



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:38 pm GMT

PDB ID : 3VLY  
Title : Assimilatory nitrite reductase (Nii3) - N226K mutant - SO3 partial complex from tobacco leaf  
Authors : Nakano, S.; Takahashi, M.; Sakamoto, A.; Morikawa, H.; Katayanagi, K.  
Deposited on : 2011-12-05  
Resolution : 1.55 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	:	trunk28620
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)	:	recalc28949

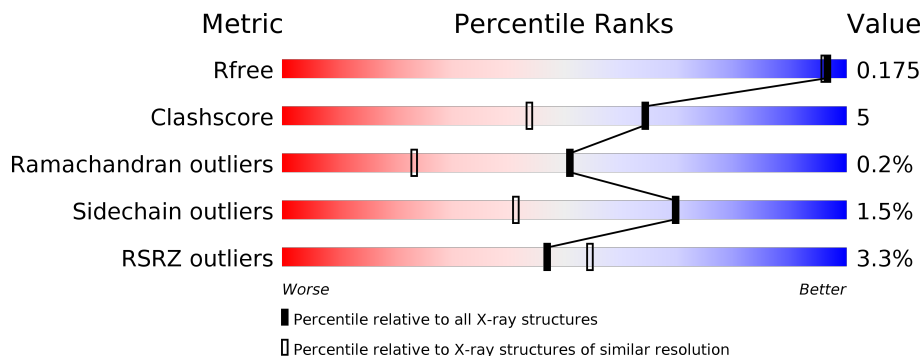
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	1088 (1.56-1.56)
Clashscore	112137	1132 (1.56-1.56)
Ramachandran outliers	110173	1110 (1.56-1.56)
Sidechain outliers	110143	1108 (1.56-1.56)
RSRZ outliers	101464	1089 (1.56-1.56)

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	584	<div> <div>3%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5261 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.

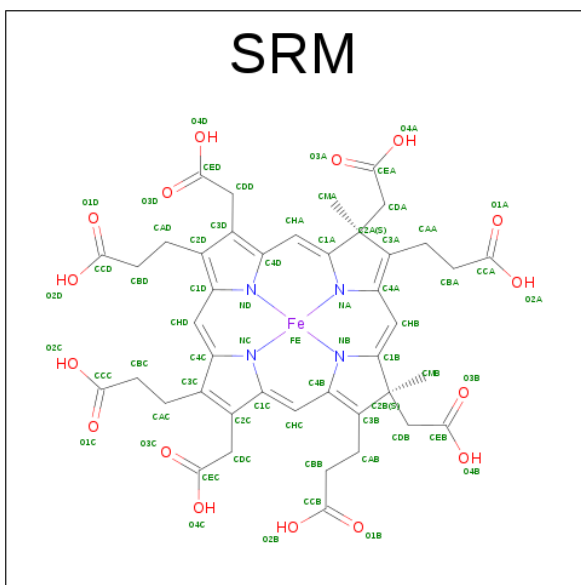
- Molecule 1 is a protein called Nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	6	0
			4261	2690	756	791	24			

There are 24 discrepancies between the modelled and reference sequences:

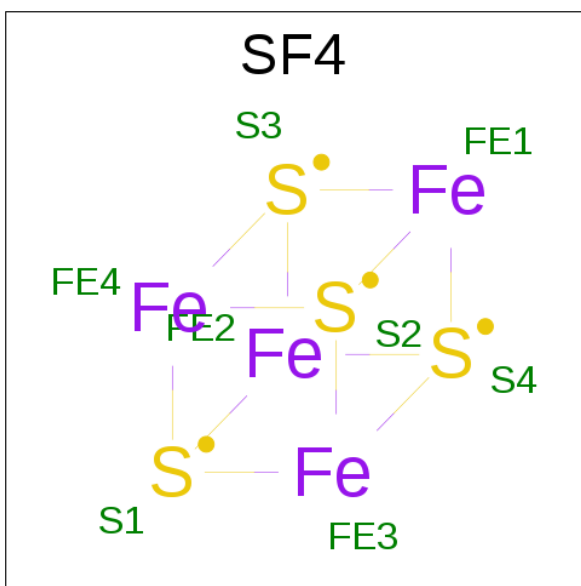
Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	EXPRESSION TAG	UNP Q76KB0
A	-27	GLY	-	EXPRESSION TAG	UNP Q76KB0
A	-26	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-25	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-24	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-23	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-22	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-21	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-20	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-19	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-18	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-17	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-16	SER	-	EXPRESSION TAG	UNP Q76KB0
A	-15	SER	-	EXPRESSION TAG	UNP Q76KB0
A	-14	GLY	-	EXPRESSION TAG	UNP Q76KB0
A	-13	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-12	ILE	-	EXPRESSION TAG	UNP Q76KB0
A	-11	GLU	-	EXPRESSION TAG	UNP Q76KB0
A	-10	GLY	-	EXPRESSION TAG	UNP Q76KB0
A	-9	ARG	-	EXPRESSION TAG	UNP Q76KB0
A	-8	HIS	-	EXPRESSION TAG	UNP Q76KB0
A	-7	MET	-	EXPRESSION TAG	UNP Q76KB0
A	226	LYS	ASN	ENGINEERED MUTATION	UNP Q76KB0
A	290	ARG	LYS	CONFLICT	UNP Q76KB0

- Molecule 2 is SIROHEME (three-letter code: SRM) (formula:  $C_{42}H_{42}FeN_4O_{16}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

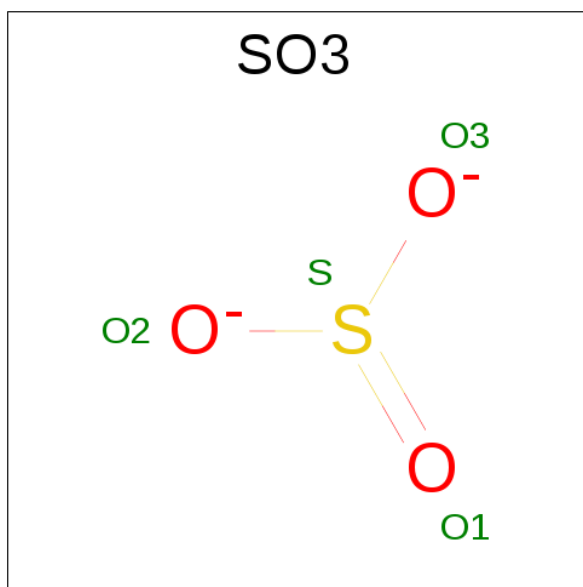
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0

- Molecule 6 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).



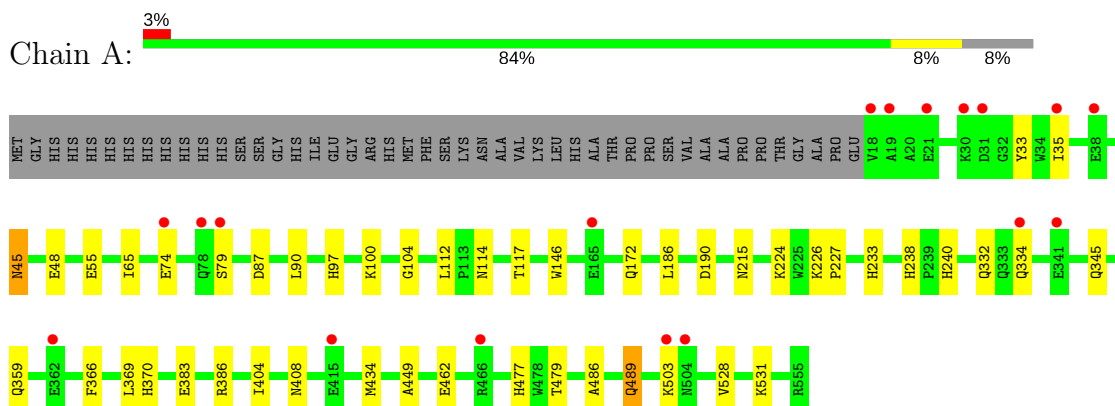
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 4 3 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	922	Total O 922 922	0	0



- Molecule 1: Nitrite reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.66Å 133.66Å 77.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.99 – 1.55 35.98 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.99-1.55) 99.6 (35.98-1.55)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.164 , 0.176 0.161 , 0.175	Depositor DCC
$R_{free}$ test set	5048 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: K, SRM, SF4, SO3, 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	0.44	0/4378	0.59	0/5920

There are no bond length outliers.

There are no bond angle outliers.

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	4261	0	4295	42	0
2	A	63	0	34	1	0
3	A	8	0	0	1	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	4	0	0	1	0
7	A	922	0	0	10	1
All	All	5261	0	4329	42	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 5.

All (42) 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:97:HIS:HE1	1:A:104:GLY:H	1.17	0.89
1:A:383:GLU:OE1	1:A:386:ARG:NH2	2.05	0.88
1:A:359:GLN:HE22	1:A:408:ASN:H	1.25	0.85
1:A:233:HIS:HD2	1:A:345:GLN:H	1.25	0.80
1:A:359:GLN:NE2	1:A:408:ASN:H	1.85	0.75
1:A:233:HIS:CD2	1:A:345:GLN:H	2.06	0.72
1:A:74:GLU:HG2	7:A:1330:HOH:O	1.91	0.70
1:A:489:GLN:HE21	1:A:489:GLN:H	1.43	0.67
1:A:224[B]:LYS:CE	1:A:226:LYS:HE3	2.25	0.65
1:A:224[B]:LYS:NZ	6:A:606:SO3:O3	2.29	0.64
1:A:117[A]:THR:HG21	1:A:146:TRP:HE1	1.63	0.63
1:A:112:LEU:HD11	1:A:117[A]:THR:HG22	1.83	0.60
1:A:477:HIS:HD2	1:A:486:ALA:O	1.88	0.56
1:A:172:GLN:HE22	1:A:215:ASN:H	1.54	0.56
1:A:238:HIS:HE1	7:A:1006:HOH:O	1.89	0.56
1:A:489:GLN:NE2	1:A:489:GLN:H	2.02	0.55
1:A:117[A]:THR:HG21	1:A:146:TRP:NE1	2.22	0.55
1:A:224[B]:LYS:HE2	1:A:226:LYS:HE3	1.88	0.55
1:A:240:HIS:HE1	7:A:1025:HOH:O	1.90	0.55
1:A:35:ILE:HG22	7:A:1411:HOH:O	2.06	0.55
1:A:359:GLN:HE22	1:A:408:ASN:N	2.01	0.54
1:A:370:HIS:HD2	7:A:1019:HOH:O	1.90	0.54
1:A:87:ASP:OD2	1:A:97:HIS:HD2	1.92	0.53
1:A:112:LEU:HD21	1:A:117[A]:THR:CG2	2.38	0.52
1:A:238:HIS:HD2	7:A:1034:HOH:O	1.94	0.51
1:A:112:LEU:HD21	1:A:117[A]:THR:HG23	1.93	0.50
1:A:97:HIS:CE1	1:A:104:GLY:H	2.10	0.49
1:A:477:HIS:HE1	7:A:1007:HOH:O	1.95	0.49
1:A:359:GLN:HE21	1:A:366:PHE:HB3	1.76	0.49
1:A:528:VAL:HG11	1:A:531:LYS:HD3	1.93	0.48
1:A:186:LEU:HB3	1:A:190:ASP:HB2	1.96	0.47
1:A:369:LEU:HD12	1:A:404[A]:ILE:HD11	1.97	0.47
1:A:45:ASN:ND2	1:A:48:GLU:H	2.13	0.46
1:A:100:LYS:NZ	7:A:1481:HOH:O	2.48	0.46
1:A:434:MET:CE	1:A:462:GLU:HG3	2.46	0.45
1:A:477:HIS:CD2	1:A:486:ALA:O	2.69	0.45
1:A:332:GLN:NE2	7:A:1722:HOH:O	2.46	0.44
1:A:449:ALA:HB2	3:A:602:SF4:S3	2.58	0.43
1:A:65:ILE:HD13	1:A:90:LEU:HD21	1.99	0.43
1:A:33:TYR:CD1	1:A:55:GLU:HG2	2.54	0.43
1:A:224[A]:LYS:NZ	2:A:601:SRM:HBD2	2.35	0.42
1:A:370:HIS:HE1	7:A:1042:HOH:O	2.03	0.41

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)
7:A:1191:HOH:O	7:A:1906:HOH:O[7_555]	2.13	0.07

## 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	542/584 (93%)	529 (98%)	12 (2%)	1 (0%)	51 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	PRO

### 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	469/500 (94%)	462 (98%)	7 (2%)	70 41

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	79	SER

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Mol	Chain	Res	Type
1	A	114	ASN
1	A	334	GLN
1	A	479	THR
1	A	489	GLN
1	A	503	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	97	HIS
1	A	101	ASN
1	A	172	GLN
1	A	177	ASN
1	A	202	ASN
1	A	233	HIS
1	A	238	HIS
1	A	240	HIS
1	A	306	GLN
1	A	332	GLN
1	A	359	GLN
1	A	370	HIS
1	A	377	GLN
1	A	467	GLN
1	A	477	HIS
1	A	489	GLN
1	A	524	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 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	$\# Z  > 2$
2	SRM	A	601	1,6	34,70,70	1.31	5 (14%)	34,112,112	2.22	7 (20%)
3	SF4	A	602	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SO3	A	606	2	1,3,3	0.52	0	0,3,3	0.00	-

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	SRM	A	601	1,6	-	0/22/126/126	0/0/8/8
3	SF4	A	602	1	-	0/0/48/48	0/6/5/5
6	SO3	A	606	2	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	SRM	C4A-NA	-2.45	1.34	1.39
2	A	601	SRM	CHA-C1A	2.05	1.39	1.36
2	A	601	SRM	FE-NA	2.54	2.05	1.95
2	A	601	SRM	C3D-C2D	3.11	1.46	1.39
2	A	601	SRM	C3C-C2C	3.12	1.46	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	SRM	CAB-C3B-C2B	-7.76	114.75	123.52
2	A	601	SRM	CAA-C3A-C2A	-6.47	116.21	123.52
2	A	601	SRM	CED-CDD-C3D	-3.06	110.19	116.14
2	A	601	SRM	C2A-CDA-CEA	-2.12	112.25	115.39
2	A	601	SRM	C4D-CHA-C1A	-2.08	126.00	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	SRM	C4B-NB-C1B	2.91	108.33	106.37
2	A	601	SRM	C4A-NA-C1A	3.83	108.95	106.37

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
2	A	601	SRM	1	0
3	A	602	SF4	1	0
6	A	606	SO3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	538/584 (92%)	-0.06	18 (3%) 47 54	7, 12, 22, 34	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	VAL	7.4
1	A	503	LYS	4.0
1	A	38	GLU	3.9
1	A	341	GLU	3.7
1	A	19	ALA	3.5
1	A	334	GLN	3.5
1	A	31	ASP	3.1
1	A	504	ASN	3.1
1	A	74	GLU	3.0
1	A	78	GLN	2.8
1	A	30	LYS	2.4
1	A	21	GLU	2.3
1	A	165	GLU	2.3
1	A	466	ARG	2.1
1	A	35	ILE	2.1
1	A	415	GLU	2.1
1	A	79	SER	2.1
1	A	362	GLU	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( $\text{\AA}^2$ )	Q<0.9
2	SRM	A	601	63/63	0.97	0.10	-0.14	6,8,16,25	0
6	SO3	A	606	4/4	0.98	0.09	-0.99	12,15,17,18	0
3	SF4	A	602	8/8	1.00	0.05	-1.19	8,8,9,9	0
5	CL	A	605	1/1	0.98	0.04	-2.02	17,17,17,17	0
4	K	A	603	1/1	1.00	0.03	-4.65	11,11,11,11	0
5	CL	A	604	1/1	0.97	0.07	-	25,25,25,25	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.