



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 01:57 PM EDT

PDB ID : 2XXF  
Title : Cu metallated H254F mutant of nitrite reductase  
Authors : Hough, M.A.; Eady, R.R.; Hasnain, S.S.  
Deposited on : 2010-11-10  
Resolution : 1.50 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

<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) : 1.20.1  
EDS : 2.36.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

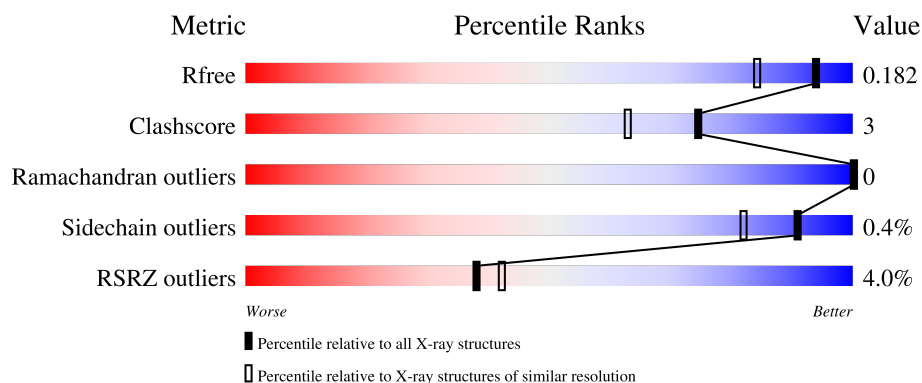
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\leq 5\%$ . 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	336	<div> <div>4%</div> <div>94%</div> <div>6%</div> </div>
1	B	336	<div> <div>4%</div> <div>95%</div> <div>5%</div> </div>

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
4	PEG	A	1347	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5899 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 DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	2	0
			2574	1643	444	475	12			
1	B	335	Total	C	N	O	S	0	3	0
			2580	1648	445	475	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP O68601
A	254	PHE	HIS	engineered mutation	UNP O68601
B	1	GLU	-	expression tag	UNP O68601
B	254	PHE	HIS	engineered mutation	UNP O68601

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

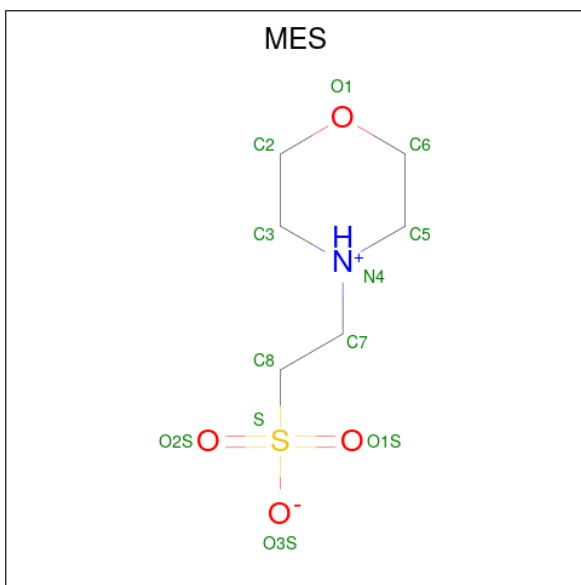
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		
3	B	3	Total	Zn	0	0
			3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



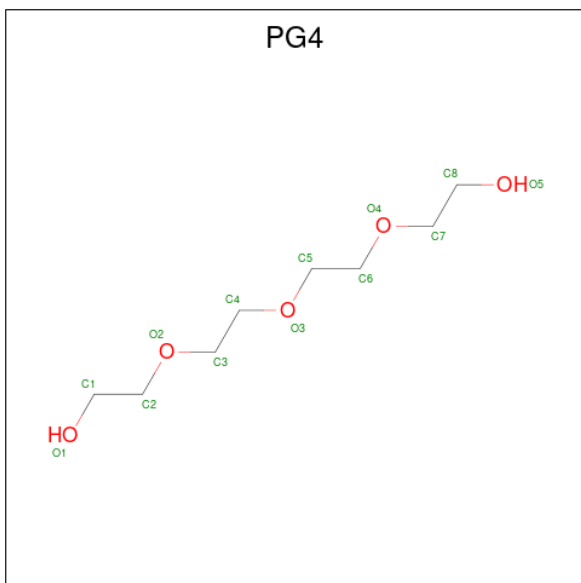
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	294	Total	O	0	1
			295	295		
7	B	319	Total	O	0	0
			319	319		

### 3 Residue-property plots

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 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: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain A: 



#### • Molecule 1: DISSIMILATORY COPPER-CONTAINING NITRITE REDUCTASE

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.33Å 89.33Å 287.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.78 – 1.50 26.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (95.78-1.50) 91.9 (26.00-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.145 , 0.176 0.153 , 0.182	Depositor DCC
$R_{free}$ test set	6310 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 60.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h-k,k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	5899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5759e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PG4, PEG, MES, CU, ZN

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	0.89	2/2651 (0.1%)	0.88	1/3609 (0.0%)
1	B	0.88	0/2660	0.97	11/3620 (0.3%)
All	All	0.88	2/5311 (0.0%)	0.93	12/7229 (0.2%)

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
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	GLY	N-CA	5.90	1.54	1.46
1	A	133	GLU	CG-CD	5.15	1.59	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135[A]	MET	CG-SD-CE	13.44	121.70	100.20
1	B	135[B]	MET	CG-SD-CE	13.44	121.70	100.20
1	B	189	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	214	PHE	CB-CG-CD1	5.86	124.90	120.80
1	B	122	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	153	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	244[A]	ARG	NE-CZ-NH2	-5.30	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244[B]	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	158	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	214	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	B	153	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	189	ASP	CB-CG-OD2	-5.12	113.70	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	HIS	Peptide
1	B	300	HIS	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	2574	0	2541	17	0
1	B	2580	0	2554	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	19	0	24	11	0
4	B	28	0	40	9	0
5	A	24	0	24	0	0
5	B	24	0	24	0	0
6	A	13	0	18	0	0
6	B	13	0	18	0	0
7	A	295	0	0	2	0
7	B	319	0	0	3	2
All	All	5899	0	5243	34	2

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 (34) 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:244[A]:ARG:NH1	7:A:2224:HOH:O	1.58	1.28
1:A:165:HIS:HB3	4:A:1347:PEG:H32	1.48	0.95
1:B:135[A]:MET:HE2	7:B:2110:HOH:O	1.78	0.82
1:B:35:PHE:O	4:B:1343:PEG:C4	2.37	0.73
1:B:135[A]:MET:CE	1:B:139:HIS:HE2	2.01	0.73
1:B:135[A]:MET:HG3	1:B:139:HIS:CD2	2.32	0.65
1:B:35:PHE:O	4:B:1343:PEG:H42	1.98	0.64
1:A:163:PRO:HB2	4:A:1347:PEG:H42	1.81	0.63
1:A:165:HIS:CB	4:A:1347:PEG:H32	2.26	0.63
1:A:157:LYS:NZ	7:A:2142:HOH:O	2.33	0.62
1:B:35:PHE:O	4:B:1343:PEG:H41	2.00	0.61
1:B:135[A]:MET:HE3	1:B:139:HIS:HE2	1.67	0.59
1:B:88:PRO:HG2	7:B:2110:HOH:O	2.03	0.58
1:B:194:ALA:HB1	4:B:1345:PEG:H21	1.84	0.58
1:B:21:PRO:HD2	4:B:1342:PEG:O2	2.05	0.56
1:B:22:HIS:HA	4:B:1341:PEG:H21	1.91	0.53
1:B:135[A]:MET:CE	7:B:2110:HOH:O	2.49	0.52
1:A:165:HIS:ND1	4:A:1347:PEG:C3	2.75	0.50
1:B:12:THR:HB	4:B:1342:PEG:H21	1.92	0.50
1:A:163:PRO:CB	4:A:1347:PEG:H12	2.44	0.47
1:A:165:HIS:HD1	4:A:1347:PEG:C3	2.28	0.47
1:A:130:CYS:SG	1:A:132:PRO:HD3	2.55	0.47
1:A:164:LEU:C	4:A:1347:PEG:H41	2.35	0.47
1:A:165:HIS:CG	4:A:1347:PEG:H32	2.50	0.46
1:B:39:ILE:HD13	1:B:89:HIS:HB2	1.97	0.46
1:A:163:PRO:HB3	4:A:1347:PEG:H12	1.98	0.44
1:A:165:HIS:HD1	4:A:1347:PEG:C4	2.32	0.43
1:B:12:THR:O	4:B:1342:PEG:C2	2.66	0.43
1:B:39:ILE:HD13	1:B:89:HIS:CB	2.49	0.43
1:A:299:ASN:O	1:A:305:ALA:HB2	2.19	0.43
4:B:1341:PEG:H22	4:B:1341:PEG:H41	1.66	0.41
1:A:135[B]:MET:CE	4:A:1340:PEG:O1	2.70	0.40
1:A:75:VAL:O	1:A:117:ARG:HA	2.22	0.40
1:A:3:ALA:HB2	1:A:74:TYR:CE2	2.56	0.40

All (2) 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:B:2254:HOH:O	7:B:2262:HOH:O[3_665]	1.99	0.21
7:B:2251:HOH:O	7:B:2251:HOH:O[2_655]	2.05	0.15

## 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	335/336 (100%)	329 (98%)	6 (2%)	0	100	100
1	B	336/336 (100%)	330 (98%)	6 (2%)	0	100	100
All	All	671/672 (100%)	659 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	271/271 (100%)	270 (100%)	1 (0%)	91	82
1	B	272/271 (100%)	271 (100%)	1 (0%)	91	82
All	All	543/542 (100%)	541 (100%)	2 (0%)	91	82

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

Mol	Chain	Res	Type
1	A	247	ARG
1	B	247	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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$
4	PEG	A	1346	-	4,4,6	0.91	0	3,3,5	0.06	0
5	MES	A	1343	-	12,12,12	2.05	2 (16%)	15,16,16	3.79	9 (60%)
4	PEG	B	1345	-	6,6,6	0.49	0	5,5,5	0.96	0
5	MES	B	1346	-	12,12,12	1.70	1 (8%)	15,16,16	4.00	9 (60%)
4	PEG	A	1347	-	6,6,6	1.14	0	5,5,5	1.29	1 (20%)
6	PG4	B	1347	-	12,12,12	0.57	0	11,11,11	0.54	0
5	MES	A	1342	-	12,12,12	1.69	1 (8%)	15,16,16	3.74	8 (53%)
4	PEG	B	1342	-	6,6,6	1.27	0	5,5,5	1.36	1 (20%)
4	PEG	B	1341	-	6,6,6	0.65	0	5,5,5	0.58	0
4	PEG	B	1343	-	6,6,6	1.45	1 (16%)	5,5,5	1.34	0
4	PEG	A	1340	-	6,6,6	0.46	0	5,5,5	0.81	0
5	MES	B	1339	-	12,12,12	1.26	1 (8%)	15,16,16	3.53	9 (60%)
6	PG4	A	1344	-	12,12,12	0.51	0	11,11,11	0.63	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
4	PEG	A	1346	-	-	1/2/2/4	-
5	MES	A	1343	-	-	0/6/14/14	0/1/1/1
4	PEG	B	1345	-	-	3/4/4/4	-
5	MES	B	1346	-	-	2/6/14/14	0/1/1/1
4	PEG	A	1347	-	-	4/4/4/4	-
6	PG4	B	1347	-	-	1/10/10/10	-
5	MES	A	1342	-	-	1/6/14/14	0/1/1/1
4	PEG	B	1342	-	-	2/4/4/4	-
4	PEG	B	1341	-	-	2/4/4/4	-
4	PEG	B	1343	-	-	1/4/4/4	-
4	PEG	A	1340	-	-	2/4/4/4	-
5	MES	B	1339	-	-	1/6/14/14	0/1/1/1
6	PG4	A	1344	-	-	0/10/10/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1343	MES	C8-S	-5.81	1.69	1.77
5	A	1342	MES	C8-S	-5.40	1.70	1.77
5	B	1346	MES	C8-S	-5.04	1.70	1.77
5	B	1339	MES	C8-S	-3.86	1.72	1.77
5	A	1343	MES	O1S-S	3.29	1.54	1.45
4	B	1343	PEG	O2-C3	2.05	1.51	1.42

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1339	MES	O1S-S-C8	-8.49	93.90	106.73
5	A	1343	MES	O1S-S-C8	-8.34	94.12	106.73
5	A	1342	MES	O2S-S-C8	-7.65	95.16	106.73
5	B	1346	MES	O1S-S-C8	-7.01	96.14	106.73
5	B	1346	MES	C5-N4-C3	6.59	123.03	108.84
5	A	1343	MES	O3S-S-O1S	6.27	127.08	111.40
5	A	1342	MES	C5-N4-C3	6.12	122.02	108.84
5	A	1342	MES	O3S-S-C8	-6.03	94.21	106.00
5	B	1346	MES	O2S-S-C8	-5.73	98.07	106.73
5	B	1346	MES	O3S-S-O2S	5.64	125.52	111.40
5	B	1346	MES	O3S-S-C8	-5.61	95.02	106.00
5	B	1339	MES	C7-N4-C5	5.28	125.31	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1339	MES	C5-N4-C3	4.84	119.28	108.84
5	A	1343	MES	O2S-S-C8	-4.83	99.43	106.73
5	A	1343	MES	C5-N4-C3	4.78	119.15	108.84
5	A	1342	MES	O1S-S-C8	-4.54	99.87	106.73
5	A	1343	MES	C7-N4-C5	4.44	123.08	111.24
5	B	1346	MES	O3S-S-O1S	4.37	122.34	111.40
5	A	1342	MES	C7-N4-C5	4.22	122.50	111.24
5	A	1342	MES	C2-C3-N4	4.00	116.19	110.12
5	B	1339	MES	O3S-S-O1S	3.74	120.76	111.40
5	A	1343	MES	C2-C3-N4	3.72	115.78	110.12
5	B	1346	MES	C7-N4-C5	3.39	120.27	111.24
5	B	1339	MES	O2S-S-C8	-3.31	101.72	106.73
5	B	1339	MES	C6-C5-N4	3.29	115.13	110.12
5	A	1343	MES	C6-C5-N4	3.07	114.78	110.12
5	A	1342	MES	O3S-S-O2S	2.82	118.46	111.40
5	B	1339	MES	C2-C3-N4	2.80	114.37	110.12
5	B	1346	MES	C2-C3-N4	2.71	114.23	110.12
5	A	1342	MES	O2S-S-O1S	2.67	122.51	113.82
5	B	1339	MES	O3S-S-C8	-2.66	100.81	106.00
4	A	1347	PEG	O2-C2-C1	-2.40	99.52	110.11
4	B	1342	PEG	O2-C2-C1	2.29	120.19	110.11
5	B	1346	MES	C6-C5-N4	2.24	113.52	110.12
5	A	1343	MES	O3S-S-O2S	2.20	116.91	111.40
5	B	1339	MES	O1-C6-C5	2.13	116.35	111.77
5	A	1343	MES	O3S-S-C8	-2.12	101.87	106.00

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1342	MES	C8-C7-N4-C5
5	B	1339	MES	C8-C7-N4-C5
5	B	1346	MES	C8-C7-N4-C5
4	A	1340	PEG	O1-C1-C2-O2
4	B	1341	PEG	O1-C1-C2-O2
4	B	1343	PEG	O1-C1-C2-O2
4	A	1346	PEG	O1-C1-C2-O2
4	B	1345	PEG	O2-C3-C4-O4
4	B	1341	PEG	C4-C3-O2-C2
4	A	1347	PEG	O2-C3-C4-O4
4	B	1342	PEG	O1-C1-C2-O2
4	B	1345	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	1347	PEG	O1-C1-C2-O2
4	B	1342	PEG	C1-C2-O2-C3
4	A	1340	PEG	C1-C2-O2-C3
6	B	1347	PG4	C8-C7-O4-C6
4	A	1347	PEG	C1-C2-O2-C3
4	A	1347	PEG	C4-C3-O2-C2
4	B	1345	PEG	C1-C2-O2-C3
5	B	1346	MES	C8-C7-N4-C3

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1345	PEG	1	0
4	A	1347	PEG	10	0
4	B	1342	PEG	3	0
4	B	1341	PEG	2	0
4	B	1343	PEG	3	0
4	A	1340	PEG	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, 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	335/336 (99%)	0.06	15 (4%) 33 36	13, 23, 36, 56	2 (0%)
1	B	335/336 (99%)	-0.01	12 (3%) 42 47	12, 22, 33, 57	3 (0%)
All	All	670/672 (99%)	0.02	27 (4%) 38 42	12, 23, 36, 57	5 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LYS	6.6
1	A	5	LYS	5.8
1	A	335	PRO	5.4
1	B	2	ASP	5.0
1	A	336	ARG	4.8
1	A	334	ILE	4.5
1	B	336	ARG	4.4
1	B	335	PRO	4.3
1	A	2	ASP	3.9
1	B	183	PRO	3.8
1	A	183	PRO	3.5
1	A	328	ILE	3.2
1	B	333	PRO	3.1
1	A	27	LYS	3.0
1	A	83	ALA	2.8
1	B	83	ALA	2.6
1	A	111	GLY	2.5
1	A	224	ALA	2.5
1	A	10	LYS	2.5
1	B	27	LYS	2.4
1	B	224	ALA	2.2
1	A	319	LYS	2.2
1	B	10	LYS	2.1
1	B	4	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	333	PRO	2.1
1	A	91	VAL	2.0
1	B	319	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 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( $\text{\AA}^2$ )	Q<0.9
4	PEG	B	1342	7/7	0.73	0.27	46,51,57,57	0
4	PEG	A	1340	7/7	0.80	0.22	53,54,58,58	0
4	PEG	B	1341	7/7	0.82	0.32	61,62,63,64	0
3	ZN	A	1345	1/1	0.87	0.15	70,70,70,70	1
4	PEG	A	1346	5/7	0.88	0.18	56,57,58,59	0
4	PEG	B	1345	7/7	0.89	0.14	51,52,52,54	0
4	PEG	B	1343	7/7	0.90	0.23	34,48,54,54	0
4	PEG	A	1347	7/7	0.91	0.36	30,34,41,43	0
6	PG4	A	1344	13/13	0.93	0.09	29,33,43,47	0
6	PG4	B	1347	13/13	0.94	0.08	28,32,42,49	0
5	MES	A	1342	12/12	0.95	0.15	26,33,36,38	2
5	MES	B	1339	12/12	0.95	0.12	24,27,33,36	0
5	MES	A	1343	12/12	0.96	0.10	24,27,37,38	0
5	MES	B	1346	12/12	0.96	0.15	27,29,34,34	2
3	ZN	B	1348	1/1	0.99	0.03	46,46,46,46	1
3	ZN	B	1338	1/1	1.00	0.04	18,18,18,18	1
3	ZN	B	1344	1/1	1.00	0.03	25,25,25,25	0
2	CU	A	1338	1/1	1.00	0.05	14,14,14,14	1
2	CU	B	1337	1/1	1.00	0.04	23,23,23,23	0
2	CU	B	1340	1/1	1.00	0.05	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	1339	1/1	1.00	0.05	15,15,15,15	1
3	ZN	A	1341	1/1	1.00	0.02	26,26,26,26	0
2	CU	A	1337	1/1	1.00	0.03	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.