



# wwPDB X-ray Structure Validation Summary Report

Jul 12, 2022 – 01:12 pm BST


PDB ID : 7NWU  
Title : Co-crystal structure of UPF3B-RRM-NOPS-L with UPF2-MIF4GIII  
Authors : Powers, K.T.; Bufton, J.C.; Szeto, J.A.; Schaffitzel, C.  
Deposited on : 2021-03-17  
Resolution : 2.60 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

<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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

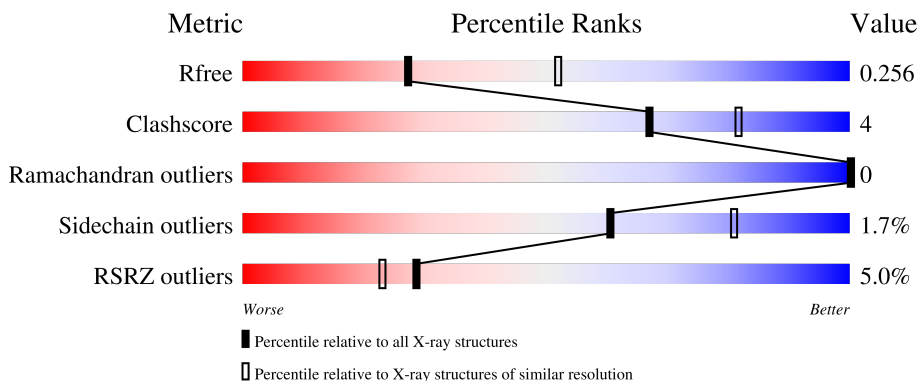
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



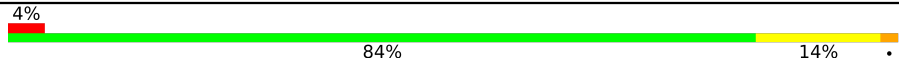
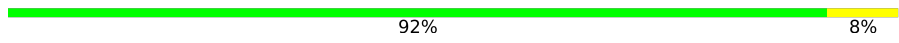
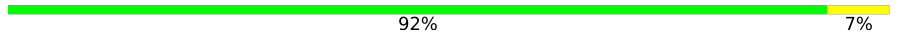
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	122	 15% 89% 11%
1	C	122	 20% 74% 18% 6%
1	E	122	 7% 83% 10% 7%
1	G	122	 7% 81% 13% 6%
2	B	251	 % 92% 8%

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Mol	Chain	Length	Quality of chain
2	D	251	 4% 84% 14%
2	F	251	 92% 8%
2	H	251	 92% 7%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12248 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 Regulator of nonsense transcripts 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	122	996	644	163	187	2	0	0	0
1	C	115	942	612	156	172	2	0	0	0
1	E	114	952	617	154	179	2	0	0	0
1	G	115	935	607	152	174	2	0	0	0

- Molecule 2 is a protein called Regulator of nonsense transcripts 2.

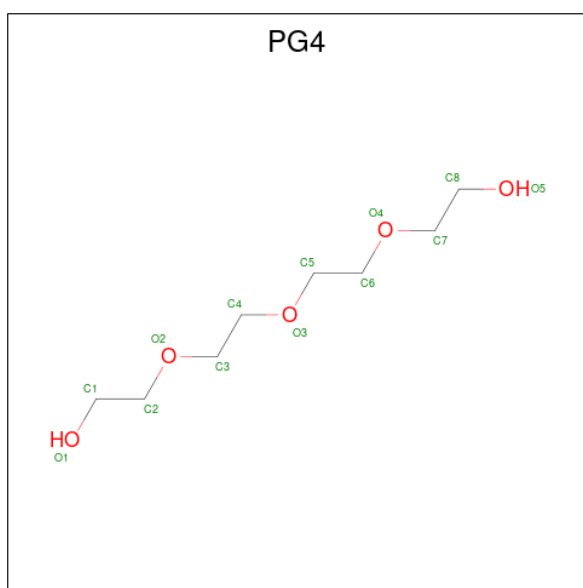
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	250	2059	1331	350	366	12	0	0	0
2	D	250	2050	1321	347	370	12	0	0	0
2	F	250	2059	1331	350	366	12	0	0	0
2	H	250	2050	1321	347	370	12	0	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	C O	0	0
			16	10 6		
3	H	1	Total	C O	0	0
			16	10 6		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	C O	0	0
			13	8 5		

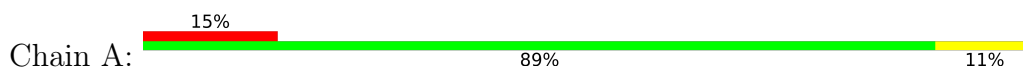
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	36	Total O 36 36	0	0
5	C	3	Total O 3 3	0	0
5	D	20	Total O 20 20	0	0
5	E	4	Total O 4 4	0	0
5	F	48	Total O 48 48	0	0
5	G	7	Total O 7 7	0	0
5	H	36	Total O 36 36	0	0

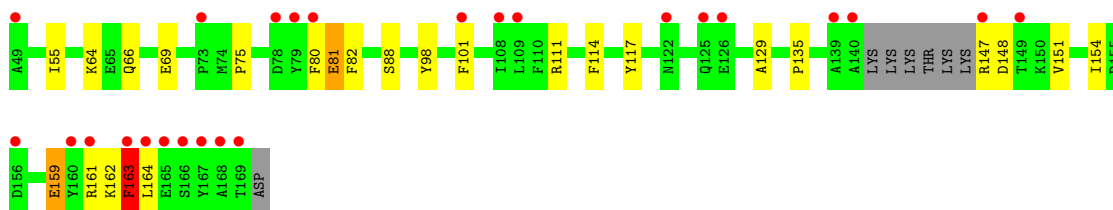
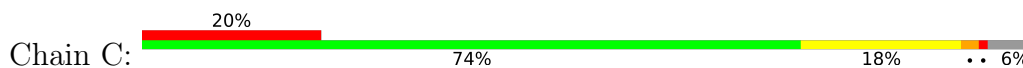
### 3 Residue-property plots [i](#)

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 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.

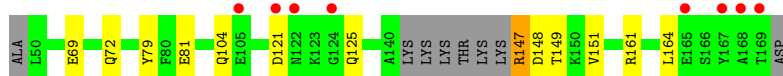
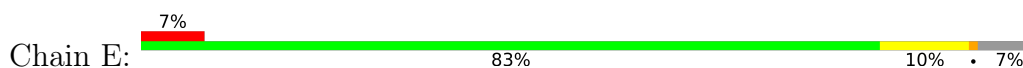
- Molecule 1: Regulator of nonsense transcripts 3B



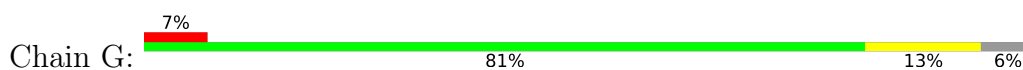
- Molecule 1: Regulator of nonsense transcripts 3B



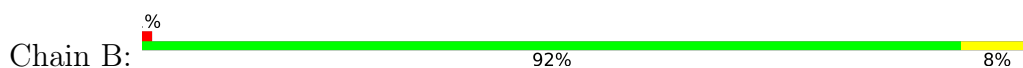
- Molecule 1: Regulator of nonsense transcripts 3B

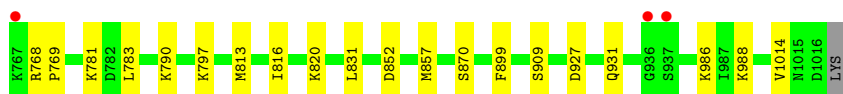


- Molecule 1: Regulator of nonsense transcripts 3B

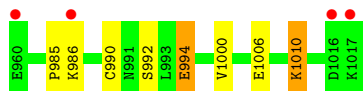
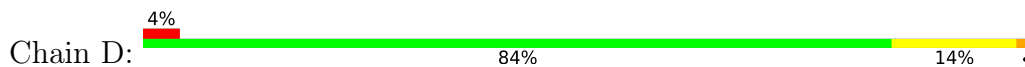


- Molecule 2: Regulator of nonsense transcripts 2

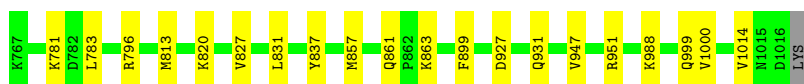




• Molecule 2: Regulator of nonsense transcripts 2



• Molecule 2: Regulator of nonsense transcripts 2



• Molecule 2: Regulator of nonsense transcripts 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.59Å 130.59Å 267.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.60) 100.0 (30.00-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, $R_{free}$	0.217 , 0.256 0.216 , 0.256	Depositor DCC
$R_{free}$ test set	3568 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.44 % 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 4.6575e-03. 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 1PE

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	0.28	0/1024	0.43	0/1389
1	C	0.40	1/969 (0.1%)	0.48	0/1315
1	E	0.27	0/979	0.43	0/1327
1	G	0.28	0/962	0.44	0/1308
2	B	0.27	0/2106	0.39	0/2851
2	D	0.27	0/2097	0.39	0/2844
2	F	0.27	0/2106	0.39	0/2851
2	H	0.27	0/2097	0.39	0/2844
All	All	0.28	1/12340 (0.0%)	0.41	0/16729

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	PHE	CE1-CZ	-5.80	1.26	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	81	GLU	Peptide

## 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	996	0	928	7	0
1	C	942	0	884	18	0
1	E	952	0	897	9	0
1	G	935	0	861	8	0
2	B	2059	0	2072	11	0
2	D	2050	0	2037	27	0
2	F	2059	0	2072	12	0
2	H	2050	0	2037	11	0
3	D	16	0	22	1	0
3	H	16	0	22	1	0
4	F	13	0	18	0	0
5	A	6	0	0	0	0
5	B	36	0	0	1	0
5	C	3	0	0	0	0
5	D	20	0	0	1	0
5	E	4	0	0	0	0
5	F	48	0	0	1	0
5	G	7	0	0	0	0
5	H	36	0	0	2	0
All	All	12248	0	11850	94	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 4.

The worst 5 of 94 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:C:159:GLU:HA	1:C:162:LYS:HD2	1.58	0.85
1:C:154:ILE:HB	2:D:797:LYS:HB3	1.60	0.83
2:D:775:VAL:HG11	2:D:809:VAL:HG12	1.68	0.74
2:D:882:ARG:HE	3:D:1101:1PE:H232	1.51	0.74
1:C:135:PRO:HB2	2:D:850:LEU:HD13	1.72	0.70

There are no symmetry-related clashes.

## 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	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	C	111/122 (91%)	104 (94%)	7 (6%)	0	100	100
1	E	110/122 (90%)	106 (96%)	4 (4%)	0	100	100
1	G	111/122 (91%)	106 (96%)	5 (4%)	0	100	100
2	B	248/251 (99%)	243 (98%)	5 (2%)	0	100	100
2	D	248/251 (99%)	236 (95%)	12 (5%)	0	100	100
2	F	248/251 (99%)	243 (98%)	5 (2%)	0	100	100
2	H	248/251 (99%)	241 (97%)	7 (3%)	0	100	100
All	All	1444/1492 (97%)	1393 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	103/111 (93%)	101 (98%)	2 (2%)	57	79
1	C	97/111 (87%)	93 (96%)	4 (4%)	30	56
1	E	102/111 (92%)	99 (97%)	3 (3%)	42	68
1	G	96/111 (86%)	95 (99%)	1 (1%)	76	90
2	B	231/237 (98%)	227 (98%)	4 (2%)	60	81
2	D	230/237 (97%)	224 (97%)	6 (3%)	46	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	231/237 (98%)	230 (100%)	1 (0%)	91	97
2	H	230/237 (97%)	228 (99%)	2 (1%)	78	91
All	All	1320/1392 (95%)	1297 (98%)	23 (2%)	60	81

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	994	GLU
1	E	147	ARG
1	E	104	GLN
1	E	149	THR
1	C	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
2	D	822	ASN
2	F	861	GLN
2	F	931	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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
3	1PE	D	1101	-	15,15,15	0.53	0	14,14,14	0.26	0
3	1PE	H	1101	-	15,15,15	0.53	0	14,14,14	0.26	0
4	PG4	F	1101	-	12,12,12	0.51	0	11,11,11	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
3	1PE	D	1101	-	-	10/13/13/13	-
3	1PE	H	1101	-	-	10/13/13/13	-
4	PG4	F	1101	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1101	1PE	OH5-C14-C24-OH4
3	H	1101	1PE	OH4-C13-C23-OH3
3	D	1101	1PE	OH7-C16-C26-OH6
4	F	1101	PG4	O2-C3-C4-O3
3	H	1101	1PE	OH2-C12-C22-OH3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1101	1PE	1	0
3	H	1101	1PE	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	122/122 (100%)	0.62	18 (14%) 2 1	47, 75, 107, 135	0
1	C	115/122 (94%)	1.01	25 (21%) 0 0	55, 85, 118, 139	0
1	E	114/122 (93%)	0.35	8 (7%) 16 12	42, 70, 95, 113	0
1	G	115/122 (94%)	0.20	9 (7%) 13 9	39, 64, 96, 121	0
2	B	250/251 (99%)	-0.07	3 (1%) 79 76	38, 50, 68, 100	0
2	D	250/251 (99%)	0.22	9 (3%) 42 35	41, 58, 94, 110	0
2	F	250/251 (99%)	-0.12	0 100 100	35, 49, 68, 98	0
2	H	250/251 (99%)	-0.07	1 (0%) 92 91	35, 49, 69, 87	0
All	All	1466/1492 (98%)	0.17	73 (4%) 28 23	35, 56, 98, 139	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	168	ALA	6.4
1	C	169	THR	6.3
1	C	167	TYR	6.2
1	A	144	THR	5.5
2	D	839	GLU	5.3

### 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
3	1PE	H	1101	16/16	0.89	0.21	50,55,63,64	16
3	1PE	D	1101	16/16	0.95	0.13	66,71,97,102	16
4	PG4	F	1101	13/13	0.95	0.19	47,51,60,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.