



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 09:11 PM 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 wwPDB validation summary 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/ValidationPDFNotes.html>

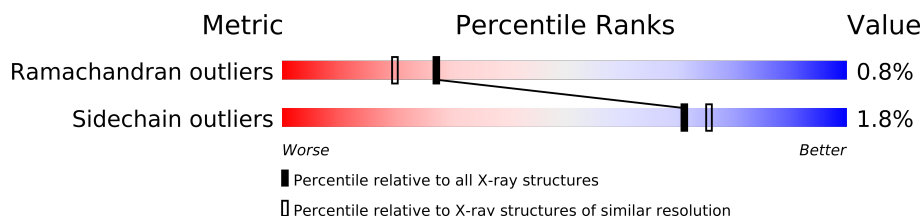
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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))
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	253	
1	1-B	253	
1	10-A	253	
1	10-B	253	
1	11-A	253	
1	11-B	253	
1	12-A	253	
1	12-B	253	
1	13-A	253	
1	13-B	253	
1	14-A	253	
1	14-B	253	
1	15-A	253	
1	15-B	253	
1	16-A	253	
1	16-B	253	
1	2-A	253	
1	2-B	253	
1	3-A	253	

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Mol	Chain	Length	Quality of chain
1	3-B	253	
1	4-A	253	
1	4-B	253	
1	5-A	253	
1	5-B	253	
1	6-A	253	
1	6-B	253	
1	7-A	253	
1	7-B	253	
1	8-A	253	
1	8-B	253	
1	9-A	253	
1	9-B	253	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 66192 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a 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	1-B	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	2-B	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	3-B	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	4-B	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	5-B	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	6-B	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	7-B	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	8-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			

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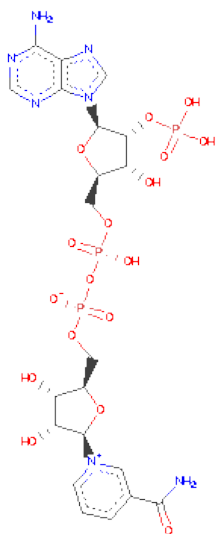
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	9-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	9-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	10-A	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	10-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	11-A	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-A	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-A	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-A	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-A	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-A	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-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-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-A	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-A	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-A	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-A	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-A	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-A	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		

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	12-A	147	Total 147	O 147	0	0
3	12-B	222	Total 222	O 222	0	0
3	13-A	146	Total 146	O 146	0	0
3	13-B	223	Total 223	O 223	0	0
3	14-A	146	Total 146	O 146	0	0
3	14-B	223	Total 223	O 223	0	0
3	15-A	147	Total 147	O 147	0	0
3	15-B	222	Total 222	O 222	0	0
3	16-A	147	Total 147	O 147	0	0
3	16-B	222	Total 222	O 222	0	0

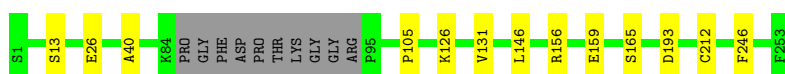
3 Residue-property plots

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

Note EDS failed to run properly.

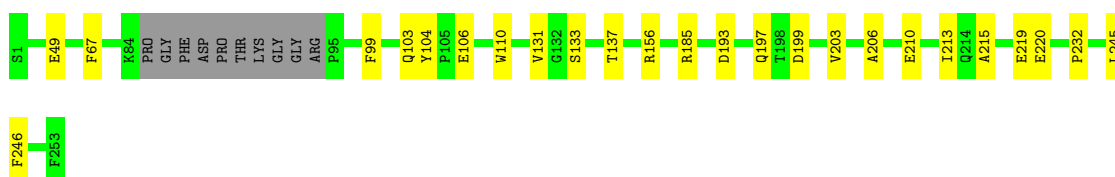
- Molecule 1: Protein At5g02240

Chain 1-A: 



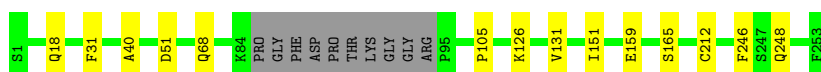
- Molecule 1: Protein At5g02240

Chain 1-B: 



- Molecule 1: Protein At5g02240

Chain 2-A: 



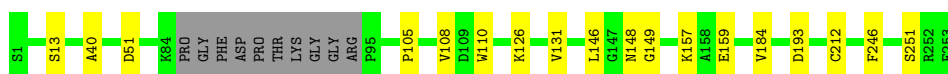
- Molecule 1: Protein At5g02240

Chain 2-B: 



- Molecule 1: Protein At5g02240

Chain 3-A: 



- Molecule 1: Protein At5g02240

Chain 3-B: 



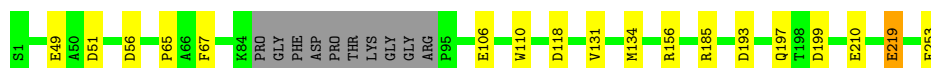
- Molecule 1: Protein At5g02240

Chain 4-A:



- Molecule 1: Protein At5g02240

Chain 4-B:



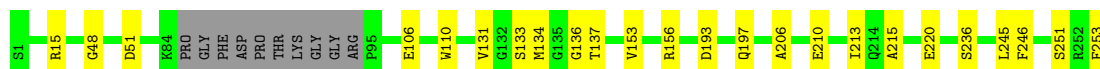
- Molecule 1: Protein At5g02240

Chain 5-A:



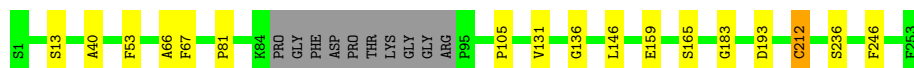
- Molecule 1: Protein At5g02240

Chain 5-B:



- Molecule 1: Protein At5g02240

Chain 6-A:



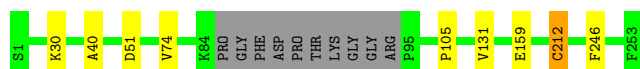
- Molecule 1: Protein At5g02240

Chain 6-B:



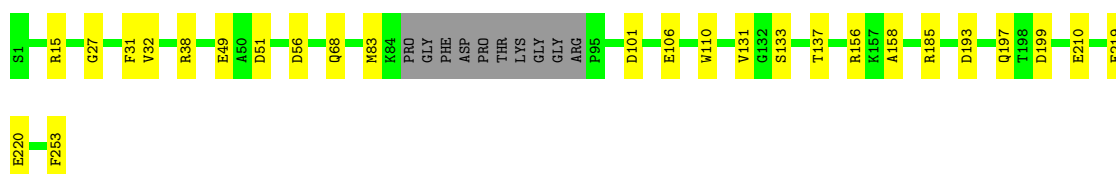
- Molecule 1: Protein At5g02240

Chain 7-A:



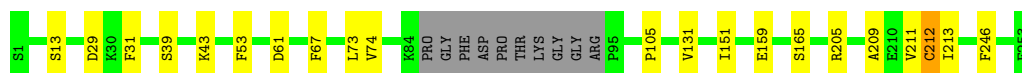
- Molecule 1: Protein At5g02240

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:



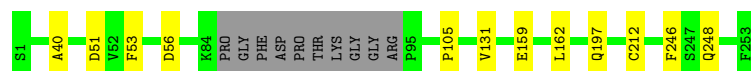
- Molecule 1: Protein At5g02240

Chain 11-B:



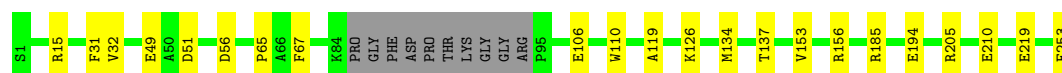
- Molecule 1: Protein At5g02240

Chain 12-A:



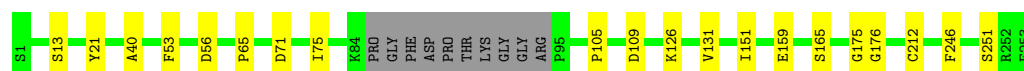
- Molecule 1: Protein At5g02240

Chain 12-B:



- Molecule 1: Protein At5g02240

Chain 13-A:



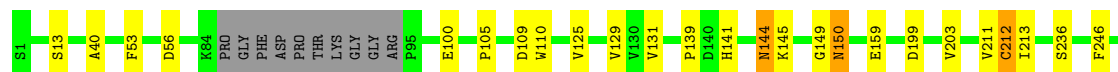
- Molecule 1: Protein At5g02240

Chain 13-B:



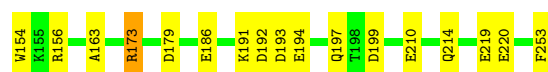
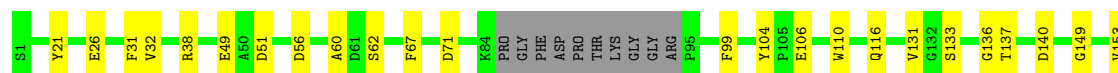
- Molecule 1: Protein At5g02240

Chain 14-A:



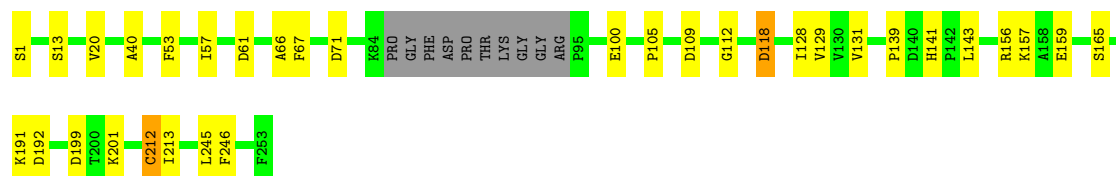
- Molecule 1: Protein At5g02240

Chain 14-B:



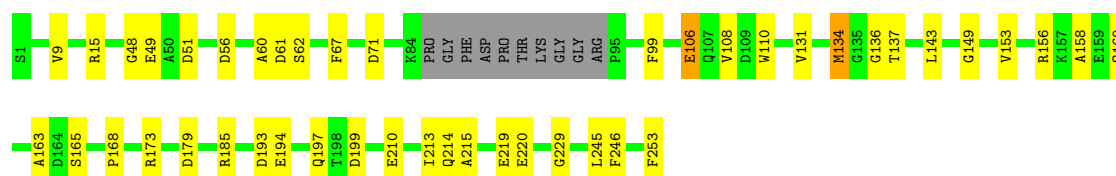
- Molecule 1: Protein At5g02240

Chain 15-A:



- Molecule 1: Protein At5g02240

Chain 15-B:



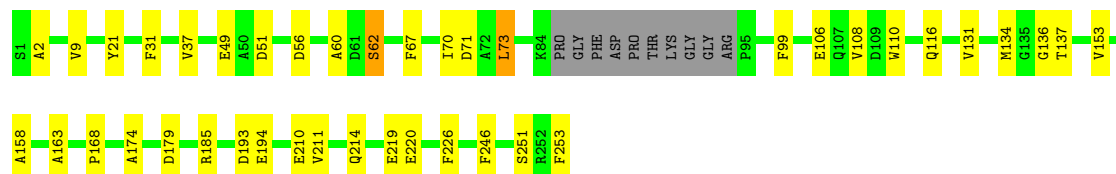
- Molecule 1: Protein At5g02240

Chain 16-A:



- Molecule 1: Protein At5g02240

Chain 16-B:



4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	92.9 (29.09-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.16 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.257	Depositor
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.045	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29855 reflections	Xtriage
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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The worst 5 of 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

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1
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
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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	15-A	147	0	0	0	3
3	15-B	222	0	0	0	2
3	16-A	147	0	0	0	2
3	16-B	222	0	0	0	2
All	All	66192	0	60467	0	33

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

The worst 5 of 33 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:511:HOH:O	3:B:568:HOH:O[3_646]	1.89	0.31
3:A:512:HOH:O	3:B:567:HOH:O[3_646]	1.89	0.31
3:A:512:HOH:O	3:B:567:HOH:O[3_646]	1.89	0.31
3:A:511:HOH:O	3:B:568:HOH:O[3_646]	1.89	0.31
3:A:512:HOH:O	3:B:567:HOH:O[3_646]	1.89	0.31

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	239/253 (94%)	224 (94%)	12 (5%)	3 (1%)	18	10
1	1-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	43	39
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%)	43	39
1	3-A	239/253 (94%)	214 (90%)	21 (9%)	4 (2%)	14	6
1	3-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	43	39
1	4-A	239/253 (94%)	220 (92%)	16 (7%)	3 (1%)	18	10
1	4-B	239/253 (94%)	228 (95%)	11 (5%)	0	100	100
1	5-A	239/253 (94%)	218 (91%)	20 (8%)	1 (0%)	43	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-B	239/253 (94%)	225 (94%)	11 (5%)	3 (1%)	18	10
1	6-A	239/253 (94%)	215 (90%)	17 (7%)	7 (3%)	7	2
1	6-B	239/253 (94%)	227 (95%)	11 (5%)	1 (0%)	43	39
1	7-A	239/253 (94%)	220 (92%)	18 (8%)	1 (0%)	43	39
1	7-B	239/253 (94%)	229 (96%)	8 (3%)	2 (1%)	27	20
1	8-A	239/253 (94%)	214 (90%)	22 (9%)	3 (1%)	18	10
1	8-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	43	39
1	9-A	239/253 (94%)	223 (93%)	15 (6%)	1 (0%)	43	39
1	9-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	43	39
1	10-A	239/253 (94%)	222 (93%)	16 (7%)	1 (0%)	43	39
1	10-B	239/253 (94%)	229 (96%)	9 (4%)	1 (0%)	43	39
1	11-A	239/253 (94%)	218 (91%)	17 (7%)	4 (2%)	14	6
1	11-B	239/253 (94%)	223 (93%)	15 (6%)	1 (0%)	43	39
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%)	43	39
1	14-A	239/253 (94%)	209 (87%)	21 (9%)	9 (4%)	5	1
1	14-B	239/253 (94%)	228 (95%)	10 (4%)	1 (0%)	43	39
1	15-A	239/253 (94%)	206 (86%)	29 (12%)	4 (2%)	14	6
1	15-B	239/253 (94%)	225 (94%)	12 (5%)	2 (1%)	27	20
1	16-A	239/253 (94%)	222 (93%)	16 (7%)	1 (0%)	43	39
1	16-B	239/253 (94%)	220 (92%)	19 (8%)	0	100	100
All	All	7648/8096 (94%)	7109 (93%)	480 (6%)	59 (1%)	27	20

5 of 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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	1-B	196/203 (97%)	192 (98%)	4 (2%)	68	72
1	2-A	196/203 (97%)	191 (97%)	5 (3%)	59	62
1	2-B	196/203 (97%)	193 (98%)	3 (2%)	76	81
1	3-A	196/203 (97%)	191 (97%)	5 (3%)	59	62
1	3-B	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	4-A	196/203 (97%)	192 (98%)	4 (2%)	68	72
1	4-B	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	5-A	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	5-B	196/203 (97%)	195 (100%)	1 (0%)	94	96
1	6-A	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	6-B	196/203 (97%)	193 (98%)	3 (2%)	76	81
1	7-A	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	7-B	196/203 (97%)	192 (98%)	4 (2%)	68	72
1	8-A	196/203 (97%)	191 (97%)	5 (3%)	59	62
1	8-B	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	9-A	196/203 (97%)	193 (98%)	3 (2%)	76	81
1	9-B	196/203 (97%)	190 (97%)	6 (3%)	52	54
1	10-A	196/203 (97%)	193 (98%)	3 (2%)	76	81
1	10-B	196/203 (97%)	195 (100%)	1 (0%)	94	96
1	11-A	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	11-B	196/203 (97%)	193 (98%)	3 (2%)	76	81
1	12-A	196/203 (97%)	192 (98%)	4 (2%)	68	72
1	12-B	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	13-A	196/203 (97%)	192 (98%)	4 (2%)	68	72
1	13-B	196/203 (97%)	193 (98%)	3 (2%)	76	81
1	14-A	196/203 (97%)	191 (97%)	5 (3%)	59	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	14-B	196/203 (97%)	194 (99%)	2 (1%)	85	90
1	15-A	196/203 (97%)	185 (94%)	11 (6%)	30	25
1	15-B	196/203 (97%)	193 (98%)	3 (2%)	76	81
1	16-A	196/203 (97%)	191 (97%)	5 (3%)	59	62
1	16-B	196/203 (97%)	191 (97%)	5 (3%)	59	62
All	All	6272/6496 (97%)	6162 (98%)	110 (2%)	71	75

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9-A	126	LYS
1	11-A	105	PRO
1	16-A	126	LYS
1	9-B	49	GLU
1	9-B	143	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-A	18	GLN
1	10-B	64	ASN
1	15-A	150	ASN
1	9-A	64	ASN
1	9-B	18	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	-	52,52,52	2.58	16 (30%)	80,80,80	3.51	28 (35%)
2	NAP	1-B	401	-	52,52,52	3.07	20 (38%)	80,80,80	3.46	29 (36%)
2	NAP	10-A	400	-	52,52,52	2.55	17 (32%)	80,80,80	3.49	24 (30%)
2	NAP	10-B	401	-	52,52,52	3.04	21 (40%)	80,80,80	3.70	27 (33%)
2	NAP	11-A	400	-	52,52,52	2.62	17 (32%)	80,80,80	3.33	21 (26%)
2	NAP	11-B	401	-	52,52,52	2.94	16 (30%)	80,80,80	3.70	28 (35%)
2	NAP	12-A	400	-	52,52,52	2.67	22 (42%)	80,80,80	3.40	26 (32%)
2	NAP	12-B	401	-	52,52,52	3.80	21 (40%)	80,80,80	4.02	30 (37%)
2	NAP	13-A	400	-	52,52,52	2.83	20 (38%)	80,80,80	3.27	26 (32%)
2	NAP	13-B	401	-	52,52,52	4.76	29 (55%)	80,80,80	3.43	24 (30%)
2	NAP	14-A	400	-	52,52,52	2.72	19 (36%)	80,80,80	3.28	25 (31%)
2	NAP	14-B	401	-	52,52,52	4.71	21 (40%)	80,80,80	4.92	34 (42%)
2	NAP	15-A	400	-	52,52,52	2.65	20 (38%)	80,80,80	3.30	25 (31%)
2	NAP	15-B	401	-	52,52,52	4.27	22 (42%)	80,80,80	4.71	34 (42%)
2	NAP	16-A	400	-	52,52,52	2.70	21 (40%)	80,80,80	3.18	23 (28%)
2	NAP	16-B	401	-	52,52,52	3.74	18 (34%)	80,80,80	4.01	30 (37%)
2	NAP	2-A	400	-	52,52,52	2.57	17 (32%)	80,80,80	3.50	25 (31%)
2	NAP	2-B	401	-	52,52,52	2.96	17 (32%)	80,80,80	3.73	28 (35%)
2	NAP	3-A	400	-	52,52,52	2.82	18 (34%)	80,80,80	3.51	25 (31%)
2	NAP	3-B	401	-	52,52,52	3.83	18 (34%)	80,80,80	4.03	30 (37%)
2	NAP	4-A	400	-	52,52,52	2.65	15 (28%)	80,80,80	3.50	28 (35%)
2	NAP	4-B	401	-	52,52,52	2.93	15 (28%)	80,80,80	3.56	30 (37%)
2	NAP	5-A	400	-	52,52,52	2.79	19 (36%)	80,80,80	3.52	26 (32%)
2	NAP	5-B	401	-	52,52,52	3.89	18 (34%)	80,80,80	4.05	30 (37%)
2	NAP	6-A	400	-	52,52,52	2.97	19 (36%)	80,80,80	3.44	25 (31%)
2	NAP	6-B	401	-	52,52,52	2.95	17 (32%)	80,80,80	3.72	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	7-A	400	-	52,52,52	2.54	19 (36%)	80,80,80	3.39	25 (31%)
2	NAP	7-B	401	-	52,52,52	3.81	18 (34%)	80,80,80	3.99	29 (36%)
2	NAP	8-A	400	-	52,52,52	2.98	15 (28%)	80,80,80	3.45	28 (35%)
2	NAP	8-B	401	-	52,52,52	2.97	22 (42%)	80,80,80	3.40	27 (33%)
2	NAP	9-A	400	-	52,52,52	2.40	15 (28%)	80,80,80	3.40	25 (31%)
2	NAP	9-B	401	-	52,52,52	2.94	18 (34%)	80,80,80	3.51	28 (35%)

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	0/35/67/67	0/3/5/5
2	NAP	1-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	10-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	10-B	401	-	1/1/12/12	1/35/67/67	0/3/5/5
2	NAP	11-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	11-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	12-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	12-B	401	-	1/1/12/12	1/35/67/67	0/3/5/5
2	NAP	13-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	13-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	14-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	14-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	15-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	15-B	401	-	-	1/35/67/67	0/3/5/5
2	NAP	16-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	16-B	401	-	-	0/35/67/67	0/3/5/5
2	NAP	2-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	2-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	3-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	3-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	4-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	4-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	5-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	5-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	6-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	6-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	7-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	7-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	8-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	8-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	9-A	400	-	1/1/12/12	0/35/67/67	0/3/5/5
2	NAP	9-B	401	-	1/1/12/12	0/35/67/67	0/3/5/5

The worst 5 of 600 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-B	401	NAP	O4B-C4B	26.05	2.06	1.45
2	15-B	401	NAP	O4B-C4B	22.46	1.97	1.45
2	16-B	401	NAP	O4B-C4B	18.04	1.87	1.45
2	13-B	401	NAP	O4B-C4B	16.01	1.82	1.45
2	12-B	401	NAP	O3B-C3B	15.22	1.79	1.43

The worst 5 of 871 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-B	401	NAP	O4B-C1B-N9A	22.93	129.77	108.44
2	15-B	401	NAP	O4B-C1B-N9A	22.56	129.42	108.44
2	16-B	401	NAP	O4B-C1B-N9A	20.38	127.40	108.44
2	14-B	401	NAP	O4B-C4B-C3B	-18.49	67.69	105.17
2	5-B	401	NAP	O4B-C1B-C2B	-18.37	89.77	106.95

5 of 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

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	15-B	401	NAP	C2D-C1D-N1N-C6N
2	12-B	401	NAP	C2D-C1D-N1N-C6N
2	10-B	401	NAP	C2D-C1D-N1N-C6N

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.