



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 05:52 PM EST

PDB ID : 3D1L  
Title : Crystal structure of putative NADP oxidoreductase BF3122 from *Bacteroides fragilis*  
Authors : Chang, C.; Hendricks, R.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2008-05-06  
Resolution : 2.19 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

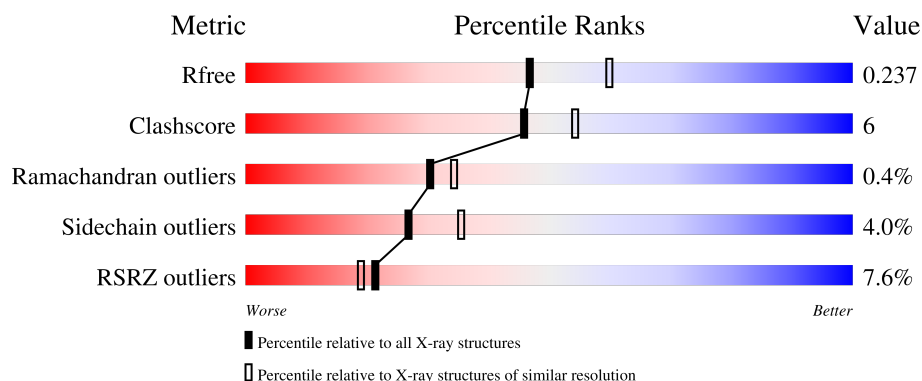
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	266	<div> <div>9%</div> <div>82%</div> <div>12%</div> <div>• •</div> </div>
1	B	266	<div> <div>5%</div> <div>82%</div> <div>15%</div> <div>•</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4447 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.

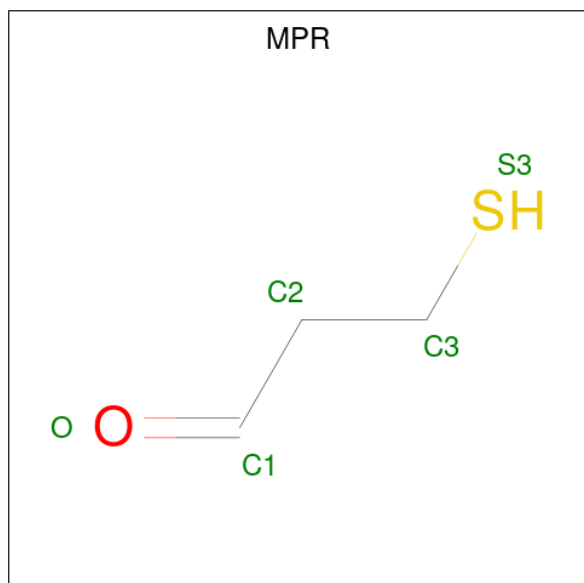
- Molecule 1 is a protein called Putative NADP oxidoreductase BF3122.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	257	2056	1312	350	386	1	7	0	5	0
1	B	259	2149	1370	366	405	1	7	0	13	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5LAQ6
A	-1	ASN	-	expression tag	UNP Q5LAQ6
A	0	ALA	-	expression tag	UNP Q5LAQ6
B	-2	SER	-	expression tag	UNP Q5LAQ6
B	-1	ASN	-	expression tag	UNP Q5LAQ6
B	0	ALA	-	expression tag	UNP Q5LAQ6

- Molecule 2 is 2-MERCAPTO-PROPION ALDEHYDE (three-letter code: MPR) (formula:  $C_3H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			5	3	1	1		
2	B	1	Total	C	O	S	0	0
			5	3	1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

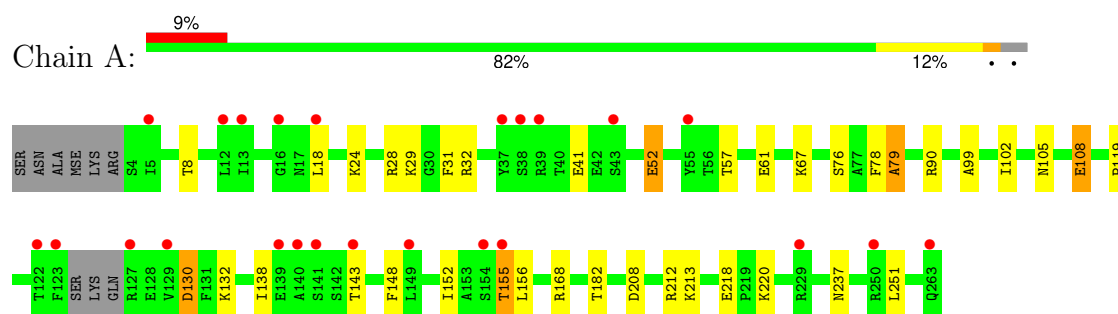
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	114	Total	O	0	0
			114	114		

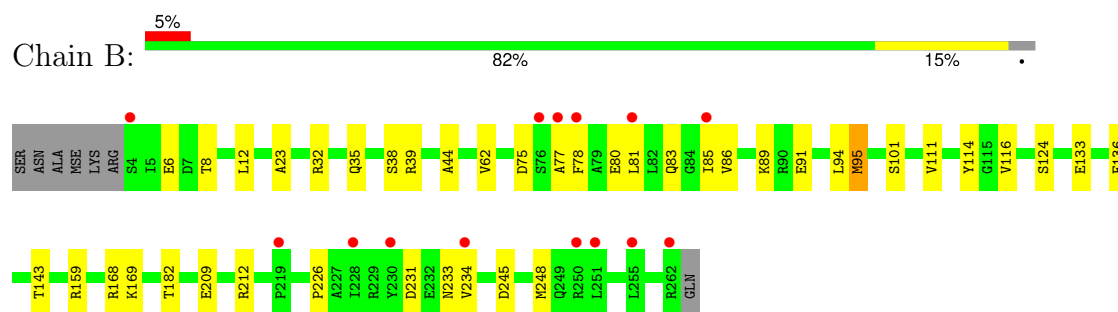
### 3 Residue-property plots [i](#)

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. 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. 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: Putative NADP oxidoreductase BF3122



- Molecule 1: Putative NADP oxidoreductase BF3122



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.00Å 155.00Å 54.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.71 – 2.19 33.71 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.2 (33.71-2.19) 98.2 (33.71-2.19)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.239 0.184 , 0.237	Depositor DCC
$R_{free}$ test set	1662 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MPR

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	0.97	3/2105 (0.1%)	0.76	2/2840 (0.1%)
1	B	0.63	1/2215 (0.0%)	0.69	1/2987 (0.0%)
All	All	0.81	4/4320 (0.1%)	0.73	3/5827 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	GLU	CG-CD	27.40	1.93	1.51
1	A	52	GLU	CD-OE2	-20.11	1.03	1.25
1	B	233	ASN	CG-OD1	7.38	1.40	1.24
1	A	132	LYS	C-O	6.61	1.35	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	52	GLU	OE1-CD-OE2	15.27	141.63	123.30
1	A	52	GLU	CG-CD-OE1	-12.54	93.21	118.30
1	B	94	LEU	CA-CB-CG	5.51	127.98	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	78	PHE	Peptide

## 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	2056	0	2046	22	0
1	B	2149	0	2142	27	0
2	A	5	0	5	0	0
2	B	5	0	6	0	0
3	B	1	0	0	0	0
4	A	117	0	0	3	0
4	B	114	0	0	6	0
All	All	4447	0	4199	47	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 6.

All (47) 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:52:GLU:CD	1:A:52:GLU:CG	1.93	1.37
1:B:12:LEU:HD11	1:B:23:ALA:HB2	1.47	0.94
1:A:31:PHE:HE1	1:A:155:THR:HG21	1.43	0.83
1:B:32:ARG:HD3	4:B:388:HOH:O	1.80	0.81
1:B:95:MSE:HG2	1:B:111:VAL:HG21	1.63	0.80
1:B:101:SER:OG	4:B:403:HOH:O	2.06	0.73
1:A:52:GLU:CG	1:A:52:GLU:OE1	2.37	0.72
1:A:31:PHE:CE1	1:A:155:THR:HG21	2.28	0.66
1:A:76:SER:O	1:A:79:ALA:HB3	1.99	0.63
1:B:95:MSE:CG	1:B:111:VAL:HG21	2.32	0.60
1:A:182:THR:HG23	1:B:182:THR:HG23	1.86	0.57
1:B:85:ILE:O	1:B:89:LYS:HE3	2.06	0.55
1:B:245:ASP:OD2	1:B:248:MSE:HE3	2.07	0.54
1:B:80:GLU:HG2	1:B:81:LEU:HD23	1.90	0.54
1:B:83[A]:GLN:HA	1:B:86:VAL:HG22	1.91	0.53
1:A:32:ARG:CZ	1:A:32:ARG:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:SER:HB3	1:B:44:ALA:HB2	1.91	0.52
1:B:86:VAL:O	4:B:373:HOH:O	2.19	0.52
1:A:61:GLU:HG3	4:A:334:HOH:O	2.08	0.52
1:B:12:LEU:CD1	1:B:23:ALA:HB2	2.31	0.51
1:B:133:GLU:OE1	1:B:159[B]:ARG:NH2	2.42	0.51
1:B:226:PRO:HB3	1:B:234:VAL:HG21	1.95	0.49
1:A:130:ASP:OD2	1:A:130:ASP:C	2.51	0.49
1:B:83[B]:GLN:HA	1:B:86:VAL:HG22	1.95	0.49
1:B:226:PRO:CB	1:B:234:VAL:HG21	2.43	0.48
1:A:90:ARG:HB2	4:A:403:HOH:O	2.13	0.48
1:B:39[A]:ARG:NH2	4:B:396:HOH:O	2.46	0.47
1:A:208:ASP:HB3	1:A:212[A]:ARG:HH12	1.81	0.45
1:B:133:GLU:OE1	1:B:159[B]:ARG:NE	2.49	0.45
1:A:32:ARG:CZ	1:A:32:ARG:CB	2.93	0.45
1:B:116:VAL:HG11	1:B:168:ARG:CZ	2.47	0.45
1:A:29:LYS:HG3	1:A:156:LEU:HD23	1.99	0.44
1:A:24:LYS:HE3	1:A:28:ARG:HH22	1.82	0.44
1:A:213:LYS:CE	1:B:124:SER:OG	2.66	0.44
1:A:105:ASN:O	1:A:108:GLU:HB3	2.18	0.44
1:B:77:ALA:O	1:B:81:LEU:HG	2.18	0.44
1:A:8:THR:HG23	1:A:67:LYS:HB3	2.01	0.43
1:A:99:ALA:HB3	1:A:102:ILE:HD12	2.00	0.43
1:B:95:MSE:O	1:B:114:TYR:HA	2.19	0.43
1:A:168:ARG:HD3	4:A:399:HOH:O	2.19	0.43
1:A:218:GLU:OE2	1:A:220[B]:LYS:HE2	2.19	0.42
1:A:148:PHE:O	1:A:152:ILE:HG12	2.19	0.42
1:B:8:THR:O	4:B:383:HOH:O	2.22	0.41
1:B:35:GLN:OE1	1:B:62:VAL:HA	2.21	0.41
1:B:209[B]:GLU:OE1	1:B:209[B]:GLU:HA	2.21	0.41
1:A:18:LEU:HD11	1:A:119:PRO:HG2	2.01	0.41
1:B:169:LYS:HG2	4:B:403:HOH:O	2.20	0.41

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	258/266 (97%)	250 (97%)	7 (3%)	1 (0%)	30	34
1	B	270/266 (102%)	261 (97%)	8 (3%)	1 (0%)	30	34
All	All	528/532 (99%)	511 (97%)	15 (3%)	2 (0%)	30	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	ALA
1	B	231	ASP

### 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	218/218 (100%)	209 (96%)	9 (4%)	26	34
1	B	230/218 (106%)	221 (96%)	9 (4%)	27	37
All	All	448/436 (103%)	430 (96%)	18 (4%)	27	35

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	57	THR
1	A	108	GLU
1	A	130	ASP
1	A	138	ILE
1	A	143	THR
1	A	155	THR
1	A	237	ASN
1	A	251	LEU
1	B	6	GLU
1	B	75	ASP

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Mol	Chain	Res	Type
1	B	78	PHE
1	B	91	GLU
1	B	95	MSE
1	B	136	PHE
1	B	143	THR
1	B	212[A]	ARG
1	B	212[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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	MPR	B	301	1	2,4,4	0.93	0	1,3,3	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MPR	A	301	1	2,4,4	0.59	0	1,3,3	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	MPR	B	301	1	-	0/1/2/2	-
2	MPR	A	301	1	-	0/1/2/2	-

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 ⓘ

**Warning:** The R factor obtained from EDS is 0.2388, which does not match the depositor's R factor of 0.18532. Please interpret the results in this section carefully.

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	250/266 (93%)	0.86	24 (9%)	15 12	21, 50, 64, 73	5 (2%)
1	B	252/266 (94%)	0.53	14 (5%)	31 28	22, 44, 62, 69	13 (5%)
All	All	502/532 (94%)	0.70	38 (7%)	21 19	21, 47, 64, 73	18 (3%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	4.3
1	A	123	PHE	3.8
1	A	18	LEU	3.5
1	A	37	TYR	3.5
1	A	12	LEU	3.4
1	A	140	ALA	3.4
1	B	4	SER	3.2
1	A	13	ILE	3.0
1	B	251	LEU	3.0
1	A	229[A]	ARG	3.0
1	A	263	GLN	3.0
1	B	76	SER	2.8
1	A	5	ILE	2.8
1	B	77	ALA	2.8
1	B	234	VAL	2.8
1	A	154	SER	2.7
1	B	85	ILE	2.7
1	A	38	SER	2.6
1	A	39	ARG	2.6
1	A	129	VAL	2.5
1	B	230	TYR	2.5
1	B	250	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	255	LEU	2.4
1	A	155	THR	2.4
1	A	141	SER	2.4
1	A	127	ARG	2.4
1	A	139	GLU	2.3
1	A	122	THR	2.3
1	A	143	THR	2.3
1	B	262	ARG	2.3
1	A	149	LEU	2.3
1	B	219	PRO	2.2
1	B	78	PHE	2.2
1	A	250	ARG	2.1
1	A	43	SER	2.1
1	B	228	ILE	2.1
1	A	16	GLY	2.0
1	A	55	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	MPR	A	301	5/5	0.65	0.31	52,54,54,54	5
3	CL	B	302	1/1	0.86	0.20	50,50,50,50	1
2	MPR	B	301	5/5	0.88	0.17	53,54,55,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.