



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:43 AM UTC

PDB ID : 8ACU / pdb_00008acu
Title : Structure of Bacillus subtilis Rel in complex with DarB
Authors : Garcia-Pino, A.
Deposited on : 2022-07-06
Resolution : 2.97 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

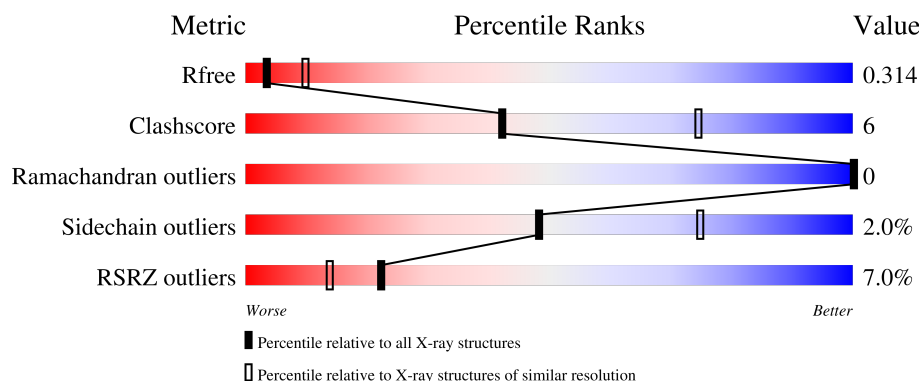
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	373	5% 81% 12% 6%
1	B	373	12% 72% 16% • 11%
2	E	147	2% 80% 14% 5%
2	F	147	2% 80% 16% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7219 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 GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2635	1679	453	493	10			
1	B	331	Total	C	N	O	S	0	0	0
			2371	1507	406	447	11			

- Molecule 2 is a protein called CBS domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	139	Total	C	N	O	S	0	1	0
			1091	697	187	200	7			
2	F	140	Total	C	N	O	S	0	0	0
			1078	689	179	203	7			

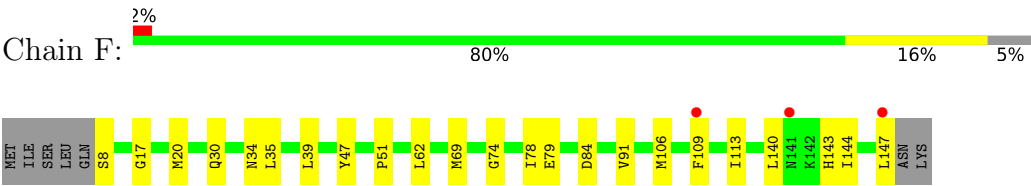
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	17	Total	O	0	0
			17	17		
4	E	7	Total	O	0	0
			7	7		
4	F	2	Total	O	0	0
			2	2		

● Molecule 2: CBS domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.40Å 98.14Å 126.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.72 – 2.97 75.72 – 2.97	Depositor EDS
% Data completeness (in resolution range)	90.0 (75.72-2.97) 90.1 (75.72-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.260 , 0.315 0.261 , 0.314	Depositor DCC
R_{free} test set	1118 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.15	0/2686	0.38	1/3657 (0.0%)
1	B	0.24	0/2416	0.52	2/3303 (0.1%)
2	E	0.09	0/1111	0.27	0/1503
2	F	0.11	0/1095	0.32	0/1485
All	All	0.17	0/7308	0.41	3/9948 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	ASN	N-CA-C	-6.15	105.47	114.39
1	B	30	LYS	N-CA-C	-5.81	104.95	111.28
1	B	69	SER	N-CA-C	-5.59	105.18	111.28

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	2635	0	2445	25	0
1	B	2371	0	2096	37	0
2	E	1091	0	1099	18	0
2	F	1078	0	1062	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	16	0	0	1	0
4	B	17	0	0	1	0
4	E	7	0	0	1	0
4	F	2	0	0	0	0
All	All	7219	0	6702	88	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 6.

All (88) 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:B:79:VAL:O	1:B:83:THR:HG22	1.67	0.95
1:B:221:VAL:HG21	1:B:323:LEU:HD13	1.57	0.87
1:B:79:VAL:O	1:B:83:THR:CG2	2.28	0.80
1:B:28:VAL:O	1:B:31:ALA:HB3	1.97	0.65
1:B:229:VAL:HG22	1:B:234:ILE:HB	1.79	0.63
2:E:144:ILE:HG12	2:F:109:PHE:HE2	1.62	0.63
2:F:144:ILE:HD12	2:F:147:LEU:HD12	1.81	0.63
2:E:39:LEU:HD21	2:F:69:MET:HE2	1.83	0.61
2:E:28:HIS:HE1	2:E:30:GLN:HE21	1.49	0.60
1:A:207:MET:SD	4:A:516:HOH:O	2.56	0.60
1:A:126:LYS:HZ1	1:A:177:ARG:HH21	1.49	0.59
1:A:292:MET:HE3	1:A:295:ARG:HG3	1.86	0.58
1:B:275:ILE:HD13	2:E:24:ASP:HB3	1.86	0.58
1:B:77:HIS:HB2	1:B:105:VAL:HG11	1.85	0.58
1:B:35:ALA:HB1	1:B:51:ILE:HD11	1.84	0.57
1:A:83:THR:HG22	1:A:84:ASP:H	1.70	0.57
2:E:69:MET:HE2	2:F:39:LEU:HD21	1.87	0.56
1:A:181:SER:HB3	1:A:337:GLU:HA	1.86	0.56
1:B:53:HIS:HB3	1:B:54:PRO:HD3	1.89	0.55
2:E:89:GLU:HA	2:E:92:MET:HG2	1.90	0.54
1:B:108:LEU:HD11	1:B:132:ALA:HB2	1.90	0.54
1:A:199:GLN:HA	1:A:202:ARG:HD3	1.90	0.52
1:B:134:ASP:HB3	1:B:137:VAL:HG23	1.91	0.51
2:F:8:SER:HA	2:F:143:HIS:HE1	1.75	0.51
1:A:299:TYR:HB2	1:A:310:SER:H	1.74	0.51
2:E:144:ILE:CG1	2:F:109:PHE:HE2	2.24	0.51
1:A:83:THR:HG22	1:A:84:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:SER:HB2	1:B:185:TRP:CZ2	2.47	0.49
1:A:243:LYS:HB3	1:A:248:ILE:HD11	1.95	0.49
2:E:144:ILE:HG12	2:F:109:PHE:CE2	2.46	0.49
1:B:66:MET:HE3	1:B:67:ASP:H	1.77	0.49
1:B:52:ILE:O	1:B:56:GLN:HG2	2.13	0.49
1:A:19:TYR:CZ	1:A:65:GLU:HA	2.49	0.48
1:A:190:THR:HA	1:A:193:ARG:HG2	1.95	0.48
2:F:17:GLY:HA2	2:F:20:MET:HG2	1.96	0.48
1:A:60:ILE:HD13	1:A:146:LEU:HD23	1.96	0.48
1:A:53:HIS:HB3	1:A:54:PRO:HD3	1.94	0.48
1:B:124:HIS:ND1	1:B:170:ILE:HD11	2.29	0.47
1:B:170:ILE:O	1:B:174:LEU:HB2	2.14	0.47
1:B:35:ALA:HB1	1:B:51:ILE:CD1	2.44	0.47
1:B:176:HIS:HB2	1:B:184:LYS:HE3	1.95	0.47
2:E:144:ILE:HD13	2:F:106:MET:HE1	1.97	0.47
1:A:37:ASP:HA	1:A:40:ARG:HH11	1.79	0.47
1:A:126:LYS:HZ1	1:A:177:ARG:NH2	2.13	0.46
1:A:180:ILE:HG12	1:A:338:TYR:O	2.15	0.46
1:B:178:LEU:HD23	1:B:340:VAL:HB	1.96	0.46
1:A:252:MET:O	1:A:255:GLN:O	2.33	0.46
1:B:22:ASP:C	1:B:24:HIS:H	2.23	0.46
1:B:221:VAL:HG13	1:B:289:TRP:CH2	2.51	0.46
1:B:91:LYS:HG3	1:B:96:GLU:HA	1.97	0.45
2:F:74:GLY:HA3	2:F:79:GLU:OE2	2.15	0.45
1:A:241:ARG:HB3	1:A:267:ALA:HB3	1.98	0.45
2:F:51:PRO:HA	2:F:62:LEU:HD23	1.98	0.45
2:F:109:PHE:CE1	2:F:140:LEU:HD21	2.51	0.45
2:E:45:THR:HG23	2:E:47:TYR:H	1.81	0.45
2:F:34:ASN:HD22	2:F:84:ASP:HA	1.82	0.45
1:B:309:GLN:HG2	1:B:332:MET:SD	2.57	0.45
1:A:304:LYS:HE2	1:A:308:TYR:CD2	2.52	0.44
1:B:97:GLU:HG2	1:B:98:VAL:N	2.31	0.44
1:A:25:ILE:HA	1:A:28:VAL:HG22	2.00	0.44
2:E:112:VAL:HG21	2:E:136:VAL:HG21	2.00	0.44
1:B:150:ARG:HB2	4:B:513:HOH:O	2.18	0.43
1:B:271:LEU:HA	1:B:328:ARG:O	2.18	0.43
1:B:292:MET:HE2	1:B:316:ILE:HD12	2.00	0.43
1:B:221:VAL:HG21	1:B:323:LEU:CD1	2.40	0.42
2:E:12:LEU:HA	2:E:105:ILE:HD11	2.00	0.42
2:E:134:ARG:HG3	2:F:113:ILE:O	2.19	0.42
1:B:134:ASP:OD2	1:B:136:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:TYR:HA	1:B:252:MET:HE2	2.00	0.42
1:B:309:GLN:O	1:B:328:ARG:HG3	2.18	0.42
1:B:79:VAL:O	1:B:83:THR:HG23	2.18	0.42
1:B:346:TYR:O	1:B:347:LYS:C	2.62	0.42
1:B:51:ILE:HD12	1:B:51:ILE:HA	1.77	0.42
1:A:207:MET:O	1:A:211:ARG:HG3	2.20	0.41
1:B:223:ASN:O	1:B:227:LYS:HG2	2.20	0.41
2:E:82:LYS:NZ	4:E:201:HOH:O	2.53	0.41
2:E:34:ASN:HD22	2:E:84:ASP:HA	1.86	0.41
2:F:35:LEU:HD11	2:F:91:VAL:HG21	2.02	0.41
1:B:152:LEU:HD11	1:B:163:ILE:HD12	2.02	0.41
2:E:144:ILE:CD1	2:F:109:PHE:HE2	2.34	0.41
1:A:289:TRP:HB3	1:A:317:GLY:H	1.86	0.41
1:A:152:LEU:HG	1:A:160:GLN:HG2	2.03	0.41
1:B:293:PRO:HG3	2:F:78:ILE:HG12	2.03	0.41
1:A:184:LYS:HE2	1:A:188:GLU:OE2	2.20	0.40
1:A:14:ASP:HA	1:A:17:ARG:HG3	2.03	0.40
2:E:17:GLY:HA2	2:E:20:MET:HG2	2.02	0.40
2:E:140:LEU:HD13	2:F:140:LEU:HD23	2.03	0.40
2:F:8:SER:HA	2:F:143:HIS:CE1	2.54	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	343/373 (92%)	335 (98%)	8 (2%)	0	100	100
1	B	325/373 (87%)	312 (96%)	13 (4%)	0	100	100
2	E	138/147 (94%)	137 (99%)	1 (1%)	0	100	100
2	F	138/147 (94%)	137 (99%)	1 (1%)	0	100	100
All	All	944/1040 (91%)	921 (98%)	23 (2%)	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	252/328 (77%)	249 (99%)	3 (1%)	63	82
1	B	209/328 (64%)	200 (96%)	9 (4%)	26	58
2	E	120/132 (91%)	120 (100%)	0	100	100
2	F	117/132 (89%)	115 (98%)	2 (2%)	53	77
All	All	698/920 (76%)	684 (98%)	14 (2%)	48	75

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	A	208	LYS
1	A	232	VAL
1	B	27	PHE
1	B	34	TYR
1	B	67	ASP
1	B	88	ASP
1	B	117	GLU
1	B	133	GLN
1	B	185	TRP
1	B	308	TYR
1	B	316	ILE
2	F	30	GLN
2	F	47	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	176	HIS
1	B	56	GLN

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Mol	Chain	Res	Type
1	B	176	HIS
1	B	309	GLN
2	E	28	HIS
2	E	125	GLN
2	F	28	HIS
2	F	143	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	349/373 (93%)	0.57	18 (5%) 33 20	41, 89, 143, 178	0
1	B	331/373 (88%)	1.05	43 (12%) 7 5	46, 102, 144, 176	0
2	E	139/147 (94%)	0.09	3 (2%) 62 43	38, 62, 111, 148	1 (0%)
2	F	140/147 (95%)	0.24	3 (2%) 63 44	39, 67, 112, 143	0
All	All	959/1040 (92%)	0.62	67 (6%) 22 14	38, 86, 141, 178	1 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	HIS	7.5
1	B	31	ALA	5.8
1	B	28	VAL	4.8
1	B	264	ASP	4.6
1	A	365	PHE	4.4
1	B	245	ILE	4.2
1	B	35	ALA	4.2
1	B	13	ILE	3.8
1	B	68	PRO	3.8
1	B	203	ILE	3.7
1	A	188	GLU	3.6
1	B	204	VAL	3.6
1	A	25	ILE	3.5
1	B	97	GLU	3.4
1	B	146	LEU	3.3
1	A	254	LEU	3.3
1	A	258	GLN	3.2
1	A	190	THR	3.2
1	B	86	THR	3.1
1	A	165	ASN	3.0
1	B	32	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	265	LEU	2.9
1	B	22	ASP	2.9
1	B	262	ILE	2.9
1	B	94	PHE	2.9
1	A	294	GLY	2.8
1	B	50	TYR	2.8
1	B	259	PHE	2.7
2	E	147	LEU	2.7
2	F	109	PHE	2.7
1	A	192	LEU	2.6
1	B	45	LYS	2.6
1	A	41	GLU	2.6
1	B	76	LEU	2.6
1	B	27	PHE	2.6
1	A	249	TYR	2.5
1	B	98	VAL	2.5
1	B	75	PHE	2.5
1	A	14	ASP	2.5
1	B	101	LEU	2.4
1	A	118	GLU	2.4
1	B	99	ALA	2.4
1	B	20	LEU	2.4
1	A	130	ALA	2.4
1	A	175	ALA	2.4
1	B	132	ALA	2.4
1	B	205	ASN	2.3
2	E	10	GLN	2.3
1	B	57	VAL	2.3
1	B	218	VAL	2.3
1	B	12	VAL	2.3
1	B	25	ILE	2.2
1	A	253	VAL	2.2
2	E	11	LEU	2.1
2	F	141	ASN	2.1
1	B	67	ASP	2.1
2	F	147	LEU	2.1
1	B	9	ALA	2.1
1	B	7	LEU	2.1
1	B	70	THR	2.1
1	B	46	SER	2.0
1	A	90	LEU	2.0
1	B	177	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	111	ILE	2.0
1	B	142	LEU	2.0
1	B	152	LEU	2.0
1	A	121	ALA	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	A	401	1/1	0.96	0.10	99,99,99,99	0
3	MN	B	401	1/1	0.97	0.13	114,114,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.