



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:45 pm GMT

PDB ID : 1PQ9  
Title : HUMAN LXR BETA HORMONE RECEPTOR COMPLEXED WITH  
T0901317 COMPLEX  
Authors : Farnegardh, M.; Bonn, T.; Sun, S.; Ljunggren, J.; Ahola, H.; Wilhelmsson, A.;  
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Deposited on : 2003-06-18  
Resolution : 2.10 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	:	1.7.2 (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

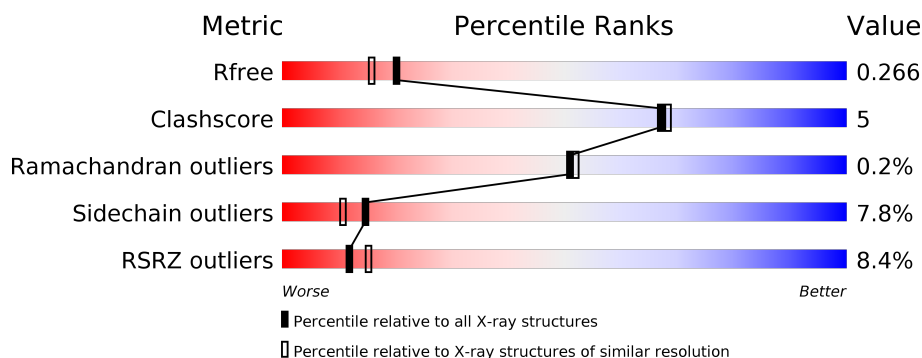
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	253	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 8%</div> </div> </div>
1	B	253	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	C	253	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>• 9%</div> </div> </div>
1	D	253	<div> <div>14%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>• 13%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BNS	C	3500	-	-	-	X
2	BNS	D	4500	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7779 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.

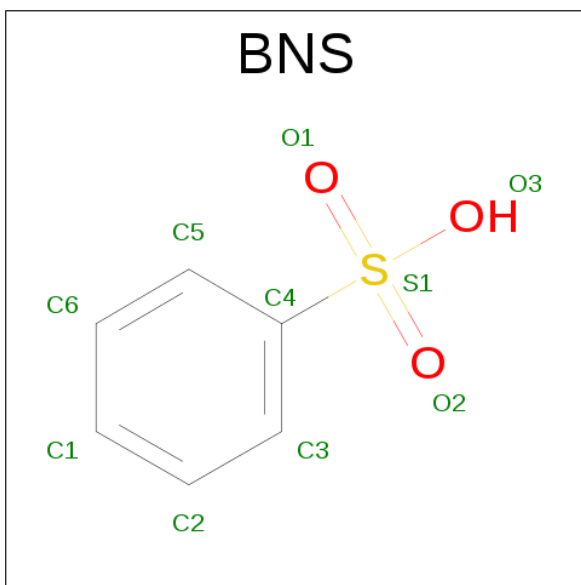
- Molecule 1 is a protein called Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1891	1210	331	343	7			
1	B	238	Total	C	N	O	S	0	0	0
			1925	1230	337	351	7			
1	C	231	Total	C	N	O	S	0	0	0
			1884	1204	333	340	7			
1	D	219	Total	C	N	O	S	0	0	0
			1774	1133	313	321	7			

There are 16 discrepancies between the modelled and reference sequences:

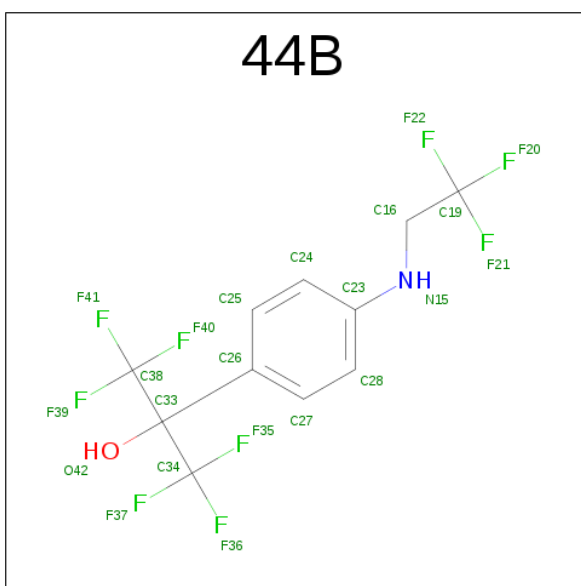
Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	CLONING ARTIFACT	UNP P55055
A	210	SER	-	CLONING ARTIFACT	UNP P55055
A	211	HIS	-	CLONING ARTIFACT	UNP P55055
A	212	MET	-	CLONING ARTIFACT	UNP P55055
B	209	GLY	-	CLONING ARTIFACT	UNP P55055
B	210	SER	-	CLONING ARTIFACT	UNP P55055
B	211	HIS	-	CLONING ARTIFACT	UNP P55055
B	212	MET	-	CLONING ARTIFACT	UNP P55055
C	209	GLY	-	CLONING ARTIFACT	UNP P55055
C	210	SER	-	CLONING ARTIFACT	UNP P55055
C	211	HIS	-	CLONING ARTIFACT	UNP P55055
C	212	MET	-	CLONING ARTIFACT	UNP P55055
D	209	GLY	-	CLONING ARTIFACT	UNP P55055
D	210	SER	-	CLONING ARTIFACT	UNP P55055
D	211	HIS	-	CLONING ARTIFACT	UNP P55055
D	212	MET	-	CLONING ARTIFACT	UNP P55055

- Molecule 2 is BENZENESULFONIC ACID (three-letter code: BNS) (formula: C<sub>6</sub>H<sub>6</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			9	6	2	1		
2	B	1	Total	C	O	S	0	0
			9	6	2	1		
2	C	1	Total	C	O	S	0	0
			9	6	2	1		
2	D	1	Total	C	O	S	0	0
			9	6	2	1		

- Molecule 3 is 1,1,1,3,3,3-HEXAFLUORO-2-{4-[(2,2,2-TRIFLUOROETHYL)AMINO]PHE  
NYL}PROPAN-2-OL (three-letter code: 44B) (formula: C<sub>11</sub>H<sub>8</sub>F<sub>9</sub>NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	B	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	C	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	D	1	Total	C	F	N	O	0	0
			22	11	9	1	1		

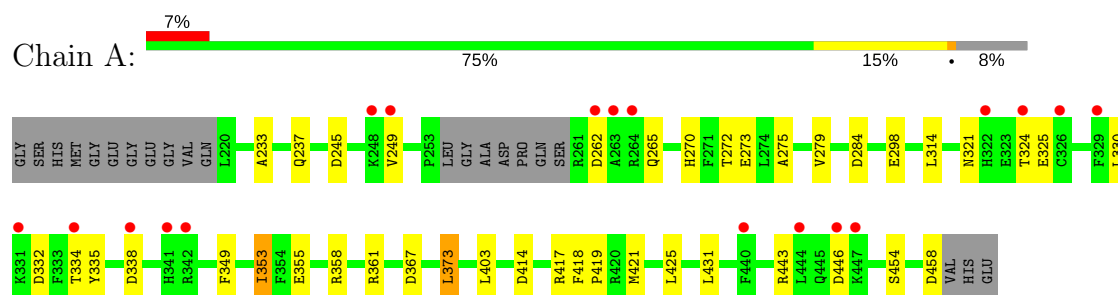
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	73	Total	O	0	0
			73	73		
4	C	52	Total	O	0	0
			52	52		
4	D	21	Total	O	0	0
			21	21		

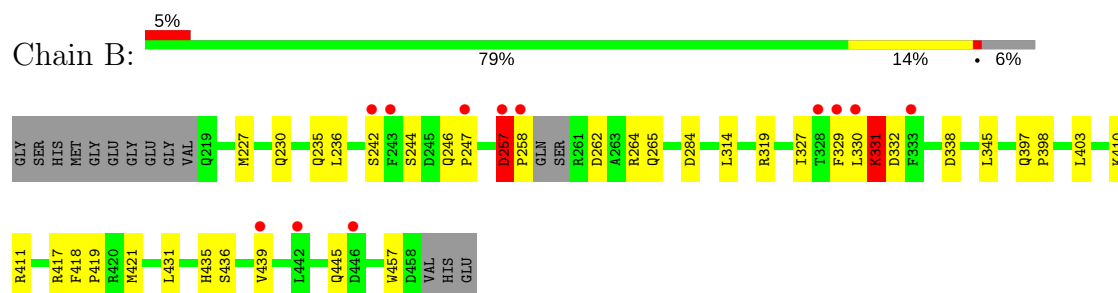
### 3 Residue-property plots [i](#)

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

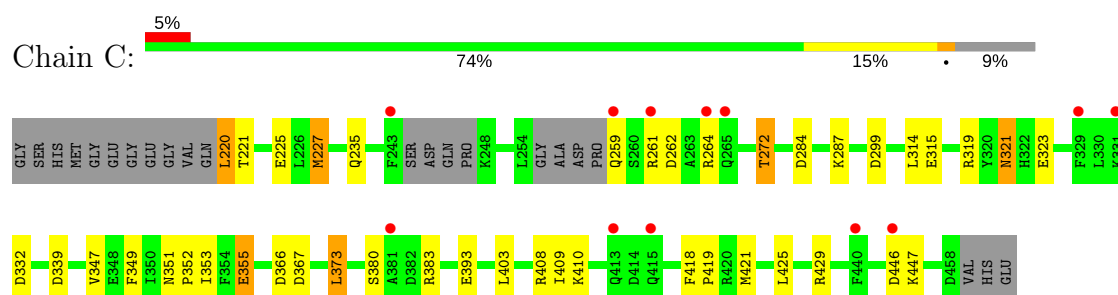
#### • Molecule 1: Oxysterols receptor LXR-beta



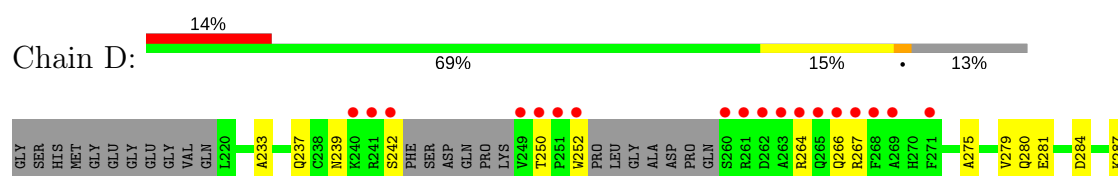
#### • Molecule 1: Oxysterols receptor LXR-beta

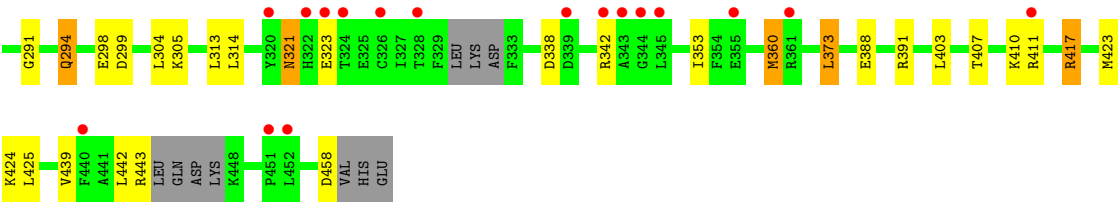


#### • Molecule 1: Oxysterols receptor LXR-beta



#### • Molecule 1: Oxysterols receptor LXR-beta







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.87Å 103.61Å 176.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.84 – 2.10 55.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (55.84-2.10) 99.7 (55.84-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.28	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.214 , 0.254 0.268 , 0.266	Depositor DCC
$R_{free}$ test set	3222 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.9	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	0.92	EDS
Total number of atoms	7779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: BNS, 44B

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	0.62	0/1928	0.80	8/2607 (0.3%)
1	B	0.66	0/1963	0.82	4/2656 (0.2%)
1	C	0.68	1/1919 (0.1%)	0.84	10/2591 (0.4%)
1	D	0.59	0/1804	0.75	4/2436 (0.2%)
All	All	0.64	1/7614 (0.0%)	0.80	26/10290 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	THR	CB-CG2	-5.35	1.34	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	MET	CG-SD-CE	-8.11	87.23	100.20
1	B	284	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	338	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	332	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	446	ASP	CB-CG-OD2	5.81	123.53	118.30

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	1891	0	1913	12	0
1	B	1925	0	1936	16	0
1	C	1884	0	1905	18	0
1	D	1774	0	1788	19	0
2	A	9	0	5	1	0
2	B	9	0	5	1	0
2	C	9	0	5	2	0
2	D	9	0	5	1	0
3	A	22	0	8	1	0
3	B	22	0	8	0	0
3	C	22	0	8	2	0
3	D	22	0	8	1	0
4	A	35	0	0	0	0
4	B	73	0	0	0	0
4	C	52	0	0	0	0
4	D	21	0	0	0	0
All	All	7779	0	7594	69	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 5.

The worst 5 of 69 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:352:PRO:HA	1:C:355:GLU:HG3	1.49	0.94
1:D:233:ALA:O	1:D:237:GLN:HG3	1.87	0.74
1:D:360:MET:HE1	1:D:424:LYS:HD2	1.72	0.72
2:C:3500:BNS:O1	3:C:3501:44B:N15	2.25	0.70
1:C:351:ASN:O	1:C:355:GLU:HG2	1.93	0.69

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	228/253 (90%)	224 (98%)	4 (2%)	0	100	100
1	B	234/253 (92%)	229 (98%)	3 (1%)	2 (1%)	20	14
1	C	225/253 (89%)	221 (98%)	4 (2%)	0	100	100
1	D	209/253 (83%)	202 (97%)	7 (3%)	0	100	100
All	All	896/1012 (88%)	876 (98%)	18 (2%)	2 (0%)	51	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	ASP
1	B	331	LYS

### 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	206/222 (93%)	193 (94%)	13 (6%)	21	17
1	B	208/222 (94%)	191 (92%)	17 (8%)	13	9
1	C	204/222 (92%)	188 (92%)	16 (8%)	15	11
1	D	191/222 (86%)	174 (91%)	17 (9%)	11	7
All	All	809/888 (91%)	746 (92%)	63 (8%)	15	11

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	431	LEU
1	C	264	ARG
1	D	417	ARG
1	B	445	GLN
1	C	227	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	230	GLN
1	C	259	GLN
1	D	266	GLN
1	B	288	GLN
1	D	280	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

8 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	BNS	A	1500	-	7,9,10	2.10	4 (57%)	8,11,14	1.15	1 (12%)
3	44B	A	1501	-	22,22,22	1.53	3 (13%)	33,36,36	1.20	3 (9%)
2	BNS	B	2500	-	7,9,10	2.02	2 (28%)	8,11,14	0.79	0
3	44B	B	2501	-	22,22,22	1.69	6 (27%)	33,36,36	0.99	1 (3%)
2	BNS	C	3500	-	7,9,10	2.21	2 (28%)	8,11,14	0.46	0
3	44B	C	3501	-	22,22,22	1.72	5 (22%)	33,36,36	1.11	4 (12%)
2	BNS	D	4500	-	7,9,10	2.19	3 (42%)	8,11,14	1.04	1 (12%)
3	44B	D	4501	-	22,22,22	1.87	8 (36%)	33,36,36	1.28	5 (15%)

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	BNS	A	1500	-	-	0/4/4/6	0/1/1/1
3	44B	A	1501	-	-	0/30/30/30	0/1/1/1
2	BNS	B	2500	-	-	0/4/4/6	0/1/1/1
3	44B	B	2501	-	-	0/30/30/30	0/1/1/1
2	BNS	C	3500	-	-	0/4/4/6	0/1/1/1
3	44B	C	3501	-	-	0/30/30/30	0/1/1/1
2	BNS	D	4500	-	-	0/4/4/6	0/1/1/1
3	44B	D	4501	-	-	0/30/30/30	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	BNS	C4-S1	-2.25	1.76	1.80
3	B	2501	44B	C24-C25	2.02	1.42	1.38
2	D	4500	BNS	C2-C1	2.02	1.42	1.38
3	D	4501	44B	O42-C33	2.13	1.46	1.42
2	A	1500	BNS	C6-C5	2.13	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2501	44B	C38-C33-C34	-2.95	107.91	110.39
3	A	1501	44B	C38-C33-C26	-2.90	106.58	110.20
3	D	4501	44B	C38-C33-C34	-2.74	108.09	110.39
3	D	4501	44B	C24-C23-N15	-2.37	116.26	121.03
3	C	3501	44B	C38-C33-C26	-2.26	107.38	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	BNS	1	0
3	A	1501	44B	1	0
2	B	2500	BNS	1	0
2	C	3500	BNS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3501	44B	2	0
2	D	4500	BNS	1	0
3	D	4501	44B	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	232/253 (91%)	0.70	18 (7%) 14 18	9, 20, 32, 36	0
1	B	238/253 (94%)	0.61	12 (5%) 30 36	8, 19, 40, 51	0
1	C	231/253 (91%)	0.59	12 (5%) 28 34	7, 19, 35, 57	0
1	D	219/253 (86%)	0.87	35 (15%) 2 3	11, 19, 30, 43	0
All	All	920/1012 (90%)	0.69	77 (8%) 12 15	7, 19, 34, 57	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	PHE	6.5
1	A	263	ALA	6.0
1	D	241	ARG	5.7
1	D	263	ALA	5.4
1	B	243	PHE	5.0

### 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	BNS	D	4500	9/10	0.79	0.42	6.58	46,46,50,51	0
2	BNS	C	3500	9/10	0.87	0.27	2.71	48,49,54,55	0
2	BNS	B	2500	9/10	0.81	0.23	0.72	48,50,53,53	0
2	BNS	A	1500	9/10	0.92	0.18	0.56	33,34,39,39	0
3	44B	C	3501	22/22	0.95	0.15	0.07	15,21,27,28	0
3	44B	D	4501	22/22	0.92	0.17	0.06	12,18,25,26	0
3	44B	B	2501	22/22	0.94	0.11	-1.22	13,17,28,29	0
3	44B	A	1501	22/22	0.94	0.11	-1.28	9,14,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.