



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:23 AM UTC

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

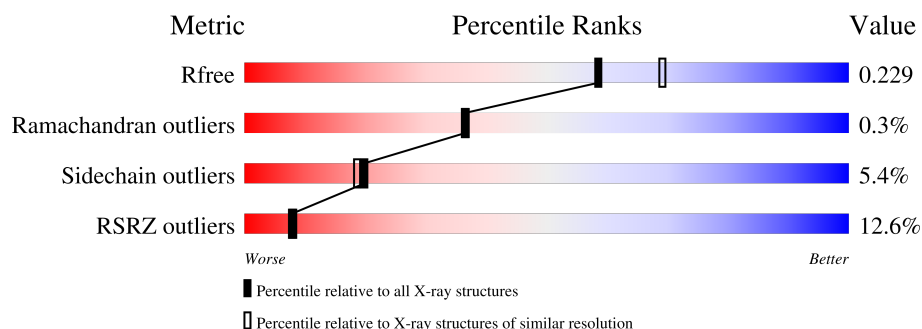
1 Overall quality at a glance

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.



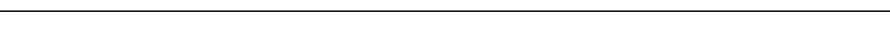
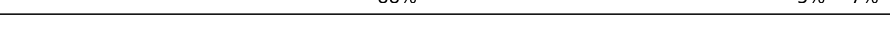
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	318	14% 85% 11%
1	1-B	318	9% 88% 5% 7%
1	10-A	318	85% 11%
1	10-B	318	88% 5% 7%
1	11-A	318	85% 11%
1	11-B	318	87% 6% 7%
1	12-A	318	85% 11%

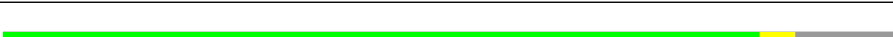
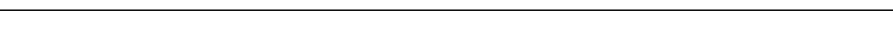
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Mol	Chain	Length	Quality of chain
1	12-B	318	 87%5%7%
1	13-A	318	 85%11%
1	13-B	318	 88%5%7%
1	14-A	318	 85%11%
1	14-B	318	 87%5%7%
1	15-A	318	 85%11%
1	15-B	318	 88%5%7%
1	16-A	318	 85%11%
1	16-B	318	 88%5%7%
1	17-A	318	 85%11%
1	17-B	318	 87%6%7%
1	18-A	318	 85%11%
1	18-B	318	 87%6%7%
1	19-A	318	 85%11%
1	19-B	318	 88%5%7%
1	2-A	318	 85%11%
1	2-B	318	 88%5%7%
1	20-A	318	 85%11%
1	20-B	318	 88%5%7%
1	21-A	318	 85%11%
1	21-B	318	 87%5%7%
1	22-A	318	 85%11%
1	22-B	318	 88%5%7%
1	23-A	318	 85%11%
1	23-B	318	 88%5%7%

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Mol	Chain	Length	Quality of chain
1	3-A	318	 85% 5% 11%
1	3-B	318	 88% 5% 7%
1	4-A	318	 85% 5% 11%
1	4-B	318	 87% 6% 7%
1	5-A	318	 85% 5% 11%
1	5-B	318	 87% 6% 7%
1	6-A	318	 84% 5% 11%
1	6-B	318	 88% 5% 7%
1	7-A	318	 85% 5% 11%
1	7-B	318	 88% 5% 7%
1	8-A	318	 85% 5% 11%
1	8-B	318	 87% 5% 7%
1	9-A	318	 85% 5% 11%
1	9-B	318	 88% 5% 7%

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:

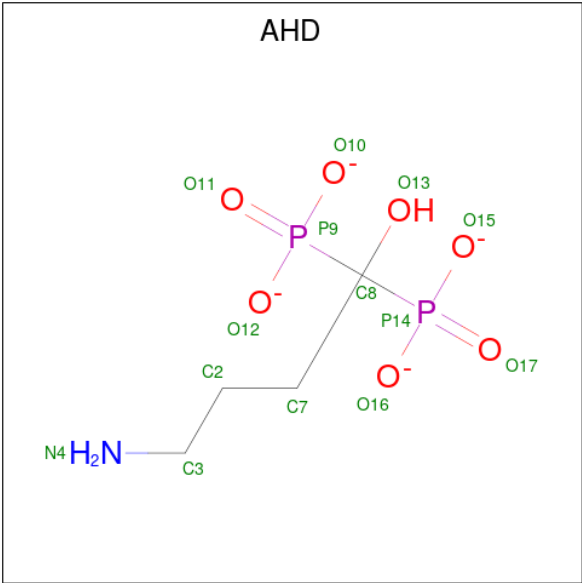
Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ALA	-	expression tag	UNP C9K1X5
A	309	ALA	-	expression tag	UNP C9K1X5
A	310	ALA	-	expression tag	UNP C9K1X5
A	311	LEU	-	expression tag	UNP C9K1X5
A	312	GLU	-	expression tag	UNP C9K1X5
A	313	HIS	-	expression tag	UNP C9K1X5
A	314	HIS	-	expression tag	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 14	C 4	N 1	O 7	P 2	0	0
2	10-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	11-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	12-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	13-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	14-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	15-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	16-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	17-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	18-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	19-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	20-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	21-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	22-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
2	23-B	1	Total 14	C 4	N 1	O 7	P 2	0	0

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

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

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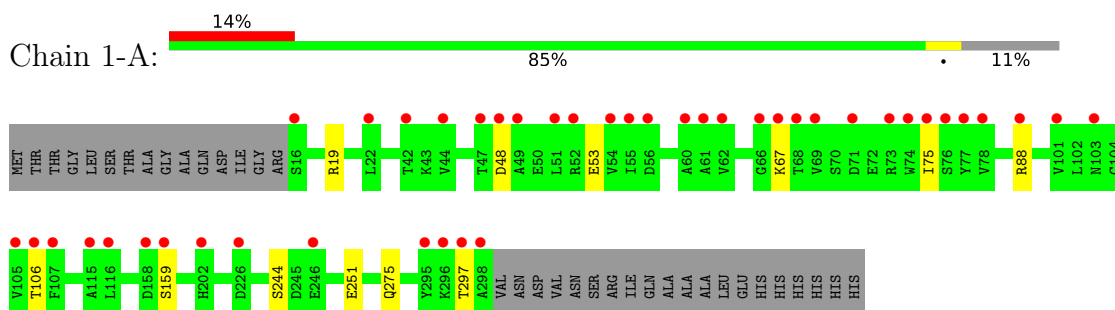
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	20-B	149	Total 149	O 149	0	0
4	21-B	146	Total 146	O 146	0	0
4	22-B	153	Total 153	O 153	0	0
4	23-B	153	Total 153	O 153	0	0

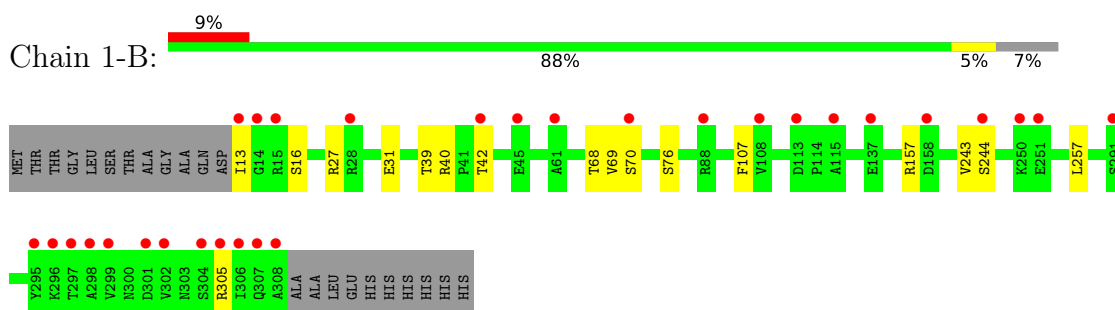
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

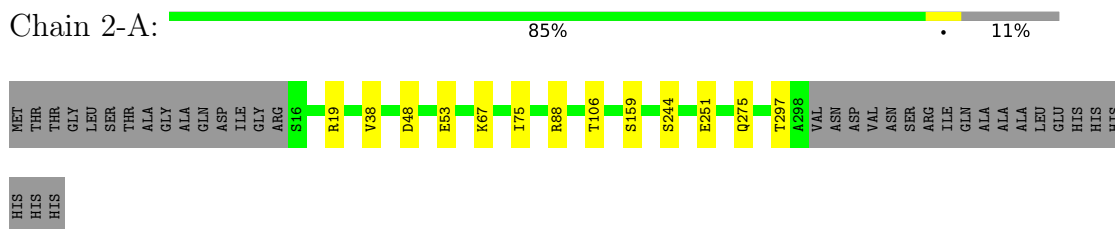
- Molecule 1: Cyclooctat-9-en-7-ol synthase



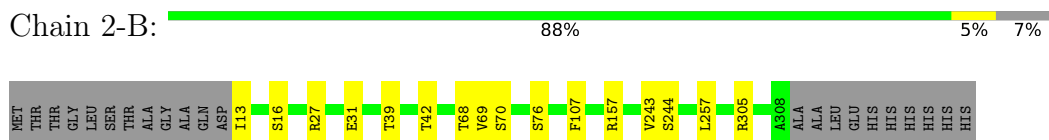
- Molecule 1: Cyclooctat-9-en-7-ol synthase



- Molecule 1: Cyclooctat-9-en-7-ol synthase



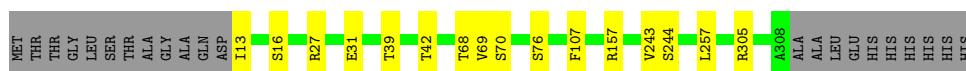
- Molecule 1: Cyclooctat-9-en-7-ol synthase



• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 3-A:  85% 11%

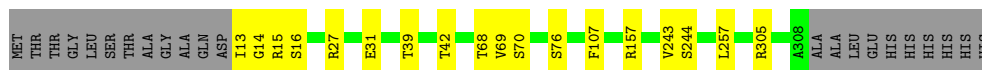
• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 3-B:  88% 5% 7%

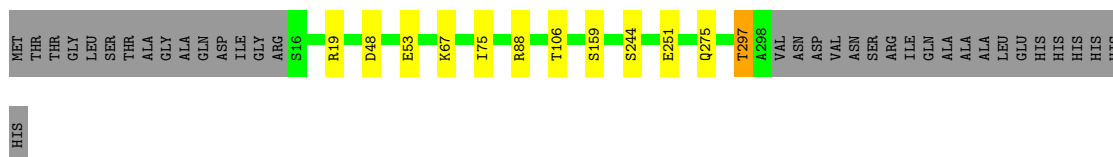
• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 4-A:  85% 11%

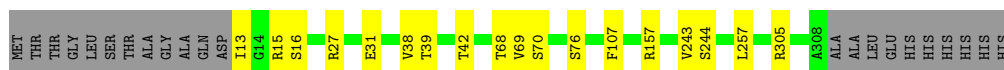
• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 4-B:  87% 6% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 5-A:  85% 11%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 5-B:  87% 6% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

HIS		MET	
HIS	THR	THR	THR
HIS	GLY	GLY	GLY
HIS	LEU	LEU	LEU
HIS	SER	SER	SER
HIS	ALA	ALA	ALA
	GLY	GLY	GLY
	GLN	GLN	GLN
	ASP	ASP	ASP
	ILE	ILE	ILE
	GLY	GLY	GLY
	ARG	ARG	ARG
		\$16	
		R19	
		V38	
		D48	
		E53	
		K67	
		I75	
		R88	
		T106	
		D158	
		S159	
		S244	
		E251	
		Q275	
		Y295	
		K296	
		T297	
		A298	
		VAL	ASN
		ASP	ASP
		VAL	VAL
		ASN	ASN
		SER	SER
		ARG	ARG
		ILE	ILE
		GLN	GLN
		ALA	ALA
		ALA	ALA
		LEU	LEU
		CYS	CYS

- | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | THR | THR | GLY | LEU | SER | THR | ALA | GLY | ALA | GLN | ASP | I13 | G14 | R15 | S16 | R27 | E31 | T39 | T42 | T68 | V69 | S70 | S76 | F107 | R157 | V243 | S244 | L257 | R305 | A308 | ALA | ALA | LEU | GLU | HIS | HIS | HIS | HIS | HIS | HIS |
|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- | HIS | | HIS | |
|------|--|-----|--|
| MET | | | |
| THR | | | |
| GLY | | | |
| LEU | | | |
| SER | | | |
| THR | | | |
| ALA | | | |
| GLY | | | |
| GLN | | | |
| ASP | | | |
| ILE | | | |
| GLY | | | |
| ARG | | | |
| S16 | | | |
| R19 | | | |
| D48 | | | |
| E53 | | | |
| K67 | | | |
| I75 | | | |
| R88 | | | |
| T106 | | | |
| S159 | | | |
| S244 | | | |
| E251 | | | |
| Q275 | | | |
| K296 | | | |
| T297 | | | |
| K298 | | | |
| VAL | | | |
| ASN | | | |
| ASP | | | |
| VAL | | | |
| ASN | | | |
| SER | | | |
| ARG | | | |
| ILE | | | |
| GLN | | | |
| ALA | | | |
| ALA | | | |
| LEU | | | |
| GLU | | | |
| HIS | | | |
| HIS | | | |
| HIS | | | |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | THR | THR | GLY | LEU | SER | THR | ALA | ALA | GLN | ASP | I113 | I115 | S16 | R27 | E31 | R35 | T39 | T42 | T68 | V69 | S70 | S76 | F107 | R157 | V243 | S244 | L257 | R305 | A308 | ALA | ALA | LEU | GLU | HIS | HIS | HIS | HIS | HIS | HIS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- | | | |
|-----|------|---|
| HIS | MET | 1 |
| HIS | THR | 1 |
| HIS | GLY | 1 |
| HIS | LEU | 1 |
| | SER | 1 |
| | THR | 1 |
| | ALA | 1 |
| | GLY | 1 |
| | ALA | 1 |
| | GLN | 1 |
| | ASP | 1 |
| | ILE | 1 |
| | GLY | 1 |
| | ARG | 1 |
| | S16 | 1 |
| | R19 | 1 |
| | D48 | 1 |
| | E53 | 1 |
| | K67 | 1 |
| | D71 | 1 |
| | I75 | 1 |
| | R88 | 1 |
| | T106 | 1 |
| | D158 | 1 |
| | S159 | 1 |
| | S244 | 1 |
| | E251 | 1 |
| | Q275 | 1 |
| | T297 | 1 |
| | A298 | 1 |
| | VAL | 1 |
| | ASN | 1 |
| | ASP | 1 |
| | VAL | 1 |
| | ASN | 1 |
| | SER | 1 |
| | ILE | 1 |
| | GLN | 1 |
| | ALA | 1 |
| | ALA | 1 |
| | LEU | 1 |
| | GLU | 1 |
| | HIS | 1 |
| | HIS | 1 |

- | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | THR | THR | GLY | LEU | SER | THR | ALA | GLY | ALA | GLN | ASP | I13 | S16 | R27 | E31 | T39 | T42 | D48 | T68 | V69 | S70 | S76 | F107 | R157 | V243 | S244 | L257 | A298 | R305 | A308 | ALA | LEU | GLU | HIS | HIS | HIS | HIS | HIS | THR |
|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

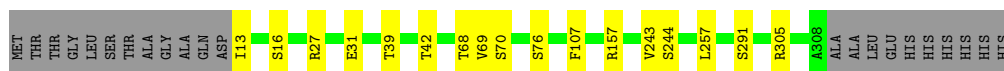
- WORLDWIDE
 **PDB**
PROTEIN DATA BANK

Chain 9-A:  85% 11%



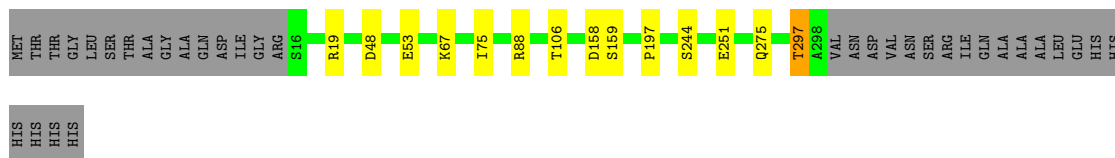
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 9-B:  88% 5% 7%



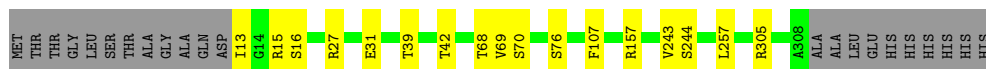
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 10-A:  85% 11%



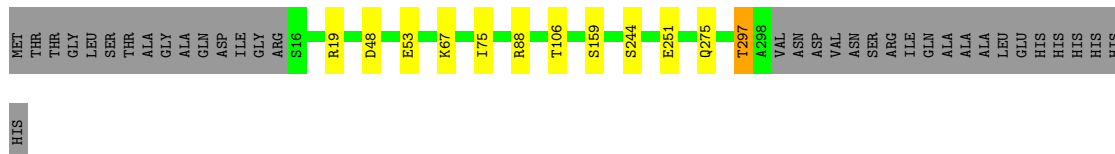
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 10-B:  88% 5% 7%



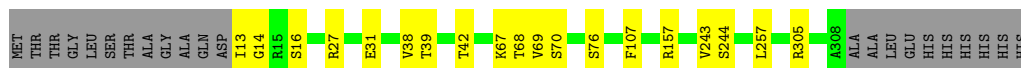
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 11-A:  85% 11%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 11-B:  87% 6% 7%



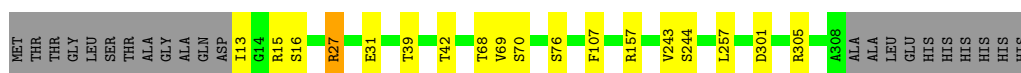
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 12-A:  85% 11%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 12-B:  87% 5% 7%



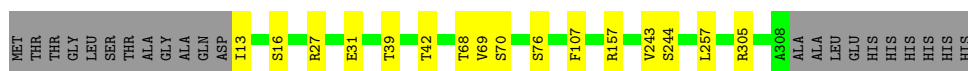
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 13-A:  85% 11%



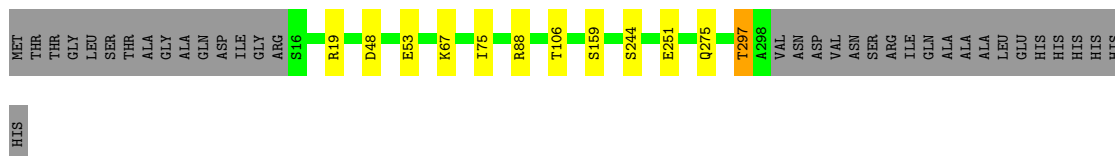
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 13-B:  88% 5% 7%



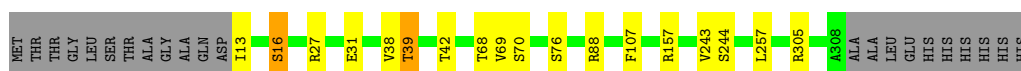
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 14-A:  85% 11%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 14-B:  87% 5% 7%



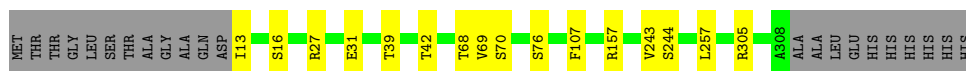
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 15-A:  85% 11%



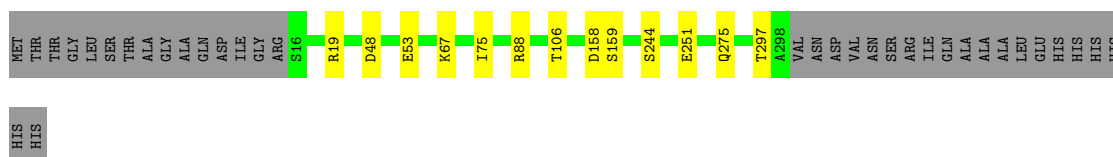
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 15-B:  88% 5% 7%



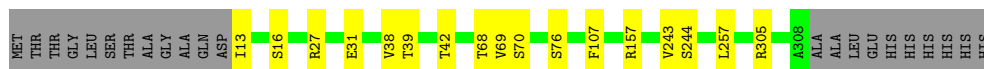
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 16-A:  85% 11%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 16-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 17-A:  85% 11%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 17-B:  87% 6% 7%



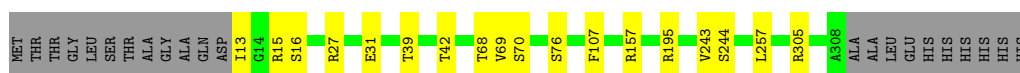
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 18-A:  85% 11%



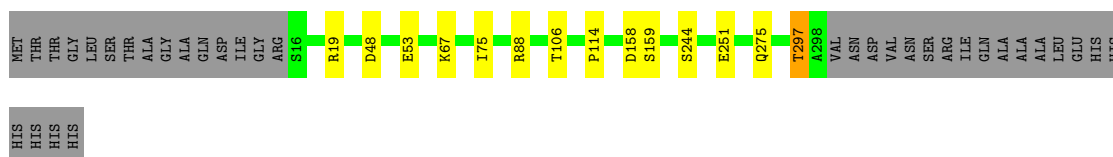
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 18-B:  87% 6% 7%



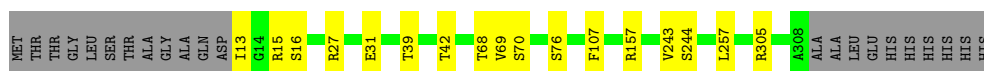
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 19-A:  85% 11%



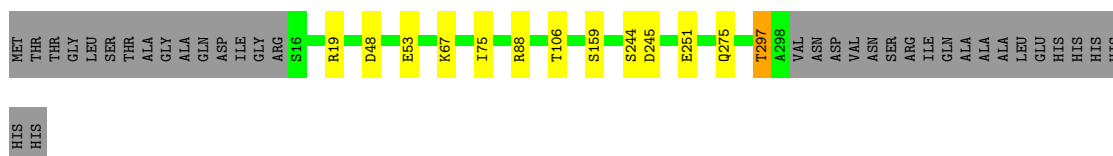
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 19-B:  88% 5% 7%



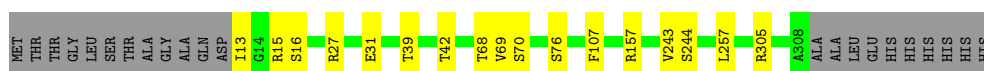
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 20-A:  85% 11%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 20-B:  88% 5% 7%



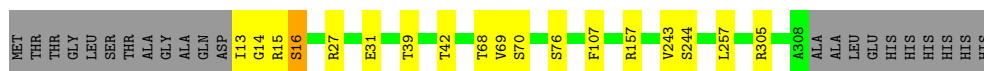
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 21-A:  85% 11%



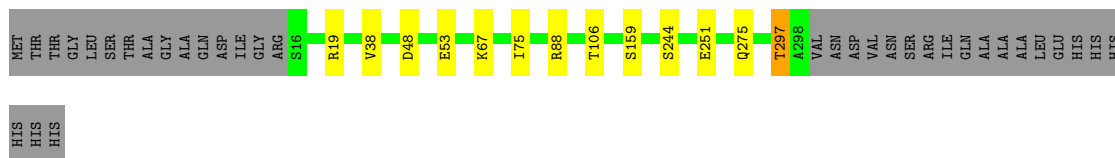
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 21-B:  87% 5% 7%



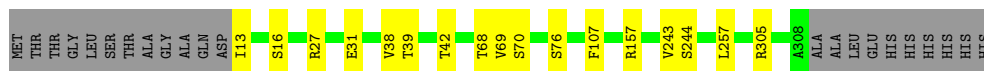
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 22-A:  85% 11%



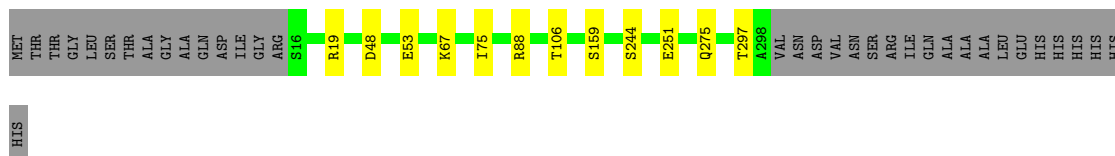
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 22-B:  88% 5% 7%



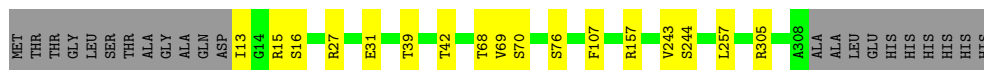
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 23-A:  85% 11%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 23-B:  88% 5% 7%



4 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.

5 Model quality

5.1 Standard geometry

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

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-A	0.12	0/2375	0.19	0/3221
1	1-B	0.14	0/2475	0.23	0/3356
1	2-A	0.12	0/2375	0.19	0/3221
1	2-B	0.14	0/2475	0.23	0/3356
1	3-A	0.12	0/2375	0.19	0/3221
1	3-B	0.14	0/2475	0.23	0/3356
1	4-A	0.12	0/2375	0.19	0/3221
1	4-B	0.14	0/2475	0.23	0/3356
1	5-A	0.12	0/2375	0.19	0/3221
1	5-B	0.14	0/2475	0.23	0/3356
1	6-A	0.12	0/2375	0.19	0/3221
1	6-B	0.14	0/2475	0.23	0/3356
1	7-A	0.12	0/2375	0.19	0/3221
1	7-B	0.14	0/2475	0.23	0/3356
1	8-A	0.12	0/2375	0.19	0/3221
1	8-B	0.14	0/2475	0.23	0/3356
1	9-A	0.12	0/2375	0.19	0/3221
1	9-B	0.14	0/2475	0.23	0/3356
1	10-A	0.12	0/2375	0.19	0/3221
1	10-B	0.14	0/2475	0.23	0/3356
1	11-A	0.12	0/2375	0.19	0/3221
1	11-B	0.14	0/2475	0.23	0/3356
1	12-A	0.12	0/2375	0.19	0/3221
1	12-B	0.14	0/2475	0.23	0/3356
1	13-A	0.12	0/2375	0.19	0/3221
1	13-B	0.14	0/2475	0.23	0/3356
1	14-A	0.12	0/2375	0.19	0/3221
1	14-B	0.14	0/2475	0.23	0/3356
1	15-A	0.12	0/2375	0.19	0/3221
1	15-B	0.14	0/2475	0.23	0/3356
1	16-A	0.12	0/2375	0.19	0/3221
1	16-B	0.14	0/2475	0.23	0/3356

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	17-A	0.12	0/2375	0.19	0/3221
1	17-B	0.14	0/2475	0.23	0/3356
1	18-A	0.12	0/2375	0.19	0/3221
1	18-B	0.14	0/2475	0.23	0/3356
1	19-A	0.12	0/2375	0.19	0/3221
1	19-B	0.14	0/2475	0.23	0/3356
1	20-A	0.12	0/2375	0.19	0/3221
1	20-B	0.14	0/2475	0.23	0/3356
1	21-A	0.12	0/2375	0.19	0/3221
1	21-B	0.14	0/2475	0.23	0/3356
1	22-A	0.12	0/2375	0.19	0/3221
1	22-B	0.14	0/2475	0.23	0/3356
1	23-A	0.12	0/2375	0.19	0/3221
1	23-B	0.14	0/2475	0.23	0/3356
All	All	0.13	0/111550	0.21	0/151271

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-B	0	1
1	3-A	0	1
1	5-B	0	1
1	6-A	0	1
1	6-B	0	1
1	7-A	0	1
1	7-B	0	1
1	8-B	0	1
1	12-B	0	2
1	14-B	0	2
1	17-A	0	1
1	18-B	0	1
1	19-B	0	1
1	21-B	0	1
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-B	40	ARG	Sidechain
1	12-B	15	ARG	Sidechain
1	12-B	27	ARG	Sidechain
1	14-B	16	SER	Peptide
1	14-B	88	ARG	Sidechain
1	17-A	297	THR	Peptide
1	18-B	195	ARG	Sidechain
1	19-B	15	ARG	Peptide
1	21-B	16	SER	Peptide
1	3-A	296	LYS	Peptide
1	5-B	15	ARG	Peptide
1	6-A	295	TYR	Peptide
1	6-B	27	ARG	Sidechain
1	7-A	296	LYS	Peptide
1	7-B	35	ARG	Sidechain
1	8-B	157	ARG	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2317	0	2232	0	0
1	1-B	2417	0	2335	0	0
1	2-A	2317	0	2232	0	0
1	2-B	2417	0	2335	0	0
1	3-A	2317	0	2232	0	0
1	3-B	2417	0	2335	0	0
1	4-A	2317	0	2232	0	0
1	4-B	2417	0	2335	0	0
1	5-A	2317	0	2232	0	0
1	5-B	2417	0	2335	0	0
1	6-A	2317	0	2231	0	0
1	6-B	2417	0	2335	0	0
1	7-A	2317	0	2232	0	0
1	7-B	2417	0	2335	0	0
1	8-A	2317	0	2232	0	0
1	8-B	2417	0	2335	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9-A	2317	0	2231	0	0
1	9-B	2417	0	2335	0	0
1	10-A	2317	0	2232	0	0
1	10-B	2417	0	2335	0	0
1	11-A	2317	0	2232	0	0
1	11-B	2417	0	2335	0	0
1	12-A	2317	0	2232	0	0
1	12-B	2417	0	2335	0	0
1	13-A	2317	0	2232	0	0
1	13-B	2417	0	2335	0	0
1	14-A	2317	0	2231	0	0
1	14-B	2417	0	2335	0	0
1	15-A	2317	0	2232	0	0
1	15-B	2417	0	2335	0	0
1	16-A	2317	0	2232	0	0
1	16-B	2417	0	2335	0	0
1	17-A	2317	0	2232	0	0
1	17-B	2417	0	2335	0	0
1	18-A	2317	0	2232	0	0
1	18-B	2417	0	2335	0	0
1	19-A	2317	0	2232	0	0
1	19-B	2417	0	2335	0	0
1	20-A	2317	0	2232	0	0
1	20-B	2417	0	2335	0	0
1	21-A	2317	0	2232	0	0
1	21-B	2417	0	2335	0	0
1	22-A	2317	0	2231	0	0
1	22-B	2417	0	2335	0	0
1	23-A	2317	0	2231	0	0
1	23-B	2417	0	2335	0	0
2	1-A	14	0	9	0	0
2	1-B	14	0	9	0	0
2	2-A	14	0	9	0	0
2	2-B	14	0	9	0	0
2	3-A	14	0	9	0	0
2	3-B	14	0	9	0	0
2	4-A	14	0	9	0	0
2	4-B	14	0	9	0	0
2	5-A	14	0	9	0	0
2	5-B	14	0	9	0	0
2	6-A	14	0	9	0	0
2	6-B	14	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	7-A	14	0	9	0	0
2	7-B	14	0	9	0	0
2	8-A	14	0	9	0	0
2	8-B	14	0	9	0	0
2	9-A	14	0	9	0	0
2	9-B	14	0	9	0	0
2	10-A	14	0	9	0	0
2	10-B	14	0	9	0	0
2	11-A	14	0	9	0	0
2	11-B	14	0	9	0	0
2	12-A	14	0	9	0	0
2	12-B	14	0	9	0	0
2	13-A	14	0	9	0	0
2	13-B	14	0	9	0	0
2	14-A	14	0	9	0	0
2	14-B	14	0	9	0	0
2	15-A	14	0	9	0	0
2	15-B	14	0	9	0	0
2	16-A	14	0	9	0	0
2	16-B	14	0	9	0	0
2	17-A	14	0	9	0	0
2	17-B	14	0	9	0	0
2	18-A	14	0	9	0	0
2	18-B	14	0	9	0	0
2	19-A	14	0	9	0	0
2	19-B	14	0	9	0	0
2	20-A	14	0	9	0	0
2	20-B	14	0	9	0	0
2	21-A	14	0	9	0	0
2	21-B	14	0	9	0	0
2	22-A	14	0	9	0	0
2	22-B	14	0	9	0	0
2	23-A	14	0	9	0	0
2	23-B	14	0	9	0	0
3	1-A	3	0	0	0	0
3	1-B	3	0	0	0	0
3	2-A	3	0	0	0	0
3	2-B	3	0	0	0	0
3	3-A	3	0	0	0	0
3	3-B	3	0	0	0	0
3	4-A	3	0	0	0	0
3	4-B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	5-A	3	0	0	0	0
3	5-B	3	0	0	0	0
3	6-A	3	0	0	0	0
3	6-B	3	0	0	0	0
3	7-A	3	0	0	0	0
3	7-B	3	0	0	0	0
3	8-A	3	0	0	0	0
3	8-B	3	0	0	0	0
3	9-A	3	0	0	0	0
3	9-B	3	0	0	0	0
3	10-A	3	0	0	0	0
3	10-B	3	0	0	0	0
3	11-A	3	0	0	0	0
3	11-B	3	0	0	0	0
3	12-A	3	0	0	0	0
3	12-B	3	0	0	0	0
3	13-A	3	0	0	0	0
3	13-B	3	0	0	0	0
3	14-A	3	0	0	0	0
3	14-B	3	0	0	0	0
3	15-A	3	0	0	0	0
3	15-B	3	0	0	0	0
3	16-A	3	0	0	0	0
3	16-B	3	0	0	0	0
3	17-A	3	0	0	0	0
3	17-B	3	0	0	0	0
3	18-A	3	0	0	0	0
3	18-B	3	0	0	0	0
3	19-A	3	0	0	0	0
3	19-B	3	0	0	0	0
3	20-A	3	0	0	0	0
3	20-B	3	0	0	0	0
3	21-A	3	0	0	0	0
3	21-B	3	0	0	0	0
3	22-A	3	0	0	0	0
3	22-B	3	0	0	0	0
3	23-A	3	0	0	0	0
3	23-B	3	0	0	0	0
4	1-A	62	0	0	0	0
4	1-B	149	0	0	0	0
4	2-A	67	0	0	0	0
4	2-B	154	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3-A	72	0	0	0	0
4	3-B	167	0	0	0	0
4	4-A	62	0	0	0	0
4	4-B	149	0	0	0	0
4	5-A	60	0	0	0	0
4	5-B	143	0	0	0	0
4	6-A	66	0	0	0	0
4	6-B	153	0	0	0	0
4	7-A	62	0	0	0	0
4	7-B	147	0	0	0	0
4	8-A	62	0	0	0	0
4	8-B	147	0	0	0	0
4	9-A	61	0	0	0	0
4	9-B	143	0	0	0	0
4	10-A	62	0	0	0	0
4	10-B	149	0	0	0	0
4	11-A	60	0	0	0	0
4	11-B	143	0	0	0	0
4	12-A	71	0	0	0	0
4	12-B	163	0	0	0	0
4	13-A	56	0	0	0	0
4	13-B	131	0	0	0	0
4	14-A	60	0	0	0	0
4	14-B	143	0	0	0	0
4	15-A	61	0	0	0	0
4	15-B	146	0	0	0	0
4	16-A	67	0	0	0	0
4	16-B	161	0	0	0	0
4	17-A	61	0	0	0	0
4	17-B	145	0	0	0	0
4	18-A	63	0	0	0	0
4	18-B	149	0	0	0	0
4	19-A	59	0	0	0	0
4	19-B	133	0	0	0	0
4	20-A	65	0	0	0	0
4	20-B	149	0	0	0	0
4	21-A	61	0	0	0	0
4	21-B	146	0	0	0	0
4	22-A	67	0	0	0	0
4	22-B	153	0	0	0	0
4	23-A	66	0	0	0	0
4	23-B	153	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	114533	0	105450	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	281/318 (88%)	275 (98%)	6 (2%)	0	100	100
1	1-B	294/318 (92%)	287 (98%)	7 (2%)	0	100	100
1	2-A	281/318 (88%)	270 (96%)	10 (4%)	1 (0%)	30	28
1	2-B	294/318 (92%)	284 (97%)	10 (3%)	0	100	100
1	3-A	281/318 (88%)	278 (99%)	3 (1%)	0	100	100
1	3-B	294/318 (92%)	286 (97%)	8 (3%)	0	100	100
1	4-A	281/318 (88%)	273 (97%)	8 (3%)	0	100	100
1	4-B	294/318 (92%)	283 (96%)	9 (3%)	2 (1%)	18	15
1	5-A	281/318 (88%)	271 (96%)	9 (3%)	1 (0%)	30	28
1	5-B	294/318 (92%)	288 (98%)	5 (2%)	1 (0%)	36	36
1	6-A	281/318 (88%)	271 (96%)	8 (3%)	2 (1%)	18	15
1	6-B	294/318 (92%)	282 (96%)	11 (4%)	1 (0%)	36	36
1	7-A	281/318 (88%)	270 (96%)	10 (4%)	1 (0%)	30	28
1	7-B	294/318 (92%)	287 (98%)	7 (2%)	0	100	100
1	8-A	281/318 (88%)	272 (97%)	7 (2%)	2 (1%)	18	15
1	8-B	294/318 (92%)	286 (97%)	6 (2%)	2 (1%)	18	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-A	281/318 (88%)	271 (96%)	10 (4%)	0	100	100
1	9-B	294/318 (92%)	286 (97%)	7 (2%)	1 (0%)	36	36
1	10-A	281/318 (88%)	269 (96%)	9 (3%)	3 (1%)	11	8
1	10-B	294/318 (92%)	287 (98%)	6 (2%)	1 (0%)	36	36
1	11-A	281/318 (88%)	270 (96%)	10 (4%)	1 (0%)	30	28
1	11-B	294/318 (92%)	281 (96%)	10 (3%)	3 (1%)	12	9
1	12-A	281/318 (88%)	275 (98%)	4 (1%)	2 (1%)	18	15
1	12-B	294/318 (92%)	285 (97%)	8 (3%)	1 (0%)	36	36
1	13-A	281/318 (88%)	268 (95%)	13 (5%)	0	100	100
1	13-B	294/318 (92%)	281 (96%)	13 (4%)	0	100	100
1	14-A	281/318 (88%)	271 (96%)	9 (3%)	1 (0%)	30	28
1	14-B	294/318 (92%)	284 (97%)	8 (3%)	2 (1%)	18	15
1	15-A	281/318 (88%)	271 (96%)	10 (4%)	0	100	100
1	15-B	294/318 (92%)	284 (97%)	10 (3%)	0	100	100
1	16-A	281/318 (88%)	272 (97%)	8 (3%)	1 (0%)	30	28
1	16-B	294/318 (92%)	289 (98%)	4 (1%)	1 (0%)	36	36
1	17-A	281/318 (88%)	269 (96%)	11 (4%)	1 (0%)	30	28
1	17-B	294/318 (92%)	285 (97%)	7 (2%)	2 (1%)	18	15
1	18-A	281/318 (88%)	273 (97%)	8 (3%)	0	100	100
1	18-B	294/318 (92%)	285 (97%)	8 (3%)	1 (0%)	36	36
1	19-A	281/318 (88%)	269 (96%)	9 (3%)	3 (1%)	11	8
1	19-B	294/318 (92%)	286 (97%)	8 (3%)	0	100	100
1	20-A	281/318 (88%)	269 (96%)	10 (4%)	2 (1%)	18	15
1	20-B	294/318 (92%)	285 (97%)	8 (3%)	1 (0%)	36	36
1	21-A	281/318 (88%)	265 (94%)	16 (6%)	0	100	100
1	21-B	294/318 (92%)	282 (96%)	10 (3%)	2 (1%)	18	15
1	22-A	281/318 (88%)	272 (97%)	7 (2%)	2 (1%)	18	15
1	22-B	294/318 (92%)	288 (98%)	5 (2%)	1 (0%)	36	36
1	23-A	281/318 (88%)	274 (98%)	7 (2%)	0	100	100
1	23-B	294/318 (92%)	286 (97%)	7 (2%)	1 (0%)	36	36
All	All	13225/14628 (90%)	12795 (97%)	384 (3%)	46 (0%)	36	36

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	7-A	297	THR
1	9-B	291	SER
1	10-A	297	THR
1	12-A	297	THR
1	18-B	15	ARG
1	19-A	158	ASP
1	20-A	297	THR
1	23-B	15	ARG
1	4-B	14	GLY
1	4-B	15	ARG
1	12-A	245	ASP
1	12-B	301	ASP
1	14-A	297	THR
1	17-B	14	GLY
1	19-A	297	THR
1	20-B	15	ARG
1	5-A	297	THR
1	8-A	158	ASP
1	8-B	48	ASP
1	10-B	15	ARG
1	11-A	297	THR
1	6-A	158	ASP
1	6-B	15	ARG
1	8-A	71	ASP
1	11-B	67	LYS
1	14-B	39	THR
1	16-A	158	ASP
1	20-A	245	ASP
1	21-B	15	ARG
1	8-B	298	ALA
1	10-A	158	ASP
1	10-A	197	PRO
1	17-A	39	THR
1	6-A	38	VAL
1	11-B	14	GLY
1	22-A	297	THR
1	11-B	38	VAL
1	21-B	14	GLY
1	5-B	38	VAL
1	14-B	38	VAL
1	2-A	38	VAL
1	17-B	38	VAL

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Mol	Chain	Res	Type
1	19-A	114	PRO
1	22-B	38	VAL
1	22-A	38	VAL
1	16-B	38	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	1-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	2-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	2-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	3-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	3-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	4-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	4-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	5-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	5-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	6-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	6-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	7-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	7-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	8-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	8-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	9-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	9-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	10-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	10-B	265/281 (94%)	249 (94%)	16 (6%)	17	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	11-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	12-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	12-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	13-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	13-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	14-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	14-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	15-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	15-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	16-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	16-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	17-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	17-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	18-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	18-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	19-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	19-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	20-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	20-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	21-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	21-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	22-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	22-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
1	23-A	254/281 (90%)	242 (95%)	12 (5%)	23	24
1	23-B	265/281 (94%)	249 (94%)	16 (6%)	17	15
All	All	11937/12926 (92%)	11293 (95%)	644 (5%)	20	18

All (644) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	19	ARG
1	1-A	48	ASP

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Mol	Chain	Res	Type
1	1-A	53	GLU
1	1-A	67	LYS
1	1-A	75	ILE
1	1-A	88	ARG
1	1-A	106	THR
1	1-A	159	SER
1	1-A	244	SER
1	1-A	251	GLU
1	1-A	275	GLN
1	1-A	297	THR
1	1-B	13	ILE
1	1-B	16	SER
1	1-B	27	ARG
1	1-B	31	GLU
1	1-B	39	THR
1	1-B	42	THR
1	1-B	68	THR
1	1-B	69	VAL
1	1-B	70	SER
1	1-B	76	SER
1	1-B	107	PHE
1	1-B	157	ARG
1	1-B	243	VAL
1	1-B	244	SER
1	1-B	257	LEU
1	1-B	305	ARG
1	2-A	19	ARG
1	2-A	48	ASP
1	2-A	53	GLU
1	2-A	67	LYS
1	2-A	75	ILE
1	2-A	88	ARG
1	2-A	106	THR
1	2-A	159	SER
1	2-A	244	SER
1	2-A	251	GLU
1	2-A	275	GLN
1	2-A	297	THR
1	2-B	13	ILE
1	2-B	16	SER
1	2-B	27	ARG
1	2-B	31	GLU

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Mol	Chain	Res	Type
1	2-B	39	THR
1	2-B	42	THR
1	2-B	68	THR
1	2-B	69	VAL
1	2-B	70	SER
1	2-B	76	SER
1	2-B	107	PHE
1	2-B	157	ARG
1	2-B	243	VAL
1	2-B	244	SER
1	2-B	257	LEU
1	2-B	305	ARG
1	3-A	19	ARG
1	3-A	48	ASP
1	3-A	53	GLU
1	3-A	67	LYS
1	3-A	75	ILE
1	3-A	88	ARG
1	3-A	106	THR
1	3-A	159	SER
1	3-A	244	SER
1	3-A	251	GLU
1	3-A	275	GLN
1	3-A	297	THR
1	3-B	13	ILE
1	3-B	16	SER
1	3-B	27	ARG
1	3-B	31	GLU
1	3-B	39	THR
1	3-B	42	THR
1	3-B	68	THR
1	3-B	69	VAL
1	3-B	70	SER
1	3-B	76	SER
1	3-B	107	PHE
1	3-B	157	ARG
1	3-B	243	VAL
1	3-B	244	SER
1	3-B	257	LEU
1	3-B	305	ARG
1	4-A	19	ARG
1	4-A	48	ASP

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Mol	Chain	Res	Type
1	4-A	53	GLU
1	4-A	67	LYS
1	4-A	75	ILE
1	4-A	88	ARG
1	4-A	106	THR
1	4-A	159	SER
1	4-A	244	SER
1	4-A	251	GLU
1	4-A	275	GLN
1	4-A	297	THR
1	4-B	13	ILE
1	4-B	16	SER
1	4-B	27	ARG
1	4-B	31	GLU
1	4-B	39	THR
1	4-B	42	THR
1	4-B	68	THR
1	4-B	69	VAL
1	4-B	70	SER
1	4-B	76	SER
1	4-B	107	PHE
1	4-B	157	ARG
1	4-B	243	VAL
1	4-B	244	SER
1	4-B	257	LEU
1	4-B	305	ARG
1	5-A	19	ARG
1	5-A	48	ASP
1	5-A	53	GLU
1	5-A	67	LYS
1	5-A	75	ILE
1	5-A	88	ARG
1	5-A	106	THR
1	5-A	159	SER
1	5-A	244	SER
1	5-A	251	GLU
1	5-A	275	GLN
1	5-A	297	THR
1	5-B	13	ILE
1	5-B	16	SER
1	5-B	27	ARG
1	5-B	31	GLU

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Mol	Chain	Res	Type
1	5-B	39	THR
1	5-B	42	THR
1	5-B	68	THR
1	5-B	69	VAL
1	5-B	70	SER
1	5-B	76	SER
1	5-B	107	PHE
1	5-B	157	ARG
1	5-B	243	VAL
1	5-B	244	SER
1	5-B	257	LEU
1	5-B	305	ARG
1	6-A	19	ARG
1	6-A	48	ASP
1	6-A	53	GLU
1	6-A	67	LYS
1	6-A	75	ILE
1	6-A	88	ARG
1	6-A	106	THR
1	6-A	159	SER
1	6-A	244	SER
1	6-A	251	GLU
1	6-A	275	GLN
1	6-A	297	THR
1	6-B	13	ILE
1	6-B	16	SER
1	6-B	27	ARG
1	6-B	31	GLU
1	6-B	39	THR
1	6-B	42	THR
1	6-B	68	THR
1	6-B	69	VAL
1	6-B	70	SER
1	6-B	76	SER
1	6-B	107	PHE
1	6-B	157	ARG
1	6-B	243	VAL
1	6-B	244	SER
1	6-B	257	LEU
1	6-B	305	ARG
1	7-A	19	ARG
1	7-A	48	ASP

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Mol	Chain	Res	Type
1	7-A	53	GLU
1	7-A	67	LYS
1	7-A	75	ILE
1	7-A	88	ARG
1	7-A	106	THR
1	7-A	159	SER
1	7-A	244	SER
1	7-A	251	GLU
1	7-A	275	GLN
1	7-A	297	THR
1	7-B	13	ILE
1	7-B	16	SER
1	7-B	27	ARG
1	7-B	31	GLU
1	7-B	39	THR
1	7-B	42	THR
1	7-B	68	THR
1	7-B	69	VAL
1	7-B	70	SER
1	7-B	76	SER
1	7-B	107	PHE
1	7-B	157	ARG
1	7-B	243	VAL
1	7-B	244	SER
1	7-B	257	LEU
1	7-B	305	ARG
1	8-A	19	ARG
1	8-A	48	ASP
1	8-A	53	GLU
1	8-A	67	LYS
1	8-A	75	ILE
1	8-A	88	ARG
1	8-A	106	THR
1	8-A	159	SER
1	8-A	244	SER
1	8-A	251	GLU
1	8-A	275	GLN
1	8-A	297	THR
1	8-B	13	ILE
1	8-B	16	SER
1	8-B	27	ARG
1	8-B	31	GLU

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Mol	Chain	Res	Type
1	8-B	39	THR
1	8-B	42	THR
1	8-B	68	THR
1	8-B	69	VAL
1	8-B	70	SER
1	8-B	76	SER
1	8-B	107	PHE
1	8-B	157	ARG
1	8-B	243	VAL
1	8-B	244	SER
1	8-B	257	LEU
1	8-B	305	ARG
1	9-A	19	ARG
1	9-A	48	ASP
1	9-A	53	GLU
1	9-A	67	LYS
1	9-A	75	ILE
1	9-A	88	ARG
1	9-A	106	THR
1	9-A	159	SER
1	9-A	244	SER
1	9-A	251	GLU
1	9-A	275	GLN
1	9-A	297	THR
1	9-B	13	ILE
1	9-B	16	SER
1	9-B	27	ARG
1	9-B	31	GLU
1	9-B	39	THR
1	9-B	42	THR
1	9-B	68	THR
1	9-B	69	VAL
1	9-B	70	SER
1	9-B	76	SER
1	9-B	107	PHE
1	9-B	157	ARG
1	9-B	243	VAL
1	9-B	244	SER
1	9-B	257	LEU
1	9-B	305	ARG
1	10-A	19	ARG
1	10-A	48	ASP

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Mol	Chain	Res	Type
1	10-A	53	GLU
1	10-A	67	LYS
1	10-A	75	ILE
1	10-A	88	ARG
1	10-A	106	THR
1	10-A	159	SER
1	10-A	244	SER
1	10-A	251	GLU
1	10-A	275	GLN
1	10-A	297	THR
1	10-B	13	ILE
1	10-B	16	SER
1	10-B	27	ARG
1	10-B	31	GLU
1	10-B	39	THR
1	10-B	42	THR
1	10-B	68	THR
1	10-B	69	VAL
1	10-B	70	SER
1	10-B	76	SER
1	10-B	107	PHE
1	10-B	157	ARG
1	10-B	243	VAL
1	10-B	244	SER
1	10-B	257	LEU
1	10-B	305	ARG
1	11-A	19	ARG
1	11-A	48	ASP
1	11-A	53	GLU
1	11-A	67	LYS
1	11-A	75	ILE
1	11-A	88	ARG
1	11-A	106	THR
1	11-A	159	SER
1	11-A	244	SER
1	11-A	251	GLU
1	11-A	275	GLN
1	11-A	297	THR
1	11-B	13	ILE
1	11-B	16	SER
1	11-B	27	ARG
1	11-B	31	GLU

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Mol	Chain	Res	Type
1	11-B	39	THR
1	11-B	42	THR
1	11-B	68	THR
1	11-B	69	VAL
1	11-B	70	SER
1	11-B	76	SER
1	11-B	107	PHE
1	11-B	157	ARG
1	11-B	243	VAL
1	11-B	244	SER
1	11-B	257	LEU
1	11-B	305	ARG
1	12-A	19	ARG
1	12-A	48	ASP
1	12-A	53	GLU
1	12-A	67	LYS
1	12-A	75	ILE
1	12-A	88	ARG
1	12-A	106	THR
1	12-A	159	SER
1	12-A	244	SER
1	12-A	251	GLU
1	12-A	275	GLN
1	12-A	297	THR
1	12-B	13	ILE
1	12-B	16	SER
1	12-B	27	ARG
1	12-B	31	GLU
1	12-B	39	THR
1	12-B	42	THR
1	12-B	68	THR
1	12-B	69	VAL
1	12-B	70	SER
1	12-B	76	SER
1	12-B	107	PHE
1	12-B	157	ARG
1	12-B	243	VAL
1	12-B	244	SER
1	12-B	257	LEU
1	12-B	305	ARG
1	13-A	19	ARG
1	13-A	48	ASP

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Mol	Chain	Res	Type
1	13-A	53	GLU
1	13-A	67	LYS
1	13-A	75	ILE
1	13-A	88	ARG
1	13-A	106	THR
1	13-A	159	SER
1	13-A	244	SER
1	13-A	251	GLU
1	13-A	275	GLN
1	13-A	297	THR
1	13-B	13	ILE
1	13-B	16	SER
1	13-B	27	ARG
1	13-B	31	GLU
1	13-B	39	THR
1	13-B	42	THR
1	13-B	68	THR
1	13-B	69	VAL
1	13-B	70	SER
1	13-B	76	SER
1	13-B	107	PHE
1	13-B	157	ARG
1	13-B	243	VAL
1	13-B	244	SER
1	13-B	257	LEU
1	13-B	305	ARG
1	14-A	19	ARG
1	14-A	48	ASP
1	14-A	53	GLU
1	14-A	67	LYS
1	14-A	75	ILE
1	14-A	88	ARG
1	14-A	106	THR
1	14-A	159	SER
1	14-A	244	SER
1	14-A	251	GLU
1	14-A	275	GLN
1	14-A	297	THR
1	14-B	13	ILE
1	14-B	16	SER
1	14-B	27	ARG
1	14-B	31	GLU

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Mol	Chain	Res	Type
1	14-B	39	THR
1	14-B	42	THR
1	14-B	68	THR
1	14-B	69	VAL
1	14-B	70	SER
1	14-B	76	SER
1	14-B	107	PHE
1	14-B	157	ARG
1	14-B	243	VAL
1	14-B	244	SER
1	14-B	257	LEU
1	14-B	305	ARG
1	15-A	19	ARG
1	15-A	48	ASP
1	15-A	53	GLU
1	15-A	67	LYS
1	15-A	75	ILE
1	15-A	88	ARG
1	15-A	106	THR
1	15-A	159	SER
1	15-A	244	SER
1	15-A	251	GLU
1	15-A	275	GLN
1	15-A	297	THR
1	15-B	13	ILE
1	15-B	16	SER
1	15-B	27	ARG
1	15-B	31	GLU
1	15-B	39	THR
1	15-B	42	THR
1	15-B	68	THR
1	15-B	69	VAL
1	15-B	70	SER
1	15-B	76	SER
1	15-B	107	PHE
1	15-B	157	ARG
1	15-B	243	VAL
1	15-B	244	SER
1	15-B	257	LEU
1	15-B	305	ARG
1	16-A	19	ARG
1	16-A	48	ASP

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Mol	Chain	Res	Type
1	16-A	53	GLU
1	16-A	67	LYS
1	16-A	75	ILE
1	16-A	88	ARG
1	16-A	106	THR
1	16-A	159	SER
1	16-A	244	SER
1	16-A	251	GLU
1	16-A	275	GLN
1	16-A	297	THR
1	16-B	13	ILE
1	16-B	16	SER
1	16-B	27	ARG
1	16-B	31	GLU
1	16-B	39	THR
1	16-B	42	THR
1	16-B	68	THR
1	16-B	69	VAL
1	16-B	70	SER
1	16-B	76	SER
1	16-B	107	PHE
1	16-B	157	ARG
1	16-B	243	VAL
1	16-B	244	SER
1	16-B	257	LEU
1	16-B	305	ARG
1	17-A	19	ARG
1	17-A	48	ASP
1	17-A	53	GLU
1	17-A	67	LYS
1	17-A	75	ILE
1	17-A	88	ARG
1	17-A	106	THR
1	17-A	159	SER
1	17-A	244	SER
1	17-A	251	GLU
1	17-A	275	GLN
1	17-A	297	THR
1	17-B	13	ILE
1	17-B	16	SER
1	17-B	27	ARG
1	17-B	31	GLU

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Mol	Chain	Res	Type
1	17-B	39	THR
1	17-B	42	THR
1	17-B	68	THR
1	17-B	69	VAL
1	17-B	70	SER
1	17-B	76	SER
1	17-B	107	PHE
1	17-B	157	ARG
1	17-B	243	VAL
1	17-B	244	SER
1	17-B	257	LEU
1	17-B	305	ARG
1	18-A	19	ARG
1	18-A	48	ASP
1	18-A	53	GLU
1	18-A	67	LYS
1	18-A	75	ILE
1	18-A	88	ARG
1	18-A	106	THR
1	18-A	159	SER
1	18-A	244	SER
1	18-A	251	GLU
1	18-A	275	GLN
1	18-A	297	THR
1	18-B	13	ILE
1	18-B	16	SER
1	18-B	27	ARG
1	18-B	31	GLU
1	18-B	39	THR
1	18-B	42	THR
1	18-B	68	THR
1	18-B	69	VAL
1	18-B	70	SER
1	18-B	76	SER
1	18-B	107	PHE
1	18-B	157	ARG
1	18-B	243	VAL
1	18-B	244	SER
1	18-B	257	LEU
1	18-B	305	ARG
1	19-A	19	ARG
1	19-A	48	ASP

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Mol	Chain	Res	Type
1	19-A	53	GLU
1	19-A	67	LYS
1	19-A	75	ILE
1	19-A	88	ARG
1	19-A	106	THR
1	19-A	159	SER
1	19-A	244	SER
1	19-A	251	GLU
1	19-A	275	GLN
1	19-A	297	THR
1	19-B	13	ILE
1	19-B	16	SER
1	19-B	27	ARG
1	19-B	31	GLU
1	19-B	39	THR
1	19-B	42	THR
1	19-B	68	THR
1	19-B	69	VAL
1	19-B	70	SER
1	19-B	76	SER
1	19-B	107	PHE
1	19-B	157	ARG
1	19-B	243	VAL
1	19-B	244	SER
1	19-B	257	LEU
1	19-B	305	ARG
1	20-A	19	ARG
1	20-A	48	ASP
1	20-A	53	GLU
1	20-A	67	LYS
1	20-A	75	ILE
1	20-A	88	ARG
1	20-A	106	THR
1	20-A	159	SER
1	20-A	244	SER
1	20-A	251	GLU
1	20-A	275	GLN
1	20-A	297	THR
1	20-B	13	ILE
1	20-B	16	SER
1	20-B	27	ARG
1	20-B	31	GLU

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Mol	Chain	Res	Type
1	20-B	39	THR
1	20-B	42	THR
1	20-B	68	THR
1	20-B	69	VAL
1	20-B	70	SER
1	20-B	76	SER
1	20-B	107	PHE
1	20-B	157	ARG
1	20-B	243	VAL
1	20-B	244	SER
1	20-B	257	LEU
1	20-B	305	ARG
1	21-A	19	ARG
1	21-A	48	ASP
1	21-A	53	GLU
1	21-A	67	LYS
1	21-A	75	ILE
1	21-A	88	ARG
1	21-A	106	THR
1	21-A	159	SER
1	21-A	244	SER
1	21-A	251	GLU
1	21-A	275	GLN
1	21-A	297	THR
1	21-B	13	ILE
1	21-B	16	SER
1	21-B	27	ARG
1	21-B	31	GLU
1	21-B	39	THR
1	21-B	42	THR
1	21-B	68	THR
1	21-B	69	VAL
1	21-B	70	SER
1	21-B	76	SER
1	21-B	107	PHE
1	21-B	157	ARG
1	21-B	243	VAL
1	21-B	244	SER
1	21-B	257	LEU
1	21-B	305	ARG
1	22-A	19	ARG
1	22-A	48	ASP

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Mol	Chain	Res	Type
1	22-A	53	GLU
1	22-A	67	LYS
1	22-A	75	ILE
1	22-A	88	ARG
1	22-A	106	THR
1	22-A	159	SER
1	22-A	244	SER
1	22-A	251	GLU
1	22-A	275	GLN
1	22-A	297	THR
1	22-B	13	ILE
1	22-B	16	SER
1	22-B	27	ARG
1	22-B	31	GLU
1	22-B	39	THR
1	22-B	42	THR
1	22-B	68	THR
1	22-B	69	VAL
1	22-B	70	SER
1	22-B	76	SER
1	22-B	107	PHE
1	22-B	157	ARG
1	22-B	243	VAL
1	22-B	244	SER
1	22-B	257	LEU
1	22-B	305	ARG
1	23-A	19	ARG
1	23-A	48	ASP
1	23-A	53	GLU
1	23-A	67	LYS
1	23-A	75	ILE
1	23-A	88	ARG
1	23-A	106	THR
1	23-A	159	SER
1	23-A	244	SER
1	23-A	251	GLU
1	23-A	275	GLN
1	23-A	297	THR
1	23-B	13	ILE
1	23-B	16	SER
1	23-B	27	ARG
1	23-B	31	GLU

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Mol	Chain	Res	Type
1	23-B	39	THR
1	23-B	42	THR
1	23-B	68	THR
1	23-B	69	VAL
1	23-B	70	SER
1	23-B	76	SER
1	23-B	107	PHE
1	23-B	157	ARG
1	23-B	243	VAL
1	23-B	244	SER
1	23-B	257	LEU
1	23-B	305	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	89	HIS
1	1-A	220	ASN
1	1-A	285	ASN
1	1-B	30	GLN
1	1-B	292	ASN
1	2-A	125	GLN
1	2-A	220	ASN
1	2-A	285	ASN
1	2-B	85	GLN
1	2-B	307	GLN
1	3-A	220	ASN
1	3-A	272	GLN
1	3-A	275	GLN
1	3-A	285	ASN
1	3-B	292	ASN
1	4-A	220	ASN
1	4-A	254	GLN
1	4-A	272	GLN
1	4-A	275	GLN
1	4-A	285	ASN
1	4-B	233	GLN
1	4-B	254	GLN
1	5-A	272	GLN
1	5-A	285	ASN
1	5-B	85	GLN
1	5-B	196	HIS

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Mol	Chain	Res	Type
1	5-B	233	GLN
1	5-B	254	GLN
1	5-B	275	GLN
1	5-B	292	ASN
1	6-A	125	GLN
1	6-A	202	HIS
1	6-A	285	ASN
1	7-A	125	GLN
1	7-A	196	HIS
1	7-A	285	ASN
1	7-B	30	GLN
1	7-B	36	HIS
1	7-B	103	ASN
1	7-B	292	ASN
1	7-B	307	GLN
1	8-A	125	GLN
1	8-A	272	GLN
1	8-A	275	GLN
1	8-A	285	ASN
1	9-A	125	GLN
1	9-A	196	HIS
1	9-A	275	GLN
1	9-A	285	ASN
1	9-B	125	GLN
1	9-B	275	GLN
1	10-A	103	ASN
1	10-A	202	HIS
1	10-B	125	GLN
1	10-B	233	GLN
1	11-A	125	GLN
1	11-A	275	GLN
1	11-B	307	GLN
1	12-A	30	GLN
1	12-A	220	ASN
1	12-A	285	ASN
1	12-B	30	GLN
1	12-B	285	ASN
1	13-A	125	GLN
1	13-A	196	HIS
1	13-A	275	GLN
1	13-A	285	ASN
1	13-B	30	GLN

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Mol	Chain	Res	Type
1	13-B	275	GLN
1	14-A	89	HIS
1	14-A	103	ASN
1	14-A	202	HIS
1	14-A	275	GLN
1	14-A	285	ASN
1	14-B	59	ASN
1	14-B	254	GLN
1	15-A	125	GLN
1	15-A	172	GLN
1	15-A	220	ASN
1	15-A	275	GLN
1	15-A	285	ASN
1	15-B	196	HIS
1	15-B	233	GLN
1	15-B	254	GLN
1	15-B	285	ASN
1	15-B	307	GLN
1	16-A	85	GLN
1	16-A	103	ASN
1	16-A	196	HIS
1	16-A	220	ASN
1	16-A	272	GLN
1	16-A	285	ASN
1	16-B	254	GLN
1	16-B	275	GLN
1	17-A	59	ASN
1	17-A	125	GLN
1	17-A	202	HIS
1	17-A	220	ASN
1	17-A	272	GLN
1	17-A	285	ASN
1	17-B	85	GLN
1	17-B	303	ASN
1	18-A	125	GLN
1	18-A	272	GLN
1	18-A	285	ASN
1	18-B	307	GLN
1	19-A	196	HIS
1	19-A	220	ASN
1	19-A	285	ASN
1	19-B	30	GLN

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Mol	Chain	Res	Type
1	19-B	202	HIS
1	19-B	307	GLN
1	20-A	220	ASN
1	20-A	272	GLN
1	20-A	275	GLN
1	20-A	285	ASN
1	20-B	233	GLN
1	20-B	285	ASN
1	20-B	307	GLN
1	21-A	220	ASN
1	21-A	272	GLN
1	21-B	233	GLN
1	21-B	307	GLN
1	22-A	125	GLN
1	22-A	202	HIS
1	22-A	285	ASN
1	22-B	233	GLN
1	22-B	275	GLN
1	22-B	285	ASN
1	22-B	307	GLN
1	23-A	85	GLN
1	23-A	125	GLN
1	23-A	272	GLN
1	23-A	275	GLN
1	23-A	285	ASN
1	23-B	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	4-A	401	3	13,13,13	1.24	1 (7%)	19,21,21	2.34	7 (36%)
2	AHD	15-B	401	3	13,13,13	1.54	2 (15%)	19,21,21	1.43	5 (26%)
2	AHD	8-A	401	3	13,13,13	1.33	1 (7%)	19,21,21	2.47	7 (36%)
2	AHD	6-B	401	3	13,13,13	1.64	2 (15%)	19,21,21	1.28	2 (10%)
2	AHD	13-B	401	3	13,13,13	1.72	3 (23%)	19,21,21	1.62	4 (21%)
2	AHD	18-B	401	3	13,13,13	1.46	1 (7%)	19,21,21	1.69	4 (21%)
2	AHD	9-B	401	3	13,13,13	1.73	3 (23%)	19,21,21	1.69	4 (21%)
2	AHD	9-A	401	3	13,13,13	1.53	1 (7%)	19,21,21	1.94	7 (36%)
2	AHD	13-A	401	3	13,13,13	1.45	2 (15%)	19,21,21	1.93	5 (26%)
2	AHD	19-A	401	3	13,13,13	1.38	1 (7%)	19,21,21	1.60	2 (10%)
2	AHD	3-A	401	3	13,13,13	1.38	1 (7%)	19,21,21	1.91	4 (21%)
2	AHD	20-A	401	3	13,13,13	1.61	1 (7%)	19,21,21	1.68	6 (31%)
2	AHD	16-B	401	3	13,13,13	1.48	1 (7%)	19,21,21	1.83	5 (26%)
2	AHD	5-A	401	3	13,13,13	1.43	1 (7%)	19,21,21	1.68	3 (15%)
2	AHD	18-A	401	3	13,13,13	1.24	1 (7%)	19,21,21	1.91	6 (31%)
2	AHD	16-A	401	3	13,13,13	1.43	2 (15%)	19,21,21	1.84	6 (31%)
2	AHD	1-A	401	3	13,13,13	1.50	1 (7%)	19,21,21	1.81	3 (15%)
2	AHD	19-B	401	3	13,13,13	1.54	2 (15%)	19,21,21	1.58	4 (21%)
2	AHD	10-A	401	3	13,13,13	1.66	2 (15%)	19,21,21	1.26	2 (10%)
2	AHD	22-B	401	3	13,13,13	1.56	3 (23%)	19,21,21	1.60	4 (21%)
2	AHD	21-A	401	3	13,13,13	1.43	1 (7%)	19,21,21	1.94	6 (31%)
2	AHD	7-B	401	3	13,13,13	1.52	3 (23%)	19,21,21	1.63	5 (26%)
2	AHD	2-A	401	3	13,13,13	1.61	2 (15%)	19,21,21	1.91	5 (26%)
2	AHD	3-B	401	3	13,13,13	1.55	2 (15%)	19,21,21	1.56	4 (21%)
2	AHD	7-A	401	3	13,13,13	1.51	1 (7%)	19,21,21	1.98	4 (21%)
2	AHD	20-B	401	3	13,13,13	1.68	2 (15%)	19,21,21	1.38	4 (21%)

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	1.56	1 (7%)	19,21,21	1.46	4 (21%)
2	AHD	11-A	401	3	13,13,13	1.47	1 (7%)	19,21,21	1.80	4 (21%)
2	AHD	12-B	401	3	13,13,13	1.61	3 (23%)	19,21,21	1.65	3 (15%)
2	AHD	23-B	401	3	13,13,13	1.60	3 (23%)	19,21,21	1.58	4 (21%)
2	AHD	15-A	401	3	13,13,13	1.35	1 (7%)	19,21,21	1.71	4 (21%)
2	AHD	12-A	401	3	13,13,13	1.31	1 (7%)	19,21,21	1.83	5 (26%)
2	AHD	14-A	401	3	13,13,13	1.44	1 (7%)	19,21,21	1.57	2 (10%)
2	AHD	17-B	401	3	13,13,13	1.60	2 (15%)	19,21,21	1.41	4 (21%)
2	AHD	10-B	401	3	13,13,13	1.68	2 (15%)	19,21,21	1.50	4 (21%)
2	AHD	21-B	401	3	13,13,13	1.56	1 (7%)	19,21,21	1.52	5 (26%)
2	AHD	4-B	401	3	13,13,13	1.59	2 (15%)	19,21,21	1.61	4 (21%)
2	AHD	8-B	401	3	13,13,13	1.54	1 (7%)	19,21,21	1.52	4 (21%)
2	AHD	6-A	401	3	13,13,13	1.55	2 (15%)	19,21,21	1.81	4 (21%)
2	AHD	23-A	401	3	13,13,13	1.31	1 (7%)	19,21,21	1.83	5 (26%)
2	AHD	17-A	401	3	13,13,13	1.40	1 (7%)	19,21,21	1.96	6 (31%)
2	AHD	22-A	401	3	13,13,13	1.40	1 (7%)	19,21,21	1.91	3 (15%)
2	AHD	11-B	401	3	13,13,13	1.59	3 (23%)	19,21,21	1.56	4 (21%)
2	AHD	2-B	401	3	13,13,13	1.51	1 (7%)	19,21,21	1.36	4 (21%)
2	AHD	14-B	401	3	13,13,13	1.61	1 (7%)	19,21,21	1.60	4 (21%)
2	AHD	5-B	401	3	13,13,13	1.51	1 (7%)	19,21,21	1.55	4 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AHD	4-A	401	3	-	4/23/23/23	-
2	AHD	15-B	401	3	-	0/23/23/23	-
2	AHD	8-A	401	3	-	5/23/23/23	-
2	AHD	6-B	401	3	-	2/23/23/23	-
2	AHD	13-B	401	3	-	2/23/23/23	-
2	AHD	18-B	401	3	-	3/23/23/23	-
2	AHD	9-B	401	3	-	2/23/23/23	-
2	AHD	9-A	401	3	-	3/23/23/23	-
2	AHD	13-A	401	3	-	3/23/23/23	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AHD	14-B	401	3	-	2/23/23/23	-
2	AHD	5-B	401	3	-	3/23/23/23	-

All (73) 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
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	-4.21	1.39	1.44
2	9-A	401	AHD	O13-C8	-4.11	1.39	1.44
2	13-B	401	AHD	O13-C8	-4.11	1.39	1.44
2	6-A	401	AHD	O13-C8	-4.08	1.39	1.44
2	20-B	401	AHD	O13-C8	-4.06	1.39	1.44
2	2-A	401	AHD	O13-C8	-4.04	1.39	1.44
2	1-A	401	AHD	O13-C8	-4.04	1.39	1.44
2	9-B	401	AHD	O13-C8	-3.94	1.39	1.44
2	14-A	401	AHD	O13-C8	-3.93	1.39	1.44
2	11-A	401	AHD	O13-C8	-3.93	1.39	1.44
2	5-A	401	AHD	O13-C8	-3.91	1.39	1.44
2	7-A	401	AHD	O13-C8	-3.90	1.39	1.44
2	12-B	401	AHD	O13-C8	-3.88	1.39	1.44
2	3-A	401	AHD	O13-C8	-3.84	1.39	1.44
2	11-B	401	AHD	O13-C8	-3.80	1.39	1.44
2	1-B	401	AHD	O13-C8	-3.78	1.40	1.44
2	15-B	401	AHD	O13-C8	-3.77	1.40	1.44
2	5-B	401	AHD	O13-C8	-3.75	1.40	1.44
2	17-B	401	AHD	O13-C8	-3.74	1.40	1.44
2	19-B	401	AHD	O13-C8	-3.73	1.40	1.44
2	19-A	401	AHD	O13-C8	-3.70	1.40	1.44
2	21-B	401	AHD	O13-C8	-3.67	1.40	1.44
2	22-B	401	AHD	O13-C8	-3.67	1.40	1.44
2	17-A	401	AHD	O13-C8	-3.67	1.40	1.44
2	7-B	401	AHD	O13-C8	-3.66	1.40	1.44
2	6-B	401	AHD	O13-C8	-3.66	1.40	1.44
2	14-B	401	AHD	O13-C8	-3.61	1.40	1.44
2	12-A	401	AHD	O13-C8	-3.60	1.40	1.44
2	16-B	401	AHD	O13-C8	-3.59	1.40	1.44
2	23-B	401	AHD	O13-C8	-3.58	1.40	1.44
2	23-A	401	AHD	O13-C8	-3.57	1.40	1.44
2	8-B	401	AHD	O13-C8	-3.57	1.40	1.44
2	4-B	401	AHD	O13-C8	-3.54	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-B	401	AHD	O13-C8	-3.51	1.40	1.44
2	15-A	401	AHD	O13-C8	-3.48	1.40	1.44
2	2-B	401	AHD	O13-C8	-3.45	1.40	1.44
2	22-A	401	AHD	O13-C8	-3.45	1.40	1.44
2	13-A	401	AHD	O13-C8	-3.33	1.40	1.44
2	8-A	401	AHD	O13-C8	-3.24	1.40	1.44
2	16-A	401	AHD	O13-C8	-3.23	1.40	1.44
2	18-B	401	AHD	O13-C8	-3.21	1.40	1.44
2	18-A	401	AHD	O13-C8	-2.98	1.41	1.44
2	4-A	401	AHD	O13-C8	-2.75	1.41	1.44
2	10-A	401	AHD	P14-C8	2.53	1.86	1.85
2	2-A	401	AHD	P14-C8	2.44	1.86	1.85
2	9-B	401	AHD	P14-O17	2.44	1.54	1.50
2	9-B	401	AHD	P9-O12	-2.26	1.49	1.54
2	10-B	401	AHD	P14-O15	-2.25	1.49	1.54
2	12-B	401	AHD	P9-O12	-2.23	1.49	1.54
2	16-A	401	AHD	P14-C8	2.20	1.86	1.85
2	22-B	401	AHD	P9-O12	-2.19	1.49	1.54
2	20-B	401	AHD	P9-O12	-2.18	1.49	1.54
2	7-B	401	AHD	P14-O15	-2.17	1.49	1.54
2	13-B	401	AHD	P14-C8	-2.15	1.83	1.85
2	13-B	401	AHD	P9-O12	-2.15	1.49	1.54
2	11-B	401	AHD	P14-O15	-2.14	1.49	1.54
2	4-B	401	AHD	P14-O15	-2.14	1.49	1.54
2	11-B	401	AHD	P9-O12	-2.14	1.49	1.54
2	6-B	401	AHD	P14-O15	-2.13	1.49	1.54
2	7-B	401	AHD	P9-O12	-2.10	1.49	1.54
2	3-B	401	AHD	P9-O10	-2.08	1.49	1.54
2	13-A	401	AHD	P14-C8	2.07	1.86	1.85
2	6-A	401	AHD	P14-C8	2.07	1.86	1.85
2	15-B	401	AHD	P14-O15	-2.06	1.49	1.54
2	23-B	401	AHD	P9-O12	-2.05	1.49	1.54
2	19-B	401	AHD	P9-O12	-2.03	1.49	1.54
2	17-B	401	AHD	P14-O15	-2.02	1.49	1.54
2	12-B	401	AHD	P14-O15	-2.02	1.49	1.54
2	22-B	401	AHD	P14-O15	-2.02	1.49	1.54
2	23-B	401	AHD	P9-C8	2.01	1.86	1.85

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	401	AHD	P14-C8-P9	-5.85	102.24	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12-A	401	AHD	C2-C7-C8	-5.84	105.88	116.02
2	3-A	401	AHD	C2-C7-C8	-5.81	105.93	116.02
2	6-A	401	AHD	C2-C7-C8	-5.45	106.56	116.02
2	2-A	401	AHD	C2-C7-C8	-5.42	106.61	116.02
2	8-A	401	AHD	O10-P9-O11	-5.14	100.38	112.96
2	4-A	401	AHD	C2-C7-C8	-5.07	107.22	116.02
2	23-A	401	AHD	C2-C7-C8	-4.79	107.70	116.02
2	16-B	401	AHD	P14-C8-P9	-4.76	104.19	112.72
2	22-A	401	AHD	O15-P14-C8	4.67	116.47	106.19
2	14-A	401	AHD	C2-C7-C8	-4.63	107.98	116.02
2	22-A	401	AHD	C2-C7-C8	-4.50	108.21	116.02
2	19-A	401	AHD	C2-C7-C8	-4.48	108.24	116.02
2	4-A	401	AHD	P14-C8-P9	-4.45	104.75	112.72
2	1-A	401	AHD	O10-P9-C8	4.43	115.95	106.19
2	18-B	401	AHD	P14-C8-P9	-4.41	104.82	112.72
2	21-A	401	AHD	C2-C7-C8	-4.32	108.52	116.02
2	11-A	401	AHD	P14-C8-P9	-4.29	105.04	112.72
2	13-A	401	AHD	P14-C8-P9	-4.28	105.05	112.72
2	5-A	401	AHD	C2-C7-C8	-4.26	108.61	116.02
2	16-B	401	AHD	C2-C7-C8	-4.16	108.79	116.02
2	3-B	401	AHD	C2-C7-C8	-4.09	108.91	116.02
2	14-B	401	AHD	P14-C8-P9	-4.05	105.47	112.72
2	16-A	401	AHD	O15-P14-C8	4.02	115.03	106.19
2	12-B	401	AHD	C2-C7-C8	-3.96	109.13	116.02
2	8-A	401	AHD	C2-C7-C8	-3.88	109.28	116.02
2	17-A	401	AHD	C7-C2-C3	-3.86	104.59	112.21
2	20-A	401	AHD	P14-C8-P9	-3.86	105.80	112.72
2	16-A	401	AHD	O10-P9-C8	3.86	114.68	106.19
2	8-B	401	AHD	C2-C7-C8	-3.84	109.34	116.02
2	9-A	401	AHD	O10-P9-C8	3.84	114.64	106.19
2	19-B	401	AHD	C2-C7-C8	-3.80	109.42	116.02
2	9-B	401	AHD	P14-C8-P9	-3.78	105.95	112.72
2	4-A	401	AHD	O10-P9-O11	-3.76	103.76	112.96
2	8-A	401	AHD	P14-C8-P9	-3.75	106.01	112.72
2	15-A	401	AHD	O10-P9-C8	3.75	114.43	106.19
2	9-A	401	AHD	P14-C8-P9	-3.75	106.01	112.72
2	1-A	401	AHD	O15-P14-C8	3.74	114.41	106.19
2	18-A	401	AHD	C2-C7-C8	-3.73	109.54	116.02
2	17-B	401	AHD	C2-C7-C8	-3.63	109.72	116.02
2	7-B	401	AHD	C2-C7-C8	-3.62	109.73	116.02
2	13-B	401	AHD	P14-C8-P9	-3.57	106.32	112.72
2	15-A	401	AHD	C2-C7-C8	-3.56	109.84	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12-B	401	AHD	P14-C8-P9	-3.56	106.35	112.72
2	7-B	401	AHD	P14-C8-P9	-3.53	106.40	112.72
2	18-A	401	AHD	P14-C8-P9	-3.52	106.42	112.72
2	19-B	401	AHD	P14-C8-P9	-3.52	106.42	112.72
2	22-B	401	AHD	P14-C8-P9	-3.47	106.51	112.72
2	17-A	401	AHD	O10-P9-C8	3.46	113.79	106.19
2	4-B	401	AHD	O16-P14-C8	3.44	113.76	106.19
2	9-B	401	AHD	C2-C7-C8	-3.43	110.07	116.02
2	8-A	401	AHD	O10-P9-C8	3.41	113.69	106.19
2	22-B	401	AHD	C2-C7-C8	-3.40	110.11	116.02
2	11-A	401	AHD	C2-C7-C8	-3.40	110.12	116.02
2	10-B	401	AHD	C2-C7-C8	-3.37	110.17	116.02
2	4-B	401	AHD	P14-C8-P9	-3.35	106.72	112.72
2	4-A	401	AHD	O10-P9-C8	3.28	113.42	106.19
2	11-B	401	AHD	P14-C8-P9	-3.27	106.86	112.72
2	18-A	401	AHD	O10-P9-O11	-3.26	104.98	112.96
2	23-B	401	AHD	P14-C8-P9	-3.25	106.90	112.72
2	2-A	401	AHD	O15-P14-C8	3.24	113.31	106.19
2	1-B	401	AHD	P14-C8-P9	-3.23	106.93	112.72
2	17-A	401	AHD	O10-P9-O11	-3.23	105.05	112.96
2	5-B	401	AHD	P14-C8-P9	-3.23	106.94	112.72
2	9-A	401	AHD	C2-C7-C8	-3.22	110.43	116.02
2	13-A	401	AHD	O10-P9-O11	-3.17	105.20	112.96
2	7-A	401	AHD	O15-P14-C8	3.14	113.11	106.19
2	6-A	401	AHD	P14-C8-P9	-3.10	107.16	112.72
2	20-B	401	AHD	C2-C7-C8	-3.09	110.66	116.02
2	3-B	401	AHD	P14-C8-P9	-3.08	107.21	112.72
2	23-B	401	AHD	C2-C7-C8	-3.07	110.68	116.02
2	1-B	401	AHD	C2-C7-C8	-3.05	110.72	116.02
2	7-A	401	AHD	O10-P9-O11	-3.04	105.52	112.96
2	5-A	401	AHD	O15-P14-C8	3.03	112.86	106.19
2	23-B	401	AHD	O16-P14-C8	3.03	112.86	106.19
2	21-B	401	AHD	C2-C7-C8	-3.03	110.75	116.02
2	5-B	401	AHD	C2-C7-C8	-3.02	110.78	116.02
2	3-A	401	AHD	P14-C8-P9	-3.01	107.32	112.72
2	8-A	401	AHD	O15-P14-C8	3.01	112.82	106.19
2	13-A	401	AHD	O15-P14-C8	3.01	112.81	106.19
2	18-B	401	AHD	C2-C7-C8	-3.01	110.80	116.02
2	13-B	401	AHD	O16-P14-C8	3.00	112.79	106.19
2	21-A	401	AHD	O10-P9-O11	-2.98	105.65	112.96
2	13-B	401	AHD	C2-C7-C8	-2.97	110.86	116.02
2	15-B	401	AHD	P14-C8-P9	-2.97	107.40	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-B	401	AHD	C2-C7-C8	-2.96	110.88	116.02
2	21-B	401	AHD	O16-P14-C8	2.96	112.69	106.19
2	18-A	401	AHD	O17-P14-C8	-2.95	102.25	109.82
2	17-A	401	AHD	P9-C8-O13	2.95	114.18	107.42
2	14-B	401	AHD	C2-C7-C8	-2.95	110.89	116.02
2	8-A	401	AHD	P9-C8-O13	2.94	114.14	107.42
2	11-B	401	AHD	C2-C7-C8	-2.92	110.94	116.02
2	8-B	401	AHD	P14-C8-P9	-2.92	107.49	112.72
2	16-A	401	AHD	P14-C8-P9	-2.92	107.49	112.72
2	8-A	401	AHD	O12-P9-C8	2.92	112.60	106.19
2	6-B	401	AHD	O16-P14-C8	2.91	112.60	106.19
2	7-A	401	AHD	C2-C7-C8	-2.91	110.96	116.02
2	11-A	401	AHD	O10-P9-O11	-2.89	105.87	112.96
2	3-A	401	AHD	O15-P14-C8	2.85	112.46	106.19
2	21-A	401	AHD	O15-P14-C8	2.85	112.45	106.19
2	23-A	401	AHD	P14-C8-P9	-2.85	107.62	112.72
2	2-B	401	AHD	O16-P14-C8	2.82	112.39	106.19
2	20-A	401	AHD	O10-P9-O11	-2.79	106.12	112.96
2	9-A	401	AHD	C7-C2-C3	-2.78	106.72	112.21
2	21-A	401	AHD	O17-P14-C8	-2.77	102.71	109.82
2	17-A	401	AHD	O15-P14-C8	2.77	112.29	106.19
2	21-A	401	AHD	O10-P9-C8	2.77	112.28	106.19
2	15-B	401	AHD	C2-C7-C8	-2.76	111.22	116.02
2	23-A	401	AHD	O10-P9-O11	-2.75	106.22	112.96
2	13-A	401	AHD	C2-C7-C8	-2.75	111.24	116.02
2	4-B	401	AHD	C2-C7-C8	-2.75	111.24	116.02
2	7-B	401	AHD	O16-P14-C8	2.73	112.20	106.19
2	6-B	401	AHD	C2-C7-C8	-2.71	111.31	116.02
2	19-A	401	AHD	O10-P9-C8	2.70	112.12	106.19
2	3-B	401	AHD	O16-P14-C8	2.69	112.11	106.19
2	15-A	401	AHD	O15-P14-C8	2.67	112.07	106.19
2	4-A	401	AHD	O17-P14-C8	-2.65	103.02	109.82
2	17-A	401	AHD	P14-C8-P9	-2.65	107.97	112.72
2	16-A	401	AHD	O10-P9-O11	-2.64	106.49	112.96
2	10-A	401	AHD	C2-C7-C8	-2.63	111.46	116.02
2	2-A	401	AHD	O10-P9-C8	2.60	111.91	106.19
2	5-A	401	AHD	O10-P9-C8	2.60	111.91	106.19
2	6-A	401	AHD	O15-P14-C8	2.59	111.89	106.19
2	17-B	401	AHD	O16-P14-C8	2.58	111.86	106.19
2	11-B	401	AHD	O16-P14-C8	2.57	111.83	106.19
2	19-B	401	AHD	O16-P14-C8	2.55	111.80	106.19
2	5-B	401	AHD	O16-P14-C8	2.55	111.80	106.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-B	401	AHD	O16-P14-O17	-2.55	106.72	112.96
2	18-B	401	AHD	O16-P14-C8	2.54	111.77	106.19
2	22-B	401	AHD	O16-P14-C8	2.52	111.74	106.19
2	14-A	401	AHD	P14-C8-P9	-2.52	108.21	112.72
2	9-A	401	AHD	O15-P14-C8	2.48	111.65	106.19
2	20-A	401	AHD	O10-P9-C8	2.47	111.62	106.19
2	11-A	401	AHD	O17-P14-C8	-2.46	103.51	109.82
2	21-B	401	AHD	O16-P14-O17	-2.46	106.94	112.96
2	20-B	401	AHD	P14-C8-P9	-2.46	108.32	112.72
2	1-B	401	AHD	O16-P14-C8	2.46	111.59	106.19
2	12-B	401	AHD	O16-P14-O17	-2.42	107.03	112.96
2	20-A	401	AHD	C7-C2-C3	-2.41	107.45	112.21
2	20-A	401	AHD	O15-P14-C8	2.40	111.46	106.19
2	20-B	401	AHD	O16-P14-O17	-2.38	107.14	112.96
2	23-A	401	AHD	O15-P14-C8	2.36	111.38	106.19
2	8-B	401	AHD	O16-P14-O17	-2.35	107.21	112.96
2	16-B	401	AHD	O16-P14-O17	-2.33	107.24	112.96
2	12-A	401	AHD	P14-C8-P9	-2.33	108.55	112.72
2	14-B	401	AHD	O16-P14-O17	-2.32	107.28	112.96
2	16-A	401	AHD	P9-C8-O13	2.32	112.72	107.42
2	3-A	401	AHD	O10-P9-O11	-2.31	107.29	112.96
2	16-B	401	AHD	O10-P9-O12	2.31	114.76	108.24
2	14-B	401	AHD	O16-P14-C8	2.30	111.26	106.19
2	18-A	401	AHD	O10-P9-C8	2.30	111.25	106.19
2	23-B	401	AHD	O16-P14-O17	-2.29	107.34	112.96
2	9-B	401	AHD	O16-P14-C8	2.29	111.22	106.19
2	4-A	401	AHD	O10-P9-O12	2.28	114.67	108.24
2	1-B	401	AHD	O16-P14-O17	-2.26	107.42	112.96
2	23-A	401	AHD	O17-P14-C8	-2.26	104.03	109.82
2	10-B	401	AHD	C7-C2-C3	-2.26	107.75	112.21
2	3-B	401	AHD	O16-P14-O17	-2.25	107.44	112.96
2	10-B	401	AHD	P14-C8-P9	-2.24	108.70	112.72
2	13-A	401	AHD	C7-C2-C3	-2.24	107.78	112.21
2	21-A	401	AHD	P14-C8-P9	-2.24	108.70	112.72
2	2-B	401	AHD	O16-P14-O17	-2.24	107.48	112.96
2	4-B	401	AHD	O16-P14-O17	-2.21	107.55	112.96
2	10-A	401	AHD	P14-C8-P9	-2.20	108.78	112.72
2	18-B	401	AHD	O16-P14-O17	-2.19	107.58	112.96
2	20-B	401	AHD	O16-P14-C8	2.19	111.01	106.19
2	5-B	401	AHD	O16-P14-O17	-2.19	107.60	112.96
2	12-A	401	AHD	O10-P9-O11	-2.18	107.62	112.96
2	18-A	401	AHD	O15-P14-C8	2.17	110.97	106.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-B	401	AHD	O16-P14-C8	2.17	110.97	106.19
2	11-B	401	AHD	O10-P9-O12	2.17	114.35	108.24
2	1-A	401	AHD	P14-C8-P9	-2.17	108.84	112.72
2	10-B	401	AHD	O16-P14-O17	-2.17	107.65	112.96
2	16-B	401	AHD	O16-P14-C8	2.17	110.96	106.19
2	22-A	401	AHD	O10-P9-O11	-2.15	107.70	112.96
2	2-B	401	AHD	P14-C8-P9	-2.15	108.88	112.72
2	17-B	401	AHD	O16-P14-O17	-2.14	107.72	112.96
2	2-A	401	AHD	P14-C8-P9	-2.14	108.89	112.72
2	2-A	401	AHD	O12-P9-C8	2.13	110.88	106.19
2	7-B	401	AHD	O16-P14-O17	-2.11	107.78	112.96
2	15-B	401	AHD	O16-P14-C8	2.10	110.82	106.19
2	22-B	401	AHD	O10-P9-O12	2.10	114.17	108.24
2	7-B	401	AHD	O10-P9-O12	2.10	114.15	108.24
2	12-A	401	AHD	O15-P14-C8	2.10	110.80	106.19
2	21-B	401	AHD	P14-C8-P9	-2.09	108.97	112.72
2	20-A	401	AHD	O15-P14-O17	-2.09	107.84	112.96
2	15-B	401	AHD	C7-C2-C3	-2.09	108.08	112.21
2	17-B	401	AHD	P14-C8-P9	-2.07	109.01	112.72
2	4-A	401	AHD	O15-P14-C8	2.05	110.71	106.19
2	9-A	401	AHD	P9-C8-O13	2.05	112.12	107.42
2	19-B	401	AHD	O16-P14-O17	-2.04	107.95	112.96
2	21-B	401	AHD	O17-P14-C8	-2.04	104.59	109.82
2	6-A	401	AHD	O10-P9-O11	-2.03	107.98	112.96
2	16-A	401	AHD	C2-C7-C8	-2.03	112.50	116.02
2	12-A	401	AHD	O10-P9-C8	2.02	110.64	106.19
2	15-A	401	AHD	O10-P9-O11	-2.01	108.03	112.96
2	9-A	401	AHD	O10-P9-O11	-2.01	108.04	112.96
2	15-B	401	AHD	O16-P14-O17	-2.01	108.04	112.96
2	13-B	401	AHD	P9-C8-O13	2.01	112.02	107.42

There are no chirality outliers.

All (150) 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

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Mol	Chain	Res	Type	Atoms
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	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	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	22-A	401	AHD	C2-C7-C8-P14
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

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Mol	Chain	Res	Type	Atoms
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
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-O13
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-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	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

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Mol	Chain	Res	Type	Atoms
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	12-A	401	AHD	C7-C8-P14-O17
2	12-A	401	AHD	P9-C8-P14-O15
2	12-A	401	AHD	P9-C8-P14-O17
2	15-A	401	AHD	C7-C8-P14-O17
2	18-A	401	AHD	C7-C8-P14-O17
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	17-A	401	AHD	C2-C7-C8-P14
2	4-B	401	AHD	C2-C7-C8-P9
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	10-B	401	AHD	C2-C7-C8-P9
2	13-B	401	AHD	C2-C7-C8-P14
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-P14
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	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	18-A	401	AHD	P9-C8-P14-O15
2	18-A	401	AHD	O13-C8-P14-O15
2	1-B	401	AHD	C2-C7-C8-P14
2	5-B	401	AHD	C2-C7-C8-P9
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
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	15-A	401	AHD	C7-C2-C3-N4
2	13-A	401	AHD	C3-C2-C7-C8

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Mol	Chain	Res	Type	Atoms
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	10-A	401	AHD	O13-C8-P9-O11
2	13-A	401	AHD	C7-C8-P14-O17
2	14-A	401	AHD	C7-C8-P14-O17
2	18-A	401	AHD	P9-C8-P14-O16
2	18-A	401	AHD	P9-C8-P14-O17
2	20-A	401	AHD	O13-C8-P9-O11
2	3-A	401	AHD	C2-C7-C8-P14
2	12-A	401	AHD	C2-C7-C8-P14
2	3-B	401	AHD	C2-C7-C8-P14
2	19-B	401	AHD	C2-C7-C8-P9
2	20-B	401	AHD	C2-C7-C8-P14
2	22-B	401	AHD	C2-C7-C8-P9
2	17-A	401	AHD	C7-C2-C3-N4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 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%)	1.06	43 (15%) 5 5	1, 1, 2, 2	283 (100%)
1	1-B	296/318 (93%)	0.78	30 (10%) 12 13	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%)	0.92	73 (12%) 8 8	1, 1, 2, 2	579 (100%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	13	ILE	7.1
1	1-A	158	ASP	7.0
1	1-B	14	GLY	6.8
1	1-A	49	ALA	5.7
1	1-A	298	ALA	5.3
1	1-B	307	GLN	4.6
1	1-B	15	ARG	4.4
1	1-A	297	THR	4.3
1	1-B	301	ASP	4.2
1	1-B	305	ARG	4.0
1	1-B	302	VAL	3.7
1	1-A	68	THR	3.7
1	1-A	48	ASP	3.5
1	1-A	295	TYR	3.4
1	1-A	69	VAL	3.2
1	1-A	77	TYR	3.2
1	1-B	158	ASP	3.2
1	1-A	106	THR	3.2
1	1-A	103	ASN	3.1
1	1-B	298	ALA	3.1
1	1-A	71	ASP	3.1
1	1-A	60	ALA	3.1
1	1-B	299	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	297	THR	3.0
1	1-A	76	SER	3.0
1	1-A	16	SER	3.0
1	1-A	42	THR	3.0
1	1-A	115	ALA	2.9
1	1-A	47	THR	2.9
1	1-B	244	SER	2.8
1	1-B	308	ALA	2.8
1	1-A	62	VAL	2.8
1	1-B	250	LYS	2.8
1	1-B	42	THR	2.7
1	1-B	45	GLU	2.7
1	1-A	74	TRP	2.6
1	1-A	246	GLU	2.6
1	1-A	66	GLY	2.6
1	1-A	75	ILE	2.6
1	1-A	159	SER	2.6
1	1-B	304	SER	2.6
1	1-A	105	VAL	2.5
1	1-A	22	LEU	2.5
1	1-A	107	PHE	2.5
1	1-B	113	ASP	2.5
1	1-A	61	ALA	2.5
1	1-A	116	LEU	2.5
1	1-A	54	VAL	2.5
1	1-A	88	ARG	2.5
1	1-B	61	ALA	2.4
1	1-A	78	VAL	2.4
1	1-A	73	ARG	2.4
1	1-B	296	LYS	2.4
1	1-A	51	LEU	2.3
1	1-B	306	ILE	2.3
1	1-B	137	GLU	2.3
1	1-B	295	TYR	2.3
1	1-A	67	LYS	2.3
1	1-A	44	VAL	2.2
1	1-B	88	ARG	2.2
1	1-B	115	ALA	2.2
1	1-A	226	ASP	2.2
1	1-A	52	ARG	2.2
1	1-A	296	LYS	2.2
1	1-B	28	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	251	GLU	2.1
1	1-A	55	ILE	2.1
1	1-B	70	SER	2.1
1	1-A	56	ASP	2.1
1	1-A	202	HIS	2.1
1	1-A	101	VAL	2.0
1	1-B	108	VAL	2.0
1	1-B	291	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	23-B	404	1/1	-	-	31,31,31,31	1

6.5 Other polymers [i](#)

There are no such residues in this entry.