



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:01 PM GMT

PDB ID : 4NIE  
Title : Crystal structure of the orphan nuclear receptor ROR(gamma)t ligand-binding domain in complex with small molecule ligand  
Authors : Ma, Y.L.; Yang, L.Q.  
Deposited on : 2013-11-06  
Resolution : 2.01 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.

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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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

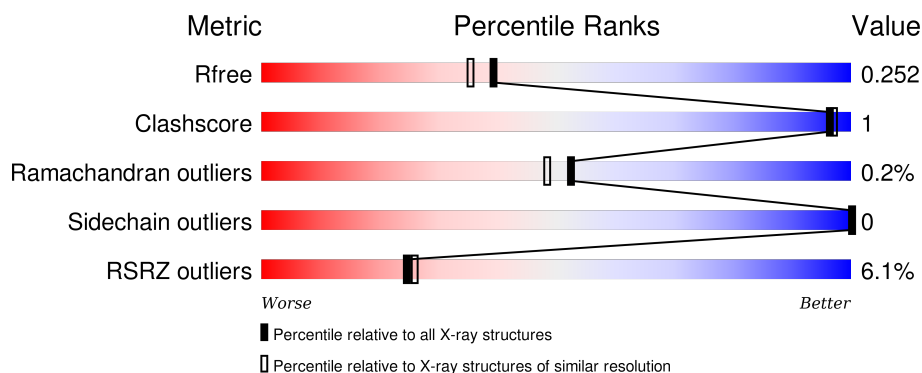
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	262	<div> <div>3%</div> <div>92%</div> <div>6%</div> </div>
1	B	262	<div> <div>7%</div> <div>87%</div> <div>6%</div> <div>6%</div> </div>
2	C	12	<div> <div>25%</div> <div>75%</div> <div>25%</div> </div>
2	D	12	<div> <div>75%</div> <div>8%</div> <div>17%</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
3	NBH	A	601	-	-	-	X
3	NBH	B	601	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4437 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 Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	5	0
			2008	1287	352	354	15			
1	B	245	Total	C	N	O	S	0	2	0
			1978	1265	343	355	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	MET	-	EXPRESSION TAG	UNP P51449
A	249	LYS	-	EXPRESSION TAG	UNP P51449
A	250	LYS	-	EXPRESSION TAG	UNP P51449
A	251	HIS	-	EXPRESSION TAG	UNP P51449
A	252	HIS	-	EXPRESSION TAG	UNP P51449
A	253	HIS	-	EXPRESSION TAG	UNP P51449
A	254	HIS	-	EXPRESSION TAG	UNP P51449
A	255	HIS	-	EXPRESSION TAG	UNP P51449
A	256	HIS	-	EXPRESSION TAG	UNP P51449
A	257	LEU	-	EXPRESSION TAG	UNP P51449
A	258	VAL	-	EXPRESSION TAG	UNP P51449
A	259	PRO	-	EXPRESSION TAG	UNP P51449
A	260	ARG	-	EXPRESSION TAG	UNP P51449
A	261	GLY	-	EXPRESSION TAG	UNP P51449
A	262	SER	-	EXPRESSION TAG	UNP P51449
B	248	MET	-	EXPRESSION TAG	UNP P51449
B	249	LYS	-	EXPRESSION TAG	UNP P51449
B	250	LYS	-	EXPRESSION TAG	UNP P51449
B	251	HIS	-	EXPRESSION TAG	UNP P51449
B	252	HIS	-	EXPRESSION TAG	UNP P51449
B	253	HIS	-	EXPRESSION TAG	UNP P51449
B	254	HIS	-	EXPRESSION TAG	UNP P51449
B	255	HIS	-	EXPRESSION TAG	UNP P51449
B	256	HIS	-	EXPRESSION TAG	UNP P51449
B	257	LEU	-	EXPRESSION TAG	UNP P51449

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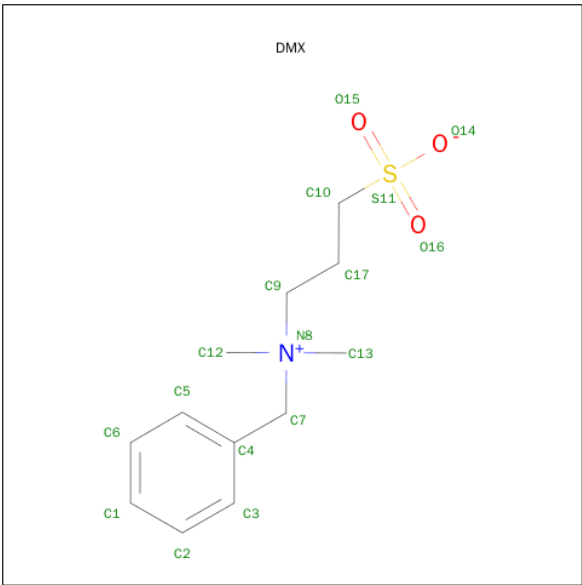
Chain	Residue	Modelled	Actual	Comment	Reference
B	258	VAL	-	EXPRESSION TAG	UNP P51449
B	259	PRO	-	EXPRESSION TAG	UNP P51449
B	260	ARG	-	EXPRESSION TAG	UNP P51449
B	261	GLY	-	EXPRESSION TAG	UNP P51449
B	262	SER	-	EXPRESSION TAG	UNP P51449

- | Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2   | C     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 75    | 50 | 16 | 9  |         |         |       |
| 2   | D     | 10       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 89    | 57 | 19 | 13 |         |         |       |

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- The ORTEP diagram shows the molecular structure of compound NBH. The molecule consists of two benzene rings connected by a methylene group (-CH<sub>2</sub>-). One benzene ring is substituted with a methyl group (-CH<sub>3</sub>) and a dimethylamino group (-N(CH<sub>3</sub>)<sub>2</sub>). The other benzene ring is substituted with a methyl group (-CH<sub>3</sub>) and a dimethylsulfonyl group (-SO<sub>2</sub>(CH<sub>3</sub>)<sub>2</sub>). The atoms are labeled as follows: C01-C10 for the carbon atoms, O01-O08 for the oxygen atoms, N01 for the nitrogen atom, and S01 for the sulfur atom.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 33	C 27	N 2	O 3	S 1	0	0
3	B	1	Total 33	C 27	N 2	O 3	S 1	0	0

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- WORLD WIDE  
PDB  
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			16	11	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			16	11	1	3	1		

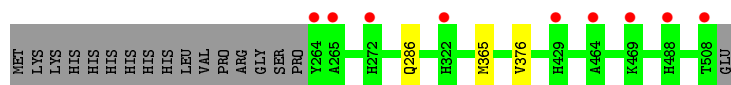
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	71	Total	O	0	0
			71	71		
5	C	1	Total	O	0	0
			1	1		
5	D	2	Total	O	0	0
			2	2		

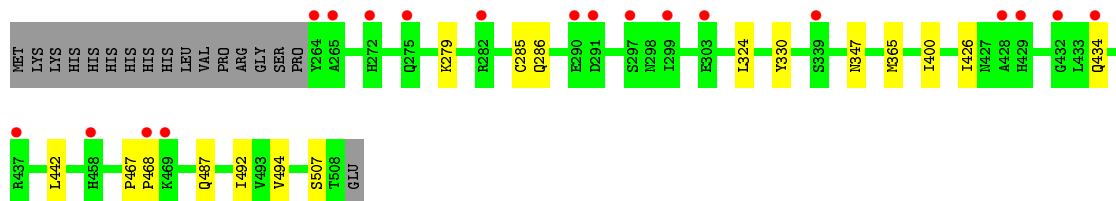
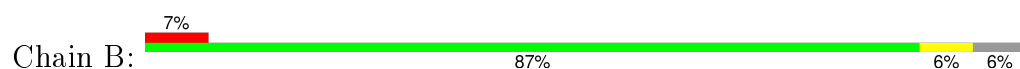
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

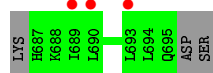
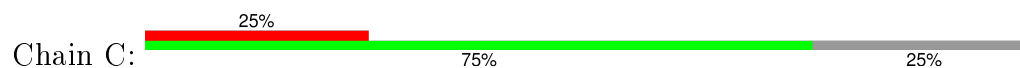
- Molecule 1: Nuclear receptor ROR-gamma



- Molecule 1: Nuclear receptor ROR-gamma



- Molecule 2: Peptide from Nuclear receptor coactivator 2



- Molecule 2: Peptide from Nuclear receptor coactivator 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.08Å 86.35Å 91.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.01 25.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-2.01) 99.7 (25.00-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.208 , 0.247 0.212 , 0.252	Depositor DCC
$R_{free}$ test set	1807 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 36252 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4437	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DMX, NBH

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	0.38	0/2062	0.50	0/2782
1	B	0.38	0/2022	0.50	1/2733 (0.0%)
2	C	0.32	0/76	0.41	0/101
2	D	0.42	0/90	0.52	0/119
All	All	0.38	0/4250	0.50	1/5735 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	CYS	CA-CB-SG	-5.46	104.18	114.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2008	0	1990	1	0
1	B	1978	0	1931	11	0
2	C	75	0	78	0	0
2	D	89	0	95	1	0
3	A	33	0	32	0	0
3	B	33	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	16	0	16	0	0
4	B	16	0	16	0	0
5	A	115	0	0	0	0
5	B	71	0	0	1	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
All	All	4437	0	4190	12	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 1.

The worst 5 of 12 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:B:279:LYS:CG	5:B:771:HOH:O	2.56	0.53
1:B:487[B]:GLN:NE2	1:B:507:SER:OG	2.45	0.49
1:B:347:ASN:ND2	1:B:434:GLN:HG3	2.29	0.48
1:B:492:ILE:HD12	2:D:692:ARG:HB3	1.98	0.46
1:B:487[B]:GLN:HE21	1:B:494:VAL:HG11	1.81	0.45

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	248/262 (95%)	243 (98%)	4 (2%)	1 (0%)	39	33
1	B	245/262 (94%)	242 (99%)	3 (1%)	0	100	100
2	C	7/12 (58%)	7 (100%)	0	0	100	100
2	D	8/12 (67%)	8 (100%)	0	0	100	100
All	All	508/548 (93%)	500 (98%)	7 (1%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	GLN

### 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	216/235 (92%)	216 (100%)	0	100	100
1	B	211/235 (90%)	211 (100%)	0	100	100
2	C	7/12 (58%)	7 (100%)	0	100	100
2	D	10/12 (83%)	10 (100%)	0	100	100
All	All	444/494 (90%)	444 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	A	488	HIS
1	B	347	ASN
2	D	687	HIS
2	D	695	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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$
3	NBH	A	601	-	34,35,35	1.43	3 (8%)	46,47,47	2.02	4 (8%)
4	DMX	A	602	-	15,16,17	1.17	3 (20%)	19,21,24	2.41	6 (31%)
3	NBH	B	601	-	34,35,35	1.44	5 (14%)	46,47,47	2.02	3 (6%)
4	DMX	B	602	-	15,16,17	1.08	2 (13%)	19,21,24	2.18	4 (21%)

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	NBH	A	601	-	-	0/28/28/28	0/3/3/3
4	DMX	A	602	-	-	0/11/11/13	0/1/1/1
3	NBH	B	601	-	-	0/28/28/28	0/3/3/3
4	DMX	B	602	-	-	0/11/11/13	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NBH	C25-C24	2.06	1.42	1.38
3	B	601	NBH	C23-C22	2.11	1.42	1.38
4	B	602	DMX	C2-C1	2.13	1.43	1.38
4	A	602	DMX	C2-C1	2.14	1.43	1.38
3	B	601	NBH	C26-C21	2.14	1.43	1.38

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	B	601	NBH	O29-S27-O28	-10.95	103.93	118.40
3	A	601	NBH	O29-S27-O28	-10.72	104.23	118.40
4	B	602	DMX	O14-S11-O15	-4.72	100.63	111.61
4	A	602	DMX	O14-S11-O15	-4.04	102.20	111.61
4	A	602	DMX	C17-C9-N8	2.03	120.46	113.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NBH	3	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	245/262 (93%)	0.09	9 (3%) 45 47	17, 25, 36, 42	0
1	B	245/262 (93%)	0.36	19 (7%) 16 17	19, 31, 48, 64	0
2	C	9/12 (75%)	1.63	3 (33%) 0 1	61, 72, 91, 96	0
2	D	10/12 (83%)	0.82	0 100 100	27, 35, 44, 55	0
All	All	509/548 (92%)	0.26	31 (6%) 25 26	17, 28, 47, 96	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	272	HIS	4.3
1	B	297	SER	3.9
1	B	469	LYS	3.6
1	B	264	TYR	3.5
1	B	290	GLU	3.4

### 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
3	NBH	A	601	33/33	0.89	0.17	2.43	37,41,44,44	0
3	NBH	B	601	33/33	0.88	0.17	2.07	37,39,42,43	0
4	DMX	B	602	16/17	0.95	0.12	0.92	35,38,41,41	0
4	DMX	A	602	16/17	0.92	0.16	0.89	40,47,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.