



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:42 PM UTC

PDB ID : 5VID / pdb_00005vid
Title : Receptor binding domain of BoNT/B in complex with mini-protein binder Bot.0671.2
Authors : Jin, R.; Lam, K.; Yao, G.
Deposited on : 2017-04-15
Resolution : 2.75 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

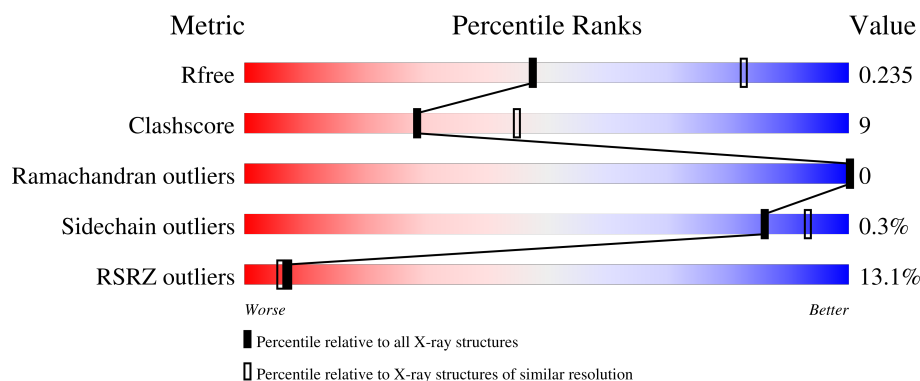
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	438	11% 78% 16% 5%
1	B	438	9% 75% 18% 6%
1	C	438	10% 78% 19% .
1	D	438	7% 79% 16% .
1	E	438	17% 73% 19% 8%

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Mol	Chain	Length	Quality of chain
2	F	66	17% 44% 15% 39%
2	G	66	21% 36% 21% 41%
2	H	66	32% 44% 12% 44%
2	I	66	14% 47% 12% 41%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19064 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 B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	420	Total	C	N	O	S	0	2	0
			3596	2326	587	675	8			
1	B	412	Total	C	N	O	S	0	1	0
			3527	2278	578	663	8			
1	C	426	Total	C	N	O	S	0	2	0
			3631	2342	596	685	8			
1	A	415	Total	C	N	O	S	0	2	0
			3543	2294	577	664	8			
1	E	405	Total	C	N	O	S	0	2	0
			3442	2233	560	641	8			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	854	GLY	-	expression tag	UNP P10844
D	855	PRO	-	expression tag	UNP P10844
D	856	LEU	-	expression tag	UNP P10844
D	857	GLY	-	expression tag	UNP P10844
D	858	SER	-	expression tag	UNP P10844
B	854	GLY	-	expression tag	UNP P10844
B	855	PRO	-	expression tag	UNP P10844
B	856	LEU	-	expression tag	UNP P10844
B	857	GLY	-	expression tag	UNP P10844
B	858	SER	-	expression tag	UNP P10844
C	854	GLY	-	expression tag	UNP P10844
C	855	PRO	-	expression tag	UNP P10844
C	856	LEU	-	expression tag	UNP P10844
C	857	GLY	-	expression tag	UNP P10844
C	858	SER	-	expression tag	UNP P10844
A	854	GLY	-	expression tag	UNP P10844
A	855	PRO	-	expression tag	UNP P10844
A	856	LEU	-	expression tag	UNP P10844
A	857	GLY	-	expression tag	UNP P10844

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Chain	Residue	Modelled	Actual	Comment	Reference
A	858	SER	-	expression tag	UNP P10844
E	854	GLY	-	expression tag	UNP P10844
E	855	PRO	-	expression tag	UNP P10844
E	856	LEU	-	expression tag	UNP P10844
E	857	GLY	-	expression tag	UNP P10844
E	858	SER	-	expression tag	UNP P10844

- Molecule 2 is a protein called Bot.0671.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	40	Total	C	N	O	S	0	1	0
			336	213	60	62	1			
2	G	39	Total	C	N	O		0	0	0
			318	202	59	57				
2	H	37	Total	C	N	O		0	0	0
			282	180	50	52				
2	I	39	Total	C	N	O		0	0	0
			315	198	59	58				

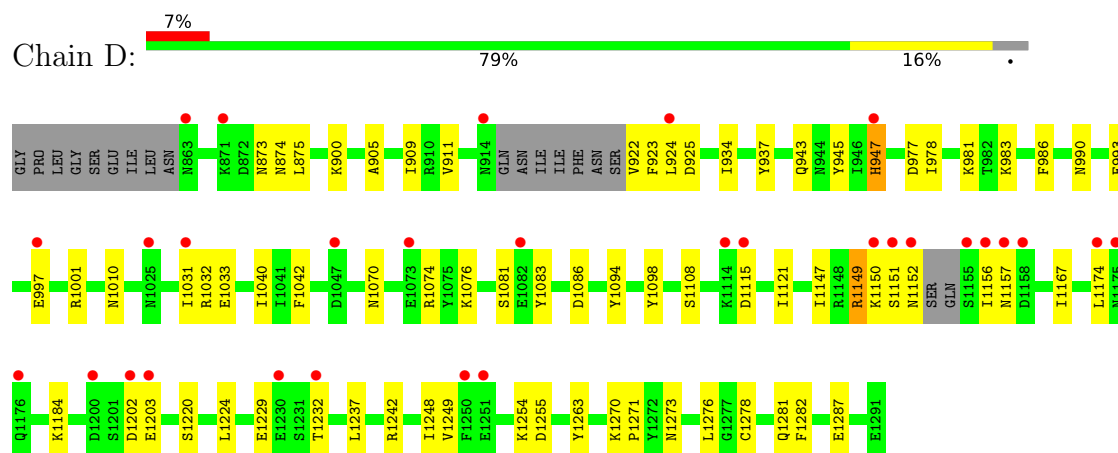
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	25	Total	O	0	0
			25	25		
3	B	11	Total	O	0	0
			11	11		
3	C	15	Total	O	0	0
			15	15		
3	A	22	Total	O	0	0
			22	22		
3	E	1	Total	O	0	0
			1	1		

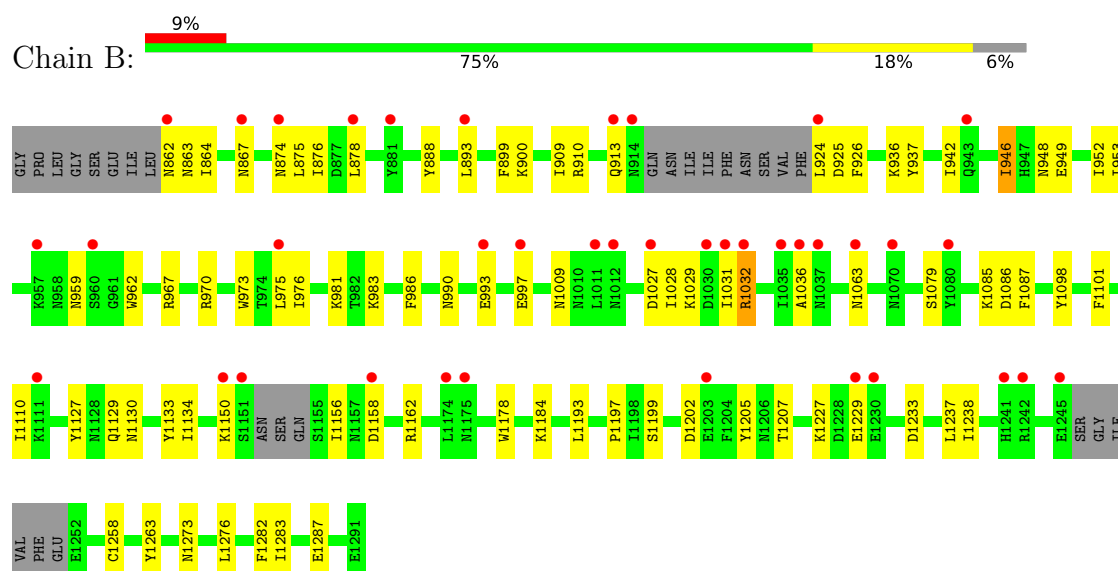
3 Residue-property plots [i](#)

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.

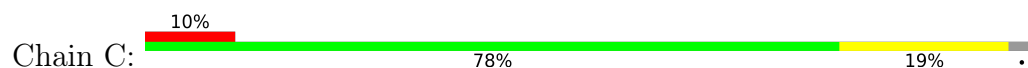
• Molecule 1: Botulinum neurotoxin type B

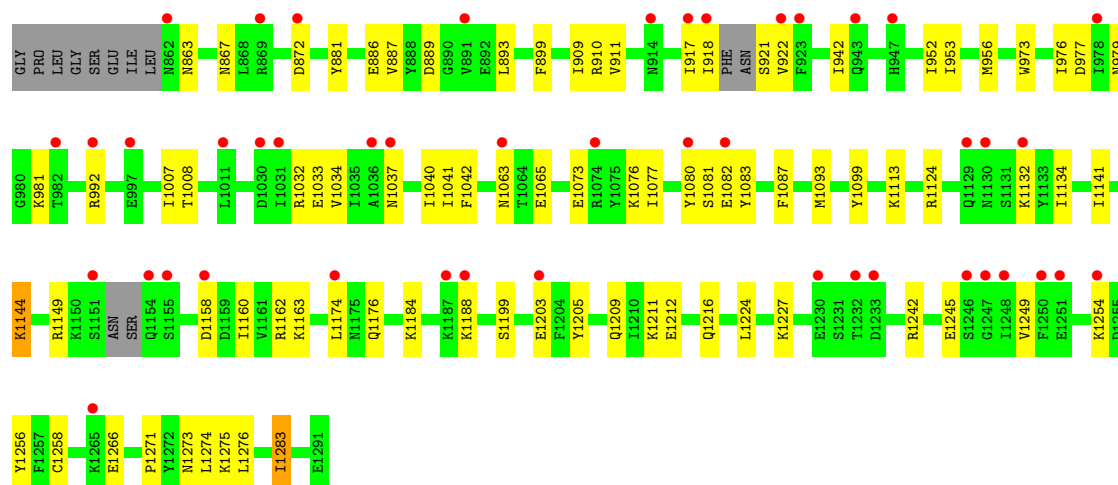


• Molecule 1: Botulinum neurotoxin type B

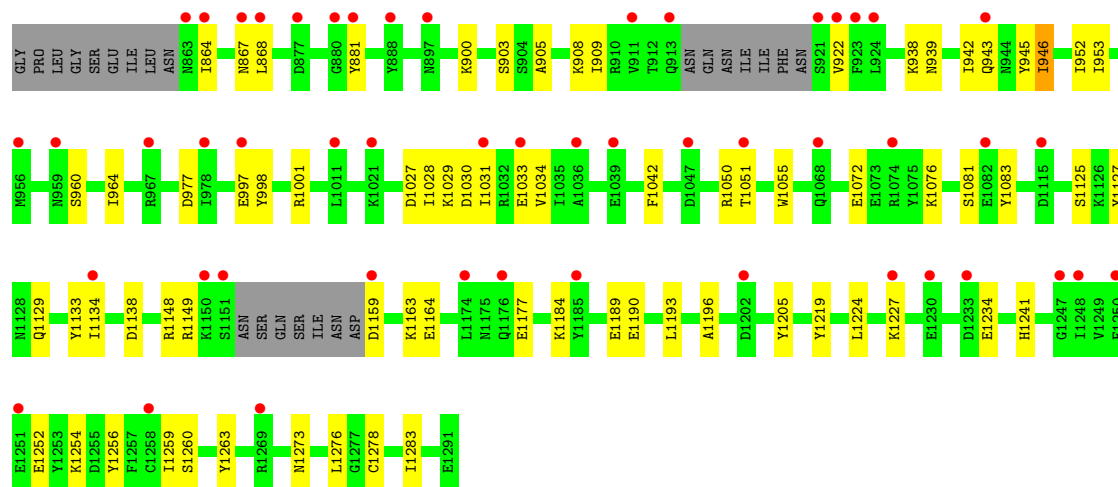
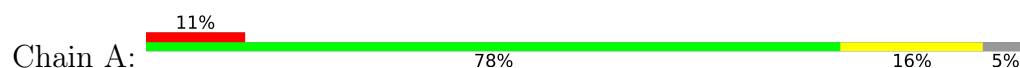


• Molecule 1: Botulinum neurotoxin type B

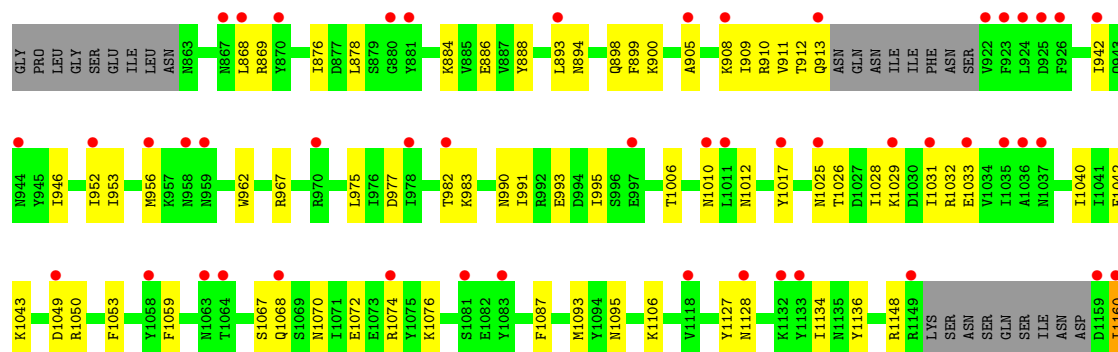
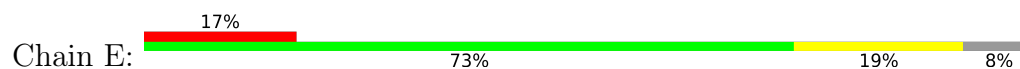




• Molecule 1: Botulinum neurotoxin type B

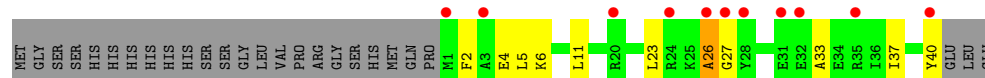


• Molecule 1: Botulinum neurotoxin type B

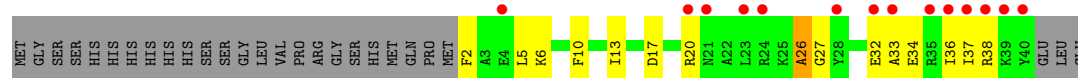
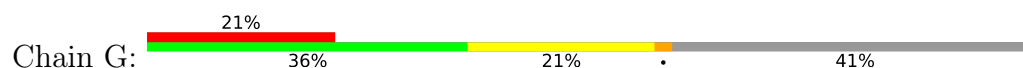




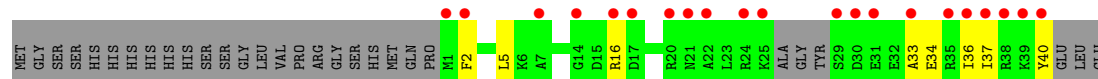
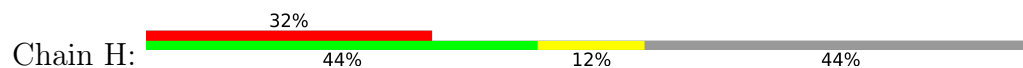
• Molecule 2: Bot.0671.2



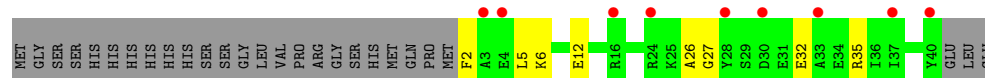
• Molecule 2: Bot.0671.2



• Molecule 2: Bot.0671.2



• Molecule 2: Bot.0671.2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	140.89Å 87.31Å 148.46Å 90.00° 114.53° 90.00°	Depositor
Resolution (Å)	67.53 – 2.75 67.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (67.53-2.75) 99.9 (67.53-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.219 , 0.232 0.223 , 0.235	Depositor DCC
R_{free} test set	4279 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19064	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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

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	0.61	0/3627	0.92	4/4888 (0.1%)
1	B	0.61	1/3609 (0.0%)	0.93	9/4861 (0.2%)
1	C	0.59	0/3714	0.95	6/5006 (0.1%)
1	D	0.72	0/3681	0.96	5/4960 (0.1%)
1	E	0.42	0/3524	0.86	4/4753 (0.1%)
2	F	0.55	0/343	0.96	1/454 (0.2%)
2	G	0.50	0/322	0.92	1/427 (0.2%)
2	H	0.59	0/284	0.96	0/378
2	I	0.47	0/318	0.92	0/421
All	All	0.59	1/19422 (0.0%)	0.93	30/26148 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	981	LYS	CA-C	5.76	1.60	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	947	HIS	N-CA-C	8.52	120.65	111.36
1	E	1128	ASN	N-CA-C	7.08	118.79	111.14
1	C	1188	LYS	N-CA-C	-6.75	101.03	110.35
1	B	1130	ASN	N-CA-C	6.39	120.72	112.41
1	B	1032	ARG	CB-CA-C	-6.36	107.18	116.53
2	F	26	ALA	N-CA-C	6.33	118.17	111.28
1	C	1266	GLU	N-CA-C	6.30	119.13	111.82
1	C	1283	ILE	CA-C-N	6.20	126.38	120.31
1	C	1283	ILE	C-N-CA	6.20	126.38	120.31
1	B	1156	ILE	N-CA-C	6.15	116.97	107.99
1	A	946	ILE	N-CA-C	6.06	116.84	110.72
1	D	934	ILE	CA-C-N	5.98	125.89	119.85
1	D	934	ILE	C-N-CA	5.98	125.89	119.85
1	B	1110	ILE	CB-CA-C	-5.88	103.62	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	26	ALA	N-CA-C	5.82	117.63	111.28
1	B	1258	CYS	N-CA-C	5.77	117.74	109.14
1	B	946	ILE	N-CA-C	5.68	116.46	110.72
1	A	1196	ALA	N-CA-C	5.63	113.08	108.07
1	B	997	GLU	N-CA-C	-5.61	106.39	113.18
1	B	948	ASN	N-CA-C	5.49	117.25	108.41
1	C	1082	GLU	N-CA-C	-5.41	105.38	111.28
1	E	1160	ILE	N-CA-C	5.38	116.72	108.71
1	A	881	TYR	N-CA-C	-5.32	106.46	113.17
1	C	1258	CYS	N-CA-C	5.29	117.02	109.14
1	B	1134	ILE	N-CA-C	5.28	117.47	108.86
1	E	956	MET	N-CA-C	5.28	117.84	109.50
1	A	1283	ILE	N-CA-C	5.19	113.15	107.60
1	D	905	ALA	N-CA-C	5.17	117.66	111.71
1	E	1247	GLY	N-CA-C	-5.11	102.80	112.51
1	D	986	PHE	N-CA-C	5.09	116.92	109.24

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	3543	0	3452	71	0
1	B	3527	0	3438	58	0
1	C	3631	0	3536	68	0
1	D	3596	0	3503	61	0
1	E	3442	0	3334	64	0
2	F	336	0	339	7	0
2	G	318	0	317	8	0
2	H	282	0	267	5	0
2	I	315	0	314	6	0
3	A	22	0	0	0	0
3	B	11	0	0	0	0
3	C	15	0	0	1	0
3	D	25	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
All	All	19064	0	18500	330	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 9.

All (330) 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:1184:LYS:HE3	1:A:1205:TYR:CE1	1.82	1.13
1:D:983:LYS:HG2	1:D:1031:ILE:HD11	1.29	1.13
1:A:942:ILE:HG12	1:A:1134:ILE:HD11	1.13	1.07
1:A:942:ILE:HG12	1:A:1134:ILE:CD1	1.83	1.07
1:E:1170:ASP:OD1	1:E:1179:ARG:HG2	1.54	1.06
1:E:1249:VAL:HG12	1:E:1250:PHE:CD2	1.90	1.05
1:D:1094:TYR:CE2	1:D:1149:ARG:NH1	2.24	1.04
1:E:1249:VAL:HG12	1:E:1250:PHE:HD2	1.20	1.04
1:E:908:LYS:HE2	1:E:1043:LYS:HD2	1.40	1.03
1:A:939:ASN:O	1:A:942:ILE:HD12	1.65	0.95
1:E:1028:ILE:O	1:E:1031:ILE:HG22	1.69	0.91
1:E:977:ASP:HB2	1:E:1033:GLU:O	1.71	0.90
1:E:977:ASP:OD2	1:E:1031:ILE:O	1.90	0.88
1:A:1184:LYS:HE3	1:A:1205:TYR:CZ	2.10	0.87
1:D:983:LYS:CG	1:D:1031:ILE:HD11	2.04	0.86
1:A:942:ILE:CG1	1:A:1134:ILE:HD11	2.04	0.84
1:B:864:ILE:HD11	1:B:867:ASN:HB3	1.61	0.82
1:A:997:GLU:OE2	1:A:998:TYR:CE2	2.39	0.76
1:A:938:LYS:NZ	1:A:1051:THR:HG21	2.02	0.75
1:A:1184:LYS:CE	1:A:1205:TYR:CE1	2.67	0.74
1:A:939:ASN:O	1:A:942:ILE:CD1	2.35	0.74
1:B:983:LYS:HG3	1:B:1028:ILE:HG22	1.70	0.74
1:A:1133:TYR:HB2	1:A:1134:ILE:HD12	1.70	0.73
1:C:918:ILE:HB	1:C:1063:ASN:OD1	1.90	0.71
1:A:1273:ASN:HB3	1:A:1276:LEU:HG	1.71	0.71
1:B:1199:SER:HB3	2:H:2:PHE:CE1	2.26	0.71
1:A:1051:THR:O	1:A:1051:THR:HG22	1.89	0.71
1:C:881:TYR:CD2	1:C:917:ILE:HG22	2.25	0.70
1:E:1012:ASN:HB3	1:E:1029:LYS:HG2	1.72	0.70
1:C:1158:ASP:OD2	1:C:1162:ARG:NH2	2.24	0.70
2:I:32:GLU:HA	2:I:35:ARG:HD3	1.73	0.70
1:E:977:ASP:CB	1:E:1033:GLU:O	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1174:LEU:HD21	1:A:1050:ARG:O	1.92	0.69
1:E:1028:ILE:O	1:E:1031:ILE:CG2	2.40	0.69
1:C:1076:LYS:HE2	1:C:1216:GLN:OE1	1.93	0.69
1:C:1245:GLU:OE1	1:C:1254:LYS:HG2	1.93	0.68
1:E:995:ILE:HG13	1:E:1106:LYS:HB2	1.75	0.68
2:G:17:ASP:OD1	2:G:20:ARG:NH2	2.26	0.68
1:D:1031:ILE:HG22	1:D:1032:ARG:N	2.07	0.68
1:A:1189:GLU:HG3	1:A:1190:GLU:OE1	1.94	0.68
1:A:864:ILE:HG21	1:A:867:ASN:ND2	2.10	0.67
1:A:1125:SER:OG	1:A:1138:ASP:OD2	2.09	0.67
1:A:1149:ARG:HH21	1:A:1159:ASP:HB3	1.60	0.67
1:B:942:ILE:HG13	1:B:946:ILE:HD12	1.77	0.66
1:E:908:LYS:HE2	1:E:1043:LYS:CD	2.23	0.66
1:B:973:TRP:HE1	1:B:975:LEU:HD11	1.59	0.66
1:A:1184:LYS:HE3	1:A:1205:TYR:HE1	1.55	0.65
1:B:924:LEU:HD12	1:B:924:LEU:O	1.96	0.65
1:C:921:SER:HB2	1:C:1037:ASN:ND2	2.12	0.65
1:A:942:ILE:CG1	1:A:1134:ILE:CD1	2.70	0.65
1:E:946:ILE:O	1:E:967:ARG:NH2	2.30	0.65
1:B:990:ASN:HD22	1:B:993:GLU:HG3	1.61	0.65
1:E:1163:LYS:HG2	1:E:1164:GLU:HG2	1.79	0.65
1:D:978:ILE:HG23	1:D:1033:GLU:O	1.96	0.64
1:E:1025:ASN:HD22	1:E:1026:THR:N	1.93	0.64
1:D:1150:LYS:HG2	1:D:1229:GLU:OE2	1.98	0.63
1:D:1149:ARG:CZ	3:D:1303:HOH:O	2.47	0.62
1:B:1158:ASP:OD2	1:B:1162:ARG:NH2	2.32	0.62
1:A:938:LYS:HZ3	1:A:1051:THR:HG21	1.64	0.62
1:E:869:ARG:HB2	1:E:878:LEU:HD13	1.80	0.62
1:E:1012:ASN:CG	1:E:1029:LYS:HA	2.25	0.61
1:D:1273:ASN:HB3	1:D:1276:LEU:HG	1.83	0.61
2:H:16:ARG:NH2	2:H:34:GLU:OE2	2.34	0.61
1:C:881:TYR:CE2	1:C:917:ILE:HG22	2.37	0.60
1:D:1149:ARG:HB3	1:D:1151:SER:O	2.02	0.59
1:D:1149:ARG:HH21	1:C:1077:ILE:HG12	1.67	0.59
1:E:962:TRP:HB3	1:E:975:LEU:HD23	1.84	0.59
1:A:1027:ASP:OD1	1:A:1029:LYS:HG2	2.03	0.58
1:B:913:GLN:NE2	1:B:1036:ALA:O	2.36	0.58
1:E:876:ILE:HG13	1:E:878:LEU:CD1	2.33	0.58
1:D:937:TYR:HB3	1:D:945:TYR:CD1	2.38	0.58
1:E:884:LYS:N	1:E:912:THR:O	2.34	0.58
1:E:1049:ASP:OD1	1:E:1050:ARG:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:SER:OG	1:A:1050:ARG:HG3	2.03	0.58
1:C:979:ASN:OD1	1:C:981:LYS:NZ	2.36	0.58
2:G:26:ALA:N	2:G:27:GLY:HA2	2.17	0.58
1:D:900:LYS:NZ	1:D:1287:GLU:OE2	2.29	0.57
1:B:949:GLU:HB2	1:B:967:ARG:HE	1.68	0.57
1:D:1156:ILE:HG22	1:D:1157:ASN:N	2.18	0.57
1:B:990:ASN:ND2	1:B:993:GLU:HG3	2.18	0.57
1:C:909:ILE:HG22	1:C:910:ARG:N	2.20	0.57
1:E:1247:GLY:HA3	1:E:1252:GLU:OE1	2.05	0.57
1:E:884:LYS:HB3	1:E:912:THR:HB	1.87	0.56
1:E:1012:ASN:HB3	1:E:1029:LYS:CG	2.34	0.56
1:D:1157:ASN:CB	1:C:867:ASN:HD21	2.17	0.56
1:D:1149:ARG:NH2	3:D:1303:HOH:O	2.37	0.56
1:A:997:GLU:HA	1:A:1001:ARG:NH1	2.21	0.56
1:A:1001:ARG:HH21	1:A:1219:TYR:HD2	1.53	0.56
1:E:1067:SER:OG	1:E:1070:ASN:OD1	2.17	0.56
1:B:888:TYR:OH	1:B:910:ARG:NH2	2.39	0.55
1:C:992:ARG:NH2	1:C:1132:LYS:O	2.40	0.55
1:E:1068[A]:GLN:NE2	1:E:1072:GLU:OE1	2.40	0.55
2:H:33:ALA:O	2:H:37:ILE:HG13	2.07	0.55
1:C:1113:LYS:NZ	2:I:12:GLU:OE2	2.37	0.55
1:C:886:GLU:HB2	1:C:910:ARG:HB3	1.89	0.55
1:C:1274:LEU:HD12	1:C:1274:LEU:C	2.32	0.54
1:A:997:GLU:HA	1:A:1001:ARG:HH11	1.71	0.54
2:H:36:ILE:CG2	2:H:40:TYR:CZ	2.90	0.54
1:B:1184:LYS:HD2	1:B:1205:TYR:CZ	2.43	0.54
1:A:945:TYR:CD2	1:A:946:ILE:CD1	2.90	0.54
1:E:869:ARG:HG3	1:E:878:LEU:HD22	1.89	0.54
1:E:909:ILE:HB	1:E:1042:PHE:HB2	1.90	0.54
1:C:1076:LYS:O	1:C:1080:TYR:CE1	2.60	0.54
1:A:864:ILE:HG21	1:A:867:ASN:HD21	1.72	0.54
1:D:1151:SER:HB3	1:C:1073:GLU:HG3	1.90	0.54
1:B:874:ASN:OD1	1:B:875:LEU:N	2.35	0.53
1:B:975:LEU:HD11	1:B:1009:ASN:OD1	2.08	0.53
1:E:1093:MET:SD	1:E:1160:ILE:HG12	2.49	0.53
1:B:1101:PHE:HB2	1:B:1283:ILE:HD11	1.90	0.53
1:A:952:ILE:HG13	1:A:953:ILE:HG13	1.91	0.53
1:A:997:GLU:OE2	1:A:998:TYR:HE2	1.91	0.53
1:C:1254:LYS:HG3	1:C:1256:TYR:CE1	2.43	0.53
2:F:33:ALA:O	2:F:37:ILE:HG13	2.08	0.53
1:D:1202:ASP:HA	1:B:1032:ARG:HH21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:26:ALA:N	2:I:27:GLY:HA2	2.22	0.53
1:C:911:VAL:HB	1:C:1040:ILE:HB	1.91	0.53
1:A:945:TYR:HD2	1:A:946:ILE:CD1	2.22	0.53
1:C:909:ILE:HG22	1:C:910:ARG:H	1.72	0.53
1:C:1245:GLU:HG2	1:C:1249:VAL:HG11	1.89	0.53
1:A:1163:LYS:HG2	1:A:1164:GLU:HG2	1.90	0.53
1:E:952:ILE:HG13	1:E:953:ILE:HG13	1.91	0.53
1:D:1094:TYR:HE2	1:D:1149:ARG:HH12	1.54	0.53
1:A:1051:THR:O	1:A:1051:THR:CG2	2.56	0.53
1:E:942:ILE:HD11	1:E:1134:ILE:HD13	1.89	0.52
1:E:1127:TYR:CE2	1:E:1134:ILE:HD11	2.44	0.52
1:C:1093:MET:SD	1:C:1160:ILE:HG12	2.49	0.52
1:C:1273:ASN:HB3	1:C:1276:LEU:HG	1.91	0.52
1:A:909:ILE:HB	1:A:1042:PHE:HB2	1.91	0.52
1:E:1127:TYR:CZ	1:E:1134:ILE:HD11	2.44	0.52
1:C:1245:GLU:OE1	1:C:1254:LYS:CG	2.55	0.52
1:D:1151:SER:O	1:D:1152:ASN:HB2	2.08	0.51
1:B:924:LEU:HD12	1:B:924:LEU:C	2.34	0.51
1:E:1127:TYR:HB2	1:E:1136:TYR:CE2	2.45	0.51
2:F:4[A]:GLU:OE2	2:F:40:TYR:OH	2.28	0.51
1:E:884:LYS:HE2	1:E:886:GLU:OE2	2.10	0.51
1:B:946:ILE:HD13	1:B:1133:TYR:CD2	2.45	0.51
1:C:1132:LYS:O	1:C:1132:LYS:HG3	2.10	0.51
1:C:1184:LYS:HG3	1:C:1203:GLU:C	2.36	0.51
1:A:1184:LYS:HG2	1:A:1205:TYR:CE1	2.45	0.51
2:H:2:PHE:O	2:H:5:LEU:N	2.44	0.51
1:D:990:ASN:HB3	1:D:993:GLU:HG2	1.92	0.51
1:A:938:LYS:HZ1	1:A:1051:THR:HG21	1.74	0.51
1:B:1150:LYS:NZ	1:B:1207:THR:OG1	2.32	0.51
1:C:921:SER:HB2	1:C:1037:ASN:HD22	1.75	0.51
1:E:1006:THR:HB	1:E:1017:TYR:HB2	1.93	0.50
1:D:1031:ILE:HG22	1:D:1032:ARG:H	1.75	0.50
1:D:1242:ARG:HG2	1:D:1255:ASP:OD1	2.12	0.50
1:D:909:ILE:HB	1:D:1042:PHE:HB2	1.92	0.50
1:C:1124:ARG:HG2	1:C:1141:ILE:HD11	1.94	0.50
1:A:1184:LYS:HG2	1:A:1205:TYR:CZ	2.47	0.50
1:D:1031:ILE:CG2	1:D:1032:ARG:N	2.73	0.50
1:A:942:ILE:O	1:A:946:ILE:HG12	2.12	0.50
1:E:905:ALA:O	1:E:908:LYS:HE3	2.12	0.49
1:D:1156:ILE:CG2	1:D:1157:ASN:N	2.75	0.49
1:B:952:ILE:HG13	1:B:953:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1099:TYR:CZ	1:C:1144:LYS:HD3	2.47	0.49
1:C:956:MET:HE1	1:C:976:ILE:HD12	1.93	0.49
1:E:1025:ASN:HD22	1:E:1025:ASN:C	2.20	0.49
1:B:862:ASN:OD1	1:B:863:ASN:N	2.45	0.49
1:A:922:VAL:HG13	1:A:1034:VAL:O	2.12	0.49
1:E:894:ASN:HD21	1:E:898:GLN:HB2	1.77	0.49
1:A:1263:TYR:CD2	1:A:1278:CYS:HB3	2.48	0.48
1:A:945:TYR:CD2	1:A:946:ILE:HD13	2.48	0.48
2:G:33:ALA:O	2:G:37:ILE:HG13	2.13	0.48
1:C:1174:LEU:O	1:C:1176:GLN:HG3	2.13	0.48
1:C:1254:LYS:HG3	1:C:1256:TYR:HE1	1.77	0.48
1:A:1224:LEU:HD11	1:A:1234:GLU:HB3	1.95	0.48
1:E:876:ILE:HG13	1:E:878:LEU:HD11	1.95	0.48
1:E:888:TYR:OH	1:E:910:ARG:NH2	2.47	0.48
1:D:1232:THR:HG22	1:D:1232:THR:O	2.13	0.48
1:C:1149:ARG:NH2	1:C:1158:ASP:O	2.44	0.48
1:D:873:ASN:ND2	1:C:872:ASP:OD1	2.37	0.48
1:D:943[B]:GLN:O	1:D:947:HIS:ND1	2.27	0.48
1:A:938:LYS:NZ	1:A:1051:THR:CG2	2.76	0.48
1:E:1012:ASN:OD1	1:E:1029:LYS:HA	2.14	0.48
1:D:923:PHE:HE1	1:D:1033:GLU:HA	1.79	0.47
1:B:1193:LEU:HD11	1:B:1238:ILE:HG23	1.95	0.47
1:A:1081:SER:HB2	1:A:1083:TYR:CE2	2.48	0.47
2:F:2:PHE:HE2	2:F:6:LYS:HE3	1.79	0.47
1:D:1070:ASN:OD1	1:D:1074:ARG:NH1	2.44	0.47
1:B:1087:PHE:CB	1:B:1283:ILE:HG12	2.44	0.47
1:D:1115:ASP:OD1	1:A:905:ALA:HB2	2.14	0.47
1:D:1151:SER:CB	1:C:1073:GLU:HG3	2.45	0.47
1:B:986:PHE:CZ	1:C:1271:PRO:HD2	2.49	0.47
1:B:1127:TYR:CZ	1:B:1129:GLN:HB2	2.50	0.47
1:D:1108:SER:HB3	1:D:1121:ILE:CG2	2.45	0.47
1:B:1079:SER:O	1:B:1085:LYS:NZ	2.48	0.47
1:D:1149:ARG:NH2	1:C:1077:ILE:HG12	2.30	0.46
1:C:1087:PHE:CB	1:C:1283:ILE:HG12	2.44	0.46
1:D:923:PHE:CE1	1:D:1033:GLU:HA	2.50	0.46
1:C:1008:THR:HB	1:C:1065:GLU:HG3	1.97	0.46
1:B:959:ASN:O	1:B:976:ILE:CG2	2.63	0.46
1:C:889:ASP:CG	3:C:1301:HOH:O	2.57	0.46
1:C:1081:SER:OG	1:C:1083:TYR:O	2.28	0.46
1:E:1087:PHE:CB	1:E:1283:ILE:HG12	2.45	0.46
2:G:10:PHE:HA	2:G:13:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:991:ILE:HD12	1:E:1134:ILE:HG22	1.98	0.46
1:E:1070:ASN:HD22	1:E:1074:ARG:HH22	1.64	0.46
1:D:1202:ASP:OD1	1:B:1032:ARG:NE	2.39	0.46
1:D:925:ASP:OD1	1:D:1010:ASN:HA	2.16	0.46
1:C:1274:LEU:HD12	1:C:1275:LYS:HG2	1.98	0.46
1:A:1241:HIS:HE1	1:A:1260:SER:CB	2.29	0.46
1:D:922:VAL:HG12	1:D:924:LEU:HG	1.98	0.46
1:D:1081:SER:HB2	1:D:1083:TYR:CE2	2.51	0.46
1:D:1184:LYS:HG3	1:D:1203:GLU:C	2.41	0.46
1:D:1254:LYS:HE2	1:D:1254:LYS:HB3	1.66	0.46
1:B:925:ASP:O	1:B:926:PHE:HB3	2.16	0.46
1:B:1086:ASP:HB2	1:B:1282:PHE:O	2.16	0.46
1:D:943[A]:GLN:O	1:D:947:HIS:ND1	2.27	0.45
1:C:922:VAL:HG11	1:C:1033:GLU:HG2	1.97	0.45
1:C:1205:TYR:CZ	1:C:1227:LYS:HG2	2.51	0.45
1:B:878:LEU:HG	1:B:878:LEU:O	2.16	0.45
1:A:943[B]:GLN:H	1:A:943[B]:GLN:CD	2.24	0.45
1:A:1028:ILE:O	1:A:1031:ILE:HG22	2.16	0.45
1:E:893:LEU:HD23	1:E:899:PHE:HB3	1.98	0.45
1:D:997:GLU:HA	1:D:1001:ARG:HH11	1.82	0.45
1:D:1270:LYS:HA	1:D:1271:PRO:C	2.42	0.45
1:A:1127:TYR:CZ	1:A:1129:GLN:HB2	2.50	0.45
1:E:900:LYS:HE3	1:E:1053:PHE:CD1	2.52	0.45
1:B:986:PHE:HZ	1:C:1271:PRO:HD2	1.80	0.45
1:A:942:ILE:HG21	1:A:1134:ILE:HD11	1.98	0.45
1:A:997:GLU:OE1	1:A:997:GLU:N	2.49	0.45
1:B:1028:ILE:HB	1:B:1031:ILE:CG1	2.47	0.45
1:C:1163:LYS:HE2	1:C:1212:GLU:HB3	1.99	0.45
1:A:1241:HIS:HE1	1:A:1260:SER:OG	2.00	0.45
1:B:893:LEU:HD23	1:B:899:PHE:HB3	1.98	0.45
1:B:1027:ASP:OD1	1:B:1029:LYS:HG3	2.17	0.45
1:B:1273:ASN:HB3	1:B:1276:LEU:HG	1.99	0.45
1:C:1245:GLU:OE1	1:C:1254:LYS:CD	2.65	0.44
2:G:5:LEU:HD23	2:G:5:LEU:HA	1.81	0.44
1:D:874:ASN:OD1	1:D:875:LEU:N	2.47	0.44
1:B:926:PHE:HZ	1:B:975:LEU:HD21	1.82	0.44
1:B:1150:LYS:HE2	1:B:1229:GLU:OE2	2.16	0.44
1:B:863:ASN:HB3	1:B:1063:ASN:OD1	2.17	0.44
1:C:1209:GLN:OE1	1:C:1211:LYS:NZ	2.38	0.44
2:F:26:ALA:N	2:F:27:GLY:HA2	2.32	0.44
1:C:1245:GLU:CD	1:C:1254:LYS:HE3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:LYS:HE3	1:A:1205:TYR:OH	2.16	0.44
1:E:1249:VAL:O	1:E:1250:PHE:CD2	2.70	0.44
1:E:1184:LYS:HA	1:E:1205:TYR:CE2	2.52	0.44
1:B:962:TRP:HB3	1:B:975:LEU:HD23	1.99	0.44
1:C:942:ILE:HD11	1:C:1134:ILE:HD13	2.00	0.44
1:E:911:VAL:HB	1:E:1040:ILE:HB	1.99	0.44
1:A:900:LYS:HD2	1:A:1055:TRP:CZ2	2.53	0.44
1:E:1194:PHE:CE2	1:E:1196:ALA:HB2	2.53	0.44
1:A:1072:GLU:HG2	1:A:1076:LYS:HE3	1.99	0.44
1:E:1220:SER:HA	1:E:1281:GLN:HG2	1.99	0.44
1:D:1224:LEU:HA	1:D:1237:LEU:HD23	1.99	0.44
1:C:977:ASP:HA	1:C:1034:VAL:HG22	2.00	0.43
1:B:1229:GLU:OE1	1:B:1229:GLU:N	2.48	0.43
1:A:1189:GLU:CG	1:A:1190:GLU:OE1	2.65	0.43
1:B:1098:TYR:CG	1:B:1282:PHE:HB3	2.54	0.43
1:C:909:ILE:HB	1:C:1042:PHE:HB2	2.00	0.43
1:C:1203:GLU:OE1	2:I:6:LYS:NZ	2.44	0.43
1:A:977:ASP:HA	1:A:1033:GLU:O	2.18	0.43
1:A:1205:TYR:CZ	1:A:1227:LYS:HG2	2.53	0.43
1:E:990:ASN:HD21	1:E:993:GLU:HG3	1.83	0.43
1:D:911:VAL:HB	1:D:1040:ILE:HB	2.00	0.43
1:A:942:ILE:CD1	1:A:1134:ILE:HD13	2.48	0.43
1:E:1010:ASN:OD1	1:E:1012:ASN:N	2.42	0.43
1:D:1220:SER:HA	1:D:1281:GLN:HG2	2.00	0.43
1:A:1193:LEU:HD21	1:A:1259:ILE:HB	2.01	0.43
1:D:983:LYS:HG2	1:D:1031:ILE:CD1	2.22	0.43
1:B:1129:GLN:O	1:C:1242:ARG:HD3	2.19	0.43
1:C:1205:TYR:CE1	1:C:1227:LYS:HA	2.53	0.43
1:A:1254:LYS:HG3	1:A:1256:TYR:CE1	2.54	0.43
1:B:1184:LYS:NZ	1:B:1202:ASP:O	2.50	0.42
1:A:977:ASP:HB3	1:A:1031:ILE:HG13	2.01	0.42
1:D:1086:ASP:HB2	1:D:1282:PHE:O	2.19	0.42
1:B:936:LYS:HG2	1:B:937:TYR:O	2.18	0.42
1:A:1241:HIS:CE1	1:A:1260:SER:HB2	2.54	0.42
1:A:868:LEU:HD23	1:A:868:LEU:HA	1.83	0.42
1:B:900:LYS:NZ	1:B:1287:GLU:OE2	2.46	0.42
1:D:1076:LYS:HE2	1:D:1076:LYS:HB3	1.79	0.42
1:B:875:LEU:O	1:B:876:ILE:HD13	2.19	0.42
1:C:1199:SER:HB3	2:I:2:PHE:CE1	2.54	0.42
1:C:953:ILE:HA	1:C:1041:ILE:O	2.20	0.42
1:E:868:LEU:HA	1:E:868:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:LEU:HD12	1:B:909:ILE:HD13	2.00	0.42
1:B:924:LEU:O	1:B:924:LEU:CD1	2.66	0.42
1:C:1211:LYS:HZ3	1:C:1224:LEU:HD23	1.85	0.42
1:E:908:LYS:HA	1:E:1042:PHE:O	2.20	0.42
1:B:936:LYS:HE2	1:B:937:TYR:CE1	2.54	0.41
1:B:970:ARG:HG3	1:B:986:PHE:CD1	2.55	0.41
1:C:981:LYS:NZ	1:C:1032:ARG:HG3	2.35	0.41
1:D:977:ASP:OD2	1:D:981:LYS:HB3	2.19	0.41
1:D:1147:ILE:HG23	1:D:1167:ILE:HD12	2.01	0.41
1:C:952:ILE:HG13	1:C:953:ILE:HG13	2.02	0.41
1:C:977:ASP:OD2	1:C:981:LYS:NZ	2.42	0.41
1:C:887:VAL:HG11	1:C:893:LEU:HD11	2.01	0.41
1:A:1184:LYS:HG2	1:A:1205:TYR:CD1	2.55	0.41
1:E:982:THR:O	1:E:983:LYS:HD3	2.20	0.41
1:C:909:ILE:CG2	1:C:910:ARG:N	2.82	0.41
1:E:1012:ASN:HA	1:E:1028:ILE:HG13	2.01	0.41
2:F:23:LEU:O	2:F:27:GLY:HA2	2.19	0.41
2:G:32:GLU:O	2:G:36:ILE:HG13	2.20	0.41
2:I:5:LEU:HD23	2:I:5:LEU:HA	1.83	0.41
1:D:1202:ASP:HA	1:B:1032:ARG:NH2	2.34	0.41
1:C:973:TRP:CG	1:C:1007:ILE:HG21	2.56	0.41
1:C:909:ILE:CG2	1:C:910:ARG:H	2.34	0.41
2:F:11:LEU:CD2	2:F:37:ILE:HG23	2.50	0.41
1:B:1227:LYS:NZ	1:B:1233:ASP:OD2	2.36	0.41
1:A:1029:LYS:HG3	1:A:1030:ASP:OD1	2.21	0.41
1:D:937:TYR:HB3	1:D:945:TYR:CE1	2.55	0.41
1:D:1094:TYR:CZ	1:D:1149:ARG:NH1	2.85	0.41
1:B:942:ILE:CG1	1:B:946:ILE:HD12	2.47	0.41
1:C:863:ASN:OD1	1:C:863:ASN:N	2.53	0.41
1:C:973:TRP:CD2	1:C:1007:ILE:HG21	2.55	0.41
1:A:960:SER:OG	1:A:977:ASP:O	2.37	0.41
2:G:2:PHE:HE2	2:G:6:LYS:HE3	1.85	0.41
1:D:1263:TYR:CG	1:D:1278:CYS:HB3	2.56	0.41
1:E:1031:ILE:HG23	1:E:1032:ARG:N	2.36	0.41
1:E:1095:ASN:OD1	1:E:1148:ARG:NH1	2.46	0.41
1:A:1050:ARG:HH11	1:A:1050:ARG:HD3	1.76	0.40
1:C:893:LEU:HD23	1:C:899:PHE:HB3	2.03	0.40
1:A:953:ILE:HD12	1:A:964:ILE:HD12	2.03	0.40
1:E:1042:PHE:HZ	1:E:1059:PHE:CD2	2.39	0.40
1:E:1179:ARG:CZ	1:E:1198:ILE:HG23	2.51	0.40
2:F:5:LEU:HA	2:F:5:LEU:HD23	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:LYS:HA	1:A:1042:PHE:O	2.22	0.40
1:E:1017:TYR:HE2	1:E:1068[A]:GLN:HA	1.87	0.40
1:D:1031:ILE:CG2	1:D:1032:ARG:H	2.34	0.40
1:D:1098:TYR:CG	1:D:1282:PHE:HB3	2.56	0.40
1:B:1178:TRP:CE2	1:B:1197:PRO:HG3	2.56	0.40
1:B:1184:LYS:HD2	1:B:1205:TYR:CE1	2.57	0.40
1:B:1237:LEU:HD12	1:B:1263:TYR:CB	2.51	0.40
1:A:1148:ARG:HH21	1:A:1177:GLU:CD	2.27	0.40
2:G:34:GLU:HG2	2:G:38:ARG:HH21	1.86	0.40
1:D:1184:LYS:NZ	3:D:1307:HOH:O	2.53	0.40
1:E:1180:VAL:O	1:E:1225:PHE:HZ	2.04	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	411/438 (94%)	397 (97%)	14 (3%)	0	100	100
1	B	405/438 (92%)	389 (96%)	16 (4%)	0	100	100
1	C	422/438 (96%)	409 (97%)	13 (3%)	0	100	100
1	D	416/438 (95%)	401 (96%)	15 (4%)	0	100	100
1	E	399/438 (91%)	386 (97%)	13 (3%)	0	100	100
2	F	39/66 (59%)	38 (97%)	1 (3%)	0	100	100
2	G	37/66 (56%)	36 (97%)	1 (3%)	0	100	100
2	H	33/66 (50%)	31 (94%)	2 (6%)	0	100	100
2	I	37/66 (56%)	34 (92%)	3 (8%)	0	100	100
All	All	2199/2454 (90%)	2121 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	389/411 (95%)	388 (100%)	1 (0%)	86	93
1	B	389/411 (95%)	389 (100%)	0	100	100
1	C	400/411 (97%)	399 (100%)	1 (0%)	86	93
1	D	396/411 (96%)	393 (99%)	3 (1%)	73	84
1	E	374/411 (91%)	372 (100%)	2 (0%)	81	89
2	F	32/54 (59%)	32 (100%)	0	100	100
2	G	29/54 (54%)	29 (100%)	0	100	100
2	H	24/54 (44%)	24 (100%)	0	100	100
2	I	29/54 (54%)	29 (100%)	0	100	100
All	All	2062/2271 (91%)	2055 (100%)	7 (0%)	86	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1149	ARG
1	D	1248	ILE
1	D	1249	VAL
1	C	1144	LYS
1	A	1252	GLU
1	E	913	GLN
1	E	1076	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	863	ASN
1	D	954	ASN
1	D	1052	GLN
1	D	1209	GLN
1	D	1216	GLN
1	B	979	ASN

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Mol	Chain	Res	Type
1	B	1105	ASN
1	B	1216	GLN
1	A	867	ASN
1	A	913	GLN
1	A	954	ASN
1	A	1052	GLN
1	A	1105	ASN
1	A	1129	GLN
1	A	1281	GLN
1	E	897	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	415/438 (94%)	0.65	50 (12%) 9 7	23, 46, 99, 124	2 (0%)
1	B	412/438 (94%)	0.64	39 (9%) 14 13	29, 48, 87, 118	1 (0%)
1	C	426/438 (97%)	0.67	45 (10%) 11 10	25, 50, 101, 127	2 (0%)
1	D	420/438 (95%)	0.34	30 (7%) 22 22	16, 34, 78, 127	2 (0%)
1	E	405/438 (92%)	1.30	74 (18%) 3 2	43, 87, 124, 142	2 (0%)
2	F	40/66 (60%)	1.40	11 (27%) 1 1	31, 62, 135, 146	1 (2%)
2	G	39/66 (59%)	1.48	14 (35%) 1 0	34, 89, 127, 141	0
2	H	37/66 (56%)	2.18	21 (56%) 0 0	44, 80, 131, 146	0
2	I	39/66 (59%)	1.44	9 (23%) 2 1	43, 85, 128, 136	0
All	All	2233/2454 (90%)	0.78	293 (13%) 7 6	16, 53, 114, 146	10 (0%)

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1156	ILE	7.2
1	B	924	LEU	6.6
1	C	918	ILE	6.5
1	D	1157	ASN	6.4
1	C	1082	GLU	6.0
1	B	1242	ARG	5.9
1	D	1151	SER	5.7
1	E	1249	VAL	5.6
2	H	40	TYR	5.5
1	A	1250	PHE	5.5
1	D	1152	ASN	5.4
1	A	913	GLN	5.4
1	C	1158	ASP	5.3
1	C	1132	LYS	5.3
1	E	1248	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	922	VAL	5.0
1	E	1183	TYR	4.9
1	E	1180	VAL	4.9
1	C	1154	GLN	4.9
1	D	914	ASN	4.9
1	C	869	ARG	4.9
2	H	38	ARG	4.8
1	E	1049	ASP	4.6
1	C	1080	TYR	4.5
2	F	24	ARG	4.5
2	H	35	ARG	4.4
1	A	1033	GLU	4.4
1	C	1011	LEU	4.2
1	D	863	ASN	4.2
2	G	37	ILE	4.2
1	A	922	VAL	4.2
2	F	1	MET	4.1
2	H	1	MET	4.1
1	C	1130	ASN	4.1
2	H	29	SER	4.0
1	D	1082	GLU	4.0
1	E	881	TYR	4.0
1	C	923	PHE	4.0
1	E	1011	LEU	3.9
1	E	1033	GLU	3.9
2	F	32	GLU	3.9
2	G	38	ARG	3.9
2	H	31	GLU	3.9
1	A	1174	LEU	3.9
1	E	1036	ALA	3.9
2	H	33	ALA	3.9
1	E	1083	TYR	3.9
1	E	1174	LEU	3.9
1	D	1158	ASP	3.9
1	E	1226	LYS	3.8
1	E	1253	TYR	3.8
2	F	26	ALA	3.8
1	C	1151	SER	3.7
1	A	1151	SER	3.7
1	D	1155	SER	3.7
1	B	1030	ASP	3.6
2	G	40	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	1250	PHE	3.6
1	B	997	GLU	3.6
1	A	1051	THR	3.5
1	D	1115	ASP	3.5
2	F	28	TYR	3.5
1	C	947	HIS	3.5
1	E	924	LEU	3.5
2	I	33	ALA	3.5
1	B	1031	ILE	3.5
1	E	867	ASN	3.5
1	D	924	LEU	3.5
1	B	1032	ARG	3.5
1	D	1031	ILE	3.4
1	A	1068[A]	GLN	3.4
1	C	1155	SER	3.4
1	D	1175	ASN	3.4
1	C	1251	GLU	3.4
1	E	923	PHE	3.4
2	I	30	ASP	3.4
1	C	922	VAL	3.4
2	I	40	TYR	3.4
2	H	16	ARG	3.3
1	C	1232	THR	3.3
1	E	870	TYR	3.3
1	A	943[A]	GLN	3.3
2	I	4	GLU	3.3
1	A	867	ASN	3.3
1	C	1248	ILE	3.2
1	E	1179	ARG	3.2
1	B	914	ASN	3.2
1	A	1202	ASP	3.2
1	E	1159	ASP	3.2
2	I	28	TYR	3.2
1	C	1063	ASN	3.1
1	E	958	ASN	3.1
1	E	1149	ARG	3.1
1	A	924	LEU	3.1
1	D	947	HIS	3.1
1	B	1229	GLU	3.1
1	B	1151	SER	3.1
1	B	943	GLN	3.1
2	H	37	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	1037	ASN	3.1
2	H	30	ASP	3.1
1	E	1235	ILE	3.0
1	B	1036	ALA	3.0
1	E	1068[A]	GLN	3.0
2	H	36	ILE	3.0
2	G	21	ASN	3.0
1	E	1133	TYR	3.0
1	C	1129	GLN	2.9
1	B	1070	ASN	2.9
1	B	1035	ILE	2.9
1	E	1074	ARG	2.9
2	F	40	TYR	2.9
2	G	28	TYR	2.9
1	E	908	LYS	2.9
2	H	39	LYS	2.9
1	B	913	GLN	2.9
1	B	1012	ASN	2.9
1	E	978	ILE	2.9
1	B	1158	ASP	2.9
1	B	1080	TYR	2.9
1	B	975	LEU	2.9
1	C	997	GLU	2.8
1	C	1230	GLU	2.8
2	I	37	ILE	2.8
1	C	1036	ALA	2.8
1	C	1254	LYS	2.8
1	D	1230	GLU	2.8
1	A	863	ASN	2.8
1	C	982	THR	2.8
1	B	1111	LYS	2.8
1	B	862	ASN	2.8
1	E	1118	VAL	2.8
1	C	1188	LYS	2.7
2	G	36	ILE	2.7
2	F	35	ARG	2.7
1	E	1081	SER	2.7
1	D	1232	THR	2.7
1	A	1036	ALA	2.7
1	C	1187	LYS	2.7
1	A	921	SER	2.7
2	F	31	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	1200	ASP	2.7
1	C	1233	ASP	2.7
2	H	17	ASP	2.7
1	B	881	TYR	2.7
1	A	1031	ILE	2.7
1	B	1175	ASN	2.7
1	E	959	ASN	2.7
1	E	1186	PHE	2.7
1	E	1187	LYS	2.7
1	E	1031	ILE	2.6
1	C	1074	ARG	2.6
1	A	923	PHE	2.6
1	E	1205	TYR	2.6
1	B	878	LEU	2.6
1	D	1150	LYS	2.6
1	E	1025	ASN	2.6
1	E	926	PHE	2.6
1	E	1198	ILE	2.6
1	C	1174	LEU	2.6
1	A	1039	GLU	2.6
1	E	913	GLN	2.6
1	C	872	ASP	2.6
1	B	1011	LEU	2.6
1	E	1213	TYR	2.6
1	E	1269	ARG	2.6
1	E	1029	LYS	2.6
1	C	1203	GLU	2.6
1	E	1254	LYS	2.5
2	H	7	ALA	2.5
2	I	3	ALA	2.5
1	A	978	ILE	2.5
2	I	16	ARG	2.5
1	D	1073	GLU	2.5
1	A	997	GLU	2.5
2	G	33	ALA	2.5
1	A	1134	ILE	2.5
2	G	24	ARG	2.5
2	H	24	ARG	2.5
2	G	4	GLU	2.5
1	E	956	MET	2.5
1	A	897	ASN	2.5
1	A	1258	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	1132	LYS	2.5
1	A	1248	ILE	2.5
1	C	1030	ASP	2.5
1	B	1241	HIS	2.5
2	H	25	LYS	2.4
2	H	20	ARG	2.4
1	A	1115	ASP	2.4
1	B	1230	GLU	2.4
2	G	32	GLU	2.4
1	A	888	TYR	2.4
1	B	957	LYS	2.4
1	C	943[A]	GLN	2.4
1	A	1074	ARG	2.4
1	E	1193	LEU	2.4
1	E	1185	TYR	2.4
1	C	1250	PHE	2.4
1	D	1203	GLU	2.4
1	D	871	LYS	2.4
2	G	39	LYS	2.4
1	E	1236	GLY	2.4
1	E	1017	TYR	2.4
1	E	1172	PHE	2.4
1	E	1204	PHE	2.4
1	D	1251	GLU	2.4
1	A	1247	GLY	2.4
1	B	1037	ASN	2.3
1	C	1037	ASN	2.3
1	A	1233	ASP	2.3
1	A	1269	ARG	2.3
2	H	22	ALA	2.3
1	A	1251	GLU	2.3
1	E	997	GLU	2.3
2	G	23	LEU	2.3
2	H	2	PHE	2.3
1	C	978	ILE	2.3
1	E	1035	ILE	2.3
1	E	1064	THR	2.3
1	B	1203	GLU	2.3
1	B	960	SER	2.3
1	B	893	LEU	2.3
1	A	868	LEU	2.3
1	C	1265	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	993	GLU	2.3
1	A	1150	LYS	2.2
2	H	21	ASN	2.2
1	C	992	ARG	2.2
1	E	1128	ASN	2.2
1	A	1082	GLU	2.2
2	G	20	ARG	2.2
1	E	1058	TYR	2.2
1	A	877	ASP	2.2
1	A	1047	ASP	2.2
1	E	880	GLY	2.2
1	A	911	VAL	2.2
1	C	862	ASN	2.2
1	A	1227	LYS	2.2
1	E	1275	LYS	2.2
1	A	1159	ASP	2.2
1	E	905	ALA	2.1
2	F	20	ARG	2.1
1	E	1063	ASN	2.1
1	A	881	TYR	2.1
1	A	1011	LEU	2.1
1	E	893	LEU	2.1
2	H	14	GLY	2.1
1	C	891	VAL	2.1
1	C	1246	SER	2.1
1	E	952	ILE	2.1
2	F	3	ALA	2.1
1	E	970	ARG	2.1
1	D	1176	GLN	2.1
1	B	874	ASN	2.1
1	E	1160	ILE	2.1
2	G	35	ARG	2.1
1	B	1174	LEU	2.1
1	E	1169	LEU	2.1
2	F	27	GLY	2.1
1	C	917	ILE	2.1
1	C	1031	ILE	2.1
1	E	925	ASP	2.1
1	B	1245	GLU	2.1
1	A	1021	LYS	2.1
1	E	982	THR	2.1
1	B	867	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1010	ASN	2.1
1	A	864	ILE	2.1
1	A	1185	TYR	2.1
1	D	1202	ASP	2.0
1	B	1027	ASP	2.0
1	D	1114	LYS	2.0
1	B	1150	LYS	2.0
1	E	1182	THR	2.0
1	A	956	MET	2.0
1	B	1063	ASN	2.0
1	A	959	ASN	2.0
1	A	880	GLY	2.0
1	E	1256	TYR	2.0
1	D	997	GLU	2.0
1	D	1047	ASP	2.0
1	A	1230	GLU	2.0
1	D	1174	LEU	2.0
1	A	1176	GLN	2.0
1	E	868	LEU	2.0
1	D	1025	ASN	2.0
1	C	914	ASN	2.0
1	C	1247	GLY	2.0
1	E	942	ILE	2.0
1	E	944	ASN	2.0
1	A	967	ARG	2.0
2	I	24	ARG	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.