



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:21 PM UTC

PDB ID : 5BQN / pdb_00005bqn
Title : Crystal structure of the LHn fragment of botulinum neurotoxin type D, mutant H233Y E230Q
Authors : Masuyer, G.; Davies, J.R.; Moore, K.; Chaddock, J.A.; Acharya, K.R.
Deposited on : 2015-05-29
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

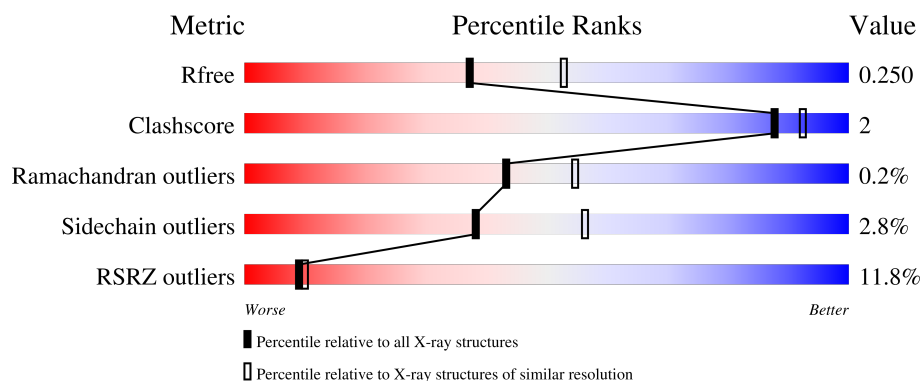
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	885	11% 87% 7% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6920 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 D, Botulinum neurotoxin type D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	838	Total	C	N	O	S	0	2	0
			6708	4301	1091	1298	18			

There are 37 discrepancies between the modelled and reference sequences:

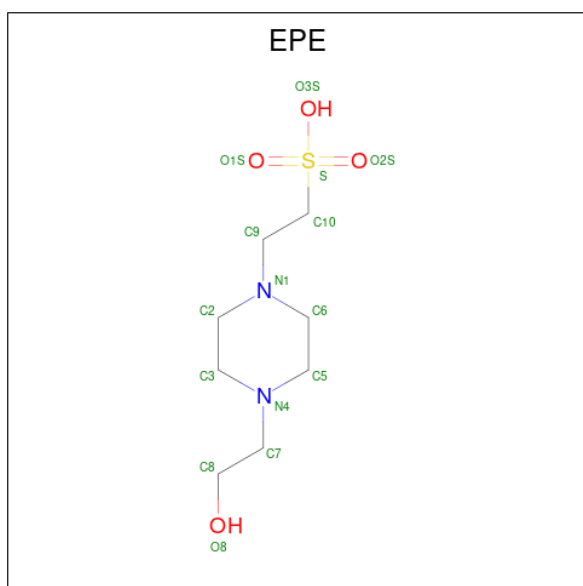
Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLN	GLU	conflict	UNP P19321
A	233	TYR	HIS	conflict	UNP P19321
A	438	VAL	-	linker	UNP P19321
A	439	ASP	-	linker	UNP P19321
A	440	LYS	-	linker	UNP P19321
A	441	SER	-	linker	UNP P19321
A	442	GLU	-	linker	UNP P19321
A	443	GLU	-	linker	UNP P19321
A	444	LYS	-	linker	UNP P19321
A	445	LEU	-	linker	UNP P19321
A	446	TYR	-	linker	UNP P19321
A	447	ASP	-	linker	UNP P19321
A	448	ASP	-	linker	UNP P19321
A	449	ASP	-	linker	UNP P19321
A	450	ASP	-	linker	UNP P19321
A	451	LYS	-	linker	UNP P19321
A	452	ASP	-	linker	UNP P19321
A	453	ARG	-	linker	UNP P19321
A	454	TRP	-	linker	UNP P19321
A	455	GLY	-	linker	UNP P19321
A	456	SER	-	linker	UNP P19321
A	457	SER	-	linker	UNP P19321
A	458	LEU	-	linker	UNP P19321
A	459	GLN	-	linker	UNP P19321
A	873	LEU	-	expression tag	UNP P19321
A	874	GLU	-	expression tag	UNP P19321
A	875	ALA	-	expression tag	UNP P19321

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Chain	Residue	Modelled	Actual	Comment	Reference
A	876	HIS	-	expression tag	UNP P19321
A	877	HIS	-	expression tag	UNP P19321
A	878	HIS	-	expression tag	UNP P19321
A	879	HIS	-	expression tag	UNP P19321
A	880	HIS	-	expression tag	UNP P19321
A	881	HIS	-	expression tag	UNP P19321
A	882	HIS	-	expression tag	UNP P19321
A	883	HIS	-	expression tag	UNP P19321
A	884	HIS	-	expression tag	UNP P19321
A	885	HIS	-	expression tag	UNP P19321

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

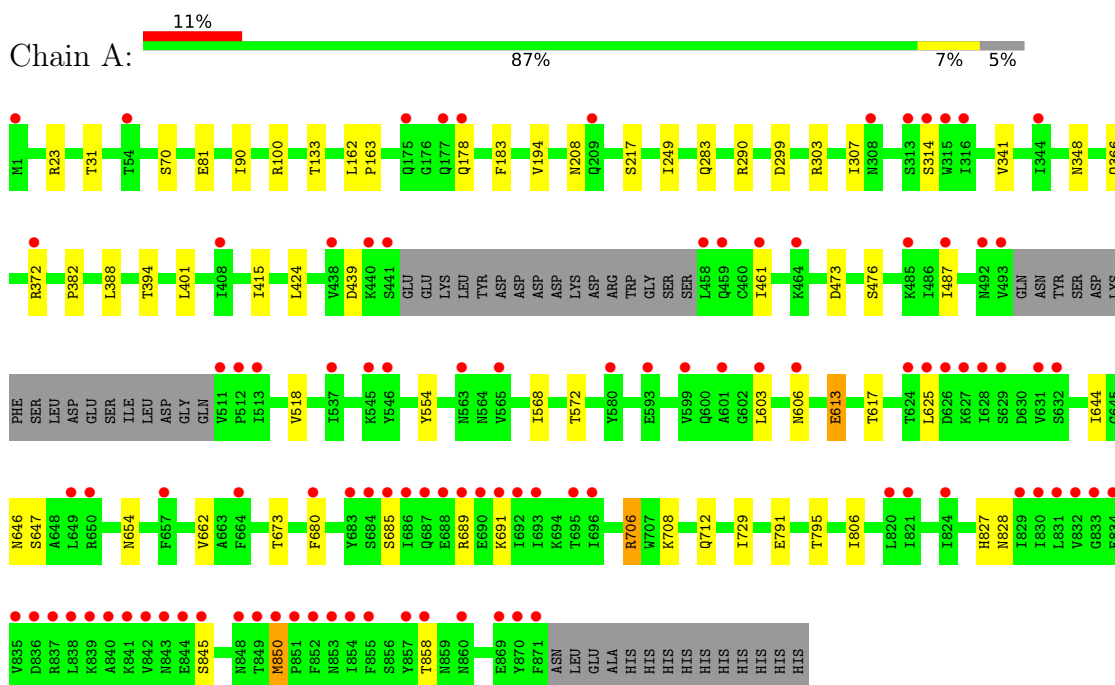
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total	O	0	0
			197	197		

3 Residue-property plots [i](#)

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 D,Botulinum neurotoxin type D



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	173.54Å 173.54Å 222.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	150.00 – 2.30 150.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (150.00-2.30) 98.4 (150.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.220 , 0.247 0.225 , 0.250	Depositor DCC
R_{free} test set	4277 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6920	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: EPE

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	0.78	0/6858	0.96	5/9318 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	806	ILE	N-CA-CB	5.88	117.43	110.55
1	A	706	ARG	N-CA-C	5.79	117.67	111.36
1	A	70	SER	N-CA-C	5.58	118.32	109.50
1	A	568	ILE	N-CA-C	5.43	117.00	109.45
1	A	662	VAL	N-CA-C	5.21	116.56	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	691	LYS	Peptide

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	6708	0	6548	26	0
2	A	15	0	18	0	0
3	A	197	0	0	1	0
All	All	6920	0	6566	26	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 2.

All (26) 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:382:PRO:HG2	1:A:424:LEU:HD12	1.73	0.71
1:A:249:ILE:HA	1:A:476:SER:OG	1.96	0.65
1:A:487:ILE:HD11	1:A:680:PHE:CD1	2.33	0.64
1:A:283:GLN:HE21	1:A:712:GLN:HE22	1.46	0.63
1:A:372[A]:ARG:HB2	1:A:372[A]:ARG:HH11	1.66	0.61
1:A:487:ILE:HD11	1:A:680:PHE:CG	2.38	0.58
1:A:290:ARG:HH11	1:A:348:ASN:HD22	1.53	0.55
1:A:461:ILE:HD12	1:A:554:TYR:CD1	2.42	0.55
1:A:461:ILE:HD12	1:A:554:TYR:CE1	2.45	0.51
1:A:473:ASP:O	1:A:476:SER:HB3	2.12	0.50
1:A:372[A]:ARG:HH11	1:A:372[A]:ARG:CB	2.26	0.49
1:A:133:THR:HG22	1:A:178:GLN:HG2	1.94	0.48
1:A:613:GLU:O	1:A:617:THR:HG22	2.13	0.48
1:A:644:ILE:O	1:A:647:SER:HB2	2.17	0.45
1:A:100:ARG:HD2	1:A:366:GLN:O	2.18	0.44
1:A:791:GLU:O	1:A:795:THR:HG23	2.19	0.43
1:A:23:ARG:NH1	1:A:31:THR:O	2.51	0.42
1:A:299:ASP:HB3	3:A:1039:HOH:O	2.18	0.42
1:A:850:MET:HE3	1:A:850:MET:HB3	1.94	0.42
1:A:603:LEU:HB2	1:A:606:ASN:HD22	1.85	0.41
1:A:303:ARG:O	1:A:307:ILE:HG13	2.21	0.41
1:A:394:THR:HG23	1:A:401:LEU:HD21	2.03	0.41
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.96	0.40
1:A:685:SER:O	1:A:827:HIS:NE2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LYS:HE3	1:A:858:THR:HG21	2.03	0.40
1:A:162:LEU:HB3	1:A:163:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	834/885 (94%)	803 (96%)	29 (4%)	2 (0%)	43 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ASP
1	A	689	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	754/823 (92%)	733 (97%)	21 (3%)	38 56

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	90	ILE
1	A	183	PHE
1	A	194	VAL
1	A	208	ASN
1	A	217	SER
1	A	314	SER
1	A	341	VAL
1	A	415	ILE
1	A	518	VAL
1	A	572	THR
1	A	613	GLU
1	A	625	LEU
1	A	646	ASN
1	A	654	ASN
1	A	673	THR
1	A	706	ARG
1	A	729	ILE
1	A	828	ASN
1	A	845	SER
1	A	850	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	283	GLN
1	A	296	HIS
1	A	348	ASN
1	A	356	ASN
1	A	466	ASN
1	A	582	ASN
1	A	606	ASN
1	A	654	ASN
1	A	717	ASN
1	A	766	GLN
1	A	783	ASN
1	A	786	ASN
1	A	859	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EPE	A	901	-	15,15,15	1.65	1 (6%)	19,20,20	4.50	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	A	901	-	-	2/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	EPE	C10-S	-5.97	1.69	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	901	EPE	O3S-S-C10	-12.56	81.43	106.00
2	A	901	EPE	O2S-S-C10	-11.09	89.97	106.73
2	A	901	EPE	O1S-S-C10	-8.12	94.45	106.73
2	A	901	EPE	O3S-S-O2S	3.56	120.30	111.40
2	A	901	EPE	O3S-S-O1S	3.39	119.89	111.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	EPE	C10-C9-N1-C2
2	A	901	EPE	C10-C9-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	838/885 (94%)	0.72	99 (11%) 9 10	32, 73, 128, 182	2 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	871	PHE	10.0
1	A	511	VAL	7.7
1	A	1	MET	6.8
1	A	838	LEU	6.8
1	A	870	TYR	6.5
1	A	842	VAL	6.4
1	A	843	ASN	6.3
1	A	512	PRO	6.2
1	A	835	VAL	5.6
1	A	440	LYS	5.5
1	A	493	VAL	5.5
1	A	829	ILE	5.3
1	A	687	GLN	5.3
1	A	692	ILE	5.3
1	A	686	ILE	5.2
1	A	840	ALA	5.1
1	A	438	VAL	4.8
1	A	684	SER	4.7
1	A	848	ASN	4.6
1	A	565	VAL	4.6
1	A	831	LEU	4.5
1	A	458	LEU	4.2
1	A	625	LEU	4.2
1	A	441	SER	4.1
1	A	854	ILE	4.1
1	A	850	MET	4.1
1	A	408	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	372[A]	ARG	3.8
1	A	849	THR	3.8
1	A	628	ILE	3.7
1	A	178	GLN	3.7
1	A	832	VAL	3.7
1	A	830	ILE	3.6
1	A	513	ILE	3.6
1	A	845	SER	3.5
1	A	841	LYS	3.5
1	A	688	GLU	3.5
1	A	869	GLU	3.4
1	A	691	LYS	3.4
1	A	175	GLN	3.3
1	A	685	SER	3.3
1	A	627	LYS	3.2
1	A	855	PHE	3.1
1	A	632	SER	3.1
1	A	857	TYR	3.0
1	A	690	GLU	3.0
1	A	650	ARG	2.9
1	A	833	GLY	2.9
1	A	858	THR	2.9
1	A	492	ASN	2.9
1	A	563	ASN	2.9
1	A	836	ASP	2.9
1	A	852	PHE	2.9
1	A	624	THR	2.9
1	A	851	PRO	2.8
1	A	629	SER	2.8
1	A	487	ILE	2.7
1	A	689	ARG	2.7
1	A	315	TRP	2.7
1	A	839	LYS	2.6
1	A	631	VAL	2.6
1	A	314	SER	2.6
1	A	693	ILE	2.6
1	A	649	LEU	2.6
1	A	599	VAL	2.5
1	A	683	TYR	2.5
1	A	834	GLU	2.5
1	A	820	LEU	2.5
1	A	601	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	844	GLU	2.4
1	A	821	ILE	2.4
1	A	664	PHE	2.4
1	A	177	GLN	2.3
1	A	209	GLN	2.3
1	A	459	GLN	2.3
1	A	580	TYR	2.3
1	A	485	LYS	2.3
1	A	461	ILE	2.2
1	A	696	ILE	2.2
1	A	824	ILE	2.2
1	A	545	LYS	2.2
1	A	593	GLU	2.2
1	A	680	PHE	2.1
1	A	54	THR	2.1
1	A	626	ASP	2.1
1	A	860	ASN	2.1
1	A	837	ARG	2.1
1	A	313	SER	2.1
1	A	603	LEU	2.1
1	A	344	ILE	2.1
1	A	537	ILE	2.1
1	A	606	ASN	2.1
1	A	546	TYR	2.1
1	A	308	ASN	2.0
1	A	853	ASN	2.0
1	A	657	PHE	2.0
1	A	695	THR	2.0
1	A	316	ILE	2.0
1	A	464	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	EPE	A	901	15/15	0.82	0.27	114,119,127,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.