



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:35 PM UTC

PDB ID : 1ZL5 / pdb_00001zl5
Title : Crystal structure of Glu335Gln mutant of Clostridium botulinum neurotoxin E catalytic domain
Authors : Agarwal, R.; Binz, T.; Swaminathan, S.
Deposited on : 2005-05-05
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

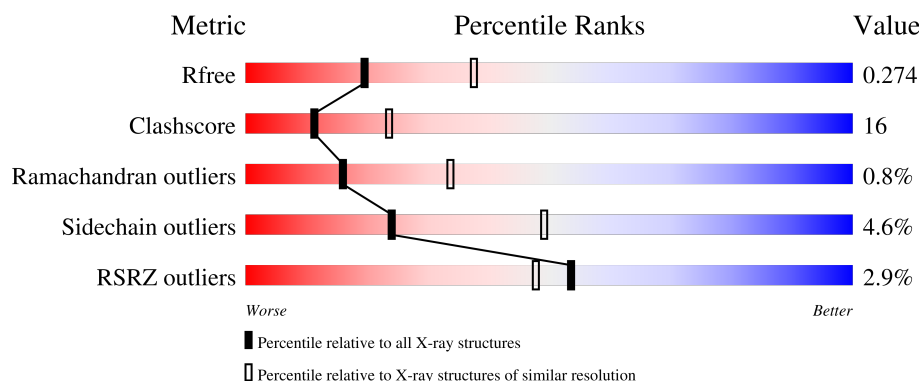
1 Overall quality at a glance

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	
1	B	420	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	602	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6575 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	400	Total	C	N	O	S	0	0	0
			3207	2052	534	613	8			
1	B	387	Total	C	N	O	S	0	0	0
			3110	1992	517	594	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	GLN	GLU	engineered mutation	UNP Q00496
B	335	GLN	GLU	engineered mutation	UNP Q00496

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Cl	0	0
			6	6		
2	B	2	Total	Cl	0	0
			2	2		

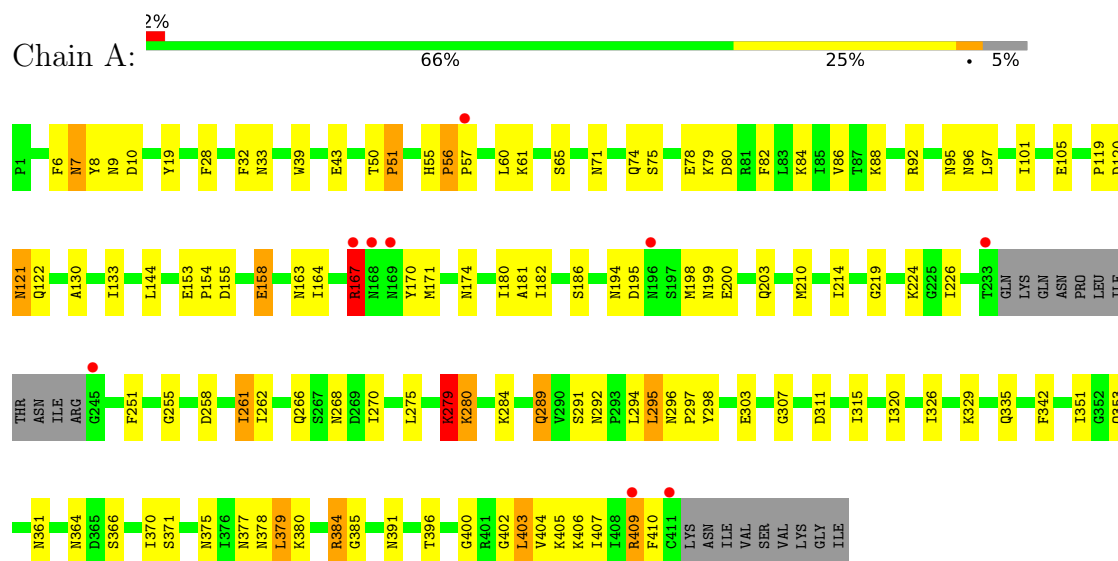
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		
3	B	114	Total	O	0	0
			114	114		

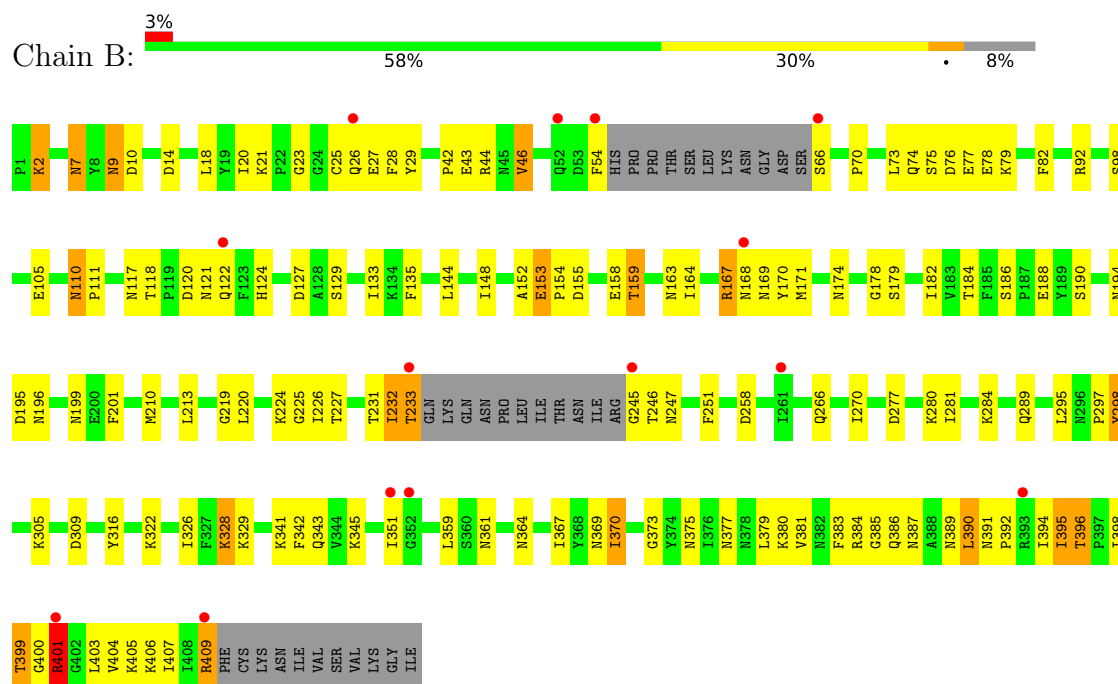
3 Residue-property plots

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	88.95Å 144.57Å 83.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.60 46.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.3 (46.55-2.60) 84.3 (46.55-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.271 0.214 , 0.274	Depositor DCC
R_{free} test set	422 reflections (1.36%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: 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	0.49	1/3279 (0.0%)	1.00	18/4440 (0.4%)
1	B	0.49	2/3177 (0.1%)	0.96	17/4299 (0.4%)
All	All	0.49	3/6456 (0.0%)	0.98	35/8739 (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	-9.92	1.42	1.53
1	B	170	TYR	N-CA	-7.30	1.37	1.45
1	A	170	TYR	N-CA	5.50	1.52	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	THR	N-CA-C	7.43	122.06	112.92
1	A	371	SER	N-CA-C	7.39	120.39	111.82
1	B	401	ARG	N-CA-C	-7.03	103.70	111.36
1	A	320	ILE	N-CA-C	6.87	117.62	110.62
1	A	7	ASN	N-CA-C	-6.69	99.31	109.95
1	B	398	ILE	N-CA-C	-6.64	98.00	108.95
1	A	198	MET	N-CA-C	6.31	120.26	111.74
1	B	7	ASN	N-CA-C	-6.14	99.39	109.40
1	A	391	ASN	CA-C-N	6.13	125.75	119.56
1	A	391	ASN	C-N-CA	6.13	125.75	119.56
1	A	409	ARG	N-CA-C	6.06	123.72	110.80
1	A	186	SER	CA-C-N	5.97	125.65	119.56
1	A	186	SER	C-N-CA	5.97	125.65	119.56
1	A	158	GLU	N-CA-C	5.87	118.96	110.28
1	A	303	GLU	N-CA-C	-5.76	104.91	111.07
1	B	74	GLN	N-CA-C	-5.68	106.02	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	GLN	N-CA-C	5.66	118.28	110.35
1	B	117	ASN	N-CA-C	5.64	119.25	112.93
1	A	65	SER	N-CA-C	-5.58	106.52	113.55
1	A	57	PRO	N-CA-C	-5.53	105.85	113.53
1	B	158	GLU	N-CA-C	5.49	118.20	109.96
1	A	56	PRO	N-CA-C	5.45	117.34	110.70
1	B	23	GLY	N-CA-C	-5.41	104.19	111.54
1	B	396	THR	CA-C-N	5.39	126.14	120.11
1	B	396	THR	C-N-CA	5.39	126.14	120.11
1	B	152	ALA	N-CA-C	5.31	117.15	110.24
1	B	370	ILE	N-CA-C	5.29	115.50	110.53
1	A	120	ASP	N-CA-C	5.25	117.69	111.33
1	A	279	LYS	N-CA-C	-5.25	105.64	111.36
1	B	110	ASN	N-CA-C	5.23	116.00	109.57
1	B	186	SER	CA-C-N	5.16	124.61	119.24
1	B	186	SER	C-N-CA	5.16	124.61	119.24
1	A	121	ASN	N-CA-C	5.15	119.43	113.20
1	B	169	ASN	CA-C-N	-5.14	114.59	122.87
1	B	169	ASN	C-N-CA	-5.14	114.59	122.87

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	3207	0	3160	97	0
1	B	3110	0	3070	108	0
2	A	6	0	0	4	0
2	B	2	0	0	0	0
3	A	136	0	0	13	0
3	B	114	0	0	9	0
All	All	6575	0	6230	203	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 16.

All (203) 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:B:167:ARG:HB2	1:B:167:ARG:HH11	1.37	0.87
1:B:75:SER:HB3	1:B:78:GLU:HG3	1.58	0.83
1:B:233:THR:HA	1:B:245:GLY:HA2	1.60	0.81
1:A:284:LYS:HB2	3:A:744:HOH:O	1.83	0.78
1:B:196:ASN:HA	3:B:715:HOH:O	1.84	0.77
1:A:275:LEU:O	1:A:279:LYS:HG2	1.84	0.77
1:B:409:ARG:HH11	1:B:409:ARG:HA	1.54	0.72
1:B:375:ASN:HB3	1:B:380:LYS:HA	1.71	0.71
1:A:292:ASN:O	1:A:295:LEU:HD22	1.91	0.71
1:B:75:SER:HB3	1:B:78:GLU:CG	2.22	0.70
1:B:46:VAL:HG22	3:B:659:HOH:O	1.91	0.70
1:B:385:GLY:HA2	1:B:391:ASN:HD22	1.58	0.69
1:B:21:LYS:HD3	1:B:25:CYS:O	1.93	0.69
1:B:409:ARG:HH11	1:B:409:ARG:CA	2.06	0.68
1:A:153:GLU:HG2	2:A:602:CL:CL	2.31	0.68
1:A:153:GLU:HB2	1:A:154:PRO:CD	2.25	0.67
1:A:289:GLN:HG3	1:A:291:SER:H	1.58	0.67
1:B:21:LYS:HG2	1:B:27:GLU:O	1.94	0.66
1:B:227:THR:HG22	1:B:270:ILE:HD12	1.78	0.66
1:A:194:ASN:ND2	1:A:200:GLU:HG2	2.11	0.65
1:B:400:GLY:O	1:B:404:VAL:HG23	1.97	0.65
1:A:105:GLU:CD	1:A:329:LYS:HD2	2.23	0.64
1:B:153:GLU:HB2	1:B:154:PRO:CD	2.28	0.64
1:B:54:PHE:O	1:B:70:PRO:HG3	1.97	0.63
1:A:171:MET:HE2	3:A:689:HOH:O	2.00	0.62
1:A:194:ASN:HD21	1:A:200:GLU:HG2	1.64	0.62
1:A:153:GLU:HB2	1:A:154:PRO:HD2	1.80	0.61
1:A:280:LYS:HD3	3:A:744:HOH:O	1.99	0.61
1:B:381:VAL:O	1:B:384:ARG:HG3	1.99	0.61
1:B:409:ARG:N	1:B:409:ARG:HD2	2.15	0.61
1:A:261:ILE:HD12	1:A:261:ILE:N	2.15	0.60
1:B:167:ARG:HH11	1:B:167:ARG:CB	2.13	0.60
1:B:2:LYS:HB3	3:B:713:HOH:O	2.03	0.59
1:B:2:LYS:HD3	1:B:2:LYS:H	1.68	0.59
1:B:395:ILE:HD12	1:B:395:ILE:N	2.18	0.59
1:A:75:SER:OG	1:A:78:GLU:HG3	2.03	0.58
1:B:381:VAL:HG23	3:B:652:HOH:O	2.03	0.58
1:B:251:PHE:HD2	1:B:258:ASP:HB3	1.67	0.58
1:A:210:MET:O	1:A:214:ILE:HG13	2.04	0.58
1:B:289:GLN:HB2	3:B:677:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:O	1:B:380:LYS:HG2	2.04	0.57
1:B:233:THR:HA	1:B:245:GLY:CA	2.34	0.57
1:A:171:MET:CE	3:A:689:HOH:O	2.52	0.56
1:B:396:THR:HG21	3:B:710:HOH:O	2.03	0.56
1:B:387:ASN:HB3	1:B:390:LEU:HB3	1.87	0.56
1:B:266:GLN:O	1:B:270:ILE:HG12	2.05	0.56
1:A:33:ASN:HB2	1:A:39:TRP:CZ2	2.40	0.55
1:A:266:GLN:O	1:A:270:ILE:HG12	2.06	0.55
1:A:19:TYR:HB3	1:A:28:PHE:HB3	1.89	0.55
1:A:311:ASP:OD2	1:A:315:ILE:HB	2.05	0.55
1:A:155:ASP:O	2:A:602:CL:CL	2.62	0.55
1:A:195:ASP:OD2	1:A:199:ASN:HB2	2.06	0.55
1:A:97:LEU:O	1:A:101:ILE:HG12	2.07	0.55
1:A:261:ILE:HD12	1:A:261:ILE:H	1.72	0.54
1:A:130:ALA:HB2	1:A:144:LEU:CD2	2.37	0.54
1:B:379:LEU:HD13	1:B:391:ASN:ND2	2.22	0.54
1:B:44:ARG:HD3	1:B:73:LEU:HB2	1.89	0.54
1:B:148:ILE:HB	1:B:182:ILE:HD13	1.90	0.54
1:B:29:TYR:CD1	1:B:43:GLU:HG3	2.43	0.53
1:A:262:ILE:HD12	1:A:262:ILE:H	1.74	0.53
1:B:168:ASN:HD22	1:B:168:ASN:N	2.07	0.53
1:B:92:ARG:HA	1:B:370:ILE:HG23	1.90	0.52
1:B:9:ASN:C	1:B:9:ASN:HD22	2.17	0.52
1:A:403:LEU:HD22	1:A:407:ILE:HD11	1.92	0.51
1:A:182:ILE:HD12	1:A:182:ILE:N	2.25	0.51
1:B:385:GLY:HA2	1:B:391:ASN:ND2	2.25	0.51
1:A:33:ASN:HB2	1:A:39:TRP:CH2	2.46	0.51
1:A:119:PRO:HG2	1:A:122:GLN:HG2	1.93	0.51
1:A:158:GLU:O	2:A:602:CL:CL	2.66	0.51
1:A:375:ASN:HB3	1:A:380:LYS:HA	1.93	0.51
1:A:400:GLY:HA2	1:A:403:LEU:HD12	1.93	0.50
1:A:378:ASN:ND2	1:A:384:ARG:HH12	2.09	0.50
1:A:50:THR:HG22	1:A:51:PRO:HD2	1.93	0.50
1:B:118:THR:HG21	1:B:124:HIS:CD2	2.47	0.50
1:B:394:ILE:HG13	1:B:395:ILE:CD1	2.42	0.50
1:A:80:ASP:CG	1:A:84:LYS:HZ3	2.19	0.50
1:B:409:ARG:HH11	1:B:409:ARG:N	2.10	0.49
1:B:210:MET:HE1	1:B:342:PHE:CD2	2.47	0.49
1:A:182:ILE:HG23	3:A:693:HOH:O	2.12	0.49
1:B:14:ASP:OD1	1:B:135:PHE:HB3	2.12	0.49
1:A:377:ASN:O	1:A:380:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASN:HD22	1:B:10:ASP:N	2.11	0.49
1:A:6:PHE:CD2	1:A:32:PHE:HB3	2.48	0.49
1:B:73:LEU:HD21	1:B:82:PHE:HB2	1.95	0.49
1:B:395:ILE:HD12	1:B:395:ILE:H	1.78	0.49
1:A:7:ASN:HB2	1:A:10:ASP:OD1	2.13	0.49
1:B:163:ASN:HD22	1:B:224:LYS:NZ	2.11	0.49
1:A:251:PHE:HB2	1:A:262:ILE:HD11	1.95	0.48
1:B:251:PHE:HB3	1:B:258:ASP:O	2.13	0.48
1:B:129:SER:O	1:B:144:LEU:HD13	2.13	0.48
1:B:322:LYS:O	1:B:326:ILE:HG13	2.12	0.48
1:A:284:LYS:HD2	3:A:744:HOH:O	2.14	0.48
1:B:190:SER:HB3	1:B:359:LEU:HD21	1.96	0.48
1:B:232:ILE:O	1:B:233:THR:O	2.32	0.48
1:B:226:ILE:CG2	1:B:270:ILE:HD13	2.44	0.48
1:A:409:ARG:HA	1:A:409:ARG:HD3	1.71	0.47
1:B:309:ASP:O	1:B:316:TYR:HA	2.14	0.47
1:B:163:ASN:ND2	1:B:219:GLY:HA3	2.29	0.47
1:B:7:ASN:HB2	1:B:10:ASP:OD1	2.15	0.47
1:B:2:LYS:HD3	1:B:2:LYS:N	2.27	0.47
1:B:20:ILE:HG12	1:B:133:ILE:HG22	1.96	0.47
1:B:163:ASN:ND2	1:B:224:LYS:NZ	2.63	0.47
1:A:262:ILE:HD12	1:A:262:ILE:N	2.29	0.47
1:A:174:ASN:ND2	1:A:224:LYS:C	2.74	0.46
1:A:180:ILE:HG22	1:A:182:ILE:HD12	1.97	0.46
1:A:43:GLU:OE2	1:A:79:LYS:NZ	2.47	0.46
1:A:307:GLY:HA2	3:A:687:HOH:O	2.16	0.46
1:A:370:ILE:HG12	3:A:673:HOH:O	2.14	0.46
1:B:42:PRO:O	1:B:79:LYS:HG2	2.15	0.46
1:B:381:VAL:HG11	1:B:384:ARG:HH21	1.79	0.46
1:A:255:GLY:O	1:A:258:ASP:HB2	2.16	0.46
1:B:98:SER:OG	1:B:341:LYS:HD3	2.16	0.46
1:B:231:THR:HG22	1:B:247:ASN:HA	1.96	0.46
1:B:391:ASN:N	1:B:392:PRO:HD3	2.30	0.46
1:A:9:ASN:O	1:A:10:ASP:C	2.58	0.46
1:A:251:PHE:CZ	1:A:351:ILE:HD11	2.51	0.46
1:A:261:ILE:H	1:A:261:ILE:CD1	2.28	0.46
1:A:163:ASN:OD1	1:A:219:GLY:HA3	2.15	0.45
1:B:29:TYR:CG	1:B:43:GLU:HG3	2.51	0.45
1:A:105:GLU:OE1	1:A:329:LYS:HD2	2.15	0.45
1:B:26:GLN:HG2	3:B:718:HOH:O	2.15	0.45
1:B:110:ASN:O	1:B:305:LYS:NZ	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:SER:HB2	1:B:155:ASP:CG	2.41	0.45
1:B:105:GLU:CD	1:B:329:LYS:HD2	2.41	0.45
1:B:403:LEU:O	1:B:407:ILE:HG13	2.17	0.45
1:A:195:ASP:CG	1:A:199:ASN:HB2	2.41	0.45
1:B:153:GLU:HB2	1:B:154:PRO:HD2	1.99	0.45
1:B:399:THR:C	1:B:401:ARG:H	2.25	0.45
1:B:403:LEU:O	1:B:406:LYS:HB2	2.16	0.45
1:B:194:ASN:HA	1:B:199:ASN:O	2.17	0.45
1:A:71:ASN:O	1:A:74:GLN:HG2	2.16	0.44
1:B:328:LYS:NZ	1:B:328:LYS:HB3	2.32	0.44
1:A:153:GLU:CB	1:A:154:PRO:CD	2.95	0.44
1:A:194:ASN:HA	1:A:199:ASN:O	2.17	0.44
1:B:159:THR:HA	1:B:184:THR:O	2.17	0.44
1:B:178:GLY:HA3	1:B:220:LEU:O	2.16	0.44
1:B:21:LYS:HB2	1:B:28:PHE:CE1	2.52	0.44
1:A:130:ALA:HB2	1:A:144:LEU:HD23	1.99	0.44
1:A:167:ARG:H	1:A:167:ARG:HG3	1.61	0.44
1:B:21:LYS:HB2	1:B:28:PHE:CD1	2.52	0.44
1:A:61:LYS:HG2	1:A:61:LYS:O	2.18	0.44
1:B:232:ILE:HD11	1:B:251:PHE:CE1	2.53	0.44
1:A:88:LYS:HG3	1:A:370:ILE:CD1	2.48	0.44
1:A:261:ILE:N	1:A:261:ILE:CD1	2.81	0.44
1:B:127:ASP:O	1:B:164:ILE:HG21	2.17	0.44
1:A:164:ILE:HD11	1:A:182:ILE:HD11	2.00	0.44
1:A:364:ASN:OD1	1:A:366:SER:HB2	2.18	0.44
1:B:195:ASP:OD1	1:B:199:ASN:HB2	2.18	0.44
1:B:163:ASN:ND2	1:B:224:LYS:HZ1	2.16	0.43
1:A:378:ASN:C	1:A:380:LYS:H	2.26	0.43
1:B:345:LYS:HB2	1:B:383:PHE:CD2	2.53	0.43
1:A:409:ARG:C	3:A:697:HOH:O	2.61	0.43
1:A:297:PRO:HB2	1:B:297:PRO:HB2	2.01	0.43
1:B:168:ASN:N	1:B:168:ASN:ND2	2.66	0.43
1:B:232:ILE:N	1:B:232:ILE:HD13	2.34	0.43
1:A:181:ALA:C	1:A:182:ILE:HD12	2.43	0.43
1:A:226:ILE:CG2	1:A:270:ILE:HD13	2.49	0.43
1:B:246:THR:OG1	1:B:351:ILE:HD11	2.19	0.43
1:B:295:LEU:O	1:B:298:TYR:HB2	2.19	0.43
1:B:174:ASN:HB3	1:B:225:GLY:HA2	2.01	0.42
1:A:105:GLU:OE2	1:A:329:LYS:HD2	2.18	0.42
1:B:280:LYS:O	1:B:280:LYS:HD3	2.19	0.42
1:B:381:VAL:HG11	1:B:384:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:TYR:O	1:A:133:ILE:HA	2.20	0.42
1:A:396:THR:HG22	3:A:663:HOH:O	2.18	0.42
1:B:110:ASN:HA	1:B:111:PRO:HD3	1.93	0.42
1:B:277:ASP:O	1:B:281:ILE:HG13	2.18	0.42
1:B:364:ASN:HB3	1:B:367:ILE:HD12	2.00	0.42
1:A:379:LEU:HB3	1:A:385:GLY:CA	2.48	0.42
1:A:405:LYS:HB3	1:A:405:LYS:HE2	1.70	0.42
1:B:163:ASN:HB3	1:B:179:SER:OG	2.20	0.42
1:B:120:ASP:OD1	1:B:284:LYS:HG2	2.20	0.42
1:B:403:LEU:O	1:B:403:LEU:HD22	2.18	0.42
1:A:180:ILE:HG22	1:A:182:ILE:CD1	2.49	0.42
1:B:210:MET:HE1	1:B:342:PHE:CE2	2.55	0.42
1:B:369:ASN:O	1:B:373:GLY:HA2	2.20	0.42
1:A:88:LYS:HG3	1:A:370:ILE:HD11	2.01	0.42
1:A:402:GLY:O	1:A:406:LYS:HD3	2.20	0.42
1:A:55:HIS:HA	1:A:56:PRO:HD3	1.90	0.42
1:A:410:PHE:N	3:A:697:HOH:O	2.52	0.42
1:B:9:ASN:C	1:B:9:ASN:ND2	2.78	0.42
1:A:82:PHE:O	1:A:86:VAL:HG23	2.21	0.41
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.85	0.41
1:A:95:ASN:HA	3:A:659:HOH:O	2.18	0.41
1:B:188:GLU:HB2	3:B:626:HOH:O	2.20	0.41
1:A:280:LYS:HA	1:A:280:LYS:HE2	2.02	0.41
1:B:213:LEU:HD23	1:B:213:LEU:HA	1.94	0.41
1:A:50:THR:CG2	1:A:51:PRO:HD2	2.51	0.41
1:A:158:GLU:HB2	2:A:602:CL:CL	2.58	0.41
1:A:8:TYR:HB2	1:A:80:ASP:HA	2.03	0.41
1:A:60:LEU:N	1:A:60:LEU:HD12	2.36	0.41
1:A:294:LEU:HD13	1:B:295:LEU:HD11	2.03	0.41
1:B:201:PHE:HA	1:B:386:GLN:O	2.21	0.41
1:B:381:VAL:HB	1:B:384:ARG:CZ	2.51	0.41
1:B:409:ARG:HH11	1:B:409:ARG:H	1.69	0.41
1:A:32:PHE:CD2	1:A:32:PHE:N	2.89	0.40
1:B:121:ASN:HB3	3:B:664:HOH:O	2.20	0.40
1:A:96:ASN:HB3	1:A:342:PHE:CZ	2.56	0.40
1:A:203:GLN:HE22	1:A:335:GLN:NE2	2.19	0.40
1:A:167:ARG:HD2	3:A:710:HOH:O	2.21	0.40
1:A:326:ILE:HA	1:A:329:LYS:HE3	2.03	0.40
1:A:296:ASN:N	1:A:297:PRO:CD	2.85	0.40
1:A:375:ASN:HD22	1:A:385:GLY:HA3	1.86	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	396/420 (94%)	373 (94%)	19 (5%)	4 (1%)	12	28
1	B	381/420 (91%)	351 (92%)	28 (7%)	2 (0%)	24	46
All	All	777/840 (92%)	724 (93%)	47 (6%)	6 (1%)	16	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ARG
1	A	361	ASN
1	A	379	LEU
1	B	361	ASN
1	A	51	PRO
1	B	153	GLU

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	361/380 (95%)	349 (97%)	12 (3%)	33	61
1	B	349/380 (92%)	328 (94%)	21 (6%)	17	37
All	All	710/760 (93%)	677 (95%)	33 (5%)	24	49

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	167	ARG
1	A	261	ILE
1	A	268	ASN
1	A	279	LYS
1	A	280	LYS
1	A	295	LEU
1	A	298	TYR
1	A	353	GLN
1	A	384	ARG
1	A	403	LEU
1	A	404	VAL
1	B	2	LYS
1	B	9	ASN
1	B	18	LEU
1	B	46	VAL
1	B	76	ASP
1	B	77	GLU
1	B	122	GLN
1	B	159	THR
1	B	167	ARG
1	B	171	MET
1	B	232	ILE
1	B	233	THR
1	B	298	TYR
1	B	328	LYS
1	B	343	GLN
1	B	389	ASN
1	B	390	LEU
1	B	395	ILE
1	B	401	ARG
1	B	405	LYS
1	B	409	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	71	ASN
1	A	117	ASN
1	A	121	ASN
1	A	140	GLN
1	A	174	ASN

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Mol	Chain	Res	Type
1	A	175	HIS
1	A	194	ASN
1	A	199	ASN
1	A	296	ASN
1	A	335	GLN
1	A	353	GLN
1	A	375	ASN
1	A	378	ASN
1	A	389	ASN
1	B	9	ASN
1	B	71	ASN
1	B	95	ASN
1	B	124	HIS
1	B	163	ASN
1	B	168	ASN
1	B	174	ASN
1	B	260	ASN
1	B	296	ASN
1	B	335	GLN
1	B	348	GLN
1	B	375	ASN
1	B	377	ASN
1	B	378	ASN
1	B	382	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 8 ligands modelled in this entry, 8 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	400/420 (95%)	-0.26	9 (2%) 61 55	13, 29, 50, 72	0
1	B	387/420 (92%)	0.13	14 (3%) 46 40	17, 38, 64, 90	0
All	All	787/840 (93%)	-0.07	23 (2%) 53 48	13, 33, 60, 90	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	THR	5.2
1	B	245	GLY	3.6
1	B	54	PHE	3.3
1	A	167	ARG	3.2
1	B	393	ARG	3.0
1	A	196	ASN	2.9
1	B	66	SER	2.9
1	A	245	GLY	2.7
1	A	233	THR	2.6
1	B	351	ILE	2.5
1	B	122	GLN	2.5
1	B	409	ARG	2.4
1	A	411	CYS	2.4
1	A	57	PRO	2.4
1	A	409	ARG	2.3
1	A	168	ASN	2.3
1	B	168	ASN	2.3
1	B	401	ARG	2.2
1	A	169	ASN	2.2
1	B	261	ILE	2.1
1	B	26	GLN	2.0
1	B	52	GLN	2.0
1	B	352	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
2	CL	A	601	1/1	0.95	0.11	35,35,35,35	0
2	CL	A	602	1/1	0.96	0.25	63,63,63,63	0
2	CL	A	607	1/1	0.96	0.12	34,34,34,34	0
2	CL	A	605	1/1	0.97	0.11	19,19,19,19	0
2	CL	A	609	1/1	0.97	0.06	38,38,38,38	0
2	CL	B	606	1/1	0.97	0.11	28,28,28,28	0
2	CL	B	608	1/1	0.98	0.04	35,35,35,35	0
2	CL	A	604	1/1	0.99	0.03	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.