



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 11:44 pm GMT

PDB ID : 2HPY  
Title : Crystallographic model of lumirhodopsin  
Authors : Nakamichi, H.; Okada, T.  
Deposited on : 2006-07-18  
Resolution : 2.80 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

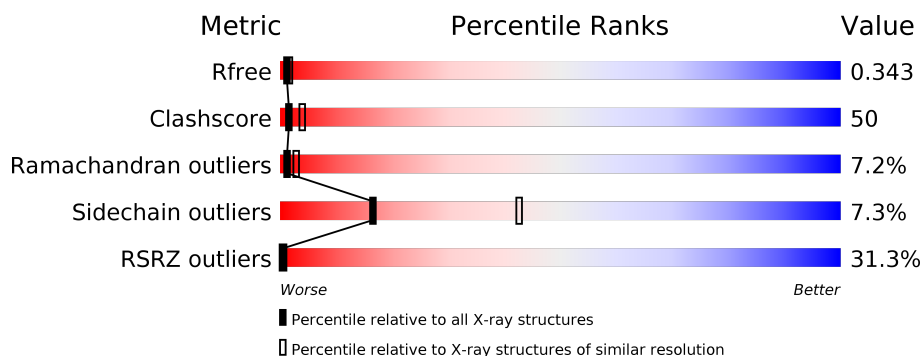
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	349	<div> <div>28%</div> <div>38%</div> <div>53%</div> <div>9%</div> </div>
1	B	349	<div> <div>34%</div> <div>34%</div> <div>55%</div> <div>10%</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
10	HTG	A	1507	-	-	-	X
10	HTG	B	1509	-	-	-	X
6	ZN	B	963	-	-	-	X
7	RET	A	1296	-	-	-	X
7	RET	B	1296	-	-	-	X
8	PLM	A	1322	-	-	-	X
8	PLM	B	1322	-	-	-	X
8	PLM	B	1323	-	-	-	X
8	PLM	B	1407	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5948 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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			
1	B	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

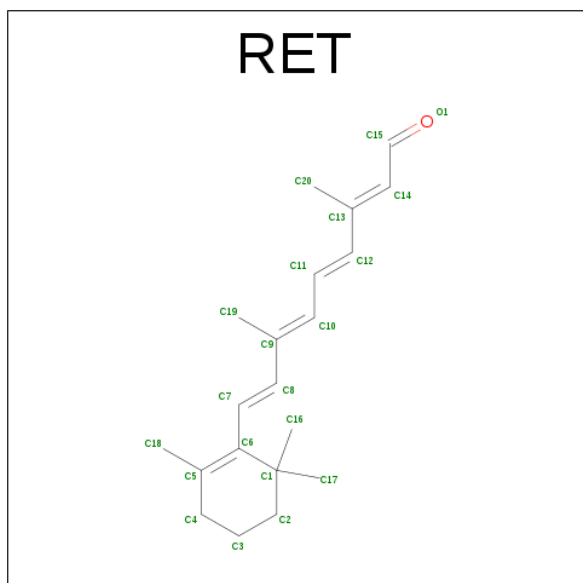
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Hg	0	0
			3	3		
5	A	3	Total	Hg	0	0
			3	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

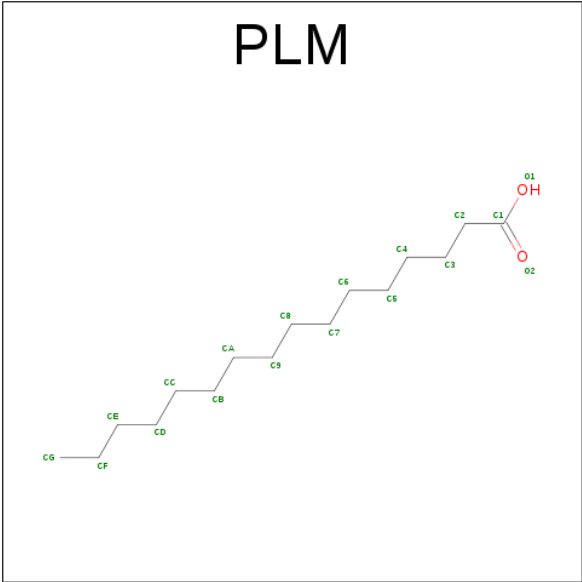
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Zn	0	0
			3	3		
6	A	4	Total	Zn	0	0
			4	4		

- Molecule 7 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



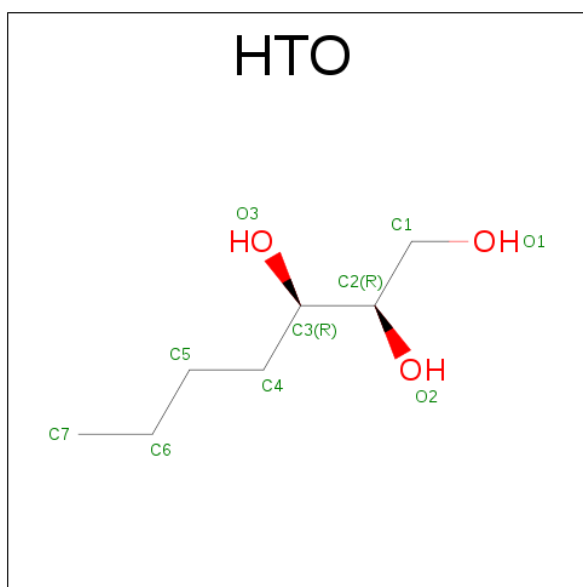
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C	0	0
			20	20		
7	B	1	Total	C	0	0
			20	20		

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



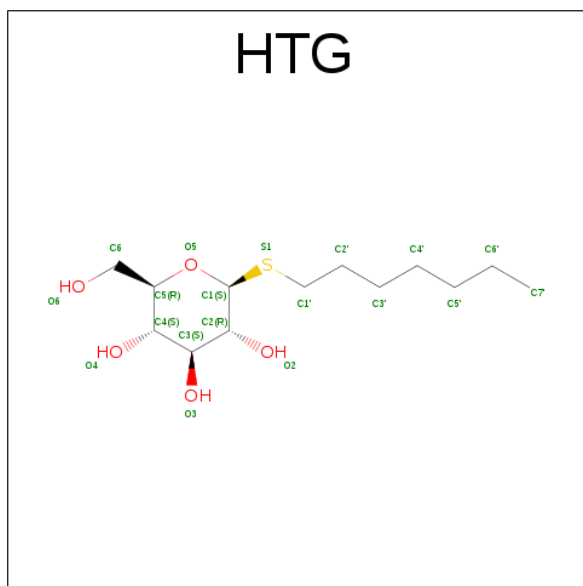
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	16	1		
8	A	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C		0	0
			16	16			
8	A	1	Total	C		0	0
			16	16			

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	O	S	0	0
			19	13	5	1		
10	A	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	S	0	0
			19	13	5	1		
10	B	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 11 is water.

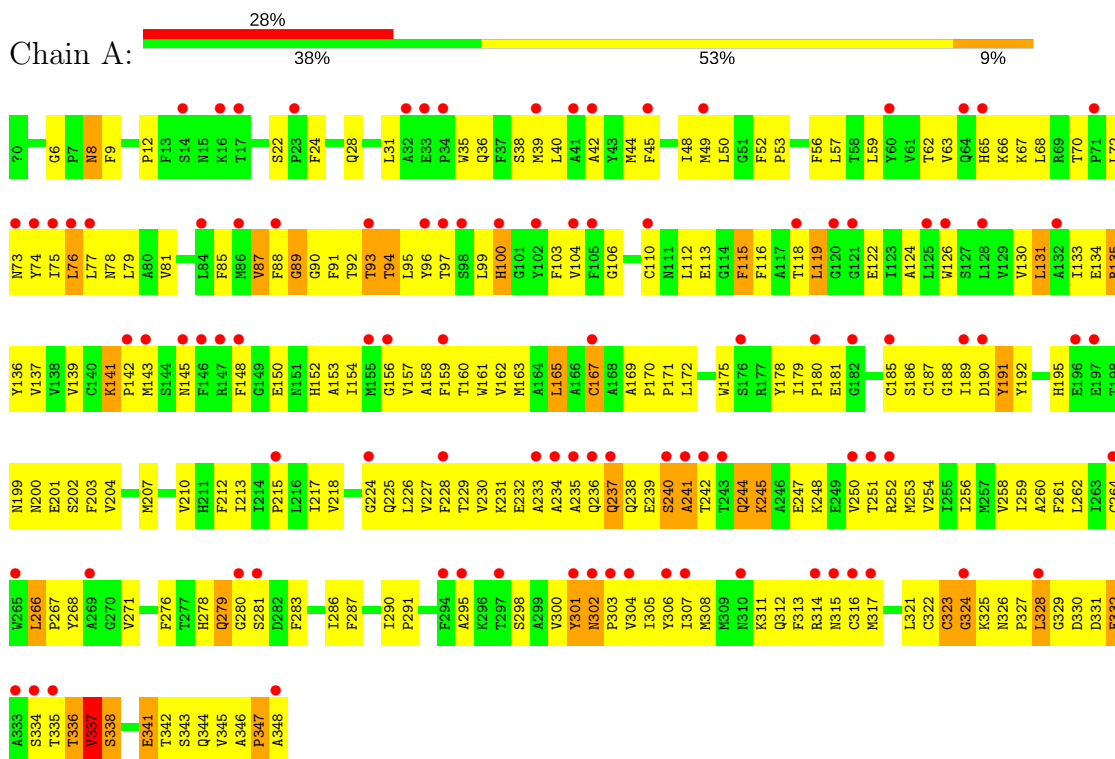
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	37	Total	O	0	0
			37	37		
11	B	29	Total	O	0	0
			29	29		



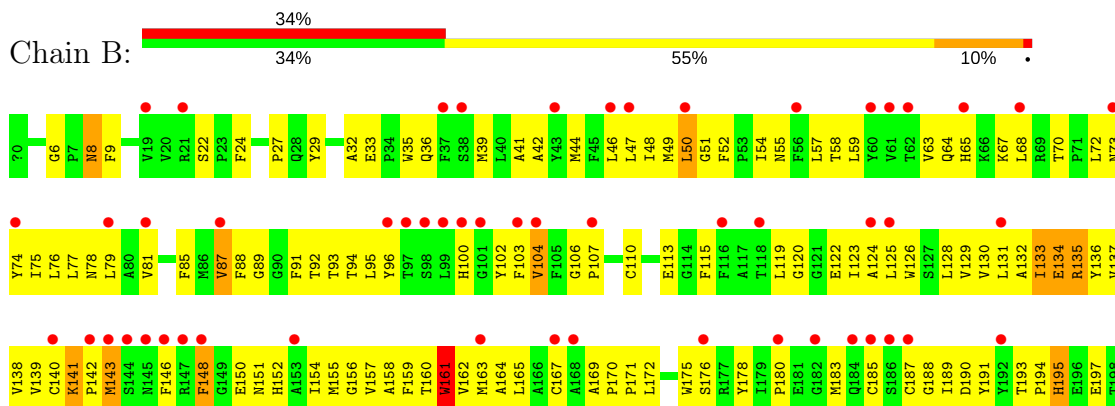
### 3 Residue-property plots [i](#)

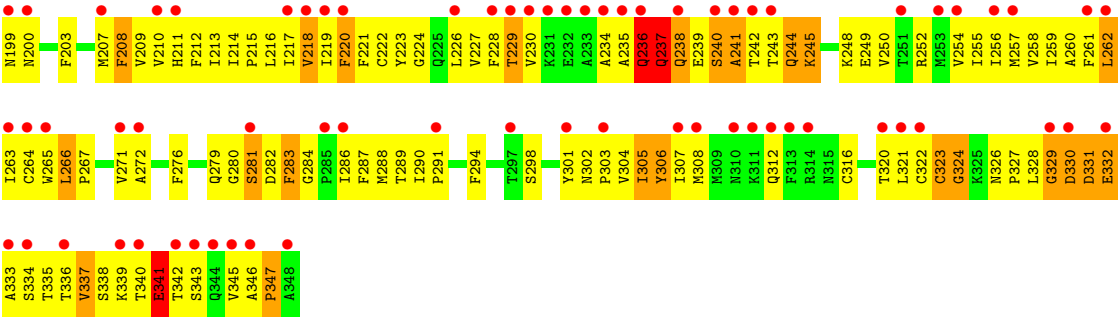
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Rhodopsin



#### • Molecule 1: Rhodopsin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.72Å 96.72Å 150.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 35.05 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 87.3 (35.05-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.238 0.350 , 0.343	Depositor DCC
$R_{free}$ test set	1530 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.15 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HTG, ZN, BMA, NAG, ACE, HTO, RET, PLM, HG, MAN

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	0.65	0/2831	0.70	0/3859
1	B	0.65	0/2831	0.68	0/3859
All	All	0.65	0/5662	0.69	0/7718

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	TYR	Sidechain

### 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	2749	0	2709	257	1
1	B	2749	0	2709	327	0
2	A	39	0	34	1	0
3	B	50	0	43	0	0
4	A	28	0	25	0	0
4	B	28	0	25	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
7	A	20	0	27	2	0
7	B	20	0	27	2	0
8	A	50	0	89	7	0
8	B	50	0	89	4	0
9	B	10	0	16	1	0
10	A	38	0	52	3	0
10	B	38	0	52	4	1
11	A	37	0	0	6	0
11	B	29	0	0	10	0
All	All	5948	0	5897	584	1

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 50.

The worst 5 of 584 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:298:SER:HA	1:A:301:TYR:CE2	1.82	1.15
1:B:298:SER:HA	1:B:301:TYR:CE2	1.81	1.15
1:A:67:LYS:HB2	1:A:337:VAL:HB	1.38	1.02
1:B:64:GLN:HG3	1:B:339:LYS:HE2	1.39	1.02
1:A:345:VAL:HG12	1:A:347:PRO:HD3	1.45	0.98

All (1) 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)
1:A:344:GLN:NE2	10:B:1509:HTG:O6[4_564]	2.19	0.01

## 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	347/349 (99%)	264 (76%)	57 (16%)	26 (8%)	1	2
1	B	347/349 (99%)	254 (73%)	69 (20%)	24 (7%)	1	3
All	All	694/698 (99%)	518 (75%)	126 (18%)	50 (7%)	1	3

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	SER
1	A	241	ALA
1	A	323	CYS
1	A	328	LEU
1	A	341	GLU

### 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	296/296 (100%)	276 (93%)	20 (7%)	18	47
1	B	296/296 (100%)	273 (92%)	23 (8%)	15	39
All	All	592/592 (100%)	549 (93%)	43 (7%)	16	42

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	SER

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Mol	Chain	Res	Type
1	B	134	GLU
1	B	283	PHE
1	B	8	ASN
1	B	50	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	B	8	ASN
1	B	237	GLN
1	A	312	GLN
1	B	151	ASN

### 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 ⓘ

11 carbohydrates 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	MAN	A	503	2	11,11,12	0.79	0	13,15,17	0.83	0
2	NAG	A	504	2	14,14,15	0.76	0	15,19,21	0.97	1 (6%)
2	NAG	A	505	1,2	14,14,15	0.62	0	15,19,21	0.84	0
4	NAG	A	704	4	14,14,15	0.61	0	15,19,21	1.04	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	705	1,4	14,14,15	0.52	0	15,19,21	0.84	1 (6%)
3	BMA	B	602	3	11,11,12	0.83	0	13,15,17	0.90	1 (7%)
3	BMA	B	603	3	11,11,12	0.82	0	13,15,17	0.72	0
3	NAG	B	604	3	14,14,15	0.64	0	15,19,21	0.98	1 (6%)
3	NAG	B	605	1,3	14,14,15	0.59	0	15,19,21	0.66	0
4	NAG	B	804	4	14,14,15	0.64	0	15,19,21	0.70	0
4	NAG	B	805	1,4	14,14,15	0.63	0	15,19,21	0.86	1 (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	MAN	A	503	2	-	0/2/19/22	0/1/1/1
2	NAG	A	504	2	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1,4	-	0/6/23/26	0/1/1/1
3	BMA	B	602	3	-	0/2/19/22	0/1/1/1
3	BMA	B	603	3	-	0/2/19/22	0/1/1/1
3	NAG	B	604	3	-	0/6/23/26	0/1/1/1
3	NAG	B	605	1,3	-	0/6/23/26	0/1/1/1
4	NAG	B	804	4	-	0/6/23/26	0/1/1/1
4	NAG	B	805	1,4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	NAG	C2-N2-C7	-2.97	118.61	122.94
3	B	604	NAG	C2-N2-C7	-2.61	119.13	122.94
4	A	705	NAG	C2-N2-C7	-2.58	119.18	122.94
4	B	805	NAG	C2-N2-C7	-2.05	119.95	122.94
2	A	504	NAG	C8-C7-N2	2.06	119.83	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	NAG	1	0
2	A	505	NAG	1	0
4	B	805	NAG	1	0

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 13 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
7	RET	A	1296	1	19,20,21	2.48	3 (15%)	27,27,28	1.98	7 (25%)
8	PLM	A	1322	1	16,16,17	0.96	1 (6%)	15,15,17	0.60	0
8	PLM	A	1323	1	16,16,17	0.96	1 (6%)	15,15,17	0.52	0
8	PLM	A	1410	-	15,15,17	1.79	3 (20%)	14,14,17	3.32	5 (35%)
10	HTG	A	1507	-	19,19,19	3.19	8 (42%)	23,24,24	2.73	2 (8%)
10	HTG	A	1508	-	19,19,19	2.44	8 (42%)	23,24,24	3.22	2 (8%)
7	RET	B	1296	1	19,20,21	2.12	3 (15%)	27,27,28	1.86	7 (25%)
8	PLM	B	1322	1	16,16,17	1.00	1 (6%)	15,15,17	0.43	0
8	PLM	B	1323	1	16,16,17	0.97	1 (6%)	15,15,17	0.44	0
9	HTO	B	1401	-	9,9,9	1.68	1 (11%)	9,10,10	1.25	1 (11%)
8	PLM	B	1407	-	15,15,17	1.74	3 (20%)	14,14,17	3.31	6 (42%)
10	HTG	B	1506	-	19,19,19	3.01	8 (42%)	23,24,24	2.38	2 (8%)
10	HTG	B	1509	-	19,19,19	2.73	8 (42%)	23,24,24	2.74	3 (13%)

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
7	RET	A	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	A	1322	1	-	0/14/14/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PLM	A	1323	1	-	0/14/14/15	0/0/0/0
8	PLM	A	1410	-	-	0/13/13/15	0/0/0/0
10	HTG	A	1507	-	-	0/10/30/30	0/1/1/1
10	HTG	A	1508	-	-	0/10/30/30	0/1/1/1
7	RET	B	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	B	1322	1	-	0/14/14/15	0/0/0/0
8	PLM	B	1323	1	-	0/14/14/15	0/0/0/0
9	HTO	B	1401	-	-	0/10/10/10	0/0/0/0
8	PLM	B	1407	-	-	0/13/13/15	0/0/0/0
10	HTG	B	1506	-	-	0/10/30/30	0/1/1/1
10	HTG	B	1509	-	-	0/10/30/30	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1410	PLM	CC-CB	-4.76	1.24	1.51
8	B	1407	PLM	CC-CB	-4.56	1.25	1.51
8	A	1322	PLM	O1-C1	-3.68	1.22	1.42
8	B	1322	PLM	O1-C1	-3.61	1.23	1.42
8	A	1323	PLM	O1-C1	-3.57	1.23	1.42

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1296	RET	C11-C10-C9	-4.87	120.36	127.31
7	B	1296	RET	C11-C10-C9	-3.76	121.94	127.31
7	B	1296	RET	C8-C9-C10	-3.72	113.23	118.94
7	A	1296	RET	C8-C9-C10	-2.99	114.36	118.94
7	A	1296	RET	C18-C5-C4	-2.47	108.77	113.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1296	RET	2	0
8	A	1322	PLM	6	0
8	A	1410	PLM	1	0
10	A	1507	HTG	2	0
10	A	1508	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1296	RET	2	0
8	B	1322	PLM	2	0
8	B	1323	PLM	2	0
9	B	1401	HTO	1	0
8	B	1407	PLM	1	0
10	B	1506	HTG	1	0
10	B	1509	HTG	3	1

## 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	348/349 (99%)	1.47	98 (28%) <b>1</b> <b>0</b>	48, 61, 135, 149	228 (65%)
1	B	348/349 (99%)	1.71	120 (34%) <b>0</b> <b>0</b>	48, 64, 154, 163	228 (65%)
All	All	696/698 (99%)	1.59	218 (31%) <b>0</b> <b>0</b>	48, 63, 147, 163	456 (65%)

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	ALA	9.9
1	B	232	GLU	9.3
1	B	344	GLN	7.6
1	B	142	PRO	7.3
1	B	342	THR	6.5

### 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](#)

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
4	NAG	B	805	14/15	0.90	0.30	0.45	65,69,71,77	0
3	NAG	B	605	14/15	0.91	0.23	-0.24	63,64,69,75	0
3	BMA	B	602	11/12	0.49	0.38	-0.24	120,122,122,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	505	14/15	0.90	0.16	-0.68	66,68,74,75	0
4	NAG	A	705	14/15	0.86	0.17	-1.48	70,75,80,84	0
3	NAG	B	604	14/15	0.82	0.32	-	77,83,90,97	0
4	NAG	A	704	14/15	0.80	0.34	-	91,94,99,101	0
2	MAN	A	503	11/12	0.83	0.29	-	94,97,97,99	0
4	NAG	B	804	14/15	0.79	0.34	-	84,89,91,92	0
3	BMA	B	603	11/12	0.64	0.30	-	104,108,112,116	0
2	NAG	A	504	14/15	0.88	0.27	-	79,82,87,92	0

## 6.4 Ligands ⓘ

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
8	PLM	A	1322	17/18	0.65	0.52	4.18	94,104,110,110	0
7	RET	A	1296	20/21	0.70	0.51	3.11	50,52,54,55	20
10	HTG	A	1507	19/19	0.76	0.40	2.27	99,113,115,116	0
8	PLM	B	1407	16/18	0.65	0.46	2.16	75,82,87,88	0
7	RET	B	1296	20/21	0.72	0.43	1.89	51,52,54,54	20
6	ZN	B	963	1/1	0.39	0.45	1.85	93,93,93,93	1
8	PLM	B	1322	17/18	0.68	0.46	1.06	105,108,109,110	0
8	PLM	B	1323	17/18	0.70	0.46	0.92	117,122,124,124	0
10	HTG	B	1506	19/19	0.73	0.37	0.76	88,93,97,99	0
8	PLM	A	1323	17/18	0.70	0.33	0.53	98,105,113,114	0
10	HTG	B	1509	19/19	0.70	0.43	0.49	93,95,100,100	0
6	ZN	A	962	1/1	0.81	0.33	0.19	80,80,80,80	1
8	PLM	A	1410	16/18	0.82	0.33	-0.05	74,77,79,79	0
5	HG	B	904	1/1	0.93	0.24	-0.44	109,109,109,109	1
5	HG	A	903	1/1	0.98	0.22	-0.44	96,96,96,96	1
10	HTG	A	1508	19/19	0.79	0.27	-0.47	72,78,82,85	0
5	HG	B	906	1/1	0.78	0.23	-0.67	121,121,121,121	1
9	HTO	B	1401	10/10	0.75	0.24	-2.07	56,60,62,63	0
5	HG	A	901	1/1	0.94	0.20	-2.80	82,82,82,82	1
5	HG	B	902	1/1	0.96	0.17	-2.83	80,80,80,80	1
6	ZN	A	959	1/1	0.94	0.04	-	92,92,92,92	1
6	ZN	A	2011	1/1	0.96	0.15	-	53,53,53,53	1
6	ZN	A	957	1/1	0.97	0.09	-	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ZN	B	958	1/1	0.96	0.11	-	43,43,43,43	1
5	HG	A	905	1/1	0.86	0.39	-	99,99,99,99	1
6	ZN	B	956	1/1	0.96	0.09	-	60,60,60,60	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.