



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:43 AM GMT

PDB ID : 4DB8
Title : Designed Armadillo-repeat Protein
Authors : Madhurantakam, C.; Varadamsetty, G.; Grutter, M.G.; Pluckthun, A.; Mittl, P.R.E.
Deposited on : 2012-01-13
Resolution : 2.50 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>

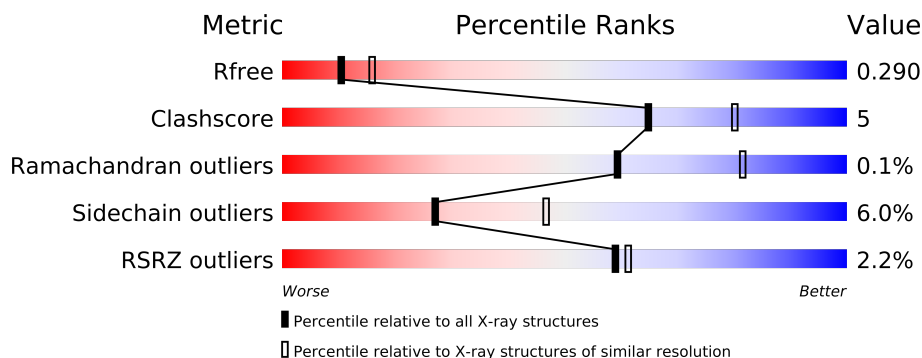
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	252	
1	B	252	
1	C	252	
1	D	252	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7385 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 Armadillo-repeat Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	1	0
			1856	1151	323	380	2			
1	B	239	Total	C	N	O	S	0	1	0
			1783	1108	304	369	2			
1	C	238	Total	C	N	O	S	0	0	0
			1763	1096	299	366	2			
1	D	246	Total	C	N	O	S	0	0	0
			1845	1145	321	377	2			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

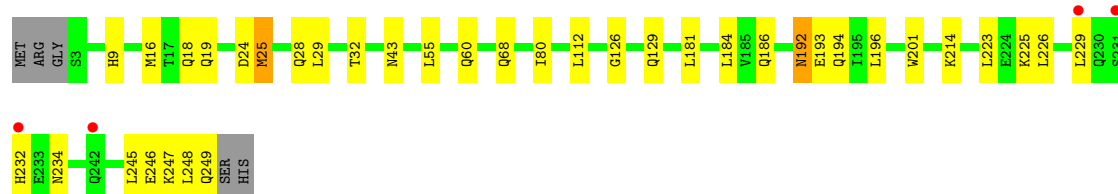
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	25	Total	O	0	0
			25	25		
3	C	35	Total	O	0	0
			35	35		
3	D	46	Total	O	0	0
			46	46		

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.

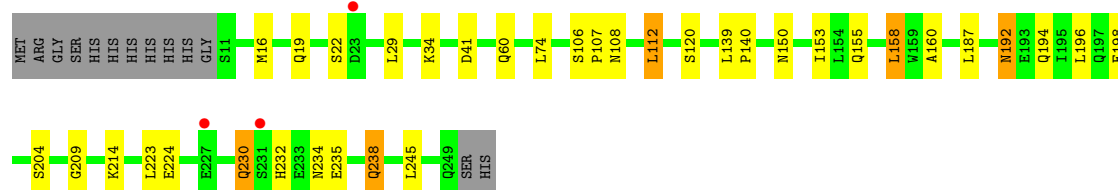
• Molecule 1: Armadillo-repeat Protein

Chain A: 



• Molecule 1: Armadillo-repeat Protein

Chain B: 



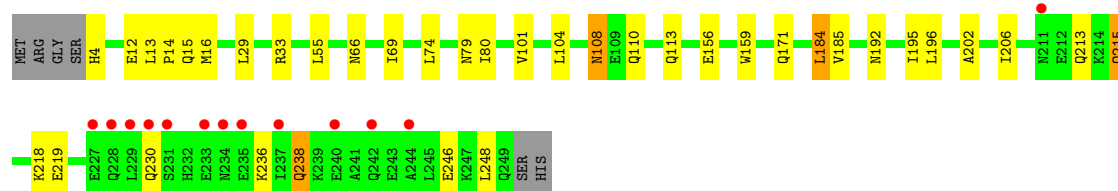
• Molecule 1: Armadillo-repeat Protein

Chain C: 



• Molecule 1: Armadillo-repeat Protein

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.00Å 113.64Å 85.59Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 39.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.00-2.50) 95.3 (39.71-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.232 , 0.299 0.235 , 0.290	Depositor DCC
R_{free} test set	1747 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.3	EDS
Estimated twinning fraction	0.078 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 35089 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7385	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: MG

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	0/1883	0.52	1/2561 (0.0%)
1	B	0.34	0/1801	0.51	1/2450 (0.0%)
1	C	0.34	0/1781	0.49	0/2426
1	D	0.33	0/1869	0.50	0/2542
All	All	0.34	0/7334	0.50	2/9979 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	25	MET	CB-CA-C	-5.09	100.21	110.40

There are no chirality outliers.

There are no planarity outliers.

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	1856	0	1832	32	0
1	B	1783	0	1778	18	0
1	C	1763	0	1745	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1845	0	1821	18	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	0	7	0
3	B	25	0	0	1	0
3	C	35	0	0	2	0
3	D	46	0	0	1	0
All	All	7385	0	7176	76	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 5.

All (76) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:247:LYS:HB2	3:A:413:HOH:O	1.71	0.88
1:C:55:LEU:HD21	1:C:80:ILE:HD13	1.61	0.82
1:C:201:TRP:HZ3	3:C:317:HOH:O	1.63	0.81
1:C:232:HIS:HD2	1:C:234:ASN:H	1.37	0.72
1:A:55:LEU:HD21	1:A:80:ILE:HD13	1.75	0.67
1:A:247:LYS:N	3:A:413:HOH:O	2.27	0.67
1:A:225:LYS:O	1:A:229:LEU:HB2	1.95	0.67
1:A:9:HIS:HD2	1:B:198:GLU:OE1	1.76	0.66
1:A:223:LEU:HB2	3:A:409:HOH:O	1.96	0.65
1:B:192:ASN:C	1:B:192:ASN:HD22	2.02	0.63
1:B:150:ASN:HB3	1:B:153:ILE:HD12	1.83	0.60
1:A:16:MET:HA	1:A:19:GLN:HE21	1.68	0.59
1:D:101:VAL:O	1:D:104:LEU:HB2	2.04	0.57
1:A:43:ASN:HD21	1:D:79:ASN:HD21	1.50	0.57
1:B:192:ASN:HD22	1:B:194:GLN:H	1.52	0.57
1:A:193:GLU:HA	1:A:196:LEU:HD12	1.87	0.57
1:A:247:LYS:CA	3:A:413:HOH:O	2.54	0.56
1:C:55:LEU:CD2	1:C:80:ILE:HD13	2.35	0.56
1:A:247:LYS:CB	3:A:413:HOH:O	2.43	0.54
1:A:24:ASP:O	1:A:25:MET:HB3	2.08	0.54
1:D:4:HIS:N	3:D:445:HOH:O	2.41	0.54
1:D:66:ASN:HD22	1:D:69:ILE:H	1.56	0.54
1:B:120:SER:HB3	1:B:160:ALA:HB2	1.91	0.53
1:A:28:GLN:O	1:A:32:THR:HG23	2.08	0.53
1:C:232:HIS:CD2	1:C:234:ASN:H	2.22	0.53
1:D:55:LEU:HD21	1:D:80:ILE:HD13	1.91	0.52
1:D:202:ALA:O	1:D:206:ILE:HD12	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:102:GLN:NE2	3:C:333:HOH:O	2.36	0.52
1:B:139:LEU:HB2	1:B:140:PRO:HD3	1.92	0.51
1:B:16:MET:HA	1:B:19:GLN:HE21	1.74	0.51
1:D:12:GLU:O	1:D:16:MET:HG3	2.12	0.49
1:B:230:GLN:HE22	1:B:245:LEU:HD22	1.78	0.49
1:B:19:GLN:O	1:B:22:SER:HB3	2.12	0.49
1:C:66:ASN:ND2	1:C:68:GLN:H	2.12	0.48
1:B:209:GLY:O	1:B:214:LYS:HE3	2.12	0.48
1:B:232:HIS:HD2	1:B:234:ASN:H	1.61	0.48
1:C:66:ASN:HD22	1:C:68:GLN:N	2.11	0.47
1:A:214:LYS:HE2	1:A:247:LYS:O	2.14	0.47
1:B:60:GLN:NE2	3:B:424:HOH:O	2.45	0.47
1:B:158:LEU:HD12	1:B:198:GLU:HG3	1.96	0.47
1:A:25:MET:HG3	1:D:69:ILE:CD1	2.45	0.47
1:A:226:LEU:HB2	1:A:245:LEU:HD13	1.96	0.46
1:A:68:GLN:HE21	1:D:33:ARG:NH2	2.14	0.46
1:A:25:MET:HA	1:A:28:GLN:HB2	1.97	0.46
1:D:113:GLN:HG3	1:D:156:GLU:HG3	1.98	0.46
1:A:25:MET:CG	1:A:25:MET:O	2.63	0.45
1:A:18:GLN:HG2	1:C:93:ASP:HA	1.97	0.45
1:D:13:LEU:HB2	1:D:14:PRO:HD3	1.98	0.45
1:A:126:GLY:H	1:A:129:GLN:HE21	1.64	0.45
1:A:186:GLN:NE2	3:A:423:HOH:O	2.49	0.45
1:A:192:ASN:HD22	1:A:192:ASN:C	2.20	0.45
1:B:232:HIS:CD2	1:B:234:ASN:H	2.34	0.45
1:B:235:GLU:HA	1:B:238:GLN:HB2	1.98	0.45
1:A:192:ASN:HD22	1:A:193:GLU:N	2.15	0.44
1:A:24:ASP:O	1:A:25:MET:CB	2.66	0.44
1:B:192:ASN:ND2	1:B:194:GLN:H	2.15	0.44
1:A:18:GLN:CG	1:C:93:ASP:HA	2.47	0.44
1:D:215:GLN:HA	1:D:218:LYS:HD2	2.00	0.43
1:D:192:ASN:HB3	1:D:195:ILE:HB	1.99	0.43
1:C:66:ASN:HD22	1:C:68:GLN:H	1.66	0.43
1:D:108:ASN:HD21	1:D:110:GLN:HG2	1.83	0.43
1:A:68:GLN:HE21	1:D:33:ARG:HH22	1.65	0.43
1:A:247:LYS:C	1:A:249:GLN:H	2.22	0.43
1:B:158:LEU:HD21	1:B:187:LEU:HD13	2.01	0.42
1:A:126:GLY:H	1:A:129:GLN:NE2	2.18	0.42
1:A:181:LEU:HD23	1:A:184:LEU:HD12	2.01	0.42
1:C:215:GLN:O	1:C:219:GLU:HB2	2.21	0.41
1:B:106:SER:HA	1:B:107:PRO:HD3	1.92	0.41
1:C:66:ASN:HD21	1:C:68:GLN:HB2	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:184:LEU:HD11	1:D:202:ALA:HB3	2.03	0.41
1:A:232:HIS:HD2	1:A:234:ASN:H	1.67	0.41
1:C:186:GLN:HE21	1:C:186:GLN:HA	1.86	0.41
1:D:246:GLU:C	1:D:248:LEU:H	2.25	0.40
1:C:112:LEU:O	1:C:116:LEU:HB2	2.22	0.40
1:A:194:GLN:NE2	3:A:412:HOH:O	2.55	0.40
1:D:230:GLN:HA	1:D:238:GLN:HG3	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	246/252 (98%)	241 (98%)	4 (2%)	1 (0%)	43	66
1	B	238/252 (94%)	235 (99%)	3 (1%)	0	100	100
1	C	236/252 (94%)	233 (99%)	3 (1%)	0	100	100
1	D	244/252 (97%)	241 (99%)	3 (1%)	0	100	100
All	All	964/1008 (96%)	950 (98%)	13 (1%)	1 (0%)	59	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	LEU

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	198/202 (98%)	192 (97%)	6 (3%)	53	80
1	B	190/202 (94%)	175 (92%)	15 (8%)	18	31
1	C	186/202 (92%)	175 (94%)	11 (6%)	28	48
1	D	196/202 (97%)	182 (93%)	14 (7%)	21	37
All	All	770/808 (95%)	724 (94%)	46 (6%)	27	47

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	60	GLN
1	A	112	LEU
1	A	192	ASN
1	A	201	TRP
1	A	246	GLU
1	B	29	LEU
1	B	34	LYS
1	B	41	ASP
1	B	74	LEU
1	B	108	ASN
1	B	112	LEU
1	B	155	GLN
1	B	158	LEU
1	B	192	ASN
1	B	196	LEU
1	B	204	SER
1	B	223	LEU
1	B	224	GLU
1	B	230	GLN
1	B	238	GLN
1	C	29	LEU
1	C	44	GLU
1	C	66	ASN
1	C	70	LEU
1	C	111	ILE
1	C	116	LEU
1	C	186	GLN
1	C	196	LEU
1	C	201	TRP
1	C	215	GLN
1	C	219	GLU
1	D	15	GLN

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Mol	Chain	Res	Type
1	D	29	LEU
1	D	74	LEU
1	D	108	ASN
1	D	159	TRP
1	D	171	GLN
1	D	184	LEU
1	D	185	VAL
1	D	196	LEU
1	D	213	GLN
1	D	215	GLN
1	D	219	GLU
1	D	236	LYS
1	D	238	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	19	GLN
1	A	43	ASN
1	A	47	GLN
1	A	68	GLN
1	A	71	GLN
1	A	79	ASN
1	A	89	GLN
1	A	129	GLN
1	A	163	ASN
1	A	169	ASN
1	A	186	GLN
1	A	192	ASN
1	A	194	GLN
1	A	232	HIS
1	B	19	GLN
1	B	43	ASN
1	B	60	GLN
1	B	108	ASN
1	B	163	ASN
1	B	192	ASN
1	B	215	GLN
1	B	230	GLN
1	B	232	HIS
1	B	238	GLN

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Mol	Chain	Res	Type
1	C	19	GLN
1	C	66	ASN
1	C	79	ASN
1	C	87	GLN
1	C	113	GLN
1	C	152	GLN
1	C	163	ASN
1	C	186	GLN
1	C	197	GLN
1	C	232	HIS
1	D	66	ASN
1	D	68	GLN
1	D	79	ASN
1	D	87	GLN
1	D	108	ASN
1	D	113	GLN
1	D	152	GLN
1	D	169	ASN
1	D	171	GLN
1	D	232	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 ⓘ

Of 4 ligands modelled in this entry, 4 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.

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	247/252 (98%)	0.12	4 (1%) 68 71	24, 39, 75, 78	0
1	B	239/252 (94%)	0.07	3 (1%) 74 76	26, 36, 59, 61	0
1	C	238/252 (94%)	0.11	1 (0%) 90 92	27, 35, 51, 54	0
1	D	246/252 (97%)	0.38	13 (5%) 25 26	24, 43, 95, 98	0
All	All	970/1008 (96%)	0.17	21 (2%) 59 61	24, 37, 73, 98	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	ILE	4.7
1	D	231	SER	3.8
1	D	233	GLU	3.7
1	C	23	ASP	3.5
1	D	229	LEU	3.2
1	D	234	ASN	3.2
1	A	231	SER	3.0
1	D	211	ASN	3.0
1	D	230	GLN	2.8
1	D	228	GLN	2.6
1	B	227	GLU	2.4
1	B	231	SER	2.4
1	D	242	GLN	2.3
1	D	240	GLU	2.3
1	D	244	ALA	2.2
1	D	227	GLU	2.2
1	A	242	GLN	2.2
1	A	229	LEU	2.2
1	D	235	GLU	2.2
1	B	23	ASP	2.1
1	A	232	HIS	2.1

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	MG	B	301	1/1	0.15	-0.34	30,30,30,30	0
2	MG	A	301	1/1	0.11	-2.80	30,30,30,30	0
2	MG	D	301	1/1	0.08	-3.41	36,36,36,36	0
2	MG	B	302	1/1	0.08	-3.85	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.