



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:44 am GMT

PDB ID : 4EBF  
Title : SeMet thermostable phosphite dehydrogenase Glu175-Ala mutant  
Authors : Zou, Y.; Zhang, H.; Nair, S.K.  
Deposited on : 2012-03-23  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

---

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

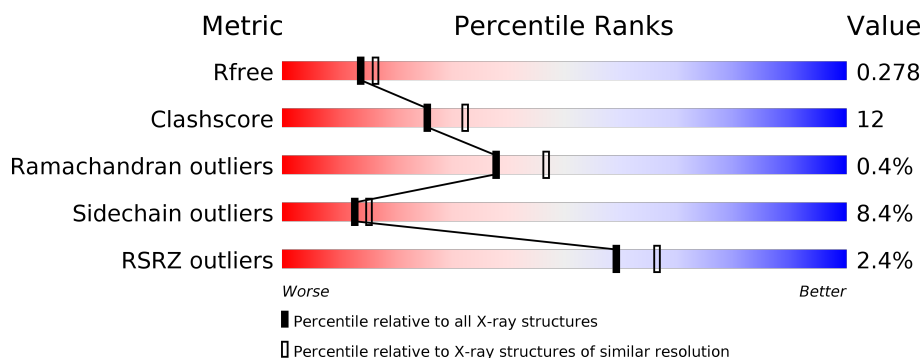
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	334	<div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	B	334	<div> <div>71%</div> <div>24%</div> <div>..</div> </div>
1	C	334	<div> <div>%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	D	334	<div> <div>76%</div> <div>19%</div> <div>..</div> </div>
1	E	334	<div> <div>12%</div> <div>70%</div> <div>22%</div> <div>..</div> </div>
1	F	334	<div> <div>%</div> <div>69%</div> <div>24%</div> <div>5%</div> <div>.</div> </div>

2 Entry composition [i](#)

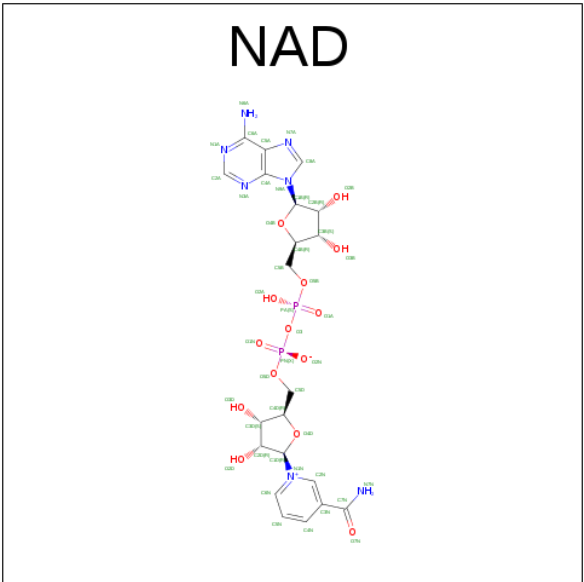
There are 3 unique types of molecules in this entry. The entry contains 15960 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thermostable phosphite dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	Se	0	0	0
			2536	1601	461	460	8	6			
1	B	330	Total	C	N	O	S	Se	0	0	0
			2524	1594	458	457	8	7			
1	C	329	Total	C	N	O	S	Se	0	0	0
			2512	1585	456	456	8	7			
1	D	330	Total	C	N	O	S	Se	0	0	0
			2521	1592	458	457	8	6			
1	E	321	Total	C	N	O	S	Se	0	0	0
			2449	1548	443	444	8	6			
1	F	326	Total	C	N	O	S	Se	0	0	0
			2488	1570	453	451	8	6			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

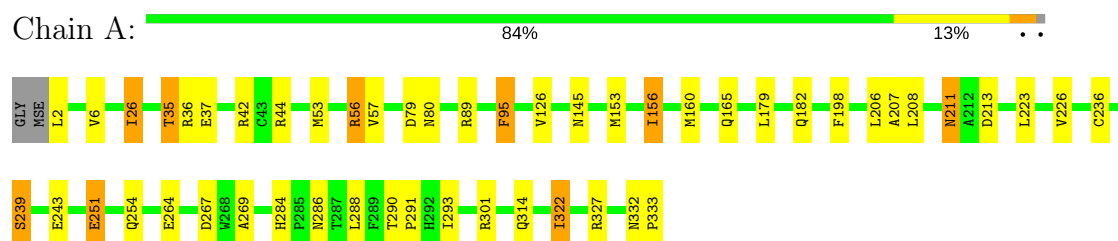
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		
3	B	137	Total	O	0	0
			137	137		
3	C	99	Total	O	0	0
			99	99		
3	D	125	Total	O	0	0
			125	125		
3	E	110	Total	O	0	0
			110	110		
3	F	128	Total	O	0	0
			128	128		

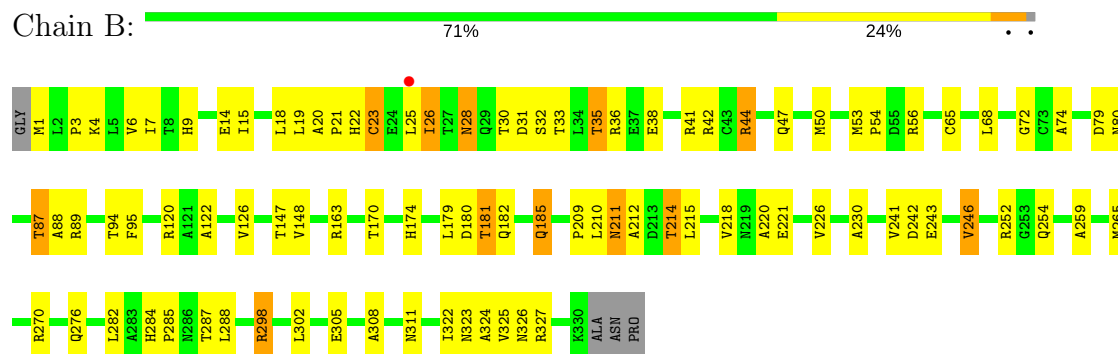
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

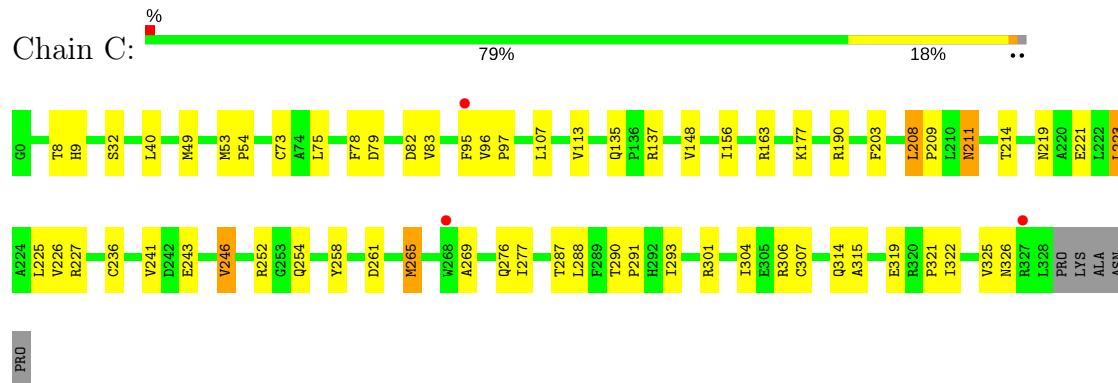
- Molecule 1: Thermostable phosphite dehydrogenase



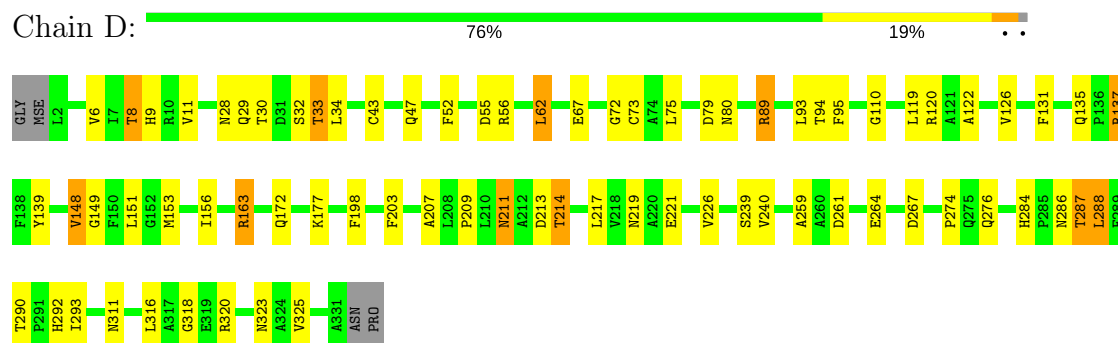
- Molecule 1: Thermostable phosphite dehydrogenase



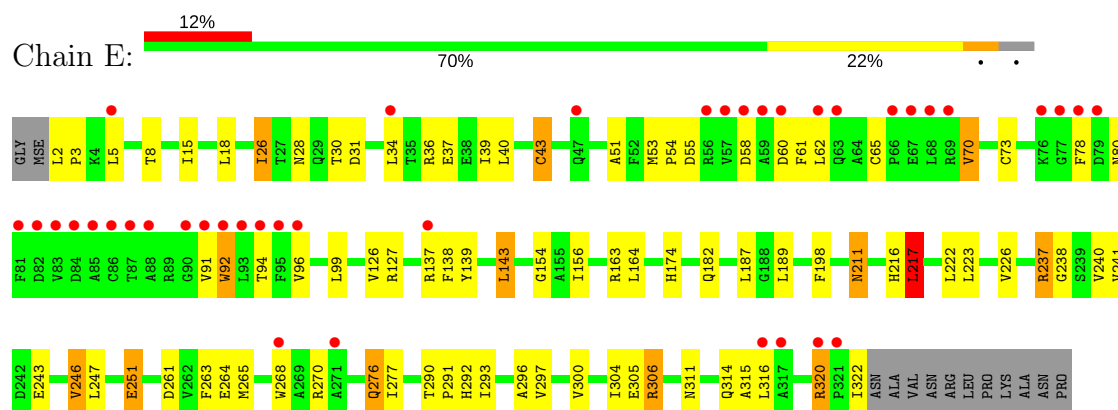
- Molecule 1: Thermostable phosphite dehydrogenase



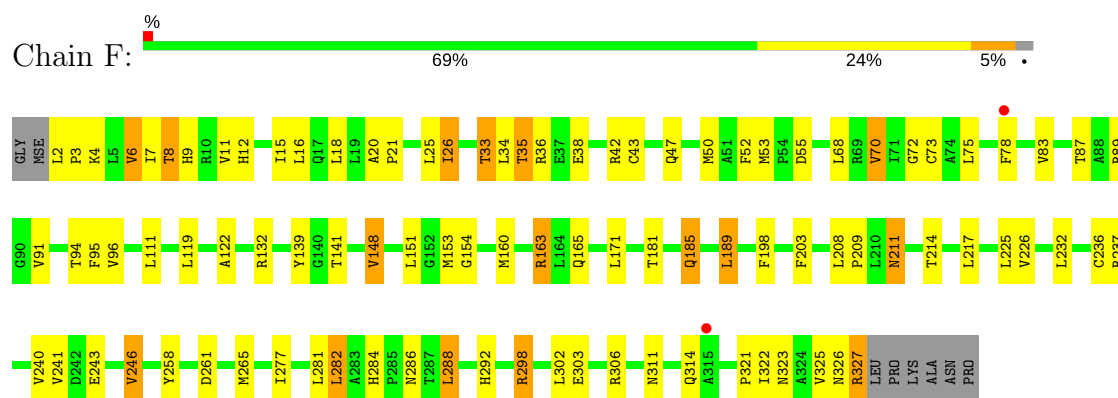
- Molecule 1: Thermostable phosphite dehydrogenase



• Molecule 1: Thermostable phosphite dehydrogenase



• Molecule 1: Thermostable phosphite dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.22Å 122.58Å 135.01Å 90.00° 96.36° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 47.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.4 (25.00-2.30) 96.3 (47.31-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.207 , 0.274 0.219 , 0.278	Depositor DCC
$R_{free}$ test set	4850 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: NAD

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	0.63	0/2578	0.73	0/3499
1	B	0.57	0/2565	0.72	1/3479 (0.0%)
1	C	0.62	0/2551	0.68	2/3458 (0.1%)
1	D	0.62	1/2562 (0.0%)	0.71	1/3476 (0.0%)
1	E	0.61	0/2489	0.72	2/3377 (0.1%)
1	F	0.66	2/2528 (0.1%)	0.76	3/3430 (0.1%)
All	All	0.62	3/15273 (0.0%)	0.72	9/20719 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	160	MSE	CG-SE	-5.13	1.77	1.95
1	D	153	MSE	CG-SE	-5.04	1.78	1.95
1	F	265	MSE	CG-SE	-5.03	1.78	1.95

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	163	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	D	163	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	E	163	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	F	163	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	E	217	LEU	CA-CB-CG	5.65	128.29	115.30

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	2536	0	2553	48	0
1	B	2524	0	2547	70	0
1	C	2512	0	2530	53	0
1	D	2521	0	2540	65	0
1	E	2449	0	2461	63	0
1	F	2488	0	2500	85	0
2	A	44	0	26	4	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	155	0	0	7	0
3	B	137	0	0	12	0
3	C	99	0	0	1	0
3	D	125	0	0	8	0
3	E	110	0	0	13	0
3	F	128	0	0	13	0
All	All	15960	0	15235	362	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 12.

The worst 5 of 362 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:F:87:THR:HG22	1:F:326:ASN:HD22	1.08	1.10
1:D:156:ILE:HB	3:D:1024:HOH:O	1.56	1.06
1:C:290:THR:CG2	1:C:293:ILE:HG12	1.87	1.03
1:B:53:MSE:HE3	3:B:910:HOH:O	1.55	1.03
1:D:9:HIS:HE2	1:D:33:THR:HB	1.26	1.00

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	330/334 (99%)	317 (96%)	13 (4%)	0	100	100
1	B	328/334 (98%)	305 (93%)	19 (6%)	4 (1%)	15	16
1	C	327/334 (98%)	311 (95%)	14 (4%)	2 (1%)	28	34
1	D	328/334 (98%)	313 (95%)	15 (5%)	0	100	100
1	E	319/334 (96%)	294 (92%)	24 (8%)	1 (0%)	44	55
1	F	324/334 (97%)	306 (94%)	18 (6%)	0	100	100
All	All	1956/2004 (98%)	1846 (94%)	103 (5%)	7 (0%)	38	47

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	CYS
1	B	31	ASP
1	C	269	ALA
1	E	138	PHE
1	B	44	ARG

### 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	260/254 (102%)	245 (94%)	15 (6%)	23	31
1	B	259/254 (102%)	237 (92%)	22 (8%)	12	15
1	C	257/254 (101%)	240 (93%)	17 (7%)	19	25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	258/254 (102%)	239 (93%)	19 (7%)	16	20
1	E	250/254 (98%)	218 (87%)	32 (13%)	5	5
1	F	254/254 (100%)	230 (91%)	24 (9%)	10	12
All	All	1538/1524 (101%)	1409 (92%)	129 (8%)	13	15

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	56	ARG
1	D	288	LEU
1	F	225	LEU
1	D	79	ASP
1	D	148	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	29	GLN
1	D	286	ASN
1	F	284	HIS
1	D	47	GLN
1	D	165	GLN

### 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

4 ligands are modelled in this entry.

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	NAD	A	800	-	41,48,48	0.78	2 (4%)	43,73,73	1.77	4 (9%)
2	NAD	B	800	-	41,48,48	0.74	1 (2%)	43,73,73	1.90	4 (9%)
2	NAD	C	800	-	41,48,48	0.71	1 (2%)	43,73,73	1.77	4 (9%)
2	NAD	D	800	-	41,48,48	0.73	0	43,73,73	1.76	3 (6%)

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	NAD	A	800	-	-	0/22/62/62	0/5/5/5
2	NAD	B	800	-	-	0/22/62/62	0/5/5/5
2	NAD	C	800	-	-	0/22/62/62	0/5/5/5
2	NAD	D	800	-	-	0/22/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	NAD	C2A-N3A	2.01	1.35	1.32
2	A	800	NAD	C2A-N3A	2.26	1.36	1.32
2	A	800	NAD	O4B-C1B	2.38	1.44	1.41
2	C	800	NAD	O4B-C1B	2.60	1.44	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	NAD	N3A-C2A-N1A	-9.51	120.58	128.86
2	A	800	NAD	N3A-C2A-N1A	-9.40	120.67	128.86
2	D	800	NAD	N3A-C2A-N1A	-9.16	120.88	128.86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	NAD	N3A-C2A-N1A	-8.89	121.12	128.86
2	D	800	NAD	C1B-N9A-C4A	-3.71	120.23	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	NAD	4	0
2	C	800	NAD	1	0
2	D	800	NAD	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	326/334 (97%)	-0.12	0 <span>100</span> <span>100</span>	21, 32, 48, 61	0
1	B	323/334 (96%)	0.10	1 (0%) <span>93</span> <span>96</span>	21, 41, 61, 66	0
1	C	322/334 (96%)	-0.06	3 (0%) <span>84</span> <span>87</span>	25, 39, 58, 69	0
1	D	324/334 (97%)	-0.02	0 <span>100</span> <span>100</span>	22, 37, 54, 57	0
1	E	315/334 (94%)	0.52	40 (12%) <span>4</span> <span>6</span>	23, 45, 82, 86	0
1	F	320/334 (95%)	-0.05	2 (0%) <span>89</span> <span>92</span>	20, 36, 50, 57	0
All	All	1930/2004 (96%)	0.06	46 (2%) <span>59</span> <span>66</span>	20, 38, 62, 86	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	88	ALA	8.0
1	E	268	TRP	5.0
1	E	57	VAL	4.6
1	E	81	PHE	4.6
1	E	84	ASP	4.5

### 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
2	NAD	D	800	44/44	0.95	0.12	0.04	29,36,59,60	0
2	NAD	A	800	44/44	0.97	0.11	-0.18	25,32,46,47	0
2	NAD	B	800	44/44	0.97	0.11	-0.34	22,27,45,47	0
2	NAD	C	800	44/44	0.93	0.12	-0.43	36,47,56,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.