



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 10:38 AM GMT

PDB ID : 3DTD
Title : Crystal structure of invasion associated protein b from bartonella henselae
Authors : Patskovsky, Y.; Ozyurt, S.; Freeman, J.; Slocombe, A.; Groshong, C.; Koss, J.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-07-14
Resolution : 2.35 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

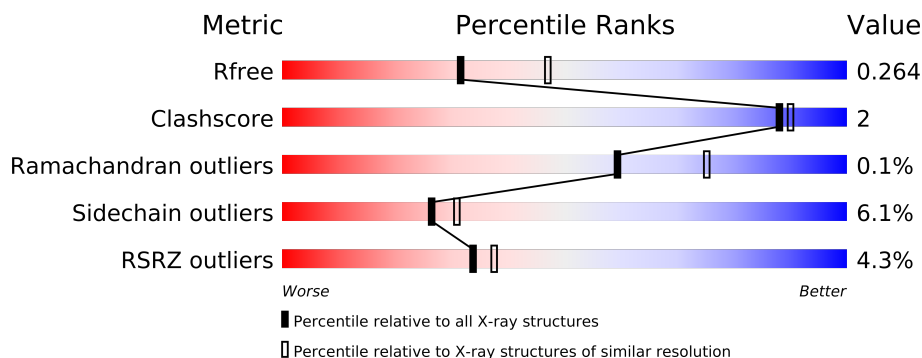
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	
1	C	175	
1	D	175	
1	E	175	
1	F	175	
1	G	175	
1	H	175	
1	I	175	
1	J	175	
1	K	175	
1	L	175	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	B	1	-	X
2	GOL	B	194	-	X
2	GOL	C	1	-	X
2	GOL	C	194	-	X
2	GOL	C	195	-	X
2	GOL	C	196	-	X
2	GOL	D	1	-	X
2	GOL	F	1	-	X
2	GOL	G	1	-	X
2	GOL	H	1	-	X
2	GOL	I	1	-	X
2	GOL	I	194	-	X
2	GOL	I	195	-	X
2	GOL	J	1	-	X
2	GOL	K	1	-	X
2	GOL	L	1	-	X
2	GOL	L	194	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13760 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Invasion-associated protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1074	685	188	194	7			
1	B	146	Total	C	N	O	S	0	2	0
			1113	708	197	201	7			
1	C	147	Total	C	N	O	S	0	1	0
			1113	708	196	202	7			
1	D	145	Total	C	N	O	S	0	2	0
			1109	706	196	200	7			
1	E	143	Total	C	N	O	S	0	1	0
			1091	696	193	195	7			
1	F	142	Total	C	N	O	S	0	2	0
			1090	695	194	194	7			
1	G	143	Total	C	N	O	S	0	2	0
			1097	699	193	198	7			
1	H	146	Total	C	N	O	S	0	2	0
			1115	709	197	202	7			
1	I	145	Total	C	N	O	S	0	2	0
			1108	707	195	199	7			
1	J	145	Total	C	N	O	S	0	2	0
			1107	705	195	200	7			
1	K	145	Total	C	N	O	S	0	2	0
			1112	708	198	199	7			
1	L	145	Total	C	N	O	S	0	2	0
			1107	705	195	200	7			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP Q6G4Y3
A	20	SER	-	expression tag	UNP Q6G4Y3
A	21	LEU	-	expression tag	UNP Q6G4Y3
A	186	GLU	-	expression tag	UNP Q6G4Y3
A	187	GLY	-	expression tag	UNP Q6G4Y3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	HIS	-	expression tag	UNP Q6G4Y3
A	189	HIS	-	expression tag	UNP Q6G4Y3
A	190	HIS	-	expression tag	UNP Q6G4Y3
A	191	HIS	-	expression tag	UNP Q6G4Y3
A	192	HIS	-	expression tag	UNP Q6G4Y3
A	193	HIS	-	expression tag	UNP Q6G4Y3
B	19	MET	-	expression tag	UNP Q6G4Y3
B	20	SER	-	expression tag	UNP Q6G4Y3
B	21	LEU	-	expression tag	UNP Q6G4Y3
B	186	GLU	-	expression tag	UNP Q6G4Y3
B	187	GLY	-	expression tag	UNP Q6G4Y3
B	188	HIS	-	expression tag	UNP Q6G4Y3
B	189	HIS	-	expression tag	UNP Q6G4Y3
B	190	HIS	-	expression tag	UNP Q6G4Y3
B	191	HIS	-	expression tag	UNP Q6G4Y3
B	192	HIS	-	expression tag	UNP Q6G4Y3
B	193	HIS	-	expression tag	UNP Q6G4Y3
C	19	MET	-	expression tag	UNP Q6G4Y3
C	20	SER	-	expression tag	UNP Q6G4Y3
C	21	LEU	-	expression tag	UNP Q6G4Y3
C	186	GLU	-	expression tag	UNP Q6G4Y3
C	187	GLY	-	expression tag	UNP Q6G4Y3
C	188	HIS	-	expression tag	UNP Q6G4Y3
C	189	HIS	-	expression tag	UNP Q6G4Y3
C	190	HIS	-	expression tag	UNP Q6G4Y3
C	191	HIS	-	expression tag	UNP Q6G4Y3
C	192	HIS	-	expression tag	UNP Q6G4Y3
C	193	HIS	-	expression tag	UNP Q6G4Y3
D	19	MET	-	expression tag	UNP Q6G4Y3
D	20	SER	-	expression tag	UNP Q6G4Y3
D	21	LEU	-	expression tag	UNP Q6G4Y3
D	186	GLU	-	expression tag	UNP Q6G4Y3
D	187	GLY	-	expression tag	UNP Q6G4Y3
D	188	HIS	-	expression tag	UNP Q6G4Y3
D	189	HIS	-	expression tag	UNP Q6G4Y3
D	190	HIS	-	expression tag	UNP Q6G4Y3
D	191	HIS	-	expression tag	UNP Q6G4Y3
D	192	HIS	-	expression tag	UNP Q6G4Y3
D	193	HIS	-	expression tag	UNP Q6G4Y3
E	19	MET	-	expression tag	UNP Q6G4Y3
E	20	SER	-	expression tag	UNP Q6G4Y3
E	21	LEU	-	expression tag	UNP Q6G4Y3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	186	GLU	-	expression tag	UNP Q6G4Y3
E	187	GLY	-	expression tag	UNP Q6G4Y3
E	188	HIS	-	expression tag	UNP Q6G4Y3
E	189	HIS	-	expression tag	UNP Q6G4Y3
E	190	HIS	-	expression tag	UNP Q6G4Y3
E	191	HIS	-	expression tag	UNP Q6G4Y3
E	192	HIS	-	expression tag	UNP Q6G4Y3
E	193	HIS	-	expression tag	UNP Q6G4Y3
F	19	MET	-	expression tag	UNP Q6G4Y3
F	20	SER	-	expression tag	UNP Q6G4Y3
F	21	LEU	-	expression tag	UNP Q6G4Y3
F	186	GLU	-	expression tag	UNP Q6G4Y3
F	187	GLY	-	expression tag	UNP Q6G4Y3
F	188	HIS	-	expression tag	UNP Q6G4Y3
F	189	HIS	-	expression tag	UNP Q6G4Y3
F	190	HIS	-	expression tag	UNP Q6G4Y3
F	191	HIS	-	expression tag	UNP Q6G4Y3
F	192	HIS	-	expression tag	UNP Q6G4Y3
F	193	HIS	-	expression tag	UNP Q6G4Y3
G	19	MET	-	expression tag	UNP Q6G4Y3
G	20	SER	-	expression tag	UNP Q6G4Y3
G	21	LEU	-	expression tag	UNP Q6G4Y3
G	186	GLU	-	expression tag	UNP Q6G4Y3
G	187	GLY	-	expression tag	UNP Q6G4Y3
G	188	HIS	-	expression tag	UNP Q6G4Y3
G	189	HIS	-	expression tag	UNP Q6G4Y3
G	190	HIS	-	expression tag	UNP Q6G4Y3
G	191	HIS	-	expression tag	UNP Q6G4Y3
G	192	HIS	-	expression tag	UNP Q6G4Y3
G	193	HIS	-	expression tag	UNP Q6G4Y3
H	19	MET	-	expression tag	UNP Q6G4Y3
H	20	SER	-	expression tag	UNP Q6G4Y3
H	21	LEU	-	expression tag	UNP Q6G4Y3
H	186	GLU	-	expression tag	UNP Q6G4Y3
H	187	GLY	-	expression tag	UNP Q6G4Y3
H	188	HIS	-	expression tag	UNP Q6G4Y3
H	189	HIS	-	expression tag	UNP Q6G4Y3
H	190	HIS	-	expression tag	UNP Q6G4Y3
H	191	HIS	-	expression tag	UNP Q6G4Y3
H	192	HIS	-	expression tag	UNP Q6G4Y3
H	193	HIS	-	expression tag	UNP Q6G4Y3
I	19	MET	-	expression tag	UNP Q6G4Y3

Continued on next page...

Continued from previous page...

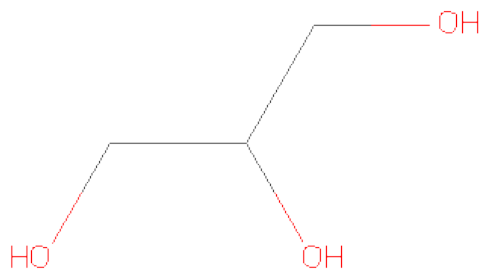
Chain	Residue	Modelled	Actual	Comment	Reference
I	20	SER	-	expression tag	UNP Q6G4Y3
I	21	LEU	-	expression tag	UNP Q6G4Y3
I	186	GLU	-	expression tag	UNP Q6G4Y3
I	187	GLY	-	expression tag	UNP Q6G4Y3
I	188	HIS	-	expression tag	UNP Q6G4Y3
I	189	HIS	-	expression tag	UNP Q6G4Y3
I	190	HIS	-	expression tag	UNP Q6G4Y3
I	191	HIS	-	expression tag	UNP Q6G4Y3
I	192	HIS	-	expression tag	UNP Q6G4Y3
I	193	HIS	-	expression tag	UNP Q6G4Y3
J	19	MET	-	expression tag	UNP Q6G4Y3
J	20	SER	-	expression tag	UNP Q6G4Y3
J	21	LEU	-	expression tag	UNP Q6G4Y3
J	186	GLU	-	expression tag	UNP Q6G4Y3
J	187	GLY	-	expression tag	UNP Q6G4Y3
J	188	HIS	-	expression tag	UNP Q6G4Y3
J	189	HIS	-	expression tag	UNP Q6G4Y3
J	190	HIS	-	expression tag	UNP Q6G4Y3
J	191	HIS	-	expression tag	UNP Q6G4Y3
J	192	HIS	-	expression tag	UNP Q6G4Y3
J	193	HIS	-	expression tag	UNP Q6G4Y3
K	19	MET	-	expression tag	UNP Q6G4Y3
K	20	SER	-	expression tag	UNP Q6G4Y3
K	21	LEU	-	expression tag	UNP Q6G4Y3
K	186	GLU	-	expression tag	UNP Q6G4Y3
K	187	GLY	-	expression tag	UNP Q6G4Y3
K	188	HIS	-	expression tag	UNP Q6G4Y3
K	189	HIS	-	expression tag	UNP Q6G4Y3
K	190	HIS	-	expression tag	UNP Q6G4Y3
K	191	HIS	-	expression tag	UNP Q6G4Y3
K	192	HIS	-	expression tag	UNP Q6G4Y3
K	193	HIS	-	expression tag	UNP Q6G4Y3
L	19	MET	-	expression tag	UNP Q6G4Y3
L	20	SER	-	expression tag	UNP Q6G4Y3
L	21	LEU	-	expression tag	UNP Q6G4Y3
L	186	GLU	-	expression tag	UNP Q6G4Y3
L	187	GLY	-	expression tag	UNP Q6G4Y3
L	188	HIS	-	expression tag	UNP Q6G4Y3
L	189	HIS	-	expression tag	UNP Q6G4Y3
L	190	HIS	-	expression tag	UNP Q6G4Y3
L	191	HIS	-	expression tag	UNP Q6G4Y3
L	192	HIS	-	expression tag	UNP Q6G4Y3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	193	HIS	-	expression tag	UNP Q6G4Y3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

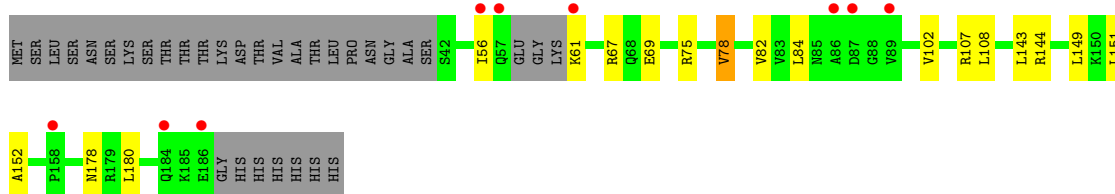
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	46	Total	O	0	0
			46	46		
3	C	44	Total	O	0	0
			44	44		
3	D	35	Total	O	0	0
			35	35		
3	E	28	Total	O	0	0
			28	28		
3	F	44	Total	O	0	0
			44	44		
3	G	39	Total	O	0	0
			39	39		
3	H	25	Total	O	0	0
			25	25		
3	I	35	Total	O	0	0
			35	35		
3	J	32	Total	O	0	0
			32	32		
3	K	32	Total	O	0	0
			32	32		
3	L	25	Total	O	0	0
			25	25		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

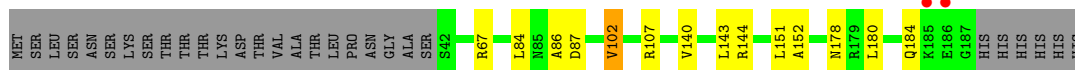
- Molecule 1: Invasion-associated protein B

Chain A: 



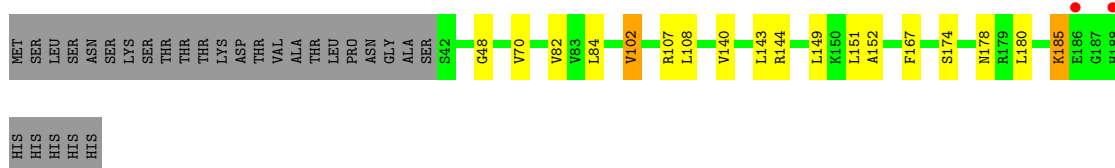
- Molecule 1: Invasion-associated protein B

Chain B: 



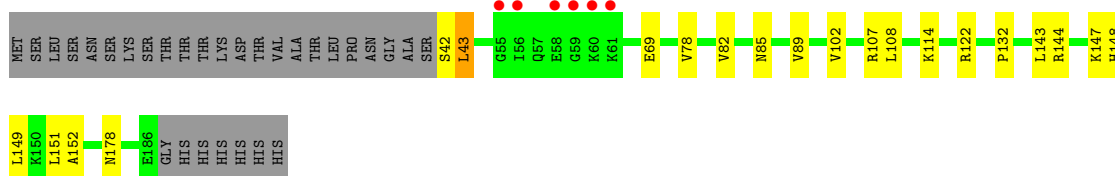
- Molecule 1: Invasion-associated protein B

Chain C: 



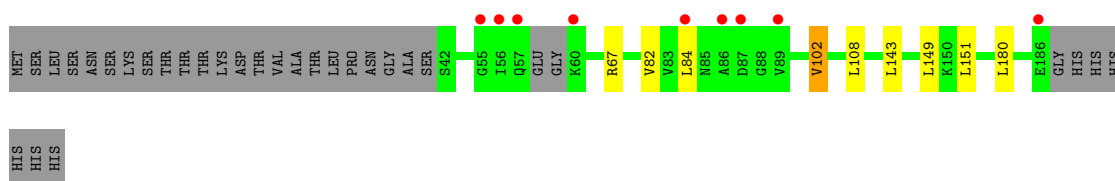
- Molecule 1: Invasion-associated protein B

Chain D: 



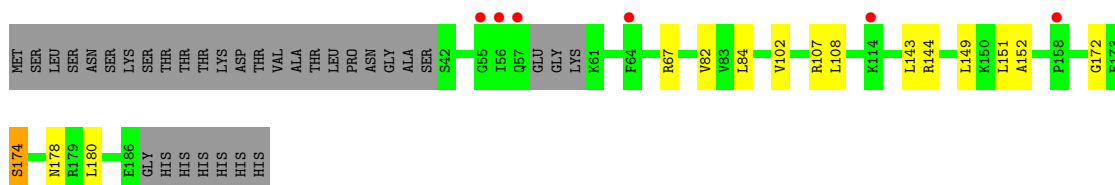
- Molecule 1: Invasion-associated protein B

Chain E: 



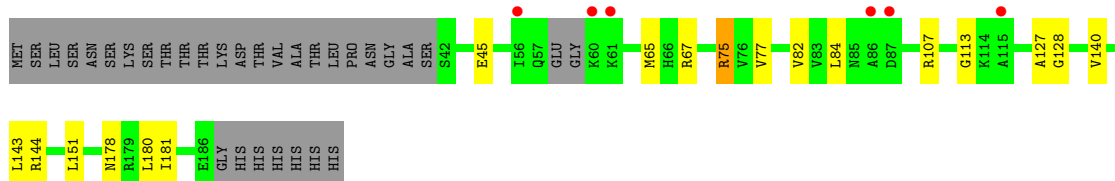
- Molecule 1: Invasion-associated protein B

Chain F:



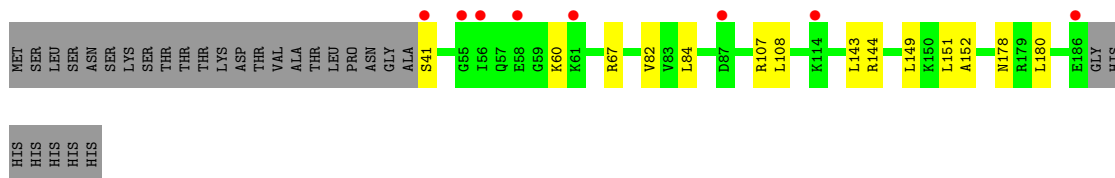
- Molecule 1: Invasion-associated protein B

Chain G:



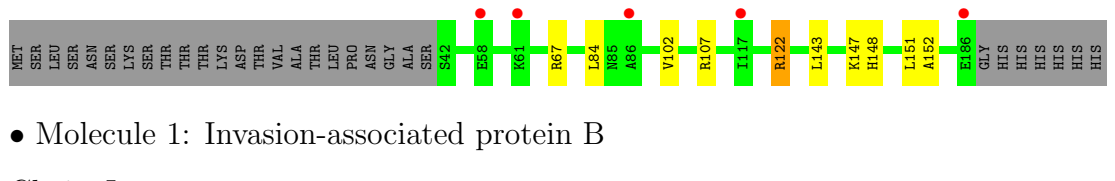
- Molecule 1: Invasion-associated protein B

Chain H:



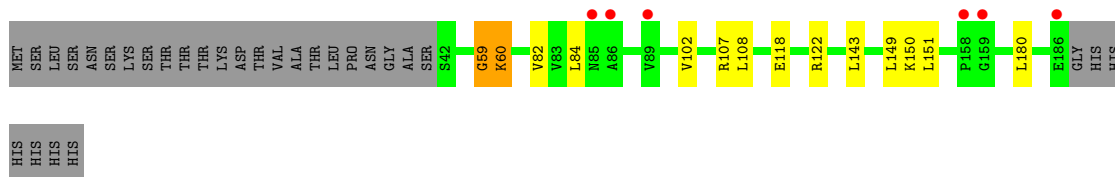
- Molecule 1: Invasion-associated protein B

Chain I:

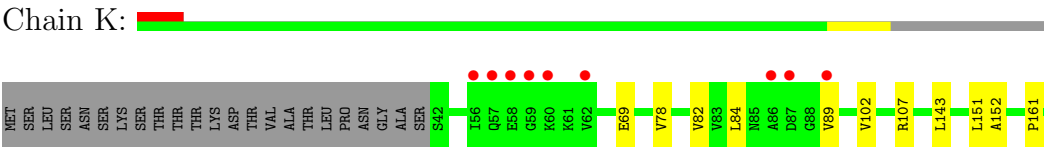


- Molecule 1: Invasion-associated protein B

Chain J:

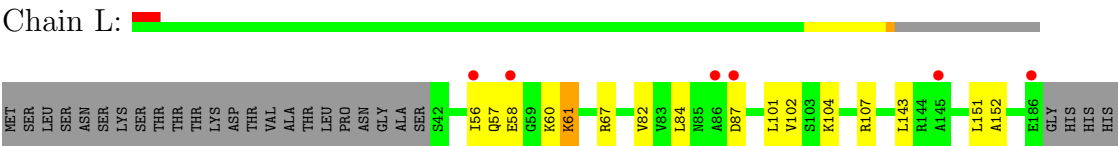


● Molecule 1: Invasion-associated protein B



GLY
HIS
HIS
HIS
HIS
HIS
HIS

● Molecule 1: Invasion-associated protein B



HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.71Å 139.95Å 179.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 36.76 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.35) 99.3 (36.76-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.265 0.232 , 0.264	Depositor DCC
R_{free} test set	3005 reflections (3.10%)	DCC
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 99857 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13760	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.40	0/1090	0.61	0/1480
1	B	0.39	0/1136	0.61	0/1541
1	C	0.43	0/1134	0.63	0/1539
1	D	0.37	0/1132	0.61	0/1536
1	E	0.38	0/1110	0.59	0/1505
1	F	0.40	0/1112	0.62	0/1508
1	G	0.42	0/1116	0.63	0/1514
1	H	0.37	0/1138	0.61	0/1544
1	I	0.40	0/1131	0.60	0/1535
1	J	0.45	0/1130	0.61	0/1533
1	K	0.42	0/1135	0.61	0/1539
1	L	0.40	0/1130	0.61	0/1533
All	All	0.40	0/13494	0.61	0/18307

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	J	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	59	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1074	0	1110	5	0
1	B	1113	0	1155	5	0
1	C	1113	0	1148	12	0
1	D	1109	0	1152	8	0
1	E	1091	0	1136	2	0
1	F	1090	0	1136	8	0
1	G	1097	0	1137	11	0
1	H	1115	0	1157	3	0
1	I	1108	0	1155	3	0
1	J	1107	0	1151	7	0
1	K	1112	0	1159	3	0
1	L	1107	0	1151	7	0
2	B	12	0	16	0	0
2	C	24	0	31	2	0
2	D	6	0	8	0	0
2	F	6	0	8	5	0
2	G	6	0	8	4	0
2	H	12	0	16	0	0
2	I	18	0	24	1	0
2	J	6	0	8	0	0
2	K	6	0	8	0	0
2	L	12	0	16	0	0
3	A	31	0	0	0	0
3	B	46	0	0	0	0
3	C	44	0	0	0	0
3	D	35	0	0	0	0
3	E	28	0	0	0	0
3	F	44	0	0	0	0
3	G	39	0	0	0	0
3	H	25	0	0	0	0
3	I	35	0	0	0	0
3	J	32	0	0	0	0
3	K	32	0	0	0	0
3	L	25	0	0	0	0
All	All	13760	0	13890	65	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (65) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:185:LYS:HE2	1:J:60:LYS:HE3	1.29	1.09
1:L:61:LYS:O	1:L:61:LYS:HG2	1.66	0.95
1:C:185:LYS:CE	1:J:60:LYS:HE3	2.03	0.88
1:F:174:SER:H	2:F:1:GOL:H31	1.46	0.80
1:L:61:LYS:CG	1:L:61:LYS:O	2.30	0.80
1:F:174:SER:HB3	2:F:1:GOL:H32	1.63	0.79
1:C:185:LYS:HE2	1:J:60:LYS:CE	2.16	0.72
1:C:144:ARG:NH2	1:C:178:ASN:OD1	2.29	0.64
1:B:144:ARG:NH2	1:B:178:ASN:OD1	2.31	0.64
1:F:172:GLY:HA2	2:F:1:GOL:H12	1.80	0.63
1:F:172:GLY:CA	2:F:1:GOL:H12	2.28	0.62
1:F:144[B]:ARG:NH1	1:F:178:ASN:OD1	2.33	0.61
1:B:86:ALA:HA	1:B:184:GLN:HE22	1.67	0.58
1:I:122[A]:ARG:HB2	2:I:194:GOL:H2	1.87	0.55
1:C:167:PHE:CZ	1:G:45:GLU:HG2	2.41	0.55
1:F:174:SER:HB3	2:F:1:GOL:C3	2.35	0.55
1:A:144:ARG:NH2	1:A:178:ASN:OD1	2.40	0.54
1:G:181:ILE:HG21	1:L:60:LYS:HG3	1.91	0.53
1:G:77:VAL:O	2:G:1:GOL:H12	2.08	0.53
1:F:107:ARG:HB3	1:F:152:ALA:HB3	1.92	0.52
1:A:107:ARG:HB3	1:A:152:ALA:HB3	1.91	0.51
1:L:57:GLN:O	1:L:58:GLU:C	2.48	0.51
1:C:107:ARG:HB3	1:C:152:ALA:HB3	1.92	0.51
1:H:144:ARG:NH2	1:H:178:ASN:OD1	2.44	0.51
1:C:102:VAL:HG13	1:E:102:VAL:HG13	1.93	0.50
1:C:70:VAL:HG22	2:C:1:GOL:H32	1.93	0.50
1:A:69:GLU:HB2	1:A:78:VAL:HG13	1.93	0.50
1:C:140:VAL:O	1:C:144:ARG:HG3	2.12	0.50
1:C:167:PHE:HZ	1:G:45:GLU:HG2	1.78	0.48
1:L:56:ILE:HG13	1:L:56:ILE:O	2.13	0.48
1:D:147:LYS:O	1:D:148:HIS:HD2	1.96	0.48
1:B:107:ARG:HB3	1:B:152:ALA:HB3	1.97	0.47
1:F:108:LEU:HD23	1:F:149:LEU:HD21	1.97	0.47
1:G:144:ARG:NH2	1:G:178:ASN:OD1	2.47	0.46
1:I:107:ARG:HB3	1:I:152:ALA:HB3	1.98	0.46
1:D:85:ASN:HD22	1:D:89:VAL:HB	1.80	0.46
1:K:107:ARG:HB3	1:K:152:ALA:HB3	1.96	0.46
1:D:122[B]:ARG:HD2	1:D:132:PRO:HG3	1.98	0.46
1:G:75:ARG:NH1	2:G:1:GOL:O2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:101:LEU:HD23	1:L:104:LYS:HG3	1.97	0.44
1:H:108:LEU:HD23	1:H:149:LEU:HD21	1.99	0.44
1:D:144:ARG:NH2	1:D:178:ASN:OD1	2.50	0.44
1:J:107[B]:ARG:HG3	1:J:118:GLU:HG3	1.99	0.44
1:C:48:GLY:N	2:C:195:GOL:H2	2.33	0.44
1:B:140:VAL:O	1:B:144:ARG:HG3	2.17	0.43
1:E:108:LEU:HD23	1:E:149:LEU:HD21	1.99	0.43
1:D:107:ARG:HB3	1:D:152:ALA:HB3	2.00	0.43
1:B:102:VAL:HB	1:J:122:ARG:O	2.19	0.43
1:H:107:ARG:HB3	1:H:152:ALA:HB3	2.01	0.43
1:K:69:GLU:HB2	1:K:78:VAL:HG13	2.00	0.42
1:G:140:VAL:O	1:G:144:ARG:HG3	2.20	0.42
1:C:108:LEU:HD23	1:C:149:LEU:HD21	2.01	0.42
1:D:43:LEU:HD12	1:D:43:LEU:HA	1.79	0.42
1:G:65:MET:HB2	1:G:180:LEU:HD11	2.02	0.41
1:A:56:ILE:HA	1:A:61:LYS:HA	2.02	0.41
1:J:108:LEU:HD23	1:J:149:LEU:HD21	2.02	0.41
1:I:147:LYS:O	1:I:148:HIS:HD2	2.03	0.41
1:D:69:GLU:HB2	1:D:78:VAL:HG13	2.03	0.41
1:G:127:ALA:O	2:G:1:GOL:H31	2.20	0.41
1:G:113:GLY:HA2	1:K:161:PRO:HA	2.02	0.41
1:L:107:ARG:HB3	1:L:152:ALA:HB3	2.02	0.41
1:D:108:LEU:HD23	1:D:149:LEU:HD21	2.02	0.41
1:A:108:LEU:HD23	1:A:149:LEU:HD21	2.02	0.40
1:G:128:GLY:HA3	2:G:1:GOL:H31	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	138/175 (79%)	137 (99%)	1 (1%)	0	100	100
1	B	146/175 (83%)	143 (98%)	3 (2%)	0	100	100
1	C	146/175 (83%)	143 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	145/175 (83%)	142 (98%)	3 (2%)	0	100	100
1	E	140/175 (80%)	139 (99%)	1 (1%)	0	100	100
1	F	140/175 (80%)	140 (100%)	0	0	100	100
1	G	141/175 (81%)	140 (99%)	1 (1%)	0	100	100
1	H	146/175 (83%)	144 (99%)	2 (1%)	0	100	100
1	I	145/175 (83%)	145 (100%)	0	0	100	100
1	J	145/175 (83%)	142 (98%)	2 (1%)	1 (1%)	30	34
1	K	145/175 (83%)	142 (98%)	3 (2%)	0	100	100
1	L	145/175 (83%)	141 (97%)	4 (3%)	0	100	100
All	All	1722/2100 (82%)	1698 (99%)	23 (1%)	1 (0%)	59	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	59	GLY

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	119/147 (81%)	110 (92%)	9 (8%)	19	21
1	B	123/147 (84%)	116 (94%)	7 (6%)	29	34
1	C	123/147 (84%)	115 (94%)	8 (6%)	24	27
1	D	123/147 (84%)	116 (94%)	7 (6%)	29	34
1	E	121/147 (82%)	114 (94%)	7 (6%)	28	33
1	F	121/147 (82%)	113 (93%)	8 (7%)	24	26
1	G	122/147 (83%)	115 (94%)	7 (6%)	29	34
1	H	124/147 (84%)	116 (94%)	8 (6%)	24	27
1	I	123/147 (84%)	116 (94%)	7 (6%)	29	34
1	J	123/147 (84%)	116 (94%)	7 (6%)	29	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	123/147 (84%)	116 (94%)	7 (6%)	29	34
1	L	123/147 (84%)	115 (94%)	8 (6%)	24	27
All	All	1468/1764 (83%)	1378 (94%)	90 (6%)	26	31

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	75	ARG
1	A	78	VAL
1	A	82	VAL
1	A	84	LEU
1	A	102	VAL
1	A	143	LEU
1	A	151	LEU
1	A	180	LEU
1	B	67	ARG
1	B	84	LEU
1	B	87	ASP
1	B	102	VAL
1	B	143	LEU
1	B	151	LEU
1	B	180	LEU
1	C	82	VAL
1	C	84	LEU
1	C	102	VAL
1	C	143	LEU
1	C	151	LEU
1	C	174	SER
1	C	180	LEU
1	C	185	LYS
1	D	42	SER
1	D	43	LEU
1	D	82	VAL
1	D	102	VAL
1	D	114	LYS
1	D	143	LEU
1	D	151	LEU
1	E	67	ARG
1	E	82	VAL
1	E	84	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	102	VAL
1	E	143	LEU
1	E	151	LEU
1	E	180	LEU
1	F	67	ARG
1	F	82	VAL
1	F	84	LEU
1	F	102	VAL
1	F	143	LEU
1	F	151	LEU
1	F	174	SER
1	F	180	LEU
1	G	67	ARG
1	G	75	ARG
1	G	82	VAL
1	G	84	LEU
1	G	107	ARG
1	G	143	LEU
1	G	151	LEU
1	H	41	SER
1	H	60	LYS
1	H	67	ARG
1	H	82	VAL
1	H	84	LEU
1	H	143	LEU
1	H	151	LEU
1	H	180	LEU
1	I	67	ARG
1	I	84	LEU
1	I	102	VAL
1	I	122[A]	ARG
1	I	122[B]	ARG
1	I	143	LEU
1	I	151	LEU
1	J	60	LYS
1	J	82	VAL
1	J	84	LEU
1	J	143	LEU
1	J	150	LYS
1	J	151	LEU
1	J	180	LEU
1	K	82	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	84	LEU
1	K	89	VAL
1	K	102	VAL
1	K	143	LEU
1	K	151	LEU
1	K	180	LEU
1	L	61	LYS
1	L	67	ARG
1	L	82	VAL
1	L	84	LEU
1	L	87	ASP
1	L	102	VAL
1	L	143	LEU
1	L	151	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	B	85	ASN
1	B	148	HIS
1	B	184	GLN
1	C	68	GLN
1	C	85	ASN
1	C	148	HIS
1	D	53	ASN
1	D	85	ASN
1	D	148	HIS
1	E	85	ASN
1	E	148	HIS
1	F	148	HIS
1	G	148	HIS
1	H	57	GLN
1	H	148	HIS
1	I	148	HIS
1	J	148	HIS
1	J	184	GLN
1	K	148	HIS
1	L	148	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 ligands are 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	GOL	B	1	-	5,5,5	0.34	0	5,5,5	0.37	0
2	GOL	B	194	-	5,5,5	0.31	0	5,5,5	0.26	0
2	GOL	C	1	-	5,5,5	0.33	0	5,5,5	0.46	0
2	GOL	C	194	-	5,5,5	0.31	0	5,5,5	0.63	0
2	GOL	C	195	-	5,5,5	1.04	1 (20%)	5,5,5	0.61	0
2	GOL	C	196	-	5,5,5	0.37	0	5,5,5	0.35	0
2	GOL	D	1	-	5,5,5	0.35	0	5,5,5	0.44	0
2	GOL	F	1	-	5,5,5	0.71	0	5,5,5	0.53	0
2	GOL	G	1	-	5,5,5	0.78	0	5,5,5	0.82	0
2	GOL	H	1	-	5,5,5	0.35	0	5,5,5	0.29	0
2	GOL	H	194	-	5,5,5	0.33	0	5,5,5	0.26	0
2	GOL	I	1	-	5,5,5	0.29	0	5,5,5	0.52	0
2	GOL	I	194	-	5,5,5	0.32	0	5,5,5	0.19	0
2	GOL	I	195	-	5,5,5	0.33	0	5,5,5	0.26	0
2	GOL	J	1	-	5,5,5	0.74	0	5,5,5	0.48	0
2	GOL	K	1	-	5,5,5	0.33	0	5,5,5	0.29	0
2	GOL	L	1	-	5,5,5	0.33	0	5,5,5	0.23	0
2	GOL	L	194	-	5,5,5	0.33	0	5,5,5	0.23	0

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	GOL	B	1	-	-	0/4/4/4	0/0/0/0
2	GOL	B	194	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1	-	-	0/4/4/4	0/0/0/0
2	GOL	C	194	-	-	0/4/4/4	0/0/0/0
2	GOL	C	195	-	-	0/4/4/4	0/0/0/0
2	GOL	C	196	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1	-	-	0/4/4/4	0/0/0/0
2	GOL	F	1	-	-	0/4/4/4	0/0/0/0
2	GOL	G	1	-	-	0/4/4/4	0/0/0/0
2	GOL	H	1	-	-	0/4/4/4	0/0/0/0
2	GOL	H	194	-	-	0/4/4/4	0/0/0/0
2	GOL	I	1	-	-	0/4/4/4	0/0/0/0
2	GOL	I	194	-	-	0/4/4/4	0/0/0/0
2	GOL	I	195	-	-	0/4/4/4	0/0/0/0
2	GOL	J	1	-	-	0/4/4/4	0/0/0/0
2	GOL	K	1	-	-	0/4/4/4	0/0/0/0
2	GOL	L	1	-	-	0/4/4/4	0/0/0/0
2	GOL	L	194	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	195	GOL	O2-C2	-2.17	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	142/175 (81%)	0.52	9 (6%) 19 22	32, 46, 80, 108	0
1	B	146/175 (83%)	0.25	2 (1%) 72 76	32, 45, 73, 87	0
1	C	147/175 (84%)	0.40	2 (1%) 72 76	31, 45, 73, 108	0
1	D	145/175 (82%)	0.43	6 (4%) 35 39	31, 46, 83, 111	0
1	E	143/175 (81%)	0.41	9 (6%) 19 22	32, 45, 80, 116	0
1	F	142/175 (81%)	0.37	6 (4%) 35 38	31, 45, 71, 104	0
1	G	143/175 (81%)	0.40	6 (4%) 35 38	32, 46, 77, 98	0
1	H	146/175 (83%)	0.21	8 (5%) 24 27	32, 47, 81, 113	0
1	I	145/175 (82%)	0.28	5 (3%) 43 47	32, 46, 78, 86	0
1	J	145/175 (82%)	0.34	6 (4%) 35 39	31, 46, 77, 96	0
1	K	145/175 (82%)	0.30	9 (6%) 20 22	32, 46, 91, 119	0
1	L	145/175 (82%)	0.25	6 (4%) 35 39	32, 46, 92, 128	0
All	All	1734/2100 (82%)	0.35	74 (4%) 34 37	31, 46, 81, 128	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	86	ALA	8.4
1	E	56	ILE	6.7
1	K	56	ILE	6.0
1	K	86	ALA	5.7
1	D	56	ILE	5.2
1	H	58	GLU	4.4
1	G	60	LYS	4.3
1	L	56	ILE	4.3
1	E	60	LYS	4.2
1	H	41	SER	4.1
1	K	87	ASP	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	87	ASP	4.0
1	K	58	GLU	3.9
1	A	56	ILE	3.9
1	J	158	PRO	3.8
1	F	57	GLN	3.8
1	H	56	ILE	3.8
1	L	58	GLU	3.7
1	D	58	GLU	3.7
1	F	56	ILE	3.6
1	E	186	GLU	3.6
1	I	186	GLU	3.5
1	D	61	LYS	3.5
1	J	159	GLY	3.5
1	G	56	ILE	3.4
1	L	87	ASP	3.4
1	L	86	ALA	3.3
1	K	60	LYS	3.3
1	C	188	HIS	3.2
1	E	86	ALA	3.2
1	H	186	GLU	3.0
1	E	57	GLN	3.0
1	H	114	LYS	3.0
1	A	158	PRO	2.9
1	I	58	GLU	2.9
1	F	114	LYS	2.9
1	H	55	GLY	2.9
1	A	186	GLU	2.9
1	G	61	LYS	2.8
1	A	87	ASP	2.8
1	D	59	GLY	2.8
1	K	57	GLN	2.7
1	G	86	ALA	2.6
1	I	86	ALA	2.6
1	A	86	ALA	2.5
1	E	55	GLY	2.5
1	A	61	LYS	2.5
1	H	87	ASP	2.5
1	J	186	GLU	2.5
1	A	57	GLN	2.5
1	A	184	GLN	2.5
1	L	186	GLU	2.4
1	E	84	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	115	ALA	2.4
1	B	186	GLU	2.4
1	D	55	GLY	2.4
1	K	62	VAL	2.3
1	D	60	LYS	2.3
1	A	89	VAL	2.3
1	F	158	PRO	2.3
1	F	55	GLY	2.3
1	H	61	LYS	2.3
1	J	85	ASN	2.3
1	E	89	VAL	2.2
1	I	61	LYS	2.2
1	I	117	ILE	2.2
1	L	145	ALA	2.2
1	K	59	GLY	2.1
1	C	186	GLU	2.1
1	B	185	LYS	2.1
1	J	89	VAL	2.0
1	G	87	ASP	2.0
1	K	89	VAL	2.0
1	F	64	PHE	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	L	1	6/6	0.38	23.66	70,77,78,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	C	1	6/6	0.34	19.87	45,52,59,69	0
2	GOL	J	1	6/6	0.34	15.31	55,70,75,75	0
2	GOL	D	1	6/6	0.46	13.51	54,69,71,78	0
2	GOL	C	195	6/6	0.36	11.32	34,61,63,66	0
2	GOL	F	1	6/6	0.31	6.91	49,53,60,68	0
2	GOL	L	194	6/6	0.26	6.89	81,88,89,92	0
2	GOL	H	1	6/6	0.34	6.55	61,70,75,78	0
2	GOL	B	194	6/6	0.30	5.43	73,75,79,84	0
2	GOL	I	194	6/6	0.24	5.00	73,81,84,88	0
2	GOL	I	1	6/6	0.28	4.67	65,70,73,81	0
2	GOL	C	194	6/6	0.25	3.89	46,53,60,63	0
2	GOL	K	1	6/6	0.20	3.73	72,75,76,79	0
2	GOL	I	195	6/6	0.26	3.62	55,60,63,65	0
2	GOL	B	1	6/6	0.31	3.24	75,84,86,87	0
2	GOL	C	196	6/6	0.26	3.22	68,77,85,87	0
2	GOL	G	1	6/6	0.25	2.77	64,77,81,83	0
2	GOL	H	194	6/6	0.22	1.86	66,73,78,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.