



# wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 07:50 PM BST

PDB ID : 3O2Z  
Title : Yeast 80S ribosome. This entry consists of the 40S subunit of the first 80S in the asymmetric unit.  
Authors : Ben-Shem, A.; Jenner, L.; Yusupova, G.; Yusupov, M.  
Deposited on : 2010-07-23  
Resolution : 4.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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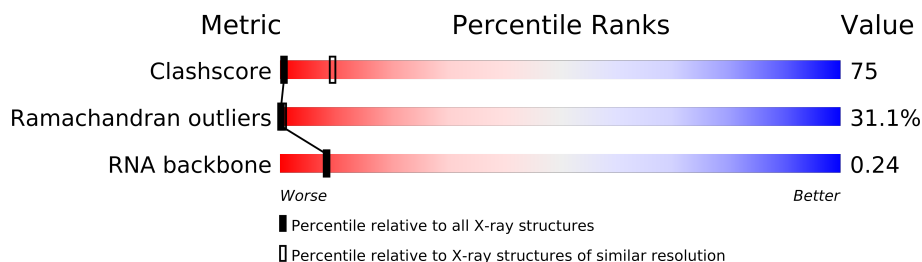
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 4.00 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))
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
RNA backbone	1838	1018 (5.00-2.80)


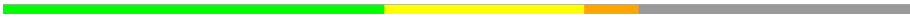




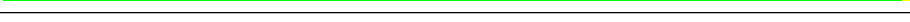

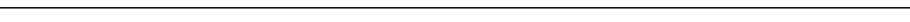


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	1800	
2	A	252	
3	B	254	
4	C	240	
5	D	225	
6	E	197	
7	F	156	
8	G	151	
9	H	137	
10	I	142	
11	J	143	
12	K	136	
13	L	146	
14	M	144	
15	N	121	
16	O	130	
17	P	145	

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Mol	Chain	Length	Quality of chain
18	Q	108	
19	R	67	
20	S	56	
21	T	319	
22	a	20	
23	b	105	
24	c	93	
25	d	35	
26	e	21	
27	f	11	
28	h	41	

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 55248 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	1789	Total	C	N	O	P	0	0	0
			38107	17037	6732	12549	1789			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	220	Total	C	N	O	0	0	0
			1090	650	220	220			

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	219	Total	C	N	O	0	0	0
			1074	636	219	219			

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	189	Total	C	N	O	0	0	0
			928	550	189	189			

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	169	Total	C	N	O	0	0	0
			836	498	169	169			

- Molecule 6 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	157	Total	C	N	O	0	0	0
			777	463	157	157			

- Molecule 7 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	F	77	Total	C	N	O	0	0	0
			382	228	77	77			

- Molecule 8 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	G	117	Total	C	N	O	0	0	0
			580	346	117	117			

- Molecule 9 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	H	128	Total	C	N	O	0	0	0
			627	371	128	128			

- Molecule 10 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	121	Total	C	N	O	0	0	0
			596	354	121	121			

- Molecule 11 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	134	Total	C	N	O	0	0	0
			658	390	134	134			

- Molecule 12 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	K	67	Total	C	N	O	0	0	0
			332	198	67	67			

- Molecule 13 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	120	Total	C	N	O	0	0	0
			591	351	120	120			

- Molecule 14 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	106	Total	C	N	O	0	0	0
			521	309	106	106			

- Molecule 15 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	N	111	Total	C	N	O	0	0	0
			551	329	111	111			

- Molecule 16 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	127	Total	C	N	O	0	0	0
			622	368	127	127			

- Molecule 17 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	116	Total	C	N	O	0	0	0
			566	334	116	116			

- Molecule 18 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Q	67	Total	C	N	O	0	0	0
			332	198	67	67			

- Molecule 19 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	47	Total	C	N	O	0	0	0
			230	136	47	47			

- Molecule 20 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	S	39	Total	C	N	O	0	0	0
			190	112	39	39			

- Molecule 21 is a protein called Guanine nucleotide-binding protein subunit beta-like protein; RACK-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	313	Total	C	N	O	0	0	0
			1543	917	313	313			

- Molecule 22 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	a	20	Total	C	N	O	0	0	0
			100	60	20	20			

- Molecule 23 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	b	105	Total	C	N	O	0	0	0
			525	315	105	105			

- Molecule 24 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	c	93	Total	C	N	O	0	0	0
			465	279	93	93			

- Molecule 25 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	d	35	Total	C	N	O	0	0	0
			175	105	35	35			

- Molecule 26 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	e	21	Total	C	N	O	0	0	0
			105	63	21	21			

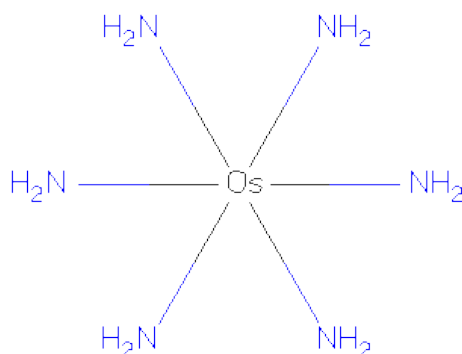
- Molecule 27 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	f	11	Total	C	N	O	0	0	0
			55	33	11	11			

- Molecule 28 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	h	41	Total	C	N	O	0	0	0
			205	123	41	41			

- Molecule 29 is OSMIUM (III) HEXAMMINE (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
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29	1	1	Total 7	N 6	Os 1	0	0
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29	g	1	Total 7	N 6	Os 1	0	0
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29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
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29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
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29	g	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
29	G	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
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29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
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29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
29	e	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
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			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
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29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	T	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	S	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	e	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	g	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0
29	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	e	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	1	1	Total	N	Os	0	0
			7	6	1		

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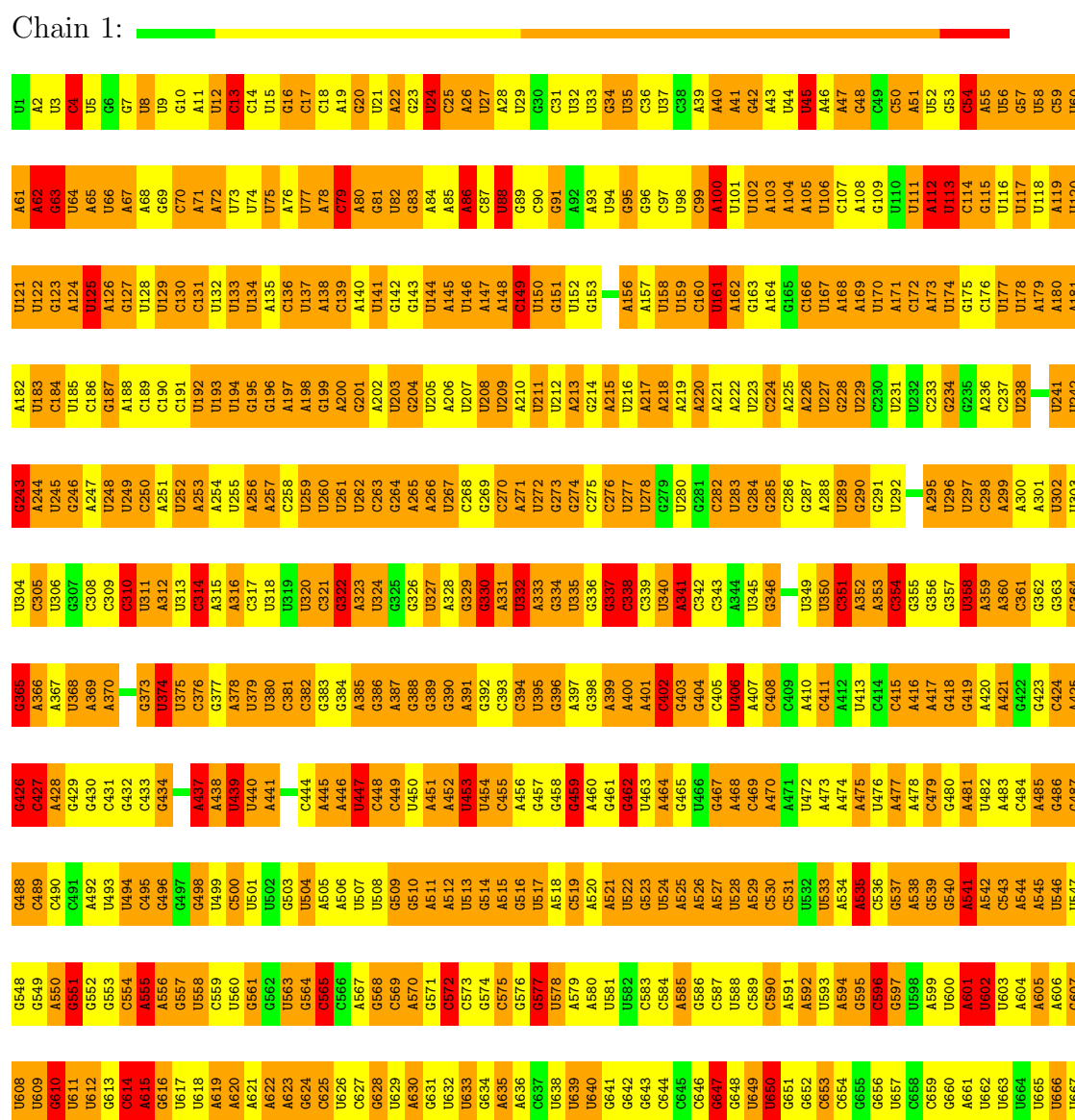
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	1	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		
29	g	1	Total	N	Os	0	0
			7	6	1		

### 3 Residue-property plots

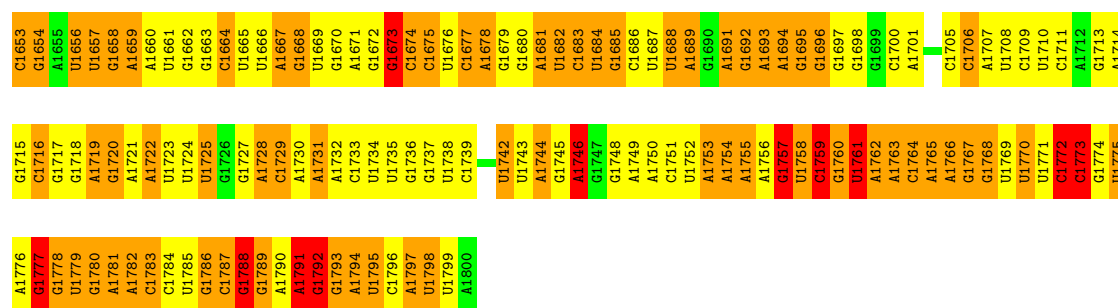
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: 18S ribosomal RNA

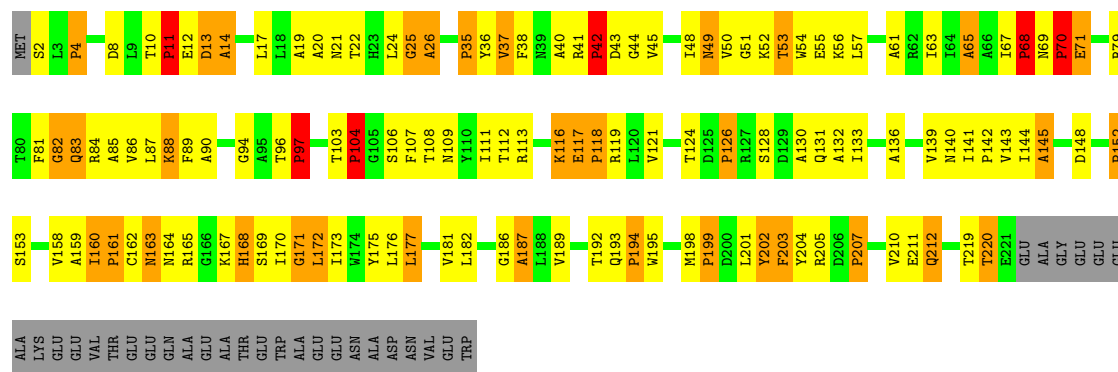


A1592	G1531	A1471	C1342	U1282	A1221	C1160	G1100	A1039	G976	U912	C852	U790	G729	C
A1593	U1532	C1472	U1343	U1283	C1222	C1161	G1101	G1040	A977	G913	C853	U791	G730	G
G1594	G1408	U1473	A1344	C1284	A1223	C1162	G1102	G1041	A978	G914	U854	U792	G731	U
U1595	G1409	A1345	A1345	U1285	A1224	C1163	U1103	G1042	A979	A915	A855	G802	G732	G
C1596	A1410	U1346	U1225	U1286	U1225	C1164	U1104	A1043	G980	U916	A856	U793	A793	U
A1597	A1411	U1347	A1226	A1287	A1226	G1165	C1105	U1044	U981	U917	A857	U794	A734	A
U1598	G1412	G1477	C1288	G1288	A1227	A1166	U1106	C1045	U982	U918	G858	U795	C735	C
C1599	U1413	U1348	U1289	U1289	G1228	G1167	G1107	G1046	A983	U920	A859	U796	C736	U
A1600	U1414	U1350	U1290	U1290	G1229	U1168	G1108	G1047	U921	U921	U860	U800	A737	G
G1601	G1415	G1351	G1291	G1291	G1229	G1169	G1109	G1048	G985	A922	U861	G802	G738	A
C1602	U1416	G1352	G1292	G1292	U1231	G1170	G1110	U1049	G986	A923	A862	G803	G739	G
U1603	U1417	U1353	G1293	G1293	G1233	A1171	G1111	G1050	G987	A926	A863	A803	A740	U
G1604	G1418	G1354	G1294	G1294	U1234	C1172	G1112	G1051	A988	U926	U864	A804	C741	A
G1605	C1355	C1355	G1295	G1295	A1234	C1173	A1113	U1052	U989	C927	A865	U805	U742	U
C1606	U1296	U1296	G1296	G1296	G1228	G1167	G1107	G1046	A983	U920	G866	A906	U743	C
G1607	G1358	C1359	G1297	G1297	G1229	U1168	G1108	G1047	U921	U921	U860	U800	A737	G
U1608	C1359	U1298	G1298	G1298	G1229	G1169	G1109	G1048	G985	A922	U861	G802	G738	A
G1610	U1361	U1361	U1299	U1299	U1231	G1170	G1110	U1049	G986	A923	A862	G803	G739	G
A1611	U1362	U1362	U1301	U1301	U1240	G1178	G1118	U1056	A993	C931	A869	A809	A746	U
U1612	G1428	G1428	U1302	U1302	G1241	G1179	G1119	U1057	G994	U932	C870	G810	C747	C
C1613	U1429	U1430	U1363	U1363	U1241	G1180	G1120	U1058	A995	A933	G871	A811	U748	C
A1614	C1431	U1364	G1364	G1364	A1242	U1181	C1121	U1059	G997	C934	G872	A812	U749	C
C1615	U1432	U1365	U1365	U1365	A1243	U1182	G1122	U1060	A998	U935	U873	A813	U750	C
G1616	G1433	G1366	U1306	U1306	A1244	A1183	C1123	U1061	U999	U936	C874	A814	G751	C
U1617	U1434	G1367	U1307	U1307	C1246	U1185	A1125	G1064	C1000	A939	G876	G815	A752	C
C1618	U1435	U1369	G1308	G1308	U1247	U1186	G1126	A1065	A1001	A940	C877	A817	A754	C
U1619	G1436	U1370	U1309	U1309	C1248	U1187	G1127	C1066	G1002	C942	G878	C818	A755	C
G1620	U1437	A1371	U1310	U1310	U1249	G1188	C1128	C1068	A1003	G949	U879	G819	A756	C
U1621	U1438	U1372	U1311	U1311	U1250	G1189	U1129	U1069	U1004	C943	C880	U820	A757	C
C1622	C1373	U1373	A1312	A1312	U1251	C1190	G1130	C1070	C1006	U945	A881	U821	A758	C
G1623	C1374	C1374	A1313	A1313	C1252	U1191	A1131	U1071	C1007	U946	C883	U822	U759	C
C1624	U1442	U1443	U1314	U1314	C1253	C1192	A1132	U1072	G1008	U947	A884	G824	A760	C
G1625	G1444	U1444	U1315	U1315	U1254	A1193	C1133	G1073	U1009	G948	G885	U825	A762	C
U1626	G1445	G1445	G1316	G1316	U1255	A1194	A1134	C1074	C1010	C949	U886	U826	A763	C
C1627	U1446	U1446	U1317	U1317	A1256	C1195	U1135	C1075	G1011	C950	A887	C927	U764	C
U1628	G1447	G1447	U1378	U1378	U1257	A1196	U1136	A1076	U1012	A951	U888	U828	G765	C
G1629	U1448	U1448	U1380	U1380	U1258	C1197	A1137	C1077	A1013	A952	U889	A829	U766	C
U1630	U1449	U1449	U1381	U1381	U1259	G1198	A1138	C1078	G1014	G953	C890	U830	U767	C
A1631	U1450	U1450	A1382	A1321	U1260	G1199	A1139	U1079	U1015	C954	A891	U831	C768	C
C1632	U1451	C1451	G1383	A1322	U1261	G1200	G1140	U1080	A955	A955	A892	U832	A769	C
G1633	U1452	U1452	A1384	A1323	G1263	A1142	A1141	A1081	U1018	U957	U894	U833	U772	C
C1634	G1453	G1453	G1385	G1324	G1264	A1202	A1142	G1082	A1019	U958	G895	U834	C773	C
A1635	U1454	G1454	G1386	A1325	G1265	A1203	A1143	G1083	U1022	U959	U896	U836	A774	C
C1636	G1455	G1455	G1387	A1326	U1266	A1204	U1144	A1084	A1023	U960	C897	U837	G775	C
C1637	U1456	C1456	C1388	C1327	G1267	U1205	U1145	G1085	U1024	U961	A898	G838	G776	C
G1638	C1457	C1457	C1389	G1328	G1268	U1206	A1147	A1086	A1025	C962	G899	U839	C777	C
C1639	U1458	U1458	U1390	A1329	U1269	C1207	A1147	A1087	A1026	A963	A900	U840	C778	C
U1640	G1459	A1391	G1390	G1330	G1270	A1208	C1148	U1088	A1027	U964	G901	U841	U779	C
C1641	U1460	U1392	U1392	A1331	G1271	C1209	G1149	U1089	C1028	U965	G902	C842	A780	C
U1642	C1461	C1393	C1393	C1332	U1272	C1210	G1150	C1090	U1029	U966	U903	C842	U781	C
G1643	U1462	G1462	U1394	U1334	U1273	A1211	A1151	A1091	C1028	A967	G904	U844	U782	C
C1644	C1463	G1463	U1394	U1334	C1274	G1212	A1152	A1092	A1030	A967	A905	G845	U783	C
G1645	U1397	U1397	U1395	U1335	A1275	G1154	G1154	U1094	C1032	A970	A906	G846	G723	C
U1646	U1398	U1398	A1336	A1337	G1276	U1155	G1155	U1095	C1033	A971	A907	A847	U784	C
C1647	G1465	G1465	U1399	A1337	G1277	C1217	C1156	C1096	C1034	G972	U908	C848	U785	C
G1648	U1400	U1400	A1400	C1338	G1278	A1217	C1156	C1096	C1034	A973	U909	C849	C786	C
U1649	C1467	C1467	A1401	U1339	G1279	G1218	A1157	U1097	A1035	A974	U910	A850	A787	C
C1650	U1468	U1468	G1402	C1390	C1280	A1219	C1158	C1097	A1036	C975	G888	U727	G788	C
A1651	G1469	G1469	G1402	U1390	C1280	A1219	C1158	C1097	A1036	C975	U911	U851	A789	C
C1652	C1470	C1470	A1403	A1341	G1281	C1220	C1159	U1099	U1099	C975	U911	U851	A789	C



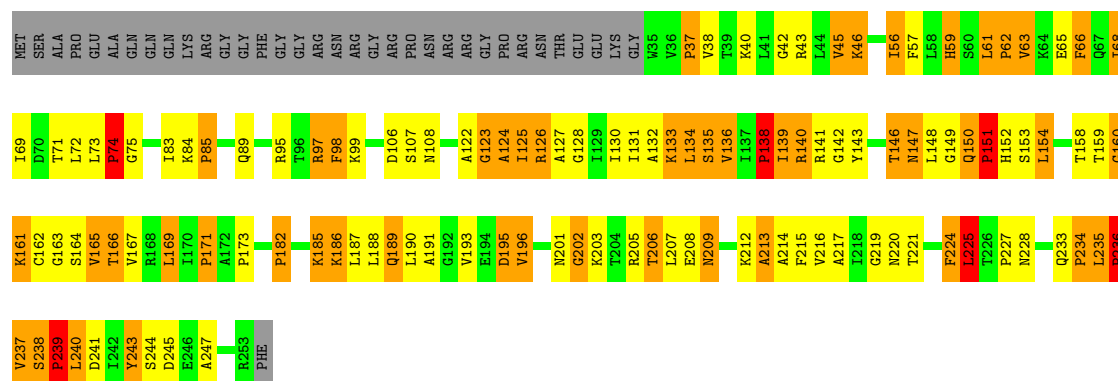
• Molecule 2: 40S ribosomal protein S0-A

Chain A:



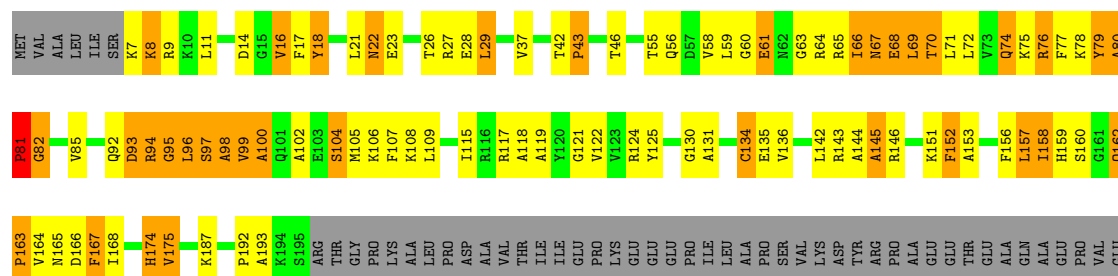
• Molecule 3: 40S ribosomal protein S2

Chain B:



• Molecule 4: 40S ribosomal protein S3

Chain C:



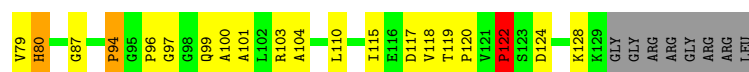
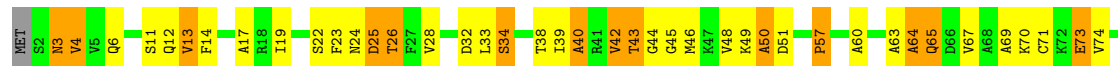
Chain D:





• Molecule 9: 40S ribosomal protein S14-A

Chain H:



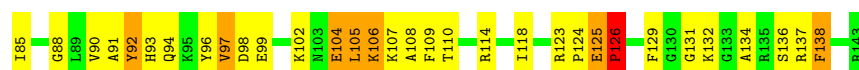
• Molecule 10: 40S ribosomal protein S15

Chain I:



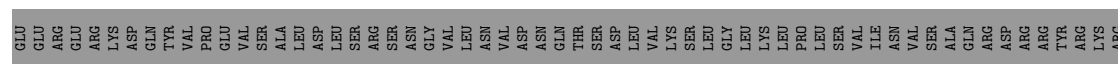
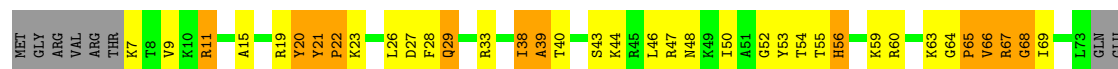
• Molecule 11: 40S ribosomal protein S16

Chain J:



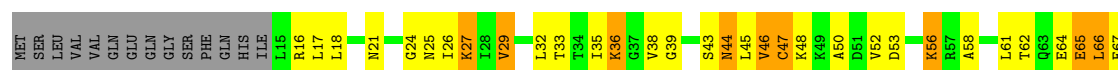
• Molecule 12: 40S ribosomal protein S17-A

Chain K:



• Molecule 13: 40S ribosomal protein S18

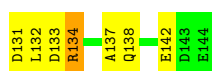
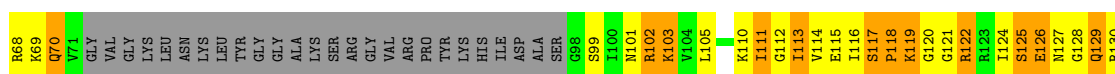
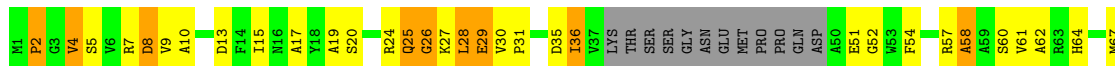
Chain L:





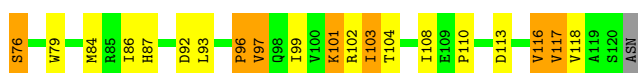
• Molecule 14: 40S ribosomal protein S19-A

Chain M:



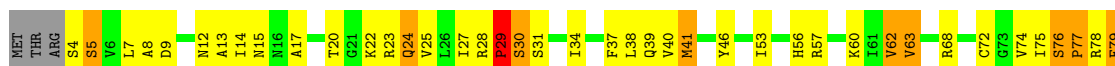
• Molecule 15: 40S ribosomal protein S20

Chain N:



• Molecule 16: 40S ribosomal protein S22-A

Chain O:



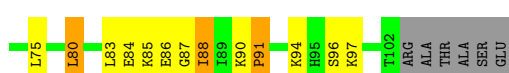
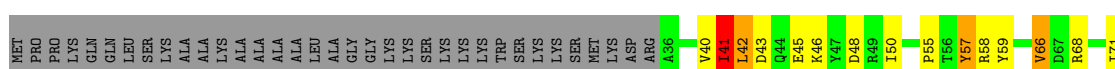
• Molecule 17: 40S ribosomal protein S23

Chain P:



• Molecule 18: 40S ribosomal protein S25-A

Chain Q:



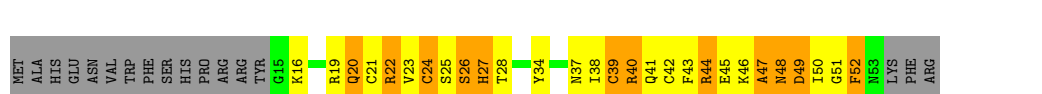
- Molecule 19: 40S ribosomal protein S28-A

Chain R:



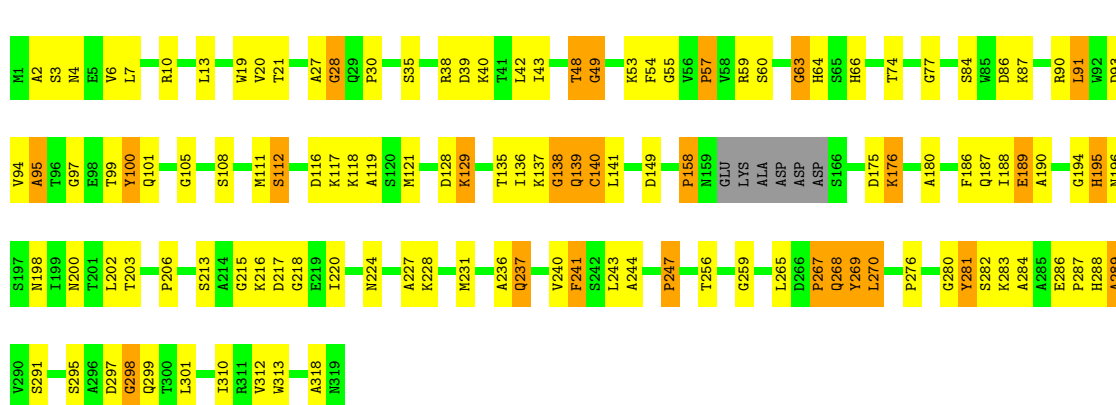
- Molecule 20: 40S ribosomal protein S29-A

Chain S:



- Molecule 21: Guanine nucleotide-binding protein subunit beta-like protein; RACK-1

Chain T:



- Molecule 22: Unassigned secondary structure

Chain a:



There are no outlier residues recorded for this chain.

- Molecule 23: Unassigned secondary structure

Chain b:



- Molecule 24: Unassigned secondary structure

Chain c:



- Molecule 25: Unassigned secondary structure

Chain d:



There are no outlier residues recorded for this chain.

- Molecule 26: Unassigned secondary structure



Chain e: 

There are no outlier residues recorded for this chain.

- Molecule 27: Unassigned secondary structure

Chain f: 

There are no outlier residues recorded for this chain.

- Molecule 28: Unassigned secondary structure

Chain h: 

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	437.11Å 288.38Å 306.56Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	268.00 – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) (268.00-4.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 4.02Å)	Xtriage
Refinement program	Phenix	Depositor
R, $R_{free}$	0.278 , 0.341	Depositor
Wilson B-factor (Å <sup>2</sup> )	147.1	Xtriage
Anisotropy	0.257	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 617642 reflections	Xtriage
Total number of atoms	55248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OHX

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	1	0.77	20/42619 (0.0%)	1.32	552/66408 (0.8%)
2	A	0.45	0/1089	0.86	16/1517 (1.1%)
3	B	0.54	0/1073	0.91	13/1488 (0.9%)
4	C	0.50	0/927	0.68	4/1286 (0.3%)
5	D	0.45	0/834	0.71	5/1159 (0.4%)
6	E	0.49	0/775	0.70	3/1077 (0.3%)
7	F	0.60	0/381	0.88	3/530 (0.6%)
8	G	0.51	0/579	0.78	5/806 (0.6%)
9	H	0.43	0/626	0.71	4/867 (0.5%)
10	I	0.45	0/595	0.90	8/826 (1.0%)
11	J	0.49	0/657	0.78	5/911 (0.5%)
12	K	0.44	0/331	0.74	2/460 (0.4%)
13	L	0.47	0/589	0.70	2/816 (0.2%)
14	M	0.54	0/518	0.83	3/715 (0.4%)
15	N	0.51	0/550	0.84	5/766 (0.7%)
16	O	0.53	0/621	0.83	3/860 (0.3%)
17	P	0.61	0/565	0.92	4/781 (0.5%)
18	Q	0.41	0/331	0.68	2/460 (0.4%)
19	R	0.40	0/229	0.63	1/316 (0.3%)
20	S	0.54	0/189	0.70	0/260
21	T	0.43	0/1541	0.61	8/2141 (0.4%)
All	All	0.72	20/55619 (0.0%)	1.23	648/84450 (0.8%)

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
3	B	0	2
17	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	Q	0	1
23	b	0	1
24	c	0	1
All	All	0	6

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1421	A	N9-C4	10.64	1.44	1.37
1	1	825	U	C2-O2	-9.58	1.13	1.22
1	1	391	A	N9-C4	-6.63	1.33	1.37
1	1	243	G	C1'-N9	-6.55	1.37	1.46
1	1	1030	A	N9-C4	-5.94	1.34	1.37

The worst 5 of 648 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1455	G	N3-C2-N2	-28.67	99.83	119.90
1	1	1455	G	N1-C6-O6	28.06	136.74	119.90
1	1	1455	G	N1-C2-N2	23.87	137.69	116.20
1	1	1455	G	C5-C6-O6	-19.72	116.77	128.60
1	1	1455	G	C5-C6-N1	-19.63	101.69	111.50

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	224	PHE	Peptide
3	B	225	LEU	Peptide
17	P	28	ASN	Peptide
18	Q	41	ILE	Peptide
23	b	14	UNK	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	38107	0	61	3135	0
2	A	1090	0	0	72	0
3	B	1074	0	0	74	0
4	C	928	0	0	51	0
5	D	836	0	0	69	0
6	E	777	0	0	58	0
7	F	382	0	0	16	0
8	G	580	0	0	42	0
9	H	627	0	0	26	0
10	I	596	0	0	25	0
11	J	658	0	0	39	0
12	K	332	0	0	15	0
13	L	591	0	0	50	0
14	M	521	0	0	47	0
15	N	551	0	0	36	0
16	O	622	0	0	44	0
17	P	566	0	0	41	0
18	Q	332	0	0	9	0
19	R	230	0	0	3	0
20	S	190	0	0	36	0
21	T	1543	0	0	53	0
22	a	100	0	25	0	0
23	b	525	0	141	0	0
24	c	465	0	122	0	0
25	d	175	0	39	0	0
26	e	105	0	25	0	0
27	f	55	0	15	0	0
28	h	205	0	51	0	0
29	l	854	0	0	98	0
29	G	7	0	0	0	0
29	L	7	0	0	0	0
29	S	7	0	0	18	0
29	T	7	0	0	0	0
29	c	7	0	0	0	0
29	e	21	0	0	0	0
29	g	1575	0	0	0	0
All	All	55248	0	479	3920	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 75.

The worst 5 of 3920 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:825:U:C5	1:1:847:A:N1	1.82	1.45
1:1:243:G:C2	1:1:251:A:N1	2.07	1.22
1:1:66:U:N3	1:1:71:A:N6	1.92	1.18
1:1:992:A:C2	1:1:1012:U:N3	2.14	1.16
1:1:650:U:N3	1:1:684:A:N6	1.93	1.16

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	
2	A	218/252 (86%)	75 (34%)	68 (31%)	75 (34%)	0	0
3	B	217/254 (85%)	85 (39%)	54 (25%)	78 (36%)	0	0
4	C	187/240 (78%)	72 (38%)	56 (30%)	59 (32%)	0	0
5	D	165/225 (73%)	55 (33%)	46 (28%)	64 (39%)	0	0
6	E	153/197 (78%)	48 (31%)	54 (35%)	51 (33%)	0	0
7	F	75/156 (48%)	32 (43%)	18 (24%)	25 (33%)	0	0
8	G	115/151 (76%)	46 (40%)	38 (33%)	31 (27%)	0	1
9	H	126/137 (92%)	52 (41%)	38 (30%)	36 (29%)	0	1
10	I	119/142 (84%)	38 (32%)	40 (34%)	41 (34%)	0	0
11	J	132/143 (92%)	57 (43%)	33 (25%)	42 (32%)	0	0
12	K	65/136 (48%)	27 (42%)	16 (25%)	22 (34%)	0	0
13	L	116/146 (80%)	48 (41%)	34 (29%)	34 (29%)	0	1
14	M	100/144 (69%)	38 (38%)	28 (28%)	34 (34%)	0	0
15	N	109/121 (90%)	49 (45%)	30 (28%)	30 (28%)	0	1
16	O	125/130 (96%)	48 (38%)	40 (32%)	37 (30%)	0	1
17	P	114/145 (79%)	48 (42%)	24 (21%)	42 (37%)	0	0
18	Q	65/108 (60%)	28 (43%)	21 (32%)	16 (25%)	0	2
19	R	45/67 (67%)	17 (38%)	12 (27%)	16 (36%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	S	37/56 (66%)	8 (22%)	14 (38%)	15 (40%)	0	0
21	T	309/319 (97%)	180 (58%)	71 (23%)	58 (19%)	0	4
All	All	2592/3269 (79%)	1051 (40%)	735 (28%)	806 (31%)	0	0

5 of 806 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	11	PRO
2	A	13	ASP
2	A	14	ALA
2	A	21	ASN
2	A	24	LEU

### 5.3.2 Protein sidechains ⓘ

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1787/1800 (99%)	1003 (56%)	148 (8%)

5 of 1003 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	3	U
1	1	4	C
1	1	7	G
1	1	8	U

5 of 148 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	607	G
1	1	846	G
1	1	1633	A
1	1	659	C
1	1	765	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

355 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	$\# Z  > 2$
29	OHX	1	1801	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1802	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1803	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1804	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1805	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1806	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1807	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1808	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1809	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1810	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1811	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1812	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1813	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1814	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1815	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1816	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1817	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1818	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1819	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1820	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1821	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1822	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OHX	1	1823	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1824	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1825	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1826	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1827	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1828	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1829	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1830	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1831	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1832	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1833	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1834	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1835	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1836	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1837	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1838	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1839	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1840	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1841	1	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1842	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1843	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1844	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1845	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1846	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1847	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1848	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1849	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1850	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1851	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1852	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1853	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1854	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1855	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1856	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1857	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1858	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1859	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1860	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1861	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1862	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1863	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1864	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1865	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OHX	1	1866	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1867	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1868	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1869	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1870	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1871	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1872	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1873	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1874	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1875	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1876	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1877	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1878	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1879	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1880	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1881	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1882	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1883	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1884	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1885	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1886	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1887	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1888	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1889	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1890	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1891	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1892	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1893	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1894	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1895	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1896	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1897	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1898	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1899	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1900	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1908	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OHX	1	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	1	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	G	189	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	L	277	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	S	534	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	T	433	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	c	100	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	e	305	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	e	564	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	e	670	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	1	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	106	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	109	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	11	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	116	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	119	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	120	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	130	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	133	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	135	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	137	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	138	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	139	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	14	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	140	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	144	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	146	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	148	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	149	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	15	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	151	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OHX	g	158	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	160	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	161	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	17	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	170	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	171	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	173	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	18	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	181	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	183	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	188	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	19	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	191	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	193	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	195	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	196	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	197	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	200	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	204	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	211	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	216	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	221	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	222	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	227	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	228	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	23	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	240	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	241	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	245	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	246	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	248	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	253	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	258	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	259	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	265	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	266	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	267	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	270	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	271	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	273	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	279	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	282	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	286	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OHX	g	288	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	289	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	295	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	299	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	3	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	30	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	307	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	309	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	312	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	317	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	323	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	327	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	328	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	33	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	331	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	333	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	336	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	338	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	343	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	345	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	348	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	35	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	351	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	353	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	354	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	356	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	357	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	36	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	366	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	369	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	370	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	375	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	377	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	378	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	38	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	381	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	384	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	387	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	388	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	395	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	398	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	399	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	40	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OHX	g	400	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	401	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	402	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	406	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	407	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	414	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	419	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	420	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	422	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	424	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	425	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	427	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	430	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	432	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	441	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	445	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	451	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	456	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	457	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	461	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	465	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	466	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	469	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	471	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	476	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	478	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	483	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	489	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	49	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	490	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	492	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	496	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	499	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	503	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	504	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	507	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	513	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	514	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	515	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	518	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	52	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	520	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	521	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OHX	g	528	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	532	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	535	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	536	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	54	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	540	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	547	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	55	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	550	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	551	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	552	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	553	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	554	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	56	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	569	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	571	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	575	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	576	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	577	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	580	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	581	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	588	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	589	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	590	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	593	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	6	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	603	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	607	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	61	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	611	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	613	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	614	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	620	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	621	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	622	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	625	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	627	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	634	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	638	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	641	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	643	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	650	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	66	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OHX	g	661	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	664	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	665	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	67	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	671	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	678	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	680	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	681	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	689	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	690	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	692	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	693	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	694	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	698	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	699	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	7	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	70	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	700	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	705	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	706	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	707	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	711	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	72	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	81	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	82	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	83	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	85	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	86	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	9	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	91	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	96	-	0,6,6	0.00	-	0,15,15	0.00	-
29	OHX	g	98	-	0,6,6	0.00	-	0,15,15	0.00	-

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
29	OHX	1	1801	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1802	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1803	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1804	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	1	1805	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1806	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1807	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1808	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1809	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1810	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1811	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1812	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1813	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1814	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1815	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1816	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1817	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1818	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1819	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1820	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1821	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1822	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1823	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1824	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1825	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1826	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1827	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1828	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1829	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1830	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1831	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1832	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1833	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1834	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1835	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1836	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1837	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1838	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1839	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1840	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1841	1	-	0/0/0/0	0/0/0/0
29	OHX	1	1842	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1843	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1844	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1845	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1846	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	1	1847	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1848	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1849	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1850	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1851	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1852	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1853	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1854	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1855	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1856	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1857	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1858	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1859	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1860	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1861	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1862	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1863	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1864	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1865	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1866	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1867	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1868	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1869	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1870	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1871	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1872	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1873	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1874	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1875	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1876	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1877	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1878	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1879	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1880	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1881	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1882	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1883	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1884	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1885	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1886	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1887	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1888	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	1	1889	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1890	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1891	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1892	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1893	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1894	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1895	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1896	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1897	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1898	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1899	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1900	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1901	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1902	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1903	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1904	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1905	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1906	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1907	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1908	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1909	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1910	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1911	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1912	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1913	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1914	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1915	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1916	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1917	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1918	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1919	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1920	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1921	-	-	0/0/0/0	0/0/0/0
29	OHX	1	1922	-	-	0/0/0/0	0/0/0/0
29	OHX	G	189	-	-	0/0/0/0	0/0/0/0
29	OHX	L	277	-	-	0/0/0/0	0/0/0/0
29	OHX	S	534	-	-	0/0/0/0	0/0/0/0
29	OHX	T	433	-	-	0/0/0/0	0/0/0/0
29	OHX	c	100	-	-	0/0/0/0	0/0/0/0
29	OHX	e	305	-	-	0/0/0/0	0/0/0/0
29	OHX	e	564	-	-	0/0/0/0	0/0/0/0
29	OHX	e	670	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	g	1	-	-	0/0/0/0	0/0/0/0
29	OHX	g	106	-	-	0/0/0/0	0/0/0/0
29	OHX	g	109	-	-	0/0/0/0	0/0/0/0
29	OHX	g	11	-	-	0/0/0/0	0/0/0/0
29	OHX	g	116	-	-	0/0/0/0	0/0/0/0
29	OHX	g	119	-	-	0/0/0/0	0/0/0/0
29	OHX	g	120	-	-	0/0/0/0	0/0/0/0
29	OHX	g	130	-	-	0/0/0/0	0/0/0/0
29	OHX	g	133	-	-	0/0/0/0	0/0/0/0
29	OHX	g	135	-	-	0/0/0/0	0/0/0/0
29	OHX	g	137	-	-	0/0/0/0	0/0/0/0
29	OHX	g	138	-	-	0/0/0/0	0/0/0/0
29	OHX	g	139	-	-	0/0/0/0	0/0/0/0
29	OHX	g	14	-	-	0/0/0/0	0/0/0/0
29	OHX	g	140	-	-	0/0/0/0	0/0/0/0
29	OHX	g	144	-	-	0/0/0/0	0/0/0/0
29	OHX	g	146	-	-	0/0/0/0	0/0/0/0
29	OHX	g	148	-	-	0/0/0/0	0/0/0/0
29	OHX	g	149	-	-	0/0/0/0	0/0/0/0
29	OHX	g	15	-	-	0/0/0/0	0/0/0/0
29	OHX	g	151	-	-	0/0/0/0	0/0/0/0
29	OHX	g	158	-	-	0/0/0/0	0/0/0/0
29	OHX	g	160	-	-	0/0/0/0	0/0/0/0
29	OHX	g	161	-	-	0/0/0/0	0/0/0/0
29	OHX	g	17	-	-	0/0/0/0	0/0/0/0
29	OHX	g	170	-	-	0/0/0/0	0/0/0/0
29	OHX	g	171	-	-	0/0/0/0	0/0/0/0
29	OHX	g	173	-	-	0/0/0/0	0/0/0/0
29	OHX	g	18	-	-	0/0/0/0	0/0/0/0
29	OHX	g	181	-	-	0/0/0/0	0/0/0/0
29	OHX	g	183	-	-	0/0/0/0	0/0/0/0
29	OHX	g	188	-	-	0/0/0/0	0/0/0/0
29	OHX	g	19	-	-	0/0/0/0	0/0/0/0
29	OHX	g	191	-	-	0/0/0/0	0/0/0/0
29	OHX	g	193	-	-	0/0/0/0	0/0/0/0
29	OHX	g	195	-	-	0/0/0/0	0/0/0/0
29	OHX	g	196	-	-	0/0/0/0	0/0/0/0
29	OHX	g	197	-	-	0/0/0/0	0/0/0/0
29	OHX	g	200	-	-	0/0/0/0	0/0/0/0
29	OHX	g	204	-	-	0/0/0/0	0/0/0/0
29	OHX	g	211	-	-	0/0/0/0	0/0/0/0
29	OHX	g	216	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	g	221	-	-	0/0/0/0	0/0/0/0
29	OHX	g	222	-	-	0/0/0/0	0/0/0/0
29	OHX	g	227	-	-	0/0/0/0	0/0/0/0
29	OHX	g	228	-	-	0/0/0/0	0/0/0/0
29	OHX	g	23	-	-	0/0/0/0	0/0/0/0
29	OHX	g	240	-	-	0/0/0/0	0/0/0/0
29	OHX	g	241	-	-	0/0/0/0	0/0/0/0
29	OHX	g	245	-	-	0/0/0/0	0/0/0/0
29	OHX	g	246	-	-	0/0/0/0	0/0/0/0
29	OHX	g	248	-	-	0/0/0/0	0/0/0/0
29	OHX	g	253	-	-	0/0/0/0	0/0/0/0
29	OHX	g	258	-	-	0/0/0/0	0/0/0/0
29	OHX	g	259	-	-	0/0/0/0	0/0/0/0
29	OHX	g	265	-	-	0/0/0/0	0/0/0/0
29	OHX	g	266	-	-	0/0/0/0	0/0/0/0
29	OHX	g	267	-	-	0/0/0/0	0/0/0/0
29	OHX	g	270	-	-	0/0/0/0	0/0/0/0
29	OHX	g	271	-	-	0/0/0/0	0/0/0/0
29	OHX	g	273	-	-	0/0/0/0	0/0/0/0
29	OHX	g	279	-	-	0/0/0/0	0/0/0/0
29	OHX	g	282	-	-	0/0/0/0	0/0/0/0
29	OHX	g	286	-	-	0/0/0/0	0/0/0/0
29	OHX	g	288	-	-	0/0/0/0	0/0/0/0
29	OHX	g	289	-	-	0/0/0/0	0/0/0/0
29	OHX	g	295	-	-	0/0/0/0	0/0/0/0
29	OHX	g	299	-	-	0/0/0/0	0/0/0/0
29	OHX	g	3	-	-	0/0/0/0	0/0/0/0
29	OHX	g	30	-	-	0/0/0/0	0/0/0/0
29	OHX	g	307	-	-	0/0/0/0	0/0/0/0
29	OHX	g	309	-	-	0/0/0/0	0/0/0/0
29	OHX	g	312	-	-	0/0/0/0	0/0/0/0
29	OHX	g	317	-	-	0/0/0/0	0/0/0/0
29	OHX	g	323	-	-	0/0/0/0	0/0/0/0
29	OHX	g	327	-	-	0/0/0/0	0/0/0/0
29	OHX	g	328	-	-	0/0/0/0	0/0/0/0
29	OHX	g	33	-	-	0/0/0/0	0/0/0/0
29	OHX	g	331	-	-	0/0/0/0	0/0/0/0
29	OHX	g	333	-	-	0/0/0/0	0/0/0/0
29	OHX	g	336	-	-	0/0/0/0	0/0/0/0
29	OHX	g	338	-	-	0/0/0/0	0/0/0/0
29	OHX	g	343	-	-	0/0/0/0	0/0/0/0
29	OHX	g	345	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	g	348	-	-	0/0/0/0	0/0/0/0
29	OHX	g	35	-	-	0/0/0/0	0/0/0/0
29	OHX	g	351	-	-	0/0/0/0	0/0/0/0
29	OHX	g	353	-	-	0/0/0/0	0/0/0/0
29	OHX	g	354	-	-	0/0/0/0	0/0/0/0
29	OHX	g	356	-	-	0/0/0/0	0/0/0/0
29	OHX	g	357	-	-	0/0/0/0	0/0/0/0
29	OHX	g	36	-	-	0/0/0/0	0/0/0/0
29	OHX	g	366	-	-	0/0/0/0	0/0/0/0
29	OHX	g	369	-	-	0/0/0/0	0/0/0/0
29	OHX	g	370	-	-	0/0/0/0	0/0/0/0
29	OHX	g	375	-	-	0/0/0/0	0/0/0/0
29	OHX	g	377	-	-	0/0/0/0	0/0/0/0
29	OHX	g	378	-	-	0/0/0/0	0/0/0/0
29	OHX	g	38	-	-	0/0/0/0	0/0/0/0
29	OHX	g	381	-	-	0/0/0/0	0/0/0/0
29	OHX	g	384	-	-	0/0/0/0	0/0/0/0
29	OHX	g	387	-	-	0/0/0/0	0/0/0/0
29	OHX	g	388	-	-	0/0/0/0	0/0/0/0
29	OHX	g	395	-	-	0/0/0/0	0/0/0/0
29	OHX	g	398	-	-	0/0/0/0	0/0/0/0
29	OHX	g	399	-	-	0/0/0/0	0/0/0/0
29	OHX	g	40	-	-	0/0/0/0	0/0/0/0
29	OHX	g	400	-	-	0/0/0/0	0/0/0/0
29	OHX	g	401	-	-	0/0/0/0	0/0/0/0
29	OHX	g	402	-	-	0/0/0/0	0/0/0/0
29	OHX	g	406	-	-	0/0/0/0	0/0/0/0
29	OHX	g	407	-	-	0/0/0/0	0/0/0/0
29	OHX	g	414	-	-	0/0/0/0	0/0/0/0
29	OHX	g	419	-	-	0/0/0/0	0/0/0/0
29	OHX	g	420	-	-	0/0/0/0	0/0/0/0
29	OHX	g	422	-	-	0/0/0/0	0/0/0/0
29	OHX	g	424	-	-	0/0/0/0	0/0/0/0
29	OHX	g	425	-	-	0/0/0/0	0/0/0/0
29	OHX	g	427	-	-	0/0/0/0	0/0/0/0
29	OHX	g	430	-	-	0/0/0/0	0/0/0/0
29	OHX	g	432	-	-	0/0/0/0	0/0/0/0
29	OHX	g	441	-	-	0/0/0/0	0/0/0/0
29	OHX	g	445	-	-	0/0/0/0	0/0/0/0
29	OHX	g	451	-	-	0/0/0/0	0/0/0/0
29	OHX	g	456	-	-	0/0/0/0	0/0/0/0
29	OHX	g	457	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	g	461	-	-	0/0/0/0	0/0/0/0
29	OHX	g	465	-	-	0/0/0/0	0/0/0/0
29	OHX	g	466	-	-	0/0/0/0	0/0/0/0
29	OHX	g	469	-	-	0/0/0/0	0/0/0/0
29	OHX	g	471	-	-	0/0/0/0	0/0/0/0
29	OHX	g	476	-	-	0/0/0/0	0/0/0/0
29	OHX	g	478	-	-	0/0/0/0	0/0/0/0
29	OHX	g	483	-	-	0/0/0/0	0/0/0/0
29	OHX	g	489	-	-	0/0/0/0	0/0/0/0
29	OHX	g	49	-	-	0/0/0/0	0/0/0/0
29	OHX	g	490	-	-	0/0/0/0	0/0/0/0
29	OHX	g	492	-	-	0/0/0/0	0/0/0/0
29	OHX	g	496	-	-	0/0/0/0	0/0/0/0
29	OHX	g	499	-	-	0/0/0/0	0/0/0/0
29	OHX	g	503	-	-	0/0/0/0	0/0/0/0
29	OHX	g	504	-	-	0/0/0/0	0/0/0/0
29	OHX	g	507	-	-	0/0/0/0	0/0/0/0
29	OHX	g	513	-	-	0/0/0/0	0/0/0/0
29	OHX	g	514	-	-	0/0/0/0	0/0/0/0
29	OHX	g	515	-	-	0/0/0/0	0/0/0/0
29	OHX	g	518	-	-	0/0/0/0	0/0/0/0
29	OHX	g	52	-	-	0/0/0/0	0/0/0/0
29	OHX	g	520	-	-	0/0/0/0	0/0/0/0
29	OHX	g	521	-	-	0/0/0/0	0/0/0/0
29	OHX	g	528	-	-	0/0/0/0	0/0/0/0
29	OHX	g	532	-	-	0/0/0/0	0/0/0/0
29	OHX	g	535	-	-	0/0/0/0	0/0/0/0
29	OHX	g	536	-	-	0/0/0/0	0/0/0/0
29	OHX	g	54	-	-	0/0/0/0	0/0/0/0
29	OHX	g	540	-	-	0/0/0/0	0/0/0/0
29	OHX	g	547	-	-	0/0/0/0	0/0/0/0
29	OHX	g	55	-	-	0/0/0/0	0/0/0/0
29	OHX	g	550	-	-	0/0/0/0	0/0/0/0
29	OHX	g	551	-	-	0/0/0/0	0/0/0/0
29	OHX	g	552	-	-	0/0/0/0	0/0/0/0
29	OHX	g	553	-	-	0/0/0/0	0/0/0/0
29	OHX	g	554	-	-	0/0/0/0	0/0/0/0
29	OHX	g	56	-	-	0/0/0/0	0/0/0/0
29	OHX	g	569	-	-	0/0/0/0	0/0/0/0
29	OHX	g	571	-	-	0/0/0/0	0/0/0/0
29	OHX	g	575	-	-	0/0/0/0	0/0/0/0
29	OHX	g	576	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	g	577	-	-	0/0/0/0	0/0/0/0
29	OHX	g	580	-	-	0/0/0/0	0/0/0/0
29	OHX	g	581	-	-	0/0/0/0	0/0/0/0
29	OHX	g	588	-	-	0/0/0/0	0/0/0/0
29	OHX	g	589	-	-	0/0/0/0	0/0/0/0
29	OHX	g	590	-	-	0/0/0/0	0/0/0/0
29	OHX	g	593	-	-	0/0/0/0	0/0/0/0
29	OHX	g	6	-	-	0/0/0/0	0/0/0/0
29	OHX	g	603	-	-	0/0/0/0	0/0/0/0
29	OHX	g	607	-	-	0/0/0/0	0/0/0/0
29	OHX	g	61	-	-	0/0/0/0	0/0/0/0
29	OHX	g	611	-	-	0/0/0/0	0/0/0/0
29	OHX	g	613	-	-	0/0/0/0	0/0/0/0
29	OHX	g	614	-	-	0/0/0/0	0/0/0/0
29	OHX	g	620	-	-	0/0/0/0	0/0/0/0
29	OHX	g	621	-	-	0/0/0/0	0/0/0/0
29	OHX	g	622	-	-	0/0/0/0	0/0/0/0
29	OHX	g	625	-	-	0/0/0/0	0/0/0/0
29	OHX	g	627	-	-	0/0/0/0	0/0/0/0
29	OHX	g	634	-	-	0/0/0/0	0/0/0/0
29	OHX	g	638	-	-	0/0/0/0	0/0/0/0
29	OHX	g	641	-	-	0/0/0/0	0/0/0/0
29	OHX	g	643	-	-	0/0/0/0	0/0/0/0
29	OHX	g	650	-	-	0/0/0/0	0/0/0/0
29	OHX	g	66	-	-	0/0/0/0	0/0/0/0
29	OHX	g	661	-	-	0/0/0/0	0/0/0/0
29	OHX	g	664	-	-	0/0/0/0	0/0/0/0
29	OHX	g	665	-	-	0/0/0/0	0/0/0/0
29	OHX	g	67	-	-	0/0/0/0	0/0/0/0
29	OHX	g	671	-	-	0/0/0/0	0/0/0/0
29	OHX	g	678	-	-	0/0/0/0	0/0/0/0
29	OHX	g	680	-	-	0/0/0/0	0/0/0/0
29	OHX	g	681	-	-	0/0/0/0	0/0/0/0
29	OHX	g	689	-	-	0/0/0/0	0/0/0/0
29	OHX	g	690	-	-	0/0/0/0	0/0/0/0
29	OHX	g	692	-	-	0/0/0/0	0/0/0/0
29	OHX	g	693	-	-	0/0/0/0	0/0/0/0
29	OHX	g	694	-	-	0/0/0/0	0/0/0/0
29	OHX	g	698	-	-	0/0/0/0	0/0/0/0
29	OHX	g	699	-	-	0/0/0/0	0/0/0/0
29	OHX	g	7	-	-	0/0/0/0	0/0/0/0
29	OHX	g	70	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OHX	g	700	-	-	0/0/0/0	0/0/0/0
29	OHX	g	705	-	-	0/0/0/0	0/0/0/0
29	OHX	g	706	-	-	0/0/0/0	0/0/0/0
29	OHX	g	707	-	-	0/0/0/0	0/0/0/0
29	OHX	g	711	-	-	0/0/0/0	0/0/0/0
29	OHX	g	72	-	-	0/0/0/0	0/0/0/0
29	OHX	g	81	-	-	0/0/0/0	0/0/0/0
29	OHX	g	82	-	-	0/0/0/0	0/0/0/0
29	OHX	g	83	-	-	0/0/0/0	0/0/0/0
29	OHX	g	85	-	-	0/0/0/0	0/0/0/0
29	OHX	g	86	-	-	0/0/0/0	0/0/0/0
29	OHX	g	9	-	-	0/0/0/0	0/0/0/0
29	OHX	g	91	-	-	0/0/0/0	0/0/0/0
29	OHX	g	96	-	-	0/0/0/0	0/0/0/0
29	OHX	g	98	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.