



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:27 PM UTC

PDB ID : 4BJM / pdb_00004bjm
Title : Crystal structure of the flax-rust effector avrM
Authors : Ve, T.; Williams, S.J.; Kobe, B.
Deposited on : 2013-04-19
Resolution : 2.60 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

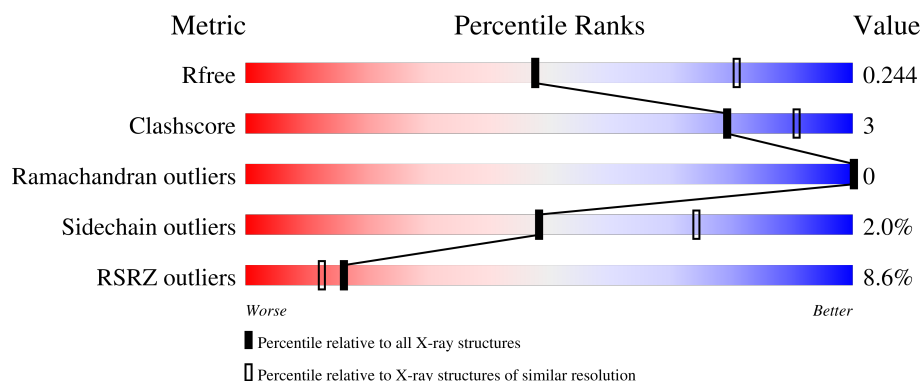
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	238	0% 87% 7% 5%
1	B	238	7% 84% 9% 7%
1	C	238	4% 82% 8% 10%
1	D	238	19% 80% 8% 12%

2 Entry composition

There are 3 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 AVR.M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1835	1153	321	357	4			
1	B	222	Total	C	N	O	S	0	0	0
			1802	1128	317	354	3			
1	C	215	Total	C	N	O	S	0	0	0
			1746	1094	304	345	3			
1	D	210	Total	C	N	O	S	0	0	0
			1709	1074	298	334	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	SER	-	expression tag	UNP Q2MV46
A	44	ASN	-	expression tag	UNP Q2MV46
A	45	ALA	-	expression tag	UNP Q2MV46
B	43	SER	-	expression tag	UNP Q2MV46
B	44	ASN	-	expression tag	UNP Q2MV46
B	45	ALA	-	expression tag	UNP Q2MV46
C	43	SER	-	expression tag	UNP Q2MV46
C	44	ASN	-	expression tag	UNP Q2MV46
C	45	ALA	-	expression tag	UNP Q2MV46
D	43	SER	-	expression tag	UNP Q2MV46
D	44	ASN	-	expression tag	UNP Q2MV46
D	45	ALA	-	expression tag	UNP Q2MV46

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total 66	O 66	0	0
3	B	35	Total 35	O 35	0	0
3	C	18	Total 18	O 18	0	0
3	D	7	Total 7	O 7	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.

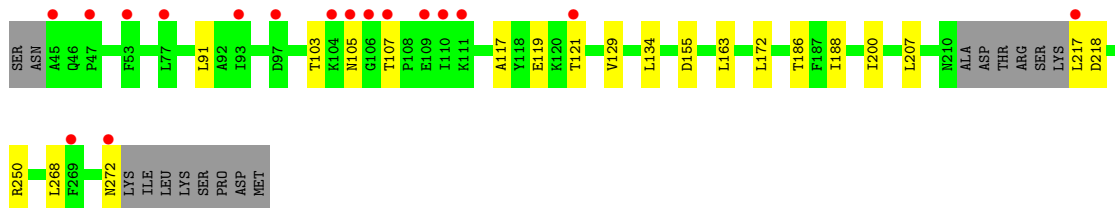
• Molecule 1: AVR

Chain A: 



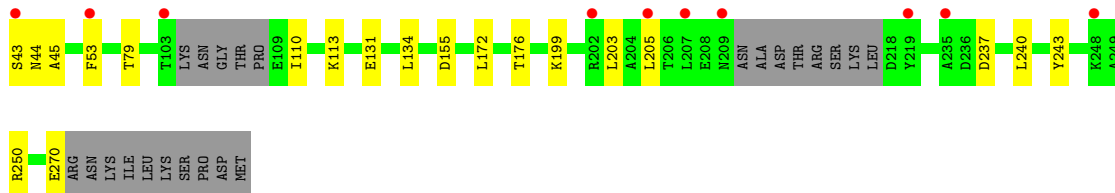
• Molecule 1: AVR

Chain B: 



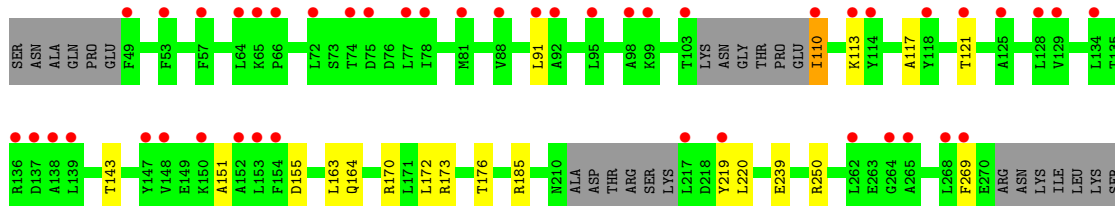
• Molecule 1: AVR

Chain C: 



• Molecule 1: AVR

Chain D: 



PRO
ASP
MET

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.47Å 125.61Å 128.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.14 – 2.60 26.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (26.14-2.60) 99.8 (26.14-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.60Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.209 , 0.233 0.222 , 0.244	Depositor DCC
R_{free} test set	2259 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: CL

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	0.88	1/1858 (0.1%)	1.40	9/2492 (0.4%)
1	B	0.85	0/1824	1.39	5/2448 (0.2%)
1	C	0.82	0/1766	1.40	4/2368 (0.2%)
1	D	0.80	0/1728	1.39	8/2316 (0.3%)
All	All	0.84	1/7176 (0.0%)	1.40	26/9624 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	MET	SD-CE	-7.74	1.60	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	CA-CB-CG	7.22	119.82	112.60
1	D	220	LEU	CA-C-N	5.98	129.80	120.82
1	D	220	LEU	C-N-CA	5.98	129.80	120.82
1	D	163	LEU	CA-C-N	5.91	128.12	120.44
1	D	163	LEU	C-N-CA	5.91	128.12	120.44
1	B	155	ASP	CA-C-N	5.86	128.06	120.44
1	B	155	ASP	C-N-CA	5.86	128.06	120.44
1	A	241	ASN	CA-CB-CG	-5.67	106.94	112.60
1	A	155	ASP	CA-C-N	5.62	127.75	120.44
1	A	155	ASP	C-N-CA	5.62	127.75	120.44
1	D	164	GLN	CA-C-N	5.59	127.71	120.44
1	D	164	GLN	C-N-CA	5.59	127.71	120.44
1	D	155	ASP	CA-C-N	5.54	127.64	120.44
1	D	155	ASP	C-N-CA	5.54	127.64	120.44
1	B	103	THR	CA-C-N	5.51	128.11	120.29
1	B	103	THR	C-N-CA	5.51	128.11	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	ASP	CA-C-N	5.34	127.39	120.44
1	C	155	ASP	C-N-CA	5.34	127.39	120.44
1	C	131	GLU	CA-C-N	5.34	127.44	120.28
1	C	131	GLU	C-N-CA	5.34	127.44	120.28
1	B	272	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	144	GLU	CA-C-N	5.14	127.43	120.44
1	A	144	GLU	C-N-CA	5.14	127.43	120.44
1	A	269	PHE	CA-C-N	5.11	129.40	122.19
1	A	269	PHE	C-N-CA	5.11	129.40	122.19
1	A	239	GLU	CB-CG-CD	5.07	121.22	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	1835	0	1863	12	0
1	B	1802	0	1813	14	0
1	C	1746	0	1751	12	0
1	D	1709	0	1725	9	0
2	B	1	0	0	0	0
3	A	66	0	0	2	0
3	B	35	0	0	0	0
3	C	18	0	0	0	0
3	D	7	0	0	0	0
All	All	7219	0	7152	38	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 3.

All (38) 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:A:81:MET:HE1	1:A:153:LEU:HD22	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:MET:HE3	1:A:81:MET:HA	1.60	0.84
1:C:172:LEU:O	1:C:176:THR:HG23	1.80	0.81
1:B:207:LEU:HG	1:B:217:LEU:HD23	1.64	0.79
1:B:188:ILE:HD11	1:C:45:ALA:HB2	1.65	0.78
1:B:91:LEU:HB3	1:B:121:THR:HG22	1.72	0.69
1:B:188:ILE:CD1	1:C:45:ALA:HB2	2.24	0.67
1:B:200:ILE:HG21	1:C:43:SER:HB3	1.76	0.67
1:D:173:ARG:O	1:D:176:THR:HG22	1.98	0.62
1:A:160:ARG:NH1	3:A:2047:HOH:O	2.32	0.61
1:C:199:LYS:O	1:C:203:LEU:HD13	2.01	0.61
1:A:89:ARG:NH1	1:B:186:THR:HG22	2.18	0.58
1:A:81:MET:CE	1:A:153:LEU:HD22	2.33	0.54
1:D:173:ARG:HG2	1:D:219:TYR:HB2	1.90	0.53
1:D:91:LEU:HB3	1:D:121:THR:HG22	1.89	0.53
1:A:81:MET:HE2	1:A:128:LEU:HD13	1.91	0.53
1:A:89:ARG:HH12	1:B:186:THR:HG22	1.75	0.52
1:C:176:THR:HG22	1:C:243:TYR:OH	2.10	0.52
1:A:144:GLU:HB3	1:A:258:MET:HE3	1.94	0.49
1:B:188:ILE:CD1	1:C:45:ALA:CB	2.91	0.49
1:C:110:ILE:HG13	1:C:113:LYS:HD2	1.96	0.48
1:D:110:ILE:HG13	1:D:113:LYS:HD2	1.96	0.47
1:C:53:PHE:HD1	1:C:79:THR:HG23	1.80	0.46
1:B:117:ALA:O	1:B:121:THR:HG23	2.17	0.45
1:D:172:LEU:HG	1:D:250:ARG:HG2	1.99	0.45
1:C:172:LEU:HG	1:C:250:ARG:HG2	1.99	0.44
1:B:217:LEU:HG	1:B:218:ASP:N	2.33	0.44
1:A:99:LYS:HD2	3:A:2002:HOH:O	2.18	0.43
1:B:105:ASN:OD1	1:B:107:THR:HG23	2.18	0.43
1:A:185:ARG:HH12	1:D:185:ARG:HH11	1.65	0.43
1:B:172:LEU:HG	1:B:250:ARG:HG2	2.00	0.43
1:A:239:GLU:HG3	1:B:163:LEU:HD21	2.01	0.43
1:C:237:ASP:OD2	1:C:240:LEU:HD13	2.18	0.42
1:C:43:SER:OG	1:C:44:ASN:N	2.50	0.42
1:A:201:GLU:CD	1:D:170:ARG:HG3	2.45	0.42
1:B:217:LEU:HG	1:B:218:ASP:H	1.83	0.42
1:D:117:ALA:O	1:D:121:THR:HG23	2.21	0.41
1:D:151:ALA:HB2	1:D:269:PHE:HE2	1.85	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	222/238 (93%)	220 (99%)	2 (1%)	0	100	100
1	B	218/238 (92%)	216 (99%)	2 (1%)	0	100	100
1	C	209/238 (88%)	207 (99%)	2 (1%)	0	100	100
1	D	204/238 (86%)	203 (100%)	1 (0%)	0	100	100
All	All	853/952 (90%)	846 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/204 (95%)	189 (97%)	5 (3%)	40	68
1	B	189/204 (93%)	185 (98%)	4 (2%)	47	73
1	C	183/204 (90%)	180 (98%)	3 (2%)	55	79
1	D	179/204 (88%)	176 (98%)	3 (2%)	53	78
All	All	745/816 (91%)	730 (98%)	15 (2%)	48	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	129	VAL

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Mol	Chain	Res	Type
1	A	141	GLU
1	A	165	ARG
1	A	199	LYS
1	B	119	GLU
1	B	129	VAL
1	B	134	LEU
1	B	268	LEU
1	C	134	LEU
1	C	205	LEU
1	C	270	GLU
1	D	110	ILE
1	D	143	THR
1	D	239	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	229	ASN
1	C	230	GLN
1	D	164	GLN
1	D	230	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 [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, 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	226/238 (94%)	-0.18	3 (1%) 75 71	41, 63, 96, 137	0
1	B	222/238 (93%)	0.37	17 (7%) 19 15	42, 86, 176, 217	0
1	C	215/238 (90%)	0.36	10 (4%) 36 30	51, 97, 165, 188	0
1	D	210/238 (88%)	1.01	45 (21%) 2 2	49, 139, 205, 234	0
All	All	873/952 (91%)	0.38	75 (8%) 16 12	41, 86, 188, 234	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	64	LEU	5.4
1	B	45	ALA	4.4
1	C	103	THR	4.3
1	D	219	TYR	4.3
1	D	78	ILE	3.9
1	D	217	LEU	3.8
1	C	207	LEU	3.8
1	D	268	LEU	3.7
1	D	77	LEU	3.6
1	D	118	TYR	3.6
1	D	139	LEU	3.6
1	D	98	ALA	3.4
1	D	134	LEU	3.4
1	D	99	LYS	3.3
1	B	47	PRO	3.3
1	C	205	LEU	3.2
1	C	43	SER	3.2
1	D	262	LEU	3.2
1	D	265	ALA	3.2
1	B	53	PHE	3.1
1	C	209	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	47	PRO	3.1
1	B	93	ILE	3.1
1	B	105	ASN	3.1
1	D	103	THR	3.1
1	D	110	ILE	3.0
1	D	152	ALA	2.9
1	B	111	LYS	2.9
1	D	264	GLY	2.8
1	D	65	LYS	2.8
1	B	97	ASP	2.8
1	A	217	LEU	2.7
1	B	109	GLU	2.7
1	D	129	VAL	2.7
1	D	150	LYS	2.7
1	C	202	ARG	2.7
1	D	148	VAL	2.7
1	B	121	THR	2.6
1	C	235	ALA	2.6
1	D	113	LYS	2.5
1	D	49	PHE	2.5
1	D	121	THR	2.5
1	A	205	LEU	2.5
1	B	110	ILE	2.5
1	B	217	LEU	2.5
1	D	147	TYR	2.5
1	D	88	VAL	2.5
1	D	114	TYR	2.4
1	B	269	PHE	2.4
1	D	92	ALA	2.4
1	D	75	ASP	2.4
1	D	138	ALA	2.4
1	D	81	MET	2.4
1	D	269	PHE	2.4
1	D	128	LEU	2.3
1	D	53	PHE	2.3
1	B	107	THR	2.3
1	B	106	GLY	2.3
1	D	154	PHE	2.3
1	D	72	LEU	2.2
1	B	272	ASN	2.2
1	D	137	ASP	2.2
1	D	91	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	66	PRO	2.2
1	C	248	LYS	2.1
1	B	77	LEU	2.1
1	D	95	LEU	2.1
1	D	57	PHE	2.1
1	D	125	ALA	2.1
1	D	153	LEU	2.1
1	C	53	PHE	2.1
1	D	136	ARG	2.0
1	B	104	LYS	2.0
1	D	74	THR	2.0
1	C	219	TYR	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
2	CL	B	1273	1/1	0.98	0.07	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.