLU:O	2.14	0.47
1:B:403:LEU:C	1:B:403:LEU:HD13	2.40	0.47
1:A:195:ASP:OD1	1:A:199:ASN:HB2	2.15	0.47
1:A:153:GLU:CB	1:A:154:PRO:CD	2.90	0.47
1:B:2:LYS:HD3	1:B:2:LYS:H	1.80	0.47
1:B:50:THR:O	1:B:53:ASP:N	2.42	0.47
1:B:262:ILE:HD12	1:B:262:ILE:N	2.28	0.46
1:A:33:ASN:ND2	4:A:648:HOH:O	2.47	0.46
1:B:77:GLU:HA	1:B:77:GLU:OE1	2.15	0.46
1:B:309:ASP:OD2	1:B:319:ASN:ND2	2.48	0.46
1:A:232:ILE:HA	1:A:236:GLN:OE1	2.16	0.46
1:B:128:ALA:O	1:B:180:ILE:HG13	2.16	0.46
1:B:66:SER:HA	1:B:157:PHE:CD2	2.51	0.46
1:A:241:THR:HG21	1:A:245:GLY:HA2	1.97	0.46
1:A:130:ALA:HB2	1:A:144:LEU:HD23	1.98	0.45
1:B:290:VAL:HG23	1:B:290:VAL:O	2.16	0.45
1:A:44:ARG:HD3	1:A:73:LEU:HB2	1.97	0.45
1:B:104:GLU:OE1	1:B:108:LYS:HE3	2.16	0.45
1:A:163:ASN:HB3	1:A:179:SER:OG	2.16	0.45
1:A:118:THR:HG21	1:A:124:HIS:CD2	2.51	0.45
1:B:255:GLY:O	1:B:258:ASP:HB2	2.17	0.45
1:A:105:GLU:OE1	1:A:329:LYS:HD2	2.17	0.45
1:B:328:LYS:HB3	1:B:328:LYS:NZ	2.32	0.45
1:B:362:LEU:HG	4:B:838:HOH:O	2.17	0.45
1:A:10:ASP:HA	4:A:681:HOH:O	2.17	0.45
1:A:63:GLY:O	1:A:401:ARG:HD2	2.17	0.45
1:A:234:GLN:NE2	1:A:243:ILE:CA	2.75	0.45
1:A:71:ASN:O	1:A:74:GLN:HG2	2.17	0.44
1:A:190:SER:OG	1:A:203:GLN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLN:O	1:A:237:ASN:CG	2.60	0.44
1:A:297:PRO:HG2	1:B:298:TYR:CD2	2.53	0.44
1:B:50:THR:O	1:B:51:PRO:C	2.59	0.44
1:A:166:LEU:O	1:A:167:ARG:C	2.60	0.44
1:B:256:GLY:C	1:B:258:ASP:N	2.74	0.44
1:B:393:ARG:HB2	4:B:860:HOH:O	2.18	0.44
1:A:277:ASP:O	1:A:280:LYS:HB3	2.18	0.44
1:B:191:PHE:CD2	1:B:191:PHE:N	2.86	0.44
1:B:309:ASP:OD2	1:B:319:ASN:HB2	2.17	0.44
1:A:63:GLY:C	1:A:401:ARG:HD2	2.43	0.43
1:A:174:ASN:HD22	1:A:224:LYS:HB2	1.82	0.43
1:B:7:ASN:O	1:B:8:TYR:C	2.61	0.43
1:A:337:ASP:O	1:A:340:THR:HB	2.17	0.43
1:B:50:THR:HG23	1:B:52:GLN:OE1	2.18	0.43
1:A:125:ILE:HD11	1:B:294:LEU:HD13	1.99	0.43
1:B:90:PHE:CE1	1:B:209:LEU:HD21	2.53	0.43
1:B:227:THR:HG22	1:B:270:ILE:HD12	2.00	0.43
1:B:251:PHE:HB2	1:B:262:ILE:HD11	2.00	0.43
1:A:96:ASN:HB3	1:A:342:PHE:CZ	2.53	0.43
1:A:133:ILE:HD11	1:A:141:ASP:HB3	2.01	0.43
1:B:173:SER:HA	1:B:178:GLY:HA2	2.01	0.43
1:A:98:SER:OG	1:A:341:LYS:HD3	2.19	0.43
1:A:262:ILE:HG23	1:A:266:GLN:NE2	2.33	0.43
1:A:311:ASP:OD1	1:A:311:ASP:C	2.62	0.43
1:A:153:GLU:HB2	1:A:154:PRO:HD3	2.00	0.42
1:A:236:GLN:C	1:A:237:ASN:CG	2.87	0.42
1:A:360:SER:O	1:A:361:ASN:C	2.62	0.42
1:A:396:THR:HG22	4:A:529:HOH:O	2.19	0.42
1:A:165:SER:CB	1:A:171:MET:HG2	2.50	0.42
1:B:370:ILE:HG22	1:B:371:SER:N	2.34	0.42
1:A:179:SER:O	1:A:180:ILE:C	2.62	0.42
1:A:263:THR:H	1:A:266:GLN:NE2	2.17	0.42
1:B:93:ILE:O	1:B:99:GLY:HA3	2.20	0.42
1:A:296:ASN:HB2	1:A:297:PRO:HD3	2.02	0.42
1:B:89:ILE:O	1:B:93:ILE:HG13	2.19	0.42
1:A:33:ASN:HB2	1:A:39:TRP:CZ2	2.55	0.42
1:A:119:PRO:HG2	1:A:122:GLN:CG	2.47	0.42
1:B:209:LEU:O	1:B:213:LEU:HG	2.19	0.42
1:A:375:ASN:HB3	1:A:380:LYS:HA	2.01	0.42
1:A:391:ASN:N	1:A:392:PRO:CD	2.82	0.42
1:B:394:ILE:HG13	1:B:395:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:THR:HA	1:B:397:PRO:HD3	1.87	0.41
1:A:133:ILE:HG21	1:A:143:LEU:HB2	2.02	0.41
1:A:33:ASN:HB2	1:A:39:TRP:CH2	2.55	0.41
1:B:381:VAL:O	1:B:382:ASN:C	2.63	0.41
1:A:409:ARG:N	1:A:409:ARG:HD3	2.35	0.41
1:B:44:ARG:NH1	1:B:72:TYR:HB3	2.35	0.41
1:A:226:ILE:CG2	1:A:270:ILE:HD13	2.51	0.41
1:B:50:THR:N	1:B:53:ASP:OD2	2.53	0.41
1:B:112:TYR:HA	1:B:302:PHE:CE1	2.55	0.41
1:B:405:LYS:HA	1:B:405:LYS:HD2	1.91	0.41
1:A:263:THR:HG23	4:A:662:HOH:O	2.20	0.41
1:A:343:GLN:HA	4:A:581:HOH:O	2.20	0.41
1:B:360:SER:O	1:B:361:ASN:C	2.64	0.41
1:A:199:ASN:ND2	4:A:649:HOH:O	2.53	0.41
1:A:233:THR:C	1:A:235:LYS:H	2.29	0.41
1:B:337:ASP:OD2	1:B:341:LYS:HE3	2.21	0.41
1:B:379:LEU:HD13	1:B:391:ASN:ND2	2.36	0.41
1:A:50:THR:O	1:A:51:PRO:C	2.64	0.40
1:A:171:MET:O	1:A:175:HIS:CD2	2.74	0.40
1:A:375:ASN:HD22	1:A:385:GLY:CA	2.34	0.40
1:A:127:ASP:O	1:A:164:ILE:HG21	2.21	0.40
1:B:29:TYR:CG	1:B:43:GLU:HG3	2.57	0.40
1:B:272:THR:CA	4:B:953:HOH:O	2.64	0.40
1:B:378:ASN:ND2	1:B:384:ARG:HH22	2.20	0.40
1:A:167:ARG:H	1:A:167:ARG:HG3	1.68	0.40
1:A:266:GLN:O	1:A:270:ILE:HG12	2.22	0.40
1:A:393:ARG:H	1:A:393:ARG:HG3	1.63	0.40
1:A:410:PHE:O	1:A:411:CYS:HB2	2.21	0.40
1:A:398:ILE:HG13	4:A:574:HOH:O	2.20	0.40
1:B:309:ASP:O	1:B:316:TYR:HA	2.21	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	409/420 (97%)	380 (93%)	22 (5%)	7 (2%)	7	15
1	B	381/420 (91%)	346 (91%)	30 (8%)	5 (1%)	9	21
All	All	790/840 (94%)	726 (92%)	52 (7%)	12 (2%)	8	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	167	ARG
1	A	236	GLN
1	A	243	ILE
1	B	8	TYR
1	B	390	LEU
1	B	408	ILE
1	A	361	ASN
1	B	51	PRO
1	A	153	GLU
1	B	361	ASN
1	A	408	ILE

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	371/379 (98%)	355 (96%)	16 (4%)	26	51
1	B	348/379 (92%)	329 (94%)	19 (6%)	19	41
All	All	719/758 (95%)	684 (95%)	35 (5%)	22	47

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU

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Mol	Chain	Res	Type
1	A	52	GLN
1	A	73	LEU
1	A	121	ASN
1	A	237	ASN
1	A	238	PRO
1	A	243	ILE
1	A	244	ARG
1	A	298	TYR
1	A	301	VAL
1	A	353	GLN
1	A	393	ARG
1	A	396	THR
1	A	401	ARG
1	A	406	LYS
1	A	410	PHE
1	B	2	LYS
1	B	9	ASN
1	B	50	THR
1	B	97	LEU
1	B	154	PRO
1	B	196	ASN
1	B	266	GLN
1	B	289	GLN
1	B	291	SER
1	B	292	ASN
1	B	294	LEU
1	B	295	LEU
1	B	298	TYR
1	B	328	LYS
1	B	348	GLN
1	B	380	LYS
1	B	403	LEU
1	B	405	LYS
1	B	409	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	71	ASN
1	A	117	ASN
1	A	121	ASN

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Mol	Chain	Res	Type
1	A	163	ASN
1	A	174	ASN
1	A	175	HIS
1	A	194	ASN
1	A	199	ASN
1	A	211	HIS
1	A	234	GLN
1	A	266	GLN
1	A	268	ASN
1	A	324	ASN
1	A	353	GLN
1	A	375	ASN
1	A	389	ASN
1	B	9	ASN
1	B	95	ASN
1	B	121	ASN
1	B	163	ASN
1	B	168	ASN
1	B	174	ASN
1	B	199	ASN
1	B	266	GLN
1	B	292	ASN
1	B	296	ASN
1	B	378	ASN
1	B	391	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	411/420 (97%)	-0.17	11 (2%) 56 50	20, 34, 55, 77	0
1	B	387/420 (92%)	0.09	9 (2%) 61 55	26, 42, 59, 68	0
All	All	798/840 (95%)	-0.04	20 (2%) 58 52	20, 37, 59, 77	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ASN	5.2
1	A	243	ILE	3.9
1	B	290	VAL	3.7
1	A	238	PRO	3.3
1	A	196	ASN	3.1
1	A	409	ARG	3.0
1	B	393	ARG	2.8
1	B	408	ILE	2.8
1	A	167	ARG	2.6
1	B	233	THR	2.6
1	A	239	LEU	2.3
1	A	236	GLN	2.3
1	B	409	ARG	2.3
1	A	410	PHE	2.3
1	B	196	ASN	2.2
1	B	54	PHE	2.2
1	A	61	LYS	2.2
1	B	167	ARG	2.1
1	A	169	ASN	2.1
1	B	400	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	502	1/1	0.93	0.18	54,54,54,54	0
3	CL	A	503	1/1	0.94	0.17	50,50,50,50	0
3	CL	B	505	1/1	0.94	0.09	30,30,30,30	1
2	ZN	A	422	1/1	0.95	0.18	49,49,49,49	0
3	CL	A	501	1/1	0.97	0.14	36,36,36,36	0
3	CL	A	504	1/1	0.98	0.07	40,40,40,40	0
2	ZN	B	822	1/1	0.98	0.04	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.