



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2025 – 01:44 pm BST

PDB ID : 9RP1 / pdb_00009rp1
Title : Ensemble refined structure of CotB2 in complex with alendronate
Authors : Helmer, C.P.O.; Loll, B.
Deposited on : 2025-06-23
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

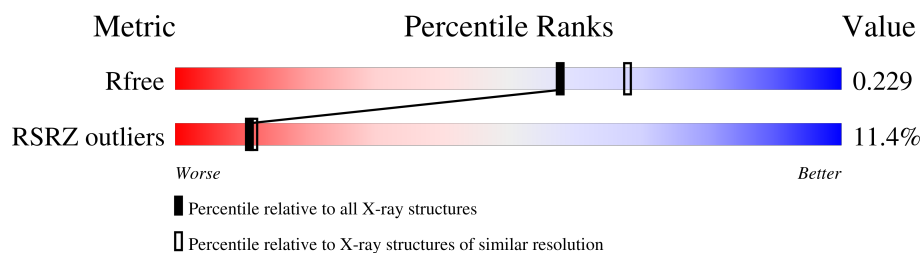
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 114533 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 Cyclooctat-9-en-7-ol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	2-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	3-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	4-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	5-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	6-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	7-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	8-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	9-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	10-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	11-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	12-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	13-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	14-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	15-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	16-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	17-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	18-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	19-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	20-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	21-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	22-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	23-A	283	Total	C	N	O	S	0	0	0
			2317	1478	387	435	17			
1	1-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	2-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	3-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	4-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	5-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	6-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	7-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	8-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	9-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	10-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	11-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	12-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	13-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	14-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	15-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	16-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	17-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	18-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	19-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	20-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	21-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	22-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			
1	23-B	296	Total	C	N	O	S	0	0	0
			2417	1537	409	454	17			

There are 22 discrepancies between the modelled and reference sequences:

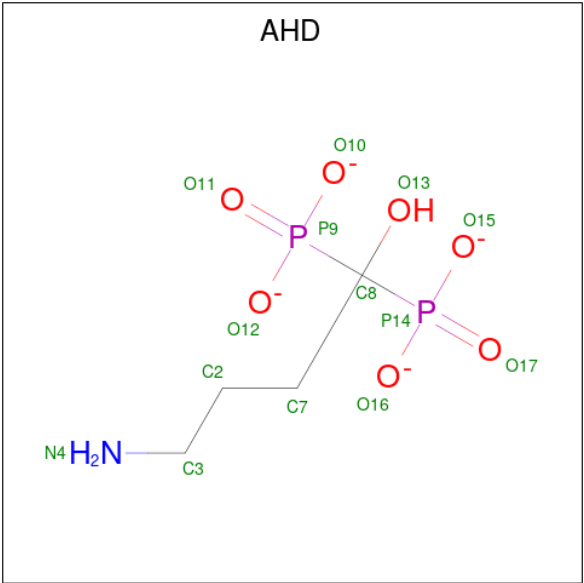
Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ALA	-	expression tag	UNP C9K1X5
A	309	ALA	-	expression tag	UNP C9K1X5
A	310	ALA	-	expression tag	UNP C9K1X5
A	311	LEU	-	expression tag	UNP C9K1X5
A	312	GLU	-	expression tag	UNP C9K1X5
A	313	HIS	-	expression tag	UNP C9K1X5
A	314	HIS	-	expression tag	UNP C9K1X5
A	315	HIS	-	expression tag	UNP C9K1X5
A	316	HIS	-	expression tag	UNP C9K1X5
A	317	HIS	-	expression tag	UNP C9K1X5
A	318	HIS	-	expression tag	UNP C9K1X5
B	308	ALA	-	expression tag	UNP C9K1X5
B	309	ALA	-	expression tag	UNP C9K1X5
B	310	ALA	-	expression tag	UNP C9K1X5
B	311	LEU	-	expression tag	UNP C9K1X5
B	312	GLU	-	expression tag	UNP C9K1X5
B	313	HIS	-	expression tag	UNP C9K1X5
B	314	HIS	-	expression tag	UNP C9K1X5
B	315	HIS	-	expression tag	UNP C9K1X5
B	316	HIS	-	expression tag	UNP C9K1X5
B	317	HIS	-	expression tag	UNP C9K1X5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	318	HIS	-	expression tag	UNP C9K1X5

- Molecule 2 is 4-AMINO-1-HYDROXYBUTANE-1,1-DIYLDIPHOSPHONATE (CCD ID: AHD) (formula: C₄H₉NO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	2-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	3-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	4-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	5-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	6-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	7-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	8-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	9-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	10-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	11-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	12-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	13-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	14-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	15-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	16-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	17-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	18-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	19-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	20-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	21-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	22-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	23-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	1-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	2-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	3-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	4-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	5-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	6-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	7-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	8-B	1	Total 14	C 4	N 1	O 7	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	9-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	10-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	11-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	12-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	13-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	14-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	15-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	16-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	17-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	18-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	19-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	20-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	21-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	22-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	23-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	3	Total	Mg	0	0
			3	3		
3	2-A	3	Total	Mg	0	0
			3	3		
3	3-A	3	Total	Mg	0	0
			3	3		
3	4-A	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	5-A	3	Total 3	Mg 3	0	0
3	6-A	3	Total 3	Mg 3	0	0
3	7-A	3	Total 3	Mg 3	0	0
3	8-A	3	Total 3	Mg 3	0	0
3	9-A	3	Total 3	Mg 3	0	0
3	10-A	3	Total 3	Mg 3	0	0
3	11-A	3	Total 3	Mg 3	0	0
3	12-A	3	Total 3	Mg 3	0	0
3	13-A	3	Total 3	Mg 3	0	0
3	14-A	3	Total 3	Mg 3	0	0
3	15-A	3	Total 3	Mg 3	0	0
3	16-A	3	Total 3	Mg 3	0	0
3	17-A	3	Total 3	Mg 3	0	0
3	18-A	3	Total 3	Mg 3	0	0
3	19-A	3	Total 3	Mg 3	0	0
3	20-A	3	Total 3	Mg 3	0	0
3	21-A	3	Total 3	Mg 3	0	0
3	22-A	3	Total 3	Mg 3	0	0
3	23-A	3	Total 3	Mg 3	0	0
3	1-B	3	Total 3	Mg 3	0	0
3	2-B	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	3-B	3	Total 3	Mg 3	0	0
3	4-B	3	Total 3	Mg 3	0	0
3	5-B	3	Total 3	Mg 3	0	0
3	6-B	3	Total 3	Mg 3	0	0
3	7-B	3	Total 3	Mg 3	0	0
3	8-B	3	Total 3	Mg 3	0	0
3	9-B	3	Total 3	Mg 3	0	0
3	10-B	3	Total 3	Mg 3	0	0
3	11-B	3	Total 3	Mg 3	0	0
3	12-B	3	Total 3	Mg 3	0	0
3	13-B	3	Total 3	Mg 3	0	0
3	14-B	3	Total 3	Mg 3	0	0
3	15-B	3	Total 3	Mg 3	0	0
3	16-B	3	Total 3	Mg 3	0	0
3	17-B	3	Total 3	Mg 3	0	0
3	18-B	3	Total 3	Mg 3	0	0
3	19-B	3	Total 3	Mg 3	0	0
3	20-B	3	Total 3	Mg 3	0	0
3	21-B	3	Total 3	Mg 3	0	0
3	22-B	3	Total 3	Mg 3	0	0
3	23-B	3	Total 3	Mg 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	62	Total O 62 62	0	0
4	2-A	67	Total O 67 67	0	0
4	3-A	72	Total O 72 72	0	0
4	4-A	62	Total O 62 62	0	0
4	5-A	60	Total O 60 60	0	0
4	6-A	66	Total O 66 66	0	0
4	7-A	62	Total O 62 62	0	0
4	8-A	62	Total O 62 62	0	0
4	9-A	61	Total O 61 61	0	0
4	10-A	62	Total O 62 62	0	0
4	11-A	60	Total O 60 60	0	0
4	12-A	71	Total O 71 71	0	0
4	13-A	56	Total O 56 56	0	0
4	14-A	60	Total O 60 60	0	0
4	15-A	61	Total O 61 61	0	0
4	16-A	67	Total O 67 67	0	0
4	17-A	61	Total O 61 61	0	0
4	18-A	63	Total O 63 63	0	0
4	19-A	59	Total O 59 59	0	0
4	20-A	65	Total O 65 65	0	0
4	21-A	61	Total O 61 61	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	22-A	67	Total 67	O 67	0	0
4	23-A	66	Total 66	O 66	0	0
4	1-B	149	Total 149	O 149	0	0
4	2-B	154	Total 154	O 154	0	0
4	3-B	167	Total 167	O 167	0	0
4	4-B	149	Total 149	O 149	0	0
4	5-B	143	Total 143	O 143	0	0
4	6-B	153	Total 153	O 153	0	0
4	7-B	147	Total 147	O 147	0	0
4	8-B	147	Total 147	O 147	0	0
4	9-B	143	Total 143	O 143	0	0
4	10-B	149	Total 149	O 149	0	0
4	11-B	143	Total 143	O 143	0	0
4	12-B	163	Total 163	O 163	0	0
4	13-B	131	Total 131	O 131	0	0
4	14-B	143	Total 143	O 143	0	0
4	15-B	146	Total 146	O 146	0	0
4	16-B	161	Total 161	O 161	0	0
4	17-B	145	Total 145	O 145	0	0
4	18-B	149	Total 149	O 149	0	0
4	19-B	133	Total 133	O 133	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	20-B	149	Total 149	O 149	0	0
4	21-B	146	Total 146	O 146	0	0
4	22-B	153	Total 153	O 153	0	0
4	23-B	153	Total 153	O 153	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.38Å 56.46Å 56.93Å 91.82° 101.66° 115.93°	Depositor
Resolution (Å)	19.83 – 2.10 19.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.83-2.10) 99.2 (19.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.173 , 0.212 0.189 , 0.229	Depositor DCC
R_{free} test set	1680 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	114533	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 138 are monoatomic - leaving 46 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$
2	AHD	1-B	401	3	13,13,13	1.82	5 (38%)	19,21,21	1.49	4 (21%)
2	AHD	6-B	401	3	13,13,13	1.92	5 (38%)	19,21,21	1.31	2 (10%)
2	AHD	8-A	401	3	13,13,13	1.51	2 (15%)	19,21,21	2.54	8 (42%)
2	AHD	23-A	401	3	13,13,13	1.51	3 (23%)	19,21,21	1.84	5 (26%)
2	AHD	9-A	401	3	13,13,13	1.74	3 (23%)	19,21,21	1.97	7 (36%)
2	AHD	17-B	401	3	13,13,13	1.88	5 (38%)	19,21,21	1.43	4 (21%)
2	AHD	12-A	401	3	13,13,13	1.50	2 (15%)	19,21,21	1.82	4 (21%)
2	AHD	16-A	401	3	13,13,13	1.64	5 (38%)	19,21,21	1.88	5 (26%)
2	AHD	14-B	401	3	13,13,13	1.86	4 (30%)	19,21,21	1.63	4 (21%)
2	AHD	21-A	401	3	13,13,13	1.61	3 (23%)	19,21,21	1.97	6 (31%)
2	AHD	4-A	401	3	13,13,13	1.44	3 (23%)	19,21,21	2.37	7 (36%)
2	AHD	10-B	401	3	13,13,13	1.97	5 (38%)	19,21,21	1.54	4 (21%)
2	AHD	7-A	401	3	13,13,13	1.72	3 (23%)	19,21,21	2.02	4 (21%)
2	AHD	1-A	401	3	13,13,13	1.67	2 (15%)	19,21,21	1.84	5 (26%)
2	AHD	20-A	401	3	13,13,13	1.79	2 (15%)	19,21,21	1.76	6 (31%)
2	AHD	15-A	401	3	13,13,13	1.55	3 (23%)	19,21,21	1.73	5 (26%)
2	AHD	22-B	401	3	13,13,13	1.84	4 (30%)	19,21,21	1.62	4 (21%)
2	AHD	23-B	401	3	13,13,13	1.88	5 (38%)	19,21,21	1.62	4 (21%)
2	AHD	3-A	401	3	13,13,13	1.57	3 (23%)	19,21,21	1.90	4 (21%)
2	AHD	19-A	401	3	13,13,13	1.58	3 (23%)	19,21,21	1.61	3 (15%)
2	AHD	5-B	401	3	13,13,13	1.79	4 (30%)	19,21,21	1.58	4 (21%)
2	AHD	18-B	401	3	13,13,13	1.75	5 (38%)	19,21,21	1.72	4 (21%)
2	AHD	22-A	401	3	13,13,13	1.61	4 (30%)	19,21,21	1.91	3 (15%)
2	AHD	5-A	401	3	13,13,13	1.61	2 (15%)	19,21,21	1.68	3 (15%)
2	AHD	19-B	401	3	13,13,13	1.80	4 (30%)	19,21,21	1.59	5 (26%)
2	AHD	13-B	401	3	13,13,13	1.98	6 (46%)	19,21,21	1.64	4 (21%)
2	AHD	10-A	401	3	13,13,13	1.82	4 (30%)	19,21,21	1.29	2 (10%)
2	AHD	7-B	401	3	13,13,13	1.80	4 (30%)	19,21,21	1.67	5 (26%)
2	AHD	15-B	401	3	13,13,13	1.80	5 (38%)	19,21,21	1.48	5 (26%)
2	AHD	18-A	401	3	13,13,13	1.46	2 (15%)	19,21,21	1.95	7 (36%)
2	AHD	9-B	401	3	13,13,13	1.96	5 (38%)	19,21,21	1.73	5 (26%)
2	AHD	20-B	401	3	13,13,13	1.96	4 (30%)	19,21,21	1.42	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AHD	14-A	401	3	13,13,13	1.65	3 (23%)	19,21,21	1.58	2 (10%)
2	AHD	16-B	401	3	13,13,13	1.71	4 (30%)	19,21,21	1.85	5 (26%)
2	AHD	11-B	401	3	13,13,13	1.87	4 (30%)	19,21,21	1.60	5 (26%)
2	AHD	17-A	401	3	13,13,13	1.63	4 (30%)	19,21,21	2.06	6 (31%)
2	AHD	13-A	401	3	13,13,13	1.64	4 (30%)	19,21,21	1.99	5 (26%)
2	AHD	21-B	401	3	13,13,13	1.82	5 (38%)	19,21,21	1.55	5 (26%)
2	AHD	2-A	401	3	13,13,13	1.80	4 (30%)	19,21,21	1.89	5 (26%)
2	AHD	4-B	401	3	13,13,13	1.89	5 (38%)	19,21,21	1.64	4 (21%)
2	AHD	8-B	401	3	13,13,13	1.81	5 (38%)	19,21,21	1.55	4 (21%)
2	AHD	2-B	401	3	13,13,13	1.81	5 (38%)	19,21,21	1.38	4 (21%)
2	AHD	12-B	401	3	13,13,13	1.91	5 (38%)	19,21,21	1.67	3 (15%)
2	AHD	6-A	401	3	13,13,13	1.73	4 (30%)	19,21,21	1.80	4 (21%)
2	AHD	3-B	401	3	13,13,13	1.86	5 (38%)	19,21,21	1.57	4 (21%)
2	AHD	11-A	401	3	13,13,13	1.64	2 (15%)	19,21,21	1.85	5 (26%)

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	AHD	1-B	401	3	-	2/23/23/23	-
2	AHD	6-B	401	3	-	2/23/23/23	-
2	AHD	8-A	401	3	-	7/23/23/23	-
2	AHD	23-A	401	3	-	5/23/23/23	-
2	AHD	9-A	401	3	-	3/23/23/23	-
2	AHD	17-B	401	3	-	2/23/23/23	-
2	AHD	12-A	401	3	-	9/23/23/23	-
2	AHD	16-A	401	3	-	5/23/23/23	-
2	AHD	14-B	401	3	-	2/23/23/23	-
2	AHD	21-A	401	3	-	5/23/23/23	-
2	AHD	4-A	401	3	-	5/23/23/23	-
2	AHD	10-B	401	3	-	3/23/23/23	-
2	AHD	7-A	401	3	-	7/23/23/23	-
2	AHD	1-A	401	3	-	4/23/23/23	-
2	AHD	20-A	401	3	-	2/23/23/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AHD	15-A	401	3	-	10/23/23/23	-
2	AHD	22-B	401	3	-	3/23/23/23	-
2	AHD	23-B	401	3	-	2/23/23/23	-
2	AHD	3-A	401	3	-	1/23/23/23	-
2	AHD	19-A	401	3	-	4/23/23/23	-
2	AHD	5-B	401	3	-	3/23/23/23	-
2	AHD	18-B	401	3	-	3/23/23/23	-
2	AHD	22-A	401	3	-	6/23/23/23	-
2	AHD	5-A	401	3	-	6/23/23/23	-
2	AHD	19-B	401	3	-	3/23/23/23	-
2	AHD	13-B	401	3	-	2/23/23/23	-
2	AHD	10-A	401	3	-	5/23/23/23	-
2	AHD	7-B	401	3	-	2/23/23/23	-
2	AHD	15-B	401	3	-	0/23/23/23	-
2	AHD	18-A	401	3	-	10/23/23/23	-
2	AHD	9-B	401	3	-	2/23/23/23	-
2	AHD	20-B	401	3	-	1/23/23/23	-
2	AHD	14-A	401	3	-	7/23/23/23	-
2	AHD	16-B	401	3	-	2/23/23/23	-
2	AHD	11-B	401	3	-	3/23/23/23	-
2	AHD	17-A	401	3	-	2/23/23/23	-
2	AHD	13-A	401	3	-	4/23/23/23	-
2	AHD	21-B	401	3	-	3/23/23/23	-
2	AHD	2-A	401	3	-	5/23/23/23	-
2	AHD	4-B	401	3	-	3/23/23/23	-
2	AHD	8-B	401	3	-	3/23/23/23	-
2	AHD	2-B	401	3	-	3/23/23/23	-
2	AHD	12-B	401	3	-	3/23/23/23	-
2	AHD	6-A	401	3	-	2/23/23/23	-
2	AHD	3-B	401	3	-	0/23/23/23	-
2	AHD	11-A	401	3	-	3/23/23/23	-

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	20-A	401	AHD	O13-C8	-4.51	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-A	401	AHD	O13-C8	-4.48	1.39	1.44
2	10-B	401	AHD	O13-C8	-4.22	1.39	1.44
2	21-A	401	AHD	O13-C8	-4.20	1.39	1.44
2	9-A	401	AHD	O13-C8	-4.10	1.39	1.44
2	13-B	401	AHD	O13-C8	-4.10	1.39	1.44
2	6-A	401	AHD	O13-C8	-4.08	1.39	1.44
2	20-B	401	AHD	O13-C8	-4.05	1.39	1.44
2	2-A	401	AHD	O13-C8	-4.03	1.39	1.44
2	1-A	401	AHD	O13-C8	-4.03	1.39	1.44
2	9-B	401	AHD	O13-C8	-3.93	1.39	1.44
2	14-A	401	AHD	O13-C8	-3.92	1.39	1.44
2	11-A	401	AHD	O13-C8	-3.92	1.39	1.44
2	5-A	401	AHD	O13-C8	-3.90	1.39	1.44
2	7-A	401	AHD	O13-C8	-3.89	1.39	1.44
2	12-B	401	AHD	O13-C8	-3.87	1.39	1.44
2	3-A	401	AHD	O13-C8	-3.83	1.39	1.44
2	11-B	401	AHD	O13-C8	-3.79	1.39	1.44
2	1-B	401	AHD	O13-C8	-3.77	1.40	1.44
2	15-B	401	AHD	O13-C8	-3.76	1.40	1.44
2	5-B	401	AHD	O13-C8	-3.74	1.40	1.44
2	17-B	401	AHD	O13-C8	-3.73	1.40	1.44
2	19-B	401	AHD	O13-C8	-3.72	1.40	1.44
2	19-A	401	AHD	O13-C8	-3.69	1.40	1.44
2	21-B	401	AHD	O13-C8	-3.66	1.40	1.44
2	22-B	401	AHD	O13-C8	-3.66	1.40	1.44
2	17-A	401	AHD	O13-C8	-3.65	1.40	1.44
2	7-B	401	AHD	O13-C8	-3.65	1.40	1.44
2	6-B	401	AHD	O13-C8	-3.64	1.40	1.44
2	14-B	401	AHD	O13-C8	-3.60	1.40	1.44
2	12-A	401	AHD	O13-C8	-3.59	1.40	1.44
2	16-B	401	AHD	O13-C8	-3.58	1.40	1.44
2	23-B	401	AHD	O13-C8	-3.57	1.40	1.44
2	23-A	401	AHD	O13-C8	-3.56	1.40	1.44
2	8-B	401	AHD	O13-C8	-3.56	1.40	1.44
2	4-B	401	AHD	O13-C8	-3.52	1.40	1.44
2	3-B	401	AHD	O13-C8	-3.50	1.40	1.44
2	15-A	401	AHD	O13-C8	-3.46	1.40	1.44
2	2-B	401	AHD	O13-C8	-3.44	1.40	1.44
2	22-A	401	AHD	O13-C8	-3.43	1.40	1.44
2	13-A	401	AHD	O13-C8	-3.32	1.40	1.44
2	8-A	401	AHD	O13-C8	-3.22	1.40	1.44
2	16-A	401	AHD	O13-C8	-3.21	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	18-B	401	AHD	O13-C8	-3.19	1.40	1.44
2	9-B	401	AHD	P9-O12	-3.14	1.49	1.54
2	10-B	401	AHD	P14-O15	-3.13	1.49	1.54
2	12-B	401	AHD	P9-O12	-3.10	1.49	1.54
2	22-B	401	AHD	P9-O12	-3.04	1.49	1.54
2	20-B	401	AHD	P9-O12	-3.02	1.49	1.54
2	7-B	401	AHD	P14-O15	-3.00	1.49	1.54
2	13-B	401	AHD	P9-O12	-2.98	1.49	1.54
2	11-B	401	AHD	P14-O15	-2.97	1.49	1.54
2	4-B	401	AHD	P14-O15	-2.96	1.49	1.54
2	11-B	401	AHD	P9-O12	-2.96	1.49	1.54
2	18-A	401	AHD	O13-C8	-2.96	1.41	1.44
2	6-B	401	AHD	P14-O15	-2.95	1.49	1.54
2	7-B	401	AHD	P9-O12	-2.91	1.49	1.54
2	3-B	401	AHD	P9-O10	-2.89	1.49	1.54
2	15-B	401	AHD	P14-O15	-2.85	1.49	1.54
2	23-B	401	AHD	P9-O12	-2.84	1.49	1.54
2	19-B	401	AHD	P9-O12	-2.80	1.49	1.54
2	17-B	401	AHD	P14-O15	-2.80	1.49	1.54
2	12-B	401	AHD	P14-O15	-2.80	1.49	1.54
2	22-B	401	AHD	P14-O15	-2.79	1.49	1.54
2	20-B	401	AHD	P14-O15	-2.77	1.49	1.54
2	4-B	401	AHD	P9-O10	-2.74	1.49	1.54
2	5-B	401	AHD	P14-O15	-2.74	1.49	1.54
2	3-B	401	AHD	P9-O12	-2.74	1.49	1.54
2	13-B	401	AHD	P14-O15	-2.73	1.49	1.54
2	4-A	401	AHD	O13-C8	-2.73	1.41	1.44
2	16-B	401	AHD	P9-O12	-2.72	1.49	1.54
2	18-B	401	AHD	P9-O12	-2.72	1.49	1.54
2	8-A	401	AHD	P9-O10	-2.71	1.49	1.54
2	20-B	401	AHD	P14-O16	-2.70	1.49	1.54
2	5-B	401	AHD	P9-O12	-2.69	1.49	1.54
2	14-B	401	AHD	P14-O15	-2.68	1.49	1.54
2	19-B	401	AHD	P14-O15	-2.68	1.49	1.54
2	17-B	401	AHD	P9-O12	-2.66	1.49	1.54
2	8-B	401	AHD	P9-O12	-2.65	1.49	1.54
2	2-B	401	AHD	P14-O16	-2.65	1.49	1.54
2	14-B	401	AHD	P9-O10	-2.64	1.49	1.54
2	2-B	401	AHD	P14-O15	-2.64	1.49	1.54
2	6-B	401	AHD	P9-O12	-2.63	1.49	1.54
2	8-B	401	AHD	P14-O15	-2.62	1.50	1.54
2	2-B	401	AHD	P9-O10	-2.62	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	18-B	401	AHD	P14-O15	-2.61	1.50	1.54
2	9-A	401	AHD	P9-O10	-2.60	1.50	1.54
2	23-B	401	AHD	P14-O15	-2.60	1.50	1.54
2	15-A	401	AHD	P9-O10	-2.60	1.50	1.54
2	1-B	401	AHD	P9-O10	-2.60	1.50	1.54
2	10-B	401	AHD	P14-O16	-2.60	1.50	1.54
2	23-B	401	AHD	P14-O16	-2.59	1.50	1.54
2	1-A	401	AHD	P9-O10	-2.58	1.50	1.54
2	4-B	401	AHD	P9-O12	-2.57	1.50	1.54
2	2-B	401	AHD	P9-O12	-2.57	1.50	1.54
2	10-B	401	AHD	P9-O12	-2.56	1.50	1.54
2	14-B	401	AHD	P9-O12	-2.56	1.50	1.54
2	16-B	401	AHD	P14-O15	-2.56	1.50	1.54
2	21-B	401	AHD	P14-O16	-2.55	1.50	1.54
2	18-B	401	AHD	P14-O16	-2.55	1.50	1.54
2	9-B	401	AHD	P14-O17	2.54	1.54	1.50
2	6-B	401	AHD	P14-O16	-2.54	1.50	1.54
2	3-B	401	AHD	P14-O16	-2.54	1.50	1.54
2	7-A	401	AHD	P9-O10	-2.53	1.50	1.54
2	7-A	401	AHD	P9-O12	-2.53	1.50	1.54
2	12-B	401	AHD	P14-O16	-2.53	1.50	1.54
2	2-A	401	AHD	P9-O10	-2.53	1.50	1.54
2	19-B	401	AHD	P14-O16	-2.52	1.50	1.54
2	22-B	401	AHD	P14-O16	-2.51	1.50	1.54
2	1-B	401	AHD	P14-O15	-2.51	1.50	1.54
2	10-A	401	AHD	P14-C8	2.51	1.86	1.85
2	14-A	401	AHD	P9-O10	-2.50	1.50	1.54
2	15-B	401	AHD	P9-O12	-2.49	1.50	1.54
2	21-B	401	AHD	P9-O12	-2.49	1.50	1.54
2	23-A	401	AHD	P9-O10	-2.49	1.50	1.54
2	16-A	401	AHD	P9-O10	-2.49	1.50	1.54
2	13-A	401	AHD	P9-O10	-2.48	1.50	1.54
2	21-B	401	AHD	P14-O15	-2.48	1.50	1.54
2	3-B	401	AHD	P14-O15	-2.47	1.50	1.54
2	9-B	401	AHD	P14-O15	-2.47	1.50	1.54
2	4-A	401	AHD	P9-O10	-2.47	1.50	1.54
2	5-B	401	AHD	P14-O16	-2.47	1.50	1.54
2	6-B	401	AHD	P9-O10	-2.47	1.50	1.54
2	10-A	401	AHD	P9-O10	-2.45	1.50	1.54
2	12-A	401	AHD	P9-O10	-2.45	1.50	1.54
2	17-B	401	AHD	P14-O16	-2.44	1.50	1.54
2	18-A	401	AHD	P9-O10	-2.44	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-B	401	AHD	P14-O16	-2.43	1.50	1.54
2	2-A	401	AHD	P14-C8	2.42	1.86	1.85
2	2-A	401	AHD	P14-O16	-2.42	1.50	1.54
2	8-B	401	AHD	P14-O16	-2.42	1.50	1.54
2	22-A	401	AHD	P9-O10	-2.41	1.50	1.54
2	11-B	401	AHD	P14-O16	-2.39	1.50	1.54
2	13-B	401	AHD	P14-O16	-2.39	1.50	1.54
2	15-B	401	AHD	P14-O16	-2.39	1.50	1.54
2	7-B	401	AHD	P14-O16	-2.39	1.50	1.54
2	17-A	401	AHD	P9-O10	-2.38	1.50	1.54
2	1-B	401	AHD	P9-O12	-2.38	1.50	1.54
2	17-B	401	AHD	P9-O10	-2.37	1.50	1.54
2	22-A	401	AHD	P14-O15	-2.36	1.50	1.54
2	20-A	401	AHD	P9-O10	-2.36	1.50	1.54
2	10-B	401	AHD	P9-O10	-2.35	1.50	1.54
2	5-A	401	AHD	P9-O10	-2.35	1.50	1.54
2	21-B	401	AHD	P9-O10	-2.34	1.50	1.54
2	4-B	401	AHD	P14-O16	-2.32	1.50	1.54
2	16-B	401	AHD	P14-O16	-2.31	1.50	1.54
2	6-A	401	AHD	P9-O10	-2.30	1.50	1.54
2	8-B	401	AHD	P9-O10	-2.30	1.50	1.54
2	9-A	401	AHD	P14-O16	-2.29	1.50	1.54
2	23-B	401	AHD	P9-O10	-2.28	1.50	1.54
2	17-A	401	AHD	P9-O12	-2.28	1.50	1.54
2	11-A	401	AHD	P9-O10	-2.26	1.50	1.54
2	12-B	401	AHD	P9-O10	-2.26	1.50	1.54
2	19-A	401	AHD	P9-O10	-2.23	1.50	1.54
2	17-A	401	AHD	P14-O16	-2.23	1.50	1.54
2	18-B	401	AHD	P9-O10	-2.20	1.50	1.54
2	21-A	401	AHD	P9-O10	-2.20	1.50	1.54
2	13-A	401	AHD	P14-O16	-2.19	1.50	1.54
2	16-A	401	AHD	P14-C8	2.18	1.86	1.85
2	16-A	401	AHD	P14-O16	-2.17	1.50	1.54
2	19-A	401	AHD	P14-O15	-2.15	1.50	1.54
2	13-B	401	AHD	P9-O10	-2.13	1.50	1.54
2	9-B	401	AHD	P9-O10	-2.13	1.50	1.54
2	15-A	401	AHD	P14-O16	-2.13	1.50	1.54
2	21-A	401	AHD	P14-O16	-2.12	1.50	1.54
2	22-A	401	AHD	P14-O16	-2.12	1.50	1.54
2	13-B	401	AHD	P14-C8	-2.09	1.83	1.85
2	10-A	401	AHD	P14-O16	-2.09	1.50	1.54
2	4-A	401	AHD	P9-O12	-2.08	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-A	401	AHD	P14-O16	-2.08	1.51	1.54
2	14-A	401	AHD	P14-O16	-2.07	1.51	1.54
2	6-A	401	AHD	P14-O16	-2.07	1.51	1.54
2	15-B	401	AHD	P9-O10	-2.07	1.51	1.54
2	23-A	401	AHD	P14-O16	-2.07	1.51	1.54
2	13-A	401	AHD	P14-C8	2.06	1.86	1.85
2	6-A	401	AHD	P14-C8	2.06	1.86	1.85
2	3-A	401	AHD	P9-O12	-2.03	1.51	1.54
2	16-A	401	AHD	P14-O15	-2.01	1.51	1.54

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	401	AHD	P14-C8-P9	-5.91	102.24	112.81
2	8-A	401	AHD	O10-P9-O11	-5.65	100.38	113.06
2	12-A	401	AHD	C2-C7-C8	-5.55	105.88	116.07
2	3-A	401	AHD	C2-C7-C8	-5.53	105.93	116.07
2	6-A	401	AHD	C2-C7-C8	-5.18	106.56	116.07
2	2-A	401	AHD	C2-C7-C8	-5.15	106.61	116.07
2	4-A	401	AHD	C2-C7-C8	-4.82	107.22	116.07
2	16-B	401	AHD	P14-C8-P9	-4.82	104.19	112.81
2	22-A	401	AHD	O15-P14-C8	4.59	116.47	106.17
2	23-A	401	AHD	C2-C7-C8	-4.56	107.70	116.07
2	4-A	401	AHD	P14-C8-P9	-4.50	104.75	112.81
2	18-B	401	AHD	P14-C8-P9	-4.46	104.82	112.81
2	14-A	401	AHD	C2-C7-C8	-4.41	107.98	116.07
2	1-A	401	AHD	O10-P9-C8	4.36	115.95	106.17
2	11-A	401	AHD	P14-C8-P9	-4.34	105.04	112.81
2	13-A	401	AHD	P14-C8-P9	-4.34	105.05	112.81
2	17-A	401	AHD	C7-C2-C3	-4.32	104.59	112.35
2	22-A	401	AHD	C2-C7-C8	-4.28	108.21	116.07
2	19-A	401	AHD	C2-C7-C8	-4.27	108.24	116.07
2	4-A	401	AHD	O10-P9-O11	-4.14	103.76	113.06
2	21-A	401	AHD	C2-C7-C8	-4.12	108.52	116.07
2	14-B	401	AHD	P14-C8-P9	-4.10	105.47	112.81
2	5-A	401	AHD	C2-C7-C8	-4.06	108.61	116.07
2	16-B	401	AHD	C2-C7-C8	-3.96	108.79	116.07
2	16-A	401	AHD	O15-P14-C8	3.95	115.03	106.17
2	20-A	401	AHD	P14-C8-P9	-3.92	105.80	112.81
2	3-B	401	AHD	C2-C7-C8	-3.90	108.91	116.07
2	9-B	401	AHD	P14-C8-P9	-3.83	105.95	112.81
2	8-A	401	AHD	P14-C8-P9	-3.80	106.01	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-A	401	AHD	P14-C8-P9	-3.80	106.01	112.81
2	16-A	401	AHD	O10-P9-C8	3.79	114.68	106.17
2	12-B	401	AHD	C2-C7-C8	-3.78	109.13	116.07
2	9-A	401	AHD	O10-P9-C8	3.78	114.64	106.17
2	8-A	401	AHD	C2-C7-C8	-3.70	109.28	116.07
2	15-A	401	AHD	O10-P9-C8	3.69	114.43	106.17
2	1-A	401	AHD	O15-P14-C8	3.68	114.41	106.17
2	8-B	401	AHD	C2-C7-C8	-3.67	109.34	116.07
2	13-B	401	AHD	P14-C8-P9	-3.62	106.32	112.81
2	19-B	401	AHD	C2-C7-C8	-3.62	109.42	116.07
2	12-B	401	AHD	P14-C8-P9	-3.61	106.35	112.81
2	18-A	401	AHD	O10-P9-O11	-3.60	104.98	113.06
2	7-B	401	AHD	P14-C8-P9	-3.58	106.40	112.81
2	18-A	401	AHD	P14-C8-P9	-3.57	106.42	112.81
2	19-B	401	AHD	P14-C8-P9	-3.57	106.42	112.81
2	17-A	401	AHD	O10-P9-O11	-3.57	105.05	113.06
2	18-A	401	AHD	C2-C7-C8	-3.56	109.54	116.07
2	22-B	401	AHD	P14-C8-P9	-3.52	106.51	112.81
2	13-A	401	AHD	O10-P9-O11	-3.50	105.20	113.06
2	17-B	401	AHD	C2-C7-C8	-3.46	109.72	116.07
2	7-B	401	AHD	C2-C7-C8	-3.45	109.73	116.07
2	4-B	401	AHD	P14-C8-P9	-3.40	106.72	112.81
2	17-A	401	AHD	O10-P9-C8	3.40	113.79	106.17
2	15-A	401	AHD	C2-C7-C8	-3.39	109.84	116.07
2	4-B	401	AHD	O16-P14-C8	3.39	113.76	106.17
2	7-A	401	AHD	O10-P9-O11	-3.36	105.52	113.06
2	8-A	401	AHD	O10-P9-C8	3.36	113.69	106.17
2	11-B	401	AHD	P14-C8-P9	-3.32	106.86	112.81
2	23-B	401	AHD	P14-C8-P9	-3.30	106.90	112.81
2	21-A	401	AHD	O10-P9-O11	-3.30	105.65	113.06
2	1-B	401	AHD	P14-C8-P9	-3.29	106.93	112.81
2	5-B	401	AHD	P14-C8-P9	-3.28	106.94	112.81
2	9-B	401	AHD	C2-C7-C8	-3.27	110.07	116.07
2	22-B	401	AHD	C2-C7-C8	-3.25	110.11	116.07
2	11-A	401	AHD	C2-C7-C8	-3.24	110.12	116.07
2	4-A	401	AHD	O10-P9-C8	3.23	113.42	106.17
2	10-B	401	AHD	C2-C7-C8	-3.21	110.17	116.07
2	11-A	401	AHD	O10-P9-O11	-3.20	105.87	113.06
2	2-A	401	AHD	O15-P14-C8	3.18	113.31	106.17
2	6-A	401	AHD	P14-C8-P9	-3.16	107.16	112.81
2	9-A	401	AHD	C7-C2-C3	-3.13	106.72	112.35
2	3-B	401	AHD	P14-C8-P9	-3.13	107.21	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	401	AHD	O15-P14-C8	3.09	113.11	106.17
2	20-A	401	AHD	O10-P9-O11	-3.09	106.12	113.06
2	9-A	401	AHD	C2-C7-C8	-3.07	110.43	116.07
2	3-A	401	AHD	P14-C8-P9	-3.07	107.32	112.81
2	23-A	401	AHD	O10-P9-O11	-3.04	106.22	113.06
2	17-A	401	AHD	P9-C8-O13	3.03	114.18	107.30
2	15-B	401	AHD	P14-C8-P9	-3.02	107.40	112.81
2	8-A	401	AHD	P9-C8-O13	3.01	114.14	107.30
2	5-A	401	AHD	O15-P14-C8	2.98	112.86	106.17
2	23-B	401	AHD	O16-P14-C8	2.98	112.86	106.17
2	8-B	401	AHD	P14-C8-P9	-2.98	107.49	112.81
2	16-A	401	AHD	P14-C8-P9	-2.97	107.49	112.81
2	8-A	401	AHD	O15-P14-C8	2.97	112.82	106.17
2	13-A	401	AHD	O15-P14-C8	2.96	112.81	106.17
2	13-B	401	AHD	O16-P14-C8	2.95	112.79	106.17
2	20-B	401	AHD	C2-C7-C8	-2.95	110.66	116.07
2	23-B	401	AHD	C2-C7-C8	-2.93	110.68	116.07
2	16-A	401	AHD	O10-P9-O11	-2.92	106.49	113.06
2	1-B	401	AHD	C2-C7-C8	-2.91	110.72	116.07
2	21-B	401	AHD	O16-P14-C8	2.91	112.69	106.17
2	18-A	401	AHD	O17-P14-C8	-2.91	102.25	109.86
2	23-A	401	AHD	P14-C8-P9	-2.90	107.62	112.81
2	21-B	401	AHD	C2-C7-C8	-2.90	110.75	116.07
2	5-B	401	AHD	C2-C7-C8	-2.88	110.78	116.07
2	18-B	401	AHD	C2-C7-C8	-2.87	110.80	116.07
2	8-A	401	AHD	O12-P9-C8	2.87	112.60	106.17
2	6-B	401	AHD	O16-P14-C8	2.87	112.60	106.17
2	13-B	401	AHD	C2-C7-C8	-2.84	110.86	116.07
2	2-B	401	AHD	C2-C7-C8	-2.83	110.88	116.07
2	14-B	401	AHD	C2-C7-C8	-2.82	110.89	116.07
2	9-B	401	AHD	O16-P14-O17	-2.82	106.72	113.06
2	3-A	401	AHD	O15-P14-C8	2.81	112.46	106.17
2	21-A	401	AHD	O15-P14-C8	2.80	112.45	106.17
2	11-B	401	AHD	C2-C7-C8	-2.79	110.94	116.07
2	7-A	401	AHD	C2-C7-C8	-2.78	110.96	116.07
2	2-B	401	AHD	O16-P14-C8	2.77	112.39	106.17
2	21-A	401	AHD	O17-P14-C8	-2.73	102.71	109.86
2	17-A	401	AHD	O15-P14-C8	2.73	112.29	106.17
2	20-A	401	AHD	C7-C2-C3	-2.73	107.45	112.35
2	21-A	401	AHD	O10-P9-C8	2.73	112.28	106.17
2	21-B	401	AHD	O16-P14-O17	-2.72	106.94	113.06
2	17-A	401	AHD	P14-C8-P9	-2.70	107.97	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-B	401	AHD	O16-P14-C8	2.69	112.20	106.17
2	12-B	401	AHD	O16-P14-O17	-2.69	107.03	113.06
2	19-A	401	AHD	O10-P9-C8	2.65	112.12	106.17
2	3-B	401	AHD	O16-P14-C8	2.65	112.11	106.17
2	15-B	401	AHD	C2-C7-C8	-2.64	111.22	116.07
2	20-B	401	AHD	O16-P14-O17	-2.64	107.14	113.06
2	13-A	401	AHD	C2-C7-C8	-2.63	111.24	116.07
2	4-B	401	AHD	C2-C7-C8	-2.63	111.24	116.07
2	15-A	401	AHD	O15-P14-C8	2.63	112.07	106.17
2	4-A	401	AHD	O17-P14-C8	-2.61	103.02	109.86
2	8-B	401	AHD	O16-P14-O17	-2.60	107.21	113.06
2	6-B	401	AHD	C2-C7-C8	-2.60	111.31	116.07
2	16-B	401	AHD	O16-P14-O17	-2.59	107.24	113.06
2	14-B	401	AHD	O16-P14-O17	-2.57	107.28	113.06
2	14-A	401	AHD	P14-C8-P9	-2.57	108.21	112.81
2	3-A	401	AHD	O10-P9-O11	-2.57	107.29	113.06
2	10-B	401	AHD	C7-C2-C3	-2.56	107.75	112.35
2	2-A	401	AHD	O10-P9-C8	2.56	111.91	106.17
2	5-A	401	AHD	O10-P9-C8	2.56	111.91	106.17
2	6-A	401	AHD	O15-P14-C8	2.55	111.89	106.17
2	13-A	401	AHD	C7-C2-C3	-2.54	107.78	112.35
2	23-B	401	AHD	O16-P14-O17	-2.54	107.34	113.06
2	17-B	401	AHD	O16-P14-C8	2.54	111.86	106.17
2	11-B	401	AHD	O16-P14-C8	2.53	111.83	106.17
2	19-B	401	AHD	O16-P14-C8	2.51	111.80	106.17
2	10-A	401	AHD	C2-C7-C8	-2.51	111.46	116.07
2	5-B	401	AHD	O16-P14-C8	2.51	111.80	106.17
2	1-B	401	AHD	O16-P14-O17	-2.51	107.42	113.06
2	20-B	401	AHD	P14-C8-P9	-2.51	108.32	112.81
2	18-B	401	AHD	O16-P14-C8	2.50	111.77	106.17
2	3-B	401	AHD	O16-P14-O17	-2.50	107.44	113.06
2	2-B	401	AHD	O16-P14-O17	-2.48	107.48	113.06
2	22-B	401	AHD	O16-P14-C8	2.48	111.74	106.17
2	4-B	401	AHD	O16-P14-O17	-2.45	107.55	113.06
2	9-A	401	AHD	O15-P14-C8	2.44	111.65	106.17
2	18-B	401	AHD	O16-P14-O17	-2.44	107.58	113.06
2	20-A	401	AHD	O10-P9-C8	2.43	111.62	106.17
2	5-B	401	AHD	O16-P14-O17	-2.43	107.60	113.06
2	11-A	401	AHD	O17-P14-C8	-2.43	103.51	109.86
2	12-A	401	AHD	O10-P9-O11	-2.42	107.62	113.06
2	1-B	401	AHD	O16-P14-C8	2.42	111.59	106.17
2	10-B	401	AHD	O16-P14-O17	-2.41	107.65	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	16-B	401	AHD	O10-P9-O12	2.40	114.76	107.99
2	16-A	401	AHD	P9-C8-O13	2.39	112.72	107.30
2	22-A	401	AHD	O10-P9-O11	-2.38	107.70	113.06
2	12-A	401	AHD	P14-C8-P9	-2.38	108.55	112.81
2	17-B	401	AHD	O16-P14-O17	-2.38	107.72	113.06
2	15-B	401	AHD	C7-C2-C3	-2.38	108.08	112.35
2	4-A	401	AHD	O10-P9-O12	2.37	114.67	107.99
2	20-A	401	AHD	O15-P14-C8	2.36	111.46	106.17
2	7-B	401	AHD	O16-P14-O17	-2.35	107.78	113.06
2	23-A	401	AHD	O15-P14-C8	2.32	111.38	106.17
2	20-A	401	AHD	O15-P14-O17	-2.32	107.84	113.06
2	10-B	401	AHD	P14-C8-P9	-2.30	108.70	112.81
2	21-A	401	AHD	P14-C8-P9	-2.29	108.70	112.81
2	11-A	401	AHD	C7-C2-C3	-2.27	108.27	112.35
2	19-B	401	AHD	O16-P14-O17	-2.27	107.95	113.06
2	14-B	401	AHD	O16-P14-C8	2.27	111.26	106.17
2	18-A	401	AHD	O10-P9-C8	2.27	111.25	106.17
2	6-A	401	AHD	O10-P9-O11	-2.26	107.98	113.06
2	11-B	401	AHD	O10-P9-O12	2.25	114.35	107.99
2	9-B	401	AHD	O16-P14-C8	2.25	111.22	106.17
2	10-A	401	AHD	P14-C8-P9	-2.25	108.78	112.81
2	15-A	401	AHD	O10-P9-O11	-2.24	108.03	113.06
2	9-A	401	AHD	O10-P9-O11	-2.23	108.04	113.06
2	15-B	401	AHD	O16-P14-O17	-2.23	108.04	113.06
2	23-A	401	AHD	O17-P14-C8	-2.23	104.03	109.86
2	8-A	401	AHD	O15-P14-O17	-2.22	108.07	113.06
2	1-A	401	AHD	P14-C8-P9	-2.22	108.84	112.81
2	1-A	401	AHD	O10-P9-O11	-2.20	108.11	113.06
2	2-B	401	AHD	P14-C8-P9	-2.20	108.88	112.81
2	22-B	401	AHD	O10-P9-O12	2.19	114.17	107.99
2	2-A	401	AHD	P14-C8-P9	-2.19	108.89	112.81
2	7-B	401	AHD	O10-P9-O12	2.18	114.15	107.99
2	20-B	401	AHD	O16-P14-C8	2.16	111.01	106.17
2	9-B	401	AHD	O12-P9-O11	-2.16	108.21	113.06
2	18-A	401	AHD	C7-C2-C3	-2.15	108.49	112.35
2	21-B	401	AHD	P14-C8-P9	-2.14	108.97	112.81
2	18-A	401	AHD	O15-P14-C8	2.14	110.97	106.17
2	8-B	401	AHD	O16-P14-C8	2.14	110.97	106.17
2	16-B	401	AHD	O16-P14-C8	2.14	110.96	106.17
2	17-B	401	AHD	P14-C8-P9	-2.13	109.01	112.81
2	9-A	401	AHD	P9-C8-O13	2.12	112.12	107.30
2	11-B	401	AHD	O16-P14-O17	-2.11	108.33	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-A	401	AHD	O12-P9-C8	2.10	110.88	106.17
2	15-B	401	AHD	O16-P14-C8	2.07	110.82	106.17
2	13-B	401	AHD	P9-C8-O13	2.07	112.02	107.30
2	12-A	401	AHD	O15-P14-C8	2.07	110.80	106.17
2	1-A	401	AHD	P9-C8-O13	2.06	111.99	107.30
2	19-A	401	AHD	O10-P9-O11	-2.06	108.44	113.06
2	15-A	401	AHD	C7-C2-C3	-2.04	108.69	112.35
2	19-B	401	AHD	O10-P9-O12	2.03	113.71	107.99
2	4-A	401	AHD	O15-P14-C8	2.02	110.71	106.17
2	21-B	401	AHD	O17-P14-C8	-2.02	104.59	109.86

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	401	AHD	C2-C7-C8-P9
2	1-A	401	AHD	C2-C7-C8-P14
2	1-A	401	AHD	C2-C7-C8-O13
2	4-A	401	AHD	C2-C7-C8-P9
2	5-A	401	AHD	C2-C7-C8-P9
2	5-A	401	AHD	C2-C7-C8-P14
2	5-A	401	AHD	C2-C7-C8-O13
2	7-A	401	AHD	C2-C7-C8-P9
2	7-A	401	AHD	C2-C7-C8-P14
2	7-A	401	AHD	C2-C7-C8-O13
2	7-A	401	AHD	O13-C8-P9-O11
2	10-A	401	AHD	C2-C7-C8-P9
2	10-A	401	AHD	C2-C7-C8-P14
2	10-A	401	AHD	C2-C7-C8-O13
2	12-A	401	AHD	C7-C8-P14-O17
2	12-A	401	AHD	P9-C8-P14-O17
2	15-A	401	AHD	C2-C7-C8-P9
2	15-A	401	AHD	C2-C7-C8-P14
2	15-A	401	AHD	C2-C7-C8-O13
2	15-A	401	AHD	C7-C8-P14-O17
2	16-A	401	AHD	C2-C7-C8-P14
2	16-A	401	AHD	C2-C7-C8-O13
2	18-A	401	AHD	C2-C7-C8-P9
2	18-A	401	AHD	C2-C7-C8-P14
2	18-A	401	AHD	C2-C7-C8-O13
2	18-A	401	AHD	C7-C8-P14-O17
2	22-A	401	AHD	C2-C7-C8-P14

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Mol	Chain	Res	Type	Atoms
2	22-A	401	AHD	C2-C7-C8-O13
2	23-A	401	AHD	C2-C7-C8-P9
2	23-A	401	AHD	C2-C7-C8-P14
2	23-A	401	AHD	C2-C7-C8-O13
2	2-A	401	AHD	C3-C2-C7-C8
2	5-A	401	AHD	C3-C2-C7-C8
2	8-A	401	AHD	C3-C2-C7-C8
2	10-A	401	AHD	C3-C2-C7-C8
2	15-A	401	AHD	C3-C2-C7-C8
2	2-A	401	AHD	C2-C7-C8-P9
2	2-A	401	AHD	C2-C7-C8-P14
2	4-A	401	AHD	C2-C7-C8-P14
2	11-A	401	AHD	C2-C7-C8-P9
2	11-A	401	AHD	C2-C7-C8-P14
2	14-A	401	AHD	C2-C7-C8-P9
2	14-A	401	AHD	C2-C7-C8-P14
2	16-A	401	AHD	C2-C7-C8-P9
2	19-A	401	AHD	C2-C7-C8-P9
2	19-A	401	AHD	C2-C7-C8-P14
2	21-A	401	AHD	C2-C7-C8-P9
2	21-A	401	AHD	C2-C7-C8-P14
2	22-A	401	AHD	C2-C7-C8-P9
2	2-B	401	AHD	C2-C7-C8-P9
2	11-B	401	AHD	C2-C7-C8-P9
2	12-B	401	AHD	C2-C7-C8-P9
2	21-B	401	AHD	C2-C7-C8-P9
2	12-A	401	AHD	P9-C8-P14-O15
2	21-A	401	AHD	C3-C2-C7-C8
2	1-A	401	AHD	C7-C2-C3-N4
2	4-A	401	AHD	C7-C2-C3-N4
2	16-A	401	AHD	C7-C2-C3-N4
2	8-A	401	AHD	C7-C8-P14-O15
2	12-A	401	AHD	C7-C8-P14-O15
2	18-A	401	AHD	C7-C8-P14-O15
2	2-A	401	AHD	C2-C7-C8-O13
2	3-A	401	AHD	C2-C7-C8-O13
2	4-A	401	AHD	C2-C7-C8-O13
2	9-A	401	AHD	C2-C7-C8-P9
2	9-A	401	AHD	C2-C7-C8-P14
2	9-A	401	AHD	C2-C7-C8-O13
2	11-A	401	AHD	C2-C7-C8-O13
2	12-A	401	AHD	C2-C7-C8-O13

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Mol	Chain	Res	Type	Atoms
2	14-A	401	AHD	C2-C7-C8-O13
2	17-A	401	AHD	C2-C7-C8-O13
2	19-A	401	AHD	C2-C7-C8-O13
2	21-A	401	AHD	C2-C7-C8-O13
2	1-B	401	AHD	C2-C7-C8-O13
2	2-B	401	AHD	C2-C7-C8-P14
2	2-B	401	AHD	C2-C7-C8-O13
2	4-B	401	AHD	C2-C7-C8-P9
2	4-B	401	AHD	C2-C7-C8-O13
2	5-B	401	AHD	C2-C7-C8-P9
2	5-B	401	AHD	C2-C7-C8-O13
2	6-B	401	AHD	C2-C7-C8-O13
2	7-B	401	AHD	C2-C7-C8-O13
2	8-B	401	AHD	C2-C7-C8-P9
2	8-B	401	AHD	C2-C7-C8-O13
2	9-B	401	AHD	C2-C7-C8-O13
2	10-B	401	AHD	C2-C7-C8-P9
2	10-B	401	AHD	C2-C7-C8-O13
2	11-B	401	AHD	C2-C7-C8-P14
2	11-B	401	AHD	C2-C7-C8-O13
2	12-B	401	AHD	C2-C7-C8-P14
2	12-B	401	AHD	C2-C7-C8-O13
2	13-B	401	AHD	C2-C7-C8-O13
2	14-B	401	AHD	C2-C7-C8-O13
2	16-B	401	AHD	C2-C7-C8-O13
2	17-B	401	AHD	C2-C7-C8-O13
2	18-B	401	AHD	C2-C7-C8-P9
2	18-B	401	AHD	C2-C7-C8-P14
2	18-B	401	AHD	C2-C7-C8-O13
2	19-B	401	AHD	C2-C7-C8-O13
2	20-B	401	AHD	C2-C7-C8-O13
2	21-B	401	AHD	C2-C7-C8-O13
2	22-B	401	AHD	C2-C7-C8-O13
2	23-B	401	AHD	C2-C7-C8-O13
2	7-A	401	AHD	C7-C8-P9-O11
2	7-A	401	AHD	P14-C8-P9-O11
2	8-A	401	AHD	C7-C8-P14-O17
2	8-A	401	AHD	P9-C8-P14-O15
2	8-A	401	AHD	O13-C8-P14-O15
2	12-A	401	AHD	P9-C8-P14-O16
2	12-A	401	AHD	O13-C8-P14-O15
2	13-A	401	AHD	C7-C8-P14-O17

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Mol	Chain	Res	Type	Atoms
2	14-A	401	AHD	C7-C8-P14-O17
2	18-A	401	AHD	P9-C8-P14-O15
2	18-A	401	AHD	P9-C8-P14-O17
2	18-A	401	AHD	O13-C8-P14-O15
2	2-A	401	AHD	C7-C2-C3-N4
2	21-A	401	AHD	C7-C2-C3-N4
2	22-A	401	AHD	C7-C2-C3-N4
2	13-A	401	AHD	C3-C2-C7-C8
2	13-A	401	AHD	C7-C2-C3-N4
2	5-A	401	AHD	C7-C2-C3-N4
2	23-A	401	AHD	C7-C2-C3-N4
2	17-A	401	AHD	C2-C7-C8-P14
2	4-B	401	AHD	C2-C7-C8-P14
2	5-B	401	AHD	C2-C7-C8-P14
2	8-B	401	AHD	C2-C7-C8-P14
2	9-B	401	AHD	C2-C7-C8-P14
2	13-B	401	AHD	C2-C7-C8-P14
2	19-B	401	AHD	C2-C7-C8-P9
2	19-B	401	AHD	C2-C7-C8-P14
2	21-B	401	AHD	C2-C7-C8-P14
2	22-B	401	AHD	C2-C7-C8-P9
2	22-B	401	AHD	C2-C7-C8-P14
2	6-A	401	AHD	P9-C8-P14-O15
2	15-A	401	AHD	P9-C8-P14-O15
2	18-A	401	AHD	P9-C8-P14-O16
2	4-A	401	AHD	C7-C8-P14-O15
2	5-A	401	AHD	C7-C8-P14-O15
2	7-A	401	AHD	C7-C8-P9-O12
2	12-A	401	AHD	C7-C8-P14-O16
2	13-A	401	AHD	C7-C8-P14-O15
2	14-A	401	AHD	C7-C8-P14-O15
2	15-A	401	AHD	C7-C8-P14-O15
2	15-A	401	AHD	C7-C8-P14-O16
2	16-A	401	AHD	C7-C8-P14-O15
2	19-A	401	AHD	C7-C8-P14-O15
2	22-A	401	AHD	C7-C8-P14-O15
2	23-A	401	AHD	C7-C8-P14-O15
2	15-A	401	AHD	C7-C2-C3-N4
2	1-B	401	AHD	C2-C7-C8-P14
2	6-B	401	AHD	C2-C7-C8-P14
2	7-B	401	AHD	C2-C7-C8-P14
2	10-B	401	AHD	C2-C7-C8-P14

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Mol	Chain	Res	Type	Atoms
2	14-B	401	AHD	C2-C7-C8-P14
2	16-B	401	AHD	C2-C7-C8-P14
2	17-B	401	AHD	C2-C7-C8-P14
2	23-B	401	AHD	C2-C7-C8-P14
2	6-A	401	AHD	P9-C8-P14-O17
2	8-A	401	AHD	P9-C8-P14-O17
2	8-A	401	AHD	O13-C8-P14-O16
2	10-A	401	AHD	O13-C8-P9-O11
2	12-A	401	AHD	O13-C8-P14-O16
2	14-A	401	AHD	P9-C8-P14-O15
2	14-A	401	AHD	P9-C8-P14-O17
2	15-A	401	AHD	P9-C8-P14-O17
2	18-A	401	AHD	O13-C8-P14-O16
2	20-A	401	AHD	C7-C8-P9-O11
2	20-A	401	AHD	O13-C8-P9-O11
2	22-A	401	AHD	C7-C8-P14-O17

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	1-A	283/318 (88%)	0.94	39 (13%) 8 8	1, 1, 2, 2	283 (100%)
1	1-B	296/318 (93%)	0.68	27 (9%) 16 17	1, 1, 2, 2	296 (100%)
1	2-A	0/318	-	-	-	-
1	2-B	0/318	-	-	-	-
1	3-A	0/318	-	-	-	-
1	3-B	0/318	-	-	-	-
1	4-A	0/318	-	-	-	-
1	4-B	0/318	-	-	-	-
1	5-A	0/318	-	-	-	-
1	5-B	0/318	-	-	-	-
1	6-A	0/318	-	-	-	-
1	6-B	0/318	-	-	-	-
1	7-A	0/318	-	-	-	-
1	7-B	0/318	-	-	-	-
1	8-A	0/318	-	-	-	-
1	8-B	0/318	-	-	-	-
1	9-A	0/318	-	-	-	-
1	9-B	0/318	-	-	-	-
1	10-A	0/318	-	-	-	-
1	10-B	0/318	-	-	-	-
1	11-A	0/318	-	-	-	-
1	11-B	0/318	-	-	-	-
1	12-A	0/318	-	-	-	-
1	12-B	0/318	-	-	-	-
1	13-A	0/318	-	-	-	-
1	13-B	0/318	-	-	-	-
1	14-A	0/318	-	-	-	-
1	14-B	0/318	-	-	-	-
1	15-A	0/318	-	-	-	-
1	15-B	0/318	-	-	-	-
1	16-A	0/318	-	-	-	-
1	16-B	0/318	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	17-A	0/318	-	-	-	-
1	17-B	0/318	-	-	-	-
1	18-A	0/318	-	-	-	-
1	18-B	0/318	-	-	-	-
1	19-A	0/318	-	-	-	-
1	19-B	0/318	-	-	-	-
1	20-A	0/318	-	-	-	-
1	20-B	0/318	-	-	-	-
1	21-A	0/318	-	-	-	-
1	21-B	0/318	-	-	-	-
1	22-A	0/318	-	-	-	-
1	22-B	0/318	-	-	-	-
1	23-A	0/318	-	-	-	-
1	23-B	0/318	-	-	-	-
All	All	579/14628 (3%)	0.81	66 (11%) 11 12	1, 1, 2, 2	579 (100%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	158	ASP	6.9
1	1-B	13	ILE	6.9
1	1-B	14	GLY	6.5
1	1-A	49	ALA	5.5
1	1-A	298	ALA	5.1
1	1-B	307	GLN	4.6
1	1-B	15	ARG	4.4
1	1-B	301	ASP	4.1
1	1-A	297	THR	4.1
1	1-B	305	ARG	4.0
1	1-B	302	VAL	3.6
1	1-A	68	THR	3.5
1	1-A	48	ASP	3.4
1	1-A	295	TYR	3.2
1	1-B	158	ASP	3.1
1	1-A	69	VAL	3.1
1	1-A	77	TYR	3.1
1	1-A	106	THR	3.0
1	1-A	103	ASN	3.0
1	1-A	71	ASP	3.0
1	1-B	298	ALA	3.0
1	1-A	76	SER	2.9
1	1-B	297	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-B	299	VAL	2.9
1	1-A	60	ALA	2.9
1	1-A	16	SER	2.9
1	1-A	42	THR	2.8
1	1-A	47	THR	2.8
1	1-A	115	ALA	2.8
1	1-B	250	LYS	2.7
1	1-B	244	SER	2.7
1	1-B	308	ALA	2.7
1	1-A	62	VAL	2.6
1	1-B	45	GLU	2.6
1	1-B	42	THR	2.6
1	1-A	246	GLU	2.6
1	1-A	159	SER	2.4
1	1-B	304	SER	2.4
1	1-A	75	ILE	2.4
1	1-A	66	GLY	2.4
1	1-A	74	TRP	2.4
1	1-B	113	ASP	2.4
1	1-A	105	VAL	2.4
1	1-A	88	ARG	2.4
1	1-A	22	LEU	2.4
1	1-A	107	PHE	2.4
1	1-A	116	LEU	2.3
1	1-A	61	ALA	2.3
1	1-A	54	VAL	2.3
1	1-B	296	LYS	2.3
1	1-A	73	ARG	2.3
1	1-B	61	ALA	2.3
1	1-B	137	GLU	2.2
1	1-A	78	VAL	2.2
1	1-B	306	ILE	2.2
1	1-A	51	LEU	2.2
1	1-A	67	LYS	2.2
1	1-B	295	TYR	2.2
1	1-B	88	ARG	2.2
1	1-A	44	VAL	2.1
1	1-A	296	LYS	2.1
1	1-A	52	ARG	2.1
1	1-A	226	ASP	2.1
1	1-B	115	ALA	2.1
1	1-B	28	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	251	GLU	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	1-B	403	1/1	0.63	0.13	31,31,31,31	1
2	AHD	2-A	401	14/14	-	-	32,33,34,35	14
2	AHD	3-A	401	14/14	-	-	32,33,34,35	14
2	AHD	4-A	401	14/14	-	-	32,33,34,35	14
2	AHD	5-A	401	14/14	-	-	32,33,34,35	14
2	AHD	6-A	401	14/14	-	-	32,33,34,35	14
2	AHD	7-A	401	14/14	-	-	32,33,34,35	14
2	AHD	8-A	401	14/14	-	-	32,33,34,35	14
2	AHD	9-A	401	14/14	-	-	32,33,34,35	14
2	AHD	10-A	401	14/14	-	-	32,33,34,35	14
2	AHD	11-A	401	14/14	-	-	32,33,34,35	14
2	AHD	12-A	401	14/14	-	-	32,33,34,35	14
2	AHD	13-A	401	14/14	-	-	32,33,34,35	14
2	AHD	14-A	401	14/14	-	-	32,33,34,35	14
2	AHD	15-A	401	14/14	-	-	32,33,34,35	14
2	AHD	16-A	401	14/14	-	-	32,33,34,35	14
2	AHD	17-A	401	14/14	-	-	32,33,34,35	14
2	AHD	18-A	401	14/14	-	-	32,33,34,35	14
2	AHD	19-A	401	14/14	-	-	32,33,34,35	14
2	AHD	20-A	401	14/14	-	-	32,33,34,35	14
2	AHD	21-A	401	14/14	-	-	32,33,34,35	14
2	AHD	22-A	401	14/14	-	-	32,33,34,35	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AHD	23-A	401	14/14	-	-	32,33,34,35	14
3	MG	1-A	404	1/1	0.69	0.14	32,32,32,32	1
2	AHD	2-B	401	14/14	-	-	30,31,32,32	14
2	AHD	3-B	401	14/14	-	-	30,31,32,32	14
2	AHD	4-B	401	14/14	-	-	30,31,32,32	14
2	AHD	5-B	401	14/14	-	-	30,31,32,32	14
2	AHD	6-B	401	14/14	-	-	30,31,32,32	14
2	AHD	7-B	401	14/14	-	-	30,31,32,32	14
2	AHD	8-B	401	14/14	-	-	30,31,32,32	14
2	AHD	9-B	401	14/14	-	-	30,31,32,32	14
2	AHD	10-B	401	14/14	-	-	30,31,32,32	14
2	AHD	11-B	401	14/14	-	-	30,31,32,32	14
2	AHD	12-B	401	14/14	-	-	30,31,32,32	14
2	AHD	13-B	401	14/14	-	-	30,31,32,32	14
2	AHD	14-B	401	14/14	-	-	30,31,32,32	14
2	AHD	15-B	401	14/14	-	-	30,31,32,32	14
2	AHD	16-B	401	14/14	-	-	30,31,32,32	14
2	AHD	17-B	401	14/14	-	-	30,31,32,32	14
2	AHD	18-B	401	14/14	-	-	30,31,32,32	14
2	AHD	19-B	401	14/14	-	-	30,31,32,32	14
2	AHD	20-B	401	14/14	-	-	30,31,32,32	14
2	AHD	21-B	401	14/14	-	-	30,31,32,32	14
2	AHD	22-B	401	14/14	-	-	30,31,32,32	14
2	AHD	23-B	401	14/14	-	-	30,31,32,32	14
3	MG	1-B	402	1/1	0.72	0.12	32,32,32,32	1
3	MG	2-A	402	1/1	-	-	34,34,34,34	1
3	MG	3-A	402	1/1	-	-	34,34,34,34	1
3	MG	4-A	402	1/1	-	-	34,34,34,34	1
3	MG	5-A	402	1/1	-	-	34,34,34,34	1
3	MG	6-A	402	1/1	-	-	34,34,34,34	1
3	MG	7-A	402	1/1	-	-	34,34,34,34	1
3	MG	8-A	402	1/1	-	-	34,34,34,34	1
3	MG	9-A	402	1/1	-	-	34,34,34,34	1
3	MG	10-A	402	1/1	-	-	34,34,34,34	1
3	MG	11-A	402	1/1	-	-	34,34,34,34	1
3	MG	12-A	402	1/1	-	-	34,34,34,34	1
3	MG	13-A	402	1/1	-	-	34,34,34,34	1
3	MG	14-A	402	1/1	-	-	34,34,34,34	1
3	MG	15-A	402	1/1	-	-	34,34,34,34	1
3	MG	16-A	402	1/1	-	-	34,34,34,34	1
3	MG	17-A	402	1/1	-	-	34,34,34,34	1
3	MG	18-A	402	1/1	-	-	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	19-A	402	1/1	-	-	34,34,34,34	1
3	MG	20-A	402	1/1	-	-	34,34,34,34	1
3	MG	21-A	402	1/1	-	-	34,34,34,34	1
3	MG	22-A	402	1/1	-	-	34,34,34,34	1
3	MG	23-A	402	1/1	-	-	34,34,34,34	1
3	MG	1-A	402	1/1	0.72	0.10	34,34,34,34	1
3	MG	2-A	403	1/1	-	-	34,34,34,34	1
3	MG	3-A	403	1/1	-	-	34,34,34,34	1
3	MG	4-A	403	1/1	-	-	34,34,34,34	1
3	MG	5-A	403	1/1	-	-	34,34,34,34	1
3	MG	6-A	403	1/1	-	-	34,34,34,34	1
3	MG	7-A	403	1/1	-	-	34,34,34,34	1
3	MG	8-A	403	1/1	-	-	34,34,34,34	1
3	MG	9-A	403	1/1	-	-	34,34,34,34	1
3	MG	10-A	403	1/1	-	-	34,34,34,34	1
3	MG	11-A	403	1/1	-	-	34,34,34,34	1
3	MG	12-A	403	1/1	-	-	34,34,34,34	1
3	MG	13-A	403	1/1	-	-	34,34,34,34	1
3	MG	14-A	403	1/1	-	-	34,34,34,34	1
3	MG	15-A	403	1/1	-	-	34,34,34,34	1
3	MG	16-A	403	1/1	-	-	34,34,34,34	1
3	MG	17-A	403	1/1	-	-	34,34,34,34	1
3	MG	18-A	403	1/1	-	-	34,34,34,34	1
3	MG	19-A	403	1/1	-	-	34,34,34,34	1
3	MG	20-A	403	1/1	-	-	34,34,34,34	1
3	MG	21-A	403	1/1	-	-	34,34,34,34	1
3	MG	22-A	403	1/1	-	-	34,34,34,34	1
3	MG	23-A	403	1/1	-	-	34,34,34,34	1
3	MG	1-A	403	1/1	0.79	0.10	34,34,34,34	1
3	MG	2-A	404	1/1	-	-	32,32,32,32	1
3	MG	3-A	404	1/1	-	-	32,32,32,32	1
3	MG	4-A	404	1/1	-	-	32,32,32,32	1
3	MG	5-A	404	1/1	-	-	32,32,32,32	1
3	MG	6-A	404	1/1	-	-	32,32,32,32	1
3	MG	7-A	404	1/1	-	-	32,32,32,32	1
3	MG	8-A	404	1/1	-	-	32,32,32,32	1
3	MG	9-A	404	1/1	-	-	32,32,32,32	1
3	MG	10-A	404	1/1	-	-	32,32,32,32	1
3	MG	11-A	404	1/1	-	-	32,32,32,32	1
3	MG	12-A	404	1/1	-	-	32,32,32,32	1
3	MG	13-A	404	1/1	-	-	32,32,32,32	1
3	MG	14-A	404	1/1	-	-	32,32,32,32	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	15-A	404	1/1	-	-	32,32,32,32	1
3	MG	16-A	404	1/1	-	-	32,32,32,32	1
3	MG	17-A	404	1/1	-	-	32,32,32,32	1
3	MG	18-A	404	1/1	-	-	32,32,32,32	1
3	MG	19-A	404	1/1	-	-	32,32,32,32	1
3	MG	20-A	404	1/1	-	-	32,32,32,32	1
3	MG	21-A	404	1/1	-	-	32,32,32,32	1
3	MG	22-A	404	1/1	-	-	32,32,32,32	1
3	MG	23-A	404	1/1	-	-	32,32,32,32	1
2	AHD	1-A	401	14/14	0.91	0.10	32,33,34,35	14
3	MG	2-B	402	1/1	-	-	32,32,32,32	1
3	MG	3-B	402	1/1	-	-	32,32,32,32	1
3	MG	4-B	402	1/1	-	-	32,32,32,32	1
3	MG	5-B	402	1/1	-	-	32,32,32,32	1
3	MG	6-B	402	1/1	-	-	32,32,32,32	1
3	MG	7-B	402	1/1	-	-	32,32,32,32	1
3	MG	8-B	402	1/1	-	-	32,32,32,32	1
3	MG	9-B	402	1/1	-	-	32,32,32,32	1
3	MG	10-B	402	1/1	-	-	32,32,32,32	1
3	MG	11-B	402	1/1	-	-	32,32,32,32	1
3	MG	12-B	402	1/1	-	-	32,32,32,32	1
3	MG	13-B	402	1/1	-	-	32,32,32,32	1
3	MG	14-B	402	1/1	-	-	32,32,32,32	1
3	MG	15-B	402	1/1	-	-	32,32,32,32	1
3	MG	16-B	402	1/1	-	-	32,32,32,32	1
3	MG	17-B	402	1/1	-	-	32,32,32,32	1
3	MG	18-B	402	1/1	-	-	32,32,32,32	1
3	MG	19-B	402	1/1	-	-	32,32,32,32	1
3	MG	20-B	402	1/1	-	-	32,32,32,32	1
3	MG	21-B	402	1/1	-	-	32,32,32,32	1
3	MG	22-B	402	1/1	-	-	32,32,32,32	1
3	MG	23-B	402	1/1	-	-	32,32,32,32	1
2	AHD	1-B	401	14/14	0.95	0.08	30,31,32,32	14
3	MG	2-B	403	1/1	-	-	31,31,31,31	1
3	MG	3-B	403	1/1	-	-	31,31,31,31	1
3	MG	4-B	403	1/1	-	-	31,31,31,31	1
3	MG	5-B	403	1/1	-	-	31,31,31,31	1
3	MG	6-B	403	1/1	-	-	31,31,31,31	1
3	MG	7-B	403	1/1	-	-	31,31,31,31	1
3	MG	8-B	403	1/1	-	-	31,31,31,31	1
3	MG	9-B	403	1/1	-	-	31,31,31,31	1
3	MG	10-B	403	1/1	-	-	31,31,31,31	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	11-B	403	1/1	-	-	31,31,31,31	1
3	MG	12-B	403	1/1	-	-	31,31,31,31	1
3	MG	13-B	403	1/1	-	-	31,31,31,31	1
3	MG	14-B	403	1/1	-	-	31,31,31,31	1
3	MG	15-B	403	1/1	-	-	31,31,31,31	1
3	MG	16-B	403	1/1	-	-	31,31,31,31	1
3	MG	17-B	403	1/1	-	-	31,31,31,31	1
3	MG	18-B	403	1/1	-	-	31,31,31,31	1
3	MG	19-B	403	1/1	-	-	31,31,31,31	1
3	MG	20-B	403	1/1	-	-	31,31,31,31	1
3	MG	21-B	403	1/1	-	-	31,31,31,31	1
3	MG	22-B	403	1/1	-	-	31,31,31,31	1
3	MG	23-B	403	1/1	-	-	31,31,31,31	1
3	MG	1-B	404	1/1	0.98	0.03	31,31,31,31	1
3	MG	2-B	404	1/1	-	-	31,31,31,31	1
3	MG	3-B	404	1/1	-	-	31,31,31,31	1
3	MG	4-B	404	1/1	-	-	31,31,31,31	1
3	MG	5-B	404	1/1	-	-	31,31,31,31	1
3	MG	6-B	404	1/1	-	-	31,31,31,31	1
3	MG	7-B	404	1/1	-	-	31,31,31,31	1
3	MG	8-B	404	1/1	-	-	31,31,31,31	1
3	MG	9-B	404	1/1	-	-	31,31,31,31	1
3	MG	10-B	404	1/1	-	-	31,31,31,31	1
3	MG	11-B	404	1/1	-	-	31,31,31,31	1
3	MG	12-B	404	1/1	-	-	31,31,31,31	1
3	MG	13-B	404	1/1	-	-	31,31,31,31	1
3	MG	14-B	404	1/1	-	-	31,31,31,31	1
3	MG	15-B	404	1/1	-	-	31,31,31,31	1
3	MG	16-B	404	1/1	-	-	31,31,31,31	1
3	MG	17-B	404	1/1	-	-	31,31,31,31	1
3	MG	18-B	404	1/1	-	-	31,31,31,31	1
3	MG	19-B	404	1/1	-	-	31,31,31,31	1
3	MG	20-B	404	1/1	-	-	31,31,31,31	1
3	MG	21-B	404	1/1	-	-	31,31,31,31	1
3	MG	22-B	404	1/1	-	-	31,31,31,31	1
3	MG	23-B	404	1/1	-	-	31,31,31,31	1

5.5 Other polymers [i](#)

There are no such residues in this entry.