Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:27 AM GMT

PDB ID	:	2Q4B
Title	:	Ensemble refinement of the protein crystal structure of selenomethionyl gene product from Arabidopsis thaliana At5g02240 in space group P21212
Authors	:	Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2007-05-31
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

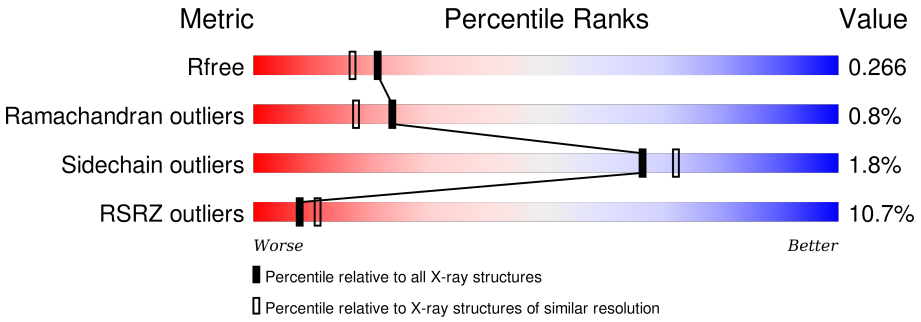
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3939 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	253	11% 91% 5% ·
1	1-B	253	8% 86% 10% ·
1	10-A	253	11% 91% 5% ·
1	10-B	253	8% 89% 8% ·
1	11-A	253	11% 91% 5% ·
1	11-B	253	8% 88% 8% ·
1	12-A	253	11% 91% 5% ·

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Mol	Chain	Length	Quality of chain
1	12-B	253	8% 87% 9%
1	13-A	253	11% 88% 8%
1	13-B	253	8% 81% 15%
1	14-A	253	11% 86% 9%
1	14-B	253	8% 80% 16%
1	15-A	253	11% 83% 12%
1	15-B	253	8% 78% 17%
1	16-A	253	11% 88% 8%
1	16-B	253	8% 80% 15%
1	2-A	253	11% 91% 6%
1	2-B	253	8% 88% 8%
1	3-A	253	11% 89% 7%
1	3-B	253	8% 87% 9%
1	4-A	253	11% 89% 7%
1	4-B	253	8% 89% 7%
1	5-A	253	11% 91% 6%
1	5-B	253	8% 87% 9%
1	6-A	253	11% 89% 6%
1	6-B	253	8% 87% 9%
1	7-A	253	11% 92%
1	7-B	253	8% 86% 10%
1	8-A	253	11% 88% 8%
1	8-B	253	8% 89% 8%
1	9-A	253	11% 92%
1	9-B	253	8% 88% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	1-A	400	X	-	-	-
2	NAP	1-B	401	X	-	-	-
2	NAP	10-A	400	X	-	-	-
2	NAP	10-B	401	X	-	-	-
2	NAP	11-A	400	X	-	-	-
2	NAP	11-B	401	X	-	-	-
2	NAP	12-A	400	X	-	-	-
2	NAP	12-B	401	X	-	-	-
2	NAP	13-A	400	X	-	-	-
2	NAP	13-B	401	X	-	-	-
2	NAP	14-A	400	X	-	-	-
2	NAP	14-B	401	X	-	-	-
2	NAP	15-A	400	X	-	-	-
2	NAP	16-A	400	X	-	-	-
2	NAP	2-A	400	X	-	-	-
2	NAP	2-B	401	X	-	-	-
2	NAP	3-A	400	X	-	-	-
2	NAP	3-B	401	X	-	-	-
2	NAP	4-A	400	X	-	-	-
2	NAP	4-B	401	X	-	-	-
2	NAP	5-A	400	X	-	-	-
2	NAP	5-B	401	X	-	-	-
2	NAP	6-A	400	X	-	-	-
2	NAP	6-B	401	X	-	-	-
2	NAP	7-A	400	X	-	-	-
2	NAP	7-B	401	X	-	-	-
2	NAP	8-A	400	X	-	-	-
2	NAP	8-B	401	X	-	-	-
2	NAP	9-A	400	X	-	-	-
2	NAP	9-B	401	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 66192 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 Protein At5g02240.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	2-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	3-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	4-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	5-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	6-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	7-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	8-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	9-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	10-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	11-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	12-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	13-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	14-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	15-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	16-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			

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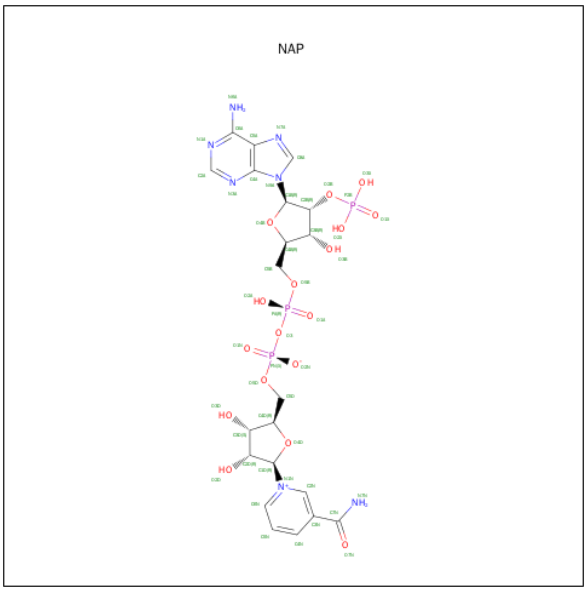
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	2-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	3-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	4-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	5-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	6-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	7-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	8-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	9-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	10-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	11-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	12-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	13-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	14-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	15-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	16-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q94EG6
B	1	SER	-	EXPRESSION TAG	UNP Q94EG6

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	2-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	3-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	4-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	5-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	6-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	7-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	8-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	9-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	10-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	11-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	12-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	13-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	14-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	15-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	16-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	1-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	2-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	3-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	4-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	5-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	6-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	7-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	8-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	9-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	10-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	11-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	12-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	13-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	14-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	15-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	16-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	146	Total	O	0	0
			146	146		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	2-A	147	Total O 147 147	0	0
3	3-A	147	Total O 147 147	0	0
3	4-A	146	Total O 146 146	0	0
3	5-A	147	Total O 147 147	0	0
3	6-A	145	Total O 145 145	0	0
3	7-A	145	Total O 145 145	0	0
3	8-A	146	Total O 146 146	0	0
3	9-A	146	Total O 146 146	0	0
3	10-A	147	Total O 147 147	0	0
3	11-A	146	Total O 146 146	0	0
3	12-A	147	Total O 147 147	0	0
3	13-A	146	Total O 146 146	0	0
3	14-A	146	Total O 146 146	0	0
3	15-A	147	Total O 147 147	0	0
3	16-A	147	Total O 147 147	0	0
3	1-B	223	Total O 223 223	0	0
3	2-B	222	Total O 222 222	0	0
3	3-B	222	Total O 222 222	0	0
3	4-B	223	Total O 223 223	0	0
3	5-B	222	Total O 222 222	0	0
3	6-B	224	Total O 224 224	0	0

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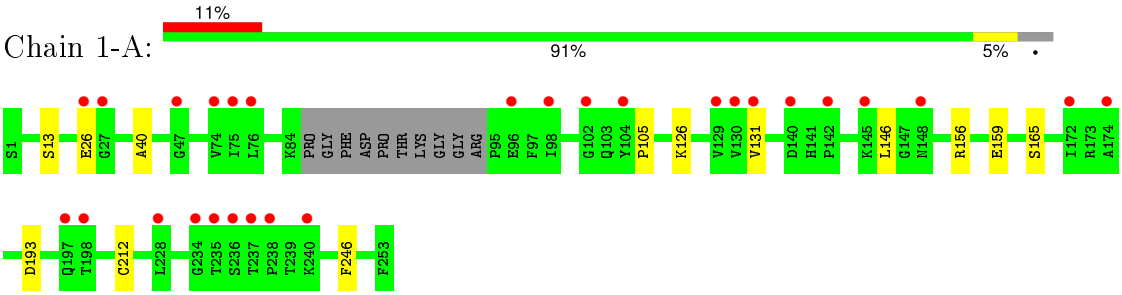
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	7-B	224	Total O 224 224	0	0
3	8-B	223	Total O 223 223	0	0
3	9-B	223	Total O 223 223	0	0
3	10-B	222	Total O 222 222	0	0
3	11-B	223	Total O 223 223	0	0
3	12-B	222	Total O 222 222	0	0
3	13-B	223	Total O 223 223	0	0
3	14-B	223	Total O 223 223	0	0
3	15-B	222	Total O 222 222	0	0
3	16-B	222	Total O 222 222	0	0

3 Residue-property plots (i)

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

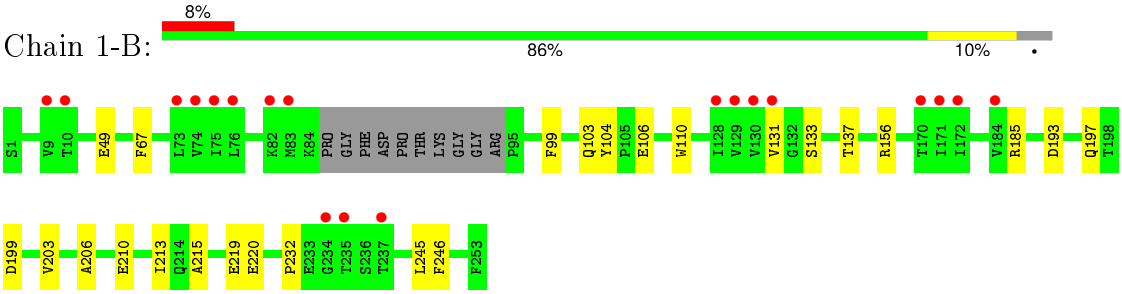
- Molecule 1: Protein At5g02240

Chain 1-A:



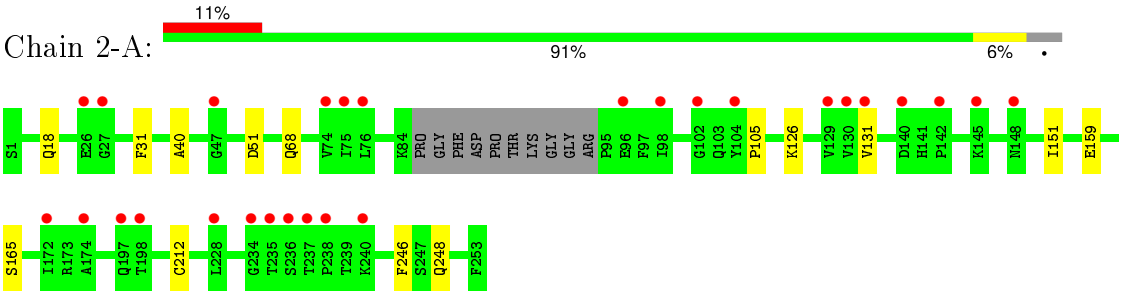
- Molecule 1: Protein At5g02240

Chain 1-B:



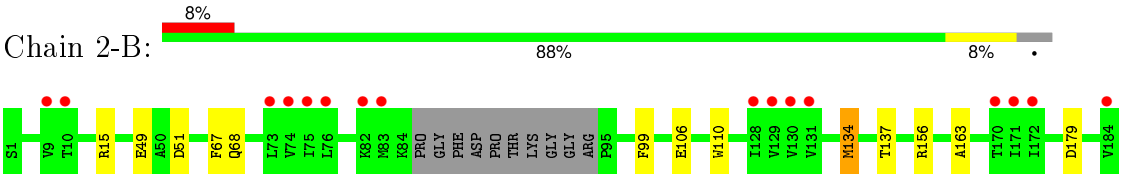
- Molecule 1: Protein At5g02240

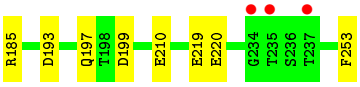
Chain 2-A:



- Molecule 1: Protein At5g02240

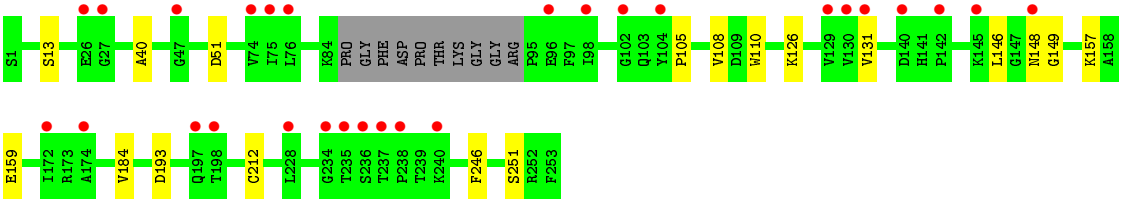
Chain 2-B:





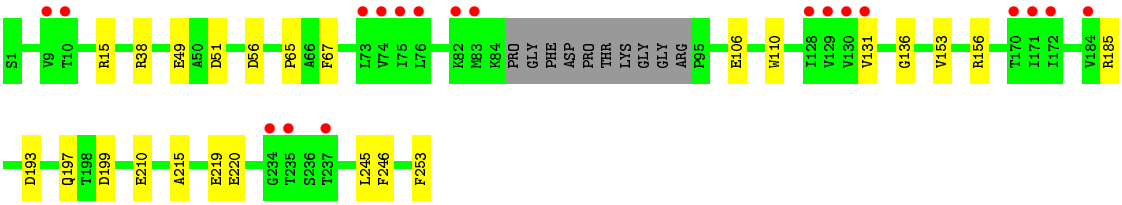
• Molecule 1: Protein At5g02240

Chain 3-A:



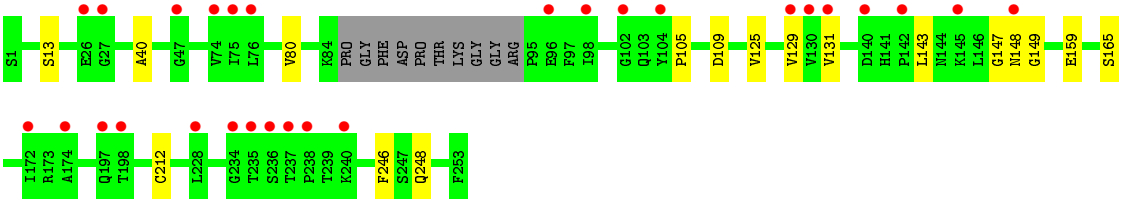
• Molecule 1: Protein At5g02240

Chain 3-B:



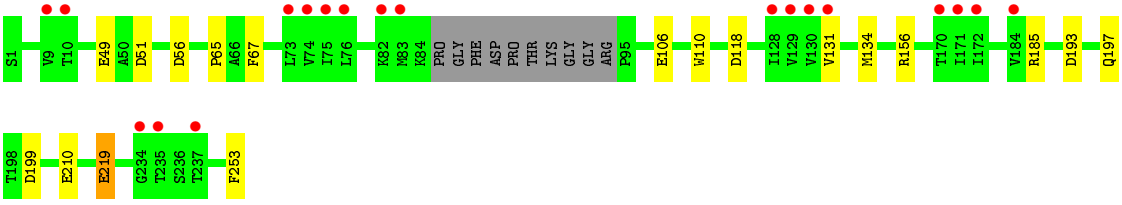
• Molecule 1: Protein At5g02240

Chain 4-A:



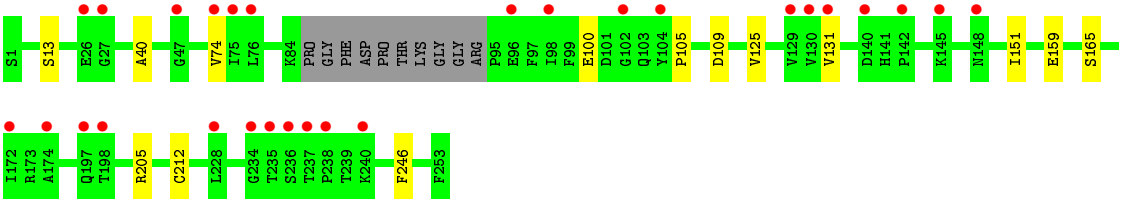
• Molecule 1: Protein At5g02240

Chain 4-B:



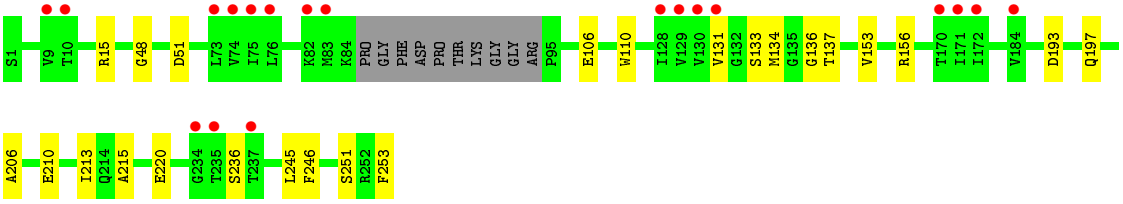
• Molecule 1: Protein At5g02240

Chain 5-A:



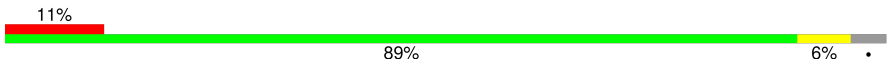
• Molecule 1: Protein At5g02240

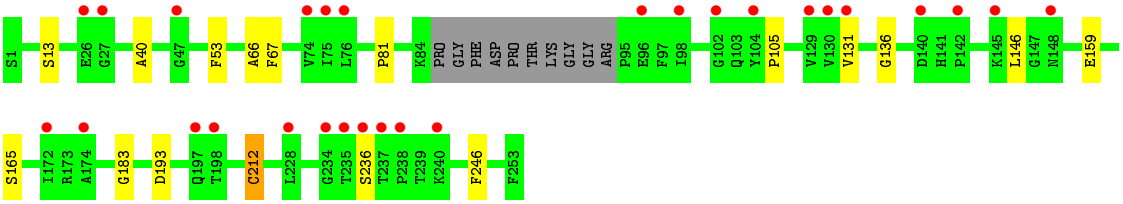
Chain 5-B:



• Molecule 1: Protein At5g02240

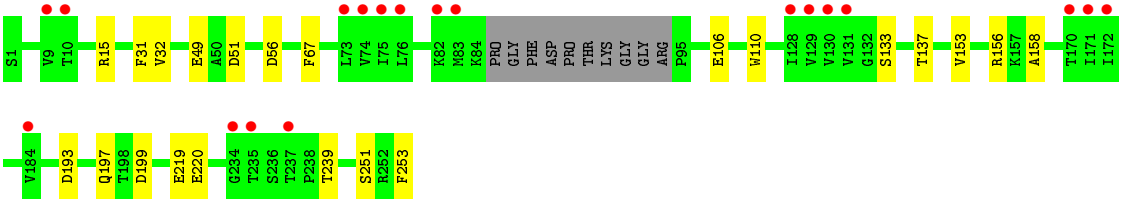
Chain 6-A:





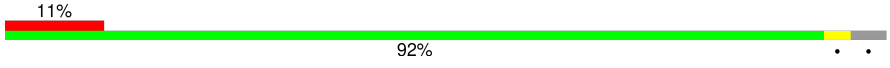
• Molecule 1: Protein At5g02240

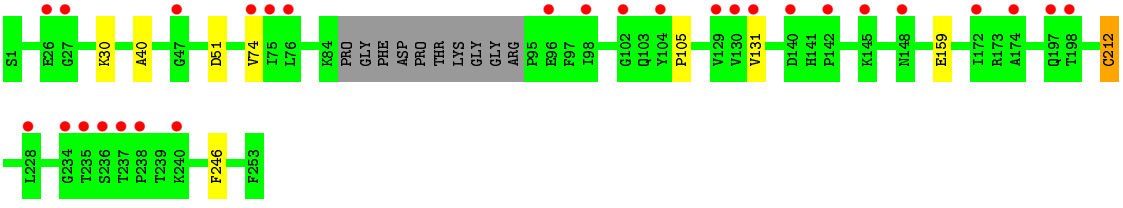
Chain 6-B:



• Molecule 1: Protein At5g02240

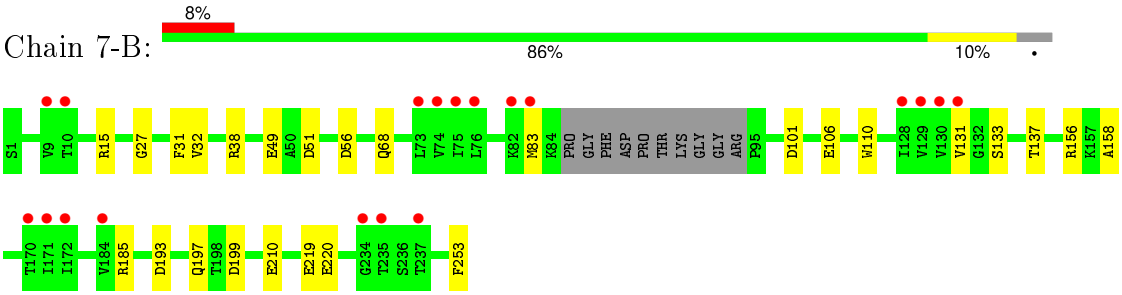
Chain 7-A:





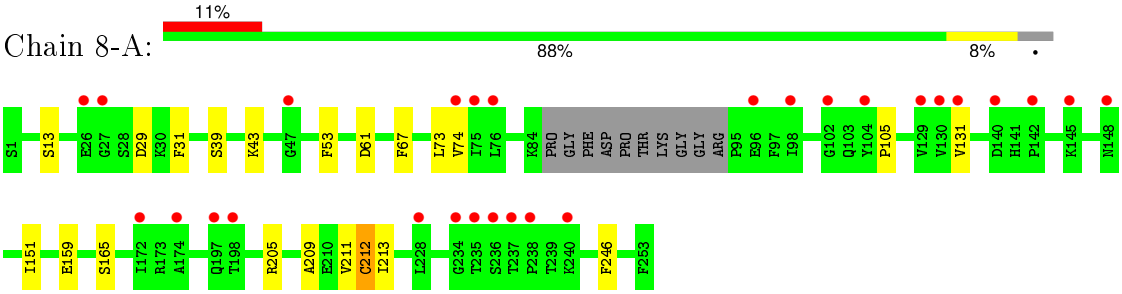
• Molecule 1: Protein At5g02240

Chain 7-B:



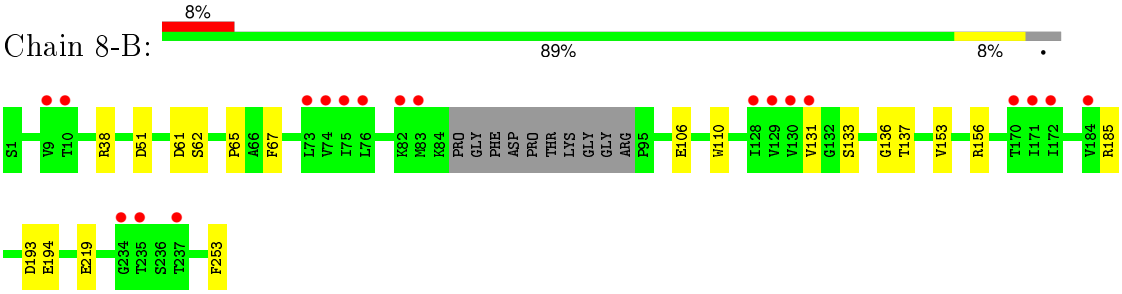
• Molecule 1: Protein At5g02240

Chain 8-A:



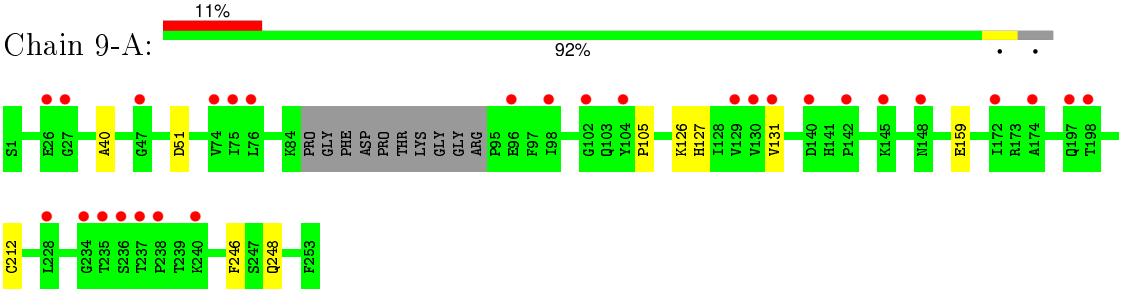
• Molecule 1: Protein At5g02240

Chain 8-B:



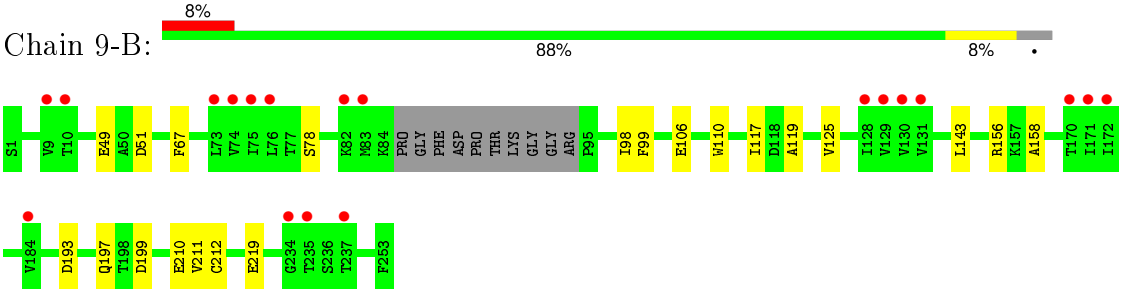
• Molecule 1: Protein At5g02240

Chain 9-A:



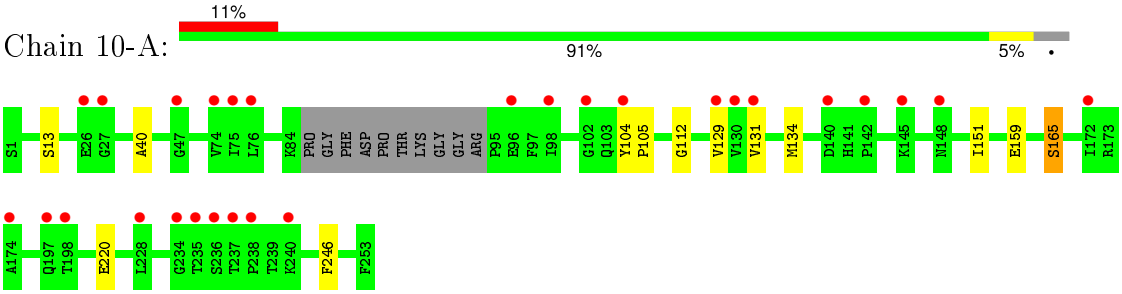
• Molecule 1: Protein At5g02240

Chain 9-B:



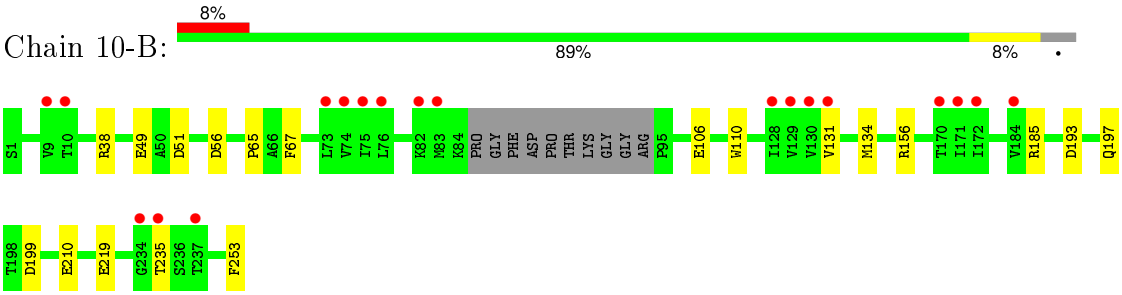
• Molecule 1: Protein At5g02240

Chain 10-A:



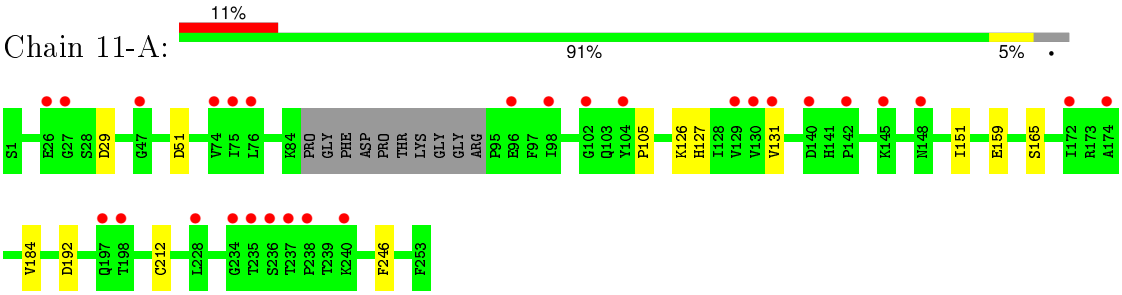
• Molecule 1: Protein At5g02240

Chain 10-B:



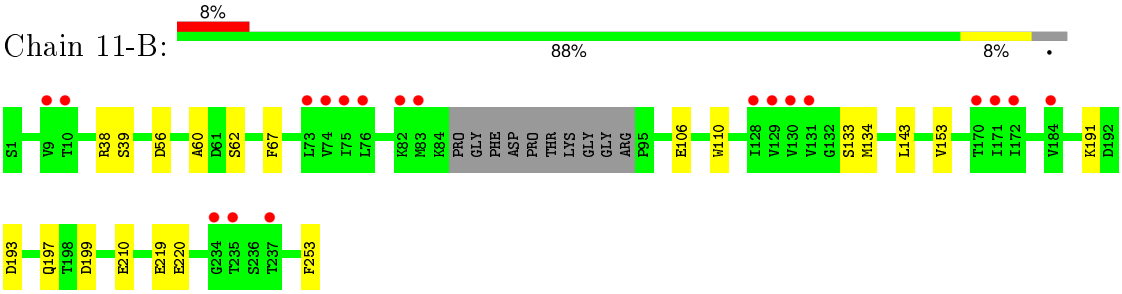
• Molecule 1: Protein At5g02240

Chain 11-A:



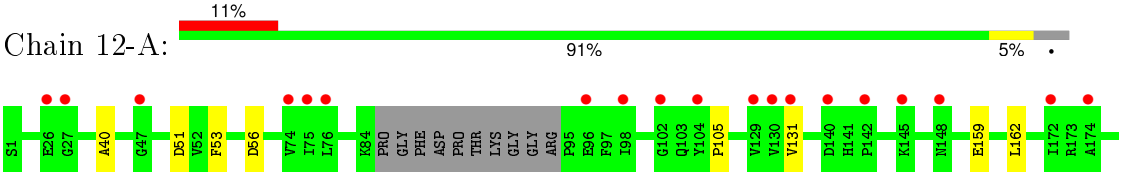
• Molecule 1: Protein At5g02240

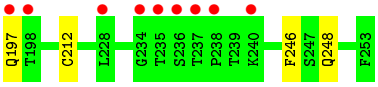
Chain 11-B:



• Molecule 1: Protein At5g02240

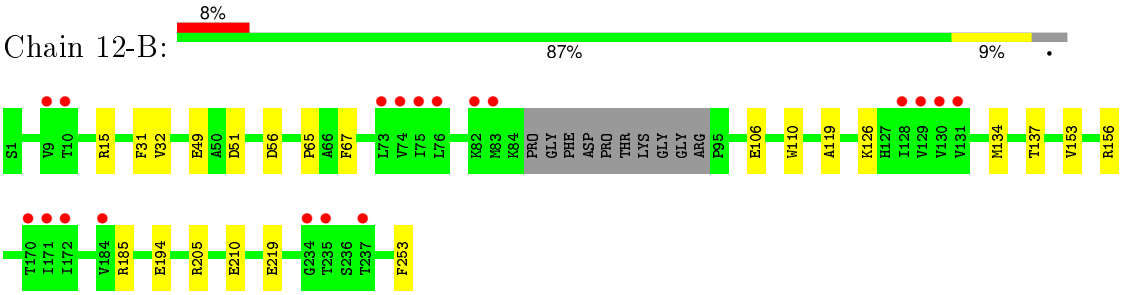
Chain 12-A:





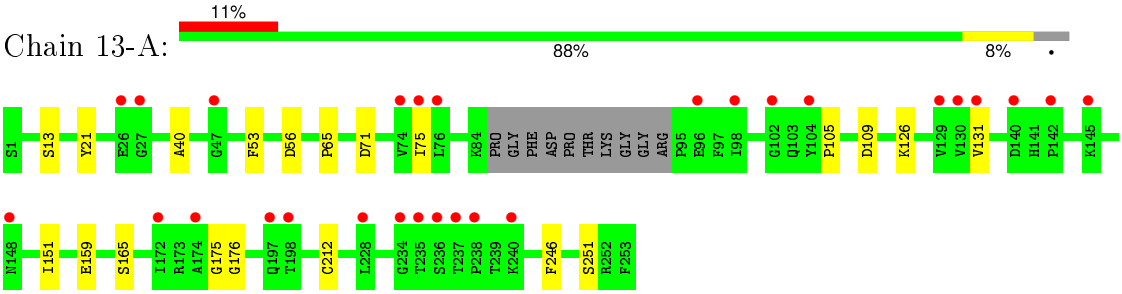
• Molecule 1: Protein At5g02240

Chain 12-B:



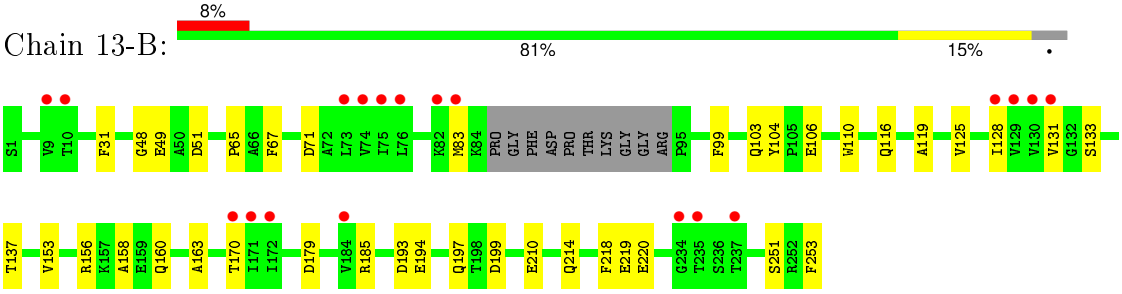
• Molecule 1: Protein At5g02240

Chain 13-A:



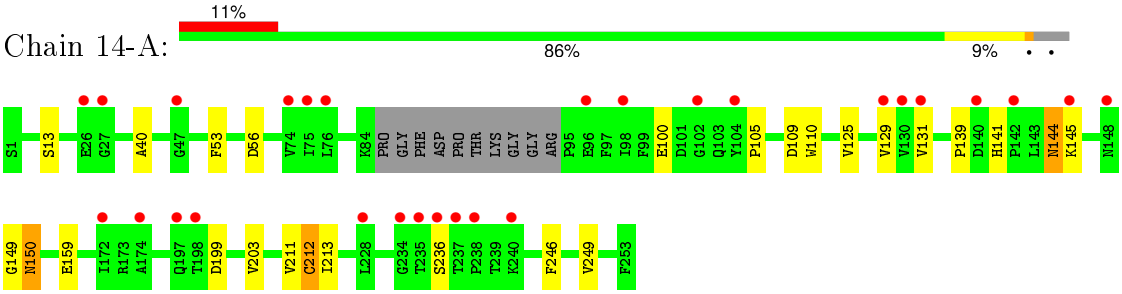
• Molecule 1: Protein At5g02240

Chain 13-B:



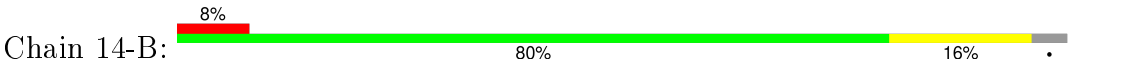
• Molecule 1: Protein At5g02240

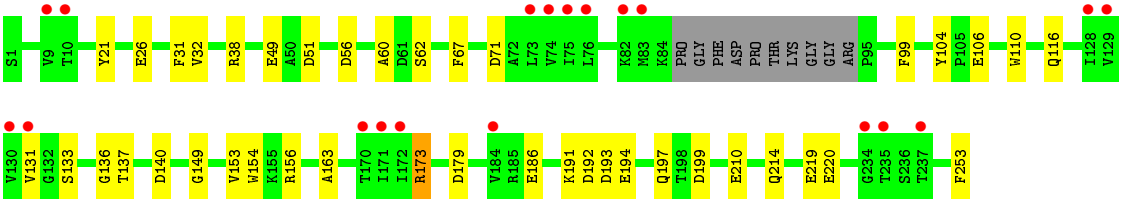
Chain 14-A:



• Molecule 1: Protein At5g02240

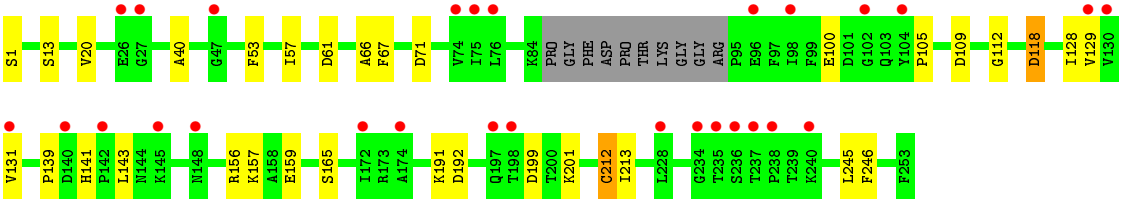
Chain 14-B:





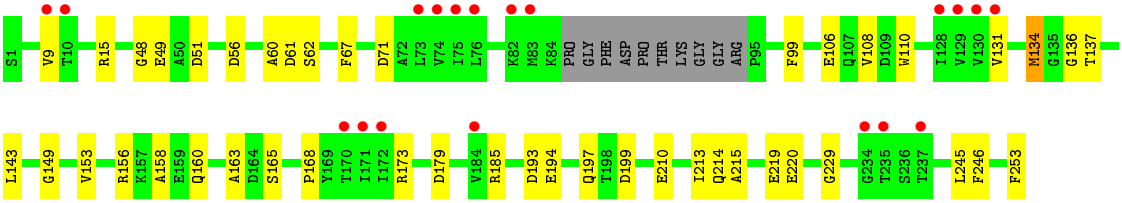
- Molecule 1: Protein At5g02240

Chain 15-A:



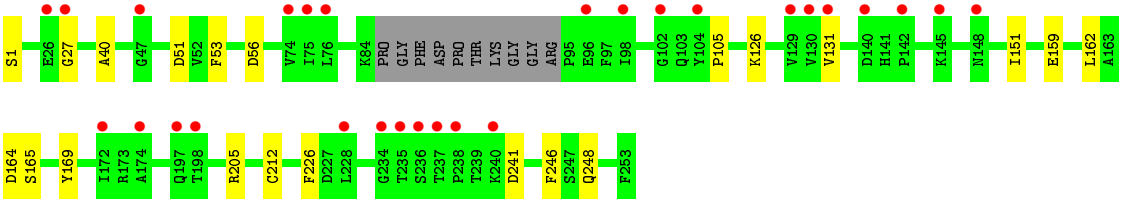
- Molecule 1: Protein At5g02240

Chain 15-B:



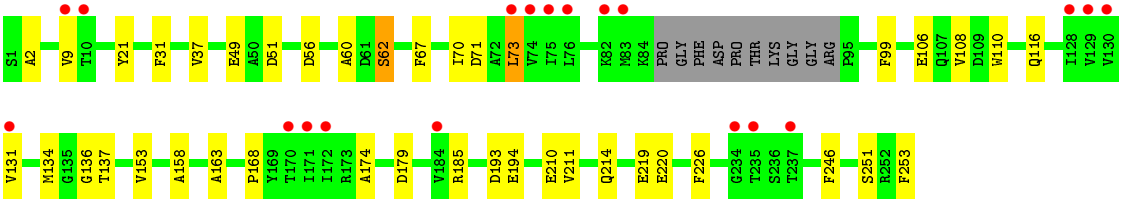
- Molecule 1: Protein At5g02240

Chain 16-A:



- Molecule 1: Protein At5g02240

Chain 16-B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.63Å 77.29Å 92.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.09 – 2.10 29.09 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.9 (29.09-2.10) 92.7 (29.09-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.16 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.257 0.189 , 0.266	Depositor DCC
R_{free} test set	1525 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 70.9	EDS
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 29855 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	66192	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP

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	1.35	9/1865 (0.5%)	1.01	1/2516 (0.0%)
1	1-B	1.60	18/1865 (1.0%)	1.12	3/2516 (0.1%)
1	2-A	1.36	11/1865 (0.6%)	1.00	1/2516 (0.0%)
1	2-B	1.59	14/1865 (0.8%)	1.10	5/2516 (0.2%)
1	3-A	1.41	8/1865 (0.4%)	1.01	3/2516 (0.1%)
1	3-B	1.60	15/1865 (0.8%)	1.13	7/2516 (0.3%)
1	4-A	1.37	10/1865 (0.5%)	1.01	2/2516 (0.1%)
1	4-B	1.60	11/1865 (0.6%)	1.11	6/2516 (0.2%)
1	5-A	1.39	12/1865 (0.6%)	1.02	2/2516 (0.1%)
1	5-B	1.59	16/1865 (0.9%)	1.11	4/2516 (0.2%)
1	6-A	1.32	9/1865 (0.5%)	1.01	1/2516 (0.0%)
1	6-B	1.59	13/1865 (0.7%)	1.10	5/2516 (0.2%)
1	7-A	1.39	8/1865 (0.4%)	1.00	2/2516 (0.1%)
1	7-B	1.59	13/1865 (0.7%)	1.12	7/2516 (0.3%)
1	8-A	1.40	15/1865 (0.8%)	1.02	1/2516 (0.0%)
1	8-B	1.57	12/1865 (0.6%)	1.11	4/2516 (0.2%)
1	9-A	1.36	7/1865 (0.4%)	1.01	1/2516 (0.0%)
1	9-B	1.58	10/1865 (0.5%)	1.11	4/2516 (0.2%)
1	10-A	1.37	12/1865 (0.6%)	0.99	0/2516
1	10-B	1.61	11/1865 (0.6%)	1.11	6/2516 (0.2%)
1	11-A	1.44	8/1865 (0.4%)	1.01	2/2516 (0.1%)
1	11-B	1.60	13/1865 (0.7%)	1.09	3/2516 (0.1%)
1	12-A	1.50	8/1865 (0.4%)	1.01	1/2516 (0.0%)
1	12-B	1.60	14/1865 (0.8%)	1.13	7/2516 (0.3%)
1	13-A	1.58	19/1865 (1.0%)	1.11	3/2516 (0.1%)
1	13-B	1.84	28/1865 (1.5%)	1.22	8/2516 (0.3%)
1	14-A	1.64	19/1865 (1.0%)	1.09	3/2516 (0.1%)
1	14-B	1.87	35/1865 (1.9%)	1.26	9/2516 (0.4%)
1	15-A	1.61	18/1865 (1.0%)	1.11	3/2516 (0.1%)
1	15-B	1.83	38/1865 (2.0%)	1.25	10/2516 (0.4%)
1	16-A	1.59	18/1865 (1.0%)	1.09	1/2516 (0.0%)
1	16-B	1.85	37/1865 (2.0%)	1.22	5/2516 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	1.56	489/59680 (0.8%)	1.09	120/80512 (0.1%)

All (489) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	12-A	212	CYS	CB-SG	-27.96	1.34	1.82
1	11-A	212	CYS	CB-SG	-21.73	1.45	1.82
1	14-A	212	CYS	CB-SG	19.59	2.15	1.82
1	3-A	212	CYS	CB-SG	-19.56	1.49	1.82
1	15-A	212	CYS	CB-SG	-18.22	1.51	1.82
1	16-A	212	CYS	CB-SG	-16.61	1.54	1.82
1	7-A	212	CYS	CB-SG	16.50	2.10	1.82
1	13-B	106	GLU	CG-CD	11.93	1.69	1.51
1	14-B	106	GLU	CG-CD	11.82	1.69	1.51
1	5-A	212	CYS	CB-SG	-11.81	1.62	1.82
1	13-A	212	CYS	CB-SG	11.49	2.01	1.82
1	16-B	106	GLU	CG-CD	11.22	1.68	1.51
1	15-B	106	GLU	CG-CD	11.12	1.68	1.51
1	8-A	212	CYS	CB-SG	-10.49	1.64	1.82
1	11-B	106	GLU	CG-CD	10.08	1.67	1.51
1	5-B	106	GLU	CG-CD	9.82	1.66	1.51
1	7-B	106	GLU	CG-CD	9.60	1.66	1.51
1	3-B	106	GLU	CG-CD	9.28	1.65	1.51
1	14-A	159	GLU	CD-OE2	9.02	1.35	1.25
1	13-A	159	GLU	CB-CG	8.95	1.69	1.52
1	14-A	131	VAL	CB-CG1	8.75	1.71	1.52
1	11-B	134	MET	SD-CE	-8.71	1.29	1.77
1	13-A	131	VAL	CB-CG1	8.70	1.71	1.52
1	2-A	212	CYS	CB-SG	-8.60	1.67	1.82
1	15-A	67	PHE	CE1-CZ	8.55	1.53	1.37
1	8-B	106	GLU	CG-CD	8.53	1.64	1.51
1	14-A	159	GLU	CB-CG	8.50	1.68	1.52
1	15-A	131	VAL	CB-CG1	8.44	1.70	1.52
1	10-B	134	MET	SD-CE	-8.41	1.30	1.77
1	2-B	134	MET	SD-CE	-8.36	1.31	1.77
1	16-A	131	VAL	CB-CG1	8.26	1.70	1.52
1	2-B	106	GLU	CG-CD	8.26	1.64	1.51
1	14-B	219	GLU	C-O	-8.26	1.07	1.23
1	14-B	210	GLU	CG-CD	8.21	1.64	1.51
1	14-B	253	PHE	CE2-CZ	8.18	1.52	1.37
1	15-A	129	VAL	CB-CG2	8.15	1.70	1.52
1	10-A	131	VAL	CB-CG1	8.14	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	159	GLU	CB-CG	8.13	1.67	1.52
1	13-B	210	GLU	CG-CD	8.09	1.64	1.51
1	9-B	110	TRP	CZ3-CH2	8.09	1.52	1.40
1	6-B	106	GLU	CG-CD	8.03	1.64	1.51
1	10-B	106	GLU	CG-CD	8.03	1.64	1.51
1	5-A	159	GLU	CB-CG	7.94	1.67	1.52
1	14-B	194	GLU	CD-OE2	7.94	1.34	1.25
1	4-B	110	TRP	CZ3-CH2	7.90	1.52	1.40
1	16-B	210	GLU	CG-CD	7.87	1.63	1.51
1	13-B	219	GLU	C-O	-7.82	1.08	1.23
1	7-A	131	VAL	CB-CG1	7.80	1.69	1.52
1	9-B	117	ILE	C-O	7.75	1.38	1.23
1	12-B	110	TRP	CZ3-CH2	7.75	1.52	1.40
1	11-A	131	VAL	CB-CG1	7.74	1.69	1.52
1	1-A	159	GLU	CB-CG	7.72	1.66	1.52
1	8-A	159	GLU	CB-CG	7.68	1.66	1.52
1	13-B	253	PHE	CE2-CZ	7.68	1.51	1.37
1	2-A	159	GLU	CB-CG	7.60	1.66	1.52
1	10-B	110	TRP	CZ3-CH2	7.57	1.52	1.40
1	6-B	110	TRP	CZ3-CH2	7.56	1.52	1.40
1	2-A	131	VAL	CB-CG1	7.53	1.68	1.52
1	9-A	131	VAL	CB-CG1	7.52	1.68	1.52
1	4-A	212	CYS	CB-SG	-7.47	1.69	1.82
1	1-B	110	TRP	CZ3-CH2	7.45	1.51	1.40
1	16-B	219	GLU	C-O	-7.39	1.09	1.23
1	5-A	131	VAL	CB-CG1	7.37	1.68	1.52
1	6-A	131	VAL	CB-CG1	7.36	1.68	1.52
1	12-B	106	GLU	CG-CD	7.36	1.62	1.51
1	15-A	159	GLU	CB-CG	7.36	1.66	1.52
1	16-A	246	PHE	CE1-CZ	7.35	1.51	1.37
1	1-B	106	GLU	CG-CD	7.35	1.62	1.51
1	3-A	131	VAL	CB-CG1	7.35	1.68	1.52
1	13-B	110	TRP	CZ3-CH2	7.34	1.51	1.40
1	16-B	110	TRP	CZ3-CH2	7.34	1.51	1.40
1	8-B	110	TRP	CZ3-CH2	7.33	1.51	1.40
1	8-A	67	PHE	CE1-CZ	7.33	1.51	1.37
1	16-A	159	GLU	CB-CG	7.29	1.66	1.52
1	10-A	165	SER	CB-OG	7.25	1.51	1.42
1	14-A	40	ALA	CA-CB	7.25	1.67	1.52
1	6-B	219	GLU	C-O	-7.24	1.09	1.23
1	2-B	210	GLU	CG-CD	7.24	1.62	1.51
1	8-A	131	VAL	CB-CG1	7.22	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	131	VAL	CB-CG1	7.21	1.68	1.52
1	4-A	131	VAL	CB-CG1	7.20	1.68	1.52
1	15-B	220	GLU	CD-OE1	7.20	1.33	1.25
1	4-B	210	GLU	CG-CD	7.19	1.62	1.51
1	10-B	210	GLU	CG-CD	7.17	1.62	1.51
1	4-B	106	GLU	CG-CD	7.17	1.62	1.51
1	12-B	210	GLU	CG-CD	7.16	1.62	1.51
1	12-B	134	MET	SD-CE	-7.16	1.37	1.77
1	16-A	40	ALA	CA-CB	7.13	1.67	1.52
1	11-B	210	GLU	CG-CD	7.12	1.62	1.51
1	7-B	210	GLU	CG-CD	7.10	1.62	1.51
1	12-A	131	VAL	CB-CG1	7.10	1.67	1.52
1	7-B	219	GLU	C-O	-7.09	1.09	1.23
1	9-B	106	GLU	CG-CD	7.05	1.62	1.51
1	1-A	212	CYS	CB-SG	-7.03	1.70	1.82
1	4-B	219	GLU	C-O	-6.98	1.10	1.23
1	11-B	253	PHE	CE2-CZ	6.98	1.50	1.37
1	6-A	159	GLU	CB-CG	6.97	1.65	1.52
1	2-B	253	PHE	CE2-CZ	6.94	1.50	1.37
1	2-B	219	GLU	C-O	-6.94	1.10	1.23
1	15-A	53	PHE	CE1-CZ	6.93	1.50	1.37
1	13-A	40	ALA	CA-CB	6.92	1.67	1.52
1	16-B	49	GLU	CD-OE1	6.86	1.33	1.25
1	13-A	246	PHE	CE1-CZ	6.85	1.50	1.37
1	10-A	159	GLU	CB-CG	6.84	1.65	1.52
1	10-A	129	VAL	CB-CG2	6.83	1.67	1.52
1	15-A	112	GLY	C-O	-6.75	1.12	1.23
1	15-B	67	PHE	CE1-CZ	6.75	1.50	1.37
1	9-A	212	CYS	CB-SG	-6.72	1.70	1.82
1	13-A	159	GLU	CG-CD	6.70	1.61	1.51
1	14-A	211	VAL	CB-CG1	6.69	1.67	1.52
1	14-B	220	GLU	CG-CD	6.69	1.61	1.51
1	11-B	219	GLU	C-O	-6.68	1.10	1.23
1	11-A	159	GLU	CB-CG	6.67	1.64	1.52
1	14-B	67	PHE	CE1-CZ	6.63	1.50	1.37
1	14-B	49	GLU	CD-OE1	6.62	1.32	1.25
1	2-B	110	TRP	CZ3-CH2	6.62	1.50	1.40
1	14-B	110	TRP	CZ3-CH2	6.58	1.50	1.40
1	4-B	253	PHE	CE2-CZ	6.55	1.49	1.37
1	14-A	246	PHE	CE1-CZ	6.55	1.49	1.37
1	9-A	159	GLU	CB-CG	6.54	1.64	1.52
1	14-A	246	PHE	CG-CD1	6.54	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-B	153	VAL	CB-CG2	6.54	1.66	1.52
1	2-B	134	MET	CG-SD	6.53	1.98	1.81
1	6-B	32	VAL	CB-CG1	6.52	1.66	1.52
1	7-B	253	PHE	CE2-CZ	6.51	1.49	1.37
1	13-B	131	VAL	CB-CG1	6.48	1.66	1.52
1	15-B	197	GLN	CG-CD	6.47	1.66	1.51
1	14-B	153	VAL	CB-CG2	6.46	1.66	1.52
1	5-B	220	GLU	CD-OE1	6.45	1.32	1.25
1	16-A	159	GLU	CG-CD	6.44	1.61	1.51
1	5-A	246	PHE	CE1-CZ	6.44	1.49	1.37
1	14-A	159	GLU	CG-CD	6.44	1.61	1.51
1	3-B	110	TRP	CZ3-CH2	6.43	1.50	1.40
1	3-A	246	PHE	CE1-CZ	6.42	1.49	1.37
1	14-A	246	PHE	CE2-CZ	6.42	1.49	1.37
1	14-B	197	GLN	CG-CD	6.42	1.65	1.51
1	2-A	40	ALA	CA-CB	6.37	1.65	1.52
1	6-B	253	PHE	CE2-CZ	6.37	1.49	1.37
1	15-B	210	GLU	CB-CG	6.36	1.64	1.52
1	10-A	134	MET	SD-CE	6.33	2.13	1.77
1	13-A	151	ILE	CB-CG2	-6.33	1.33	1.52
1	13-B	197	GLN	CG-CD	6.33	1.65	1.51
1	1-B	215	ALA	C-O	6.32	1.35	1.23
1	13-A	165	SER	CB-OG	6.32	1.50	1.42
1	2-A	31	PHE	CE1-CZ	6.31	1.49	1.37
1	7-A	159	GLU	CB-CG	6.30	1.64	1.52
1	9-B	210	GLU	CG-CD	6.30	1.61	1.51
1	8-A	246	PHE	CE1-CZ	6.29	1.49	1.37
1	11-A	246	PHE	CE1-CZ	6.29	1.49	1.37
1	15-B	163	ALA	CA-CB	6.28	1.65	1.52
1	10-A	40	ALA	CA-CB	6.27	1.65	1.52
1	12-A	246	PHE	CE1-CZ	6.26	1.49	1.37
1	4-A	246	PHE	CE1-CZ	6.26	1.49	1.37
1	5-A	40	ALA	CA-CB	6.26	1.65	1.52
1	13-A	159	GLU	CD-OE2	6.25	1.32	1.25
1	6-A	246	PHE	CE1-CZ	6.25	1.49	1.37
1	1-B	220	GLU	CD-OE1	6.25	1.32	1.25
1	1-A	40	ALA	CA-CB	6.23	1.65	1.52
1	12-A	40	ALA	CA-CB	6.22	1.65	1.52
1	9-A	246	PHE	CE1-CZ	6.21	1.49	1.37
1	10-A	246	PHE	CE1-CZ	6.20	1.49	1.37
1	3-A	40	ALA	CA-CB	6.18	1.65	1.52
1	3-B	220	GLU	CD-OE1	6.17	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	40	ALA	CA-CB	6.17	1.65	1.52
1	14-B	32	VAL	CB-CG1	6.16	1.65	1.52
1	7-B	32	VAL	CB-CG1	6.14	1.65	1.52
1	14-B	136	GLY	C-O	6.13	1.33	1.23
1	15-A	128	ILE	CB-CG2	-6.12	1.33	1.52
1	15-B	136	GLY	C-O	6.12	1.33	1.23
1	2-B	67	PHE	CE1-CZ	6.12	1.49	1.37
1	4-A	40	ALA	CA-CB	6.11	1.65	1.52
1	7-A	40	ALA	CA-CB	6.09	1.65	1.52
1	10-B	67	PHE	CE1-CZ	6.08	1.49	1.37
1	1-A	246	PHE	CE1-CZ	6.07	1.48	1.37
1	16-B	108	VAL	CB-CG1	6.07	1.65	1.52
1	13-B	67	PHE	CE1-CZ	6.06	1.48	1.37
1	1-B	49	GLU	CD-OE1	6.05	1.32	1.25
1	16-A	165	SER	CB-OG	6.05	1.50	1.42
1	5-B	110	TRP	CZ3-CH2	6.04	1.49	1.40
1	2-A	246	PHE	CE1-CZ	6.03	1.48	1.37
1	16-B	116	GLN	CB-CG	6.02	1.68	1.52
1	15-B	49	GLU	CD-OE1	6.02	1.32	1.25
1	8-A	74	VAL	CB-CG1	6.01	1.65	1.52
1	12-B	67	PHE	CE1-CZ	6.00	1.48	1.37
1	9-B	119	ALA	CA-CB	6.00	1.65	1.52
1	13-B	99	PHE	CE2-CZ	6.00	1.48	1.37
1	15-B	131	VAL	CB-CG1	5.99	1.65	1.52
1	12-A	159	GLU	CB-CG	5.99	1.63	1.52
1	13-B	49	GLU	CD-OE1	5.98	1.32	1.25
1	16-B	99	PHE	CE2-CZ	5.97	1.48	1.37
1	8-B	219	GLU	C-O	-5.97	1.12	1.23
1	5-A	159	GLU	CG-CD	5.96	1.60	1.51
1	11-B	110	TRP	CZ3-CH2	5.96	1.49	1.40
1	3-B	215	ALA	C-O	5.94	1.34	1.23
1	16-B	137	THR	CB-CG2	5.94	1.72	1.52
1	15-B	245	LEU	C-O	5.93	1.34	1.23
1	1-B	99	PHE	CE2-CZ	5.92	1.48	1.37
1	1-B	246	PHE	CE1-CZ	5.91	1.48	1.37
1	8-B	67	PHE	CE1-CZ	5.91	1.48	1.37
1	15-B	215	ALA	C-O	5.91	1.34	1.23
1	15-A	40	ALA	CA-CB	5.88	1.64	1.52
1	15-B	110	TRP	CE3-CZ3	-5.88	1.28	1.38
1	4-A	159	GLU	CG-CD	5.88	1.60	1.51
1	16-B	220	GLU	CG-CD	5.87	1.60	1.51
1	7-B	110	TRP	CZ3-CH2	5.87	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-B	194	GLU	CD-OE1	5.87	1.32	1.25
1	5-B	134	MET	CB-CG	5.86	1.70	1.51
1	13-B	137	THR	CB-CG2	5.86	1.71	1.52
1	11-A	159	GLU	CG-CD	5.84	1.60	1.51
1	13-B	116	GLN	CB-CG	5.84	1.68	1.52
1	2-A	159	GLU	CG-CD	5.84	1.60	1.51
1	1-B	104	TYR	CE2-CZ	5.83	1.46	1.38
1	14-A	129	VAL	CB-CG2	5.83	1.65	1.52
1	8-A	211	VAL	CB-CG1	-5.83	1.40	1.52
1	3-B	67	PHE	CE1-CZ	5.82	1.48	1.37
1	15-A	118	ASP	CG-OD2	5.82	1.38	1.25
1	14-B	116	GLN	CB-CG	5.82	1.68	1.52
1	14-B	131	VAL	CB-CG1	5.81	1.65	1.52
1	14-A	13	SER	CA-CB	5.80	1.61	1.52
1	13-B	158	ALA	CA-CB	5.80	1.64	1.52
1	8-A	53	PHE	CE1-CZ	5.79	1.48	1.37
1	3-B	253	PHE	CE2-CZ	5.78	1.48	1.37
1	3-B	210	GLU	CG-CD	5.78	1.60	1.51
1	5-B	215	ALA	C-O	5.78	1.34	1.23
1	15-B	246	PHE	CE1-CZ	5.78	1.48	1.37
1	15-B	158	ALA	CA-CB	5.77	1.64	1.52
1	16-A	169	TYR	CG-CD2	5.76	1.46	1.39
1	8-B	253	PHE	CE2-CZ	5.76	1.48	1.37
1	1-A	159	GLU	CG-CD	5.75	1.60	1.51
1	1-B	67	PHE	CE1-CZ	5.75	1.48	1.37
1	15-B	165	SER	CB-OG	-5.74	1.34	1.42
1	7-B	49	GLU	CD-OE1	5.74	1.31	1.25
1	6-A	40	ALA	CA-CB	5.73	1.64	1.52
1	6-B	67	PHE	CE1-CZ	5.73	1.48	1.37
1	14-B	60	ALA	C-O	5.72	1.34	1.23
1	7-B	220	GLU	CG-CD	5.71	1.60	1.51
1	11-B	220	GLU	CG-CD	5.70	1.60	1.51
1	3-B	49	GLU	CD-OE1	5.70	1.31	1.25
1	4-B	49	GLU	CD-OE1	5.68	1.31	1.25
1	9-B	67	PHE	CE1-CZ	5.68	1.48	1.37
1	15-B	62	SER	CB-OG	5.68	1.49	1.42
1	7-A	246	PHE	CE1-CZ	5.67	1.48	1.37
1	16-B	136	GLY	C-O	5.67	1.32	1.23
1	1-B	245	LEU	C-O	5.67	1.34	1.23
1	14-A	203	VAL	CA-CB	5.66	1.66	1.54
1	14-B	71	ASP	CB-CG	5.66	1.63	1.51
1	10-A	159	GLU	CG-CD	5.65	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	1	SER	CA-CB	5.65	1.61	1.52
1	8-A	159	GLU	CG-CD	5.65	1.60	1.51
1	3-B	246	PHE	CE1-CZ	5.64	1.48	1.37
1	5-B	246	PHE	CE1-CZ	5.64	1.48	1.37
1	6-B	220	GLU	CG-CD	5.64	1.60	1.51
1	15-B	149	GLY	C-O	-5.64	1.14	1.23
1	14-B	137	THR	CB-CG2	5.63	1.71	1.52
1	13-B	163	ALA	CA-CB	5.62	1.64	1.52
1	10-B	49	GLU	CD-OE1	5.62	1.31	1.25
1	5-B	210	GLU	CB-CG	5.62	1.62	1.52
1	15-B	60	ALA	C-O	5.61	1.34	1.23
1	16-B	158	ALA	CA-CB	5.61	1.64	1.52
1	1-B	210	GLU	CB-CG	5.60	1.62	1.52
1	5-A	165	SER	CB-OG	5.60	1.49	1.42
1	13-B	71	ASP	CB-CG	5.60	1.63	1.51
1	6-A	159	GLU	CG-CD	5.60	1.60	1.51
1	15-B	168	PRO	CG-CD	5.60	1.69	1.50
1	1-B	206	ALA	C-O	5.58	1.33	1.23
1	13-B	220	GLU	CG-CD	5.57	1.60	1.51
1	16-A	246	PHE	CG-CD1	5.57	1.47	1.38
1	16-B	9	VAL	CB-CG1	5.57	1.64	1.52
1	9-B	219	GLU	C-O	-5.56	1.12	1.23
1	16-B	194	GLU	CD-OE1	5.56	1.31	1.25
1	2-A	151	ILE	CB-CG2	-5.55	1.35	1.52
1	12-B	32	VAL	CB-CG1	5.55	1.64	1.52
1	15-B	246	PHE	C-O	5.55	1.33	1.23
1	16-B	226	PHE	CE2-CZ	5.54	1.47	1.37
1	8-A	165	SER	CB-OG	5.53	1.49	1.42
1	2-A	246	PHE	CG-CD1	5.53	1.47	1.38
1	12-A	53	PHE	CE1-CZ	5.53	1.47	1.37
1	4-A	165	SER	CB-OG	5.51	1.49	1.42
1	13-B	194	GLU	C-O	5.51	1.33	1.23
1	15-B	110	TRP	CZ3-CH2	5.51	1.48	1.40
1	3-B	210	GLU	CB-CG	5.51	1.62	1.52
1	4-A	129	VAL	CB-CG2	5.51	1.64	1.52
1	6-A	67	PHE	CE1-CZ	5.51	1.47	1.37
1	12-B	49	GLU	CD-OE1	5.51	1.31	1.25
1	13-B	119	ALA	CA-CB	5.51	1.64	1.52
1	15-B	153	VAL	CB-CG2	5.50	1.64	1.52
1	13-A	53	PHE	CE1-CZ	5.50	1.47	1.37
1	12-B	253	PHE	CE2-CZ	5.49	1.47	1.37
1	16-A	53	PHE	CE1-CZ	5.49	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-B	245	LEU	C-O	5.49	1.33	1.23
1	16-B	73	LEU	CG-CD2	-5.49	1.31	1.51
1	14-B	149	GLY	C-O	-5.48	1.14	1.23
1	15-B	253	PHE	CD1-CE1	5.48	1.50	1.39
1	1-A	165	SER	CB-OG	5.48	1.49	1.42
1	10-B	197	GLN	CG-CD	5.48	1.63	1.51
1	5-A	74	VAL	CB-CG1	5.48	1.64	1.52
1	5-B	197	GLN	CG-CD	5.47	1.63	1.51
1	16-B	134	MET	CB-CG	5.47	1.68	1.51
1	2-A	165	SER	CB-OG	5.47	1.49	1.42
1	8-B	131	VAL	CB-CG1	5.46	1.64	1.52
1	3-B	131	VAL	CB-CG1	5.46	1.64	1.52
1	14-B	62	SER	CB-OG	5.46	1.49	1.42
1	9-B	211	VAL	CB-CG1	5.46	1.64	1.52
1	11-B	197	GLN	CG-CD	5.46	1.63	1.51
1	16-B	71	ASP	CB-CG	5.46	1.63	1.51
1	15-B	134	MET	CG-SD	5.45	1.95	1.81
1	14-A	203	VAL	CB-CG2	5.45	1.64	1.52
1	13-A	246	PHE	CD1-CE1	5.45	1.50	1.39
1	14-B	99	PHE	CE2-CZ	5.44	1.47	1.37
1	3-B	197	GLN	CG-CD	5.44	1.63	1.51
1	10-A	151	ILE	CB-CG2	-5.44	1.35	1.52
1	1-B	131	VAL	CB-CG1	5.44	1.64	1.52
1	15-B	210	GLU	CG-CD	5.44	1.60	1.51
1	13-A	176	GLY	C-O	5.43	1.32	1.23
1	14-B	253	PHE	CD1-CE1	5.43	1.50	1.39
1	7-A	74	VAL	CB-CG1	5.42	1.64	1.52
1	2-B	49	GLU	CD-OE1	5.42	1.31	1.25
1	4-B	65	PRO	CG-CD	5.42	1.68	1.50
1	13-A	71	ASP	CB-CG	5.42	1.63	1.51
1	9-B	197	GLN	CG-CD	5.41	1.63	1.51
1	12-B	119	ALA	CA-CB	5.40	1.63	1.52
1	16-B	62	SER	CB-OG	5.39	1.49	1.42
1	16-B	174	ALA	CA-CB	5.38	1.63	1.52
1	15-B	71	ASP	CB-CG	5.37	1.63	1.51
1	5-B	206	ALA	C-O	5.37	1.33	1.23
1	16-B	131	VAL	CB-CG1	5.37	1.64	1.52
1	14-B	154	TRP	CG-CD1	5.37	1.44	1.36
1	4-B	67	PHE	CE1-CZ	5.37	1.47	1.37
1	16-B	246	PHE	C-O	5.37	1.33	1.23
1	7-A	246	PHE	CE2-CZ	5.36	1.47	1.37
1	16-B	253	PHE	CD1-CE1	5.36	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	151	ILE	CB-CG2	-5.36	1.36	1.52
1	9-A	246	PHE	CG-CD1	5.36	1.46	1.38
1	15-B	253	PHE	CE2-CZ	5.36	1.47	1.37
1	16-A	151	ILE	CB-CG2	-5.36	1.36	1.52
1	14-B	133	SER	CA-CB	5.36	1.60	1.52
1	6-B	197	GLN	CG-CD	5.35	1.63	1.51
1	7-B	197	GLN	CG-CD	5.35	1.63	1.51
1	15-A	66	ALA	C-O	-5.35	1.13	1.23
1	16-B	163	ALA	CA-CB	5.35	1.63	1.52
1	4-A	13	SER	CA-CB	5.34	1.60	1.52
1	8-A	13	SER	CA-CB	5.34	1.60	1.52
1	10-B	253	PHE	CE2-CZ	5.34	1.47	1.37
1	2-A	246	PHE	CE2-CZ	5.34	1.47	1.37
1	3-A	159	GLU	CB-CG	5.34	1.62	1.52
1	6-B	133	SER	CA-CB	5.33	1.60	1.52
1	5-A	159	GLU	CD-OE2	5.33	1.31	1.25
1	16-B	37	VAL	CB-CG1	5.33	1.64	1.52
1	6-A	13	SER	CA-CB	5.33	1.60	1.52
1	4-B	134	MET	SD-CE	5.32	2.07	1.77
1	4-B	197	GLN	CG-CD	5.32	1.63	1.51
1	7-B	131	VAL	CB-CG1	5.32	1.64	1.52
1	8-B	194	GLU	C-O	5.32	1.33	1.23
1	16-A	246	PHE	CE2-CZ	5.31	1.47	1.37
1	5-A	151	ILE	CB-CG2	-5.31	1.36	1.52
1	12-B	194	GLU	C-O	5.31	1.33	1.23
1	15-B	137	THR	CB-CG2	5.31	1.69	1.52
1	2-B	99	PHE	CE2-CZ	5.31	1.47	1.37
1	1-A	159	GLU	CD-OE2	5.30	1.31	1.25
1	16-A	56	ASP	C-O	5.30	1.33	1.23
1	16-B	21	TYR	CA-C	5.29	1.66	1.52
1	7-B	158	ALA	CA-CB	5.29	1.63	1.52
1	11-A	246	PHE	CG-CD1	5.29	1.46	1.38
1	2-B	137	THR	CB-CG2	5.28	1.69	1.52
1	1-A	13	SER	CA-CB	5.28	1.60	1.52
1	3-A	13	SER	CA-CB	5.28	1.60	1.52
1	14-B	163	ALA	CA-CB	5.27	1.63	1.52
1	11-B	67	PHE	CE1-CZ	5.26	1.47	1.37
1	7-B	137	THR	CB-CG2	5.26	1.69	1.52
1	9-B	158	ALA	CA-CB	5.26	1.63	1.52
1	15-B	99	PHE	CE2-CZ	5.26	1.47	1.37
1	6-A	165	SER	CB-OG	5.26	1.49	1.42
1	5-B	153	VAL	CB-CG2	5.25	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-B	153	VAL	CA-CB	5.25	1.65	1.54
1	13-B	214	GLN	CG-CD	5.24	1.63	1.51
1	8-A	246	PHE	CG-CD1	5.24	1.46	1.38
1	14-B	153	VAL	CA-CB	5.24	1.65	1.54
1	2-B	197	GLN	CG-CD	5.24	1.63	1.51
1	13-A	75	ILE	CB-CG2	5.24	1.69	1.52
1	16-B	153	VAL	CA-CB	5.24	1.65	1.54
1	16-B	214	GLN	CG-CD	5.23	1.63	1.51
1	12-A	246	PHE	CG-CD1	5.23	1.46	1.38
1	13-B	133	SER	CA-CB	5.23	1.60	1.52
1	15-B	108	VAL	CB-CG1	5.23	1.63	1.52
1	3-A	108	VAL	CB-CG1	5.22	1.63	1.52
1	8-A	31	PHE	CE1-CZ	5.22	1.47	1.37
1	15-A	165	SER	CB-OG	5.22	1.49	1.42
1	5-B	131	VAL	CB-CG1	5.22	1.63	1.52
1	2-B	163	ALA	CA-CB	5.21	1.63	1.52
1	4-A	246	PHE	CG-CD1	5.21	1.46	1.38
1	3-B	153	VAL	CB-CG2	5.20	1.63	1.52
1	13-B	153	VAL	CB-CG2	5.20	1.63	1.52
1	13-A	56	ASP	C-O	5.20	1.33	1.23
1	6-A	53	PHE	CE1-CZ	5.20	1.47	1.37
1	13-B	65	PRO	CG-CD	5.20	1.67	1.50
1	15-A	57	ILE	CB-CG2	5.20	1.69	1.52
1	16-B	253	PHE	CG-CD1	5.20	1.46	1.38
1	13-B	128	ILE	CB-CG2	5.20	1.69	1.52
1	1-B	197	GLN	CG-CD	5.19	1.62	1.51
1	1-B	210	GLU	CG-CD	5.19	1.59	1.51
1	11-A	165	SER	CB-OG	5.19	1.49	1.42
1	15-A	246	PHE	CD1-CE1	5.19	1.49	1.39
1	14-B	173	ARG	CZ-NH1	5.19	1.39	1.33
1	15-B	9	VAL	CB-CG1	5.18	1.63	1.52
1	8-B	62	SER	CB-OG	-5.18	1.35	1.42
1	13-B	153	VAL	CA-CB	5.18	1.65	1.54
1	2-B	220	GLU	CG-CD	5.17	1.59	1.51
1	8-B	133	SER	CA-CB	5.17	1.60	1.52
1	11-A	151	ILE	CB-CG2	-5.17	1.36	1.52
1	5-A	13	SER	CA-CB	5.16	1.60	1.52
1	16-B	67	PHE	CE1-CZ	5.16	1.47	1.37
1	5-B	245	LEU	C-O	5.16	1.33	1.23
1	11-B	62	SER	CB-OG	5.16	1.49	1.42
1	12-B	137	THR	CB-CG2	5.16	1.69	1.52
1	10-B	219	GLU	C-O	-5.16	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-B	131	VAL	CB-CG1	5.16	1.63	1.52
1	10-B	65	PRO	CG-CD	5.15	1.67	1.50
1	13-B	160	GLN	CB-CG	5.15	1.66	1.52
1	5-B	213	ILE	C-O	5.15	1.33	1.23
1	13-A	175	GLY	C-O	5.14	1.31	1.23
1	13-A	212	CYS	C-O	-5.14	1.13	1.23
1	7-A	246	PHE	CG-CD1	5.13	1.46	1.38
1	15-B	213	ILE	C-O	5.13	1.33	1.23
1	16-A	162	LEU	CG-CD2	5.13	1.70	1.51
1	13-B	218	PHE	CE1-CZ	5.13	1.47	1.37
1	14-B	104	TYR	CD1-CE1	5.13	1.47	1.39
1	3-A	159	GLU	CG-CD	5.13	1.59	1.51
1	16-B	2	ALA	C-O	5.13	1.33	1.23
1	14-B	110	TRP	CE3-CZ3	-5.13	1.29	1.38
1	8-B	153	VAL	CB-CG2	5.12	1.63	1.52
1	14-B	140	ASP	C-O	5.12	1.33	1.23
1	16-B	253	PHE	CE2-CZ	5.12	1.47	1.37
1	14-B	214	GLN	CG-CD	5.12	1.62	1.51
1	14-B	186	GLU	CD-OE2	5.12	1.31	1.25
1	16-B	211	VAL	CB-CG1	5.12	1.63	1.52
1	14-B	21	TYR	CA-C	5.12	1.66	1.52
1	11-B	133	SER	CA-CB	5.11	1.60	1.52
1	16-A	246	PHE	CD1-CE1	5.11	1.49	1.39
1	4-B	131	VAL	CB-CG1	5.10	1.63	1.52
1	5-B	137	THR	CB-CG2	5.10	1.69	1.52
1	14-A	159	GLU	C-O	-5.10	1.13	1.23
1	16-A	226	PHE	CE1-CZ	5.10	1.47	1.37
1	15-A	20	VAL	CB-CG2	5.09	1.63	1.52
1	7-B	133	SER	CA-CB	5.09	1.60	1.52
1	10-A	246	PHE	CG-CD1	5.09	1.46	1.38
1	12-B	219	GLU	C-O	-5.09	1.13	1.23
1	13-B	104	TYR	CD1-CE1	5.09	1.47	1.39
1	14-A	53	PHE	CE1-CZ	5.08	1.47	1.37
1	16-A	205	ARG	CZ-NH2	5.08	1.39	1.33
1	6-B	49	GLU	CD-OE1	5.08	1.31	1.25
1	13-B	103	GLN	CG-CD	5.08	1.62	1.51
1	14-A	56	ASP	C-O	5.08	1.32	1.23
1	5-B	133	SER	CA-CB	5.08	1.60	1.52
1	11-B	153	VAL	CB-CG2	5.07	1.63	1.52
1	3-B	65	PRO	CG-CD	5.07	1.67	1.50
1	15-B	229	GLY	CA-C	5.07	1.59	1.51
1	9-A	212	CYS	CA-CB	5.06	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-B	71	ASP	CA-CB	-5.06	1.42	1.53
1	13-A	21	TYR	CE2-CZ	-5.05	1.31	1.38
1	15-A	13	SER	CA-CB	5.05	1.60	1.52
1	8-B	137	THR	CB-CG2	5.05	1.69	1.52
1	1-B	137	THR	CB-CG2	5.05	1.69	1.52
1	16-A	1	SER	N-CA	5.05	1.56	1.46
1	8-B	65	PRO	CG-CD	5.04	1.67	1.50
1	14-B	194	GLU	CG-CD	5.04	1.59	1.51
1	16-B	168	PRO	CA-C	5.04	1.62	1.52
1	14-A	249	VAL	CA-CB	5.04	1.65	1.54
1	15-B	160	GLN	CB-CG	5.04	1.66	1.52
1	6-B	137	THR	CB-CG2	5.04	1.69	1.52
1	14-B	26	GLU	CG-CD	5.04	1.59	1.51
1	6-B	158	ALA	CA-CB	5.03	1.63	1.52
1	5-A	246	PHE	CG-CD1	5.03	1.46	1.38
1	6-B	153	VAL	CB-CG2	5.03	1.63	1.52
1	12-A	162	LEU	CG-CD2	5.03	1.70	1.51
1	10-A	13	SER	CA-CB	5.02	1.60	1.52
1	10-A	112	GLY	C-O	-5.02	1.15	1.23
1	12-B	65	PRO	CG-CD	5.02	1.67	1.50
1	15-B	106	GLU	CD-OE1	5.02	1.31	1.25
1	16-B	60	ALA	C-O	5.02	1.32	1.23
1	11-B	60	ALA	C-O	5.01	1.32	1.23
1	12-B	153	VAL	CB-CG2	5.01	1.63	1.52
1	15-A	71	ASP	CB-CG	5.01	1.62	1.51
1	1-B	213	ILE	C-O	5.01	1.32	1.23
1	8-A	209	ALA	CA-CB	5.01	1.62	1.52
1	15-B	214	GLN	CG-CD	5.01	1.62	1.51
1	13-A	13	SER	CA-CB	5.00	1.60	1.52
1	5-B	253	PHE	CE2-CZ	5.00	1.46	1.37
1	14-A	125	VAL	CB-CG2	-5.00	1.42	1.52
1	1-B	203	VAL	CB-CG2	-5.00	1.42	1.52

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	14-B	156	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	7-B	156	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	15-B	173	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	13-A	212	CYS	CA-CB-SG	-8.40	98.89	114.00
1	14-B	156	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	9-B	156	ARG	NE-CZ-NH2	-8.04	116.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	15-B	185	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	16-B	185	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	13-B	51	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	8-B	185	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	12-B	185	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	14-B	51	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	15-B	51	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	1-B	185	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	7-B	185	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	16-B	51	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	5-A	109	ASP	CB-CG-OD2	6.79	124.41	118.30
1	3-B	185	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	10-B	185	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	15-A	109	ASP	CB-CG-OD2	6.70	124.33	118.30
1	16-B	193	ASP	CB-CG-OD1	6.68	124.31	118.30
1	15-B	193	ASP	CB-CG-OD1	6.65	124.28	118.30
1	10-B	156	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	13-B	156	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	14-A	212	CYS	CB-CA-C	6.45	123.30	110.40
1	15-B	156	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	12-B	205	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	12-B	134	MET	CG-SD-CE	6.32	110.31	100.20
1	4-A	109	ASP	CB-CG-OD2	6.26	123.93	118.30
1	7-A	212	CYS	CA-CB-SG	-6.24	102.77	114.00
1	14-B	193	ASP	CB-CG-OD1	6.16	123.84	118.30
1	16-B	56	ASP	CB-CG-OD1	6.16	123.84	118.30
1	13-B	193	ASP	CB-CG-OD1	6.14	123.82	118.30
1	13-B	199	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	2-B	193	ASP	CB-CG-OD1	6.07	123.76	118.30
1	14-B	199	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	10-B	193	ASP	CB-CG-OD1	6.03	123.73	118.30
1	13-A	109	ASP	CB-CG-OD2	5.96	123.67	118.30
1	14-B	179	ASP	CB-CG-OD2	5.94	123.64	118.30
1	6-B	51	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	4-B	193	ASP	CB-CG-OD1	5.92	123.62	118.30
1	5-B	51	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	6-B	193	ASP	CB-CG-OD1	5.90	123.61	118.30
1	15-B	199	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	8-B	193	ASP	CB-CG-OD1	5.86	123.57	118.30
1	5-B	193	ASP	CB-CG-OD1	5.84	123.56	118.30
1	15-A	156	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	11-B	56	ASP	CB-CG-OD1	5.82	123.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-B	51	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	11-A	51	ASP	CB-CG-OD1	5.80	123.52	118.30
1	14-A	109	ASP	CB-CG-OD2	5.79	123.52	118.30
1	14-B	192	ASP	CB-CG-OD1	5.79	123.52	118.30
1	2-B	156	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	3-B	156	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	8-B	156	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	9-B	51	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	14-A	149	GLY	N-CA-C	5.76	127.50	113.10
1	9-B	193	ASP	CB-CG-OD1	5.75	123.48	118.30
1	12-B	51	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	13-B	185	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	5-B	156	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	7-B	193	ASP	CB-CG-OD1	5.74	123.46	118.30
1	1-B	156	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	10-B	56	ASP	CB-CG-OD1	5.71	123.44	118.30
1	4-B	185	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	3-B	51	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	5-B	15	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	4-B	51	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	7-B	56	ASP	CB-CG-OD1	5.65	123.39	118.30
1	3-B	56	ASP	CB-CG-OD1	5.65	123.39	118.30
1	13-B	179	ASP	CB-CG-OD2	5.63	123.37	118.30
1	3-B	193	ASP	CB-CG-OD1	5.62	123.36	118.30
1	10-B	51	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	4-B	156	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	3-A	212	CYS	CA-CB-SG	5.59	124.07	114.00
1	13-B	170	THR	CA-CB-CG2	-5.55	104.62	112.40
1	15-B	173	ARG	NH1-CZ-NH2	-5.55	113.29	119.40
1	14-B	56	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	5-A	205	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	4-B	199	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	16-B	179	ASP	CB-CG-OD2	5.43	123.19	118.30
1	6-A	212	CYS	CA-CB-SG	-5.43	104.23	114.00
1	15-B	179	ASP	CB-CG-OD2	5.41	123.17	118.30
1	12-B	56	ASP	CB-CG-OD1	5.41	123.17	118.30
1	6-B	156	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	8-A	205	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	11-B	199	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	15-B	15	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	2-B	15	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	8-B	51	ASP	CB-CG-OD2	-5.36	113.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3-A	51	ASP	CB-CG-OD1	5.35	123.12	118.30
1	7-A	51	ASP	CB-CG-OD1	5.34	123.11	118.30
1	9-A	51	ASP	CB-CG-OD1	5.33	123.10	118.30
1	9-B	199	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	11-A	212	CYS	CA-CB-SG	5.33	123.59	114.00
1	12-A	51	ASP	CB-CG-OD1	5.32	123.08	118.30
1	13-A	71	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	7-B	199	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	7-B	51	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	1-B	193	ASP	CB-CG-OD1	5.29	123.06	118.30
1	3-B	15	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	2-B	199	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	7-B	15	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	15-A	71	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	12-B	156	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	4-A	149	GLY	N-CA-C	5.22	126.15	113.10
1	6-B	15	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	3-A	149	GLY	N-CA-C	5.20	126.11	113.10
1	16-A	51	ASP	CB-CG-OD1	5.20	122.98	118.30
1	3-B	199	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	12-B	15	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	1-A	156	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	6-B	56	ASP	CB-CG-OD1	5.12	122.91	118.30
1	11-B	193	ASP	CB-CG-OD1	5.08	122.87	118.30
1	10-B	199	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	15-B	56	ASP	CB-CG-OD1	5.06	122.85	118.30
1	2-A	51	ASP	CB-CG-OD1	5.04	122.83	118.30
1	14-B	38	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	4-B	56	ASP	CB-CG-OD1	5.01	122.81	118.30
1	13-B	83	MET	CG-SD-CE	5.01	108.21	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1836	0	1866	0	0
1	1-B	1836	0	1866	0	0
1	2-A	1836	0	1866	0	0
1	2-B	1836	0	1866	0	0
1	3-A	1836	0	1866	0	0
1	3-B	1836	0	1866	0	0
1	4-A	1836	0	1866	0	0
1	4-B	1836	0	1866	0	0
1	5-A	1836	0	1866	0	0
1	5-B	1836	0	1866	0	0
1	6-A	1836	0	1866	0	0
1	6-B	1836	0	1866	0	0
1	7-A	1836	0	1866	0	0
1	7-B	1836	0	1866	0	0
1	8-A	1836	0	1866	0	0
1	8-B	1836	0	1866	0	0
1	9-A	1836	0	1866	0	0
1	9-B	1836	0	1866	0	0
1	10-A	1836	0	1866	0	0
1	10-B	1836	0	1866	0	0
1	11-A	1836	0	1866	0	0
1	11-B	1836	0	1866	0	0
1	12-A	1836	0	1866	0	0
1	12-B	1836	0	1866	0	0
1	13-A	1836	0	1866	0	0
1	13-B	1836	0	1866	0	0
1	14-A	1836	0	1866	0	0
1	14-B	1836	0	1866	0	0
1	15-A	1836	0	1866	0	0
1	15-B	1836	0	1866	0	0
1	16-A	1836	0	1866	0	0
1	16-B	1836	0	1866	0	0
2	1-A	48	0	24	0	0
2	1-B	48	0	23	0	0
2	2-A	48	0	24	0	0
2	2-B	48	0	24	0	0
2	3-A	48	0	24	0	0
2	3-B	48	0	24	0	0
2	4-A	48	0	24	0	0
2	4-B	48	0	24	0	0
2	5-A	48	0	24	0	0
2	5-B	48	0	24	0	0
2	6-A	48	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-B	48	0	24	0	0
2	7-A	48	0	24	0	0
2	7-B	48	0	24	0	0
2	8-A	48	0	24	0	0
2	8-B	48	0	23	0	0
2	9-A	48	0	24	0	0
2	9-B	48	0	23	0	0
2	10-A	48	0	24	0	0
2	10-B	48	0	24	0	0
2	11-A	48	0	24	0	0
2	11-B	48	0	24	0	0
2	12-A	48	0	23	0	0
2	12-B	48	0	24	0	0
2	13-A	48	0	24	0	0
2	13-B	48	0	23	0	0
2	14-A	48	0	23	0	0
2	14-B	48	0	22	0	0
2	15-A	48	0	23	0	0
2	15-B	48	0	21	0	0
2	16-A	48	0	24	0	0
2	16-B	48	0	23	0	0
3	1-A	146	0	0	0	0
3	1-B	223	0	0	0	0
3	2-A	147	0	0	0	0
3	2-B	222	0	0	0	0
3	3-A	147	0	0	0	0
3	3-B	222	0	0	0	0
3	4-A	146	0	0	0	0
3	4-B	223	0	0	0	0
3	5-A	147	0	0	0	0
3	5-B	222	0	0	0	0
3	6-A	145	0	0	0	0
3	6-B	224	0	0	0	0
3	7-A	145	0	0	0	0
3	7-B	224	0	0	0	0
3	8-A	146	0	0	0	0
3	8-B	223	0	0	0	0
3	9-A	146	0	0	0	0
3	9-B	223	0	0	0	0
3	10-A	147	0	0	0	0
3	10-B	222	0	0	0	0
3	11-A	146	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	11-B	223	0	0	0	0
3	12-A	147	0	0	0	0
3	12-B	222	0	0	0	0
3	13-A	146	0	0	0	0
3	13-B	223	0	0	0	0
3	14-A	146	0	0	0	0
3	14-B	223	0	0	0	0
3	15-A	147	0	0	0	0
3	15-B	222	0	0	0	0
3	16-A	147	0	0	0	0
3	16-B	222	0	0	0	0
All	All	66192	0	60467	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	239/253 (94%)	224 (94%)	12 (5%)	3 (1%)	15 9
1	1-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	39 37
1	2-A	239/253 (94%)	220 (92%)	19 (8%)	0	100 100
1	2-B	239/253 (94%)	228 (95%)	10 (4%)	1 (0%)	39 37
1	3-A	239/253 (94%)	214 (90%)	21 (9%)	4 (2%)	11 5
1	3-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	39 37
1	4-A	239/253 (94%)	220 (92%)	16 (7%)	3 (1%)	15 9
1	4-B	239/253 (94%)	228 (95%)	11 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	5-A	239/253 (94%)	218 (91%)	20 (8%)	1 (0%)	39 37
1	5-B	239/253 (94%)	225 (94%)	11 (5%)	3 (1%)	15 9
1	6-A	239/253 (94%)	215 (90%)	17 (7%)	7 (3%)	6 2
1	6-B	239/253 (94%)	227 (95%)	11 (5%)	1 (0%)	39 37
1	7-A	239/253 (94%)	220 (92%)	18 (8%)	1 (0%)	39 37
1	7-B	239/253 (94%)	229 (96%)	8 (3%)	2 (1%)	24 17
1	8-A	239/253 (94%)	214 (90%)	22 (9%)	3 (1%)	15 9
1	8-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	39 37
1	9-A	239/253 (94%)	223 (93%)	15 (6%)	1 (0%)	39 37
1	9-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	39 37
1	10-A	239/253 (94%)	222 (93%)	16 (7%)	1 (0%)	39 37
1	10-B	239/253 (94%)	229 (96%)	9 (4%)	1 (0%)	39 37
1	11-A	239/253 (94%)	218 (91%)	17 (7%)	4 (2%)	11 5
1	11-B	239/253 (94%)	223 (93%)	15 (6%)	1 (0%)	39 37
1	12-A	239/253 (94%)	222 (93%)	17 (7%)	0	100 100
1	12-B	239/253 (94%)	230 (96%)	9 (4%)	0	100 100
1	13-A	239/253 (94%)	221 (92%)	18 (8%)	0	100 100
1	13-B	239/253 (94%)	225 (94%)	13 (5%)	1 (0%)	39 37
1	14-A	239/253 (94%)	209 (87%)	21 (9%)	9 (4%)	4 1
1	14-B	239/253 (94%)	228 (95%)	10 (4%)	1 (0%)	39 37
1	15-A	239/253 (94%)	206 (86%)	29 (12%)	4 (2%)	11 5
1	15-B	239/253 (94%)	225 (94%)	12 (5%)	2 (1%)	24 17
1	16-A	239/253 (94%)	222 (93%)	16 (7%)	1 (0%)	39 37
1	16-B	239/253 (94%)	220 (92%)	19 (8%)	0	100 100
All	All	7648/8096 (94%)	7109 (93%)	480 (6%)	59 (1%)	24 17

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	26	GLU
1	1-A	146	LEU
1	3-A	184	VAL
1	6-A	146	LEU
1	7-A	30	LYS

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Mol	Chain	Res	Type
1	8-A	61	ASP
1	11-A	184	VAL
1	14-A	144	ASN
1	14-A	145	LYS
1	3-A	146	LEU
1	6-A	136	GLY
1	8-A	29	ASP
1	8-A	73	LEU
1	11-A	29	ASP
1	11-B	191	LYS
1	14-A	150	ASN
1	14-A	212	CYS
1	14-B	191	LYS
1	15-A	61	ASP
1	15-A	143	LEU
1	15-B	48	GLY
1	1-A	193	ASP
1	1-B	232	PRO
1	3-A	148	ASN
1	5-B	48	GLY
1	5-B	136	GLY
1	5-B	236	SER
1	6-A	193	ASP
1	7-B	27	GLY
1	13-B	48	GLY
1	14-A	139	PRO
1	14-A	236	SER
1	15-A	192	ASP
1	2-B	185	ARG
1	4-A	148	ASN
1	6-A	66	ALA
1	6-A	236	SER
1	7-B	83	MET
1	11-A	192	ASP
1	14-A	100	GLU
1	14-A	213	ILE
1	16-A	27	GLY
1	3-A	193	ASP
1	4-A	125	VAL
1	5-A	100	GLU
1	6-A	183	GLY
1	9-A	127	HIS

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Mol	Chain	Res	Type
1	10-A	165	SER
1	11-A	127	HIS
1	15-B	134	MET
1	6-A	81	PRO
1	6-B	239	THR
1	10-B	235	THR
1	14-A	141	HIS
1	15-A	139	PRO
1	3-B	136	GLY
1	9-B	98	ILE
1	4-A	147	GLY
1	8-B	136	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	196/203 (97%)	194 (99%)	2 (1%)	82	87
1	1-B	196/203 (97%)	192 (98%)	4 (2%)	63	68
1	2-A	196/203 (97%)	191 (97%)	5 (3%)	54	58
1	2-B	196/203 (97%)	193 (98%)	3 (2%)	72	78
1	3-A	196/203 (97%)	191 (97%)	5 (3%)	54	58
1	3-B	196/203 (97%)	194 (99%)	2 (1%)	82	87
1	4-A	196/203 (97%)	192 (98%)	4 (2%)	63	68
1	4-B	196/203 (97%)	194 (99%)	2 (1%)	82	87
1	5-A	196/203 (97%)	194 (99%)	2 (1%)	82	87
1	5-B	196/203 (97%)	195 (100%)	1 (0%)	92	95
1	6-A	196/203 (97%)	194 (99%)	2 (1%)	82	87
1	6-B	196/203 (97%)	193 (98%)	3 (2%)	72	78
1	7-A	196/203 (97%)	194 (99%)	2 (1%)	82	87
1	7-B	196/203 (97%)	192 (98%)	4 (2%)	63	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	8-A	196/203 (97%)	191 (97%)	5 (3%)	54 58
1	8-B	196/203 (97%)	194 (99%)	2 (1%)	82 87
1	9-A	196/203 (97%)	193 (98%)	3 (2%)	72 78
1	9-B	196/203 (97%)	190 (97%)	6 (3%)	47 50
1	10-A	196/203 (97%)	193 (98%)	3 (2%)	72 78
1	10-B	196/203 (97%)	195 (100%)	1 (0%)	92 95
1	11-A	196/203 (97%)	194 (99%)	2 (1%)	82 87
1	11-B	196/203 (97%)	193 (98%)	3 (2%)	72 78
1	12-A	196/203 (97%)	192 (98%)	4 (2%)	63 68
1	12-B	196/203 (97%)	194 (99%)	2 (1%)	82 87
1	13-A	196/203 (97%)	192 (98%)	4 (2%)	63 68
1	13-B	196/203 (97%)	193 (98%)	3 (2%)	72 78
1	14-A	196/203 (97%)	191 (97%)	5 (3%)	54 58
1	14-B	196/203 (97%)	194 (99%)	2 (1%)	82 87
1	15-A	196/203 (97%)	185 (94%)	11 (6%)	26 22
1	15-B	196/203 (97%)	193 (98%)	3 (2%)	72 78
1	16-A	196/203 (97%)	191 (97%)	5 (3%)	54 58
1	16-B	196/203 (97%)	191 (97%)	5 (3%)	54 58
All	All	6272/6496 (97%)	6162 (98%)	110 (2%)	66 72

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	105	PRO
1	1-A	126	LYS
1	1-B	103	GLN
1	1-B	133	SER
1	1-B	199	ASP
1	1-B	219	GLU
1	2-A	18	GLN
1	2-A	68	GLN
1	2-A	105	PRO
1	2-A	126	LYS
1	2-A	248	GLN
1	2-B	68	GLN
1	2-B	134	MET

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Mol	Chain	Res	Type
1	2-B	179	ASP
1	3-A	105	PRO
1	3-A	110	TRP
1	3-A	126	LYS
1	3-A	157	LYS
1	3-A	251	SER
1	3-B	38	ARG
1	3-B	219	GLU
1	4-A	80	VAL
1	4-A	105	PRO
1	4-A	143	LEU
1	4-A	248	GLN
1	4-B	118	ASP
1	4-B	219	GLU
1	5-A	105	PRO
1	5-A	125	VAL
1	5-B	251	SER
1	6-A	105	PRO
1	6-A	212	CYS
1	6-B	31	PHE
1	6-B	199	ASP
1	6-B	251	SER
1	7-A	105	PRO
1	7-A	212	CYS
1	7-B	31	PHE
1	7-B	38	ARG
1	7-B	68	GLN
1	7-B	101	ASP
1	8-A	39	SER
1	8-A	43	LYS
1	8-A	105	PRO
1	8-A	212	CYS
1	8-A	213	ILE
1	8-B	38	ARG
1	8-B	61	ASP
1	9-A	105	PRO
1	9-A	126	LYS
1	9-A	248	GLN
1	9-B	49	GLU
1	9-B	78	SER
1	9-B	99	PHE
1	9-B	125	VAL

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Mol	Chain	Res	Type
1	9-B	143	LEU
1	9-B	212	CYS
1	10-A	104	TYR
1	10-A	105	PRO
1	10-A	220	GLU
1	10-B	38	ARG
1	11-A	105	PRO
1	11-A	126	LYS
1	11-B	38	ARG
1	11-B	39	SER
1	11-B	143	LEU
1	12-A	56	ASP
1	12-A	105	PRO
1	12-A	197	GLN
1	12-A	248	GLN
1	12-B	31	PHE
1	12-B	126	LYS
1	13-A	65	PRO
1	13-A	105	PRO
1	13-A	126	LYS
1	13-A	251	SER
1	13-B	31	PHE
1	13-B	125	VAL
1	13-B	251	SER
1	14-A	105	PRO
1	14-A	110	TRP
1	14-A	144	ASN
1	14-A	150	ASN
1	14-A	199	ASP
1	14-B	31	PHE
1	14-B	173	ARG
1	15-A	100	GLU
1	15-A	105	PRO
1	15-A	118	ASP
1	15-A	141	HIS
1	15-A	157	LYS
1	15-A	191	LYS
1	15-A	199	ASP
1	15-A	201	LYS
1	15-A	212	CYS
1	15-A	213	ILE
1	15-A	245	LEU

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Mol	Chain	Res	Type
1	15-B	61	ASP
1	15-B	143	LEU
1	15-B	219	GLU
1	16-A	105	PRO
1	16-A	126	LYS
1	16-A	164	ASP
1	16-A	241	ASP
1	16-A	248	GLN
1	16-B	31	PHE
1	16-B	62	SER
1	16-B	70	ILE
1	16-B	73	LEU
1	16-B	251	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	3	ASN
1	1-A	64	ASN
1	1-B	18	GLN
1	2-A	3	ASN
1	2-A	18	GLN
1	2-A	64	ASN
1	2-B	18	GLN
1	2-B	103	GLN
1	3-A	3	ASN
1	3-A	64	ASN
1	3-A	115	ASN
1	3-A	138	ASN
1	3-A	148	ASN
1	3-B	18	GLN
1	3-B	64	ASN
1	3-B	68	GLN
1	3-B	103	GLN
1	3-B	160	GLN
1	4-A	3	ASN
1	4-A	18	GLN
1	4-A	197	GLN
1	4-B	18	GLN
1	4-B	68	GLN
1	5-A	3	ASN
1	5-A	197	GLN

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Mol	Chain	Res	Type
1	5-A	223	ASN
1	5-B	3	ASN
1	5-B	68	GLN
1	5-B	103	GLN
1	6-A	3	ASN
1	6-A	160	GLN
1	6-A	223	ASN
1	6-B	3	ASN
1	6-B	18	GLN
1	6-B	41	GLN
1	6-B	68	GLN
1	6-B	103	GLN
1	7-A	3	ASN
1	7-A	64	ASN
1	7-A	103	GLN
1	7-A	160	GLN
1	7-B	3	ASN
1	7-B	18	GLN
1	7-B	68	GLN
1	8-A	3	ASN
1	8-A	103	GLN
1	8-A	197	GLN
1	8-B	41	GLN
1	8-B	64	ASN
1	8-B	127	HIS
1	9-A	3	ASN
1	9-A	18	GLN
1	9-A	64	ASN
1	9-A	160	GLN
1	9-A	197	GLN
1	9-A	223	ASN
1	9-B	3	ASN
1	9-B	18	GLN
1	9-B	68	GLN
1	9-B	103	GLN
1	9-B	116	GLN
1	10-A	18	GLN
1	10-A	160	GLN
1	10-B	64	ASN
1	10-B	103	GLN
1	11-A	64	ASN
1	11-A	160	GLN

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Mol	Chain	Res	Type
1	11-B	68	GLN
1	11-B	103	GLN
1	12-A	3	ASN
1	12-A	18	GLN
1	12-A	64	ASN
1	12-A	160	GLN
1	12-A	223	ASN
1	12-B	3	ASN
1	12-B	64	ASN
1	12-B	68	GLN
1	12-B	103	GLN
1	13-A	3	ASN
1	13-A	18	GLN
1	13-A	64	ASN
1	13-A	197	GLN
1	13-B	3	ASN
1	13-B	41	GLN
1	13-B	68	GLN
1	13-B	127	HIS
1	14-A	3	ASN
1	14-A	18	GLN
1	14-A	138	ASN
1	14-A	141	HIS
1	14-A	144	ASN
1	14-A	150	ASN
1	14-A	160	GLN
1	14-A	248	GLN
1	14-B	68	GLN
1	14-B	103	GLN
1	14-B	160	GLN
1	15-A	3	ASN
1	15-A	18	GLN
1	15-A	103	GLN
1	15-A	138	ASN
1	15-A	141	HIS
1	15-A	144	ASN
1	15-A	148	ASN
1	15-A	150	ASN
1	15-A	160	GLN
1	15-A	197	GLN
1	15-B	3	ASN
1	15-B	68	GLN

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Mol	Chain	Res	Type
1	15-B	103	GLN
1	16-A	160	GLN
1	16-B	68	GLN
1	16-B	115	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 carbohydrates in this entry.

5.6 Ligand geometry

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	1-A	400	-	42,52,52	2.69	12 (28%)	54,80,80	3.48	21 (38%)
2	NAP	1-B	401	-	42,52,52	3.48	18 (42%)	54,80,80	3.46	22 (40%)
2	NAP	10-A	400	-	42,52,52	2.77	15 (35%)	54,80,80	3.49	20 (37%)
2	NAP	10-B	401	-	42,52,52	3.28	16 (38%)	54,80,80	3.60	20 (37%)
2	NAP	11-A	400	-	42,52,52	2.87	14 (33%)	54,80,80	3.39	19 (35%)
2	NAP	11-B	401	-	42,52,52	3.22	14 (33%)	54,80,80	3.60	23 (42%)
2	NAP	12-A	400	-	42,52,52	2.73	18 (42%)	54,80,80	3.47	22 (40%)
2	NAP	12-B	401	-	42,52,52	4.30	18 (42%)	54,80,80	3.82	24 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	13-A	400	-	42,52,52	2.98	15 (35%)	54,80,80	3.34	22 (40%)
2	NAP	13-B	401	-	42,52,52	5.18	21 (50%)	54,80,80	3.94	20 (37%)
2	NAP	14-A	400	-	42,52,52	2.86	16 (38%)	54,80,80	3.24	20 (37%)
2	NAP	14-B	401	-	42,52,52	5.35	19 (45%)	54,80,80	5.04	27 (50%)
2	NAP	15-A	400	-	42,52,52	2.78	15 (35%)	54,80,80	3.31	21 (38%)
2	NAP	15-B	401	-	42,52,52	4.77	19 (45%)	54,80,80	4.75	27 (50%)
2	NAP	16-A	400	-	42,52,52	2.78	14 (33%)	54,80,80	3.20	18 (33%)
2	NAP	16-B	401	-	42,52,52	4.00	13 (30%)	54,80,80	3.96	27 (50%)
2	NAP	2-A	400	-	42,52,52	2.80	15 (35%)	54,80,80	3.50	20 (37%)
2	NAP	2-B	401	-	42,52,52	3.23	13 (30%)	54,80,80	3.64	24 (44%)
2	NAP	3-A	400	-	42,52,52	2.96	14 (33%)	54,80,80	3.51	20 (37%)
2	NAP	3-B	401	-	42,52,52	4.32	14 (33%)	54,80,80	3.84	24 (44%)
2	NAP	4-A	400	-	42,52,52	2.81	11 (26%)	54,80,80	3.49	21 (38%)
2	NAP	4-B	401	-	42,52,52	3.28	12 (28%)	54,80,80	3.46	25 (46%)
2	NAP	5-A	400	-	42,52,52	2.94	15 (35%)	54,80,80	3.52	20 (37%)
2	NAP	5-B	401	-	42,52,52	4.36	14 (33%)	54,80,80	3.87	25 (46%)
2	NAP	6-A	400	-	42,52,52	3.04	12 (28%)	54,80,80	3.43	15 (27%)
2	NAP	6-B	401	-	42,52,52	3.21	13 (30%)	54,80,80	3.63	23 (42%)
2	NAP	7-A	400	-	42,52,52	2.68	13 (30%)	54,80,80	3.43	20 (37%)
2	NAP	7-B	401	-	42,52,52	4.31	15 (35%)	54,80,80	3.81	25 (46%)
2	NAP	8-A	400	-	42,52,52	3.08	10 (23%)	54,80,80	3.44	19 (35%)
2	NAP	8-B	401	-	42,52,52	3.38	18 (42%)	54,80,80	3.43	21 (38%)
2	NAP	9-A	400	-	42,52,52	2.54	9 (21%)	54,80,80	3.41	20 (37%)
2	NAP	9-B	401	-	42,52,52	3.32	14 (33%)	54,80,80	3.45	23 (42%)

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	NAP	1-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	1-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	10-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	10-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	11-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	11-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	12-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	12-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	13-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	13-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	14-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	14-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	15-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	15-B	401	-	-	0/27/67/67	0/5/5/5
2	NAP	16-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	16-B	401	-	-	0/27/67/67	0/5/5/5
2	NAP	2-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	2-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	3-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	3-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	4-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	4-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	5-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	5-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	6-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	6-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	7-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	7-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	8-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	8-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	9-A	400	-	1/1/12/12	0/27/67/67	0/5/5/5
2	NAP	9-B	401	-	1/1/12/12	0/27/67/67	0/5/5/5

All (469) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-B	401	NAP	O3B-C3B	-8.08	1.23	1.43
2	13-A	400	NAP	O4D-C1D	-7.67	1.31	1.41
2	14-A	400	NAP	O4D-C1D	-7.25	1.32	1.41
2	9-A	400	NAP	O4D-C1D	-6.71	1.32	1.41
2	2-A	400	NAP	O4D-C1D	-6.55	1.32	1.41
2	5-A	400	NAP	O4D-C1D	-6.54	1.32	1.41
2	11-A	400	NAP	O4D-C1D	-6.37	1.33	1.41
2	7-A	400	NAP	O4D-C1D	-6.32	1.33	1.41
2	10-A	400	NAP	O4D-C1D	-6.31	1.33	1.41
2	3-A	400	NAP	O4D-C1D	-6.25	1.33	1.41
2	4-A	400	NAP	O4D-C1D	-6.11	1.33	1.41
2	1-A	400	NAP	O4D-C1D	-5.83	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-B	401	NAP	O5B-C5B	-5.74	1.21	1.44
2	3-B	401	NAP	O5B-C5B	-5.71	1.21	1.44
2	12-B	401	NAP	O5B-C5B	-5.70	1.21	1.44
2	7-B	401	NAP	O5B-C5B	-5.68	1.21	1.44
2	8-A	400	NAP	O4D-C1D	-5.68	1.34	1.41
2	16-A	400	NAP	O4D-C1D	-5.25	1.34	1.41
2	12-A	400	NAP	O3D-C3D	-5.07	1.30	1.43
2	8-B	401	NAP	PA-O1A	-4.58	1.34	1.51
2	1-B	401	NAP	PA-O1A	-4.42	1.35	1.51
2	13-B	401	NAP	PA-O2A	-4.35	1.36	1.54
2	15-A	400	NAP	O4D-C1D	-4.20	1.35	1.41
2	7-B	401	NAP	C3B-C4B	-4.02	1.42	1.53
2	12-B	401	NAP	C3B-C4B	-4.01	1.42	1.53
2	3-B	401	NAP	C3B-C4B	-3.99	1.42	1.53
2	16-B	401	NAP	PA-O5B	-3.91	1.41	1.59
2	15-B	401	NAP	O3B-C3B	-3.85	1.33	1.43
2	5-B	401	NAP	C3B-C4B	-3.85	1.42	1.53
2	8-A	400	NAP	PA-O1A	-3.70	1.37	1.51
2	1-B	401	NAP	C5B-C4B	-3.64	1.39	1.51
2	8-B	401	NAP	C5B-C4B	-3.58	1.40	1.51
2	8-A	400	NAP	PA-O2A	-3.47	1.40	1.54
2	13-A	400	NAP	O2B-C2B	-3.40	1.33	1.44
2	9-B	401	NAP	C5B-C4B	-3.37	1.40	1.51
2	16-A	400	NAP	O2B-C2B	-3.27	1.34	1.44
2	6-A	400	NAP	PA-O1A	-3.24	1.39	1.51
2	4-B	401	NAP	C5B-C4B	-3.20	1.41	1.51
2	2-A	400	NAP	PA-O2A	-3.19	1.41	1.54
2	10-A	400	NAP	PA-O2A	-3.18	1.41	1.54
2	8-A	400	NAP	C3B-C4B	-3.13	1.44	1.53
2	4-B	401	NAP	C3B-C4B	-3.12	1.44	1.53
2	9-B	401	NAP	C3B-C4B	-3.08	1.44	1.53
2	12-A	400	NAP	O4D-C1D	-3.06	1.37	1.41
2	14-A	400	NAP	PA-O2A	-3.06	1.41	1.54
2	11-B	401	NAP	C3B-C4B	-3.05	1.44	1.53
2	15-A	400	NAP	O2B-C2B	-3.02	1.34	1.44
2	2-B	401	NAP	C3B-C4B	-3.01	1.44	1.53
2	7-A	400	NAP	C5B-C4B	-3.00	1.41	1.51
2	6-A	400	NAP	C3B-C4B	-2.98	1.45	1.53
2	6-B	401	NAP	C3B-C4B	-2.98	1.45	1.53
2	12-A	400	NAP	C5B-C4B	-2.96	1.42	1.51
2	3-A	400	NAP	PA-O1A	-2.93	1.40	1.51
2	1-B	401	NAP	C3B-C2B	-2.93	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9-A	400	NAP	C5B-C4B	-2.89	1.42	1.51
2	14-A	400	NAP	O3B-C3B	-2.85	1.36	1.43
2	3-A	400	NAP	PA-O2A	-2.85	1.42	1.54
2	15-A	400	NAP	O3B-C3B	-2.83	1.36	1.43
2	8-B	401	NAP	C3B-C2B	-2.81	1.46	1.53
2	1-B	401	NAP	C3B-C4B	-2.77	1.45	1.53
2	4-A	400	NAP	PA-O2A	-2.74	1.43	1.54
2	13-B	401	NAP	C8A-N7A	-2.72	1.29	1.34
2	5-A	400	NAP	PA-O2A	-2.68	1.43	1.54
2	9-B	401	NAP	PA-O1A	-2.66	1.41	1.51
2	1-A	400	NAP	PA-O2A	-2.66	1.43	1.54
2	10-B	401	NAP	C3B-C4B	-2.62	1.45	1.53
2	9-A	400	NAP	O2B-C2B	-2.61	1.36	1.44
2	14-B	401	NAP	C3B-C2B	-2.61	1.47	1.53
2	11-B	401	NAP	C5B-C4B	-2.58	1.43	1.51
2	13-B	401	NAP	PN-O1N	-2.58	1.41	1.51
2	6-A	400	NAP	C6N-C5N	-2.57	1.32	1.38
2	1-A	400	NAP	PA-O1A	-2.56	1.41	1.51
2	3-A	400	NAP	C3B-C4B	-2.55	1.46	1.53
2	7-A	400	NAP	O2B-C2B	-2.54	1.36	1.44
2	14-B	401	NAP	O3B-C3B	-2.53	1.36	1.43
2	16-B	401	NAP	P2B-O2X	-2.52	1.45	1.54
2	4-A	400	NAP	C3B-C4B	-2.51	1.46	1.53
2	13-B	401	NAP	O2B-C2B	-2.49	1.36	1.44
2	5-A	400	NAP	PA-O1A	-2.49	1.42	1.51
2	16-A	400	NAP	C5B-C4B	-2.48	1.43	1.51
2	5-A	400	NAP	C3B-C4B	-2.46	1.46	1.53
2	8-B	401	NAP	C3B-C4B	-2.45	1.46	1.53
2	1-A	400	NAP	C3B-C4B	-2.43	1.46	1.53
2	4-A	400	NAP	PA-O1A	-2.43	1.42	1.51
2	6-B	401	NAP	C5B-C4B	-2.41	1.43	1.51
2	13-A	400	NAP	C5B-C4B	-2.41	1.43	1.51
2	14-A	400	NAP	C3B-C4B	-2.41	1.46	1.53
2	12-A	400	NAP	PA-O1A	-2.38	1.42	1.51
2	6-A	400	NAP	PA-O2A	-2.37	1.44	1.54
2	15-A	400	NAP	C5B-C4B	-2.32	1.44	1.51
2	2-B	401	NAP	C5B-C4B	-2.30	1.44	1.51
2	9-B	401	NAP	C3B-C2B	-2.26	1.47	1.53
2	12-A	400	NAP	C2D-C3D	-2.25	1.47	1.53
2	16-A	400	NAP	O3B-C3B	-2.24	1.37	1.43
2	10-A	400	NAP	C5B-C4B	-2.20	1.44	1.51
2	2-A	400	NAP	C5B-C4B	-2.12	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-A	400	NAP	PA-O1A	-2.12	1.43	1.51
2	12-B	401	NAP	C3B-C2B	-2.10	1.48	1.53
2	7-B	401	NAP	C3B-C2B	-2.09	1.48	1.53
2	3-B	401	NAP	C3B-C2B	-2.08	1.48	1.53
2	2-A	400	NAP	C3B-C4B	-2.07	1.47	1.53
2	13-A	400	NAP	O3B-C3B	-2.07	1.38	1.43
2	12-A	400	NAP	O2B-C2B	-2.06	1.37	1.44
2	16-B	401	NAP	C2A-N1A	-2.04	1.30	1.33
2	11-A	400	NAP	C3B-C4B	-2.04	1.47	1.53
2	1-A	400	NAP	C2D-C3D	-2.04	1.47	1.53
2	10-A	400	NAP	C3B-C4B	-2.03	1.47	1.53
2	10-B	401	NAP	PA-O1A	-2.02	1.43	1.51
2	11-A	400	NAP	C5B-C4B	-2.02	1.45	1.51
2	1-B	401	NAP	C2N-C3N	2.01	1.42	1.39
2	14-B	401	NAP	C3D-C4D	2.02	1.58	1.53
2	14-B	401	NAP	C5B-C4B	2.02	1.58	1.51
2	7-A	400	NAP	C3D-C4D	2.03	1.58	1.53
2	11-B	401	NAP	C2D-C3D	2.03	1.58	1.53
2	5-B	401	NAP	O4D-C1D	2.03	1.43	1.41
2	15-B	401	NAP	C6A-N6A	2.04	1.41	1.34
2	15-B	401	NAP	PA-O2A	2.05	1.63	1.54
2	4-B	401	NAP	O4D-C1D	2.05	1.43	1.41
2	5-B	401	NAP	C2A-N3A	2.05	1.35	1.32
2	7-B	401	NAP	O4D-C1D	2.05	1.43	1.41
2	12-B	401	NAP	C2D-C3D	2.05	1.59	1.53
2	10-A	400	NAP	C3D-C4D	2.06	1.58	1.53
2	5-A	400	NAP	C2A-N3A	2.06	1.35	1.32
2	3-A	400	NAP	C3N-C7N	2.07	1.53	1.50
2	8-B	401	NAP	C2D-C3D	2.07	1.59	1.53
2	10-B	401	NAP	C2D-C3D	2.08	1.59	1.53
2	13-A	400	NAP	C3D-C4D	2.09	1.58	1.53
2	1-B	401	NAP	O4D-C1D	2.09	1.43	1.41
2	11-B	401	NAP	C3D-C4D	2.09	1.58	1.53
2	7-B	401	NAP	C3D-C4D	2.10	1.58	1.53
2	12-B	401	NAP	O4D-C1D	2.10	1.43	1.41
2	12-A	400	NAP	P2B-O2X	2.10	1.62	1.54
2	12-A	400	NAP	C6A-N6A	2.10	1.41	1.34
2	1-A	400	NAP	C3D-C4D	2.11	1.58	1.53
2	3-B	401	NAP	C3D-C4D	2.11	1.58	1.53
2	6-B	401	NAP	O4D-C1D	2.12	1.43	1.41
2	2-B	401	NAP	C3D-C4D	2.12	1.58	1.53
2	14-A	400	NAP	C3D-C4D	2.12	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-B	401	NAP	C3D-C4D	2.13	1.58	1.53
2	1-B	401	NAP	C2D-C3D	2.14	1.59	1.53
2	16-B	401	NAP	O4D-C1D	2.14	1.43	1.41
2	2-B	401	NAP	O4D-C1D	2.14	1.43	1.41
2	2-A	400	NAP	P2B-O2B	2.15	1.66	1.60
2	11-B	401	NAP	O4D-C1D	2.15	1.43	1.41
2	16-A	400	NAP	C3D-C4D	2.15	1.58	1.53
2	12-A	400	NAP	C3D-C4D	2.17	1.58	1.53
2	12-B	401	NAP	C3D-C4D	2.17	1.58	1.53
2	2-A	400	NAP	C3N-C7N	2.18	1.54	1.50
2	16-A	400	NAP	O4D-C4D	2.20	1.50	1.45
2	10-B	401	NAP	C2A-N3A	2.21	1.36	1.32
2	1-B	401	NAP	C2A-N1A	2.22	1.38	1.33
2	4-B	401	NAP	C6A-N6A	2.23	1.41	1.34
2	3-B	401	NAP	C2A-N3A	2.23	1.36	1.32
2	10-A	400	NAP	P2B-O2B	2.24	1.66	1.60
2	8-B	401	NAP	P2B-O1X	2.24	1.58	1.51
2	6-A	400	NAP	C3D-C4D	2.25	1.59	1.53
2	8-B	401	NAP	C3N-C7N	2.26	1.54	1.50
2	4-A	400	NAP	C2A-N3A	2.27	1.36	1.32
2	11-A	400	NAP	PA-O1A	2.27	1.59	1.51
2	9-B	401	NAP	C6A-N6A	2.29	1.42	1.34
2	5-A	400	NAP	C3N-C7N	2.32	1.54	1.50
2	14-B	401	NAP	C2D-C3D	2.34	1.59	1.53
2	10-B	401	NAP	C3D-C4D	2.35	1.59	1.53
2	15-B	401	NAP	C2D-C3D	2.35	1.59	1.53
2	3-A	400	NAP	C6N-N1N	2.36	1.41	1.35
2	5-B	401	NAP	C3D-C4D	2.36	1.59	1.53
2	14-B	401	NAP	O4D-C1D	2.36	1.44	1.41
2	15-A	400	NAP	P2B-O2B	2.36	1.67	1.60
2	15-B	401	NAP	C3D-C4D	2.36	1.59	1.53
2	5-A	400	NAP	C6N-N1N	2.37	1.41	1.35
2	12-B	401	NAP	C2A-N3A	2.39	1.36	1.32
2	13-B	401	NAP	O4D-C4D	2.39	1.50	1.45
2	7-B	401	NAP	C2A-N3A	2.41	1.36	1.32
2	15-B	401	NAP	O4D-C1D	2.42	1.44	1.41
2	6-B	401	NAP	C2A-N3A	2.42	1.36	1.32
2	2-B	401	NAP	C2A-N3A	2.42	1.36	1.32
2	13-A	400	NAP	C6N-N1N	2.43	1.42	1.35
2	8-B	401	NAP	C2A-N1A	2.44	1.38	1.33
2	15-B	401	NAP	C3B-C4B	2.44	1.59	1.53
2	3-A	400	NAP	C7N-N7N	2.45	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	400	NAP	C7N-N7N	2.46	1.38	1.33
2	12-A	400	NAP	C7N-N7N	2.46	1.38	1.33
2	13-A	400	NAP	C3N-C7N	2.47	1.54	1.50
2	10-A	400	NAP	C7N-N7N	2.47	1.38	1.33
2	2-A	400	NAP	C6N-N1N	2.48	1.42	1.35
2	12-A	400	NAP	C2A-N1A	2.51	1.38	1.33
2	12-B	401	NAP	O7N-C7N	2.53	1.29	1.24
2	15-B	401	NAP	C2A-N3A	2.53	1.36	1.32
2	11-B	401	NAP	C2A-N3A	2.53	1.36	1.32
2	2-A	400	NAP	C7N-N7N	2.53	1.38	1.33
2	11-A	400	NAP	C7N-N7N	2.54	1.38	1.33
2	14-A	400	NAP	C6N-N1N	2.55	1.42	1.35
2	12-B	401	NAP	O3D-C3D	2.55	1.49	1.43
2	15-A	400	NAP	C3D-C4D	2.56	1.59	1.53
2	13-B	401	NAP	C3D-C4D	2.58	1.60	1.53
2	14-B	401	NAP	C6A-N6A	2.61	1.43	1.34
2	11-A	400	NAP	C6N-N1N	2.62	1.42	1.35
2	14-A	400	NAP	C7N-N7N	2.63	1.38	1.33
2	10-B	401	NAP	O4D-C1D	2.65	1.44	1.41
2	7-A	400	NAP	C7N-N7N	2.66	1.38	1.33
2	10-B	401	NAP	O7N-C7N	2.66	1.29	1.24
2	10-B	401	NAP	P2B-O2B	2.70	1.68	1.60
2	8-B	401	NAP	C2N-C3N	2.72	1.43	1.39
2	16-B	401	NAP	C4A-N3A	2.74	1.39	1.35
2	10-A	400	NAP	C6N-N1N	2.76	1.42	1.35
2	10-B	401	NAP	O3D-C3D	2.79	1.49	1.43
2	13-B	401	NAP	C6A-N6A	2.80	1.43	1.34
2	9-B	401	NAP	C5N-C4N	2.80	1.44	1.38
2	13-B	401	NAP	C2N-C3N	2.82	1.43	1.39
2	16-B	401	NAP	O5B-C5B	2.83	1.56	1.44
2	5-A	400	NAP	P2B-O2B	2.84	1.68	1.60
2	1-A	400	NAP	P2B-O2B	2.84	1.68	1.60
2	2-B	401	NAP	P2B-O2B	2.86	1.68	1.60
2	14-A	400	NAP	C2A-N3A	2.89	1.37	1.32
2	7-A	400	NAP	C6N-N1N	2.90	1.43	1.35
2	9-B	401	NAP	O3B-C3B	2.91	1.49	1.43
2	8-B	401	NAP	C6N-N1N	2.91	1.43	1.35
2	6-B	401	NAP	P2B-O2B	2.92	1.68	1.60
2	7-B	401	NAP	C6N-N1N	2.92	1.43	1.35
2	13-A	400	NAP	C7N-N7N	2.96	1.39	1.33
2	1-A	400	NAP	C2A-N1A	2.97	1.39	1.33
2	1-B	401	NAP	C3N-C7N	2.98	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	15-A	400	NAP	C7N-N7N	3.00	1.39	1.33
2	12-B	401	NAP	C7N-N7N	3.02	1.39	1.33
2	11-B	401	NAP	C6N-N1N	3.02	1.43	1.35
2	14-B	401	NAP	PA-O2A	3.03	1.67	1.54
2	11-B	401	NAP	P2B-O2B	3.04	1.69	1.60
2	1-B	401	NAP	C6N-N1N	3.04	1.43	1.35
2	3-A	400	NAP	C2A-N1A	3.04	1.39	1.33
2	10-A	400	NAP	O7N-C7N	3.05	1.30	1.24
2	7-A	400	NAP	O7N-C7N	3.06	1.30	1.24
2	6-B	401	NAP	C6N-N1N	3.07	1.43	1.35
2	14-A	400	NAP	P2B-O2B	3.08	1.69	1.60
2	2-A	400	NAP	C2A-N1A	3.08	1.39	1.33
2	4-A	400	NAP	P2B-O2B	3.09	1.69	1.60
2	5-A	400	NAP	C2A-N1A	3.09	1.39	1.33
2	4-B	401	NAP	C5N-C4N	3.10	1.45	1.38
2	10-B	401	NAP	C7N-N7N	3.10	1.39	1.33
2	10-A	400	NAP	C2A-N1A	3.11	1.39	1.33
2	12-B	401	NAP	C2N-C3N	3.11	1.43	1.39
2	10-B	401	NAP	C2N-C3N	3.12	1.43	1.39
2	10-B	401	NAP	C6N-N1N	3.13	1.43	1.35
2	3-A	400	NAP	P2B-O2B	3.14	1.69	1.60
2	15-B	401	NAP	O7N-C7N	3.14	1.30	1.24
2	15-B	401	NAP	P2B-O2B	3.17	1.69	1.60
2	6-A	400	NAP	C3N-C7N	3.17	1.55	1.50
2	16-B	401	NAP	C6N-N1N	3.17	1.44	1.35
2	2-B	401	NAP	C6N-N1N	3.18	1.44	1.35
2	15-A	400	NAP	C5N-C4N	3.18	1.45	1.38
2	14-B	401	NAP	C6N-N1N	3.19	1.44	1.35
2	15-B	401	NAP	C2N-C3N	3.19	1.43	1.39
2	14-B	401	NAP	C2N-C3N	3.19	1.43	1.39
2	3-A	400	NAP	O7N-C7N	3.21	1.31	1.24
2	11-A	400	NAP	O7N-C7N	3.22	1.31	1.24
2	9-B	401	NAP	C6N-N1N	3.24	1.44	1.35
2	3-B	401	NAP	C6N-N1N	3.24	1.44	1.35
2	12-B	401	NAP	C6N-N1N	3.24	1.44	1.35
2	16-B	401	NAP	C5N-C4N	3.25	1.45	1.38
2	7-A	400	NAP	C2A-N1A	3.28	1.40	1.33
2	4-B	401	NAP	C6N-N1N	3.32	1.44	1.35
2	14-A	400	NAP	O7N-C7N	3.33	1.31	1.24
2	14-B	401	NAP	P2B-O2B	3.33	1.70	1.60
2	5-B	401	NAP	C6N-N1N	3.38	1.44	1.35
2	16-A	400	NAP	C2N-C3N	3.38	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	400	NAP	O7N-C7N	3.39	1.31	1.24
2	10-A	400	NAP	C2A-N3A	3.41	1.38	1.32
2	2-A	400	NAP	C2A-N3A	3.42	1.38	1.32
2	4-B	401	NAP	C2A-N3A	3.42	1.38	1.32
2	9-A	400	NAP	C2A-N1A	3.42	1.40	1.33
2	4-A	400	NAP	C2A-N1A	3.44	1.40	1.33
2	14-B	401	NAP	C2A-N3A	3.44	1.38	1.32
2	2-A	400	NAP	O7N-C7N	3.46	1.31	1.24
2	4-B	401	NAP	P2B-O2B	3.46	1.70	1.60
2	5-B	401	NAP	C7N-N7N	3.47	1.40	1.33
2	2-B	401	NAP	C2N-C3N	3.47	1.44	1.39
2	9-B	401	NAP	P2B-O2B	3.48	1.70	1.60
2	12-A	400	NAP	C5N-C4N	3.50	1.46	1.38
2	8-B	401	NAP	C7N-N7N	3.51	1.40	1.33
2	10-B	401	NAP	C4N-C3N	3.51	1.45	1.39
2	16-A	400	NAP	C5N-C4N	3.52	1.46	1.38
2	15-B	401	NAP	O3D-C3D	3.54	1.51	1.43
2	5-B	401	NAP	P2B-O2B	3.55	1.70	1.60
2	15-B	401	NAP	C6N-N1N	3.59	1.45	1.35
2	11-B	401	NAP	C7N-N7N	3.61	1.40	1.33
2	1-B	401	NAP	P2B-O2B	3.62	1.71	1.60
2	8-A	400	NAP	C2A-N1A	3.63	1.40	1.33
2	6-B	401	NAP	C7N-N7N	3.64	1.40	1.33
2	7-B	401	NAP	C7N-N7N	3.65	1.40	1.33
2	11-B	401	NAP	C2N-C3N	3.66	1.44	1.39
2	13-B	401	NAP	C6N-N1N	3.67	1.45	1.35
2	15-B	401	NAP	C7N-N7N	3.69	1.40	1.33
2	3-B	401	NAP	C7N-N7N	3.70	1.40	1.33
2	1-B	401	NAP	C7N-N7N	3.72	1.40	1.33
2	14-A	400	NAP	C2A-N1A	3.72	1.41	1.33
2	13-B	401	NAP	P2B-O2B	3.74	1.71	1.60
2	8-B	401	NAP	C4A-N3A	3.74	1.41	1.35
2	12-B	401	NAP	C4N-C3N	3.77	1.45	1.39
2	6-B	401	NAP	C2N-C3N	3.78	1.44	1.39
2	11-A	400	NAP	C2A-N3A	3.78	1.38	1.32
2	14-B	401	NAP	C7N-N7N	3.78	1.40	1.33
2	8-A	400	NAP	C4N-C3N	3.79	1.45	1.39
2	3-B	401	NAP	C2N-C3N	3.81	1.44	1.39
2	2-B	401	NAP	C7N-N7N	3.83	1.40	1.33
2	8-B	401	NAP	O3B-C3B	3.84	1.52	1.43
2	7-B	401	NAP	C2N-C3N	3.86	1.44	1.39
2	4-A	400	NAP	C4N-C3N	3.87	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	12-B	401	NAP	P2B-O2B	3.88	1.71	1.60
2	3-B	401	NAP	P2B-O2B	3.89	1.71	1.60
2	1-B	401	NAP	C4A-N3A	3.89	1.41	1.35
2	11-A	400	NAP	C2A-N1A	3.91	1.41	1.33
2	1-A	400	NAP	C4N-C3N	3.91	1.46	1.39
2	6-A	400	NAP	P2B-O2B	3.92	1.71	1.60
2	16-A	400	NAP	C2A-N1A	3.93	1.41	1.33
2	7-B	401	NAP	P2B-O2B	3.93	1.71	1.60
2	15-B	401	NAP	O5B-C5B	3.95	1.60	1.44
2	13-A	400	NAP	O7N-C7N	3.98	1.32	1.24
2	8-A	400	NAP	P2B-O2B	3.98	1.72	1.60
2	6-A	400	NAP	C2A-N1A	3.99	1.41	1.33
2	5-B	401	NAP	C2N-C3N	3.99	1.45	1.39
2	13-A	400	NAP	C2A-N1A	4.11	1.41	1.33
2	13-B	401	NAP	C3B-C2B	4.17	1.62	1.53
2	9-A	400	NAP	C4N-C3N	4.18	1.46	1.39
2	13-B	401	NAP	C2A-N3A	4.20	1.39	1.32
2	12-A	400	NAP	C4N-C3N	4.23	1.46	1.39
2	15-B	401	NAP	C4N-C3N	4.23	1.46	1.39
2	9-A	400	NAP	C2A-N3A	4.28	1.39	1.32
2	14-B	401	NAP	C3B-C4B	4.31	1.64	1.53
2	9-B	401	NAP	C2A-N3A	4.32	1.39	1.32
2	9-B	401	NAP	C4A-N3A	4.34	1.42	1.35
2	1-B	401	NAP	O3B-C3B	4.34	1.53	1.43
2	13-A	400	NAP	C2A-N3A	4.38	1.39	1.32
2	15-A	400	NAP	C6N-N1N	4.45	1.47	1.35
2	7-A	400	NAP	C2A-N3A	4.46	1.40	1.32
2	5-B	401	NAP	C4A-N3A	4.53	1.42	1.35
2	4-B	401	NAP	C4A-N3A	4.56	1.42	1.35
2	15-A	400	NAP	C2A-N1A	4.58	1.42	1.33
2	15-A	400	NAP	C2A-N3A	4.59	1.40	1.32
2	7-B	401	NAP	C4A-N3A	4.61	1.42	1.35
2	8-B	401	NAP	P2B-O2B	4.66	1.74	1.60
2	16-A	400	NAP	C6N-N1N	4.66	1.47	1.35
2	15-A	400	NAP	C4N-C3N	4.70	1.47	1.39
2	3-B	401	NAP	C4A-N3A	4.72	1.42	1.35
2	11-B	401	NAP	C4A-N3A	4.72	1.42	1.35
2	6-B	401	NAP	C4A-N3A	4.73	1.42	1.35
2	12-B	401	NAP	C4A-N3A	4.75	1.42	1.35
2	16-A	400	NAP	C2A-N3A	4.75	1.40	1.32
2	13-B	401	NAP	C4A-N3A	4.76	1.42	1.35
2	2-B	401	NAP	C4A-N3A	4.77	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9-A	400	NAP	C2N-C3N	4.80	1.46	1.39
2	10-B	401	NAP	C4A-N3A	4.82	1.42	1.35
2	12-A	400	NAP	C2N-C3N	4.85	1.46	1.39
2	12-A	400	NAP	C2A-N3A	4.86	1.40	1.32
2	14-B	401	NAP	O5B-C5B	4.87	1.64	1.44
2	3-B	401	NAP	O4B-C4B	4.88	1.56	1.45
2	5-B	401	NAP	O4B-C4B	4.90	1.56	1.45
2	11-A	400	NAP	P2B-O2B	4.90	1.74	1.60
2	12-A	400	NAP	C6N-N1N	4.92	1.48	1.35
2	1-A	400	NAP	C2N-C3N	4.92	1.46	1.39
2	7-B	401	NAP	O4B-C4B	4.97	1.56	1.45
2	12-B	401	NAP	O4B-C4B	5.00	1.56	1.45
2	8-A	400	NAP	C2N-C3N	5.00	1.46	1.39
2	13-A	400	NAP	O4B-C1B	5.02	1.47	1.41
2	4-A	400	NAP	C2N-C3N	5.04	1.46	1.39
2	16-A	400	NAP	O4B-C1B	5.04	1.47	1.41
2	6-A	400	NAP	C6N-N1N	5.08	1.49	1.35
2	15-A	400	NAP	C2N-C3N	5.09	1.46	1.39
2	14-B	401	NAP	C4A-N3A	5.19	1.43	1.35
2	7-A	400	NAP	C2N-C3N	5.24	1.46	1.39
2	1-B	401	NAP	C2A-N3A	5.25	1.41	1.32
2	15-A	400	NAP	O4B-C1B	5.25	1.47	1.41
2	15-B	401	NAP	C4A-N3A	5.26	1.43	1.35
2	16-B	401	NAP	PA-O1A	5.29	1.70	1.51
2	11-A	400	NAP	C2N-C3N	5.31	1.47	1.39
2	10-A	400	NAP	C2N-C3N	5.35	1.47	1.39
2	2-A	400	NAP	C2N-C3N	5.39	1.47	1.39
2	5-A	400	NAP	C2N-C3N	5.45	1.47	1.39
2	3-A	400	NAP	C2N-C3N	5.49	1.47	1.39
2	7-B	401	NAP	C4N-C3N	5.51	1.48	1.39
2	5-A	400	NAP	C4N-C3N	5.53	1.48	1.39
2	3-B	401	NAP	C4N-C3N	5.54	1.48	1.39
2	2-A	400	NAP	C4N-C3N	5.58	1.48	1.39
2	16-B	401	NAP	P2B-O2B	5.59	1.77	1.60
2	11-B	401	NAP	C4N-C3N	5.60	1.48	1.39
2	6-B	401	NAP	C4N-C3N	5.61	1.48	1.39
2	3-A	400	NAP	C4N-C3N	5.64	1.49	1.39
2	5-B	401	NAP	C4N-C3N	5.75	1.49	1.39
2	11-A	400	NAP	C4N-C3N	5.84	1.49	1.39
2	10-A	400	NAP	C4N-C3N	5.86	1.49	1.39
2	2-B	401	NAP	C4N-C3N	5.86	1.49	1.39
2	7-A	400	NAP	C4N-C3N	5.91	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8-B	401	NAP	C2A-N3A	5.91	1.42	1.32
2	6-A	400	NAP	C4N-C3N	5.91	1.49	1.39
2	8-B	401	NAP	C4N-C3N	5.95	1.49	1.39
2	13-B	401	NAP	O4D-C1D	5.96	1.48	1.41
2	13-A	400	NAP	C2N-C3N	6.00	1.48	1.39
2	13-A	400	NAP	C4N-C3N	6.07	1.49	1.39
2	12-A	400	NAP	O4B-C1B	6.14	1.49	1.41
2	7-A	400	NAP	O4B-C1B	6.22	1.49	1.41
2	14-A	400	NAP	C4N-C3N	6.22	1.50	1.39
2	14-A	400	NAP	C2N-C3N	6.30	1.48	1.39
2	1-B	401	NAP	C4N-C3N	6.42	1.50	1.39
2	9-A	400	NAP	O4B-C1B	6.42	1.49	1.41
2	14-A	400	NAP	O4B-C4B	6.45	1.59	1.45
2	14-B	401	NAP	C4N-C3N	6.59	1.50	1.39
2	9-B	401	NAP	C4N-C3N	6.68	1.50	1.39
2	16-A	400	NAP	C4N-C3N	6.73	1.50	1.39
2	11-A	400	NAP	O4B-C1B	7.07	1.50	1.41
2	4-B	401	NAP	C4N-C3N	7.28	1.51	1.39
2	14-A	400	NAP	O4B-C1B	7.37	1.50	1.41
2	10-A	400	NAP	O4B-C1B	7.67	1.50	1.41
2	2-A	400	NAP	O4B-C1B	7.71	1.50	1.41
2	7-A	400	NAP	O4B-C4B	7.77	1.63	1.45
2	13-B	401	NAP	C4N-C3N	7.88	1.52	1.39
2	16-B	401	NAP	C4N-C3N	7.95	1.52	1.39
2	10-A	400	NAP	O4B-C4B	8.09	1.63	1.45
2	9-A	400	NAP	O4B-C4B	8.10	1.63	1.45
2	11-A	400	NAP	O4B-C4B	8.19	1.63	1.45
2	2-A	400	NAP	O4B-C4B	8.34	1.64	1.45
2	12-A	400	NAP	O4B-C4B	8.45	1.64	1.45
2	1-A	400	NAP	O4B-C1B	8.80	1.52	1.41
2	16-A	400	NAP	O4B-C4B	8.92	1.65	1.45
2	1-A	400	NAP	O4B-C4B	8.96	1.65	1.45
2	5-A	400	NAP	O4B-C1B	8.99	1.52	1.41
2	3-A	400	NAP	O4B-C1B	9.01	1.52	1.41
2	15-A	400	NAP	O4B-C4B	9.22	1.66	1.45
2	13-B	401	NAP	O5B-C5B	9.24	1.82	1.44
2	4-A	400	NAP	O4B-C1B	9.25	1.52	1.41
2	8-B	401	NAP	O4B-C1B	9.36	1.53	1.41
2	13-A	400	NAP	O4B-C4B	9.38	1.66	1.45
2	5-A	400	NAP	O4B-C4B	9.43	1.66	1.45
2	4-A	400	NAP	O4B-C4B	9.48	1.66	1.45
2	3-A	400	NAP	O4B-C4B	9.72	1.67	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-A	400	NAP	O4B-C4B	10.11	1.68	1.45
2	13-B	401	NAP	O4B-C1B	10.21	1.54	1.41
2	8-A	400	NAP	O4B-C1B	10.32	1.54	1.41
2	10-B	401	NAP	O4B-C4B	10.51	1.69	1.45
2	6-A	400	NAP	O4B-C1B	10.70	1.54	1.41
2	16-B	401	NAP	O4B-C1B	10.82	1.54	1.41
2	1-B	401	NAP	O4B-C1B	10.99	1.55	1.41
2	9-B	401	NAP	O4B-C1B	11.05	1.55	1.41
2	2-B	401	NAP	O4B-C4B	11.14	1.70	1.45
2	6-B	401	NAP	O4B-C4B	11.24	1.71	1.45
2	8-A	400	NAP	O4B-C4B	11.25	1.71	1.45
2	4-B	401	NAP	O4B-C1B	11.30	1.55	1.41
2	11-B	401	NAP	O4B-C4B	11.50	1.71	1.45
2	13-B	401	NAP	C3B-C4B	11.97	1.85	1.53
2	1-B	401	NAP	O4B-C4B	12.06	1.72	1.45
2	11-B	401	NAP	O4B-C1B	12.25	1.56	1.41
2	9-B	401	NAP	O4B-C4B	12.29	1.73	1.45
2	4-B	401	NAP	O4B-C4B	12.32	1.73	1.45
2	8-B	401	NAP	O4B-C4B	12.33	1.73	1.45
2	6-B	401	NAP	O4B-C1B	12.51	1.57	1.41
2	2-B	401	NAP	O4B-C1B	12.69	1.57	1.41
2	13-B	401	NAP	C5B-C4B	13.93	1.96	1.51
2	10-B	401	NAP	O4B-C1B	14.12	1.59	1.41
2	5-B	401	NAP	O3B-C3B	15.13	1.79	1.43
2	7-B	401	NAP	O3B-C3B	15.29	1.79	1.43
2	3-B	401	NAP	O3B-C3B	15.30	1.79	1.43
2	12-B	401	NAP	O3B-C3B	15.35	1.79	1.43
2	15-B	401	NAP	O4B-C1B	15.36	1.60	1.41
2	13-B	401	NAP	O4B-C4B	16.24	1.82	1.45
2	14-B	401	NAP	O4B-C1B	16.37	1.61	1.41
2	7-B	401	NAP	O4B-C1B	18.13	1.64	1.41
2	3-B	401	NAP	O4B-C1B	18.21	1.64	1.41
2	12-B	401	NAP	O4B-C1B	18.23	1.64	1.41
2	16-B	401	NAP	O4B-C4B	18.31	1.87	1.45
2	5-B	401	NAP	O4B-C1B	18.47	1.64	1.41
2	15-B	401	NAP	O4B-C4B	22.79	1.97	1.45
2	14-B	401	NAP	O4B-C4B	26.44	2.06	1.45

All (698) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	14-B	401	NAP	O4B-C4B-C3B	-18.59	67.69	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	15-B	401	NAP	O4B-C4B-C3B	-16.56	71.78	105.15
2	14-B	401	NAP	O4B-C4B-C5B	-14.99	55.71	109.32
2	16-B	401	NAP	O4B-C4B-C3B	-13.40	78.14	105.15
2	15-B	401	NAP	O4B-C4B-C5B	-13.22	62.03	109.32
2	14-B	401	NAP	O5B-C5B-C4B	-13.13	60.73	109.12
2	13-B	401	NAP	O5B-C5B-C4B	-12.47	63.13	109.12
2	15-B	401	NAP	O5B-C5B-C4B	-12.14	64.35	109.12
2	13-B	401	NAP	O4B-C4B-C3B	-10.39	84.22	105.15
2	16-B	401	NAP	O4B-C4B-C5B	-10.20	72.85	109.32
2	15-B	401	NAP	O2A-PA-O1A	-9.63	60.35	112.53
2	5-B	401	NAP	O4B-C1B-C2B	-9.30	89.77	106.60
2	3-B	401	NAP	O4B-C1B-C2B	-9.28	89.81	106.60
2	12-B	401	NAP	O4B-C1B-C2B	-9.19	89.98	106.60
2	5-B	401	NAP	O3B-C3B-C4B	-9.15	83.60	111.05
2	3-B	401	NAP	O3B-C3B-C4B	-9.13	83.67	111.05
2	12-B	401	NAP	O3B-C3B-C4B	-9.12	83.69	111.05
2	7-B	401	NAP	O3B-C3B-C4B	-9.06	83.87	111.05
2	7-B	401	NAP	O4B-C1B-C2B	-9.06	90.21	106.60
2	13-B	401	NAP	C2B-C3B-C4B	-8.78	81.07	101.85
2	5-B	401	NAP	O4B-C4B-C5B	-8.51	78.88	109.32
2	12-B	401	NAP	O4B-C4B-C5B	-8.49	78.94	109.32
2	3-B	401	NAP	O4B-C4B-C5B	-8.48	78.99	109.32
2	7-B	401	NAP	O4B-C4B-C5B	-8.47	79.04	109.32
2	13-B	401	NAP	O4B-C4B-C5B	-8.32	79.56	109.32
2	16-B	401	NAP	O5B-C5B-C4B	-8.30	78.53	109.12
2	16-A	400	NAP	O5B-C5B-C4B	-8.05	79.45	109.12
2	4-B	401	NAP	O4B-C4B-C5B	-8.03	80.59	109.32
2	13-A	400	NAP	O5B-C5B-C4B	-8.02	79.56	109.12
2	10-B	401	NAP	O4B-C4B-C5B	-7.99	80.76	109.32
2	15-A	400	NAP	O5B-C5B-C4B	-7.96	79.78	109.12
2	6-B	401	NAP	O4B-C4B-C5B	-7.95	80.89	109.32
2	11-B	401	NAP	O4B-C4B-C5B	-7.94	80.92	109.32
2	8-B	401	NAP	O4B-C4B-C5B	-7.93	80.95	109.32
2	2-B	401	NAP	O4B-C4B-C5B	-7.92	81.00	109.32
2	12-A	400	NAP	O4B-C4B-C5B	-7.88	81.12	109.32
2	9-B	401	NAP	O4B-C4B-C5B	-7.84	81.27	109.32
2	11-A	400	NAP	O4B-C4B-C5B	-7.84	81.27	109.32
2	8-A	400	NAP	O4B-C4B-C3B	-7.80	89.43	105.15
2	14-A	400	NAP	O2A-PA-O1A	-7.76	70.44	112.53
2	1-B	401	NAP	O4B-C4B-C5B	-7.68	81.86	109.32
2	13-A	400	NAP	O4B-C4B-C5B	-7.65	81.96	109.32
2	15-A	400	NAP	O4B-C4B-C5B	-7.63	82.02	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	16-A	400	NAP	O4B-C4B-C5B	-7.62	82.06	109.32
2	12-A	400	NAP	O5B-C5B-C4B	-7.59	81.13	109.12
2	9-A	400	NAP	O4B-C4B-C5B	-7.54	82.35	109.32
2	7-A	400	NAP	O4B-C4B-C5B	-7.50	82.50	109.32
2	10-B	401	NAP	O2A-PA-O1A	-7.45	72.16	112.53
2	8-A	400	NAP	O5B-C5B-C4B	-7.43	81.73	109.12
2	2-A	400	NAP	O4B-C4B-C5B	-7.36	82.99	109.32
2	10-B	401	NAP	O5B-C5B-C4B	-7.29	82.22	109.12
2	5-A	400	NAP	O4B-C4B-C5B	-7.29	83.24	109.32
2	6-A	400	NAP	O5B-C5B-C4B	-7.29	82.25	109.12
2	4-A	400	NAP	O4B-C4B-C5B	-7.28	83.29	109.32
2	5-A	400	NAP	O5B-C5B-C4B	-7.27	82.30	109.12
2	14-B	401	NAP	O2A-PA-O1A	-7.27	73.12	112.53
2	10-A	400	NAP	O4B-C4B-C5B	-7.26	83.34	109.32
2	4-A	400	NAP	O5B-C5B-C4B	-7.26	82.34	109.12
2	2-B	401	NAP	O2A-PA-O1A	-7.26	73.17	112.53
2	3-A	400	NAP	O5B-C5B-C4B	-7.25	82.39	109.12
2	9-A	400	NAP	O5B-C5B-C4B	-7.24	82.42	109.12
2	6-B	401	NAP	O2A-PA-O1A	-7.22	73.37	112.53
2	3-A	400	NAP	O4B-C4B-C5B	-7.19	83.60	109.32
2	7-A	400	NAP	O5B-C5B-C4B	-7.19	82.61	109.12
2	6-A	400	NAP	O4B-C4B-C5B	-7.19	83.62	109.32
2	5-B	401	NAP	O2A-PA-O1A	-7.18	73.61	112.53
2	11-A	400	NAP	O5B-C5B-C4B	-7.15	82.78	109.12
2	1-A	400	NAP	O4B-C4B-C5B	-7.12	83.85	109.32
2	6-A	400	NAP	O4B-C4B-C3B	-7.12	90.81	105.15
2	8-A	400	NAP	O4B-C4B-C5B	-7.10	83.93	109.32
2	6-B	401	NAP	O4B-C4B-C3B	-7.09	90.87	105.15
2	11-B	401	NAP	O4B-C4B-C3B	-7.08	90.88	105.15
2	1-A	400	NAP	O5B-C5B-C4B	-7.06	83.07	109.12
2	2-B	401	NAP	O4B-C4B-C3B	-7.05	90.95	105.15
2	2-A	400	NAP	O5B-C5B-C4B	-7.03	83.19	109.12
2	3-A	400	NAP	O4B-C4B-C3B	-7.03	90.98	105.15
2	10-B	401	NAP	O4B-C4B-C3B	-7.00	91.04	105.15
2	4-A	400	NAP	O2A-PA-O1A	-7.00	74.61	112.53
2	3-B	401	NAP	O2A-PA-O1A	-6.99	74.62	112.53
2	5-A	400	NAP	O2A-PA-O1A	-6.97	74.77	112.53
2	10-A	400	NAP	O5B-C5B-C4B	-6.95	83.48	109.12
2	1-A	400	NAP	O2A-PA-O1A	-6.94	74.90	112.53
2	4-A	400	NAP	O4B-C4B-C3B	-6.93	91.17	105.15
2	4-B	401	NAP	O4B-C4B-C3B	-6.91	91.22	105.15
2	12-B	401	NAP	O2A-PA-O1A	-6.90	75.15	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-B	401	NAP	O5B-C5B-C4B	-6.89	83.71	109.12
2	5-A	400	NAP	O4B-C4B-C3B	-6.88	91.28	105.15
2	6-B	401	NAP	O5B-C5B-C4B	-6.88	83.77	109.12
2	11-B	401	NAP	O2A-PA-O1A	-6.87	75.29	112.53
2	11-B	401	NAP	O5B-C5B-C4B	-6.74	84.26	109.12
2	3-A	400	NAP	O2A-PA-O1A	-6.73	76.06	112.53
2	7-B	401	NAP	O2A-PA-O1A	-6.71	76.17	112.53
2	1-A	400	NAP	O4B-C4B-C3B	-6.58	91.89	105.15
2	15-A	400	NAP	O4B-C4B-C3B	-6.56	91.92	105.15
2	14-A	400	NAP	O5B-C5B-C4B	-6.54	85.01	109.12
2	13-A	400	NAP	O4B-C4B-C3B	-6.50	92.04	105.15
2	2-A	400	NAP	O2A-PA-O1A	-6.50	77.27	112.53
2	6-A	400	NAP	O2A-PA-O1A	-6.48	77.40	112.53
2	11-A	400	NAP	O4B-C4B-C3B	-6.47	92.11	105.15
2	10-A	400	NAP	O2A-PA-O1A	-6.45	77.56	112.53
2	4-B	401	NAP	O5B-C5B-C4B	-6.42	85.46	109.12
2	8-B	401	NAP	O5B-C5B-C4B	-6.41	85.50	109.12
2	9-B	401	NAP	O4B-C4B-C3B	-6.34	92.38	105.15
2	1-B	401	NAP	O5B-C5B-C4B	-6.33	85.77	109.12
2	16-A	400	NAP	O4B-C4B-C3B	-6.32	92.40	105.15
2	2-A	400	NAP	O4B-C4B-C3B	-6.32	92.42	105.15
2	13-B	401	NAP	C4B-O4B-C1B	-6.23	102.88	109.72
2	12-A	400	NAP	O4B-C4B-C3B	-6.22	92.62	105.15
2	14-A	400	NAP	O4B-C4B-C5B	-6.21	87.09	109.32
2	2-B	401	NAP	O4B-C1B-C2B	-6.19	95.41	106.60
2	10-A	400	NAP	O4B-C4B-C3B	-6.16	92.73	105.15
2	9-B	401	NAP	O5B-C5B-C4B	-6.14	86.47	109.12
2	6-B	401	NAP	O4B-C1B-C2B	-6.14	95.49	106.60
2	11-B	401	NAP	O4B-C1B-C2B	-6.08	95.61	106.60
2	9-A	400	NAP	O4B-C4B-C3B	-5.93	93.20	105.15
2	10-B	401	NAP	O4B-C1B-C2B	-5.89	95.94	106.60
2	8-B	401	NAP	O4B-C4B-C3B	-5.86	93.33	105.15
2	8-A	400	NAP	O2A-PA-O1A	-5.77	81.23	112.53
2	7-A	400	NAP	O4B-C4B-C3B	-5.73	93.60	105.15
2	16-B	401	NAP	O2A-PA-O1A	-5.73	81.48	112.53
2	1-B	401	NAP	O4B-C4B-C3B	-5.71	93.64	105.15
2	8-B	401	NAP	N3A-C2A-N1A	-5.44	124.73	128.89
2	4-B	401	NAP	O4B-C1B-C2B	-5.44	96.76	106.60
2	14-B	401	NAP	N3A-C2A-N1A	-5.35	124.79	128.89
2	1-B	401	NAP	N3A-C2A-N1A	-5.34	124.80	128.89
2	14-B	401	NAP	O4B-C1B-C2B	-5.33	96.96	106.60
2	5-B	401	NAP	O5B-C5B-C4B	-5.33	89.48	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	9-B	401	NAP	N3A-C2A-N1A	-5.32	124.82	128.89
2	15-B	401	NAP	O4B-C1B-C2B	-5.23	97.15	106.60
2	4-B	401	NAP	N3A-C2A-N1A	-5.11	124.98	128.89
2	13-A	400	NAP	O2A-PA-O1A	-5.01	85.40	112.53
2	13-B	401	NAP	N3A-C2A-N1A	-4.90	125.14	128.89
2	15-A	400	NAP	O2A-PA-O1A	-4.90	85.98	112.53
2	9-B	401	NAP	O4B-C1B-C2B	-4.89	97.76	106.60
2	3-B	401	NAP	O5B-C5B-C4B	-4.89	91.10	109.12
2	13-B	401	NAP	C5B-C4B-C3B	-4.86	95.92	115.21
2	4-B	401	NAP	O2A-PA-O1A	-4.85	86.22	112.53
2	12-B	401	NAP	O5B-C5B-C4B	-4.83	91.30	109.12
2	15-B	401	NAP	N3A-C2A-N1A	-4.81	125.22	128.89
2	16-A	400	NAP	O2A-PA-O1A	-4.80	86.49	112.53
2	7-B	401	NAP	O5B-C5B-C4B	-4.68	91.88	109.12
2	2-B	401	NAP	N3A-C2A-N1A	-4.67	125.32	128.89
2	11-B	401	NAP	N3A-C2A-N1A	-4.61	125.37	128.89
2	12-B	401	NAP	N3A-C2A-N1A	-4.60	125.37	128.89
2	9-A	400	NAP	O2A-PA-O1A	-4.60	87.61	112.53
2	6-B	401	NAP	N3A-C2A-N1A	-4.57	125.39	128.89
2	14-A	400	NAP	O4B-C4B-C3B	-4.57	95.94	105.15
2	16-B	401	NAP	O2A-PA-O3	-4.54	84.49	105.09
2	7-B	401	NAP	N3A-C2A-N1A	-4.54	125.42	128.89
2	1-B	401	NAP	O4B-C1B-C2B	-4.52	98.42	106.60
2	3-B	401	NAP	N3A-C2A-N1A	-4.50	125.45	128.89
2	7-A	400	NAP	O2A-PA-O1A	-4.49	88.18	112.53
2	10-B	401	NAP	N3A-C2A-N1A	-4.48	125.46	128.89
2	13-B	401	NAP	O2A-PA-O3	-4.45	84.92	105.09
2	1-B	401	NAP	O2A-PA-O3	-4.44	84.93	105.09
2	5-B	401	NAP	N3A-C2A-N1A	-4.43	125.50	128.89
2	16-B	401	NAP	O2A-PA-O5B	-4.43	86.15	108.46
2	8-B	401	NAP	O2A-PA-O3	-4.42	85.05	105.09
2	12-A	400	NAP	O2A-PA-O1A	-4.41	88.64	112.53
2	11-A	400	NAP	O3B-C3B-C4B	-4.30	98.15	111.05
2	9-A	400	NAP	O3B-C3B-C4B	-4.29	98.19	111.05
2	10-A	400	NAP	O3B-C3B-C4B	-4.26	98.27	111.05
2	13-B	401	NAP	C3B-C2B-C1B	-4.26	94.50	102.73
2	2-A	400	NAP	O3B-C3B-C4B	-4.24	98.34	111.05
2	8-B	401	NAP	O4B-C1B-C2B	-4.23	98.94	106.60
2	16-B	401	NAP	O3B-C3B-C4B	-4.23	98.35	111.05
2	7-A	400	NAP	O3B-C3B-C4B	-4.19	98.49	111.05
2	16-B	401	NAP	N3A-C2A-N1A	-4.15	125.72	128.89
2	15-A	400	NAP	O7N-C7N-C3N	-3.94	115.28	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	14-B	401	NAP	O3B-C3B-C4B	-3.94	99.25	111.05
2	16-B	401	NAP	O4B-C1B-C2B	-3.92	99.50	106.60
2	13-A	400	NAP	C3N-C7N-N7N	-3.90	113.55	117.82
2	5-A	400	NAP	C3N-C7N-N7N	-3.84	113.61	117.82
2	11-A	400	NAP	O4B-C1B-C2B	-3.81	99.71	106.60
2	16-A	400	NAP	N3A-C2A-N1A	-3.75	126.02	128.89
2	2-A	400	NAP	C3N-C7N-N7N	-3.73	113.73	117.82
2	12-A	400	NAP	O2A-PA-O3	-3.68	88.39	105.09
2	9-B	401	NAP	O2A-PA-O3	-3.67	88.44	105.09
2	9-A	400	NAP	N3A-C2A-N1A	-3.63	126.11	128.89
2	7-A	400	NAP	N3A-C2A-N1A	-3.63	126.12	128.89
2	12-A	400	NAP	O2A-PA-O5B	-3.62	90.18	108.46
2	12-A	400	NAP	O3B-C3B-C4B	-3.58	100.31	111.05
2	3-A	400	NAP	C3N-C7N-N7N	-3.55	113.93	117.82
2	14-B	401	NAP	C3N-C7N-N7N	-3.54	113.94	117.82
2	5-B	401	NAP	O7N-C7N-C3N	-3.52	115.74	119.59
2	2-A	400	NAP	O4B-C1B-C2B	-3.52	100.24	106.60
2	10-A	400	NAP	O4B-C1B-C2B	-3.52	100.24	106.60
2	11-A	400	NAP	C3N-C7N-N7N	-3.48	114.00	117.82
2	14-B	401	NAP	O7N-C7N-C3N	-3.48	115.78	119.59
2	13-A	400	NAP	N3A-C2A-N1A	-3.46	126.24	128.89
2	11-A	400	NAP	O2A-PA-O1A	-3.46	93.76	112.53
2	9-A	400	NAP	O4B-C1B-C2B	-3.45	100.36	106.60
2	14-A	400	NAP	C3N-C7N-N7N	-3.45	114.04	117.82
2	12-A	400	NAP	O7N-C7N-C3N	-3.43	115.84	119.59
2	3-A	400	NAP	O4B-C1B-C2B	-3.42	100.41	106.60
2	15-B	401	NAP	O3B-C3B-C4B	-3.41	100.83	111.05
2	12-A	400	NAP	N3A-C2A-N1A	-3.40	126.29	128.89
2	1-A	400	NAP	O4B-C1B-C2B	-3.34	100.55	106.60
2	1-A	400	NAP	O3B-C3B-C4B	-3.34	101.03	111.05
2	7-A	400	NAP	O4B-C1B-C2B	-3.32	100.59	106.60
2	5-A	400	NAP	O4B-C1B-C2B	-3.32	100.60	106.60
2	1-B	401	NAP	C3N-C7N-N7N	-3.29	114.22	117.82
2	15-B	401	NAP	C3N-C7N-N7N	-3.29	114.22	117.82
2	7-A	400	NAP	C3N-C7N-N7N	-3.28	114.23	117.82
2	10-A	400	NAP	C3N-C7N-N7N	-3.28	114.23	117.82
2	8-B	401	NAP	O3B-C3B-C4B	-3.27	101.23	111.05
2	11-A	400	NAP	N3A-C2A-N1A	-3.27	126.39	128.89
2	14-B	401	NAP	C3B-C2B-C1B	-3.27	96.41	102.73
2	4-A	400	NAP	O4B-C1B-C2B	-3.26	100.70	106.60
2	16-B	401	NAP	C3B-C2B-C1B	-3.24	96.45	102.73
2	16-B	401	NAP	C3N-C7N-N7N	-3.24	114.27	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	15-A	400	NAP	O4B-C1B-C2B	-3.24	100.74	106.60
2	1-B	401	NAP	O3B-C3B-C4B	-3.24	101.34	111.05
2	3-B	401	NAP	O7N-C7N-C3N	-3.23	116.06	119.59
2	6-B	401	NAP	O7N-C7N-C3N	-3.21	116.08	119.59
2	9-B	401	NAP	O3B-C3B-C4B	-3.21	101.41	111.05
2	8-A	400	NAP	O4B-C1B-C2B	-3.21	100.80	106.60
2	4-B	401	NAP	C3N-C7N-N7N	-3.21	114.31	117.82
2	4-A	400	NAP	O3B-C3B-C4B	-3.21	101.43	111.05
2	2-B	401	NAP	C3N-C7N-N7N	-3.20	114.32	117.82
2	11-B	401	NAP	O7N-C7N-C3N	-3.20	116.10	119.59
2	9-B	401	NAP	O2A-PA-O1A	-3.20	95.20	112.53
2	3-B	401	NAP	C3N-C7N-N7N	-3.17	114.35	117.82
2	2-B	401	NAP	O7N-C7N-C3N	-3.17	116.13	119.59
2	5-B	401	NAP	C3N-C7N-N7N	-3.16	114.35	117.82
2	8-B	401	NAP	O2A-PA-O5B	-3.16	92.55	108.46
2	11-B	401	NAP	C3N-C7N-N7N	-3.15	114.37	117.82
2	7-B	401	NAP	C3N-C7N-N7N	-3.14	114.38	117.82
2	15-B	401	NAP	C3B-C2B-C1B	-3.13	96.68	102.73
2	6-B	401	NAP	C3N-C7N-N7N	-3.13	114.39	117.82
2	15-A	400	NAP	N3A-C2A-N1A	-3.12	126.50	128.89
2	5-A	400	NAP	O3B-C3B-C4B	-3.11	101.72	111.05
2	8-B	401	NAP	C3N-C7N-N7N	-3.09	114.44	117.82
2	10-B	401	NAP	O3B-C3B-C4B	-3.08	101.83	111.05
2	7-B	401	NAP	O7N-C7N-C3N	-3.07	116.23	119.59
2	5-B	401	NAP	O3B-C3B-C2B	-3.06	102.32	111.16
2	2-A	400	NAP	N3A-C2A-N1A	-3.03	126.58	128.89
2	11-A	400	NAP	C1B-N9A-C4A	-3.03	122.38	126.94
2	3-A	400	NAP	O3B-C3B-C4B	-3.02	101.99	111.05
2	10-B	401	NAP	C3N-C7N-N7N	-3.02	114.51	117.82
2	14-B	401	NAP	O2A-PA-O5B	-3.02	93.25	108.46
2	1-B	401	NAP	O2A-PA-O5B	-3.01	93.26	108.46
2	10-A	400	NAP	N3A-C2A-N1A	-2.99	126.61	128.89
2	6-A	400	NAP	O4B-C1B-C2B	-2.98	101.20	106.60
2	3-B	401	NAP	O3B-C3B-C2B	-2.98	102.55	111.16
2	13-A	400	NAP	O4B-C1B-C2B	-2.98	101.21	106.60
2	12-B	401	NAP	O3B-C3B-C2B	-2.97	102.59	111.16
2	13-B	401	NAP	O4B-C1B-C2B	-2.96	101.25	106.60
2	2-B	401	NAP	O3B-C3B-C4B	-2.94	102.22	111.05
2	13-B	401	NAP	O7N-C7N-C3N	-2.94	116.38	119.59
2	7-B	401	NAP	O3B-C3B-C2B	-2.94	102.67	111.16
2	12-B	401	NAP	C3N-C7N-N7N	-2.94	114.60	117.82
2	9-B	401	NAP	O2A-PA-O5B	-2.91	93.79	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7-A	400	NAP	O2A-PA-O3	-2.88	92.01	105.09
2	13-A	400	NAP	O3B-C3B-C4B	-2.86	102.47	111.05
2	15-A	400	NAP	O3B-C3B-C4B	-2.83	102.57	111.05
2	16-B	401	NAP	C5N-C4N-C3N	-2.82	116.79	120.33
2	14-A	400	NAP	O4B-C1B-C2B	-2.80	101.53	106.60
2	6-B	401	NAP	O3B-C3B-C4B	-2.80	102.65	111.05
2	9-B	401	NAP	C3N-C7N-N7N	-2.79	114.76	117.82
2	14-B	401	NAP	O2A-PA-O3	-2.78	92.50	105.09
2	14-A	400	NAP	N3A-C2A-N1A	-2.76	126.78	128.89
2	11-B	401	NAP	O3B-C3B-C4B	-2.76	102.77	111.05
2	12-A	400	NAP	O4B-C1B-C2B	-2.75	101.63	106.60
2	13-B	401	NAP	O2A-PA-O1A	-2.73	97.75	112.53
2	8-A	400	NAP	C1B-N9A-C4A	-2.70	122.88	126.94
2	9-A	400	NAP	O2A-PA-O3	-2.68	92.95	105.09
2	12-B	401	NAP	O7N-C7N-C3N	-2.67	116.67	119.59
2	8-A	400	NAP	O3B-C3B-C4B	-2.67	103.04	111.05
2	13-A	400	NAP	C3N-C2N-N1N	-2.65	117.31	120.36
2	15-B	401	NAP	O7N-C7N-C3N	-2.63	116.71	119.59
2	16-A	400	NAP	O4B-C1B-C2B	-2.63	101.85	106.60
2	4-B	401	NAP	O3B-C3B-C4B	-2.61	103.21	111.05
2	6-A	400	NAP	C1B-N9A-C4A	-2.60	123.01	126.94
2	8-B	401	NAP	O7N-C7N-C3N	-2.60	116.75	119.59
2	10-B	401	NAP	O7N-C7N-C3N	-2.59	116.76	119.59
2	4-A	400	NAP	N3A-C2A-N1A	-2.58	126.92	128.89
2	3-A	400	NAP	C1B-N9A-C4A	-2.57	123.06	126.94
2	6-A	400	NAP	O3B-C3B-C4B	-2.56	103.36	111.05
2	5-B	401	NAP	O4B-C4B-C3B	-2.54	100.03	105.15
2	4-B	401	NAP	O2A-PA-O3	-2.54	93.59	105.09
2	14-A	400	NAP	C3N-C2N-N1N	-2.53	117.45	120.36
2	1-A	400	NAP	C1B-N9A-C4A	-2.52	123.14	126.94
2	16-A	400	NAP	O3B-C3B-C4B	-2.49	103.58	111.05
2	5-A	400	NAP	C1B-N9A-C4A	-2.49	123.19	126.94
2	8-A	400	NAP	C3N-C7N-N7N	-2.49	115.10	117.82
2	5-A	400	NAP	N3A-C2A-N1A	-2.48	127.00	128.89
2	4-A	400	NAP	C1B-N9A-C4A	-2.48	123.21	126.94
2	8-B	401	NAP	O2A-PA-O1A	-2.47	99.12	112.53
2	8-A	400	NAP	C5N-C4N-C3N	-2.47	117.23	120.33
2	4-B	401	NAP	C5N-C4N-C3N	-2.46	117.24	120.33
2	4-A	400	NAP	C3N-C7N-N7N	-2.46	115.13	117.82
2	7-A	400	NAP	O2A-PA-O5B	-2.45	96.09	108.46
2	1-A	400	NAP	C5N-C4N-C3N	-2.45	117.26	120.33
2	7-A	400	NAP	C3N-C2N-N1N	-2.43	117.56	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	15-A	400	NAP	PN-O3-PA	-2.42	125.94	132.73
2	13-A	400	NAP	PN-O3-PA	-2.41	125.97	132.73
2	4-A	400	NAP	C5N-C4N-C3N	-2.40	117.32	120.33
2	14-A	400	NAP	O3B-C3B-C4B	-2.40	103.86	111.05
2	1-A	400	NAP	N3A-C2A-N1A	-2.40	127.06	128.89
2	1-B	401	NAP	O2A-PA-O1A	-2.39	99.59	112.53
2	15-A	400	NAP	C1B-N9A-C4A	-2.38	123.36	126.94
2	16-A	400	NAP	O2A-PA-O3	-2.37	94.34	105.09
2	3-B	401	NAP	O4B-C4B-C3B	-2.36	100.39	105.15
2	12-B	401	NAP	O4B-C4B-C3B	-2.35	100.42	105.15
2	3-A	400	NAP	N3A-C2A-N1A	-2.33	127.11	128.89
2	7-B	401	NAP	O4B-C4B-C3B	-2.32	100.48	105.15
2	11-A	400	NAP	C3N-C2N-N1N	-2.31	117.70	120.36
2	10-A	400	NAP	C3N-C2N-N1N	-2.28	117.73	120.36
2	15-B	401	NAP	O2B-C2B-C3B	-2.27	102.67	111.51
2	14-B	401	NAP	O2B-C2B-C3B	-2.27	102.69	111.51
2	4-B	401	NAP	O2A-PA-O5B	-2.26	97.07	108.46
2	14-A	400	NAP	C1B-N9A-C4A	-2.25	123.55	126.94
2	9-A	400	NAP	O2A-PA-O5B	-2.24	97.18	108.46
2	13-A	400	NAP	O2A-PA-O3	-2.22	95.01	105.09
2	15-A	400	NAP	O2A-PA-O3	-2.21	95.06	105.09
2	2-A	400	NAP	C3N-C2N-N1N	-2.19	117.84	120.36
2	10-A	400	NAP	C1B-N9A-C4A	-2.19	123.64	126.94
2	3-A	400	NAP	C3N-C2N-N1N	-2.18	117.85	120.36
2	16-B	401	NAP	O2B-C2B-C3B	-2.17	103.06	111.51
2	1-A	400	NAP	C3N-C7N-N7N	-2.16	115.45	117.82
2	9-A	400	NAP	C5N-C4N-C3N	-2.16	117.62	120.33
2	5-A	400	NAP	C3N-C2N-N1N	-2.16	117.88	120.36
2	12-A	400	NAP	C1B-N9A-C4A	-2.14	123.71	126.94
2	1-B	401	NAP	O7N-C7N-C3N	-2.13	117.26	119.59
2	2-A	400	NAP	C1B-N9A-C4A	-2.12	123.74	126.94
2	3-B	401	NAP	O2B-C2B-C3B	-2.10	103.34	111.51
2	5-B	401	NAP	O2B-C2B-C3B	-2.09	103.38	111.51
2	13-B	401	NAP	C1B-N9A-C4A	-2.08	123.80	126.94
2	15-B	401	NAP	O2A-PA-O5B	-2.08	97.97	108.46
2	5-B	401	NAP	C5N-C4N-C3N	-2.06	117.74	120.33
2	12-B	401	NAP	O2B-C2B-C3B	-2.06	103.50	111.51
2	9-A	400	NAP	PN-O3-PA	-2.05	126.96	132.73
2	16-B	401	NAP	O7N-C7N-C3N	-2.04	117.36	119.59
2	13-A	400	NAP	C1B-N9A-C4A	-2.02	123.89	126.94
2	7-B	401	NAP	C5N-C4N-C3N	-2.02	117.80	120.33
2	7-B	401	NAP	O2B-C2B-C3B	-2.00	103.72	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	12-A	400	NAP	C4A-C5A-N7A	2.01	111.33	109.48
2	2-B	401	NAP	O4D-C1D-N1N	2.02	110.34	108.13
2	11-B	401	NAP	C4B-O4B-C1B	2.02	111.94	109.72
2	4-B	401	NAP	O4D-C1D-N1N	2.04	110.37	108.13
2	4-B	401	NAP	O2X-P2B-O1X	2.05	117.17	110.58
2	5-B	401	NAP	O3-PA-O5B	2.05	108.38	102.94
2	10-B	401	NAP	O3-PA-O5B	2.07	108.43	102.94
2	2-B	401	NAP	O3B-C3B-C2B	2.08	117.15	111.16
2	16-B	401	NAP	O4D-C4D-C5D	2.08	116.77	109.32
2	9-B	401	NAP	O3-PN-O5D	2.09	108.47	102.94
2	8-A	400	NAP	C4A-C5A-N7A	2.09	111.40	109.48
2	8-B	401	NAP	O4D-C4D-C5D	2.09	116.80	109.32
2	8-B	401	NAP	O3-PN-O5D	2.12	108.56	102.94
2	9-B	401	NAP	O4D-C1D-N1N	2.12	110.46	108.13
2	4-B	401	NAP	C2A-N1A-C6A	2.12	122.56	118.77
2	6-B	401	NAP	O3B-C3B-C2B	2.12	117.28	111.16
2	16-A	400	NAP	O7N-C7N-N7N	2.13	125.59	122.59
2	3-A	400	NAP	O3-PA-O5B	2.13	108.59	102.94
2	16-B	401	NAP	O3X-P2B-O2X	2.13	115.50	107.38
2	7-B	401	NAP	O2X-P2B-O1X	2.15	117.49	110.58
2	11-B	401	NAP	O3B-C3B-C2B	2.15	117.36	111.16
2	10-B	401	NAP	C4B-O4B-C1B	2.16	112.09	109.72
2	14-B	401	NAP	O2X-P2B-O1X	2.16	117.54	110.58
2	15-B	401	NAP	P2B-O2B-C2B	2.18	126.79	121.56
2	11-B	401	NAP	O2X-P2B-O1X	2.18	117.60	110.58
2	12-B	401	NAP	O2X-P2B-O1X	2.19	117.62	110.58
2	6-B	401	NAP	C4B-O4B-C1B	2.19	112.13	109.72
2	2-B	401	NAP	C4B-O4B-C1B	2.20	112.13	109.72
2	4-B	401	NAP	O3B-C3B-C2B	2.20	117.52	111.16
2	9-B	401	NAP	O4D-C4D-C5D	2.21	117.21	109.32
2	6-B	401	NAP	O2X-P2B-O1X	2.21	117.69	110.58
2	4-A	400	NAP	C6N-C5N-C4N	2.22	122.79	119.44
2	8-B	401	NAP	O2B-C2B-C1B	2.22	118.69	110.02
2	3-B	401	NAP	O2X-P2B-O1X	2.23	117.76	110.58
2	6-A	400	NAP	C4A-C5A-N7A	2.24	111.54	109.48
2	5-B	401	NAP	O2X-P2B-O1X	2.24	117.79	110.58
2	2-B	401	NAP	O2X-P2B-O1X	2.24	117.80	110.58
2	15-B	401	NAP	O2X-P2B-O1X	2.25	117.83	110.58
2	3-B	401	NAP	O3X-P2B-O2X	2.27	116.01	107.38
2	14-B	401	NAP	C2A-N1A-C6A	2.27	122.83	118.77
2	7-A	400	NAP	C4A-C5A-N7A	2.27	111.57	109.48
2	4-B	401	NAP	O3X-P2B-O2X	2.28	116.05	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1-B	401	NAP	O3X-P2B-O2X	2.28	116.08	107.38
2	7-B	401	NAP	O3X-P2B-O2X	2.28	116.08	107.38
2	12-B	401	NAP	O3X-P2B-O2X	2.30	116.12	107.38
2	9-B	401	NAP	O3X-P2B-O2X	2.30	116.13	107.38
2	8-A	400	NAP	C6N-C5N-C4N	2.31	122.93	119.44
2	1-A	400	NAP	C6N-C5N-C4N	2.31	122.93	119.44
2	14-A	400	NAP	O3-PA-O5B	2.32	109.09	102.94
2	11-B	401	NAP	O3X-P2B-O2X	2.32	116.22	107.38
2	9-B	401	NAP	O2B-C2B-C1B	2.32	119.08	110.02
2	5-B	401	NAP	O3X-P2B-O2X	2.33	116.25	107.38
2	6-B	401	NAP	O3X-P2B-O2X	2.33	116.25	107.38
2	1-A	400	NAP	O3-PA-O5B	2.34	109.13	102.94
2	2-B	401	NAP	O3X-P2B-O2X	2.34	116.29	107.38
2	15-A	400	NAP	C4A-C5A-N7A	2.35	111.64	109.48
2	1-B	401	NAP	O2B-C2B-C1B	2.35	119.19	110.02
2	13-B	401	NAP	O3X-P2B-O2X	2.36	116.35	107.38
2	13-B	401	NAP	C4A-C5A-N7A	2.36	111.65	109.48
2	13-A	400	NAP	O3X-P2B-O1X	2.36	118.19	110.58
2	5-A	400	NAP	O3-PA-O5B	2.36	109.21	102.94
2	16-A	400	NAP	O3X-P2B-O1X	2.37	118.20	110.58
2	4-A	400	NAP	O3-PA-O5B	2.38	109.24	102.94
2	3-A	400	NAP	C4A-C5A-N7A	2.39	111.68	109.48
2	15-B	401	NAP	O3X-P2B-O2X	2.40	116.51	107.38
2	9-A	400	NAP	C4A-C5A-N7A	2.40	111.69	109.48
2	1-A	400	NAP	O4D-C1D-N1N	2.41	110.78	108.13
2	14-B	401	NAP	P2B-O2B-C2B	2.41	127.33	121.56
2	14-B	401	NAP	O3X-P2B-O2X	2.43	116.64	107.38
2	1-A	400	NAP	C4A-C5A-N7A	2.43	111.72	109.48
2	8-A	400	NAP	O3X-P2B-O1X	2.44	118.42	110.58
2	4-A	400	NAP	C4A-C5A-N7A	2.44	111.72	109.48
2	5-A	400	NAP	C4A-C5A-N7A	2.45	111.73	109.48
2	1-B	401	NAP	O4D-C4D-C5D	2.45	118.10	109.32
2	9-A	400	NAP	O4D-C1D-N1N	2.47	110.84	108.13
2	1-B	401	NAP	O3-PN-O5D	2.47	109.48	102.94
2	4-B	401	NAP	C4D-O4D-C1D	2.47	112.43	109.72
2	10-A	400	NAP	C4A-C5A-N7A	2.49	111.77	109.48
2	4-B	401	NAP	O2B-C2B-C1B	2.49	119.73	110.02
2	6-A	400	NAP	C4B-O4B-C1B	2.50	112.46	109.72
2	12-A	400	NAP	O3X-P2B-O2X	2.50	116.91	107.38
2	11-B	401	NAP	C2A-N1A-C6A	2.51	123.24	118.77
2	15-A	400	NAP	O3X-P2B-O1X	2.51	118.67	110.58
2	13-A	400	NAP	C4A-C5A-N7A	2.51	111.79	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7-B	401	NAP	C2A-N1A-C6A	2.54	123.31	118.77
2	10-B	401	NAP	O2B-C2B-C1B	2.54	119.94	110.02
2	15-A	400	NAP	O3-PA-O5B	2.55	109.69	102.94
2	2-A	400	NAP	O3X-P2B-O1X	2.55	118.80	110.58
2	11-A	400	NAP	O2B-C2B-C1B	2.56	119.98	110.02
2	12-A	400	NAP	O7N-C7N-N7N	2.56	126.20	122.59
2	2-A	400	NAP	C4A-C5A-N7A	2.56	111.84	109.48
2	9-B	401	NAP	C4A-C5A-N7A	2.58	111.85	109.48
2	4-A	400	NAP	O4D-C1D-N1N	2.60	110.98	108.13
2	13-A	400	NAP	O3-PA-O5B	2.60	109.83	102.94
2	16-B	401	NAP	C2A-N1A-C6A	2.60	123.42	118.77
2	16-A	400	NAP	C4A-C5A-N7A	2.61	111.88	109.48
2	8-B	401	NAP	O5B-PA-O1A	2.61	119.75	109.62
2	12-A	400	NAP	O3-PA-O5B	2.61	109.87	102.94
2	8-A	400	NAP	C4B-O4B-C1B	2.62	112.60	109.72
2	5-B	401	NAP	C4D-O4D-C1D	2.62	112.60	109.72
2	12-B	401	NAP	C2A-N1A-C6A	2.65	123.50	118.77
2	6-B	401	NAP	C2A-N1A-C6A	2.66	123.52	118.77
2	3-B	401	NAP	C2A-N1A-C6A	2.66	123.52	118.77
2	10-A	400	NAP	O3X-P2B-O1X	2.69	119.23	110.58
2	16-A	400	NAP	O4D-C1D-N1N	2.70	111.09	108.13
2	3-B	401	NAP	O3-PA-O5B	2.71	110.12	102.94
2	14-A	400	NAP	C4B-O4B-C1B	2.71	112.70	109.72
2	6-B	401	NAP	O2B-C2B-C1B	2.72	120.61	110.02
2	16-B	401	NAP	C4D-O4D-C1D	2.72	112.71	109.72
2	2-B	401	NAP	C2A-N1A-C6A	2.72	123.63	118.77
2	11-B	401	NAP	O2B-C2B-C1B	2.73	120.64	110.02
2	2-B	401	NAP	O2B-C2B-C1B	2.73	120.66	110.02
2	6-A	400	NAP	O3X-P2B-O1X	2.73	119.38	110.58
2	16-A	400	NAP	O3-PA-O5B	2.74	110.20	102.94
2	1-B	401	NAP	O5B-PA-O1A	2.74	120.25	109.62
2	9-A	400	NAP	O7N-C7N-N7N	2.74	126.45	122.59
2	15-A	400	NAP	O4D-C1D-N1N	2.74	111.14	108.13
2	10-B	401	NAP	C2A-N1A-C6A	2.75	123.68	118.77
2	15-B	401	NAP	C2A-N1A-C6A	2.75	123.68	118.77
2	16-B	401	NAP	O2B-C2B-C1B	2.77	120.83	110.02
2	8-A	400	NAP	O4D-C1D-N1N	2.78	111.19	108.13
2	9-A	400	NAP	O3-PA-O5B	2.78	110.31	102.94
2	14-B	401	NAP	O2B-C2B-C1B	2.78	120.86	110.02
2	7-A	400	NAP	O3-PA-O5B	2.79	110.33	102.94
2	12-B	401	NAP	O3-PA-O5B	2.80	110.36	102.94
2	14-A	400	NAP	C4A-C5A-N7A	2.80	112.06	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	13-A	400	NAP	O4D-C1D-N1N	2.81	111.22	108.13
2	10-A	400	NAP	O5B-PA-O1A	2.83	120.59	109.62
2	8-A	400	NAP	O7N-C7N-N7N	2.83	126.58	122.59
2	2-A	400	NAP	O5B-PA-O1A	2.84	120.63	109.62
2	2-B	401	NAP	C4D-O4D-C1D	2.84	112.84	109.72
2	4-A	400	NAP	O7N-C7N-N7N	2.85	126.60	122.59
2	15-B	401	NAP	O2B-C2B-C1B	2.87	121.20	110.02
2	5-B	401	NAP	C2A-N1A-C6A	2.88	123.92	118.77
2	9-B	401	NAP	O5B-PA-O1A	2.90	120.88	109.62
2	16-A	400	NAP	O5B-PA-O1A	2.91	120.90	109.62
2	11-A	400	NAP	O3X-P2B-O2X	2.91	118.47	107.38
2	3-B	401	NAP	C4D-O4D-C1D	2.91	112.92	109.72
2	7-A	400	NAP	O4D-C1D-N1N	2.92	111.33	108.13
2	3-A	400	NAP	O3X-P2B-O1X	2.92	119.97	110.58
2	1-A	400	NAP	O7N-C7N-N7N	2.92	126.71	122.59
2	15-A	400	NAP	O7N-C7N-N7N	2.92	126.71	122.59
2	6-B	401	NAP	C4D-O4D-C1D	2.93	112.94	109.72
2	1-A	400	NAP	O3X-P2B-O1X	2.95	120.09	110.58
2	7-B	401	NAP	C4D-O4D-C1D	2.97	112.98	109.72
2	7-B	401	NAP	O3-PA-O5B	2.97	110.83	102.94
2	11-B	401	NAP	C4D-O4D-C1D	2.98	113.00	109.72
2	4-B	401	NAP	C4A-C5A-N7A	2.99	112.22	109.48
2	13-A	400	NAP	O5B-PA-O1A	2.99	121.21	109.62
2	11-A	400	NAP	O3-PA-O5B	3.01	110.93	102.94
2	5-A	400	NAP	O3X-P2B-O1X	3.04	120.36	110.58
2	4-B	401	NAP	O5B-PA-O1A	3.06	121.48	109.62
2	14-A	400	NAP	O4D-C1D-N1N	3.06	111.50	108.13
2	8-A	400	NAP	O5B-PA-O1A	3.07	121.54	109.62
2	3-A	400	NAP	O7N-C7N-N7N	3.07	126.92	122.59
2	4-A	400	NAP	O3X-P2B-O1X	3.09	120.51	110.58
2	16-B	401	NAP	C4A-C5A-N7A	3.09	112.33	109.48
2	2-B	401	NAP	O3-PA-O5B	3.10	111.17	102.94
2	15-B	401	NAP	O3-PA-O5B	3.11	111.18	102.94
2	15-A	400	NAP	O5B-PA-O1A	3.11	121.69	109.62
2	16-A	400	NAP	C4B-O4B-C1B	3.13	113.15	109.72
2	6-A	400	NAP	O5B-PA-O1A	3.13	121.78	109.62
2	10-A	400	NAP	O3-PA-O5B	3.14	111.25	102.94
2	2-A	400	NAP	O3-PA-O5B	3.14	111.26	102.94
2	5-A	400	NAP	O7N-C7N-N7N	3.15	127.02	122.59
2	10-A	400	NAP	O7N-C7N-N7N	3.17	127.06	122.59
2	14-B	401	NAP	O3-PA-O5B	3.18	111.36	102.94
2	11-A	400	NAP	O7N-C7N-N7N	3.18	127.07	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-A	400	NAP	O7N-C7N-N7N	3.18	127.07	122.59
2	6-B	401	NAP	O3-PA-O5B	3.19	111.41	102.94
2	14-A	400	NAP	O3X-P2B-O1X	3.22	120.95	110.58
2	2-A	400	NAP	O4D-C1D-N1N	3.22	111.67	108.13
2	7-A	400	NAP	O7N-C7N-N7N	3.23	127.14	122.59
2	9-A	400	NAP	O5B-PA-O1A	3.23	122.14	109.62
2	13-A	400	NAP	C4B-O4B-C1B	3.23	113.27	109.72
2	1-A	400	NAP	O5B-PA-O1A	3.24	122.20	109.62
2	14-A	400	NAP	O5B-PA-O1A	3.24	122.21	109.62
2	13-B	401	NAP	O7N-C7N-N7N	3.25	127.16	122.59
2	5-A	400	NAP	O5B-PA-O1A	3.26	122.25	109.62
2	14-A	400	NAP	O7N-C7N-N7N	3.26	127.18	122.59
2	4-A	400	NAP	O5B-PA-O1A	3.26	122.27	109.62
2	14-B	401	NAP	O5B-PA-O1A	3.27	122.30	109.62
2	3-A	400	NAP	O5B-PA-O1A	3.27	122.32	109.62
2	10-B	401	NAP	C4A-C5A-N7A	3.27	112.49	109.48
2	12-A	400	NAP	O4D-C1D-N1N	3.28	111.73	108.13
2	9-B	401	NAP	O3-PA-O5B	3.28	111.65	102.94
2	7-A	400	NAP	O5B-PA-O1A	3.29	122.37	109.62
2	10-A	400	NAP	O4D-C1D-N1N	3.29	111.74	108.13
2	14-B	401	NAP	C4A-C5A-N7A	3.29	112.51	109.48
2	15-B	401	NAP	O5B-PA-O1A	3.31	122.45	109.62
2	11-A	400	NAP	O4D-C1D-N1N	3.31	111.77	108.13
2	9-B	401	NAP	O7N-C7N-N7N	3.32	127.27	122.59
2	5-B	401	NAP	O2B-C2B-C1B	3.33	123.00	110.02
2	11-B	401	NAP	O3-PA-O5B	3.33	111.77	102.94
2	7-B	401	NAP	O2B-C2B-C1B	3.35	123.07	110.02
2	5-A	400	NAP	O4D-C1D-N1N	3.35	111.82	108.13
2	14-A	400	NAP	C2B-C3B-C4B	3.36	109.80	101.85
2	9-B	401	NAP	C4D-O4D-C1D	3.36	113.41	109.72
2	13-B	401	NAP	O4B-C1B-N9A	3.38	115.17	108.10
2	7-B	401	NAP	O5B-PA-O1A	3.38	122.73	109.62
2	11-B	401	NAP	C4A-C5A-N7A	3.39	112.60	109.48
2	12-B	401	NAP	O2B-C2B-C1B	3.39	123.24	110.02
2	6-B	401	NAP	C4A-C5A-N7A	3.39	112.60	109.48
2	2-B	401	NAP	C4A-C5A-N7A	3.40	112.61	109.48
2	11-B	401	NAP	O5B-PA-O1A	3.43	122.91	109.62
2	3-B	401	NAP	O2B-C2B-C1B	3.44	123.44	110.02
2	1-B	401	NAP	O3-PA-O5B	3.45	112.08	102.94
2	12-B	401	NAP	O5B-PA-O1A	3.45	123.00	109.62
2	4-B	401	NAP	O3-PA-O5B	3.45	112.08	102.94
2	7-B	401	NAP	C4A-C5A-N7A	3.45	112.65	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	13-A	400	NAP	O7N-C7N-N7N	3.45	127.45	122.59
2	8-B	401	NAP	O3-PA-O5B	3.46	112.11	102.94
2	12-B	401	NAP	C4A-C5A-N7A	3.47	112.67	109.48
2	3-B	401	NAP	C4A-C5A-N7A	3.50	112.70	109.48
2	3-B	401	NAP	O5B-PA-O1A	3.51	123.22	109.62
2	5-B	401	NAP	C4A-C5A-N7A	3.52	112.72	109.48
2	3-A	400	NAP	O4D-C1D-N1N	3.54	112.02	108.13
2	16-B	401	NAP	O3-PA-O5B	3.54	112.33	102.94
2	3-B	401	NAP	C2B-C3B-C4B	3.54	110.23	101.85
2	6-B	401	NAP	O5B-PA-O1A	3.55	123.41	109.62
2	12-A	400	NAP	O2B-P2B-O1X	3.56	116.00	107.11
2	2-B	401	NAP	O5B-PA-O1A	3.56	123.44	109.62
2	12-B	401	NAP	C2B-C3B-C4B	3.59	110.35	101.85
2	15-B	401	NAP	C4A-C5A-N7A	3.59	112.78	109.48
2	5-B	401	NAP	C2B-C3B-C4B	3.60	110.38	101.85
2	7-B	401	NAP	C2B-C3B-C4B	3.61	110.39	101.85
2	14-B	401	NAP	C4D-O4D-C1D	3.61	113.69	109.72
2	4-A	400	NAP	C4B-O4B-C1B	3.64	113.72	109.72
2	15-A	400	NAP	C4B-O4B-C1B	3.71	113.79	109.72
2	10-B	401	NAP	O5B-PA-O1A	3.71	124.02	109.62
2	5-B	401	NAP	O5B-PA-O1A	3.72	124.05	109.62
2	3-A	400	NAP	C4B-O4B-C1B	3.73	113.81	109.72
2	4-B	401	NAP	O7N-C7N-N7N	3.78	127.92	122.59
2	8-B	401	NAP	C4D-O4D-C1D	3.81	113.90	109.72
2	16-B	401	NAP	C4B-O4B-C1B	3.82	113.92	109.72
2	12-A	400	NAP	O5B-PA-O1A	3.85	124.57	109.62
2	5-A	400	NAP	C4B-O4B-C1B	3.86	113.96	109.72
2	10-B	401	NAP	C4D-O4D-C1D	3.87	113.97	109.72
2	1-A	400	NAP	C4B-O4B-C1B	3.95	114.06	109.72
2	12-A	400	NAP	C4B-O4B-C1B	3.96	114.07	109.72
2	1-B	401	NAP	C4D-O4D-C1D	3.99	114.10	109.72
2	5-B	401	NAP	C3B-C2B-C1B	4.03	110.53	102.73
2	3-B	401	NAP	C3B-C2B-C1B	4.07	110.60	102.73
2	16-B	401	NAP	O7N-C7N-N7N	4.07	128.33	122.59
2	7-B	401	NAP	C3B-C2B-C1B	4.08	110.62	102.73
2	7-A	400	NAP	C4B-O4B-C1B	4.09	114.22	109.72
2	12-B	401	NAP	C3B-C2B-C1B	4.10	110.66	102.73
2	12-B	401	NAP	C4D-O4D-C1D	4.11	114.23	109.72
2	9-A	400	NAP	C4B-O4B-C1B	4.16	114.29	109.72
2	1-B	401	NAP	O7N-C7N-N7N	4.16	128.45	122.59
2	11-A	400	NAP	C4B-O4B-C1B	4.21	114.34	109.72
2	15-B	401	NAP	C5B-C4B-C3B	4.32	132.37	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8-B	401	NAP	O7N-C7N-N7N	4.34	128.71	122.59
2	10-B	401	NAP	O7N-C7N-N7N	4.35	128.72	122.59
2	12-B	401	NAP	O7N-C7N-N7N	4.36	128.72	122.59
2	16-B	401	NAP	O5B-PA-O1A	4.36	126.53	109.62
2	2-A	400	NAP	C4B-O4B-C1B	4.42	114.57	109.72
2	16-A	400	NAP	C2B-C3B-C4B	4.46	112.41	101.85
2	10-A	400	NAP	C4B-O4B-C1B	4.47	114.63	109.72
2	15-B	401	NAP	O7N-C7N-N7N	4.59	129.05	122.59
2	13-A	400	NAP	C2B-C3B-C4B	4.67	112.91	101.85
2	15-A	400	NAP	C2B-C3B-C4B	4.70	112.97	101.85
2	7-B	401	NAP	O7N-C7N-N7N	4.71	129.23	122.59
2	15-B	401	NAP	C4D-O4D-C1D	4.79	114.98	109.72
2	6-B	401	NAP	O7N-C7N-N7N	4.81	129.37	122.59
2	11-B	401	NAP	O7N-C7N-N7N	4.81	129.37	122.59
2	2-B	401	NAP	O7N-C7N-N7N	4.84	129.41	122.59
2	3-B	401	NAP	O7N-C7N-N7N	4.86	129.44	122.59
2	7-A	400	NAP	C2B-C3B-C4B	4.89	113.42	101.85
2	5-B	401	NAP	O7N-C7N-N7N	5.08	129.74	122.59
2	9-A	400	NAP	C2B-C3B-C4B	5.08	113.89	101.85
2	12-A	400	NAP	C2B-C3B-C4B	5.10	113.93	101.85
2	16-B	401	NAP	C5B-C4B-C3B	5.13	135.57	115.21
2	8-B	401	NAP	C2B-C3B-C4B	5.20	114.16	101.85
2	15-B	401	NAP	O3B-C3B-C2B	5.23	126.25	111.16
2	13-B	401	NAP	O3B-C3B-C2B	5.24	126.28	111.16
2	1-B	401	NAP	C2B-C3B-C4B	5.33	114.46	101.85
2	6-B	401	NAP	C2B-C3B-C4B	5.35	114.53	101.85
2	6-A	400	NAP	O4D-C1D-N1N	5.38	114.04	108.13
2	14-B	401	NAP	O7N-C7N-N7N	5.38	130.17	122.59
2	11-B	401	NAP	C2B-C3B-C4B	5.38	114.60	101.85
2	2-B	401	NAP	C2B-C3B-C4B	5.43	114.70	101.85
2	11-A	400	NAP	C2B-C3B-C4B	5.46	114.79	101.85
2	10-B	401	NAP	C2B-C3B-C4B	5.47	114.81	101.85
2	10-A	400	NAP	C2B-C3B-C4B	5.50	114.89	101.85
2	4-B	401	NAP	C2B-C3B-C4B	5.56	115.03	101.85
2	1-A	400	NAP	C2B-C3B-C4B	5.62	115.16	101.85
2	2-A	400	NAP	C2B-C3B-C4B	5.63	115.18	101.85
2	5-A	400	NAP	C2B-C3B-C4B	5.77	115.51	101.85
2	3-A	400	NAP	C2B-C3B-C4B	5.78	115.55	101.85
2	9-B	401	NAP	C2B-C3B-C4B	5.81	115.60	101.85
2	4-A	400	NAP	C2B-C3B-C4B	5.88	115.78	101.85
2	15-B	401	NAP	C4B-O4B-C1B	5.91	116.21	109.72
2	14-B	401	NAP	C4B-O4B-C1B	6.04	116.36	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6-A	400	NAP	C2B-C3B-C4B	6.08	116.26	101.85
2	14-B	401	NAP	O3B-C3B-C2B	6.13	128.86	111.16
2	7-B	401	NAP	O4B-C1B-N9A	6.24	121.17	108.10
2	5-B	401	NAP	O4B-C1B-N9A	6.25	121.19	108.10
2	12-B	401	NAP	O4B-C1B-N9A	6.27	121.22	108.10
2	3-B	401	NAP	O4B-C1B-N9A	6.27	121.22	108.10
2	8-A	400	NAP	C2B-C3B-C4B	6.58	117.44	101.85
2	13-B	401	NAP	O3-PA-O5B	6.66	120.59	102.94
2	16-A	400	NAP	O4B-C1B-N9A	6.77	122.27	108.10
2	8-B	401	NAP	O4B-C1B-N9A	6.84	122.41	108.10
2	13-A	400	NAP	O4B-C1B-N9A	6.86	122.46	108.10
2	15-A	400	NAP	O4B-C1B-N9A	6.88	122.50	108.10
2	11-A	400	NAP	O4B-C1B-N9A	6.94	122.62	108.10
2	1-B	401	NAP	O4B-C1B-N9A	6.97	122.70	108.10
2	12-A	400	NAP	O4B-C1B-N9A	7.09	122.94	108.10
2	7-A	400	NAP	O4B-C1B-N9A	7.28	123.34	108.10
2	14-A	400	NAP	O4B-C1B-N9A	7.29	123.35	108.10
2	9-B	401	NAP	O4B-C1B-N9A	7.33	123.43	108.10
2	6-A	400	NAP	O4B-C1B-N9A	7.34	123.46	108.10
2	8-A	400	NAP	O4B-C1B-N9A	7.34	123.47	108.10
2	9-A	400	NAP	O4B-C1B-N9A	7.35	123.48	108.10
2	4-B	401	NAP	O4B-C1B-N9A	7.48	123.75	108.10
2	10-B	401	NAP	O4B-C1B-N9A	7.51	123.82	108.10
2	3-A	400	NAP	O4B-C1B-N9A	7.54	123.88	108.10
2	6-B	401	NAP	O4B-C1B-N9A	7.54	123.89	108.10
2	11-B	401	NAP	O4B-C1B-N9A	7.55	123.91	108.10
2	4-A	400	NAP	O4B-C1B-N9A	7.55	123.91	108.10
2	2-B	401	NAP	O4B-C1B-N9A	7.58	123.96	108.10
2	1-A	400	NAP	O4B-C1B-N9A	7.61	124.04	108.10
2	5-A	400	NAP	O4B-C1B-N9A	7.62	124.06	108.10
2	10-A	400	NAP	O4B-C1B-N9A	7.69	124.20	108.10
2	2-A	400	NAP	O4B-C1B-N9A	7.72	124.25	108.10
2	16-B	401	NAP	O4B-C1B-N9A	9.22	127.40	108.10
2	16-B	401	NAP	C2B-C3B-C4B	9.42	124.16	101.85
2	15-B	401	NAP	O4B-C1B-N9A	10.19	129.42	108.10
2	14-B	401	NAP	O4B-C1B-N9A	10.35	129.77	108.10
2	15-B	401	NAP	C2B-C3B-C4B	10.42	126.53	101.85
2	14-B	401	NAP	C2B-C3B-C4B	11.38	128.81	101.85
2	13-B	401	NAP	O3B-C3B-C4B	11.57	145.75	111.05
2	16-A	400	NAP	C5B-C4B-C3B	13.26	167.83	115.21
2	4-B	401	NAP	C5B-C4B-C3B	13.52	168.87	115.21
2	13-A	400	NAP	C5B-C4B-C3B	13.63	169.29	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	15-A	400	NAP	C5B-C4B-C3B	13.69	169.56	115.21
2	11-B	401	NAP	C5B-C4B-C3B	13.72	169.65	115.21
2	6-B	401	NAP	C5B-C4B-C3B	13.75	169.77	115.21
2	2-B	401	NAP	C5B-C4B-C3B	13.85	170.19	115.21
2	10-B	401	NAP	C5B-C4B-C3B	13.90	170.39	115.21
2	14-A	400	NAP	C5B-C4B-C3B	14.14	171.33	115.21
2	9-B	401	NAP	C5B-C4B-C3B	14.29	171.91	115.21
2	11-A	400	NAP	C5B-C4B-C3B	14.52	172.84	115.21
2	8-B	401	NAP	C5B-C4B-C3B	14.54	172.92	115.21
2	8-A	400	NAP	C5B-C4B-C3B	14.65	173.34	115.21
2	12-A	400	NAP	C5B-C4B-C3B	14.68	173.47	115.21
2	1-B	401	NAP	C5B-C4B-C3B	14.72	173.63	115.21
2	2-A	400	NAP	C5B-C4B-C3B	14.81	174.00	115.21
2	4-A	400	NAP	C5B-C4B-C3B	14.91	174.40	115.21
2	6-A	400	NAP	C5B-C4B-C3B	14.91	174.40	115.21
2	10-A	400	NAP	C5B-C4B-C3B	14.92	174.43	115.21
2	5-A	400	NAP	C5B-C4B-C3B	14.94	174.50	115.21
2	3-A	400	NAP	C5B-C4B-C3B	14.96	174.58	115.21
2	9-A	400	NAP	C5B-C4B-C3B	14.97	174.61	115.21
2	7-A	400	NAP	C5B-C4B-C3B	15.12	175.24	115.21
2	5-B	401	NAP	C5B-C4B-C3B	15.17	175.40	115.21
2	1-A	400	NAP	C5B-C4B-C3B	15.18	175.44	115.21
2	3-B	401	NAP	C5B-C4B-C3B	15.20	175.54	115.21
2	12-B	401	NAP	C5B-C4B-C3B	15.25	175.75	115.21
2	7-B	401	NAP	C5B-C4B-C3B	15.27	175.82	115.21

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	11-A	400	NAP	C4B
2	8-B	401	NAP	C4B
2	9-A	400	NAP	C4B
2	12-B	401	NAP	C4B
2	5-A	400	NAP	C4B
2	15-A	400	NAP	C4B
2	4-A	400	NAP	C4B
2	13-B	401	NAP	C4B
2	2-A	400	NAP	C4B
2	14-A	400	NAP	C4B
2	7-B	401	NAP	C4B
2	7-A	400	NAP	C4B
2	3-A	400	NAP	C4B

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Mol	Chain	Res	Type	Atom
2	5-B	401	NAP	C4B
2	4-B	401	NAP	C4B
2	13-A	400	NAP	C4B
2	10-A	400	NAP	C4B
2	14-B	401	NAP	C4B
2	3-B	401	NAP	C4B
2	6-A	400	NAP	C4B
2	8-A	400	NAP	C4B
2	1-B	401	NAP	C4B
2	6-B	401	NAP	C4B
2	16-A	400	NAP	C4B
2	1-A	400	NAP	C4B
2	11-B	401	NAP	C4B
2	2-B	401	NAP	C4B
2	9-B	401	NAP	C4B
2	10-B	401	NAP	C4B
2	12-A	400	NAP	C4B

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	1-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	2-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	2-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	3-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	3-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	4-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	4-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	5-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	5-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	6-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	6-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	7-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	7-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	8-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	8-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	9-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	9-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	10-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	10-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	11-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	11-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	12-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	12-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	13-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	13-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	14-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	14-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	15-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	15-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
1	16-A	243/253 (96%)	0.53	28 (11%) 6 9	16, 38, 66, 74	243 (100%)
1	16-B	243/253 (96%)	0.17	19 (7%) 16 22	20, 30, 50, 74	243 (100%)
All	All	7776/8096 (96%)	0.35	752 (9%) 8 14	16, 34, 62, 74	7776 (100%)

All (752) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	27	GLY	6.7
1	2-A	27	GLY	6.7
1	3-A	27	GLY	6.7
1	4-A	27	GLY	6.7
1	5-A	27	GLY	6.7
1	6-A	27	GLY	6.7
1	7-A	27	GLY	6.7
1	8-A	27	GLY	6.7
1	9-A	27	GLY	6.7
1	10-A	27	GLY	6.7
1	11-A	27	GLY	6.7
1	12-A	27	GLY	6.7
1	13-A	27	GLY	6.7
1	14-A	27	GLY	6.7
1	15-A	27	GLY	6.7
1	16-A	27	GLY	6.7
1	1-A	131	VAL	5.0
1	2-A	131	VAL	5.0
1	3-A	131	VAL	5.0
1	4-A	131	VAL	5.0
1	5-A	131	VAL	5.0
1	6-A	131	VAL	5.0
1	7-A	131	VAL	5.0
1	8-A	131	VAL	5.0
1	9-A	131	VAL	5.0
1	10-A	131	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	11-A	131	VAL	5.0
1	12-A	131	VAL	5.0
1	13-A	131	VAL	5.0
1	14-A	131	VAL	5.0
1	15-A	131	VAL	5.0
1	16-A	131	VAL	5.0
1	1-B	237	THR	4.6
1	2-B	237	THR	4.6
1	3-B	237	THR	4.6
1	4-B	237	THR	4.6
1	5-B	237	THR	4.6
1	6-B	237	THR	4.6
1	7-B	237	THR	4.6
1	8-B	237	THR	4.6
1	9-B	237	THR	4.6
1	10-B	237	THR	4.6
1	11-B	237	THR	4.6
1	12-B	237	THR	4.6
1	13-B	237	THR	4.6
1	14-B	237	THR	4.6
1	15-B	237	THR	4.6
1	16-B	237	THR	4.6
1	1-A	130	VAL	4.1
1	2-A	130	VAL	4.1
1	3-A	130	VAL	4.1
1	4-A	130	VAL	4.1
1	5-A	130	VAL	4.1
1	6-A	130	VAL	4.1
1	7-A	130	VAL	4.1
1	8-A	130	VAL	4.1
1	9-A	130	VAL	4.1
1	10-A	130	VAL	4.1
1	11-A	130	VAL	4.1
1	12-A	130	VAL	4.1
1	13-A	130	VAL	4.1
1	14-A	130	VAL	4.1
1	15-A	130	VAL	4.1
1	16-A	130	VAL	4.1
1	1-B	234	GLY	4.1
1	2-B	234	GLY	4.1
1	3-B	234	GLY	4.1
1	4-B	234	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	5-B	234	GLY	4.1
1	6-B	234	GLY	4.1
1	7-B	234	GLY	4.1
1	8-B	234	GLY	4.1
1	9-B	234	GLY	4.1
1	10-B	234	GLY	4.1
1	11-B	234	GLY	4.1
1	12-B	234	GLY	4.1
1	13-B	234	GLY	4.1
1	14-B	234	GLY	4.1
1	15-B	234	GLY	4.1
1	16-B	234	GLY	4.1
1	1-B	131	VAL	4.0
1	2-B	131	VAL	4.0
1	3-B	131	VAL	4.0
1	4-B	131	VAL	4.0
1	5-B	131	VAL	4.0
1	6-B	131	VAL	4.0
1	7-B	131	VAL	4.0
1	8-B	131	VAL	4.0
1	9-B	131	VAL	4.0
1	10-B	131	VAL	4.0
1	11-B	131	VAL	4.0
1	12-B	131	VAL	4.0
1	13-B	131	VAL	4.0
1	14-B	131	VAL	4.0
1	15-B	131	VAL	4.0
1	16-B	131	VAL	4.0
1	1-A	198	THR	3.9
1	2-A	198	THR	3.9
1	3-A	198	THR	3.9
1	4-A	198	THR	3.9
1	5-A	198	THR	3.9
1	6-A	198	THR	3.9
1	7-A	198	THR	3.9
1	8-A	198	THR	3.9
1	9-A	198	THR	3.9
1	10-A	198	THR	3.9
1	11-A	198	THR	3.9
1	12-A	198	THR	3.9
1	13-A	198	THR	3.9
1	14-A	198	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	15-A	198	THR	3.9
1	16-A	198	THR	3.9
1	1-B	74	VAL	3.9
1	2-B	74	VAL	3.9
1	3-B	74	VAL	3.9
1	4-B	74	VAL	3.9
1	5-B	74	VAL	3.9
1	6-B	74	VAL	3.9
1	7-B	74	VAL	3.9
1	8-B	74	VAL	3.9
1	9-B	74	VAL	3.9
1	10-B	74	VAL	3.9
1	11-B	74	VAL	3.9
1	12-B	74	VAL	3.9
1	13-B	74	VAL	3.9
1	14-B	74	VAL	3.9
1	15-B	74	VAL	3.9
1	16-B	74	VAL	3.9
1	1-B	9	VAL	3.8
1	2-B	9	VAL	3.8
1	3-B	9	VAL	3.8
1	4-B	9	VAL	3.8
1	5-B	9	VAL	3.8
1	6-B	9	VAL	3.8
1	7-B	9	VAL	3.8
1	8-B	9	VAL	3.8
1	9-B	9	VAL	3.8
1	10-B	9	VAL	3.8
1	11-B	9	VAL	3.8
1	12-B	9	VAL	3.8
1	13-B	9	VAL	3.8
1	14-B	9	VAL	3.8
1	15-B	9	VAL	3.8
1	16-B	9	VAL	3.8
1	1-B	130	VAL	3.6
1	2-B	130	VAL	3.6
1	3-B	130	VAL	3.6
1	4-B	130	VAL	3.6
1	5-B	130	VAL	3.6
1	6-B	130	VAL	3.6
1	7-B	130	VAL	3.6
1	8-B	130	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	9-B	130	VAL	3.6
1	10-B	130	VAL	3.6
1	11-B	130	VAL	3.6
1	12-B	130	VAL	3.6
1	13-B	130	VAL	3.6
1	14-B	130	VAL	3.6
1	15-B	130	VAL	3.6
1	16-B	130	VAL	3.6
1	1-A	197	GLN	3.6
1	2-A	197	GLN	3.6
1	3-A	197	GLN	3.6
1	4-A	197	GLN	3.6
1	5-A	197	GLN	3.6
1	6-A	197	GLN	3.6
1	7-A	197	GLN	3.6
1	8-A	197	GLN	3.6
1	9-A	197	GLN	3.6
1	10-A	197	GLN	3.6
1	11-A	197	GLN	3.6
1	12-A	197	GLN	3.6
1	13-A	197	GLN	3.6
1	14-A	197	GLN	3.6
1	15-A	197	GLN	3.6
1	16-A	197	GLN	3.6
1	1-A	172	ILE	3.6
1	2-A	172	ILE	3.6
1	3-A	172	ILE	3.6
1	4-A	172	ILE	3.6
1	5-A	172	ILE	3.6
1	6-A	172	ILE	3.6
1	7-A	172	ILE	3.6
1	8-A	172	ILE	3.6
1	9-A	172	ILE	3.6
1	10-A	172	ILE	3.6
1	11-A	172	ILE	3.6
1	12-A	172	ILE	3.6
1	13-A	172	ILE	3.6
1	14-A	172	ILE	3.6
1	15-A	172	ILE	3.6
1	16-A	172	ILE	3.6
1	1-B	76	LEU	3.4
1	2-B	76	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	3-B	76	LEU	3.4
1	4-B	76	LEU	3.4
1	5-B	76	LEU	3.4
1	6-B	76	LEU	3.4
1	7-B	76	LEU	3.4
1	8-B	76	LEU	3.4
1	9-B	76	LEU	3.4
1	10-B	76	LEU	3.4
1	11-B	76	LEU	3.4
1	12-B	76	LEU	3.4
1	13-B	76	LEU	3.4
1	14-B	76	LEU	3.4
1	15-B	76	LEU	3.4
1	16-B	76	LEU	3.4
1	1-A	236	SER	3.4
1	2-A	236	SER	3.4
1	3-A	236	SER	3.4
1	4-A	236	SER	3.4
1	5-A	236	SER	3.4
1	6-A	236	SER	3.4
1	7-A	236	SER	3.4
1	8-A	236	SER	3.4
1	9-A	236	SER	3.4
1	10-A	236	SER	3.4
1	11-A	236	SER	3.4
1	12-A	236	SER	3.4
1	13-A	236	SER	3.4
1	14-A	236	SER	3.4
1	15-A	236	SER	3.4
1	16-A	236	SER	3.4
1	1-A	234	GLY	3.4
1	2-A	234	GLY	3.4
1	3-A	234	GLY	3.4
1	4-A	234	GLY	3.4
1	5-A	234	GLY	3.4
1	6-A	234	GLY	3.4
1	7-A	234	GLY	3.4
1	8-A	234	GLY	3.4
1	9-A	234	GLY	3.4
1	10-A	234	GLY	3.4
1	11-A	234	GLY	3.4
1	12-A	234	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	13-A	234	GLY	3.4
1	14-A	234	GLY	3.4
1	15-A	234	GLY	3.4
1	16-A	234	GLY	3.4
1	1-A	145	LYS	3.4
1	2-A	145	LYS	3.4
1	3-A	145	LYS	3.4
1	4-A	145	LYS	3.4
1	5-A	145	LYS	3.4
1	6-A	145	LYS	3.4
1	7-A	145	LYS	3.4
1	8-A	145	LYS	3.4
1	9-A	145	LYS	3.4
1	10-A	145	LYS	3.4
1	11-A	145	LYS	3.4
1	12-A	145	LYS	3.4
1	13-A	145	LYS	3.4
1	14-A	145	LYS	3.4
1	15-A	145	LYS	3.4
1	16-A	145	LYS	3.4
1	1-A	129	VAL	3.3
1	1-B	129	VAL	3.3
1	2-A	129	VAL	3.3
1	2-B	129	VAL	3.3
1	3-A	129	VAL	3.3
1	3-B	129	VAL	3.3
1	4-A	129	VAL	3.3
1	4-B	129	VAL	3.3
1	5-A	129	VAL	3.3
1	5-B	129	VAL	3.3
1	6-A	129	VAL	3.3
1	6-B	129	VAL	3.3
1	7-A	129	VAL	3.3
1	7-B	129	VAL	3.3
1	8-A	129	VAL	3.3
1	8-B	129	VAL	3.3
1	9-A	129	VAL	3.3
1	9-B	129	VAL	3.3
1	10-A	129	VAL	3.3
1	10-B	129	VAL	3.3
1	11-A	129	VAL	3.3
1	11-B	129	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	12-A	129	VAL	3.3
1	12-B	129	VAL	3.3
1	13-A	129	VAL	3.3
1	13-B	129	VAL	3.3
1	14-A	129	VAL	3.3
1	14-B	129	VAL	3.3
1	15-A	129	VAL	3.3
1	15-B	129	VAL	3.3
1	16-A	129	VAL	3.3
1	16-B	129	VAL	3.3
1	1-B	235	THR	3.2
1	2-B	235	THR	3.2
1	3-B	235	THR	3.2
1	4-B	235	THR	3.2
1	5-B	235	THR	3.2
1	6-B	235	THR	3.2
1	7-B	235	THR	3.2
1	8-B	235	THR	3.2
1	9-B	235	THR	3.2
1	10-B	235	THR	3.2
1	11-B	235	THR	3.2
1	12-B	235	THR	3.2
1	13-B	235	THR	3.2
1	14-B	235	THR	3.2
1	15-B	235	THR	3.2
1	16-B	235	THR	3.2
1	1-B	75	ILE	3.2
1	2-B	75	ILE	3.2
1	3-B	75	ILE	3.2
1	4-B	75	ILE	3.2
1	5-B	75	ILE	3.2
1	6-B	75	ILE	3.2
1	7-B	75	ILE	3.2
1	8-B	75	ILE	3.2
1	9-B	75	ILE	3.2
1	10-B	75	ILE	3.2
1	11-B	75	ILE	3.2
1	12-B	75	ILE	3.2
1	13-B	75	ILE	3.2
1	14-B	75	ILE	3.2
1	15-B	75	ILE	3.2
1	16-B	75	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	140	ASP	3.1
1	2-A	140	ASP	3.1
1	3-A	140	ASP	3.1
1	4-A	140	ASP	3.1
1	5-A	140	ASP	3.1
1	6-A	140	ASP	3.1
1	7-A	140	ASP	3.1
1	8-A	140	ASP	3.1
1	9-A	140	ASP	3.1
1	10-A	140	ASP	3.1
1	11-A	140	ASP	3.1
1	12-A	140	ASP	3.1
1	13-A	140	ASP	3.1
1	14-A	140	ASP	3.1
1	15-A	140	ASP	3.1
1	16-A	140	ASP	3.1
1	1-B	172	ILE	3.1
1	2-B	172	ILE	3.1
1	3-B	172	ILE	3.1
1	4-B	172	ILE	3.1
1	5-B	172	ILE	3.1
1	6-B	172	ILE	3.1
1	7-B	172	ILE	3.1
1	8-B	172	ILE	3.1
1	9-B	172	ILE	3.1
1	10-B	172	ILE	3.1
1	11-B	172	ILE	3.1
1	12-B	172	ILE	3.1
1	13-B	172	ILE	3.1
1	14-B	172	ILE	3.1
1	15-B	172	ILE	3.1
1	16-B	172	ILE	3.1
1	1-A	76	LEU	3.1
1	2-A	76	LEU	3.1
1	3-A	76	LEU	3.1
1	4-A	76	LEU	3.1
1	5-A	76	LEU	3.1
1	6-A	76	LEU	3.1
1	7-A	76	LEU	3.1
1	8-A	76	LEU	3.1
1	9-A	76	LEU	3.1
1	10-A	76	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	11-A	76	LEU	3.1
1	12-A	76	LEU	3.1
1	13-A	76	LEU	3.1
1	14-A	76	LEU	3.1
1	15-A	76	LEU	3.1
1	16-A	76	LEU	3.1
1	1-A	96	GLU	2.9
1	2-A	96	GLU	2.9
1	3-A	96	GLU	2.9
1	4-A	96	GLU	2.9
1	5-A	96	GLU	2.9
1	6-A	96	GLU	2.9
1	7-A	96	GLU	2.9
1	8-A	96	GLU	2.9
1	9-A	96	GLU	2.9
1	10-A	96	GLU	2.9
1	11-A	96	GLU	2.9
1	12-A	96	GLU	2.9
1	13-A	96	GLU	2.9
1	14-A	96	GLU	2.9
1	15-A	96	GLU	2.9
1	16-A	96	GLU	2.9
1	1-A	98	ILE	2.9
1	2-A	98	ILE	2.9
1	3-A	98	ILE	2.9
1	4-A	98	ILE	2.9
1	5-A	98	ILE	2.9
1	6-A	98	ILE	2.9
1	7-A	98	ILE	2.9
1	8-A	98	ILE	2.9
1	9-A	98	ILE	2.9
1	10-A	98	ILE	2.9
1	11-A	98	ILE	2.9
1	12-A	98	ILE	2.9
1	13-A	98	ILE	2.9
1	14-A	98	ILE	2.9
1	15-A	98	ILE	2.9
1	16-A	98	ILE	2.9
1	1-A	240	LYS	2.8
1	2-A	240	LYS	2.8
1	3-A	240	LYS	2.8
1	4-A	240	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	5-A	240	LYS	2.8
1	6-A	240	LYS	2.8
1	7-A	240	LYS	2.8
1	8-A	240	LYS	2.8
1	9-A	240	LYS	2.8
1	10-A	240	LYS	2.8
1	11-A	240	LYS	2.8
1	12-A	240	LYS	2.8
1	13-A	240	LYS	2.8
1	14-A	240	LYS	2.8
1	15-A	240	LYS	2.8
1	16-A	240	LYS	2.8
1	1-A	235	THR	2.7
1	2-A	235	THR	2.7
1	3-A	235	THR	2.7
1	4-A	235	THR	2.7
1	5-A	235	THR	2.7
1	6-A	235	THR	2.7
1	7-A	235	THR	2.7
1	8-A	235	THR	2.7
1	9-A	235	THR	2.7
1	10-A	235	THR	2.7
1	11-A	235	THR	2.7
1	12-A	235	THR	2.7
1	13-A	235	THR	2.7
1	14-A	235	THR	2.7
1	15-A	235	THR	2.7
1	16-A	235	THR	2.7
1	1-B	128	ILE	2.7
1	2-B	128	ILE	2.7
1	3-B	128	ILE	2.7
1	4-B	128	ILE	2.7
1	5-B	128	ILE	2.7
1	6-B	128	ILE	2.7
1	7-B	128	ILE	2.7
1	8-B	128	ILE	2.7
1	9-B	128	ILE	2.7
1	10-B	128	ILE	2.7
1	11-B	128	ILE	2.7
1	12-B	128	ILE	2.7
1	13-B	128	ILE	2.7
1	14-B	128	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	15-B	128	ILE	2.7
1	16-B	128	ILE	2.7
1	1-B	83	MET	2.6
1	2-B	83	MET	2.6
1	3-B	83	MET	2.6
1	4-B	83	MET	2.6
1	5-B	83	MET	2.6
1	6-B	83	MET	2.6
1	7-B	83	MET	2.6
1	8-B	83	MET	2.6
1	9-B	83	MET	2.6
1	10-B	83	MET	2.6
1	11-B	83	MET	2.6
1	12-B	83	MET	2.6
1	13-B	83	MET	2.6
1	14-B	83	MET	2.6
1	15-B	83	MET	2.6
1	16-B	83	MET	2.6
1	1-A	228	LEU	2.6
1	2-A	228	LEU	2.6
1	3-A	228	LEU	2.6
1	4-A	228	LEU	2.6
1	5-A	228	LEU	2.6
1	6-A	228	LEU	2.6
1	7-A	228	LEU	2.6
1	8-A	228	LEU	2.6
1	9-A	228	LEU	2.6
1	10-A	228	LEU	2.6
1	11-A	228	LEU	2.6
1	12-A	228	LEU	2.6
1	13-A	228	LEU	2.6
1	14-A	228	LEU	2.6
1	15-A	228	LEU	2.6
1	16-A	228	LEU	2.6
1	1-A	102	GLY	2.5
1	2-A	102	GLY	2.5
1	3-A	102	GLY	2.5
1	4-A	102	GLY	2.5
1	5-A	102	GLY	2.5
1	6-A	102	GLY	2.5
1	7-A	102	GLY	2.5
1	8-A	102	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	9-A	102	GLY	2.5
1	10-A	102	GLY	2.5
1	11-A	102	GLY	2.5
1	12-A	102	GLY	2.5
1	13-A	102	GLY	2.5
1	14-A	102	GLY	2.5
1	15-A	102	GLY	2.5
1	16-A	102	GLY	2.5
1	1-A	75	ILE	2.5
1	2-A	75	ILE	2.5
1	3-A	75	ILE	2.5
1	4-A	75	ILE	2.5
1	5-A	75	ILE	2.5
1	6-A	75	ILE	2.5
1	7-A	75	ILE	2.5
1	8-A	75	ILE	2.5
1	9-A	75	ILE	2.5
1	10-A	75	ILE	2.5
1	11-A	75	ILE	2.5
1	12-A	75	ILE	2.5
1	13-A	75	ILE	2.5
1	14-A	75	ILE	2.5
1	15-A	75	ILE	2.5
1	16-A	75	ILE	2.5
1	1-A	26	GLU	2.4
1	2-A	26	GLU	2.4
1	3-A	26	GLU	2.4
1	4-A	26	GLU	2.4
1	5-A	26	GLU	2.4
1	6-A	26	GLU	2.4
1	7-A	26	GLU	2.4
1	8-A	26	GLU	2.4
1	9-A	26	GLU	2.4
1	10-A	26	GLU	2.4
1	11-A	26	GLU	2.4
1	12-A	26	GLU	2.4
1	13-A	26	GLU	2.4
1	14-A	26	GLU	2.4
1	15-A	26	GLU	2.4
1	16-A	26	GLU	2.4
1	1-B	10	THR	2.4
1	2-B	10	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	3-B	10	THR	2.4
1	4-B	10	THR	2.4
1	5-B	10	THR	2.4
1	6-B	10	THR	2.4
1	7-B	10	THR	2.4
1	8-B	10	THR	2.4
1	9-B	10	THR	2.4
1	10-B	10	THR	2.4
1	11-B	10	THR	2.4
1	12-B	10	THR	2.4
1	13-B	10	THR	2.4
1	14-B	10	THR	2.4
1	15-B	10	THR	2.4
1	16-B	10	THR	2.4
1	1-A	237	THR	2.4
1	2-A	237	THR	2.4
1	3-A	237	THR	2.4
1	4-A	237	THR	2.4
1	5-A	237	THR	2.4
1	6-A	237	THR	2.4
1	7-A	237	THR	2.4
1	8-A	237	THR	2.4
1	9-A	237	THR	2.4
1	10-A	237	THR	2.4
1	11-A	237	THR	2.4
1	12-A	237	THR	2.4
1	13-A	237	THR	2.4
1	14-A	237	THR	2.4
1	15-A	237	THR	2.4
1	16-A	237	THR	2.4
1	1-A	47	GLY	2.4
1	2-A	47	GLY	2.4
1	3-A	47	GLY	2.4
1	4-A	47	GLY	2.4
1	5-A	47	GLY	2.4
1	6-A	47	GLY	2.4
1	7-A	47	GLY	2.4
1	8-A	47	GLY	2.4
1	9-A	47	GLY	2.4
1	10-A	47	GLY	2.4
1	11-A	47	GLY	2.4
1	12-A	47	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	13-A	47	GLY	2.4
1	14-A	47	GLY	2.4
1	15-A	47	GLY	2.4
1	16-A	47	GLY	2.4
1	1-B	170	THR	2.3
1	2-B	170	THR	2.3
1	3-B	170	THR	2.3
1	4-B	170	THR	2.3
1	5-B	170	THR	2.3
1	6-B	170	THR	2.3
1	7-B	170	THR	2.3
1	8-B	170	THR	2.3
1	9-B	170	THR	2.3
1	10-B	170	THR	2.3
1	11-B	170	THR	2.3
1	12-B	170	THR	2.3
1	13-B	170	THR	2.3
1	14-B	170	THR	2.3
1	15-B	170	THR	2.3
1	16-B	170	THR	2.3
1	1-A	238	PRO	2.3
1	2-A	238	PRO	2.3
1	3-A	238	PRO	2.3
1	4-A	238	PRO	2.3
1	5-A	238	PRO	2.3
1	6-A	238	PRO	2.3
1	7-A	238	PRO	2.3
1	8-A	238	PRO	2.3
1	9-A	238	PRO	2.3
1	10-A	238	PRO	2.3
1	11-A	238	PRO	2.3
1	12-A	238	PRO	2.3
1	13-A	238	PRO	2.3
1	14-A	238	PRO	2.3
1	15-A	238	PRO	2.3
1	16-A	238	PRO	2.3
1	1-B	171	ILE	2.3
1	2-B	171	ILE	2.3
1	3-B	171	ILE	2.3
1	4-B	171	ILE	2.3
1	5-B	171	ILE	2.3
1	6-B	171	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	7-B	171	ILE	2.3
1	8-B	171	ILE	2.3
1	9-B	171	ILE	2.3
1	10-B	171	ILE	2.3
1	11-B	171	ILE	2.3
1	12-B	171	ILE	2.3
1	13-B	171	ILE	2.3
1	14-B	171	ILE	2.3
1	15-B	171	ILE	2.3
1	16-B	171	ILE	2.3
1	1-A	174	ALA	2.3
1	2-A	174	ALA	2.3
1	3-A	174	ALA	2.3
1	4-A	174	ALA	2.3
1	5-A	174	ALA	2.3
1	6-A	174	ALA	2.3
1	7-A	174	ALA	2.3
1	8-A	174	ALA	2.3
1	9-A	174	ALA	2.3
1	10-A	174	ALA	2.3
1	11-A	174	ALA	2.3
1	12-A	174	ALA	2.3
1	13-A	174	ALA	2.3
1	14-A	174	ALA	2.3
1	15-A	174	ALA	2.3
1	16-A	174	ALA	2.3
1	1-B	73	LEU	2.1
1	2-B	73	LEU	2.1
1	3-B	73	LEU	2.1
1	4-B	73	LEU	2.1
1	5-B	73	LEU	2.1
1	6-B	73	LEU	2.1
1	7-B	73	LEU	2.1
1	8-B	73	LEU	2.1
1	9-B	73	LEU	2.1
1	10-B	73	LEU	2.1
1	11-B	73	LEU	2.1
1	12-B	73	LEU	2.1
1	13-B	73	LEU	2.1
1	14-B	73	LEU	2.1
1	15-B	73	LEU	2.1
1	16-B	73	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	82	LYS	2.1
1	2-B	82	LYS	2.1
1	3-B	82	LYS	2.1
1	4-B	82	LYS	2.1
1	5-B	82	LYS	2.1
1	6-B	82	LYS	2.1
1	7-B	82	LYS	2.1
1	8-B	82	LYS	2.1
1	9-B	82	LYS	2.1
1	10-B	82	LYS	2.1
1	11-B	82	LYS	2.1
1	12-B	82	LYS	2.1
1	13-B	82	LYS	2.1
1	14-B	82	LYS	2.1
1	15-B	82	LYS	2.1
1	16-B	82	LYS	2.1
1	1-A	74	VAL	2.1
1	1-A	142	PRO	2.1
1	2-A	74	VAL	2.1
1	2-A	142	PRO	2.1
1	3-A	74	VAL	2.1
1	3-A	142	PRO	2.1
1	4-A	74	VAL	2.1
1	4-A	142	PRO	2.1
1	5-A	74	VAL	2.1
1	5-A	142	PRO	2.1
1	6-A	74	VAL	2.1
1	6-A	142	PRO	2.1
1	7-A	74	VAL	2.1
1	7-A	142	PRO	2.1
1	8-A	74	VAL	2.1
1	8-A	142	PRO	2.1
1	9-A	74	VAL	2.1
1	9-A	142	PRO	2.1
1	10-A	74	VAL	2.1
1	10-A	142	PRO	2.1
1	11-A	74	VAL	2.1
1	11-A	142	PRO	2.1
1	12-A	74	VAL	2.1
1	12-A	142	PRO	2.1
1	13-A	74	VAL	2.1
1	13-A	142	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	14-A	74	VAL	2.1
1	14-A	142	PRO	2.1
1	15-A	74	VAL	2.1
1	15-A	142	PRO	2.1
1	16-A	74	VAL	2.1
1	16-A	142	PRO	2.1
1	1-A	104	TYR	2.1
1	2-A	104	TYR	2.1
1	3-A	104	TYR	2.1
1	4-A	104	TYR	2.1
1	5-A	104	TYR	2.1
1	6-A	104	TYR	2.1
1	7-A	104	TYR	2.1
1	8-A	104	TYR	2.1
1	9-A	104	TYR	2.1
1	10-A	104	TYR	2.1
1	11-A	104	TYR	2.1
1	12-A	104	TYR	2.1
1	13-A	104	TYR	2.1
1	14-A	104	TYR	2.1
1	15-A	104	TYR	2.1
1	16-A	104	TYR	2.1
1	1-A	148	ASN	2.0
1	2-A	148	ASN	2.0
1	3-A	148	ASN	2.0
1	4-A	148	ASN	2.0
1	5-A	148	ASN	2.0
1	6-A	148	ASN	2.0
1	7-A	148	ASN	2.0
1	8-A	148	ASN	2.0
1	9-A	148	ASN	2.0
1	10-A	148	ASN	2.0
1	11-A	148	ASN	2.0
1	12-A	148	ASN	2.0
1	13-A	148	ASN	2.0
1	14-A	148	ASN	2.0
1	15-A	148	ASN	2.0
1	16-A	148	ASN	2.0
1	1-B	184	VAL	2.0
1	2-B	184	VAL	2.0
1	3-B	184	VAL	2.0
1	4-B	184	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	5-B	184	VAL	2.0
1	6-B	184	VAL	2.0
1	7-B	184	VAL	2.0
1	8-B	184	VAL	2.0
1	9-B	184	VAL	2.0
1	10-B	184	VAL	2.0
1	11-B	184	VAL	2.0
1	12-B	184	VAL	2.0
1	13-B	184	VAL	2.0
1	14-B	184	VAL	2.0
1	15-B	184	VAL	2.0
1	16-B	184	VAL	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAP	10-B	401	48/48	0.94	0.14	0.09	27,33,37,41	48
2	NAP	15-B	401	48/48	0.94	0.14	0.03	27,33,37,43	48
2	NAP	12-B	401	48/48	0.94	0.14	0.02	28,33,37,43	48
2	NAP	8-B	401	48/48	0.94	0.14	0.01	27,33,37,41	48
2	NAP	3-B	401	48/48	0.94	0.14	0.01	28,33,37,43	48
2	NAP	7-B	401	48/48	0.94	0.14	0.01	28,33,37,43	48
2	NAP	9-B	401	48/48	0.94	0.14	-0.01	27,33,38,42	48
2	NAP	11-B	401	48/48	0.94	0.14	-0.01	28,33,37,43	48
2	NAP	5-B	401	48/48	0.94	0.14	-0.02	27,33,37,43	48

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAP	4-B	401	48/48	0.94	0.14	-0.02	27,33,38,43	48
2	NAP	6-B	401	48/48	0.94	0.14	-0.02	28,33,37,43	48
2	NAP	2-B	401	48/48	0.94	0.14	-0.03	28,33,37,43	48
2	NAP	14-B	401	48/48	0.94	0.14	-0.03	27,33,38,43	48
2	NAP	1-B	401	48/48	0.94	0.14	-0.03	27,33,37,42	48
2	NAP	16-B	401	48/48	0.94	0.14	-0.05	23,33,38,43	48
2	NAP	13-B	401	48/48	0.94	0.14	-0.08	21,33,37,42	48
2	NAP	3-A	400	48/48	0.94	0.14	-0.24	28,37,45,49	48
2	NAP	9-A	400	48/48	0.94	0.14	-0.24	28,37,45,48	48
2	NAP	16-A	400	48/48	0.94	0.14	-0.24	28,37,45,48	48
2	NAP	1-A	400	48/48	0.94	0.14	-0.24	29,37,46,49	48
2	NAP	2-A	400	48/48	0.94	0.14	-0.24	31,37,45,48	48
2	NAP	14-A	400	48/48	0.94	0.14	-0.24	29,37,46,49	48
2	NAP	4-A	400	48/48	0.94	0.14	-0.24	29,37,46,49	48
2	NAP	7-A	400	48/48	0.94	0.14	-0.24	28,37,45,48	48
2	NAP	6-A	400	48/48	0.94	0.14	-0.24	28,37,45,49	48
2	NAP	13-A	400	48/48	0.94	0.14	-0.25	27,37,44,48	48
2	NAP	10-A	400	48/48	0.94	0.14	-0.26	31,37,45,48	48
2	NAP	5-A	400	48/48	0.94	0.14	-0.28	29,37,46,49	48
2	NAP	15-A	400	48/48	0.94	0.14	-0.28	27,37,45,49	48
2	NAP	12-A	400	48/48	0.94	0.14	-0.28	28,37,45,46	48
2	NAP	11-A	400	48/48	0.94	0.14	-0.29	24,37,44,47	48
2	NAP	8-A	400	48/48	0.94	0.14	-0.33	26,37,45,49	48

6.5 Other polymers

There are no such residues in this entry.