



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:02 PM GMT

PDB ID : 1W9L
Title : MYOSIN II DICTYOSTELIUM DISCOIDEUM MOTOR DOMAIN S456E
BOUND WITH MGADP-ALF4
Authors : Morris, C.A.; Coureux, P.-D.; Wells, A.L.; Houdusse, A.; Sweeney, H.L.
Deposited on : 2004-10-13
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

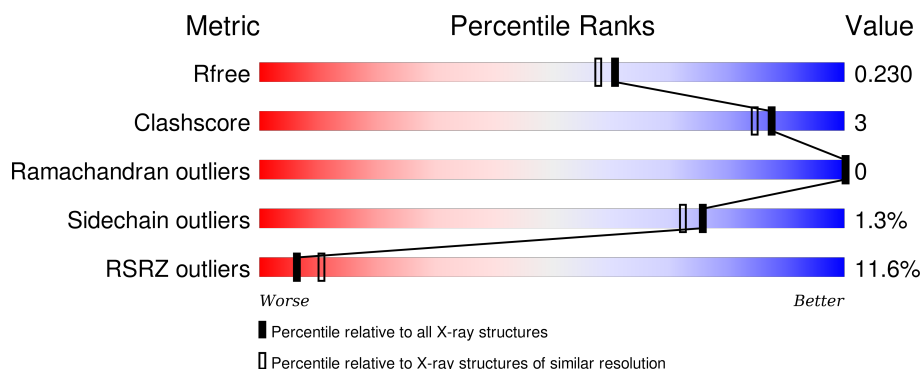
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	770	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1751	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1752	-	-	-	X
5	EDO	A	1754	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6228 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 MYOSIN II HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	1	0
			5736	3655	977	1088	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	SER	ASN	CONFLICT	UNP P08799
A	312	CYS	TYR	CONFLICT	UNP P08799
A	456	GLU	SER	ENGINEERED MUTATION	UNP P08799

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

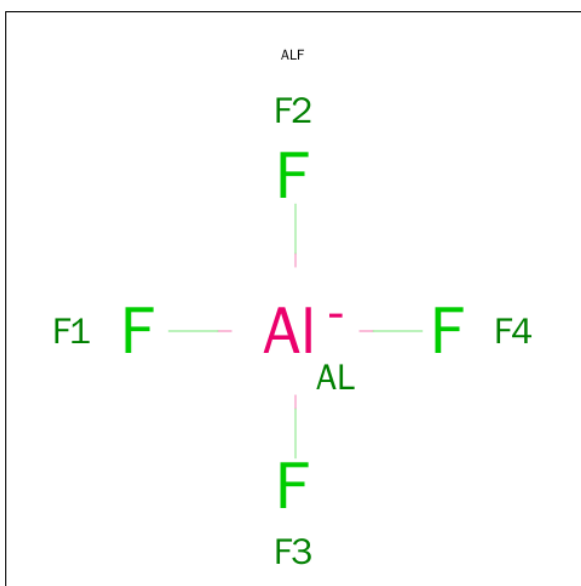
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Al	F	0
			5	1	4	

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

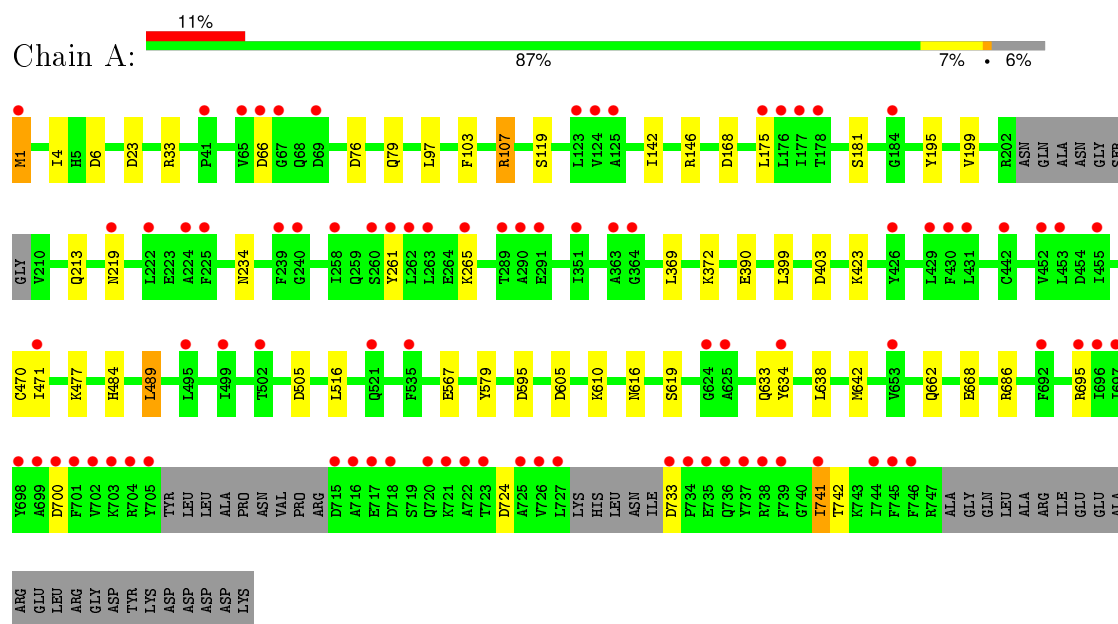
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	435	Total	O	0	0
			435	435		

3 Residue-property plots [i](#)

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: MYOSIN II HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.04Å 145.98Å 152.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 35.49 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.00-1.95) 97.8 (35.49-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.193 , 0.225 0.200 , 0.230	Depositor DCC
R_{free} test set	3525 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.3	EDS
Estimated twinning fraction	0.014 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 70083 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6228	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, MG, EDO, ADP

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	0.49	1/5850 (0.0%)	0.70	11/7910 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	SD-CE	-5.05	1.49	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	733	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	724	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	107	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	595	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	23	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	605	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	505	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	66	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	76	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	700	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	168	ASP	CB-CG-OD2	5.19	122.97	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5736	0	5566	30	0
2	A	1	0	0	0	0
3	A	27	0	12	0	0
4	A	5	0	0	1	0
5	A	24	0	36	2	0
6	A	435	0	0	8	0
All	All	6228	0	5614	30	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 (30) 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:4:ILE:HD11	1:A:142:ILE:HG23	1.61	0.83
1:A:234:ASN:H	1:A:662:GLN:HE22	1.44	0.65
1:A:181:SER:HA	4:A:1750:ALF:F1	1.87	0.65
1:A:616:ASN:ND2	6:A:2371:HOH:O	2.30	0.62
1:A:103:PHE:CE2	1:A:107:ARG:NH2	2.78	0.52
1:A:103:PHE:HE2	1:A:107:ARG:NH2	2.08	0.51
1:A:610:LYS:NZ	6:A:2368:HOH:O	2.44	0.50
1:A:265:LYS:HE3	1:A:423:LYS:HB3	1.94	0.49
1:A:97:LEU:HD23	1:A:686:ARG:HG3	1.95	0.48
1:A:638:LEU:O	1:A:642:MET:HG2	2.14	0.48
1:A:33:ARG:HH21	1:A:79:GLN:HE22	1.61	0.47
1:A:741:ILE:HG13	1:A:742:THR:HG23	1.96	0.47
1:A:633:GLN:NE2	6:A:2381:HOH:O	2.45	0.47
1:A:477:LYS:HG3	1:A:638:LEU:HD21	1.97	0.47
1:A:668:GLU:OE1	6:A:2402:HOH:O	2.20	0.46
1:A:1:MET:HE3	1:A:6:ASP:CB	2.46	0.45
1:A:234:ASN:ND2	6:A:2151:HOH:O	2.50	0.44
1:A:261:TYR:C	6:A:2167:HOH:O	2.55	0.44
1:A:369:LEU:O	1:A:372:LYS:NZ	2.50	0.44
1:A:97:LEU:CD2	1:A:686:ARG:HG3	2.48	0.43
1:A:470:CYS:HB3	1:A:634[A]:TYR:CZ	2.54	0.43
1:A:399:LEU:HA	1:A:403:ASP:O	2.19	0.42
1:A:372:LYS:NZ	1:A:390:GLU:OE2	2.51	0.42
1:A:516:LEU:HA	5:A:1755:EDO:H11	2.00	0.42
1:A:213:GLN:HG2	6:A:2135:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:TYR:CZ	1:A:199:VAL:HG11	2.55	0.42
1:A:567:GLU:HA	1:A:579:TYR:O	2.20	0.41
1:A:471:ILE:HG13	5:A:1752:EDO:H12	2.03	0.41
1:A:610:LYS:HD2	6:A:2369:HOH:O	2.21	0.40
1:A:484:HIS:CE1	1:A:489:LEU:HD13	2.56	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	719/770 (93%)	707 (98%)	12 (2%)	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	608/673 (90%)	600 (99%)	8 (1%)	76	72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	SER

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Mol	Chain	Res	Type
1	A	146	ARG
1	A	175	LEU
1	A	219	ASN
1	A	489	LEU
1	A	619	SER
1	A	695	ARG
1	A	741	ILE

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

Mol	Chain	Res	Type
1	A	79	GLN
1	A	219	ASN
1	A	234	ASN
1	A	283	GLN
1	A	338	GLN
1	A	500	ASN
1	A	582	GLN
1	A	606	ASN
1	A	662	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
3	ADP	A	1749	2,4	22,29,29	1.53	2 (9%)	27,45,45	2.68	7 (25%)
4	ALF	A	1750	3,2,6	0,4,4	0.00	-	0,6,6	0.00	-
5	EDO	A	1751	-	3,3,3	0.28	0	2,2,2	0.29	0
5	EDO	A	1752	-	3,3,3	0.28	0	2,2,2	0.56	0
5	EDO	A	1753	-	3,3,3	0.29	0	2,2,2	0.57	0
5	EDO	A	1754	-	3,3,3	0.29	0	2,2,2	0.39	0
5	EDO	A	1755	-	3,3,3	0.28	0	2,2,2	0.51	0
5	EDO	A	1756	-	3,3,3	0.32	0	2,2,2	0.40	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
3	ADP	A	1749	2,4	-	0/12/32/32	0/3/3/3
4	ALF	A	1750	3,2,6	-	0/0/0/0	0/0/0/0
5	EDO	A	1751	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1752	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1753	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1754	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1755	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1756	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1749	ADP	PA-O1A	2.52	1.60	1.51
3	A	1749	ADP	C8-N7	5.32	1.44	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1749	ADP	N3-C2-N1	-9.80	121.39	128.89
3	A	1749	ADP	C2'-C1'-N9	-5.87	105.32	114.29
3	A	1749	ADP	C1'-N9-C4	-4.54	120.09	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1749	ADP	C4-C5-N7	2.05	111.37	109.48
3	A	1749	ADP	C2-N1-C6	2.12	122.56	118.77
3	A	1749	ADP	O3B-PB-O1B	2.33	118.07	110.58
3	A	1749	ADP	O2B-PB-O1B	2.93	120.01	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1750	ALF	1	0
5	A	1752	EDO	1	0
5	A	1755	EDO	1	0

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	726/770 (94%)	0.69	84 (11%) 6 10	23, 36, 65, 94	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	726	VAL	9.8
1	A	725	ALA	7.9
1	A	722	ALA	7.8
1	A	727	LEU	7.6
1	A	705	TYR	7.4
1	A	704	ARG	7.3
1	A	746	PHE	7.2
1	A	67	GLY	7.0
1	A	263	LEU	5.9
1	A	717	GLU	5.9
1	A	737	TYR	5.8
1	A	699	ALA	5.4
1	A	734	PRO	5.3
1	A	733	ASP	4.9
1	A	723	THR	4.8
1	A	239	PHE	4.1
1	A	363	ALA	4.1
1	A	736	GLN	4.1
1	A	696	ILE	4.1
1	A	703	LYS	4.0
1	A	697	ILE	3.8
1	A	735	GLU	3.7
1	A	124	VAL	3.7
1	A	177	ILE	3.7
1	A	700	ASP	3.7
1	A	455	ILE	3.6
1	A	634[A]	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLU	3.5
1	A	290	ALA	3.5
1	A	495	LEU	3.5
1	A	739	PHE	3.5
1	A	41	PRO	3.4
1	A	698	TYR	3.4
1	A	66	ASP	3.3
1	A	430	PHE	3.3
1	A	741	ILE	3.3
1	A	123	LEU	3.3
1	A	65	VAL	3.3
1	A	502	THR	3.2
1	A	718	ASP	3.1
1	A	702	VAL	3.1
1	A	69	ASP	3.1
1	A	625	ALA	3.0
1	A	364	GLY	2.9
1	A	222	LEU	2.9
1	A	499	ILE	2.9
1	A	452	VAL	2.9
1	A	442	CYS	2.9
1	A	653	VAL	2.9
1	A	716	ALA	2.9
1	A	453	LEU	2.8
1	A	258	ILE	2.8
1	A	125	ALA	2.8
1	A	240	GLY	2.7
1	A	715	ASP	2.7
1	A	224	ALA	2.7
1	A	431	LEU	2.7
1	A	184	GLY	2.7
1	A	176	LEU	2.6
1	A	289	THR	2.6
1	A	624	GLY	2.6
1	A	720	GLN	2.6
1	A	429	LEU	2.5
1	A	701	PHE	2.4
1	A	692	PHE	2.4
1	A	745	PHE	2.3
1	A	426	TYR	2.2
1	A	261	TYR	2.2
1	A	262	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	265	LYS	2.2
1	A	225	PHE	2.1
1	A	351	ILE	2.1
1	A	471	ILE	2.1
1	A	744	ILE	2.1
1	A	178	THR	2.1
1	A	1	MET	2.1
1	A	219	ASN	2.1
1	A	175	LEU	2.1
1	A	521	GLN	2.1
1	A	695	ARG	2.1
1	A	535	PHE	2.0
1	A	738	ARG	2.0
1	A	260	SER	2.0
1	A	721	LYS	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	A	1754	4/4	0.84	0.42	4.27	58,60,61,62	0
5	EDO	A	1751	4/4	0.97	0.17	2.62	47,48,48,48	0
5	EDO	A	1752	4/4	0.91	0.36	2.02	59,61,61,62	0
5	EDO	A	1756	4/4	0.73	0.19	1.59	69,70,70,71	0
5	EDO	A	1755	4/4	0.93	0.19	1.14	58,58,58,60	0
2	MG	A	1748	1/1	0.97	0.17	0.18	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	1753	4/4	0.98	0.09	-0.74	40,40,41,43	0
4	ALF	A	1750	5/5	0.99	0.13	-0.98	24,24,25,26	0
3	ADP	A	1749	27/27	0.99	0.11	-1.17	22,29,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.