



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 11:49 AM UTC

PDB ID : 6RUT / pdb_00006rut
Title : Mycoplasma Genitalium Heterodimer Nap Complex (P140-P110 globular)
Authors : Fita, I.; Aparicio, D.
Deposited on : 2019-05-29
Resolution : 2.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

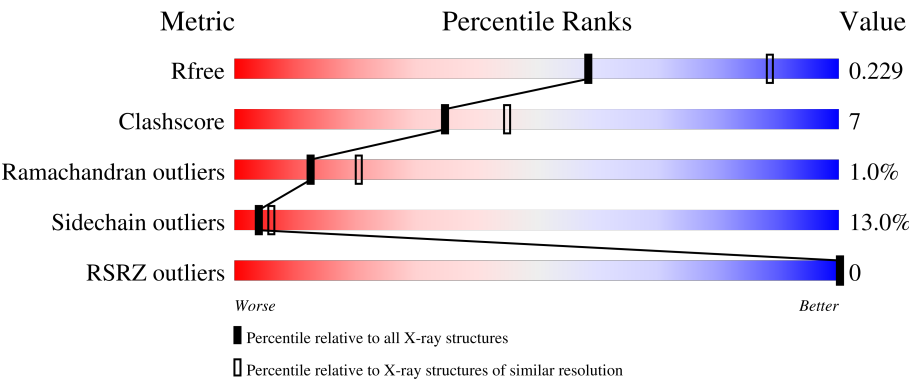
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	802	77%18%
1	C	802	73%19%
1	E	802	76%18%
1	G	802	76%18%
2	B	1334	67%24%5%5%

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Mol	Chain	Length	Quality of chain
2	D	1334	67% 23% 5% 5%
2	F	1334	65% 23% • 6%
2	H	1334	65% 24% 5% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 64181 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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6013	3758	1009	1240	6			
1	C	779	Total	C	N	O	S	0	0	0
			5999	3751	1006	1236	6			
1	E	783	Total	C	N	O	S	0	0	0
			6017	3760	1010	1241	6			
1	G	784	Total	C	N	O	S	0	0	0
			6023	3763	1011	1243	6			

- Molecule 2 is a protein called Adhesin P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1268	Total	C	N	O	S	0	0	0
			9938	6303	1679	1942	14			
2	D	1265	Total	C	N	O	S	0	0	0
			9918	6293	1676	1935	14			
2	F	1250	Total	C	N	O	S	0	0	0
			9822	6242	1658	1909	13			
2	H	1247	Total	C	N	O	S	0	0	0
			9798	6228	1654	1903	13			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	121	Total	O	0	0
			121	121		
3	C	87	Total	O	0	0
			87	87		
3	D	137	Total	O	0	0
			137	137		

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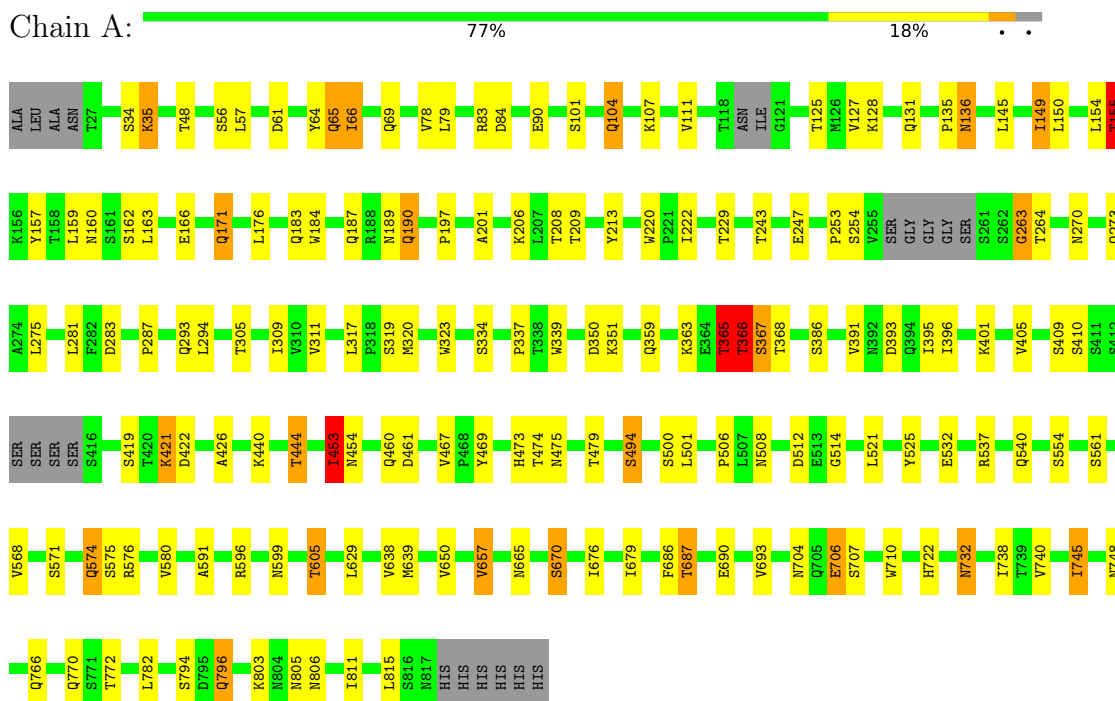
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	69	Total 69	O 69	0	0
3	F	70	Total 70	O 70	0	0
3	G	49	Total 49	O 49	0	0
3	H	58	Total 58	O 58	0	0

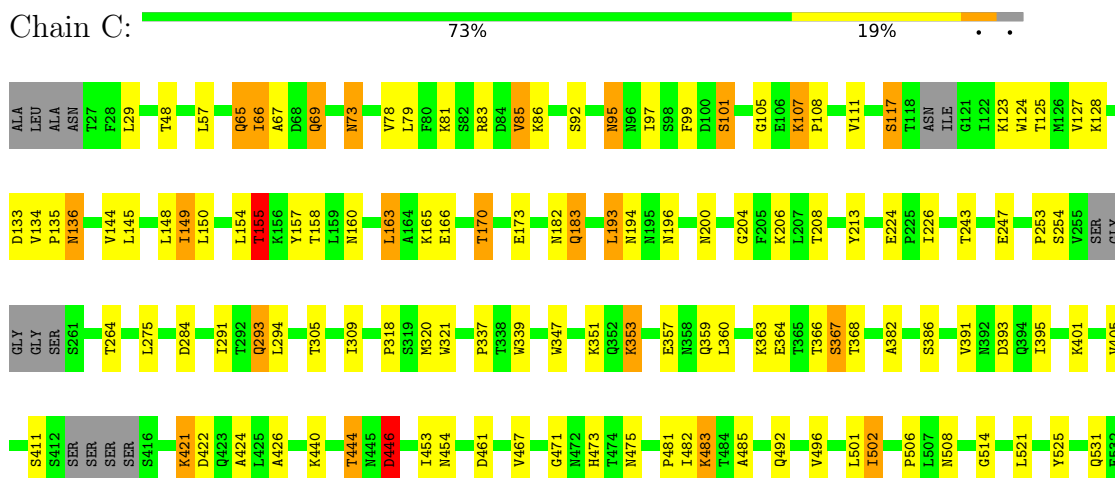
3 Residue-property plots

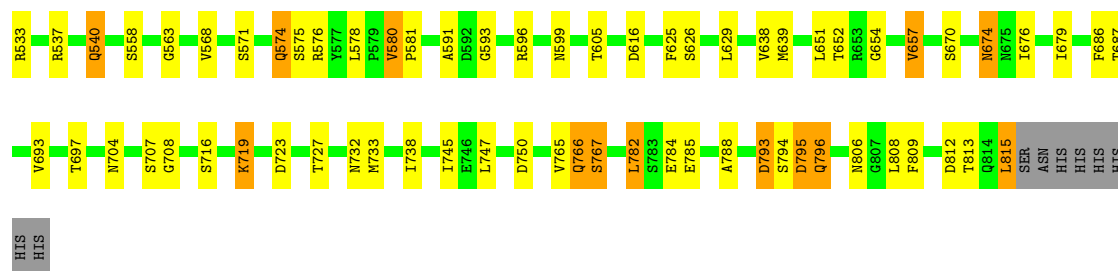
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Mgp-operon protein 3



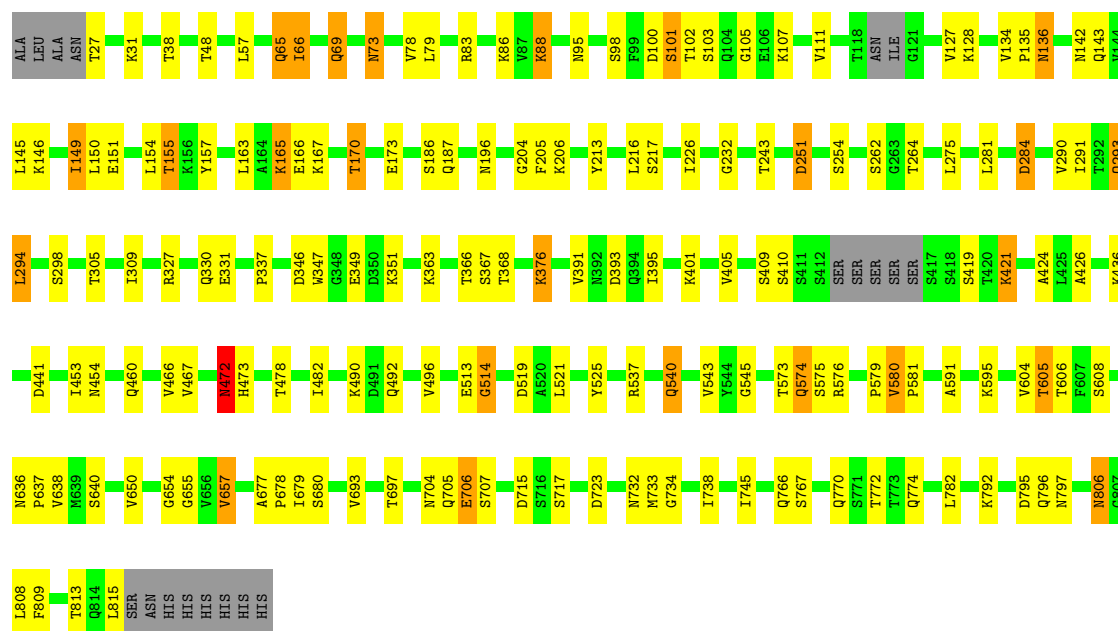
• Molecule 1: Mgp-operon protein 3





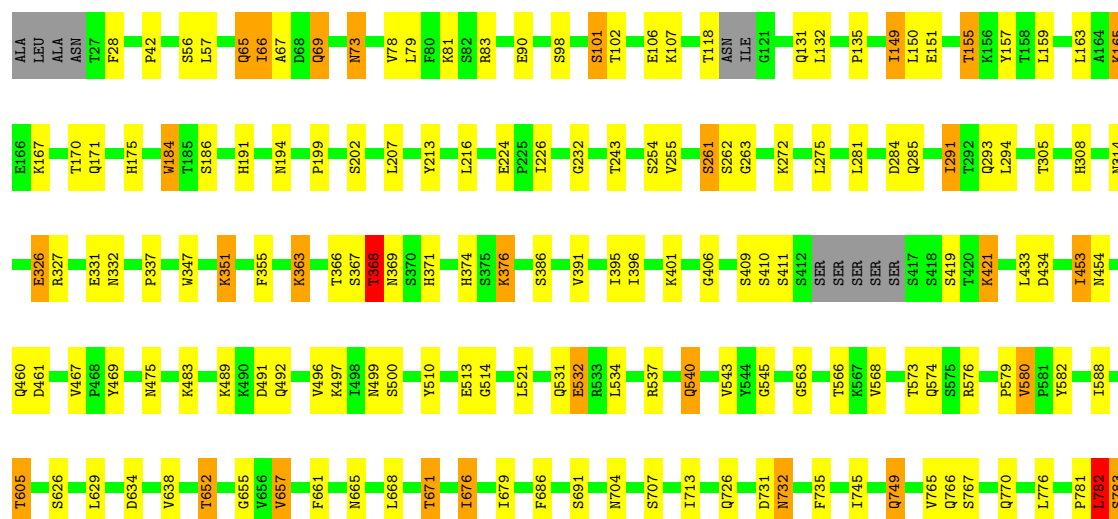
• Molecule 1: Mgp-operon protein 3

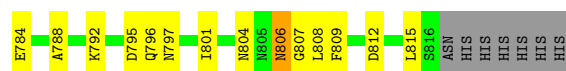
Chain E: 76% 18% . .



• Molecule 1: Mgp-operon protein 3

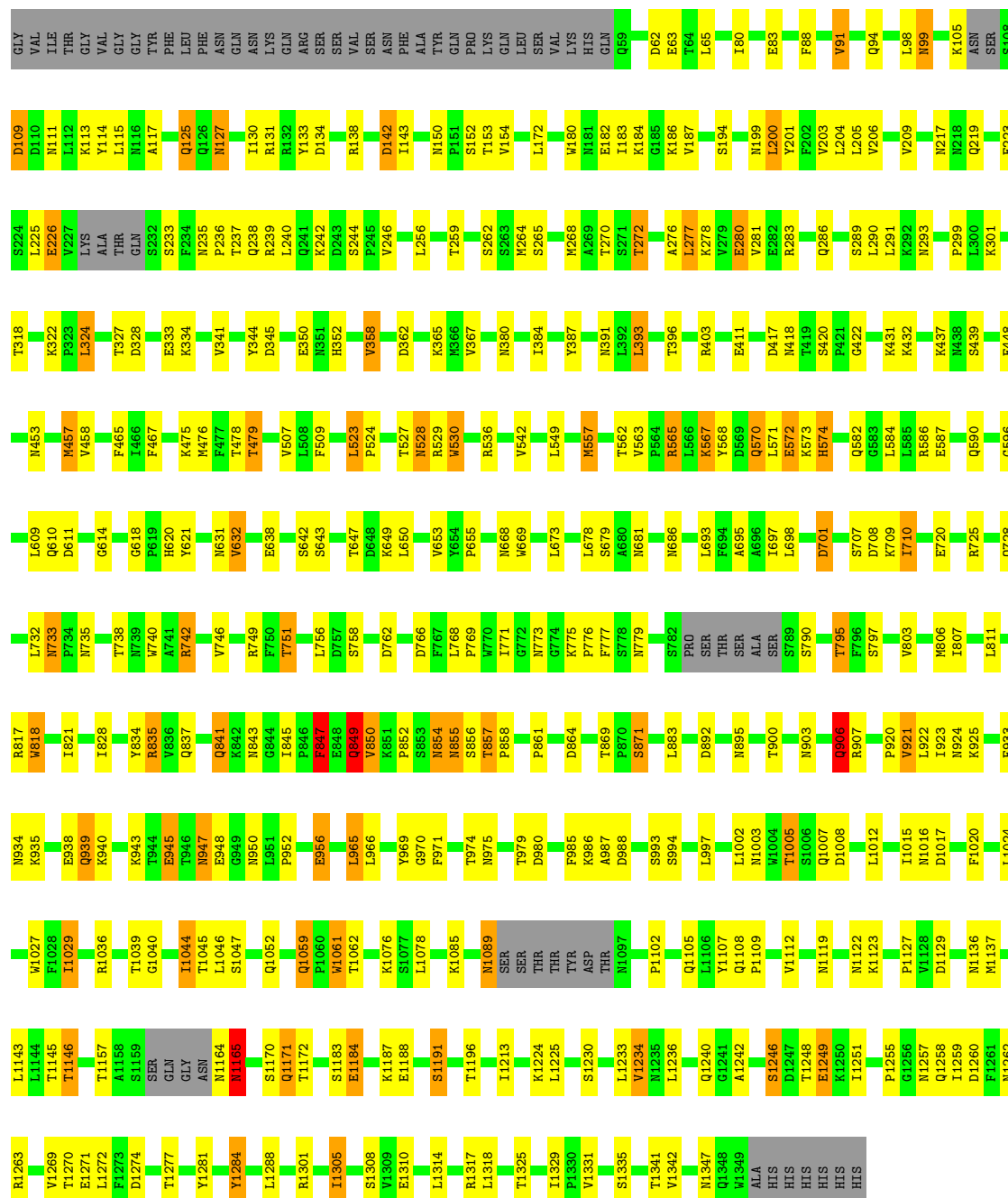
Chain G: 76% 18% . .





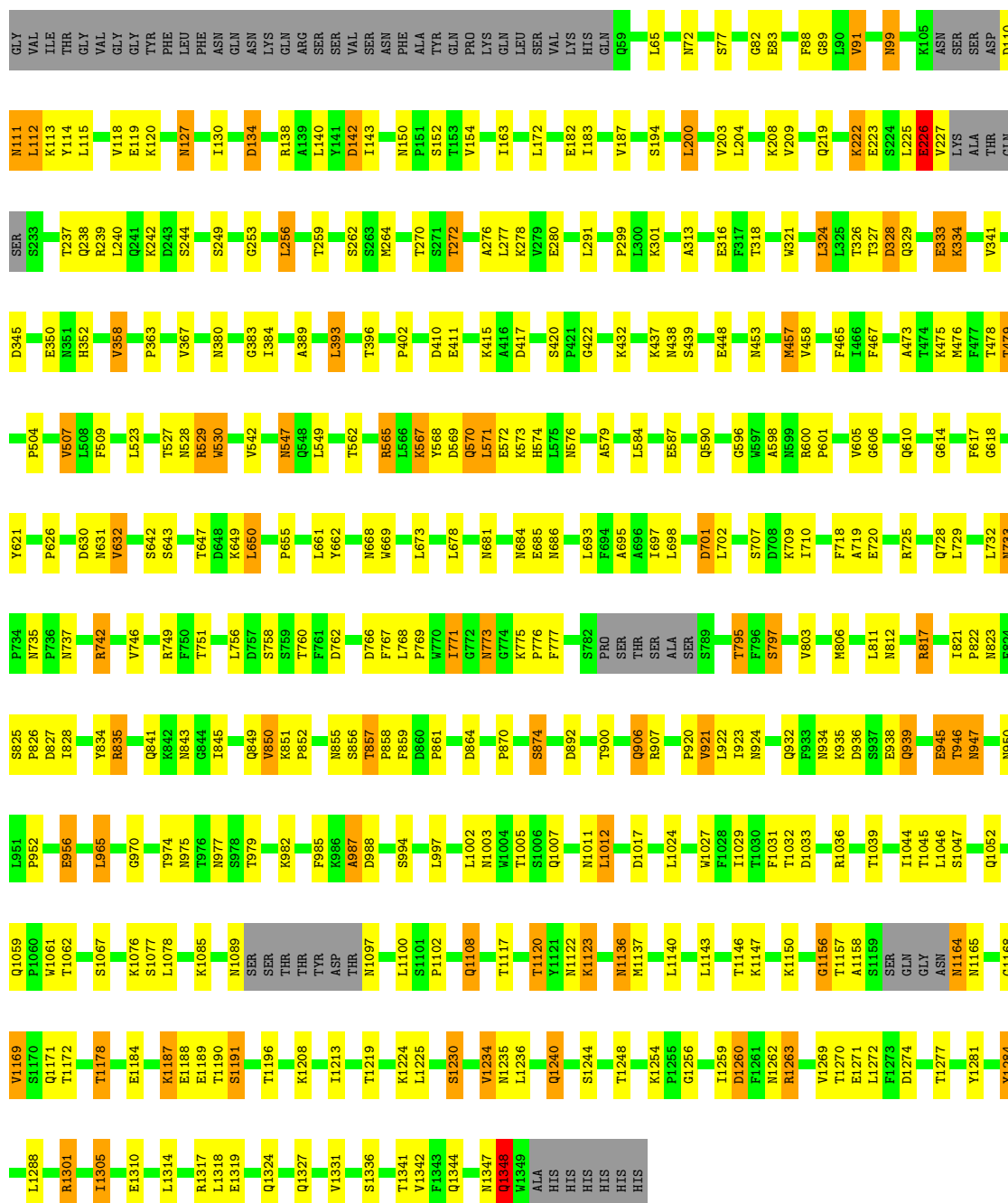
• Molecule 2: Adhesin P1

Chain B: 67% 24% 5% 5%



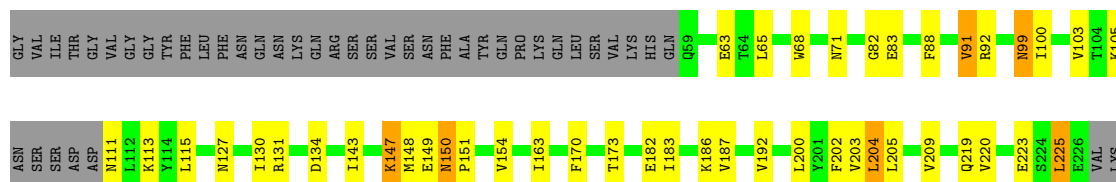
• Molecule 2: Adhesin P1

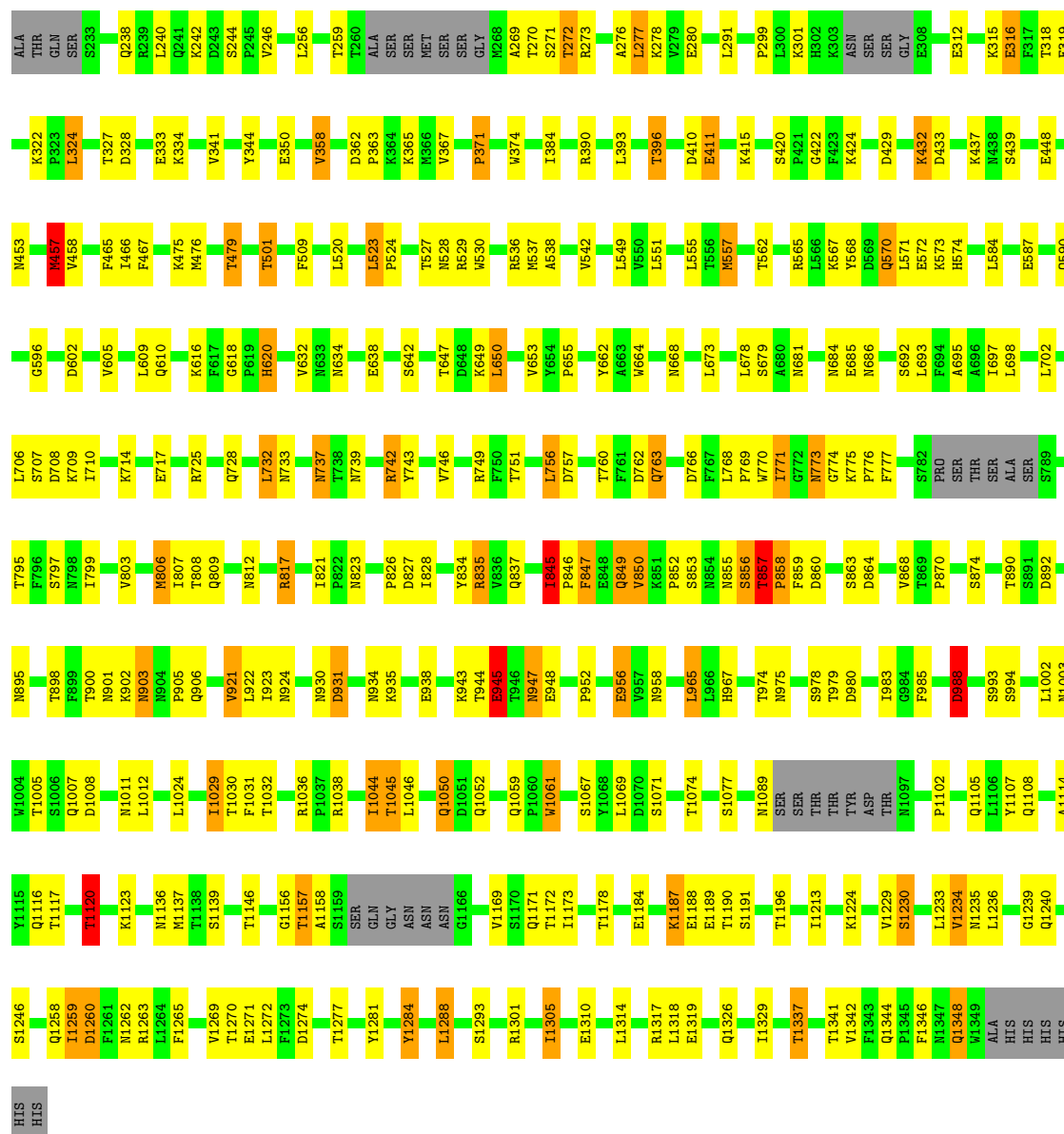
Chain D: 67% 23% 5% 5%



• Molecule 2: Adhesin P1

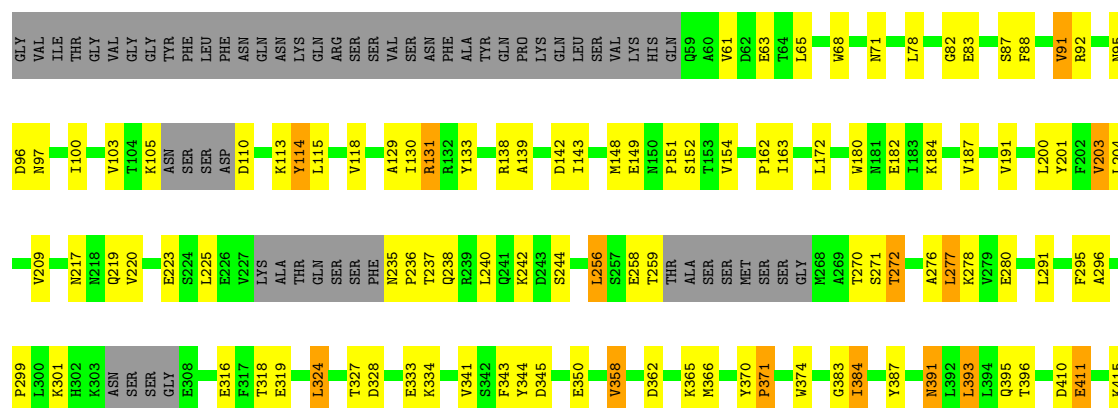
Chain F: 65% 23% 6%





• Molecule 2: Adhesin P1

Chain H: 65% 24% 5% 7%



F1343	Q1258	S1139	W1027	V921	V803	D701	L571	A416
Q1344	L1259	L1143	F1029	L922	M806	L702	D417	
P1345	D1260		I1029	I923	I807		K573	
F1346	F1261	T1146	T1030	N924	L811	S707	L584	S420
N1347	N1262	K1150	F1031	F933	N812	D768	L585	Q422
Q1348	R1263	G1156	T1032	N934	R817	K709	R586	K432
W1349	L1264	T1157	R1036	E938		I710	E587	
A1350	F1265	A1158	I1044	Q939	F820	E720	Q890	K436
HIS	L1267	SER	T1045	E945	I821	R725	P594	K437
HIS	P1268	GLN	L1046	T946	P822	Q728	N438	N438
HIS	V1269	GLY	Q1050	N947	N823		S439	
HIS	T1270	ASN	Q1051	P952	P826	L732	E448	
HIS	E1271	ASN	Q1052		D827	N737	N453	
	L1272	ASN	Q1059	E956	I828	T738	M457	
	F1273	G1156	F1060	V957		N739	V458	
	D1274		W1061	N958	Y834	P619	F465	
	T1277	V1169	S1067	L965	V836	H620	I466	
	Y1281	Q1170	Y1068	H967	Q841	V746	F467	
	Y1284	T1171	L1069	N975	N843	R749	N631	
	L1288	T1172	T1074	T976	G844	F750	V632	
		N1174		N977	I845	T751	F477	
	S1293	E1184	F1088	D980	P846	D757	T479	
	R1301	K1187	ASN				E638	
	I1305	E1188	SER		G849	D762	P504	
	S1306	E1189	SER	I983	V850		T647	
	Y1307	T1190	THR	G984	K851	D766	D648	
	S1308	S1191	TYR	F985	P852	F767	K649	
	V1309		ASP	K986	S856	L768	L520	
	E1310	T1196	THR	A987	T857	P769	L523	
	N1311	I1213	N1097	S988		V770	V653	
	Q1312			S990	D864	I771	Y654	
	T1313	M1221	P1102	S991		G772	P655	
	L1314		Q1105	S992	V868	N773	P659	
	R1317	K1224	L1106	S993	S874	G774	S659	
	L1318	L1225	Y1107	S994		K775	Y662	
	E1319	S1230	Q1108	L997	P864	P776	R536	
			A1114			F777	M537	
	D1322	V1234	Y1115	L1002	D892	F781	V542	
	Q1326	N1235	G1116	M1003		SER	L673	
	F1327	L1236	T1117	W1004	N895	PRO	L551	
	F1328	I1237	T1120	T1005		SER	L678	
	I1329	N1238	Y1121	S1006	T900	THR	S679	
	P1330	G1239	N1122	D1008	N901	ALA	A660	
	V1331	G1241	K1123	M1011	N903	SER	N651	
	S1335	A1242	L1124	L1012	Q906	S789	N654	
	S1336	D1245	M1136	D1017		T795	E685	
	T1337		M1137	L1024	L915	F796	I566	
	T1341		T1138			S797	K567	
	V1342				P920		Y568	
							A695	
							D669	
							I697	
							Q570	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.00Å 157.28Å 192.37Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	121.66 – 2.65 121.66 – 2.65	Depositor EDS
% Data completeness (in resolution range)	73.2 (121.66-2.65) 73.3 (121.66-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.187 , 0.224 0.199 , 0.229	Depositor DCC
R_{free} test set	9457 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	64181	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% 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	0.83	0/6136	1.34	32/8340 (0.4%)
1	C	0.83	1/6122 (0.0%)	1.35	50/8321 (0.6%)
1	E	0.82	0/6141	1.34	26/8347 (0.3%)
1	G	0.82	0/6147	1.34	32/8355 (0.4%)
2	B	0.86	4/10187 (0.0%)	1.37	74/13863 (0.5%)
2	D	0.85	2/10167 (0.0%)	1.37	80/13836 (0.6%)
2	F	0.82	4/10069 (0.0%)	1.34	50/13701 (0.4%)
2	H	0.84	5/10044 (0.0%)	1.34	59/13668 (0.4%)
All	All	0.84	16/65013 (0.0%)	1.35	403/88431 (0.5%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1115	TYR	CA-C	15.31	1.72	1.52
2	B	557	MET	SD-CE	-7.65	1.60	1.79
2	F	557	MET	SD-CE	-7.48	1.60	1.79
2	D	150	ASN	CA-C	6.53	1.57	1.53
2	H	812	ASN	CG-ND2	-6.01	1.20	1.33

The worst 5 of 403 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	ASN	CA-CB-CG	9.28	121.88	112.60
2	B	701	ASP	CA-CB-CG	9.28	121.88	112.60
1	G	261	SER	N-CA-C	9.16	124.40	113.23
2	H	1348	GLN	N-CA-C	-9.11	101.86	113.16
1	E	251	ASP	CA-CB-CG	8.41	121.01	112.60

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	6013	0	5805	62	0
1	C	5999	0	5794	73	0
1	E	6017	0	5809	63	0
1	G	6023	0	5814	90	0
2	B	9938	0	9645	149	0
2	D	9918	0	9631	163	0
2	F	9822	0	9548	159	0
2	H	9798	0	9529	206	0
3	A	62	0	0	0	0
3	B	121	0	0	2	0
3	C	87	0	0	0	0
3	D	137	0	0	5	0
3	E	69	0	0	0	0
3	F	70	0	0	1	0
3	G	49	0	0	0	0
3	H	58	0	0	2	0
All	All	64181	0	61575	933	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 7.

The worst 5 of 933 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:G:812:ASP:OD2	1:G:815:LEU:CD1	1.72	1.35
2:B:524:PRO:HD2	2:B:557:MET:HE2	1.31	1.12
1:G:255:VAL:HG23	1:G:726:GLN:HB3	1.19	1.11
1:G:812:ASP:OD2	1:G:815:LEU:HD13	1.36	1.09
1:G:812:ASP:OD2	1:G:815:LEU:HD12	1.54	1.06

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	773/802 (96%)	717 (93%)	50 (6%)	6 (1%)	16	27
1	C	771/802 (96%)	715 (93%)	48 (6%)	8 (1%)	12	20
1	E	777/802 (97%)	710 (91%)	60 (8%)	7 (1%)	14	24
1	G	778/802 (97%)	719 (92%)	50 (6%)	9 (1%)	10	17
2	B	1256/1334 (94%)	1162 (92%)	87 (7%)	7 (1%)	21	34
2	D	1253/1334 (94%)	1157 (92%)	84 (7%)	12 (1%)	12	20
2	F	1234/1334 (92%)	1139 (92%)	80 (6%)	15 (1%)	10	17
2	H	1231/1334 (92%)	1125 (91%)	91 (7%)	15 (1%)	10	17
All	All	8073/8544 (94%)	7444 (92%)	550 (7%)	79 (1%)	12	20

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	THR
1	A	367	SER
1	C	368	THR
2	D	618	GLY
2	D	1157	THR

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	685/701 (98%)	611 (89%)	74 (11%)	6	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	683/701 (97%)	607 (89%)	76 (11%)	6	9
1	E	684/701 (98%)	605 (88%)	79 (12%)	5	8
1	G	685/701 (98%)	615 (90%)	70 (10%)	7	10
2	B	1112/1171 (95%)	949 (85%)	163 (15%)	3	4
2	D	1109/1171 (95%)	954 (86%)	155 (14%)	3	5
2	F	1097/1171 (94%)	937 (85%)	160 (15%)	3	4
2	H	1093/1171 (93%)	943 (86%)	150 (14%)	3	5
All	All	7148/7488 (96%)	6221 (87%)	927 (13%)	4	6

5 of 927 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	1324	GLN
2	H	1024	LEU
2	F	259	THR
2	H	956	GLU
2	H	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 258 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	570	GLN
2	H	812	ASN
2	D	494	ASN
2	D	360	HIS
2	H	932	GLN

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	781/802 (97%)	-1.81	0 100 100	8, 29, 71, 112	0
1	C	779/802 (97%)	-1.82	0 100 100	9, 28, 73, 99	0
1	E	783/802 (97%)	-1.82	0 100 100	7, 29, 68, 109	0
1	G	784/802 (97%)	-1.80	0 100 100	8, 32, 69, 104	0
2	B	1268/1334 (95%)	-1.80	0 100 100	7, 29, 76, 130	0
2	D	1265/1334 (94%)	-1.83	0 100 100	6, 27, 73, 118	0
2	F	1250/1334 (93%)	-1.63	0 100 100	9, 44, 103, 136	0
2	H	1247/1334 (93%)	-1.53	0 100 100	14, 55, 115, 149	0
All	All	8157/8544 (95%)	-1.74	0 100 100	6, 34, 91, 149	0

There are no RSRZ outliers to report.

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 [i](#)

There are no such residues in this entry.