wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2024 – 02:29 PM EDT

PDB ID	:	4MR0
Title	:	Crystal structure of PfbA, a surface adhesin of Streptococcus pneumoniae
Authors	:	Ponnuraj, K.; Beulin, D.S.J.
Deposited on	:	2013-09-17
Resolution	:	1.95 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 (i) 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 (1)) were used in the production of this report:

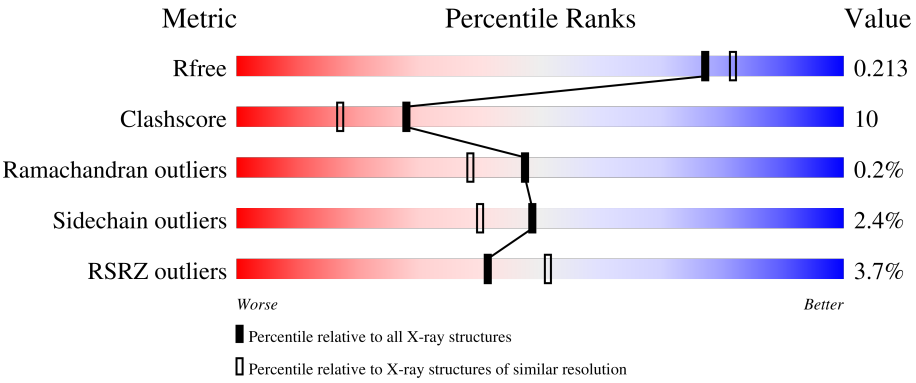
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	648	3% 56% 14% 30%
1	B	648	2% 57% 11% · 31%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7518 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 Plasmin and fibronectin-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3500	2199	599	697	5			
1	B	446	Total	C	N	O	S	0	0	0
			3430	2158	586	681	5			

There are 380 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	expression tag	UNP Q8CYC9
A	38	ARG	-	expression tag	UNP Q8CYC9
A	39	GLY	-	expression tag	UNP Q8CYC9
A	40	SER	-	expression tag	UNP Q8CYC9
A	41	HIS	-	expression tag	UNP Q8CYC9
A	42	HIS	-	expression tag	UNP Q8CYC9
A	43	HIS	-	expression tag	UNP Q8CYC9
A	44	HIS	-	expression tag	UNP Q8CYC9
A	45	HIS	-	expression tag	UNP Q8CYC9
A	46	HIS	-	expression tag	UNP Q8CYC9
A	47	GLY	-	expression tag	UNP Q8CYC9
A	48	SER	-	expression tag	UNP Q8CYC9
A	49	GLU	-	expression tag	UNP Q8CYC9
A	50	VAL	-	expression tag	UNP Q8CYC9
A	51	VAL	-	expression tag	UNP Q8CYC9
A	52	THR	-	expression tag	UNP Q8CYC9
A	53	SER	-	expression tag	UNP Q8CYC9
A	54	SER	-	expression tag	UNP Q8CYC9
A	55	SER	-	expression tag	UNP Q8CYC9
A	56	PRO	-	expression tag	UNP Q8CYC9
A	57	MET	-	expression tag	UNP Q8CYC9
A	58	ALA	-	expression tag	UNP Q8CYC9
A	59	THR	-	expression tag	UNP Q8CYC9
A	60	LYS	-	expression tag	UNP Q8CYC9
A	61	GLU	-	expression tag	UNP Q8CYC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	62	SER	-	expression tag	UNP Q8CYC9
A	63	SER	-	expression tag	UNP Q8CYC9
A	64	ASN	-	expression tag	UNP Q8CYC9
A	65	ALA	-	expression tag	UNP Q8CYC9
A	66	ILE	-	expression tag	UNP Q8CYC9
A	67	THR	-	expression tag	UNP Q8CYC9
A	68	ASN	-	expression tag	UNP Q8CYC9
A	69	ASP	-	expression tag	UNP Q8CYC9
A	70	LEU	-	expression tag	UNP Q8CYC9
A	71	ASP	-	expression tag	UNP Q8CYC9
A	72	ASN	-	expression tag	UNP Q8CYC9
A	73	SER	-	expression tag	UNP Q8CYC9
A	74	PRO	-	expression tag	UNP Q8CYC9
A	75	THR	-	expression tag	UNP Q8CYC9
A	76	VAL	-	expression tag	UNP Q8CYC9
A	77	ASN	-	expression tag	UNP Q8CYC9
A	78	GLN	-	expression tag	UNP Q8CYC9
A	79	ASN	-	expression tag	UNP Q8CYC9
A	80	ARG	-	expression tag	UNP Q8CYC9
A	81	SER	-	expression tag	UNP Q8CYC9
A	82	ALA	-	expression tag	UNP Q8CYC9
A	83	GLU	-	expression tag	UNP Q8CYC9
A	84	MET	-	expression tag	UNP Q8CYC9
A	85	ILE	-	expression tag	UNP Q8CYC9
A	86	ALA	-	expression tag	UNP Q8CYC9
A	87	SER	-	expression tag	UNP Q8CYC9
A	88	ASN	-	expression tag	UNP Q8CYC9
A	89	SER	-	expression tag	UNP Q8CYC9
A	90	THR	-	expression tag	UNP Q8CYC9
A	91	THR	-	expression tag	UNP Q8CYC9
A	92	ASN	-	expression tag	UNP Q8CYC9
A	93	GLY	-	expression tag	UNP Q8CYC9
A	94	LEU	-	expression tag	UNP Q8CYC9
A	95	ASP	-	expression tag	UNP Q8CYC9
A	96	ASN	-	expression tag	UNP Q8CYC9
A	97	SER	-	expression tag	UNP Q8CYC9
A	98	LEU	-	expression tag	UNP Q8CYC9
A	99	SER	-	expression tag	UNP Q8CYC9
A	100	VAL	-	expression tag	UNP Q8CYC9
A	101	ASN	-	expression tag	UNP Q8CYC9
A	102	SER	-	expression tag	UNP Q8CYC9
A	103	ILE	-	expression tag	UNP Q8CYC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP Q8CYC9
A	105	SER	-	expression tag	UNP Q8CYC9
A	106	ASN	-	expression tag	UNP Q8CYC9
A	107	GLY	-	expression tag	UNP Q8CYC9
A	108	THR	-	expression tag	UNP Q8CYC9
A	109	ILE	-	expression tag	UNP Q8CYC9
A	110	ARG	-	expression tag	UNP Q8CYC9
A	111	SER	-	expression tag	UNP Q8CYC9
A	112	ASN	-	expression tag	UNP Q8CYC9
A	113	SER	-	expression tag	UNP Q8CYC9
A	114	GLN	-	expression tag	UNP Q8CYC9
A	115	LEU	-	expression tag	UNP Q8CYC9
A	116	ASP	-	expression tag	UNP Q8CYC9
A	117	ASN	-	expression tag	UNP Q8CYC9
A	118	ARG	-	expression tag	UNP Q8CYC9
A	119	THR	-	expression tag	UNP Q8CYC9
A	120	VAL	-	expression tag	UNP Q8CYC9
A	121	GLU	-	expression tag	UNP Q8CYC9
A	122	SER	-	expression tag	UNP Q8CYC9
A	123	THR	-	expression tag	UNP Q8CYC9
A	124	VAL	-	expression tag	UNP Q8CYC9
A	125	THR	-	expression tag	UNP Q8CYC9
A	126	SER	-	expression tag	UNP Q8CYC9
A	127	THR	-	expression tag	UNP Q8CYC9
A	128	ASN	-	expression tag	UNP Q8CYC9
A	129	GLU	-	expression tag	UNP Q8CYC9
A	130	ASN	-	expression tag	UNP Q8CYC9
A	131	LYS	-	expression tag	UNP Q8CYC9
A	132	SER	-	expression tag	UNP Q8CYC9
A	133	TYR	-	expression tag	UNP Q8CYC9
A	134	LYS	-	expression tag	UNP Q8CYC9
A	135	GLU	-	expression tag	UNP Q8CYC9
A	136	ASP	-	expression tag	UNP Q8CYC9
A	137	VAL	-	expression tag	UNP Q8CYC9
A	138	ILE	-	expression tag	UNP Q8CYC9
A	139	SER	-	expression tag	UNP Q8CYC9
A	140	ASP	-	expression tag	UNP Q8CYC9
A	141	ARG	-	expression tag	UNP Q8CYC9
A	142	ILE	-	expression tag	UNP Q8CYC9
A	143	ILE	-	expression tag	UNP Q8CYC9
A	144	LYS	-	expression tag	UNP Q8CYC9
A	145	LYS	-	expression tag	UNP Q8CYC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	146	GLU	-	expression tag	UNP Q8CYC9
A	147	PHE	-	expression tag	UNP Q8CYC9
A	148	GLU	-	expression tag	UNP Q8CYC9
A	149	ASP	-	expression tag	UNP Q8CYC9
A	608	GLU	-	expression tag	UNP Q8CYC9
A	609	LYS	-	expression tag	UNP Q8CYC9
A	610	GLU	-	expression tag	UNP Q8CYC9
A	611	LYS	-	expression tag	UNP Q8CYC9
A	612	ASN	-	expression tag	UNP Q8CYC9
A	613	LYS	-	expression tag	UNP Q8CYC9
A	614	GLU	-	expression tag	UNP Q8CYC9
A	615	GLU	-	expression tag	UNP Q8CYC9
A	616	LYS	-	expression tag	UNP Q8CYC9
A	617	GLN	-	expression tag	UNP Q8CYC9
A	618	SER	-	expression tag	UNP Q8CYC9
A	619	ASN	-	expression tag	UNP Q8CYC9
A	620	SER	-	expression tag	UNP Q8CYC9
A	621	ASN	-	expression tag	UNP Q8CYC9
A	622	ASN	-	expression tag	UNP Q8CYC9
A	623	VAL	-	expression tag	UNP Q8CYC9
A	624	ILE	-	expression tag	UNP Q8CYC9
A	625	ASP	-	expression tag	UNP Q8CYC9
A	626	SER	-	expression tag	UNP Q8CYC9
A	627	ASN	-	expression tag	UNP Q8CYC9
A	628	GLN	-	expression tag	UNP Q8CYC9
A	629	LYS	-	expression tag	UNP Q8CYC9
A	630	ASN	-	expression tag	UNP Q8CYC9
A	631	GLY	-	expression tag	UNP Q8CYC9
A	632	GLU	-	expression tag	UNP Q8CYC9
A	633	PHE	-	expression tag	UNP Q8CYC9
A	634	ASN	-	expression tag	UNP Q8CYC9
A	635	SER	-	expression tag	UNP Q8CYC9
A	636	SER	-	expression tag	UNP Q8CYC9
A	637	LYS	-	expression tag	UNP Q8CYC9
A	638	ASP	-	expression tag	UNP Q8CYC9
A	639	ASN	-	expression tag	UNP Q8CYC9
A	640	ARG	-	expression tag	UNP Q8CYC9
A	641	GLN	-	expression tag	UNP Q8CYC9
A	642	MET	-	expression tag	UNP Q8CYC9
A	643	ASN	-	expression tag	UNP Q8CYC9
A	644	ASP	-	expression tag	UNP Q8CYC9
A	645	LYS	-	expression tag	UNP Q8CYC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	646	ILE	-	expression tag	UNP Q8CYC9
A	647	ASP	-	expression tag	UNP Q8CYC9
A	648	ASN	-	expression tag	UNP Q8CYC9
A	649	LYS	-	expression tag	UNP Q8CYC9
A	650	GLN	-	expression tag	UNP Q8CYC9
A	651	ASP	-	expression tag	UNP Q8CYC9
A	652	ASN	-	expression tag	UNP Q8CYC9
A	653	LYS	-	expression tag	UNP Q8CYC9
A	654	THR	-	expression tag	UNP Q8CYC9
A	655	GLU	-	expression tag	UNP Q8CYC9
A	656	GLU	-	expression tag	UNP Q8CYC9
A	657	VAL	-	expression tag	UNP Q8CYC9
A	658	ASN	-	expression tag	UNP Q8CYC9
A	659	TYR	-	expression tag	UNP Q8CYC9
A	660	LYS	-	expression tag	UNP Q8CYC9
A	661	ILE	-	expression tag	UNP Q8CYC9
A	662	VAL	-	expression tag	UNP Q8CYC9
A	663	GLY	-	expression tag	UNP Q8CYC9
A	664	ASP	-	expression tag	UNP Q8CYC9
A	665	GLY	-	expression tag	UNP Q8CYC9
A	666	ARG	-	expression tag	UNP Q8CYC9
A	667	GLU	-	expression tag	UNP Q8CYC9
A	668	THR	-	expression tag	UNP Q8CYC9
A	669	GLU	-	expression tag	UNP Q8CYC9
A	670	ASN	-	expression tag	UNP Q8CYC9
A	671	HIS	-	expression tag	UNP Q8CYC9
A	672	ILE	-	expression tag	UNP Q8CYC9
A	673	ASN	-	expression tag	UNP Q8CYC9
A	674	LYS	-	expression tag	UNP Q8CYC9
A	675	SER	-	expression tag	UNP Q8CYC9
A	676	LYS	-	expression tag	UNP Q8CYC9
A	677	GLU	-	expression tag	UNP Q8CYC9
A	678	ILE	-	expression tag	UNP Q8CYC9
A	679	VAL	-	expression tag	UNP Q8CYC9
A	680	ASP	-	expression tag	UNP Q8CYC9
A	681	VAL	-	expression tag	UNP Q8CYC9
A	682	LYS	-	expression tag	UNP Q8CYC9
A	683	GLN	-	expression tag	UNP Q8CYC9
A	684	LYS	-	expression tag	UNP Q8CYC9
B	37	MET	-	expression tag	UNP Q8CYC9
B	38	ARG	-	expression tag	UNP Q8CYC9
B	39	GLY	-	expression tag	UNP Q8CYC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	40	SER	-	expression tag	UNP Q8CYC9
B	41	HIS	-	expression tag	UNP Q8CYC9
B	42	HIS	-	expression tag	UNP Q8CYC9
B	43	HIS	-	expression tag	UNP Q8CYC9
B	44	HIS	-	expression tag	UNP Q8CYC9
B	45	HIS	-	expression tag	UNP Q8CYC9
B	46	HIS	-	expression tag	UNP Q8CYC9
B	47	GLY	-	expression tag	UNP Q8CYC9
B	48	SER	-	expression tag	UNP Q8CYC9
B	49	GLU	-	expression tag	UNP Q8CYC9
B	50	VAL	-	expression tag	UNP Q8CYC9
B	51	VAL	-	expression tag	UNP Q8CYC9
B	52	THR	-	expression tag	UNP Q8CYC9
B	53	SER	-	expression tag	UNP Q8CYC9
B	54	SER	-	expression tag	UNP Q8CYC9
B	55	SER	-	expression tag	UNP Q8CYC9
B	56	PRO	-	expression tag	UNP Q8CYC9
B	57	MET	-	expression tag	UNP Q8CYC9
B	58	ALA	-	expression tag	UNP Q8CYC9
B	59	THR	-	expression tag	UNP Q8CYC9
B	60	LYS	-	expression tag	UNP Q8CYC9
B	61	GLU	-	expression tag	UNP Q8CYC9
B	62	SER	-	expression tag	UNP Q8CYC9
B	63	SER	-	expression tag	UNP Q8CYC9
B	64	ASN	-	expression tag	UNP Q8CYC9
B	65	ALA	-	expression tag	UNP Q8CYC9
B	66	ILE	-	expression tag	UNP Q8CYC9
B	67	THR	-	expression tag	UNP Q8CYC9
B	68	ASN	-	expression tag	UNP Q8CYC9
B	69	ASP	-	expression tag	UNP Q8CYC9
B	70	LEU	-	expression tag	UNP Q8CYC9
B	71	ASP	-	expression tag	UNP Q8CYC9
B	72	ASN	-	expression tag	UNP Q8CYC9
B	73	SER	-	expression tag	UNP Q8CYC9
B	74	PRO	-	expression tag	UNP Q8CYC9
B	75	THR	-	expression tag	UNP Q8CYC9
B	76	VAL	-	expression tag	UNP Q8CYC9
B	77	ASN	-	expression tag	UNP Q8CYC9
B	78	GLN	-	expression tag	UNP Q8CYC9
B	79	ASN	-	expression tag	UNP Q8CYC9
B	80	ARG	-	expression tag	UNP Q8CYC9
B	81	SER	-	expression tag	UNP Q8CYC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	82	ALA	-	expression tag	UNP Q8CYC9
B	83	GLU	-	expression tag	UNP Q8CYC9
B	84	MET	-	expression tag	UNP Q8CYC9
B	85	ILE	-	expression tag	UNP Q8CYC9
B	86	ALA	-	expression tag	UNP Q8CYC9
B	87	SER	-	expression tag	UNP Q8CYC9
B	88	ASN	-	expression tag	UNP Q8CYC9
B	89	SER	-	expression tag	UNP Q8CYC9
B	90	THR	-	expression tag	UNP Q8CYC9
B	91	THR	-	expression tag	UNP Q8CYC9
B	92	ASN	-	expression tag	UNP Q8CYC9
B	93	GLY	-	expression tag	UNP Q8CYC9
B	94	LEU	-	expression tag	UNP Q8CYC9
B	95	ASP	-	expression tag	UNP Q8CYC9
B	96	ASN	-	expression tag	UNP Q8CYC9
B	97	SER	-	expression tag	UNP Q8CYC9
B	98	LEU	-	expression tag	UNP Q8CYC9
B	99	SER	-	expression tag	UNP Q8CYC9
B	100	VAL	-	expression tag	UNP Q8CYC9
B	101	ASN	-	expression tag	UNP Q8CYC9
B	102	SER	-	expression tag	UNP Q8CYC9
B	103	ILE	-	expression tag	UNP Q8CYC9
B	104	SER	-	expression tag	UNP Q8CYC9
B	105	SER	-	expression tag	UNP Q8CYC9
B	106	ASN	-	expression tag	UNP Q8CYC9
B	107	GLY	-	expression tag	UNP Q8CYC9
B	108	THR	-	expression tag	UNP Q8CYC9
B	109	ILE	-	expression tag	UNP Q8CYC9
B	110	ARG	-	expression tag	UNP Q8CYC9
B	111	SER	-	expression tag	UNP Q8CYC9
B	112	ASN	-	expression tag	UNP Q8CYC9
B	113	SER	-	expression tag	UNP Q8CYC9
B	114	GLN	-	expression tag	UNP Q8CYC9
B	115	LEU	-	expression tag	UNP Q8CYC9
B	116	ASP	-	expression tag	UNP Q8CYC9
B	117	ASN	-	expression tag	UNP Q8CYC9
B	118	ARG	-	expression tag	UNP Q8CYC9
B	119	THR	-	expression tag	UNP Q8CYC9
B	120	VAL	-	expression tag	UNP Q8CYC9
B	121	GLU	-	expression tag	UNP Q8CYC9
B	122	SER	-	expression tag	UNP Q8CYC9
B	123	THR	-	expression tag	UNP Q8CYC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	124	VAL	-	expression tag	UNP Q8CYC9
B	125	THR	-	expression tag	UNP Q8CYC9
B	126	SER	-	expression tag	UNP Q8CYC9
B	127	THR	-	expression tag	UNP Q8CYC9
B	128	ASN	-	expression tag	UNP Q8CYC9
B	129	GLU	-	expression tag	UNP Q8CYC9
B	130	ASN	-	expression tag	UNP Q8CYC9
B	131	LYS	-	expression tag	UNP Q8CYC9
B	132	SER	-	expression tag	UNP Q8CYC9
B	133	TYR	-	expression tag	UNP Q8CYC9
B	134	LYS	-	expression tag	UNP Q8CYC9
B	135	GLU	-	expression tag	UNP Q8CYC9
B	136	ASP	-	expression tag	UNP Q8CYC9
B	137	VAL	-	expression tag	UNP Q8CYC9
B	138	ILE	-	expression tag	UNP Q8CYC9
B	139	SER	-	expression tag	UNP Q8CYC9
B	140	ASP	-	expression tag	UNP Q8CYC9
B	141	ARG	-	expression tag	UNP Q8CYC9
B	142	ILE	-	expression tag	UNP Q8CYC9
B	143	ILE	-	expression tag	UNP Q8CYC9
B	144	LYS	-	expression tag	UNP Q8CYC9
B	145	LYS	-	expression tag	UNP Q8CYC9
B	146	GLU	-	expression tag	UNP Q8CYC9
B	147	PHE	-	expression tag	UNP Q8CYC9
B	148	GLU	-	expression tag	UNP Q8CYC9
B	149	ASP	-	expression tag	UNP Q8CYC9
B	608	GLU	-	expression tag	UNP Q8CYC9
B	609	LYS	-	expression tag	UNP Q8CYC9
B	610	GLU	-	expression tag	UNP Q8CYC9
B	611	LYS	-	expression tag	UNP Q8CYC9
B	612	ASN	-	expression tag	UNP Q8CYC9
B	613	LYS	-	expression tag	UNP Q8CYC9
B	614	GLU	-	expression tag	UNP Q8CYC9
B	615	GLU	-	expression tag	UNP Q8CYC9
B	616	LYS	-	expression tag	UNP Q8CYC9
B	617	GLN	-	expression tag	UNP Q8CYC9
B	618	SER	-	expression tag	UNP Q8CYC9
B	619	ASN	-	expression tag	UNP Q8CYC9
B	620	SER	-	expression tag	UNP Q8CYC9
B	621	ASN	-	expression tag	UNP Q8CYC9
B	622	ASN	-	expression tag	UNP Q8CYC9
B	623	VAL	-	expression tag	UNP Q8CYC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	624	ILE	-	expression tag	UNP Q8CYC9
B	625	ASP	-	expression tag	UNP Q8CYC9
B	626	SER	-	expression tag	UNP Q8CYC9
B	627	ASN	-	expression tag	UNP Q8CYC9
B	628	GLN	-	expression tag	UNP Q8CYC9
B	629	LYS	-	expression tag	UNP Q8CYC9
B	630	ASN	-	expression tag	UNP Q8CYC9
B	631	GLY	-	expression tag	UNP Q8CYC9
B	632	GLU	-	expression tag	UNP Q8CYC9
B	633	PHE	-	expression tag	UNP Q8CYC9
B	634	ASN	-	expression tag	UNP Q8CYC9
B	635	SER	-	expression tag	UNP Q8CYC9
B	636	SER	-	expression tag	UNP Q8CYC9
B	637	LYS	-	expression tag	UNP Q8CYC9
B	638	ASP	-	expression tag	UNP Q8CYC9
B	639	ASN	-	expression tag	UNP Q8CYC9
B	640	ARG	-	expression tag	UNP Q8CYC9
B	641	GLN	-	expression tag	UNP Q8CYC9
B	642	MET	-	expression tag	UNP Q8CYC9
B	643	ASN	-	expression tag	UNP Q8CYC9
B	644	ASP	-	expression tag	UNP Q8CYC9
B	645	LYS	-	expression tag	UNP Q8CYC9
B	646	ILE	-	expression tag	UNP Q8CYC9
B	647	ASP	-	expression tag	UNP Q8CYC9
B	648	ASN	-	expression tag	UNP Q8CYC9
B	649	LYS	-	expression tag	UNP Q8CYC9
B	650	GLN	-	expression tag	UNP Q8CYC9
B	651	ASP	-	expression tag	UNP Q8CYC9
B	652	ASN	-	expression tag	UNP Q8CYC9
B	653	LYS	-	expression tag	UNP Q8CYC9
B	654	THR	-	expression tag	UNP Q8CYC9
B	655	GLU	-	expression tag	UNP Q8CYC9
B	656	GLU	-	expression tag	UNP Q8CYC9
B	657	VAL	-	expression tag	UNP Q8CYC9
B	658	ASN	-	expression tag	UNP Q8CYC9
B	659	TYR	-	expression tag	UNP Q8CYC9
B	660	LYS	-	expression tag	UNP Q8CYC9
B	661	ILE	-	expression tag	UNP Q8CYC9
B	662	VAL	-	expression tag	UNP Q8CYC9
B	663	GLY	-	expression tag	UNP Q8CYC9
B	664	ASP	-	expression tag	UNP Q8CYC9
B	665	GLY	-	expression tag	UNP Q8CYC9

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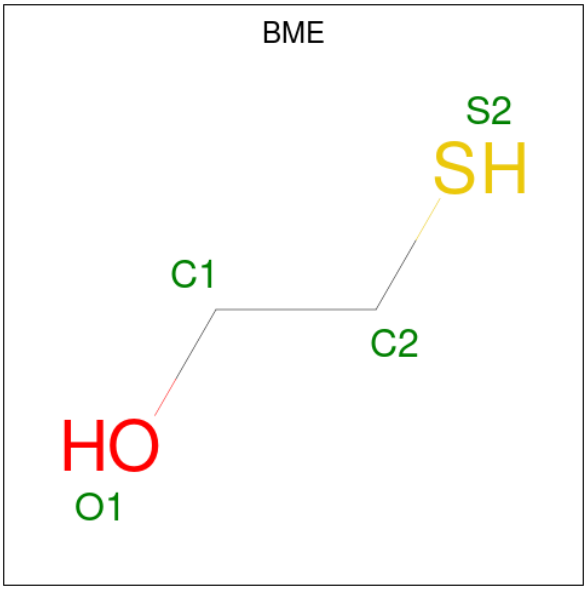
Chain	Residue	Modelled	Actual	Comment	Reference
B	666	ARG	-	expression tag	UNP Q8CYC9
B	667	GLU	-	expression tag	UNP Q8CYC9
B	668	THR	-	expression tag	UNP Q8CYC9
B	669	GLU	-	expression tag	UNP Q8CYC9
B	670	ASN	-	expression tag	UNP Q8CYC9
B	671	HIS	-	expression tag	UNP Q8CYC9
B	672	ILE	-	expression tag	UNP Q8CYC9
B	673	ASN	-	expression tag	UNP Q8CYC9
B	674	LYS	-	expression tag	UNP Q8CYC9
B	675	SER	-	expression tag	UNP Q8CYC9
B	676	LYS	-	expression tag	UNP Q8CYC9
B	677	GLU	-	expression tag	UNP Q8CYC9
B	678	ILE	-	expression tag	UNP Q8CYC9
B	679	VAL	-	expression tag	UNP Q8CYC9
B	680	ASP	-	expression tag	UNP Q8CYC9
B	681	VAL	-	expression tag	UNP Q8CYC9
B	682	LYS	-	expression tag	UNP Q8CYC9
B	683	GLN	-	expression tag	UNP Q8CYC9
B	684	LYS	-	expression tag	UNP Q8CYC9

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Mn 4 4	0	0
5	B	4	Total Mn 4 4	0	0

- Molecule 6 is water.

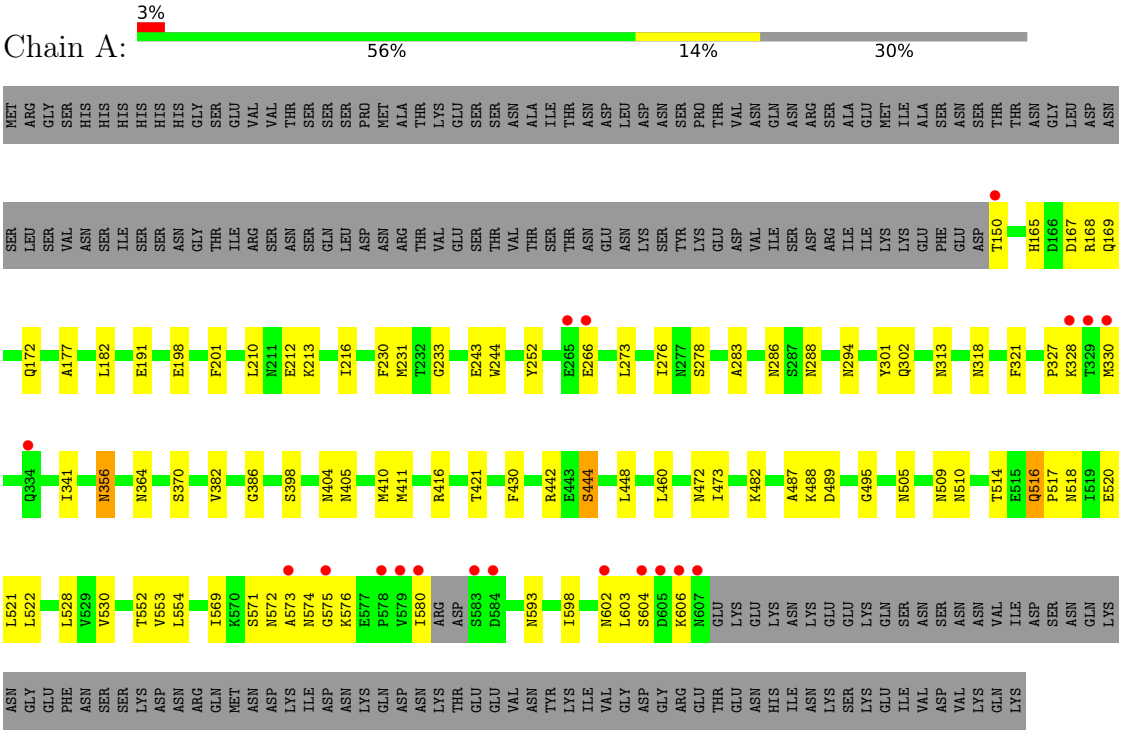
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	286	Total O 286 286	0	0
6	B	282	Total O 282 282	0	0

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.

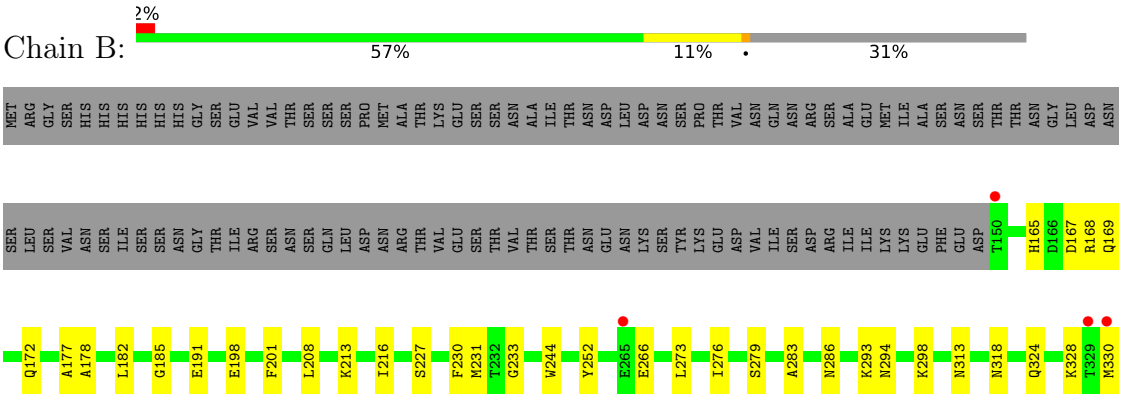
• Molecule 1: Plasmin and fibronectin-binding protein A

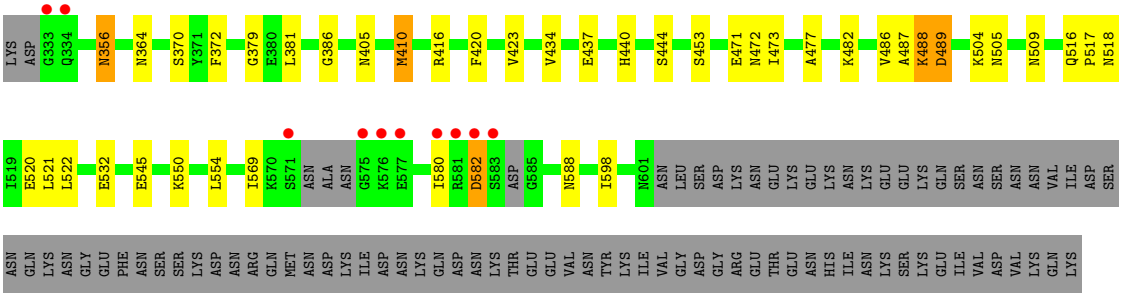
Chain A:



• Molecule 1: Plasmin and fibronectin-binding protein A

Chain B:




LYS ASP G333 Q334 N356 N364 S370 Y371 F372 G379 E380 L381 G386 N405 M410 R416 F420 V423 V434 E437 H440 S444 S453 E471 N472 I473 A477 K482 V486 A487 K488 D489 K504 N505 N509 Q516 P517 N518
I519 E520 L521 L522 E532 E545 K550 L554 I569 K570 S571 ASN ALA ASN G575 K576 E577 I580 R581 D582 S583 ASP G585 N588 I598 N601 ASN LEU SER ASP LYS ASN GLU LYS GLU LYS ASN LYS GLU GLU LYS GLN SER ASN SER ASN ASN VAL ILE ASP SER
ASN GLN LYS ASN GLY GLU PHE ASN SER SER LYS ASP ASN ARG GLN MET ASN ASP LYS ILE ASP ASN LYS GLN ASP ASN LYS THR GLU GLU VAL ASN TYR LYS ILE VAL GLY ASP GLY ARG GLU THR GLU ASN HIS ILE ASN LYS SER LYS GLU ILE VAL ASP VAL LYS GLN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.59Å 126.08Å 63.48Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 37.85 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.95) 88.3 (37.85-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 1.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.222 0.194 , 0.213	Depositor DCC
R_{free} test set	2299 reflections (2.87%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7518	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, MN, CA, BME

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	0.33	0/3553	0.69	1/4800 (0.0%)
1	B	0.32	0/3481	0.69	1/4699 (0.0%)
All	All	0.33	0/7034	0.69	2/9499 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	488	LYS	N-CA-C	-6.46	93.56	111.00
1	A	488	LYS	N-CA-C	-6.25	94.12	111.00

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	3500	0	3478	76	0
1	B	3430	0	3415	62	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	286	0	0	7	0
6	B	282	0	0	7	0
All	All	7518	0	6905	137	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 10.

The worst 5 of 137 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:172:GLN:HE22	1:B:201:PHE:H	1.10	0.98
1:B:244:TRP:H	1:B:356:ASN:HD21	1.09	0.97
1:A:172:GLN:HE22	1:A:201:PHE:H	1.02	0.96
1:A:244:TRP:H	1:A:356:ASN:HD21	1.13	0.90
1:A:575:GLY:HA3	6:A:1050:HOH:O	1.78	0.82

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	452/648 (70%)	431 (95%)	21 (5%)	0	100	100
1	B	438/648 (68%)	418 (95%)	18 (4%)	2 (0%)	29	17
All	All	890/1296 (69%)	849 (95%)	39 (4%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	582	ASP
1	B	489	ASP

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	385/568 (68%)	375 (97%)	10 (3%)	46 36
1	B	378/568 (66%)	370 (98%)	8 (2%)	53 46
All	All	763/1136 (67%)	745 (98%)	18 (2%)	49 40

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	410	MET
1	B	582	ASP
1	B	489	ASP
1	A	516	GLN
1	B	356	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	505	ASN
1	B	516	GLN
1	A	518	ASN
1	A	516	GLN
1	B	518	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

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	BME	A	701	-	3,3,3	0.52	0	1,2,2	0.12	0
2	BME	B	701	-	3,3,3	0.55	0	1,2,2	0.33	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	BME	A	701	-	-	1/1/1/1	-
2	BME	B	701	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	BME	O1-C1-C2-S2
2	B	701	BME	O1-C1-C2-S2

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	456/648 (70%)	0.04	19 (4%)	36	45	11, 22, 53, 84	0
1	B	446/648 (68%)	-0.03	14 (3%)	49	58	12, 23, 42, 73	0
All	All	902/1296 (69%)	0.01	33 (3%)	41	51	11, 22, 48, 84	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	MET	8.9
1	A	607	ASN	5.3
1	A	573	ALA	5.2
1	B	582	ASP	4.9
1	A	602	ASN	4.9

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
2	BME	A	701	4/4	0.67	0.17	36,37,39,48	0
2	BME	B	701	4/4	0.80	0.17	40,40,41,47	0
4	CL	B	703	1/1	0.88	0.07	56,56,56,56	0
3	CA	A	702	1/1	0.90	0.11	62,62,62,62	0
5	MN	B	706	1/1	0.94	0.06	39,39,39,39	0
4	CL	A	703	1/1	0.95	0.07	47,47,47,47	0
3	CA	B	702	1/1	0.96	0.15	53,53,53,53	0
5	MN	A	707	1/1	0.97	0.07	50,50,50,50	0
5	MN	A	706	1/1	0.97	0.05	46,46,46,46	0
5	MN	B	707	1/1	0.98	0.08	50,50,50,50	0
5	MN	A	705	1/1	0.99	0.03	23,23,23,23	0
5	MN	B	705	1/1	0.99	0.04	28,28,28,28	0
5	MN	B	704	1/1	1.00	0.07	18,18,18,18	0
5	MN	A	704	1/1	1.00	0.09	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.