



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:20 PM UTC

PDB ID : 8AKO / pdb_00008ako
Title : Structure of EspB-EspK complex: the non-identical twin of the PE-PPE-EspG secretion mechanism.
Authors : Gijsbers, A.; Eymery, M.; Menart, I.; Vinciauskaite, V.; Gao, Y.; Siliqi, D.; Peters, P.; Mccarthy, A.; Ravelli, R.B.G.
Deposited on : 2022-07-30
Resolution : 2.29 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

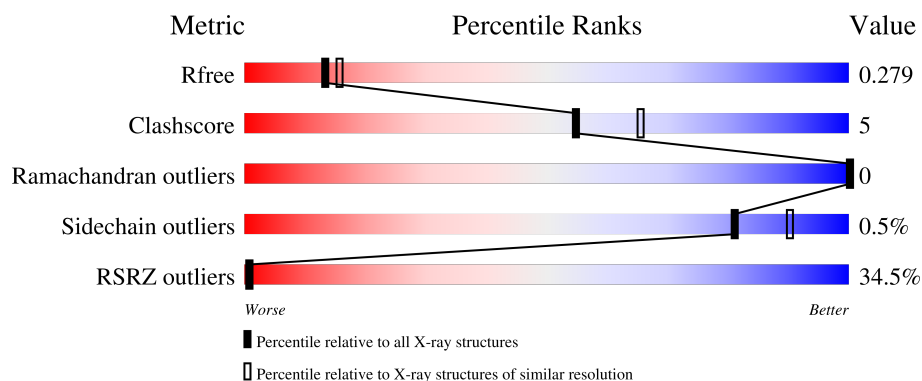
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	300	9% 78% 8% 13%
2	B	246	60% 88% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3930 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 ESX-1 secretion-associated protein EspB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2032	1269	361	395	7			

- Molecule 2 is a protein called ESX-1 secretion-associated protein EspK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	246	Total	C	N	O	S	0	0	0
			1860	1173	325	354	8			

- Molecule 3 is water.

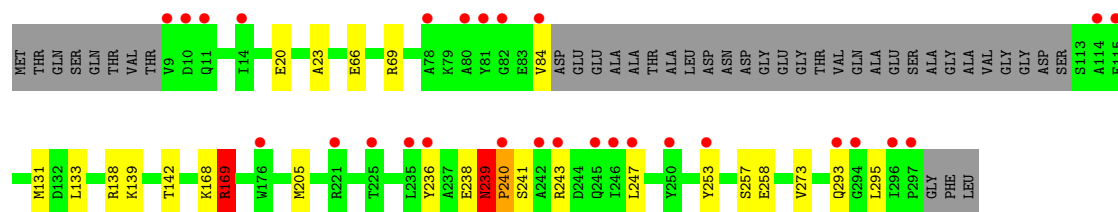
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	8	Total	O	0	0
			8	8		

3 Residue-property plots [i](#)

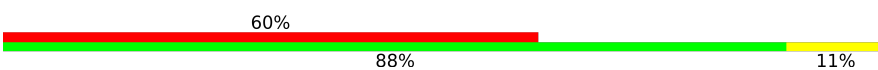
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

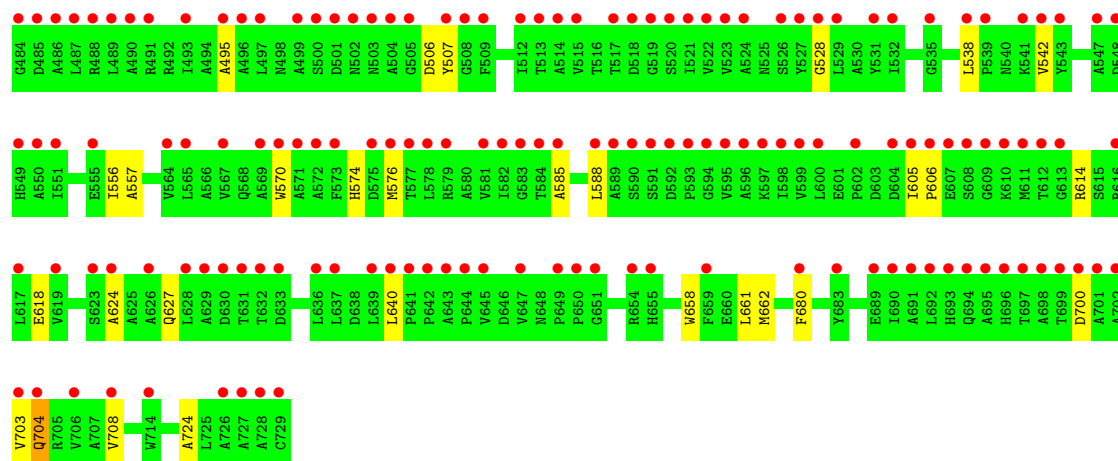
- Molecule 1: ESX-1 secretion-associated protein EspB

Chain A: 



- Molecule 2: ESX-1 secretion-associated protein EspK

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.58Å 101.58Å 377.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.82 – 2.29 85.82 – 2.29	Depositor EDS
% Data completeness (in resolution range)	53.2 (85.82-2.29) 53.2 (85.82-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.279 0.235 , 0.279	Depositor DCC
R_{free} test set	1444 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3930	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.64	1/2077 (0.0%)	1.03	6/2830 (0.2%)
2	B	0.52	0/1903	0.93	1/2606 (0.0%)
All	All	0.59	1/3980 (0.0%)	0.99	7/5436 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	SER	C-N	-6.02	1.26	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ASN	CB-CA-C	-7.46	102.89	110.65
1	A	258	GLU	CA-C-O	-5.83	114.37	120.55
2	B	704	GLN	CB-CG-CD	-5.46	103.31	112.60
1	A	240	PRO	N-CA-C	-5.44	107.68	114.20
1	A	169	ARG	N-CA-C	-5.42	106.67	113.28
1	A	257	SER	CA-C-O	5.20	126.28	120.82
1	A	169	ARG	CD-NE-CZ	-5.03	117.36	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2032	0	1979	19	0
2	B	1860	0	1816	19	0
3	A	30	0	0	3	0
3	B	8	0	0	0	0
All	All	3930	0	3795	37	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 5.

All (37) 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)
2:B:658:TRP:O	2:B:661:LEU:HB3	1.90	0.70
2:B:570:TRP:O	2:B:574:HIS:HB2	1.92	0.70
1:A:23:ALA:O	1:A:169:ARG:NH2	2.33	0.61
2:B:624:ALA:HA	2:B:627:GLN:HE21	1.67	0.60
1:A:20:GLU:HB3	3:A:406:HOH:O	2.01	0.59
1:A:247:LEU:HD23	2:B:507:TYR:HB2	1.87	0.56
2:B:658:TRP:O	2:B:662:MET:HG3	2.07	0.54
1:A:239:ASN:C	1:A:241:SER:H	2.14	0.54
1:A:240:PRO:O	1:A:243:ARG:HG2	2.07	0.54
2:B:574:HIS:HB3	2:B:576:MET:HE3	1.91	0.52
1:A:131:MET:HE1	1:A:139:LYS:HD2	1.91	0.52
1:A:239:ASN:N	1:A:239:ASN:OD1	2.43	0.52
1:A:84:VAL:O	1:A:84:VAL:HG12	2.10	0.51
1:A:239:ASN:C	1:A:241:SER:N	2.70	0.49
1:A:133:LEU:HD21	1:A:253:TYR:HB3	1.94	0.49
1:A:168:LYS:HE2	3:A:407:HOH:O	2.12	0.49
1:A:205:MET:HG2	1:A:273:VAL:HG21	1.95	0.48
1:A:238:GLU:O	1:A:240:PRO:HD3	2.12	0.48
2:B:557:ALA:HB2	2:B:724:ALA:HB1	1.94	0.48
1:A:238:GLU:HA	1:A:238:GLU:OE1	2.15	0.47
1:A:236:TYR:CE1	1:A:243:ARG:HB2	2.50	0.46
2:B:542:VAL:O	2:B:614:ARG:NH2	2.48	0.46
1:A:169:ARG:HG2	3:A:404:HOH:O	2.14	0.45
1:A:293:GLN:C	1:A:295:LEU:H	2.23	0.45
2:B:538:LEU:HD22	2:B:542:VAL:HG11	1.98	0.45
2:B:528:GLY:HA3	2:B:680:PHE:CD2	2.51	0.45
2:B:700:ASP:O	2:B:704:GLN:HG3	2.17	0.44
2:B:495:ALA:HB1	2:B:606:PRO:HD2	1.99	0.44
2:B:506:ASP:HA	2:B:662:MET:HE1	1.99	0.43
2:B:495:ALA:HA	2:B:605:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:585:ALA:HA	2:B:588:LEU:HB2	1.99	0.43
2:B:640:LEU:HD13	2:B:708:VAL:HG22	2.00	0.42
2:B:700:ASP:HB3	2:B:703:VAL:HB	2.01	0.42
2:B:556:ILE:HD13	2:B:556:ILE:HA	1.96	0.42
1:A:66:GLU:OE2	1:A:69:ARG:NH1	2.52	0.41
1:A:138:ARG:O	1:A:142:THR:OG1	2.32	0.41
2:B:614:ARG:HB3	2:B:618:GLU:HB2	2.02	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	257/300 (86%)	248 (96%)	9 (4%)	0	100	100
2	B	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
All	All	501/546 (92%)	485 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	210/237 (89%)	208 (99%)	2 (1%)	68	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	187/187 (100%)	187 (100%)	0	100	100
All	All	397/424 (94%)	395 (100%)	2 (0%)	81	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	239	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	266	ASN
2	B	627	GLN

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 ⓘ

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	261/300 (87%)	0.62	28 (10%)	11 12	30, 55, 116, 153	0
2	B	246/246 (100%)	2.41	147 (59%)	0 0	48, 108, 168, 192	0
All	All	507/546 (92%)	1.49	175 (34%)	1 1	30, 75, 156, 192	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	573	PHE	7.3
2	B	486	ALA	7.0
2	B	644	PRO	6.7
2	B	612	THR	6.7
2	B	645	VAL	6.2
2	B	593	PRO	6.0
1	A	240	PRO	6.0
2	B	606	PRO	5.6
2	B	647	VAL	5.4
2	B	608	SER	5.4
2	B	701	ALA	5.3
1	A	9	VAL	5.3
2	B	489	LEU	5.3
2	B	698	ALA	5.2
2	B	599	VAL	5.2
2	B	609	GLY	5.0
2	B	602	PRO	4.9
2	B	504	ALA	4.9
2	B	703	VAL	4.8
2	B	702	ALA	4.8
1	A	81	TYR	4.7
2	B	699	THR	4.6
2	B	497	LEU	4.6
2	B	605	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	582	ILE	4.6
2	B	543	TYR	4.5
2	B	596	ALA	4.5
2	B	535	GLY	4.5
1	A	80	ALA	4.5
2	B	503	ASN	4.4
2	B	728	ALA	4.3
2	B	570	TRP	4.2
2	B	493	ILE	4.2
2	B	629	ALA	4.0
2	B	487	LEU	4.0
2	B	505	GLY	4.0
2	B	630	ASP	4.0
2	B	611	MET	3.9
1	A	235	LEU	3.9
2	B	693	HIS	3.9
2	B	581	VAL	3.8
2	B	692	LEU	3.8
2	B	598	ILE	3.8
2	B	521	ILE	3.7
2	B	600	LEU	3.7
1	A	242	ALA	3.7
2	B	528	GLY	3.6
1	A	297	PRO	3.6
2	B	567	VAL	3.6
2	B	518	ASP	3.5
2	B	642	PRO	3.5
2	B	527	TYR	3.5
2	B	626	ALA	3.5
2	B	583	GLY	3.5
2	B	595	VAL	3.4
2	B	604	ASP	3.4
2	B	509	PHE	3.4
2	B	649	PRO	3.4
1	A	114	ALA	3.4
2	B	589	ALA	3.4
1	A	294	GLY	3.3
2	B	706	VAL	3.2
2	B	491	ARG	3.2
2	B	519	GLY	3.2
1	A	247	LEU	3.2
2	B	650	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	591	SER	3.2
2	B	695	ALA	3.2
2	B	659	PHE	3.1
2	B	607	GLU	3.1
2	B	594	GLY	3.1
2	B	577	THR	3.1
2	B	637	LEU	3.1
2	B	597	LYS	3.1
2	B	485	ASP	3.0
2	B	512	ILE	3.0
2	B	515	VAL	3.0
2	B	639	LEU	3.0
2	B	517	THR	3.0
2	B	484	GLY	3.0
2	B	550	ALA	2.9
2	B	680	PHE	2.9
2	B	542	VAL	2.9
2	B	578	LEU	2.9
2	B	655	HIS	2.9
2	B	654	ARG	2.8
2	B	636	LEU	2.8
2	B	572	ALA	2.8
2	B	576	MET	2.8
1	A	296	ILE	2.8
2	B	541	LYS	2.8
2	B	539	PRO	2.8
2	B	727	ALA	2.8
2	B	538	LEU	2.8
1	A	10	ASP	2.8
2	B	514	ALA	2.8
2	B	708	VAL	2.8
2	B	502	ASN	2.7
1	A	293	GLN	2.7
1	A	82	GLY	2.7
2	B	507	TYR	2.7
2	B	549	HIS	2.7
2	B	631	THR	2.7
2	B	697	THR	2.7
2	B	694	GLN	2.7
2	B	590	SER	2.7
2	B	704	GLN	2.6
1	A	84	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	221	ARG	2.6
2	B	488	ARG	2.6
2	B	565	LEU	2.6
2	B	651	GLY	2.6
2	B	500	SER	2.6
2	B	729	CYS	2.6
2	B	522	VAL	2.6
2	B	616	ARG	2.5
2	B	496	ALA	2.5
2	B	691	ALA	2.5
2	B	726	ALA	2.5
2	B	592	ASP	2.5
2	B	520	SER	2.5
2	B	524	ALA	2.5
1	A	245	GLN	2.5
2	B	683	TYR	2.5
2	B	585	ALA	2.5
2	B	513	THR	2.4
2	B	532	ILE	2.4
1	A	78	ALA	2.4
2	B	643	ALA	2.4
1	A	246	ILE	2.4
2	B	619	VAL	2.4
1	A	236	TYR	2.4
2	B	555	GLU	2.4
2	B	490	ALA	2.4
2	B	495	ALA	2.4
2	B	499	ALA	2.4
2	B	617	LEU	2.4
2	B	628	LEU	2.4
1	A	253	TYR	2.4
2	B	523	VAL	2.4
2	B	624	ALA	2.3
2	B	564	VAL	2.3
2	B	640	LEU	2.3
2	B	508	GLY	2.3
2	B	579	ARG	2.3
2	B	700	ASP	2.3
2	B	571	ALA	2.3
2	B	551	ILE	2.3
2	B	529	LEU	2.2
2	B	501	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	225	THR	2.2
2	B	531	TYR	2.2
2	B	610	LYS	2.2
2	B	690	ILE	2.2
2	B	613	GLY	2.2
2	B	569	ALA	2.2
2	B	632	THR	2.2
1	A	14	ILE	2.2
2	B	575	ASP	2.2
2	B	623	SER	2.2
1	A	250	TYR	2.2
1	A	243	ARG	2.2
2	B	584	THR	2.2
2	B	588	LEU	2.1
2	B	714	TRP	2.1
2	B	548	ASP	2.1
2	B	696	HIS	2.1
2	B	633	ASP	2.1
1	A	176	TRP	2.1
1	A	11	GLN	2.1
1	A	115	GLU	2.0
2	B	689	GLU	2.0
2	B	526	SER	2.0
2	B	547	ALA	2.0
2	B	641	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.