



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 09:26 PM EDT

PDB ID : 3FWY  
Title : Crystal structure of the L protein of Rhodobacter sphaeroides light-independent protochlorophyllide reductase (BchL) with MgADP bound: a homologue of the nitrogenase Fe protein  
Authors : Sarma, R.; Barney, B.M.; Hamilton, T.L.; Jones, A.; Seefeldt, L.C.; Peters, J.W.  
Deposited on : unknown  
Resolution : 1.63 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

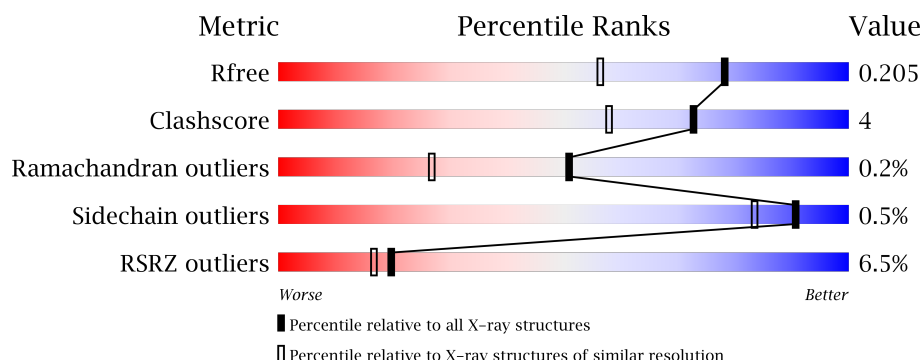
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.63 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))
$R_{free}$	100719	2211 (1.66-1.62)
Clashscore	112137	2356 (1.66-1.62)
Ramachandran outliers	110173	2315 (1.66-1.62)
Sidechain outliers	110143	2315 (1.66-1.62)
RSRZ outliers	101464	2219 (1.66-1.62)

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  $\geq 3$ , 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	314	<div> <div>4%</div> <div>79%</div> <div>6%</div> <div>15%</div> </div>
1	B	314	<div> <div>7%</div> <div>80%</div> <div>5%</div> <div>15%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4630 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 Light-independent protochlorophyllide reductase iron-sulfur ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	4	0
			2079	1313	359	397	10			
1	B	268	Total	C	N	O	S	0	5	0
			2085	1324	360	390	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	EXPRESSION TAG	UNP Q9RFD6
A	-15	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-14	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-13	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-12	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-11	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-10	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-9	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-8	GLY	-	EXPRESSION TAG	UNP Q9RFD6
A	-7	MET	-	EXPRESSION TAG	UNP Q9RFD6
A	-6	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-5	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-4	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-3	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-2	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	-1	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	0	HIS	-	EXPRESSION TAG	UNP Q9RFD6
A	1	GLY	-	EXPRESSION TAG	UNP Q9RFD6
B	-16	MET	-	EXPRESSION TAG	UNP Q9RFD6
B	-15	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-14	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-13	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-12	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-11	HIS	-	EXPRESSION TAG	UNP Q9RFD6

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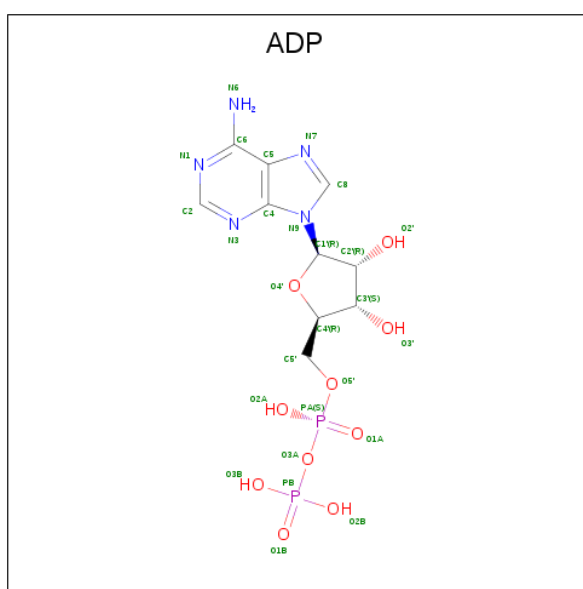
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-9	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-8	GLY	-	EXPRESSION TAG	UNP Q9RFD6
B	-7	MET	-	EXPRESSION TAG	UNP Q9RFD6
B	-6	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-5	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-4	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-3	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-2	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	-1	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	0	HIS	-	EXPRESSION TAG	UNP Q9RFD6
B	1	GLY	-	EXPRESSION TAG	UNP Q9RFD6

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

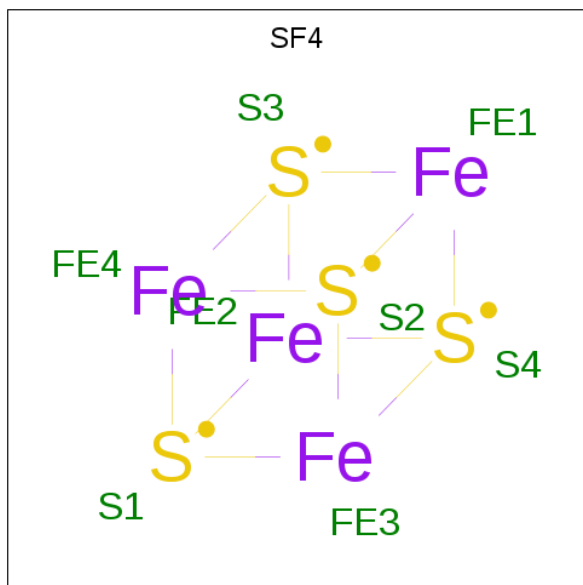
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



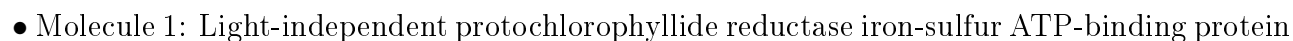
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	253	Total	O	0	0
			253	253		
5	B	149	Total	O	0	0
			149	149		



- Molecule 1: Light-independent protochlorophyllide reductase iron-sulfur ATP-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.73Å 86.62Å 117.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.02 – 1.63 32.17 – 1.63	Depositor EDS
% Data completeness (in resolution range)	96.2 (33.02-1.63) 96.2 (32.17-1.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.174 , 0.199 0.180 , 0.205	Depositor DCC
$R_{free}$ test set	3536 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, 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	0.43	0/2124	0.60	0/2876
1	B	0.35	0/2140	0.57	1/2896 (0.0%)
All	All	0.39	0/4264	0.59	1/5772 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ASP	CB-CG-OD2	5.20	122.98	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	2079	0	2051	16	0
1	B	2085	0	2086	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	0	0
4	B	8	0	0	0	0
5	A	253	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	149	0	0	3	1
All	All	4630	0	4161	33	1

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 4.

All (33) 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:124:THR:HB	5:A:458:HOH:O	1.20	1.30
1:B:234[A]:MET:HE1	1:B:262:ALA:HB1	1.25	1.06
1:B:234[A]:MET:HE2	1:B:240:ILE:HD11	1.44	0.96
1:B:188:ASN:HD21	1:B:285:LEU:H	1.22	0.85
1:A:259:VAL:HG11	5:A:635:HOH:O	1.78	0.83
1:B:234[A]:MET:CE	1:B:240:ILE:HD11	2.09	0.82
1:A:39:LYS:HE2	1:A:42:ILE:HD13	1.66	0.77
1:B:253:MET:HA	1:B:253:MET:HE2	1.65	0.76
1:B:253:MET:HA	1:B:253:MET:CE	2.16	0.75
1:B:234[A]:MET:CE	1:B:262:ALA:HB1	2.12	0.72
1:B:234[A]:MET:HE1	1:B:262:ALA:CB	2.16	0.68
1:A:182[B]:ASP:OD2	5:A:473:HOH:O	2.11	0.67
1:B:248:LYS:HD2	1:B:253:MET:HE1	1.78	0.64
1:A:50:ASN:HD21	1:A:250:LEU:H	1.46	0.63
1:B:234[A]:MET:HE3	1:B:237:LEU:HD12	1.82	0.60
1:B:51[B]:LEU:HD21	1:B:269:LEU:HD23	1.85	0.59
1:A:249:THR:O	1:A:253:MET:HG3	2.04	0.57
1:A:225:GLU:OE1	5:A:653:HOH:O	2.18	0.57
1:A:124:THR:O	1:A:125:GLY:O	2.22	0.57
1:A:211:ASN:HD21	3:A:501:ADP:HN61	1.53	0.55
1:B:92:VAL:HG13	5:B:574:HOH:O	2.07	0.54
1:A:120:PRO:HB2	1:A:124:THR:HG21	1.92	0.52
1:A:217[B]:ASP:OD1	5:A:396:HOH:O	2.19	0.50
1:A:178:ALA:HB3	1:A:180:ASP:OD2	2.13	0.48
1:A:121:PRO:HD2	1:A:124:THR:HG21	1.95	0.48
1:A:211:ASN:HD22	1:A:234:MET:HB3	1.78	0.48
1:A:211:ASN:ND2	3:A:501:ADP:HN61	2.12	0.47
1:B:248:LYS:HD2	1:B:253:MET:CE	2.45	0.47
1:B:86:ILE:HG13	1:B:90:LYS:HE3	1.97	0.46
1:B:71:HIS:HD2	5:B:355:HOH:O	2.00	0.43
1:B:140:GLN:NE2	5:B:489:HOH:O	2.54	0.40
1:B:237:LEU:CD1	1:B:262:ALA:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:HB3	1:A:118:GLY:HA2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:528:HOH:O	5:B:310:HOH:O[4_466]	1.95	0.25

## 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	270/314 (86%)	264 (98%)	5 (2%)	1 (0%)	38	16
1	B	271/314 (86%)	265 (98%)	6 (2%)	0	100	100
All	All	541/628 (86%)	529 (98%)	11 (2%)	1 (0%)	51	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	GLY

### 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	224/260 (86%)	223 (100%)	1 (0%)	93	87
1	B	226/260 (87%)	225 (100%)	1 (0%)	93	87
All	All	450/520 (86%)	448 (100%)	2 (0%)	91	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	B	97	GLU

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	50	ASN
1	A	110	ASN
1	A	141	HIS
1	A	179	ASN
1	A	200	ASN
1	A	211	ASN
1	B	71	HIS
1	B	140	GLN
1	B	188	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	501	2	25,29,29	1.01	2 (8%)	24,45,45	1.42	1 (4%)
4	SF4	B	402	1	0,12,12	0.00	-	0,24,24	0.00	-
3	ADP	B	501	2	25,29,29	1.04	2 (8%)	24,45,45	1.75	4 (16%)

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	501	2	-	0/12/32/32	0/3/3/3
4	SF4	B	402	1	-	0/0/48/48	0/6/5/5
3	ADP	B	501	2	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ADP	PB-O3A	2.04	1.63	1.60
3	A	501	ADP	PB-O3A	2.24	1.63	1.60
3	B	501	ADP	C5-C4	2.55	1.46	1.40
3	A	501	ADP	C5-C4	2.61	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	ADP	N3-C2-N1	-6.12	123.53	128.86
3	A	501	ADP	N3-C2-N1	-5.49	124.08	128.86
3	B	501	ADP	C4-C5-N7	-2.35	107.14	109.41
3	B	501	ADP	N6-C6-N1	2.01	122.75	118.77
3	B	501	ADP	O2A-PA-O1A	2.23	123.82	112.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ADP	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	268/314 (85%)	0.00	12 (4%) 34 32	10, 14, 27, 37	0
1	B	268/314 (85%)	0.37	23 (8%) 11 9	10, 16, 28, 34	0
All	All	536/628 (85%)	0.18	35 (6%) 20 17	10, 15, 27, 37	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	THR	7.9
1	B	260	LEU	4.6
1	B	256	ASP	4.3
1	B	257	GLN	4.2
1	B	100	ARG	3.6
1	B	145	ASP	3.5
1	B	246	LYS	3.5
1	B	258	ASP	3.3
1	A	257	GLN	3.2
1	B	278	ASP	3.2
1	B	198	SER	3.0
1	A	255	GLU	3.0
1	B	259	VAL	3.0
1	A	125	GLY	2.9
1	B	199	LYS	2.8
1	B	30	GLY	2.8
1	A	91	ASP	2.6
1	B	254	ASP	2.6
1	B	140	GLN	2.6
1	A	253	MET	2.5
1	B	112	VAL	2.5
1	B	280	ILE	2.4
1	B	261	ALA	2.4
1	A	100	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	259	VAL	2.2
1	B	238	ASP	2.2
1	A	98	GLU	2.2
1	B	255	GLU	2.2
1	B	279	PRO	2.2
1	B	215	ALA	2.2
1	B	253	MET	2.2
1	A	144	LEU	2.1
1	B	241	ARG	2.1
1	A	122	ALA	2.0
1	A	94	PHE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ADP	B	501	27/27	0.97	0.08	-0.99	23,28,36,39	0
4	SF4	B	402	8/8	0.99	0.03	-1.61	19,20,21,21	0
3	ADP	A	501	27/27	0.98	0.06	-1.95	18,22,26,27	0
2	MG	B	401	1/1	0.99	0.07	-2.05	24,24,24,24	0
2	MG	A	401	1/1	0.99	0.05	-3.51	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.